

Theory and Numerical Methods
for the Analysis of
Biological and Electronic Oscillators

by

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A Thesis Submitted to the
Graduate School of Engineering
in Partial Fulfillment of the Requirements for
the Degree of

Master of Science

in

Electrical & Computer Engineering

Koç University

September 2008

Koç University
Graduate School of Sciences and Engineering

This is to certify that I have examined this copy of a master's thesis by

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To my family

ABSTRACT

Oscillatory behavior is encountered in many types of systems including electronic, optical, mechanical, biological, chemical, financial, social and climatological systems. Carefully designed oscillators are intentionally introduced into many engineered systems to provide essential functionality for system operation. Oscillatory behavior in biological systems is seen in population dynamics models, in neural systems, in the motor system, and in circadian rhythms. Intracellular and intercellular oscillators of various types perform crucial functions in biological systems. Due to their essentialness, and intricate and interesting dynamic behavior, biological oscillations have been a research focus for decades. Genetic oscillators that are responsible for setting up the circadian rhythms have received particular attention. Oscillators in electronic and telecommunication systems are adversely affected by the presence of undesired disturbances such as noise. These have an impact on the spectral and timing properties of the ideally periodic signals generated by oscillators, resulting in power spreading in the spectrum and zero-crossing jitter and phase drift in the time domain. Unlike other systems which contain an implicit or explicit time reference, autonomously oscillating systems respond to noise in a peculiar and somewhat nonintuitive manner. Understanding the behavior of oscillators used in electronic systems in the presence of disturbances and noise has been a preoccupation for researchers for many decades. The behavior of biological oscillators under various types of disturbances has also been the focus of a good deal of research work in the second half of 20th century. The work on oscillator analysis in these two disparate disciplines seem to have progressed independently, without any cross-fertilization in between. In this thesis, we first decipher previous work on oscillator analysis in both biology and electronics by translating them into a common terminology and formalism. We then develop a rigorous, unifying oscillator analysis theory by using results and concepts from both domains in a synergistic manner. In doing so, we fill certain conceptual and theoretical gaps that we identify in oscillator analysis theories that have been developed both in electronics and biology that pertain to phase analysis.

We formulate a general phase analysis technique that captures both state and parametric perturbations in a unified manner. This phase analysis technique we develop can be applied to oscillators modeled with mixed differential-algebraic equations as opposed to pure differential ones. By reviewing the numerical methods that have been developed for both electronic and biological oscillator analysis, we show that the numerical techniques currently in use for biological oscillators are superseded by the ones that have been recently developed for electronic oscillator analysis. Oscillator perturbation analysis examples produced using a Matlab oscillator analysis toolbox we have developed are presented.

ÖZETÇE

Elektronik, optik, mekanik, biyolojik, kimyasal, finansal, sosyal, iklimsel ve benzeri sistemlerde osilasyonlara rastlanmaktadır. Dikkatle tasarlanmış osilatörler, mühendislerce inşa edilmiş birçok sistemde işlevsel görevleri yerine getirmektedirler. Biyolojik sistemler kapsamında osilasyonlar, popülasyon dinamiği modellerinde, nöral sistemlerde, motor sisteminde ve yirmi dört saatlik ritimlerde rol oynamaktadırlar. Hücreler arasında ve hücre içinde biyolojik osilatörler birçok önemli işlevi üstlenmektedirler. Gerekli ve temel olmaları, karmaşık ve ilgi çekici dinamik özelliklere sahip olmaları nedeniyle, biyolojik osilasyonlar, yıllardır birçok araştırmanın odağında yer almışlardır. Yirmi dört saatlik ritimleri ayarlamakla yükümlü olan genetik osilatörler, önemli derecede ilgi görmüşlerdir. Elektronik ve telekomünikasyon sistemlerindeki osilatörler, gürültü gibi istenmeyen olgulardan olumsuz yönde etkilenirler. Bu gürültüler, osilatörler tarafından oluşturulan ideal periyodik sinyallerin spektrum ve zamanlama özelliklerini bozarlar. Bu nedenle, spektrumda belli frekanslarda yoğunlaşması gereken güç, çevre frekanslara da dağılır. Ayrıca, zaman ekseninde sinyalde faz kayması gözlenir. Bir şekilde zaman referansı olan diğer sistemlerle karşılaştırıldıklarında özerk osilatörler, gürültüye karşılık bakışta akıl yürütülemeyecek derecede garip bir biçimde tepki gösterirler. Elektronik sistemlerde kullanılan osilatörlerin, gürültü var olduğu anlarda işleyişlerini anlayabilmek, araştırmacıların yıllardır kafa yordukları bir konudur. Çeşitli türlerde gürültüye maruz kalan biyolojik sistemlerin incelenmesi de yirminci yüzyılın ikinci yarısında önemli bir araştırma konusu haline gelmiştir. Birbirinden ayrık bu iki disiplinde osilatör analizi üzerine araştırmalar, bağımsız olarak ilerleyegelmişlerdir ve elektronik ile biyoloji arasında bu konu üzerine araştırmacılar arasında görüş alışverişi şimdiye dek gerçekleşmemiştir. Bu tezde, osilatör analizi üzerine elektronik ve biyolojide ortaya konmuş olan katkılar, belli bir terminoloji aracılığıyla tek bir biçime tercüme edilerek deşifre edilmektedir. Sonrasında, her iki disiplinden de sonuçlar ve kavramlar kullanılarak, kesin ve birleştirici bir osilatör analizi teorisi meydana çıkarılmaktadır. Bu katkı ortaya konulurken, elektronik ve biyolojide faz analizi kapsamında oluşmuş bazı

kavramsal ve teorik boşluklar doldurulmaktadır. Zamana bađlı, istenmeyen, hem durumsal, hem de parametrik deđişimlerin varlığında faz analizi, geliştirilen birleştirici analiz çatısı altında, birlikte ele alınabilmektedir. Bu faz analiz tekniđi, karışık diferansiyel-cebirselleştirilmiş denklemlerle modellenmiş osilatörlere uygulanabildiđi gibi sadece diferansiyel denklemler de incelenebilmektedir. Elektronik ve biyolojik osilatör analizi için geliştirilmiş nümerik yöntemler incelenerek, daha yakın zamanda geliştirilmiş olan elektronikteki yöntemlerin, biyolojideki yöntemlere göre daha üstün oldukları gösterilmektedir. Geliştirilmiş olan Matlab osilatör analizi program paketi ile osilatör analizi örnekleri oluşturulup belgelenmektedir.

ACKNOWLEDGMENTS

I would like to express my deepest gratitude to my advisor Prof. Alper Demir, for his interminable patience in answering my questions, directed to him in such an importuning manner. His punctual interventions and far-sighted guidance has prevented the rectification of the work in this thesis from turning out to be a far-fetched frivolity of an inconsequential nature. Prompted to set into action under his exacting vigilance, I was able to draw this MS study to an end, in an elated state of mind. Thanks to Prof. Demir also for granting a scholarship for a good part of my time at Koç University.

I would also like to thank the committee members Prof. Alper Erdoğan and Prof. Varga Kalantarov, for a careful evaluation of the work in this thesis, and also for their corrections and suggestions.

I was well-endowed with the perpetual support of my family, especially during the days that I was holding out for my go at a satisfactory and technically-enriched graduate study, without an actual trace of some hope for a possible grant of a likewise opportunity on my side. Encouraged by the inspirational support of some close friends as well, whose names are not to be disclosed here, I find myself fit to go on with my academic studies.

The work described in this thesis was supported by the TUBA (Turkish Academy of Sciences) GEBIP program and by TUBITAK (Scientific and Technological Research Council of Turkey) Career Award 104E057.

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NOMENCLATURE

ODE	Ordinary Differential Equation
DAE	Differential-Algebraic Equation
PPV	Perturbation Projection Vector
ISF	Impulse Sensitivity Function
LPTV	Linear Periodically Time-Varying
LTI	Linear Time-Invariant

Chapter 1

INTRODUCTION

Oscillators and their analyses have drawn considerable attention from scientists in various fields of research. These autonomous components are either engineered into systems for different purposes, or they exist naturally in, for example, biological systems. Electronic oscillators are used to generate clock signals in digital electronic systems, so that synchronization can be maintained between various components. In communication systems, the periodic signal that is generated by an electronic oscillator is used as a carrier for frequency translation of data signals. Neural [9], and circadian oscillators [6], are two types in the biological domain, which have drawn considerable research effort for decades. Neural oscillations are used for information transfer in inter-cellular activities. A living organism possesses a circadian oscillator, setting an oscillatory schedule for biological activities within the day. The daily cycle determined by the sun is twenty-four hours and modulates the circadian rhythm. The name “circadian” suggests that the period of oscillation of the oscillator maintained in an organism is about but not exactly twenty-four hours. Therefore, if an organism is forced to bear constant darkness, the circadian oscillator gradually takes control of the circadian rhythm, dictating its own period of oscillation. The circadian period of human beings is twenty-five hours.

Oscillators are plagued by perturbations and noise. Perturbations have an adverse effect on the operation of oscillators, which are expected to yield perfect periodic signals in steady-state. It happens that both the amplitude and phase of these periodic signals are affected by perturbations. Particularly, phase is an important concept that requires close attention, because in many electronic applications and biological schemes oscillators are employed as reference time generators. If the phase of an oscillator is altered through perturbations and noise, then the output periodic waveforms of oscillators cease to be perfect time references. Therefore, the study on the mathematical models, in terms of differential equations, of

oscillators, particularly targeting phase, has grown to be a preoccupation in research.

Research on oscillator phase analysis has been conducted for decades. A major accomplishment was the derivation of a differential equation, defining phase. This differential equation, which we will frequently refer to as the phase equation, was actually derived in both domains, and the derivations yielded surprisingly the same expression. It appears perfectly unnatural to obtain the same phase equation as was derived in a seemingly-detached domain, but noting that a unifying appeal over the theory of oscillator phase must surface when oscillators are expressed as differential equations, the fact that oscillator phase is defined through the same equation in both domains is comprehensible. The contributions to the theory of phase in both domains have accumulated rather independently, and intercommunication has failed to flourish between biologists and electronic engineers, researching on phase.

A thorough examination conveys that hardly any of the studies on phase has proved to be unifying and comprehensive. Derivation of the same phase equation suggests that the two independently progressing fields of research can indeed complement each other in more aspects. For example, biologists, benefitting from the contributions of interested mathematicians as well, managed to lay the grounds for precisely defining the phase of an oscillator. This intuitive and rigorous ground has been missing in the approach adopted by electronic engineers. On the other hand, in the electronic domain, the phase equation was derived intuitively, but its accuracy was justified through rigorous methods. This accuracy justification is what is missing in the works that have amassed in the biological domain. One of the contributions in this thesis is the reconciliation of biological and electronic approaches to the phase equation derivation. In this aspect, we will be unifying the two approaches, filling certain conceptual and theoretical gaps, studied over the developed theories of both domains.

The unified theory for oscillator phase analysis, which we develop in this thesis, applies to the computation of the effects of particularly two types of perturbations, on the phase of oscillators. Methods for analysis, accommodating time-varying state and parameter perturbations, are incorporated into the theory we have developed. Numerical schemes for the computation of phase, in the presence of these two types of perturbations exist in previous references. We observe that in the study of phase, numerical methods of the electronic do-

mainly supersede those of the biological world. It is shown through rigorous derivations that the theory developed by biologists, for numerical phase computations, boils down to exactly the methods that have been utilized in the electronic domain for about a decade. However, numerical methods used in biology are inefficient and somewhat ad hoc. Therefore, derivations for steady-state periodic solution computations and ensuing phase-related numerical schemes are redeveloped from scratch and documented for reference. As to the possible types of differential equations, both ODEs (Ordinary Differential Equations) and DAEs (Differential-Algebraic Equations) are accommodated. In biology, DAEs are not accounted for, whereas electronic circuits are generally modeled as DAEs. The more general theory, concerning DAEs, is the focus of more detailed derivations in the chapter on numerical methods. In addition, a MATLAB toolbox for oscillator phase analysis has been developed, based on the methods of the electronic domain. Results obtained with this toolbox, on simple oscillator models, are also presented.

The outline of the thesis is as follows. The necessary background on the mathematical methods for oscillator analysis and related theory are included in Chapter 2. In order to precisely define the phase of an oscillator, we need to make use of the invariant sets called isochrons. Isochrons and the oscillator phase definition are the focus of Chapter 3. Using the phase definition, the phase equation is derived in Chapter 4, so that the phase response of oscillators to state and parameter perturbations can be calculated. In Chapter 5, all approaches to oscillator phase analysis are unified into a single theory, which consists of the numerical computation of a vector function. The numerical methods for calculating the steady-state periodic solutions of oscillators and computing the stated vector function are presented in Chapter 6. In Chapter 7, we present results obtained with the MATLAB toolbox for oscillator phase analysis that we have developed.

Chapter 2

BACKGROUND

2.1 Mathematical Models and Properties

In this section, several properties of oscillator models are provided for reference, along with definitions and mathematical notation. The basic assumptions stated in this section are crucial in that the validity of derivations to follow throughout this work depend on these assumptions.

2.1.1 Oscillator Models

The model presented here could belong to virtually any device or mechanism that exhibits autonomous oscillatory behaviour. Whichever processes that the oscillator we have been provided may model, it is assumed that the mathematical representation of this oscillator may be translated to a system of ODEs (Ordinary Differential Equations) of the form

$$\frac{dx}{dt} = f(x). \quad (2.1)$$

If the initial value for (2.1), x at $t = 0$, $x(0)$ in brief, is given, then (2.1) can be solved through numerical techniques, for in most cases an analytical solution is not available.

The solution to (2.1), i.e. $x(t)$, is assumed to satisfy the conditions that ensure its uniqueness.

It is crucial to define a *state transition function*, Φ , associated with the system in (2.1). The following summarizes, mathematically, the functionality of Φ .

Definition 1 (State Transition Function) *The state transition function, Φ , associated with (2.1), yields the state vector, x , at time $t_0 + t_d$, given the target time $t_0 + t_d$, the initial time t_0 , and the state vector, x , at time t_0 , as in*

$$x(t_0 + t_d) = \Phi(t_0 + t_d, t_0, x(t_0)). \quad (2.2)$$

Φ merely integrates equation (2.1) from t_0 to $t_0 + t_d$, given the initial condition $x(t_0)$. Note that Φ is almost never analytically available. We evaluate Φ through numerical integration of the system in (2.1), given an initial condition $x(t_0)$.

2.1.2 Model Size

The ODE in (2.1) is M -dimensional, i.e. $x \in \mathfrak{R}^M$. We have M state variables, x_i for $1 \leq i \leq M$. Similarly, we have M nonlinear functions, $f_i: \mathfrak{R}^M \rightarrow \mathfrak{R}^1$, for $1 \leq i \leq M$. These f_i 's constitute the nonlinear vector function, $f: \mathfrak{R}^M \rightarrow \mathfrak{R}^M$. Each of these M nonlinear functions takes the state variables vector, x , as argument.

2.1.3 Model Parameters

The ODE in (2.1) has L parameters incorporated. These L parameters will be denoted by p_j for $1 \leq j \leq L$. p_j 's are the entries of the parameters vector, p . p_j 's are not included in the state variables vector, x , but changes in the values of these parameters affect the whole model in (2.1), because each particular p_j is included in the expressions that define f , though the expressions for some f_i 's may not explicitly include some particular p_j 's.

Remark 1 Note that in (2.1), we have used the notation, $f(x)$, to denote the nonlinear function, f , with its argument, x . The parameters vector, p , may be explicitly expressed as an argument to f , if needed. In such cases, we will use the notation, $f(x, p)$, to indicate that f depends on x and p . Formally, $f: \mathfrak{R}^M \times \mathfrak{R}^L \rightarrow \mathfrak{R}^M$.

2.1.4 Steady-State Periodic Solution

The generic ODE in (2.1) usually has multiple steady-state solutions. These solutions are such that each of them repeats itself over and over after a subsequent interval with a pre-determined length in time. This length in time is called the period. A formal definition for the period will follow, but the point here is that the steady-state solutions of the generic ODE in (2.1) are periodic.

Usually, only one of the steady-state solutions of (2.1) is of interest. We will temporarily call this solution $x_s(t)$. The solution of (2.1) with the initial condition $x_s(0)$ is $x_s(t)$.

An obvious property of the periodic $x_s(t)$ is that the time-shifted version $x_s(t - t_0)$, for any t_0 , is again a steady-state solution of (2.1), this time with the initial condition

$x(t = 0) = x_s(t_0)$. t_0 may be called the phase difference in units of time, between the two signals, $x_s(t)$ and $x_s(t - t_0)$.

As will be clear, the computation of $x_s(t)$ is the first task in conducting the phase analysis of (2.1). Since in most cases, there exists no analytical expression for the state transition function, Φ , $x_s(t)$ is calculated by numerical means.

2.1.5 Limit Cycle

$x_s(t)$, a periodic solution of the generic ODE in (2.1), visits a set of points in \mathfrak{R}^M , over and over. It is going to be necessary to refer to this set of points in the derivations to follow, hence the following definition.

Definition 2 (Limit Cycle) *The limit cycle, associated with $x_s(t)$, is formally defined as*

$$\gamma = \{x \in \mathfrak{R}^M \mid x = x_s(t), \forall t \in \mathfrak{R}^+\}. \quad (2.3)$$

To be consistent, we will refer to $x_s(t)$, the steady-state solution, as $x^\gamma(t)$, from this point on. γ will have to possess some assumed properties, for analyses to be carried out on the phase of γ . These properties will shortly be formally stated.

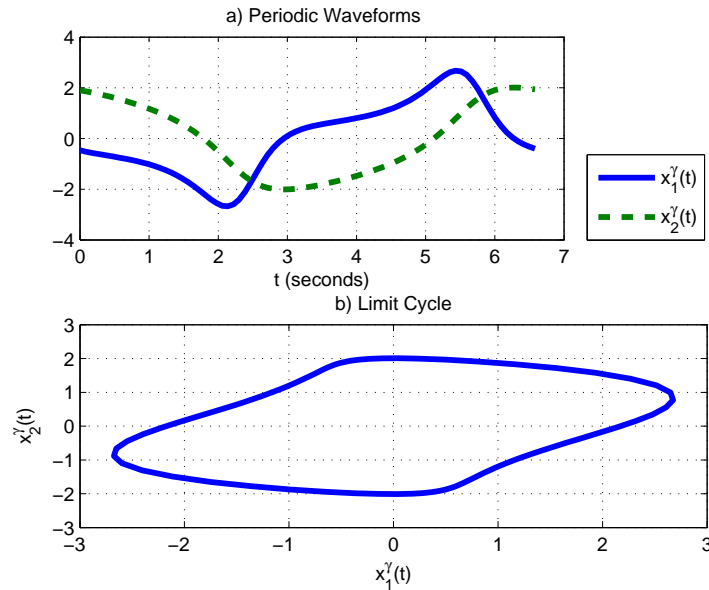


Figure 2.1: Van der Pol Oscillator. a) Steady-State Periodic Waveforms, b) Limit Cycle.

2.1.6 Period and Frequency

A crucial property, at steady-state, of autonomous oscillating systems as in (2.1), is periodicity. A periodic signal is one that repeats itself over and over, regularly, with a predefined interval, called the period of the signal. A formal definition is as follows for the period of $x^\gamma(t)$, a steady-state solution of (2.1).

Definition 3 (Period) Let $x^\gamma(t)$ be a steady-state solution of the generic ODE in (2.1), with $x^\gamma(0)$ at $t = 0$ as the initial value. Let there be a set that will be denoted by \mathcal{T} , defined as

$$\mathcal{T} = \{T^i \mid x^\gamma(t_0 + T^i) = x^\gamma(t_0), \forall t_0 \geq 0\}.$$

$x^\gamma(t_0 + T^i) = \Phi(t_0 + T^i, t_0, x^\gamma(t_0))$, where Φ is the state transition function associated with (2.1). We define T , the period of $x^\gamma(t)$, to be the smallest positive number in \mathcal{T} . We may as well refer to T as the period on γ , the limit cycle. γ is the set of points that $x^\gamma(t)$ visits through time.

It must be noted again that there can be more than one periodic solution of the generic model in (2.1). Usually, only one of these periodic solutions is of interest, and in this case, this solution is $x^\gamma(t)$.

Having defined T , the period of a particular periodic solution, $x^\gamma(t)$, we now define the frequency and angular frequency of $x^\gamma(t)$.

Definition 4 (Frequency) f_0^γ , the frequency of $\hat{x}^\gamma(t)$, is given by the reciprocal of T , the period, as in

$$f_0^\gamma = 1/T.$$

ω_0^γ , the angular frequency of $\hat{x}^\gamma(t)$, is given by

$$\omega_0^\gamma = 2\pi f_0^\gamma = 2\pi/T.$$

Figure 2.1 depicts the periodic solution and the corresponding limit cycle of the famous Van der Pol oscillator.

2.1.7 Number of Timepoints

Ideally, we would like to compute $x^\gamma(t)$ analytically. Unfortunately, $x^\gamma(t)$ is almost never analytically computable. We will represent $x^\gamma(t)$, through N samples along a single interval

of length T .

The location of these N time points along the interval depends on the numerical method that is employed. Timepoints are more frequent, along intervals on which the periodic signal, $x^\gamma(t)$, is changing at a higher rate. Some numerical methods, on the other hand, require timepoints to be uniformly separated.

2.1.8 Orbital Stability

We will now explain *orbital stability*, more commonly known as Liapunov stability, of $x^\gamma(t)$, the periodic steady-state solution of the system in (2.1). As stated before, γ is the set of points that $x^\gamma(t)$ visits repeatedly as time progresses.

In order to define orbital stability, we must first define a metric $dist$ in \mathfrak{R}^M . Let $dist(x, \gamma)$ be the distance between a point x and γ . We may assume that $dist(x, \gamma)$ is the smallest Euclidean distance between x and all the points in γ .

Let $x^0(t)$ be a solution of (2.1) in the close neighborhood of γ . If $x^\gamma(t)$ is orbitally stable, the fact that $dist(x^0(0), \gamma)$ is bounded implies that $dist(\Phi(t, 0, x^0(0)), \gamma)$ will remain bounded for $t > 0$. Note that $x^0(t) = \Phi(t, 0, x^0(0))$. Informally, nearby solutions remain near γ if $x^\gamma(t)$ is orbitally stable. A more formal definition follows.

Definition 5 (Orbital Stability) *The solution $x^\gamma(t)$ of (2.1) is said to be orbitally stable, if for any $\epsilon > 0$, there exists a $\delta > 0$ such that*

$$dist(x^0(0), \gamma) < \delta$$

implies

$$dist(\Phi(t, 0, x^0(0)), \gamma) < \epsilon,$$

where $x^0(t)$ is a solution in a neighborhood \mathcal{W} of the limit cycle γ . The set of points constituting \mathcal{W} are in turn called the domain of attraction.

Figure 2.2 is a depiction of the bounds employed in Definition 5.

We have to impose a stronger condition on $x^\gamma(t)$, for the forthcoming derivations to take effect. This condition is given by the name *asymptotic orbital stability*.

Definition 6 (Asymptotic Orbital Stability) *The solution $x^\gamma(t)$ of (2.1) is said to possess asymptotic orbital stability, if $x^\gamma(t)$ is orbitally stable and, if there exists a $\delta > 0$ such*

that $\text{dist}(x^0(0), \gamma) < \delta$ implies

$$\lim_{t \rightarrow \infty} \text{dist}(\Phi(t, 0, x^0(0)), \gamma) = 0,$$

where $x^0(t)$ is a solution in neighborhood \mathcal{W} of the limit cycle, γ .

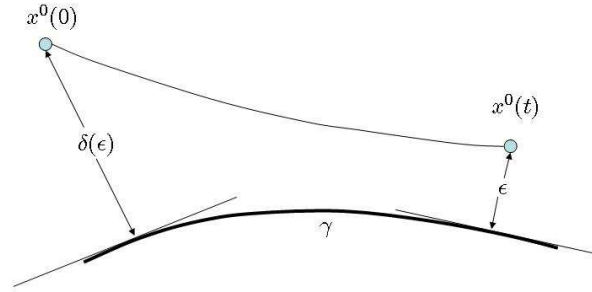


Figure 2.2: Depiction of bounds for orbital stability.

2.1.9 Asymptotic Phase

We stated that $x^\gamma(t)$ is the particular steady-state periodic solution on γ . Let us have ξ and ζ denote two points in time, such that $\xi, \zeta \in [0, T)$, where, T is the period on γ . It is known that $x^\gamma(\xi) = x^\gamma(\zeta)$ if and only if $\xi = \zeta$. Otherwise, the uniqueness of solutions property of the generic ODE in (2.1) would be ruled out. We may extend this statement to all time-shifted steady-state solutions on γ , i.e. $x^\gamma(t + \xi) = x^\gamma(t + \zeta)$ if and only if $\xi = \zeta$, for $t \geq 0$.

Let $x^0(t)$ be a solution in \mathfrak{R}^M such that $x^0(t) \in \mathcal{W}$, $\forall t \geq 0$, where \mathcal{W} is the domain of attraction associated with γ . All states in \mathcal{W} tend to the limit cycle γ as time progresses, for the system in (2.1), for γ has asymptotic orbital stability.

Note that $x^0(0)$ is the initial state of the solution $x^0(t)$, and

$$x^0(t) = \Phi(t, 0, x^0(0)).$$

$x^\gamma(t)$ has the asymptotic phase property if $x^0(t)$ tends to simultaneously hit the same points as a time-shifted version of $x^\gamma(t)$, as $t \rightarrow \infty$.

Definition 7 (Asymptotic Phase) $x^\gamma(t)$, the steady-state periodic solution of the generic ODE system in (2.1), has the asymptotic phase property if for each solution $x^0(t)$, such that $x^0(0) \in \mathcal{W}$, there is a constant $\alpha(x^0(0))$, such that

$$\lim_{t \rightarrow \infty} (\Phi(t, 0, x^0(0)) - x^\gamma(t + \alpha(x^0(0)))) = 0.$$

For (2.1) to have asymptotic phase, $\alpha(x^0(0))$ must be constant for all possible $x^0(0) \in \mathcal{W}$. Note that the solution $x^0(t)$ itself maps to some constant value $\alpha(x^0(0))$, depending on the initial state $x^0(0)$.

Figure 2.3 summarizes this review of asymptotic phase.

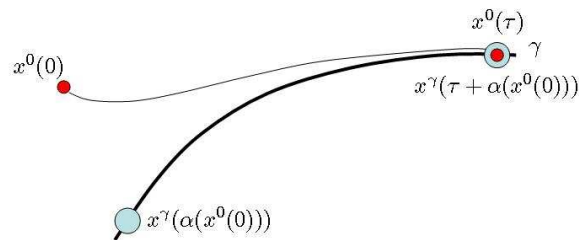


Figure 2.3: Asymptotic phase property.

2.1.10 More General Oscillator Models

In some cases, the model in (2.1) needs to be generalized. The left-hand side of this equation may need to be expressed as, not the time derivative of just x , but the time derivative of a nonlinear function of x , for example $q(x)$. Then, we will have to note the following.

- The generic model, (2.1) in Section 2.1.1, will be modified as in

$$\frac{dq(x)}{dt} = f(x). \quad (2.4)$$

- The state transition function of (2.4) will be denoted by Υ , in order to rule out confusion.
- As in Section 2.1.2, we will still maintain that the size of our dynamic system be M . In this case, $q: \mathfrak{R}^M \rightarrow \mathfrak{R}^M$, along with f , will be another vector of M nonlinear functions, each taking again x as an argument.
- The parameters vector, of size L , associated with (2.4), will still be denoted by p , as in Section 2.1.3. However, in the case of (2.4), a first group of entries in p are parameters belonging to only q . A second group of entries belongs to only f . And a third group belongs to both q and f .

The generic model in (2.4) is a DAE (Differential Algebraic Equation). The solution of DAEs require additional capabilities, as compared to ODEs (Ordinary Differential Equations). DAEs can be regarded as the more general form of ODEs, if it be noted that the nonlinear multi-dimensional function, q , taken (in a particular DAE model) as a linear function, in particular $q(x) = \mathbf{I}_M x = x$, makes the DAE an ODE. \mathbf{I}_M is the identity matrix of size $(M \times M)$.

We will frequently refer to (2.4) as the generic DAE model. Most derivations to follow will take (2.4) as the model to elaborate on, first, and simplifications will ensue, regarding ODEs, when $q(x) = x$.

2.2 Review of Floquet Theory

The steady-state periodic solution $x^\gamma(t)$ and the points that constitute the limit cycle γ are computed through numerical methods. It turns out that these steady-state periodic

solution computation algorithms use the notion of linearization around γ . We are able to define LPTV (Linear Periodically Time-Varying) systems, through linearization of the original ODE, as in (2.1), or DAE, as in (2.4).

This section is mainly about the analysis of these newly-generated LPTV systems. Our aim is to express the generic form of the state transition functions for these LPTV systems. Through Floquet theory, these generic forms are disclosed.

Before presenting a brief review of Floquet theory, however, linearization around the limit cycle has to be introduced. This is done in Section 2.2.1. As to defining state transition functions for LPTV systems, we first review how this procedure works for LTI (Linear Time Invariant) systems, in Section 2.2.2. Finally, Section 2.2.3 is a review of Floquet theory for ODEs and DAEs.

2.2.1 Linearization Around the Limit Cycle

DAE Case

Examining the generic DAE system in (2.4), let us set $x(t) = x^\gamma(t) + y(t)$. Then, Taylor expansions of both sides of (2.4) yield

$$\frac{d}{dt} \left(q(x^\gamma(t)) + \left. \frac{\partial q}{\partial x} \right|_\gamma y(t) \right) \approx f(x^\gamma(t)) + \left. \frac{\partial f}{\partial x} \right|_\gamma y(t). \quad (2.5)$$

We know that the steady-state periodic solution on γ , namely $x^\gamma(t)$, would satisfy this equation. Therefore,

$$\frac{d}{dt} [q(x^\gamma)] = f(x^\gamma). \quad (2.6)$$

Using (2.6) to cancel terms from both sides of (2.5), the linearized form is obtained as

$$\frac{d}{dt} \left(\left. \frac{\partial q}{\partial x} \right|_\gamma y \right) = \left. \frac{\partial f}{\partial x} \right|_\gamma y. \quad (2.7)$$

This process is called linearization of the generic DAE in (2.4) around $x^\gamma(t)$.

One solution out of the many, of (2.7), can be found as follows. Computing the derivatives of both sides of (2.6), with respect to t , we obtain

$$\frac{d}{dt} \left[\frac{\partial q(x^\gamma)}{\partial x^\gamma} \frac{dx^\gamma}{dt} \right] = \frac{\partial f(x^\gamma)}{\partial x^\gamma} \frac{dx^\gamma}{dt},$$

through the chain rule of partial differentiation. We define

$$\mathbf{G}(t) = \frac{\partial f(x^\gamma)}{\partial x^\gamma}, \quad \mathbf{C}(t) = \frac{\partial q(x^\gamma)}{\partial x^\gamma}.$$

Notice that $\mathbf{G}(t)$ and $\mathbf{C}(t)$ are T -periodic matrices. Then,

$$\frac{d}{dt} [\mathbf{C}(t)\dot{x}^\gamma] = \mathbf{G}(t)\dot{x}^\gamma, \quad (2.8)$$

where dot denotes differentiation with respect to time.

Therefore, $\dot{x}^\gamma(t)$ is a solution of the system of linear differential equations,

$$\frac{d}{dt} [\mathbf{C}(t)y] = \mathbf{G}(t)y. \quad (2.9)$$

(2.9) is the more compact form of (2.7) and is an LPTV (Linear Periodically Time-Varying) system, and $\dot{x}^\gamma(t)$ is a real, naturally T -periodic solution of this system. There might be other solutions that are not real or periodic, but through the simple analysis we have conducted, we can establish only $\dot{x}^\gamma(t)$ as a solution. Floquet theory yields forms of the other solutions for the system in (2.9).

We may also seek and find a few properties of the state transition function for the LPTV system in (2.9). For linear systems like (2.9), the state transition function can be numerically computed, by assigning the identity matrix as the initial condition and then solving the system forward in time.

The analysis that will disclose some properties of the state transition function for (2.9), is best conducted if we differentiate both sides of (2.6) with respect to $x^\gamma(0)$, to get

$$\frac{d}{dt} \left[\mathbf{C}(t) \frac{\partial x^\gamma(t)}{\partial x^\gamma(0)} \right] = \mathbf{G}(t) \frac{\partial x^\gamma(t)}{\partial x^\gamma(0)}.$$

Noting that

$$\frac{\partial x^\gamma(0)}{\partial x^\gamma(0)} = \mathbf{I}_M,$$

where \mathbf{I}_M is the identity matrix with size $(M \times M)$, we observe that $\partial x^\gamma(t)/\partial x^\gamma(0)$ is a legitimate state transition function for the LPTV system in (2.9). This finding leads us to declare the following.

Definition 8 (State Transition Function of DAE LPTV Systems) *The state transition function for (2.9), which is to be denoted by $\mathbf{K}(t, 0)$, is given as*

$$\mathbf{K}(t, 0) = \frac{\partial x^\gamma(t)}{\partial x^\gamma(0)}, \quad (2.10)$$

and $\mathbf{K}(t, 0)$ is computed by solving the differential equation

$$\frac{d}{dt} [\mathbf{C}(t)\mathbf{K}(t, 0)] = \mathbf{G}(t) \mathbf{K}(t, 0), \quad (2.11)$$

with

$$\mathbf{K}(0, 0) = \mathbf{I}_M.$$

It is possible to write

$$\mathbf{K}(t, 0) = \frac{\partial \Upsilon(t, 0, x^\gamma(0))}{\partial x^\gamma(0)}, \quad (2.12)$$

because $x^\gamma(t) = \Upsilon(t, 0, x^\gamma(0))$. Thus, (2.12) defines the relation between Υ and \mathbf{K} . $\mathbf{K}(t, 0)$, the state transition function of the linearized system in (2.9), is $\Upsilon(t, 0, x^\gamma(0))$, the periodic solution on γ , of the original nonlinear system in (2.4), partially differentiated with respect to $x^\gamma(0)$.

Furthermore, note the following about $\mathbf{K}(t, 0)$. $\mathbf{K}(t, 0)$ is an $(M \times M)$ -sized matrix, which takes an initial condition, $y(0)$, to $y(t)$, i.e. if the linear differential equation in (2.9) were provided with an initial condition $y(0)$ at $t = 0$, the solution of (2.9) at t would be $y(t) = \mathbf{K}(t, 0)y(0)$. Now, suppose we compute

$$\dot{x}^\gamma(T) = \mathbf{K}(T, 0)\dot{x}^\gamma(0), \quad (2.13)$$

where T is the period on γ . $\dot{x}^\gamma(t)$, the time derivative of x^γ , is T -periodic. Therefore, $\dot{x}^\gamma(0) = \mathbf{K}(T, 0)\dot{x}^\gamma(0)$. This means $\mathbf{K}(T, 0)$ must have an eigenvalue of 1, and the corresponding eigenvector is $\dot{x}^\gamma(0)$.

We have to review Floquet theory to spell out the explicit form of state transition functions for LPTV systems like (2.9). Then, the other eigenpairs associated with $\mathbf{K}(T, 0)$ can be computed. As of now, $(1, \dot{x}^\gamma(0))$ is the only eigenpair that we know belongs to $\mathbf{K}(T, 0)$.

ODE Case

We are to briefly adapt the observations in the previous section to the ODE case. Through a scheme, similar to the procedure explained for the DAE case, the linearized form of the generic ODE in (2.1) is found as

$$\frac{dy}{dt} = \frac{\partial f}{\partial x} \Big|_\gamma y. \quad (2.14)$$

Again introducing the notation $\mathbf{G}(t) = \partial f(x^\gamma(t))/\partial x^\gamma(t)$, the compact form of (2.14) is obtained as

$$\frac{dy}{dt} = \mathbf{G}(t)y. \quad (2.15)$$

Notice that in the ODE case, $\mathbf{C}(t) = \partial q(x^\gamma(t))/\partial x^\gamma(t)$ is not needed, because $q(x) = x$, and then $\mathbf{C}(t) = \mathbf{I}_M$.

A periodic solution of the LPTV system in (2.15) is $\dot{x}^\gamma(t)$. The forms of the other solutions are not available through the simple analysis we conduct here. The tools of Floquet theory are needed to express all solutions of (2.15).

The state transition function of (2.15) can be defined in a manner similar to the DAE case.

Definition 9 (State Transition Function of ODE LPTV Systems) *The state transition function for (2.15), which is to be denoted by $\mathbf{odK}(t, 0)$, is given as*

$$\mathbf{odK}(t, 0) = \frac{\partial x^\gamma(t)}{\partial x^\gamma(0)}, \quad (2.16)$$

and $\mathbf{odK}(t, 0)$ is computed by solving the differential equation

$$\frac{d}{dt} [\mathbf{odK}(t, 0)] = \mathbf{G}(t) \mathbf{odK}(t, 0), \quad (2.17)$$

with

$$\mathbf{odK}(0, 0) = \mathbf{I}_M.$$

Notice that

$$\mathbf{odK}(t, 0) = \frac{\partial \Phi(t, 0, x^\gamma(0))}{\partial x^\gamma(0)},$$

where Φ is the state transition function of the generic ODE system in (2.1).

The last note in this section is that a single eigenpair of $\mathbf{odK}(T, 0)$ is $(1, \dot{x}^\gamma(0))$.

2.2.2 State Transition Function of LTI Systems

Before presenting Floquet theory and the tools that this theory provides to help improve analysis, it is useful to recall a well-known result from the theory related to LTI (Linear Time-Invariant) dynamic systems. We will be computing the generic state-transition function for such systems and then stating the relation between the contributions of Floquet theory and this function, which is special to LTI systems.

Let

$$\frac{dx}{dt} = \mathbf{A}x \quad (2.18)$$

be an M -dimensional dynamic system, where \mathbf{A} is an $(M \times M)$ -dimensional *constant* matrix. If \mathbf{A} is diagonalizable, we can decompose it in the following manner.

$$\mathbf{A} = \mathbf{U} \Lambda \mathbf{V}^T \quad (2.19)$$

The columns of \mathbf{U} are the eigenvectors of \mathbf{A} , and these columns form a biorthonormal set with the columns of \mathbf{V} . That means, if u_i is the i^{th} column of \mathbf{U} and v_j is the j^{th} column of \mathbf{V} , then the following is true.

$$v_j^T u_i = \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \quad (2.20)$$

Alternatively, $\mathbf{U}^{-1} = \mathbf{V}^T$. It naturally follows that $\mathbf{U}\mathbf{V}^T = \mathbf{V}^T\mathbf{U} = \mathbf{I}_M$, with \mathbf{I}_M as the $(M \times M)$ -sized identity matrix. Λ is a diagonal matrix, whose diagonal entries are the eigenvalues of \mathbf{A} .

$$\Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_M \end{pmatrix} \quad (2.21)$$

Since $\mathbf{V}^T = \mathbf{U}^{-1}$, the system in (2.18) can be expressed as

$$\frac{dx}{dt} = \mathbf{U} \Lambda \mathbf{U}^{-1} x, \quad (2.22)$$

and the following is a reformulation.

$$\frac{d(\mathbf{U}^{-1}x)}{dt} = \Lambda (\mathbf{U}^{-1}x)$$

Let us define $y = \mathbf{U}^{-1}x$, and write

$$\frac{dy}{dt} = \Lambda y.$$

In fact, since Λ is a diagonal matrix, we have uncoupled equations for $1 \leq i \leq M$, as in

$$\frac{dy_i}{dt} = \lambda_i y_i.$$

We can solve the equation above for any i , independent of the others.

$$\ln y_i = \lambda_i t + c$$

Reformulating, we have

$$y_i(t) = e^{\lambda_i t} c'.$$

We solve for c' by setting $t = 0$, since we assume that an initial condition at time $t = 0$ has been provided. Then, we have

$$y_i(t) = e^{\lambda_i t} y_i(0)$$

Since the solution for each i is computed, we may now stack individual entries together to form vectors.

$$y(t) = e^{\mathbf{A}t} y(0)$$

$e^{\mathbf{A}t}$ is a diagonal matrix, with its expanded form given as below.

$$e^{\mathbf{A}t} = \begin{pmatrix} e^{\lambda_1 t} & & \\ & \ddots & \\ & & e^{\lambda_M t} \end{pmatrix}$$

Inverting the employed coordinate transformation by setting $y(t) = \mathbf{U}^{-1}x(t)$, we get

$$x(t) = \mathbf{U} e^{\mathbf{A}t} \mathbf{U}^{-1} x(0), \quad (2.23)$$

which is the solution to (2.22).

Definition 10 (State Transition Function of LTI Systems) $e^{\mathbf{A}t}$ is the state transition function of the system in (2.18), and it is expressed as in

$$e^{\mathbf{A}t} = \mathbf{U} e^{\mathbf{A}t} \mathbf{V}^T. \quad (2.24)$$

As is obvious in (2.23), $e^{\mathbf{A}t}$ transforms an initial condition $x(0)$ at time $t = 0$ into a solution $x(t)$ at time t , for $t > 0$.

Through dyadic products, the following could also be written.

$$e^{\mathbf{A}t} = \sum_{i=1}^M e^{\lambda_i t} u_i v_i^T \quad (2.25)$$

The derivation above applies to LTI systems. If \mathbf{A} had entries that periodically varied with period T , the formulation would have to be different. This is where we need to resort to *Floquet Theory* to extend our semi-analytical approach to LPTV (Linear Periodically Time-Varying) systems.

2.2.3 Floquet Theory

The most commonly known form of Floquet theory is best explained and understood in the ODE case. This is why we will provide the necessary details of Floquet theory for ODEs first, in breach of our convention of first presenting theories for systems expressed in DAEs.

ODE Systems

We explained, in Section 2.2.1, what is meant by linearization around γ . In the ODE case, out of the generic nonlinear equation in (2.1), it is simple to derive

$$\frac{dy}{dt} = \mathbf{G}(t)y, \quad (2.26)$$

where, once again, $\mathbf{G}(t) = \partial f(x^\gamma)/\partial x^\gamma$. We also found out, through the simple exploration in Section 2.2.1, that the LPTV (Linear Periodically Time-Varying) system in Section (2.26) has a state transition function, which we called $\mathbf{odK}(t, 0)$, with the following property. $(1, \dot{x}^\gamma(0))$ is an eigenpair of $\mathbf{odK}(T, 0)$. We will now present the explicit form of $\mathbf{odK}(t, 0)$, to justify this finding. Note that Floquet Theory was not needed to compute this particular eigenpair.

Through Floquet Theory, $\mathbf{odK}(t, s)$, for $t \geq s$, is expressed as

$$\mathbf{odK}(t, s) = \mathbf{U}(t) \mathbf{D}(t - s) \mathbf{V}^\top(s). \quad (2.27)$$

Above, $\mathbf{D}(t - s)$ is assumed to be a diagonal, $(M \times M)$ -sized matrix of the form

$$\mathbf{D}(t - s) = \begin{pmatrix} e^{\mu_1(t-s)} & & & \\ & \ddots & & \\ & & \ddots & \\ & & & e^{\mu_M(t-s)} \end{pmatrix}. \quad (2.28)$$

μ_i , for $1 \leq i \leq M$, are called the *Floquet exponents*.

Both $\mathbf{U}(t)$ and $\mathbf{V}(t)$ are $(M \times M)$ -sized matrices with T -periodic entries. These matrices also satisfy $\mathbf{U}(t_0) \mathbf{V}^\top(t_0) = \mathbf{V}^\top(t_0) \mathbf{U}(t_0) = \mathbf{I}_M$, for any t_0 . This condition leads to the biorthogonality property, which will be very useful in our derivations.

$$v_i^\top(t_0) u_j(t_0) = \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \quad (2.29)$$

is true for any $t_0 \geq 0$. Note that $v_i(t_0)$ is the i^{th} column of $\mathbf{V}(t_0)$, and $u_j(t_0)$ is the j^{th} column of $\mathbf{U}(t_0)$.

It must be noted here that the state transition function of the LPTV system in (2.26), defined as $\mathbf{odK}(t, 0)$, is very similar in form to the state transition function of the LTI system in (2.18), given as $e^{\mathbf{A}t}$, in Definition 10 of Section 2.2.2. However, there is a very conspicuous difference between the two functions. \mathbf{U} and \mathbf{V} , in the expanded form in (2.24),

are constant matrices. However, $\mathbf{U}(t)$ and $\mathbf{V}(t)$, in the expanded form of (2.27), are not only time-dependent, but also T -periodic.

As stated before, $(1, \dot{x}^\gamma(0))$ is an eigenpair of the matrix, $\mathbf{odK}(T, 0)$, because $\dot{x}^\gamma(t)$ is a periodic solution of the LPTV system in (2.26). It can easily be verified that $\dot{x}^\gamma(t_0)$ is an eigenvector of $\mathbf{odK}(T + t_0, t_0)$, always corresponding to the eigenvalue of 1. Furthermore, considering,

$$\mathbf{odK}(t, s)\dot{x}^\gamma(s) = \dot{x}^\gamma(t),$$

it is clear that $\dot{x}^\gamma(t)$ is one of the solutions of the LPTV system in (2.26). Then, we may call $u_1(t) = \dot{x}^\gamma(t)$, without loss of generality. As to what the corresponding Floquet exponent, μ_1 , may be, we consider

$$\mathbf{odK}(t, s)\dot{x}^\gamma(s) = e^{\mu_1(t-s)}\dot{x}^\gamma(t),$$

where $e^{\mu_1(t-s)}$ happens to remain 1 for any t and s satisfying $t \geq s \geq 0$. Then, $\mu_1 = 0$.

For the values of all Floquet exponents, we assume

$$\mu_i \begin{cases} = 0 & \text{for } i = 1 \\ < 0 & \text{for } i \in \{2, \dots, M\} \end{cases} \quad (2.30)$$

Note that for simplicity, all μ_i are real. In general, μ_i may exist as complex conjugate pairs as well. Then, on the left-hand side of the expression in (2.30), we should have not μ_i , but $\text{Re}(\mu_i)$, i.e. the real part of μ_i .

Summarizing, we assume that $x^\gamma(t)$, is a periodic solution of the generic ODE system in (2.1). We linearize (2.1) around γ , the limit cycle which consists of all the points traced by $x^\gamma(t)$, as time progresses. The resulting LPTV system represented by (2.26) has a state transition function, $\mathbf{odK}(t, s)$, given by (2.27). Furthermore, we assume that the Floquet exponents, μ_i , for $1 \leq i \leq M$, satisfy the condition in (2.30). Then, it is proven that the steady-state periodic solution, $x^\gamma(t)$, has both asymptotic orbital stability and asymptotic phase [17], reviewed in Section 2.1.8 and Section 2.1.9, respectively.

$\mathbf{odK}(t, s)$ can be expressed through dyadic products as well, as in

$$\mathbf{odK}(t, s) = \sum_{i=1}^M e^{\mu_i(t-s)} u_i(t) v_i^\top(s). \quad (2.31)$$

Supposing we would like to compute how $\mathbf{odK}(t, s)$ would transform $u_j(s)$, the compu-

tation follows as, making use of the biorthogonality property,

$$\begin{aligned} \mathbf{odK}(t, s) u_j(s) &= \sum_{i=1}^M e^{\mu_i(t-s)} u_i(t) \underbrace{v_i^\top(s) u_j(s)}_{\delta_{ij}} \\ &= e^{\mu_j(t-s)} u_j(t). \end{aligned} \quad (2.32)$$

$\mathbf{odK}(t, s)$ transforms $u_j(s)$ into a scaled version of $u_j(t)$. Note that (2.32) solves the LPTV equation in (2.26), with initial condition $u_j(s)$.

For the computations through (2.26) to be stable, we should have

$$|\exp(\mu_i(t-s))| \leq 1. \quad (2.33)$$

In (2.33), since $\mu_i \leq 0$ by our assumption in (2.30), it should be such that $s \leq t$. Therefore, forward computations in time of (2.26) are stable. Backward computations are not stable.

The matrix given by $\mathbf{odK}(T, 0)$ is called the monodromy matrix. Notice that

$$\begin{aligned} \mathbf{odK}(T, 0) &= \sum_{i=1}^M e^{\mu_i T} u_i(T) v_i^\top(0) \\ &= \sum_{i=1}^M e^{\mu_i T} u_i(0) v_i^\top(0), \end{aligned} \quad (2.34)$$

so $u_i(0)$ are the right eigenvectors, $v_i(0)$ are the left eigenvectors, and $e^{\mu_i T}$ are the corresponding eigenvalues of $\mathbf{odK}(T, 0)$, for $1 \geq i \geq M$. For convenience, $\lambda_i = \exp(\mu_i T)$ are called the *Floquet multipliers*. Note that, considering the assumption in (2.30), we have

$$|\lambda_i| = |\exp(\mu_i T)| \begin{cases} = 1 & \text{for } i = 1 \\ < 1 & \text{for } i \in \{2, \dots, M\} \end{cases} \quad (2.35)$$

All Floquet multipliers except for λ_1 are inside the unit circle on the complex plane.

There is also an adjoint LPTV equation, associated with the forward LPTV system in (2.26). This adjoint equation is given by

$$\frac{dz}{dt} = -\mathbf{G}^\top(t) z. \quad (2.36)$$

$\mathbf{odK}^\top(s, t)$, the transpose of the expression in (2.27), is the state transition function and $v_1(t)$ is a periodic solution of (2.36).

Notice that we have

$$\mathbf{odK}^\top(s, t) = \sum_{i=1}^M e^{-\mu_i(s-t)} v_i(s) u_i^\top(t), \quad (2.37)$$

where we must have

$$|\exp(-\mu_i(s-t))| \leq 1 \quad (2.38)$$

for stable computations, otherwise solutions will grow without bound. In (2.38), $\mu_i \leq 0$, so it must be such that $s-t \leq 0$. Therefore, $s \leq t$. This means forward computation in time of (2.36) is unstable. (2.36) must be solved backward in time.

In order to find out how $\mathbf{odK}^\top(s, t)$ transforms $v_j(t)$,

$$\begin{aligned} \mathbf{odK}^\top(s, t) v_j(t) &= \sum_{i=1}^M e^{-\mu_i(s-t)} v_i(s) \underbrace{u_i^\top(t) v_j(t)}_{\delta_{ij}} \\ &= e^{-\mu_j(s-t)} v_j(s). \end{aligned} \quad (2.39)$$

Note that (2.39) solves the adjoint equation (2.36) with initial condition $v_j(t)$, backward in time, i.e. $s \leq t$.

In order to relate the two LPTV equations, derived from the generic ODE in (2.1), we note the following observations. The scalar product of $z(t)$, the solution of (2.36), and the forward LPTV equation in (2.26) yields

$$z^\top(t) \frac{dy(t)}{dt} = z^\top(t) \mathbf{G}(t) y(t). \quad (2.40)$$

The scalar product of $y(t)$, the solution of (2.26), and the forward LPTV equation in (2.36) yields

$$y^\top(t) \frac{dz(t)}{dt} = -y^\top(t) \mathbf{G}^\top(t) z(t). \quad (2.41)$$

Adding (2.40) and (2.41), we obtain, after some manipulations,

$$\frac{d}{dt} [z^\top(t) y(t)] = 0. \quad (2.42)$$

This means $z^\top(t) y(t)$ is a constant for all t . We know that $y(t) = \exp(\mu_i t) u_i(t)$ is a solution for (2.26), with the initial condition $u_i(0)$ at $t = 0$. Also $z(t) = \exp(-\mu_j t) v_j(t)$ is a solution for (2.36) with the initial condition $v_j(0)$ at $t = 0$. We then have, substituting these solutions into (2.42),

$$\frac{d}{dt} [v_j^\top(t) u_i(t)] = -(\mu_i - \mu_j) [v_j^\top(t) u_i(t)]. \quad (2.43)$$

The solution of (2.43) is easily written as

$$v_j^\top(t) u_i(t) = \exp(-(\mu_i - \mu_j)t) v_j^\top(0) u_i(0). \quad (2.44)$$

Notice that in (2.44), if $i = j$, that $v_i^\top(t)u_i(t) = v_i^\top(0)u_i(0)$ is trivially satisfied, and by the biorthogonality condition in (2.29) we have $v_i^\top(t)u_i(t) = v_i^\top(0)u_i(0) = 1$. On the other hand, when $i \neq j$, that $v_j^\top(t)u_i(t) = v_j^\top(0)u_i(0)$ is true iff $v_j^\top(0)u_i(0) = 0$, and by (2.29) we have $v_j^\top(t)u_i(t) = v_j^\top(0)u_i(0) = 0$. Note that this discussion is not a proof of the biorthogonality relation but only an observation documenting the consequences of biorthogonality over the LPTV equations in (2.26) and (2.36).

DAE Systems

Demir in [3] draws attention to the fact that because of the properties of the nonlinear function q in (2.4), $x(t)$, which is a solution of (2.4), is allowed to consist of points that are only in a certain manifold in \mathfrak{R}^M . At each point on γ , this particular manifold, which is actually a subset of \mathfrak{R}^M , can be linearized into a linear subspace, so that a general solution of

$$\frac{d}{dt}(\mathbf{C}(t)y(t)) = \mathbf{G}(t)y(t), \quad (2.45)$$

at $t = t_0$ can be expressed as a linear combination of only $m < M$ vectors in \mathfrak{R}^M . (2.45) is the linearized form of the generic DAE in (2.4), with $\mathbf{C}(t) = \partial q(x^\gamma(t))/\partial x^\gamma(t)$ and $\mathbf{G}(t) = \partial f(x^\gamma(t))/\partial x^\gamma(t)$.

Demir in [3] expresses the state transition function of (2.45) as

$$\mathbf{K}(t, s) = \sum_{i=1}^m e^{\mu_i(t-s)} u_i(t) v_i^\top(s) \mathbf{C}(s), \quad (2.46)$$

for $t \geq s$. $u_i(t)$ and $v_i(t)$ are T -periodic Floquet vector functions, and μ_i are Floquet exponents, all for $1 \leq i \leq M$, associated with the LPTV system in (2.45). However, note that upper limit of the summation in (2.46) is m , not M . The reason for this will be clear shortly.

The biorthogonality condition for $u_j(t)$ and $v_i(t)$, where $1 \leq i, j \leq m$, is given as

$$v_i^\top(t_0) \mathbf{C}(t_0) u_j(t_0) = \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \quad (2.47)$$

with $t_0 \geq 0$. Using (2.47), we can compute how $\mathbf{K}(t, s)$ transforms $u_j(s)$, for $1 \leq j \leq m$.

$$\begin{aligned} \mathbf{K}(t, s) u_j(s) &= \sum_{i=1}^m e^{\mu_i(t-s)} u_i(t) \underbrace{v_i^\top(s) \mathbf{C}(s)}_{\delta_{ij}} u_j(s) \\ &= e^{\mu_j(t-s)} u_j(t) \end{aligned} \quad (2.48)$$

It is clear that (2.48) solves the forward LPTV system equation in (2.45), with initial condition $u_j(s)$. With $t \geq s$, the computation in (2.48) is stable.

From (2.48), it can be deduced that any solution $y(t)$ of (2.45) is such that $y(0)$ can be expressed as a linear combination of the vectors in $\{u_1(0), \dots, u_m(0)\}$. Then,

$$y(0) = \sum_{i=1}^m c_i u_i(0) \quad (2.49)$$

for coefficients c_i . Through (2.48)

$$y(t) = \sum_{i=1}^m c_i e^{\mu_i t} u_i(t). \quad (2.50)$$

for $t \geq 0$. As stated earlier, $x(t)$ in (2.4) resides in a subset of \mathfrak{R}^M . In turn, $y(t)$ in (2.45) at any t resides in a linear subspace of dimension m [3].

There are also other Floquet functions that constitute the set $\{u_{m+1}(t), \dots, u_M(t)\}$. These vector functions reside in the nullspace of $\mathbf{C}(t)$ [3], i.e.

$$\mathbf{C}(t) \{u_{m+1}(t), \dots, u_M(t)\} = 0. \quad (2.51)$$

This is why the upper limit in the summation expression of (2.46) is m . The components that are in the span of $\{u_{m+1}(s), \dots, u_M(s)\}$ are instantly killed by $\mathbf{K}(t, s)$ in (2.46).

The biorthogonality condition in (2.47) can then be expressed for all Floquet functions as

$$v_i^\top(t_0) \mathbf{C}(t_0) u_j(t_0) = \delta_{ij} = \begin{cases} \delta_{ij} & \text{for } 1 \leq i, j \leq m \\ 0 & \text{for } m+1 \leq i, j \leq M \end{cases} \quad (2.52)$$

for any $t_0 \geq 0$.

Following the discussion above, we may now introduce the assumed values for Floquet exponents. In Section 2.2.1, we concluded that $(1, \dot{x}^\gamma(0))$ must be an eigenpair of $\mathbf{K}(T, 0)$, whose explicit form is now easily computed through (2.46) via Floquet Theory. As in the discussion for ODE systems, we set without loss of generality $\mu_1 = 0$ and $u_1(t) = \dot{x}^\gamma(t)$. As a sufficient condition for asymptotic orbital stability and asymptotic phase to hold, we assume that all other Floquet exponents are negative [17]. Considering (2.51) and in turn (2.48), we must set the Floquet exponents that correspond to the Floquet functions in the

nullspace of $\mathbf{C}(t)$ to minus infinity. In all, we have

$$\mu_i \begin{cases} = 0 & \text{for } i = 1 \\ < 0 & \text{for } i \in \{2, \dots, m\} \\ = -\infty & \text{for } i \in \{m+1, \dots, M\} \end{cases} \quad (2.53)$$

The adjoint LPTV equation for the DAE case [3] is given by

$$\mathbf{C}^\top(t) \frac{dz}{dt} = -\mathbf{G}^\top(t)z(t). \quad (2.54)$$

The state transition function for (2.54) is not simply $\mathbf{K}^\top(s, t)$, if we are to recall the form for the ODE case. For DAEs we have

$$\mathbf{L}(s, t) = \sum_{i=1}^m e^{-\mu_i(s-t)} v_i(s) u_i^\top(t) \mathbf{C}^\top(t), \quad (2.55)$$

as the state transition function of the adjoint equation in (2.54).

We can easily determine how $\mathbf{L}(s, t)$ transforms $v_j(t)$, for $1 \leq j \leq m$.

$$\begin{aligned} \mathbf{L}(s, t) v_j(t) &= \sum_{i=1}^m e^{-\mu_i(s-t)} v_i(s) \underbrace{u_i^\top(t) \mathbf{C}^\top(t)}_{\delta_{ij}} v_j(t) \\ &= e^{-\mu_j(s-t)} v_j(s). \end{aligned} \quad (2.56)$$

(2.56) solves (2.54) with initial condition $v_j(t)$. It is also clear that with $s \leq t$, the computation in (2.56) is stable.

The following simple derivation relates the solutions of the forward LPTV equation in (2.45) to the solutions of the adjoint equation in (2.54). A similar procedure has also been included in the review for ODE systems.

The scalar product of $z(t)$, the solution of (2.54), and the forward LPTV equation in (2.45) yields

$$z^\top(t) \frac{d}{dt} (\mathbf{C}(t)y(t)) = z^\top(t) \mathbf{G}(t)y(t). \quad (2.57)$$

The scalar product of $y(t)$, the solution of (2.45), and the forward LPTV equation in (2.54) yields

$$y^\top(t) \mathbf{C}^\top(t) \frac{dz(t)}{dt} = -y^\top(t) \mathbf{G}^\top(t)z(t). \quad (2.58)$$

Adding (2.57) and (2.58), we obtain, after some manipulations,

$$\frac{d}{dt} [z^\top(t) \mathbf{C}(t)y(t)] = 0. \quad (2.59)$$

This means $z^\top(t)\mathbf{C}(t)y(t)$ is a constant for all t . Considering that $\mu_i = -\infty$ for $m+1 \leq i \leq M$, we can say that $y(t) = \exp(\mu_i t)u_i(t)$, for $1 \leq i \leq M$, is a solution for (2.54), with the initial condition $u_i(0)$ at $t = 0$. Also $z(t) = \exp(-\mu_j)v_j(t)$, for $1 \leq j \leq M$, is a solution for (2.54) with the initial condition $v_j(0)$ at $t = 0$. We then have, substituting these solutions into (2.59),

$$\frac{d}{dt} [v_j^\top(t)\mathbf{C}(t)u_i(t)] = -(\mu_i - \mu_j) [v_j^\top(t)\mathbf{C}(t)u_i(t)]. \quad (2.60)$$

The solution of (2.60) is easily written as

$$v_j^\top(t)\mathbf{C}(t)u_i(t) = \exp(-(\mu_i - \mu_j)t)v_j^\top(0)\mathbf{C}(0)u_i(0). \quad (2.61)$$

For $m+1 \leq i \leq M$, it is clear that $v_j^\top(t)\mathbf{C}(t)u_i(t) = 0$, since $\mathbf{C}(t)$ has a nullspace spanned by $\{u_{m+1}(t), \dots, u_M(t)\}$. Considering the case $1 \leq i, j \leq m$, we have $v_j^\top(t)\mathbf{C}(t)u_i(t) = v_j^\top(0)\mathbf{C}(0)u_i(0)$, when $i = j$. The biorthogonality condition in (2.52) satisfies this relation by setting $v_j^\top(t)\mathbf{C}(t)u_i(t) = v_j^\top(0)\mathbf{C}(0)u_i(0) = 1$. When $i \neq j$, $v_j^\top(t)\mathbf{C}(t)u_i(t) = v_j^\top(0)\mathbf{C}(0)u_i(0)$ iff $v_j^\top(0)\mathbf{C}(0)u_i(0) = 0$. (2.52) sets $v_j^\top(0)\mathbf{C}(0)u_i(0) = 0$. Again, this is not a proof of the biorthogonality property in (2.52), but we observe through this discussion that (2.52) satisfies (2.61).

Chapter 3

ISOCHRONS AND PHASE OF AN OSCILLATOR

Definition 7 in Section 2.1.9 is a statement of the asymptotic phase property for dynamic systems. Let us briefly recall Definition 7. This review will be most helpful before we introduce the notion of isochrons.

Let $x^0(t)$ be a solution of the generic ODE in (2.1). We will assume $x^0(0)$ to be an element of the set called the domain of attraction, \mathcal{W} , associated with γ , the limit cycle of interest. However, we will also assume that $x^0(0)$ is not on γ . Remembering that we also assume $x^\gamma(t)$, the steady-state solution on γ , to have the asymptotic orbital stability property, these conditions imply that, as $t \rightarrow \infty$, the points defined by $x^0(t)$ will tend to become elements of γ only.

Definition 7 states that any such solution $x^0(t)$ that complies with the conditions we have just stipulated is related to $x^\gamma(t)$, if $x^\gamma(t)$ has the asymptotic phase property. Definition 7 declares, provided that $x^\gamma(t)$ has asymptotic phase, the points traced by $x^\gamma(t + \alpha(x^0(0)))$ and $x^0(t)$ tend to become identical, $t \rightarrow \infty$. Moreover, $\alpha(x^0(0))$ is a constant in units of time.

For purposes of elucidation of the current matter, visualize two runners around the limit cycle, footing different tracks. Let the first runner never leave γ , and let his coordinates as a function of time be defined by $x^\gamma(t + \alpha(x^0(0)))$. Let the second runner follow the track defined by $x^0(t)$. By our assumptions, the two runners can not be at the same location at $t = 0$, as $x^0(0)$ is not on γ . However, as time progresses, the second runner approaches the set of points γ , because of asymptotic orbital stability. The first runner is always stomping along γ , but we know that eventually the second runner as well will be running along γ . By our assumptions and then through Definition 7, we are entitled to propose that there exists a constant $\alpha(x^0(0))$ that enables the two runners to eventually foot the track, or more formally trajectory, defined by γ , side by side.

The asymptotic phase property, having $x^\gamma(t + \alpha(x^0(0))) = x^0(t)$, in the limit as $t \rightarrow \infty$,

for a constant $\alpha(x^0(0))$, gives rise to the suspicion that there might be solutions other than $x^0(t)$, for example $x^1(t)$, satisfying $x^\gamma(t + \alpha(x^0(0))) = x^1(t)$, as $t \rightarrow \infty$. Notice that we have kept the constant term in the argument, $\alpha(x^0(0))$, intact, as it should be, simply because $\alpha(x^1(0)) = \alpha(x^0(0))$. Also, we require that $x^1(0)$ as well resides in \mathcal{W} , associated with γ . If as $t \rightarrow \infty$, $x^0(t)$ and $x^1(t)$ are hitting the same points simultaneously, together with $x^\gamma(t + \alpha(x^0(0)))$, we may rightfully call $x^0(t)$ and $x^1(t)$ in phase, not just for big t , but for all $t \geq 0$. Figure 3.1 shows some solutions that are in phase and suggests that these sets may indeed form a set.

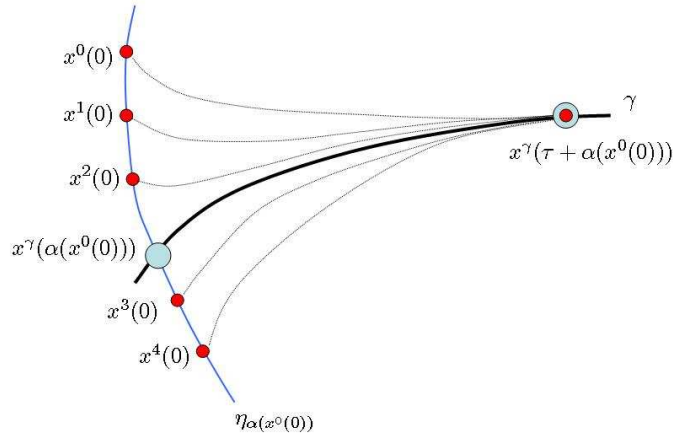


Figure 3.1: Intuitive approach leading to the discovery of isochrons.

Let us focus on $t = 0$ for the moment. By our assumptions, we know that all three of $x^0(0)$, $x^1(0)$, and $x^\gamma(\alpha(x^0(0)))$ are in phase. This observation suggests that there exists a notion of phase not just on γ , but around the limit cycle as well, possibly over the whole of \mathcal{W} . In order to develop an understanding of phase in \mathcal{W} , we will have to define the notions of period, frequency, and angular frequency in \mathcal{W} . We will sustain the likes of these notions on γ itself and will extend the existing theory to cover the whole domain of attraction. Therefore, our definitions will be for what we will call the generalized period, frequency, angular frequency, and angular phase.

Isochrons were first introduced by Winfree, who coined the term isochron and investigated into the theory of phase in oscillators around the limit cycle, through the help of isochrons, in [22] and [19], and Guckenheimer, who proved mathematically the existence of isochrons and their properties [7].

Winfree confesses that he was not aware of the notion of asymptotic phase, when he foresaw that sets of points of the same phase were foliating the domain of attraction, for γ of an oscillator [19]. Each of these sets of equal phase, Winfree called an isochron. This term literally means “of the same time”. Winfree then inaugurating a streak to publish a series of papers, the oldest of which dates back to 1967 [19], explored deeper into this new theory, which he made use of in analyzing oscillator phase under perturbations. Winfree, a renowned biologist deceased in 2002, published [22] in 1974, a work that elicited immediate response from Guckenheimer through [7] in 1975. Winfree’s intuitive questions in [22] focus on the existence of isochrons and whether or not a neighborhood of γ is partitioned into isochrons, each one of which intersects a single point on γ . Guckenheimer responds in [7] that, under certain conditions that are to be stated shortly, isochrons both exist and foliate a neighborhood of γ . Winfree’s other questions constitute an inquiry into the properties of “phaseless sets”, topological manifolds formed by the existence of isochrons [22]. Guckenheimer responds [7]. with abstract mathematical proofs.

The profundity of the abstract methods, including topology, which Guckenheimer resorted to, in proving the existence of isochrons and verifying the fact that isochrons foliate the domain of attraction, which belongs to γ , is beyond the scope of the explanations and contributions to be provided in this text. However, we note here that Guckenheimer proves the existence of isochrons, for $x^\gamma(t)$ that have characteristic multipliers, all of value less than 1 [7]. These characteristic multipliers surface in our work under the name of Floquet multipliers, i.e. $\lambda_i = \exp(\mu_i T)$, for $1 \leq i \leq M$, as defined in Section 2.2.3. It is proved in [17] that if the Floquet multipliers, associated with $x^\gamma(t)$, are such that only one of these is 1 in magnitude, and all the rest are less than 1, $x^\gamma(t)$ possesses both the asymptotic phase and the asymptotically orbital stability properties. Therefore, since we rely on these two properties in stating the forthcoming definition of isochrons, we assume that having a single Floquet multiplier as 1 and all the rest as less than 1, equivalently having the first Floquet exponent as $\mu_1 = 0$, and the rest as $\mu_i < 0$ for $2 \leq i \leq M$, assuming again that all exponents

are real, implies the existence of isochrons, at least in the close neighborhood of γ .

We will be spelling out and analyzing simple examples in this part of our work, and we will be figuring out analytical and numerical methods to illustrate the structure of isochrons over the whole domain of attraction, associated with γ . However, these methods for finding expressions of isochrons are just for demonstration purposes. Our eventual goal, the analysis of oscillator phase under perturbations, is facilitated analytically and numerically in the close neighborhood of γ , i.e. when the states vector never leaves the close neighborhood of γ . Therefore, when carrying out analyses of oscillator phase under perturbations, we will not have to make use of isochrons over the whole domain of attraction, \mathcal{W} . Analyses in the close neighborhood of γ will suffice. The accuracy of Floquet multipliers is maintained in the close neighborhood of γ only. Noting the sufficient condition that Guckenheimer specifies in [7] for the existence of isochrons, that all Floquet multipliers should be less than 1, and the proof in [17] that if only one Floquet multiplier is 1, and the rest are all less than 1, the two crucial properties, attributed to $x^\gamma(t)$, asymptotic phase and asymptotic orbital stability, exist, we rightfully assume that isochrons exist in the close neighborhood of γ , for the types of oscillators that we venture to analyze.

Guckenheimer's justified statement that there is no point in the close neighborhood of γ that is not an element of any isochron, associated with γ , i.e. that isochrons foliate the close neighborhood of γ , is also more than welcome to consolidate the veracity of our forthcoming derivations.

We will first be providing a formal definition for the sets called isochrons.

3.1 Definition

Definition 11 (Isochron) *Let $x^\eta(t)$ be a solution of the generic ODE in (2.1). $x^\gamma(t)$ is the periodic steady-state solution of (2.1). The isochron with time tag t_0 , which we call η_{t_0} , is defined to be the set*

$$\eta_{t_0} = \left\{ x^\eta(t_0) \mid \lim_{\tau \rightarrow \infty} [\Phi(\tau, t_0, x^\eta(t_0)) - x^\gamma(\tau)] = 0 \right\}, \quad (3.1)$$

where $x^\gamma(\tau) = \Phi(\tau, t_0, x^\gamma(t_0))$. Φ is the state transition function, associated with (2.1).

In Definition 7 of Section 2.1.9, γ is declared to have asymptotic phase for all solutions

$x^0(t)$ of (2.1), with $x^0(0) \in \mathcal{W}$, if there is a constant $\alpha(x^0(0))$ in units of time, such that

$$\lim_{\tau \rightarrow \infty} [x^0(\tau) - x^\gamma(\tau + \alpha(x^0(0)))] = 0.$$

In Definition 11 above, we start at $t = t_0$, not $t = 0$, and declare that $x^\eta(t_0)$ and $x^\gamma(t_0)$ are on the same isochron, provided that the stated condition is satisfied. Trivially, $x^\gamma(t_0) \in \eta_{t_0}$ as well. Figure 3.2 is an illustration of this definition.

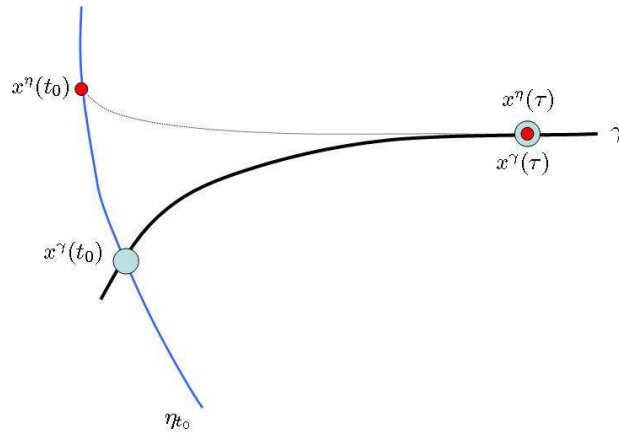


Figure 3.2: Isochron definition.

Definition 7 and Definition 11 are very similar. However, Definition 11 for isochrons introduces one particular concept that is not stated in Definition 7. Definition 7 for asymptotic phase may be interpreted as if each $x^0(0) \in \mathcal{W}$ maps to a unique $\alpha(x^0(0))$. However, Definition 11 for isochrons rules out this possibility, implying that there is a set of points that map to $\alpha(x^0(0))$, and that set is a single isochron in \mathcal{W} . Since Definition 11 introduces a stronger condition than Definition 7, it can be noted that the existence of isochrons in \mathcal{W} implies the existence of asymptotic phase in \mathcal{W} , provided that each isochron intersects a single point on γ .

Note also that in Definition 11, η_{t_0} is assumed to intersect $x^\gamma(t_0)$. The time tags are taken the same to avoid confusion only.

3.2 Properties

In this section, we present two crucial properties of isochrons. The first theorem relates isochrons to Floquet Theory. As we stated before, isochron behavior in the close neighborhood of γ is essential in the forthcoming analyses.

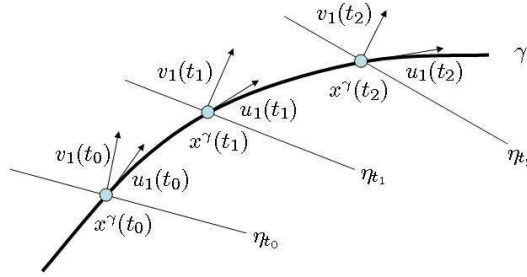


Figure 3.3: The first crucial property of isochrons.

Theorem 1 *If η_{t_0} is linearized into a hyperplane at $x^\gamma(t_0)$, then $v_1(t_0)$ is the vector orthogonal to that hyperplane.*

Proof: The definition of η_{t_0} in (3.1) suggests that the points in η_{t_0} form a nonlinear hypersurface that passes through $x^\gamma(t_0)$. The linearization of η_{t_0} at $x^\gamma(t_0)$ will naturally be a hyperplane. Hyperplanes are subspaces of dimension $(M - 1)$ in \mathfrak{R}^M . A hyperplane is defined by a single vector that is orthogonal to every vector in that hyperplane.

Our task is to linearize η_{t_0} at $x^\gamma(t_0)$. The Taylor expansion of $x^\eta(\tau) = \Phi(\tau, t_0, x^\eta(t_0))$, around $x^\gamma(t_0)$, as in

$$x^\eta(\tau) \approx \Phi(\tau, t_0, x^\gamma(t_0)) + \frac{\partial \Phi(\tau, t_0, x^\gamma(t_0))}{\partial x^\gamma(t_0)} z. \quad (3.2)$$

Notice that above, we have assumed $z = x^\eta(t_0) - x^\gamma(t_0)$.

The expression in (3.1) can then be written as, making use of the approximation in (3.2),

$$\begin{aligned} \lim_{\tau \rightarrow \infty} [\{x^\eta(\tau)\} - \{x^\gamma(\tau)\}] &= 0 \\ \lim_{\tau \rightarrow \infty} \left[\left\{ \Phi(\tau, t_0, x^\gamma(t_0)) + \frac{\partial \Phi(\tau, t_0, x^\gamma(t_0))}{\partial x^\gamma(t_0)} z \right\} - \{ \Phi(\tau, t_0, x^\gamma(t_0)) \} \right] &= 0 \\ \lim_{\tau \rightarrow \infty} \frac{\partial \Phi(\tau, t_0, x^\gamma(t_0))}{\partial x^\gamma(t_0)} z &= 0. \end{aligned} \quad (3.3)$$

Notice that (3.3) can be written as

$$\lim_{\tau \rightarrow \infty} \mathbf{odK}(\tau, t_0)z = 0,$$

where \mathbf{odK} is the state transition function of the linear equation, $\dot{y} = \mathbf{G}(t)y$, with $\mathbf{G}(t) = \partial f / \partial x$ evaluated on γ , derived from the generic ODE in (2.1). We have imposed a condition on z , and what we need to do is to determine which values z can take.

We know through Floquet Theory that

$$\mathbf{odK}(\tau, t_0) = \sum_{i=1}^M e^{\mu_i(\tau-t_0)} u_i(\tau) v_i^\top(t_0),$$

and we have

$$\lim_{\tau \gg t_0, \tau \rightarrow \infty} \mathbf{odK}(\tau, t_0) = u_1(\tau) v_1^\top(t_0), \quad (3.4)$$

since our key assumption is that $\mu_1 = 0$, and $\mu_i < 0$ for $2 \leq i \leq M$. (3.3) becomes, through (3.4),

$$\lim_{\tau \rightarrow \infty} u_1(\tau) v_1^\top(t_0) z = 0. \quad (3.5)$$

Recall that $u_1(t) = \dot{x}^\gamma(t)$. If all entries of $u_1(\tau)$ in (3.5) are zero, then $u_1(t) = \dot{x}^\gamma(t) = 0$, for $t > \tau$, i.e. oscillation stops at $t = \tau$. This is not possible, so we must have

$$v_1^\top(t_0) z = 0. \quad (3.6)$$

(3.6) above is the hyperplane expression we have been seeking. If η_{t_0} is linearized into a hyperplane at $x^\gamma(t_0)$, then (3.6) is the expression for this hyperplane.

From (3.6), we then have, because of biorthogonality,

$$z = \sum_{i=2}^M a_i u_i(t_0),$$

where not all coefficients a_i are expected to be zero. Then, it is clear that the linearization of η_{t_0} at $x^\gamma(t_0)$, i.e. the hyperplane given by (3.6), is defined by $v_1(t_0)$. ■

Figure 3.3 is an illustration of the first crucial property of isochrons. We observe that $v_1(t)$ and $u_1(t)$ are not necessarily in the same direction, but we know that $v_1(t)$ is orthogonal to the linearized form of an isochron, the linearization carried out at $x^\gamma(t)$, and that $u_1(t)$ is tangent to the trajectory we call γ , at again $x^\gamma(t)$.

The second crucial property of isochrons helps to establish periodicity not only on γ , but over the domain of attraction, \mathcal{W} . We will justify this property, but before that the following theorem has to be noted.

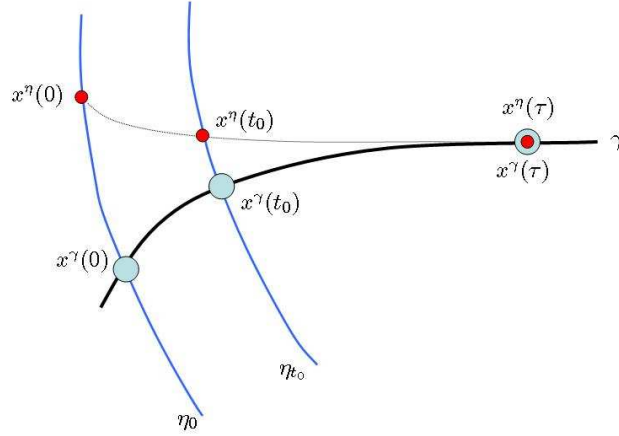


Figure 3.4: The second crucial property of isochrons.

Theorem 2 *Let the initial condition $x^\gamma(0)$ of the steady-state periodic solution $x^\gamma(t)$, of the generic ODE in (2.1), reside on the isochron η_0 . Let another solution $x^0(t)$ of (2.1) be such that $x^0(0) \in \eta_0$. Then, for all t_0 , $x^0(t_0) \in \eta_{t_0}$.*

Proof: Since $x^0(0) \in \eta_0$, by Definition 11, we have

$$\lim_{\tau \rightarrow \infty} \Phi(\tau, 0, x^0(0)) = \lim_{\tau \rightarrow \infty} \Phi(\tau, 0, x^\gamma(0)). \quad (3.7)$$

We also have

$$\Phi(\tau, t_0, x^0(t_0)) = \Phi(\tau, 0, x^0(0)), \quad (3.8)$$

for $\tau > t_0$, since

$$\Phi(\tau, t_0, x^0(t_0)) = \Phi(\tau, t_0, \Phi(t_0, 0, x^0(0))).$$

Also

$$\Phi(\tau, t_0, x^\gamma(t_0)) = \Phi(\tau, 0, x^\gamma(0)), \quad (3.9)$$

for $\tau \geq t_0$. Then, substituting the left-hand side expressions in (3.8) and (3.9) into (3.7),

$$\lim_{\tau \rightarrow \infty} \Phi(\tau, t_0, x^0(t_0)) = \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0, x^\gamma(t_0)). \quad (3.10)$$

(3.10) implies that $x^0(t_0) \in \eta_{t_0}$. ■

Figure 3.4 is an illustrative explanation of the second property of isochrons.

The following corollary follows immediately from Theorem 2.

Corollary 1 (Theorem 2) *If $x^1(t)$ and $x^2(t)$ are two solutions of (2.1) such that $x^1(0), x^2(0) \in \eta_0$, then at $t = t_0$, $x^1(t_0), x^2(t_0) \in \eta_{t_0}$.*

Corollary 1 will be necessary when explaining a numerical method for plotting the isochron portrait in the domain of attraction, associated with the limit cycle of a simple two-dimensional oscillator.

We have assumed from the beginning of our discussions that the period on the limit cycle of interest, γ , is T . Naturally, the definition of periodicity, given in Section 2.1.6, was stated, observing a generic dynamic system, oscillating only on γ . In this aspect, the periodicity definition is quite strict. The next corollary that follows from Theorem 2 is mandatory in establishing periodicity in \mathcal{W} , the domain of attraction.

Corollary 2 (Theorem 2) *Let $x^0(t)$ be a solution of the generic ODE in (2.1), and let $x^0(0)$ reside in the domain of attraction, \mathcal{W} , so that $x^0(t)$ approaches γ as time progresses. Let $x^0(t_0)$ be on the same isochron, η_{t_0} , as $x^\gamma(t_0)$, i.e. $x^0(t_0) \in \eta_{t_0}$. Then, $x^0(t_0 + nT)$, for nonnegative integers n , are also on η_{t_0} . T is the period on γ .*

Proof (Explanation of Corollary 2): By Theorem 2, $x^0(t_0 + nT) \in \eta_{t_0 + nT}$, for nonnegative integers n . $\eta_{t_0 + nT}$ is the isochron that passes through $x^\gamma(t_0 + nT)$, but $x^\gamma(t_0 + nT) = x^\gamma(t_0)$, for $x^\gamma(t)$ is the steady-state periodic solution on γ . Also by the uniqueness of solutions of the generic ODE in (2.1), and the existence of isochrons in \mathcal{W} [7], there is

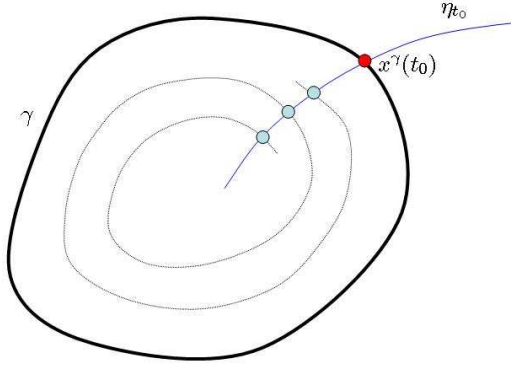


Figure 3.5: Periodicity in the domain of attraction.

a single isochron associated with $x^\gamma(t_0)$, i.e. $x^\gamma(t_0) \in \eta_{t_0}$. Therefore, $\eta_{t_0+nT} = \eta_{t_0}$, and $x^0(t_0 + nT) \in \eta_{t_0}$. ■

Proof (Alternative Proof of Corollary 2): We do not directly make of Theorem 2 while conducting this proof. This is going to be a proof by induction. The base case is that

$$\lim_{\tau \rightarrow \infty} \Phi(\tau, t_0, x^0(t_0)) = \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0, x^\gamma(t_0)). \quad (3.11)$$

This equation states that $x^0(t_0)$ are $x^\gamma(t_0)$ on the same isochron, η_{t_0} .

For the inductive step, we proceed as follows. The inductive hypothesis reads, for some nonnegative integer n ,

$$\begin{aligned} & \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + nT, x^0(t_0 + nT)) \\ &= \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + nT, x^\gamma(t_0)). \end{aligned} \quad (3.12)$$

This is a mathematical statement that $x^0(t_0 + nT)$ is assumed to be on the same isochron, η_{t_0} , as $x^\gamma(t_0)$. However, we also have

$$\begin{aligned} & \Phi(\tau, t_0 + nT, x^\gamma(t_0 + nT)) \\ &= \Phi(\tau, t_0 + nT, x^\gamma(t_0)), \end{aligned} \quad (3.13)$$

for $x^\gamma(t_0 + nT) = x^\gamma(t_0)$, because of the periodicity on γ . The previous equation is true for any $\tau \geq t_0 + nT$. Deducing through (3.12) and (3.13), we have

$$\begin{aligned} & \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + nT, x^0(t_0 + nT)) \\ &= \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + nT, x^\gamma(t_0 + nT)), \end{aligned} \quad (3.14)$$

but this is obviously a natural consequence of the base case in (3.11), noting that

$$\begin{aligned} & \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + nT, x^0(t_0 + nT)) \\ &= \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + nT, \Phi(t_0 + nT, 0, x^0(0))) \end{aligned}$$

and

$$\begin{aligned} & \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + nT, x^\gamma(t_0 + nT)) \\ &= \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + nT, \Phi(t_0 + nT, 0, x^\gamma(0))) \end{aligned}$$

So the inductive hypothesis in (3.12), at iteration number n , for some nonnegative integer n , of course, is not an assumption, but a fact.

We have

$$\begin{aligned} & \Phi(\tau, t_0 + nT, x^0(t_0 + nT)) \\ &= \Phi(\tau, t_0 + (n+1)T, x^0(t_0 + (n+1)T)), \end{aligned} \quad (3.15)$$

and

$$\begin{aligned} & \Phi(\tau, t_0 + nT, x^\gamma(t_0)) \\ &= \Phi(\tau, t_0 + (n+1)T, x^\gamma(t_0 + T)) \\ &= \Phi(\tau, t_0 + (n+1)T, x^\gamma(t_0)), \end{aligned} \quad (3.16)$$

for $\tau \geq (n+1)T$, since $x^\gamma(t)$ is periodic with T . The last two equations (3.15) and (3.16), together with the inductive hypothesis in (3.12) imply

$$\begin{aligned} & \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + (n+1)T, x^0(t_0 + (n+1)T)) \\ &= \lim_{\tau \rightarrow \infty} \Phi(\tau, t_0 + (n+1)T, x^\gamma(t_0)) \end{aligned} \quad (3.17)$$

Therefore, the inductive hypothesis, or rather the fact as we have just shown, that $x^0(t_0 + nT) \in \eta_{t_0}$ implies that $x^0(t_0 + (n+1)T) \in \eta_{t_0}$. The inductive inference is complete. \blacksquare

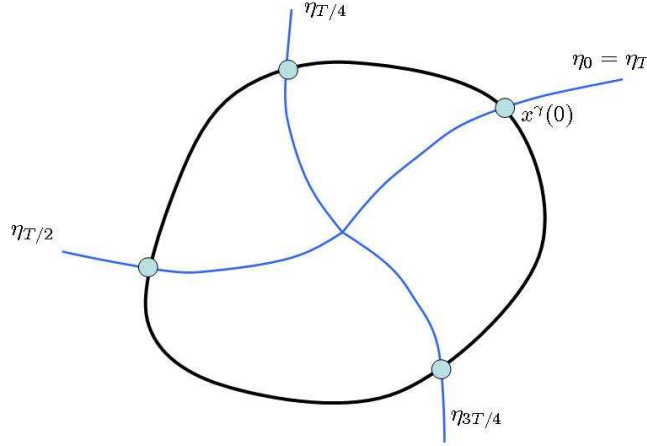


Figure 3.6: Isochron layout in the domain of attraction.

Figure 3.5 is a depiction of the periodicity in \mathcal{W} . Figure 3.6 illustrates the structure of isochrons in \mathcal{W} .

The corollary above is necessary in order to define periodicity in \mathcal{W} . We are then going to make use of periodicity to spell out a differential equation to compute the phase, associated with the generic ODE in (2.1). Then, the first theorem will be necessary to normalize this phase equation. Recall that in this part of our work about isochrons, we are only concerned in systems, with all perturbations absent, but the initial condition for a solution of (2.1) may not reside on γ , for all perturbations applied were before $t = 0$. In all, the phase equation will be applicable only to unperturbed oscillators.

3.3 Definition of Phase for an Unperturbed Oscillator

In this section, we are to define the notion of generalized period first. Definition 3 in Section 2.1.6 describes the simple procedure to compute the period on γ , the limit cycle. There, we choose a point on the limit cycle, $x^\gamma(t_0)$. Because of this choice on γ , our oscillator as given in (2.1) will never leave γ . If we record the times that our oscillator hits $x^\gamma(t_0)$ over and over, after the initial time, t_0 , we may easily calculate the difference of each hitting time

and t_0 . The smallest of these differences is going to be the period we seek.

Corollary 2, however, enables us to refine Definition 3. We now know that even if we do not start our system from an initial condition on γ , we are going to be hitting a point on the same isochron after subsequent intervals of length T , the familiar period as given by Definition 3. therefore, via isochrons, we define the generalized period as follows.

Definition 12 (Generalized Period) *Let $x^\gamma(t)$ be the steady-state periodic solution on γ , the limit cycle, of the generic ODE in (2.1). Let $x^\gamma(t_0)$, naturally a point on γ , be such that $x^\gamma(t_0) \in \eta_{t_0}$, η_{t_0} being a single isochron, associated with γ . Also let $x^0(t)$ be another solution of (2.1), and choose $x^0(0)$ such that $x^0(0) \in \mathcal{W}$, \mathcal{W} being the domain of attraction associated with γ , so that $x^0(t)$ tends to approach γ , as time progresses. Furthermore, let $x^0(t_0) \in \eta_{t_0}$. We define the set*

$$\mathcal{T} = \{T^i \mid \Phi(t_0 + T^i, t_0, x^0(t_0)) \in \eta(t_0)\},$$

and the smallest positive number in \mathcal{T} as the generalized period in \mathcal{W} , associated with γ . Note that the value of the generalized period is again T , equal to the value of the period defined on γ , as stated by Definition 3.

After formally defining the generalized period, with the help of isochrons, we proceed to define the generalized frequency and angular frequency in \mathcal{W} .

Definition 13 (Generalized Frequency) *Through T , the generalized period as given in Definition 12, we define the generalized frequency in \mathcal{W} , associated with γ , as*

$$f_0 = \frac{1}{T}.$$

Notice that we have dropped the γ notifier, as opposed to the expression given in Definition 4, for we have developed the notion of period and then phase in \mathcal{W} , not just on γ . The generalized angular frequency is defined as

$$\omega_0 = 2\pi f_0 = \frac{2\pi}{T}.$$

The transition from the generalized angular frequency to the generalized angular phase is accomplished as follows.

Definition 14 (Evolution of Angular Phase) We define the angular phase in \mathcal{W} , ϕ , as

$$\frac{d\phi}{dt} = \omega_0, \quad (3.18)$$

where ω_0 is the generalized angular frequency in \mathcal{W} .

ϕ in Definition 14 is in radians. For our purposes, we would like to have phase in units of time.

Definition 15 (Evolution of Phase in Units of Time) Let us define the phase in units of time, \hat{t} , in \mathcal{W} , associated with γ of the generic ODE in (2.1), as $\hat{t} = \phi/\omega_0$, where ω_0 is the generalized angular frequency in \mathcal{W} . The differential equation to compute \hat{t} is naturally

$$\frac{d\hat{t}}{dt} = 1. \quad (3.19)$$

This differential equation basically applies to unperturbed systems, in ODE form, as in (2.1).

Although the definitions above, except for the generalized period, may seem inessential and superfluous, we have carried out this tedious series of derivations, in order to spell out a formal definition for \hat{t} , the phase in units of time, in \mathcal{W} . Brown et al. in [2], state that they readily define the phase for unperturbed ODE system, as given in Definition 15, but in here we have based our understanding, of the generalized period in the domain of attraction, on the theory of isochrons, and then spelt out \hat{t} , after some prosaic definitions. This approach is similar to the one that Brown briefly outlines in [1].

(3.19) is a differential equation, defining the evolution of \hat{t} . The solution of this differential equation is to be trivially computed. We need an initial condition as well. Let us now formally define \hat{t} and then show that the form that is to be proposed solves (3.19).

Definition 16 (Phase in Units of Time) Let $x^\gamma(t^*)$ be the steady-state periodic solution of (2.1), $x^\gamma(t)$, evaluated at $t = t^*$. The phase in units of time of $x^\gamma(t^*)$ is defined as

$$\hat{t}(x^\gamma(t^*)) = t^*. \quad (3.20)$$

Let $x(t)$ be a solution of (2.1) such that $x(0) \notin \gamma$, but $x(0) \in \mathcal{W}$. $x(t^*)$ is $x(t)$ evaluated at $t = t^*$. Then the phase in units of time of $x(t^*)$ is defined as

$$\hat{t}(x(t^*)) = \hat{t}(x^\gamma(t')), \quad \text{such that } x(t^*), x^\gamma(t') \in \eta_\nu. \quad (3.21)$$

Examining Definition 16 above, suspicions may arise because of the periodicity of $x^\gamma(t)$. Let us assume temporarily that $0 \leq t'' < T$ and that $t' = t'' + nT$, where n is an integer and T is the period of oscillation. In (3.21), we know that $x^\gamma(t') = x^\gamma(t'' + nT) = x^\gamma(t'')$. This makes $\eta_{t'} = \eta_{t''+nT} = \eta_{t''}$, since an isochron must be associated with a single point on γ . Therefore $\eta_{t''}$ is the same set as $\eta_{t''+nT}$. However, then we have $\hat{t}(x^*(t)) = \hat{t}(x^\gamma(t')) = \hat{t}(x^\gamma(t'' + nT)) = t'' + nT$. It seems that the phase of a single point of a solution must not take more than one value. But recall that examining solutions versus running time t , $x^\gamma(t)$ is not distinguishable from $x^\gamma(t + nT)$. In fact, this is the essence of periodicity. Therefore, it is natural that the phase of a single point, i.e. $\hat{t}(x(t^*))$, is determined as a constant number t'' plus an indefinite expression nT . The important aspect of (3.21) is that whichever $x^\gamma(t') = x^\gamma(t'' + nT)$ is found to be on the same isochron $\eta_{t'}$ with $x(t^*)$, $\hat{t}(x(t^*))$ must be set to the time argument of $x^\gamma(t' = t'' + nT)$, which is t' . In all, we do not confine t' to the interval $[0, T)$.

Theorem 3 *Isochrons are the level sets of \hat{t} .*

Proof: Let $x(t)$ be a solution of (2.1) such that $x(0) \in \eta_{t_0}$. We also know that $x^\gamma(t_0) \in \eta_{t_0}$. By Definition 16, we have

$$\hat{t}(x(0)) = \hat{t}(x^\gamma(t_0)) = t_0.$$

All possible $x(0) \in \eta_{t_0}$ satisfy $\hat{t}(x(0)) = t_0$. This makes η_{t_0} the level set of \hat{t} corresponding to the value $\hat{t} = t_0$. Letting t_0 vary in the range $[0, T)$, we see that isochrons are the level sets of \hat{t} . ■

Corollary 3 (Theorem 3) *Let $x(t)$ be a solution of (2.1) such that $x(0) \in \mathcal{W}$. Then, at a particular t^* , $x(t^*)$ and $x^\gamma(\hat{t}(x(t^*)))$ are on the same isochron.*

Proof(Explanation of Corollary 3): Let us check if the phases of $x(t^*)$ and $x^\gamma(\hat{t}(x(t^*)))$ are equal. We have, by Definition 16,

$$\hat{t}(x^\gamma(\hat{t}(x(t^*)))) = \hat{t}(x(t^*)).$$

Then, we know that $x(t^*)$ and $x^\gamma(\hat{t}(x(t^*)))$ are on the same level set of \hat{t} . Isochrons are the level sets of \hat{t} , by Theorem 3. Hence the claim. ■

Theorem 3 enables us to introduce the following alternative definition for isochrons.

Definition 17 (Alternative Isochron Definition) Let $x(t)$ be a solution of (2.1) such that $x(0) \in \mathcal{W}$. η_{t_0} can then be defined as

$$\eta_{t_0} = \{x(0) \mid \hat{t}(x(0)) = t_0\}. \quad (3.22)$$

Now we can show that \hat{t} introduced in Definition 16 solves (3.19) with an appropriate initial condition.

Theorem 4 Let $x(t)$ be a solution of (2.1) such that $x(0) \in \eta_{t_0}$. Then, $\hat{t}(x(t))$ solves (3.19), as in

$$\frac{d\hat{t}}{dt} = 1, \quad \text{with} \quad \hat{t}|_0 = t_0, \quad (3.23)$$

where $\hat{t}|_0$, \hat{t} evaluated at $t = 0$, is an initial condition.

Proof: Since $x^\gamma(t_0) \in \eta_{t_0}$, we have by Definition 16

$$\hat{t}|_0 = \hat{t}(x(0)) = \hat{t}(x^\gamma(t_0)) = t_0,$$

so the initial condition in (3.23) is satisfied.

Noting that $x^\gamma(t + t_0)$ is a solution for (2.1) with the initial condition $x^\gamma(t_0)$, we know that at any time t , $x(t)$ and $x^\gamma(t + t_0)$ will instantaneously be on the same isochron, by Theorem 2. Then, by Definition 16, we have, at any time t ,

$$\hat{t}(x(t)) = \hat{t}(x^\gamma(t + t_0)) = t + t_0.$$

It is easy to compute

$$\frac{d}{dt}\hat{t}(x(t)) = \frac{d(t + t_0)}{dt} = 1,$$

which shows that $\hat{t}(x(t)) = t + t_0$ solves the differential equation in (3.23). ■

Summarizing, we visualize isochrons as the level sets of \hat{t} in \mathcal{W} , associated with γ . $\hat{t} = \hat{t}(x)$, \hat{t} depends on the states vector, x , in \mathcal{W} . The points in \mathcal{W} that satisfy $\hat{t} = t_0$, for example, form η_{t_0} , the isochron that is in phase with $x^\gamma(t_0)$. As another example, let us assume the points that satisfy $\hat{t} = t_1$ and $\hat{t} = t_2$, for $t_2 > t_1$, form the sets η_{t_1} and η_{t_2} , respectively. There is no doubt that η_{t_1} and η_{t_2} are the same set if $t_2 - t_1 = nT$, for a positive integer n , where T is the generalized period in \mathcal{W} .

Considering $\hat{t} = \hat{t}(x)$ is essential in deriving a partial differential equation. Let us rewrite $d\hat{t}/dt = 1$, as in

$$\left[\frac{\partial \hat{t}}{\partial x} \right]^\top \frac{dx}{dt} = \left[\frac{\partial \hat{t}}{\partial x} \right]^\top \cdot f(x) = 1. \quad (3.24)$$

(3.24) is a PDE (Partial Differential Equation). Since we set in Definition 16 that \hat{t} is a function of x only, $\partial\hat{t}/\partial x$ is also a function of x only. In this aspect, while computing the values for $\partial\hat{t}/\partial x$, $x \in \mathcal{W}$ to be able to compute $\partial\hat{t}/\partial x$. The same discussion is valid also for $f(x)$.

We also need boundary conditions to solve PDEs. Spelling out the boundary condition for (3.24) is simple. $\hat{t}(x^\gamma(t_0)) = t_0$ for $t_0 \in [0, T)$ is our boundary condition. This is true, because the phase in units of time on γ is expected to be the time tag of $x^\gamma(t)$ for an unperturbed oscillator. In all,

$$\left[\frac{\partial\hat{t}}{\partial x} \right]^\top f(x) = 1, \text{ with } \hat{t}(x^\gamma(t_0)) = t_0, \forall t_0 \in [0, T), \quad (3.25)$$

is the PDE to solve for \hat{t} over the whole domain of attraction, \mathcal{W} .

The next theorem associates $\partial\hat{t}/\partial x$, the phase gradient evaluated on γ , with $v_1(t)$.

Theorem 5 *The phase gradient evaluated on γ ,*

$$\frac{\partial\hat{t}(x^\gamma(t))}{\partial x^\gamma(t)} = v_1(t). \quad (3.26)$$

Proof: Let $x(t)$ be a solution of (2.1) such that $x(0) \in \eta_0$, so that $\hat{t}(x(0)) = 0$ by Definition 16. And it follows that $\hat{t}(x(t)) = t$, by Theorem 4.

Isochrons are the level sets of \hat{t} by Theorem 3. $\partial\hat{t}(x(t))/\partial x(t)$, the phase gradient at some $x(t)$, must be orthogonal to the linearization of η_t at $x(t)$. Observe that $x(t) \in \eta_t$ because of the way $x(t)$ is defined.

Now, we know that $\partial\hat{t}(x^\gamma(t))/\partial x^\gamma(t)$ must be orthogonal to the linearization of η_t at $x^\gamma(t)$. By Theorem 1, we know that $v_1(t)$ is orthogonal to the linearization of η_t at $x^\gamma(t)$. Therefore, we have $\partial\hat{t}(x^\gamma(t))/\partial x^\gamma(t) = c v_1(t)$, where the constant $c \neq 0$.

Evaluating (3.24) at $x^\gamma(t)$, and plugging in $\partial\hat{t}(x^\gamma(t))/\partial x^\gamma(t) = c v_1(t)$ and $\dot{x}^\gamma(t) = f(x^\gamma(t)) = u_1(t)$,

$$c v_1^\top(t) u_1(t) = 1.$$

But $v_1^\top(t) u_1(t) = 1$, by biorthogonality. Therefore, $c = 1$. We obtain (3.26). It can be declared that $v_1(t)$ is used to normalize the PDE in (3.24). Also note that $\partial\phi(x^\gamma(t))/\partial x^\gamma(t) = \omega_0 v_1(t)$. ■

There is one other aspect of the PDE in (3.25) to note. We may visualize dx/dt as a velocity vector. The gradient expression, $\partial\hat{t}/\partial x$, is by definition the vector defining the

linearization of an isochron, at point x , in \mathcal{W} . The linearization of an isochron is a hyperplane, and the gradient $\partial\hat{t}/\partial x$ at x is orthogonal to any vector that resides in this hyperplane. (3.25) tells us that the velocity vector, associated with the generic ODE in (2.1), never completely resides in these linearizations of isochrons. This means that dx/dt is always transverse to isochrons, over the whole domain of attraction, \mathcal{W} . Otherwise, the scalar product of the phase gradient and the velocity vector would have to be exactly zero. As an example, recalling the proof of Theorem 1, linearized form of the isochron that passes through $x^\gamma(t_0)$ is spanned by $\{u_2(t_0), \dots, u_M(t_0)\}$. $u_1(t_0)$ is the velocity vector at $x^\gamma(t_0)$. $u_1(t_0)$ cannot be expressed as a linear combination of the vectors spanning the linearized form of the isochron, because $u_i(t_0)$ for $1 \leq i \leq M$ is a linearly independent set.

Isochron structures on and around γ are best perceived through simple examples. In the next section, we explore into how expressions for isochrons can be calculated only for very simple oscillatory dynamic systems. We demonstrate particularly two methods on an example, expressed in polar coordinates.

3.4 Isochrons in DAE Systems

There are some subtleties to be considered when analyzing the structure of isochrons for systems in DAE form. The first task is to modify Definition 11 for isochrons in ODE form. This modification proves to be trivial, since only Φ is replaced by Υ . So we do not include a definition statement for the DAE case.

Definition 18 (Isochrons for DAE Systems) *Let $x^\eta(t)$ be a solution of the generic ODE in (2.4). $x^\gamma(t)$ is the periodic steady-state solution of (2.4). The isochron with time tag t_0 , which we call η_{t_0} , is defined to be the set*

$$\eta_{t_0} = \left\{ x^\eta(t_0) \mid \lim_{\tau \rightarrow \infty} [\Upsilon(\tau, t_0, x^\eta(t_0)) - x^\gamma(\tau)] = 0 \right\}, \quad (3.27)$$

where $x^\gamma(\tau) = \Upsilon(\tau, t_0, x^\gamma(t_0))$. Υ is the state transition function, associated with (2.4).

The next theorem is the modified version of Theorem 1, which was proved for the ODE case in Section 3.2.

Theorem 6 *If η_{t_0} in Definition 18 is linearized into a subspace, then $\mathbf{C}^\top(t)v_1(t_0)$ is orthogonal to that subspace.*

Proof: We stated in Section 2.2.3 that generic solutions $x(t)$ of (2.4) reside in a certain manifold of \mathfrak{R}^M , because of the properties of q , the nonlinear vector function in (2.4) [3]. Then, it can be shown that a general solution of the linearized form of (2.4),

$$\frac{d}{dt}(\mathbf{C}(t)y(t)) = \mathbf{G}(t)y(t),$$

at $t = t_0$ can be expressed as a linear combination of only $m < M$ vectors in \mathfrak{R}^M [3].

In view of the note stated above, it is clear that η_{t_0} linearized around $x^\gamma(t_0)$ is going to be a subspace spanned by $(m - 1)$ vectors. Our purpose here is to find out these $(m - 1)$ vectors and naturally the vector that is orthogonal to these vectors.

The Taylor expansion of $x^\eta(\tau) = \Upsilon(\tau, t_0, x^\eta(t_0))$, in (3.27), around $x^\gamma(t_0)$ is given by

$$x^\eta(\tau) \approx \Upsilon(\tau, t_0, x^\gamma(t_0)) + \frac{\partial \Upsilon(\tau, t_0, x^\gamma(t_0))}{\partial x^\gamma(t_0)} z, \quad (3.28)$$

where $z = x^\eta(t_0) - x^\gamma(t_0)$. Then, the expression in (3.27), making use of the approximation in (3.28), can be written as

$$\begin{aligned} \lim_{\tau \rightarrow \infty} [\{x^\eta(\tau)\} - \{x^\gamma(\tau)\}] &= 0 \\ \lim_{\tau \rightarrow \infty} \left[\left\{ x^\gamma(\tau) + \frac{\partial \Upsilon(\tau, t_0, x^\gamma(t_0))}{\partial x^\gamma(t_0)} z \right\} - \{x^\gamma(\tau)\} \right] &= 0 \\ \frac{\partial \Upsilon(\tau, t_0, x^\gamma(t_0))}{\partial x^\gamma(t_0)} z &= 0 \end{aligned} \quad (3.29)$$

Note that the last equation follows from the fact that for DAE systems

$$\begin{aligned} \frac{\partial \Upsilon(\tau, t_0, x^\gamma(t_0))}{\partial x^\gamma(t_0)} &= \mathbf{K}(\tau, t_0) \\ &= \sum_{i=1}^m \exp(\mu_i(\tau - t_0)) u_i(\tau) v_i^\top(t_0) \mathbf{C}(t_0), \end{aligned}$$

where m is the number of Floquet eigenmodes, with finite Floquet multipliers. We assume that $\mu_i > -\infty$ for $1 \leq i \leq m$. On the other hand, $\mu_i = -\infty$ for $(m + 1) \leq i \leq M$, since $\mathbf{C}(t)u_i(t) = 0$ for again $(m + 1) \leq i \leq M$, i.e. the null space of $\mathbf{C}(t)$ is spanned by $u_i(t)$ for $(m + 1) \leq i \leq M$.

For $\tau \gg t_0$, we have

$$\begin{aligned} \frac{\partial \Upsilon(\tau, t_0, x^\gamma(t_0))}{\partial x^\gamma(t_0)} &= \sum_{i=1}^m \exp(\mu_i(\tau - t_0)) u_i(\tau) v_i^\top(t_0) \mathbf{C}(t_0) \\ &\approx u_1(\tau) v_1^\top(t_0) \mathbf{C}(t_0) \end{aligned}$$

for again, we assume that $\mu_1 = 0$, and $-\infty < \mu_i < 0$ for $2 \leq i \leq m$. This is how we get (3.29) [3].

Now we proceed to analyze (3.29). Recall that $u_1(t)$ is a periodic solution of the forward LPTV equation derived from (2.4), i.e. $d/dt(\mathbf{C}(t)y) = \mathbf{G}(t)y$. Not all entries of $u_1(t)$ are allowed to be zero at the same time, for then the oscillation on γ would stop at a single point on this limit cycle. This is not one of our assumptions. We assume that γ consists of infinitely many points, not just one.

Then, the condition to make the left-hand side zero of (3.29) is given by the scalar equation

$$v_1^\top(t_0)\mathbf{C}(t_0)z = 0. \quad (3.30)$$

We have to decide now if this equation defines a hyperplane. There is no doubt that

$$v_1(t) \cdot [\mathbf{C}(t)u_2(t), \dots, \mathbf{C}(t)u_m(t)],$$

for $t \geq 0$ [3]. Therefore, z can only be written as a linear combination of $(m - 1)$ linearly independent vectors, i.e.

$$z = \sum_{i=2}^m a_i u_i(t_0).$$

This fact makes $v_1(t)$ orthogonal to a subspace of dimension $(m - 1)$. To declare $v_1(t_0)$ as the vector defining a hyperplane, we should have been able to write z as a linear combination of $(M - 1)$ linearly independent vectors. However, also note that $\dot{x}(t)$, the time-derivative of $x(t)$, is allowed to be a linear combination of the set

$$\{\exp(\mu_1 t)u_1(t), \dots, \exp(\mu_m t)u_m(t)\},$$

in the close neighborhood of γ . Therefore, $\dot{x}(t)$ does not have any components along any elements of the set

$$\{\exp(\mu_{m+1} t)u_{m+1}(t), \dots, \exp(\mu_M t)u_M(t)\},$$

in the close neighborhood of γ , because $\mu_i = -\infty$ for $(m + 1) \leq i \leq M$. That means in the region very close to γ , in the domain of attraction, the linearization of η_{t_0} cannot have components along $\{u_{m+1}(t_0), \dots, u_M(t_0)\}$, i.e. the linearized form of η_{t_0} , in the close neighborhood of γ , is a subspace only, not a hyperplane, and $v_1(t_0)$ defines this subspace, hence the claim. ■

Along with the theorem and its proof above, we need to modify the theorem about periodicity and its proof for the DAE case. However, the modification is only replacing Φ with Υ . Therefore, we state the following theorem only and not its proof.

Theorem 7 *Let $x^0(t)$ be a solution of the generic ODE in (2.1), and let $x^0(0)$ reside in the domain of attraction, \mathcal{W} , so that $x^0(t)$ approaches γ as time progresses. Let $x^0(t_0)$ be on the same isochron, η_{t_0} , as $x^\gamma(t_0)$. Then, $x^0(t_0 + nT)$, for nonnegative integers n , are also on η_{t_0} . T is the period on γ .*

With the help of Theorem 7, we are again induced to define periodicity in the domain of attraction, \mathcal{W} , associated with γ , of the system in (2.4). Therefore, we define the generalized period as in Definition 12, for the DAE case this time. Naturally, the definitions of the generalized frequency, angular phase, and phase in units of time follow as in Definitions 13, 14, and 15, respectively.

The following discussion differs from its counterpart of the ODE case. Through our definitions, we define the phase in units of time, in the domain of attraction of γ , as in

$$\frac{d\hat{t}}{dt} = 1, \text{ with } \hat{t}(0) = 0.$$

Notice that in the generic DAE of (2.4), the states vector, x , is an implicit variable. (2.4) defines the time derivative of q , the nonlinear functions vector. Let us intuitively choose to figure out then the sensitivity of \hat{t} , the phase, with respect to q , i.e. $\partial\hat{t}/\partial q$, and see where this choice leads.

The phase equation for an unperturbed oscillator, described as a DAE, can be written as

$$\frac{\partial\hat{t}}{\partial q} \cdot \frac{dq}{dt} = 1.$$

Notice that

$$\frac{\partial\hat{t}}{\partial q} \cdot f(x) = 1$$

is true over the whole domain of attraction, associated with γ . Let us evaluate these equivalent equations on γ only. We have

$$\begin{aligned} \frac{\partial\hat{t}}{\partial q} \cdot \left[\frac{\partial q}{\partial x^\gamma} \frac{dx^\gamma}{dt} \right] &= 1 \\ \frac{\partial\hat{t}}{\partial q} \cdot [\mathbf{C}(t)u_1(t)] &= 1 \end{aligned}$$

defining a normalization condition on γ . $v_1(t)$ could immediately be substituted for $\partial\hat{t}/\partial q$, on γ , since $v_1(t) \cdot (\mathbf{C}(t)u_1(t)) = 1$ [3]. However, there may be other vectors satisfying this condition. The question is how we know exactly that on γ , $v_1(t) = \partial\hat{t}/\partial q$.

\hat{t} is a spatial variable, i.e. $\hat{t} = \hat{t}(q(x(t)))$. Notice that we have expressed \hat{t} as such, because x is an implicit variable in the generic DAE of (2.4). Also we have by definition that $\hat{t}(q(x^\gamma(t))) = t$ on the limit cycle. Recall that the isochrons are actually the level sets of \hat{t} over \mathcal{W} , the domain of attraction. If we have some points x that satisfy $\hat{t}(q(x)) = t_0$, that means these points x are in phase with $x^\gamma(t_0)$, and all these points x together with $x^\gamma(t_0)$ constitute the isochron expressed as η_{t_0} .

Since we have $\hat{t} = \hat{t}(q(x(t)))$, the gradient of \hat{t} is actually given as $\partial\hat{t}/\partial q$ over \mathcal{W} . On γ , we know by Theorem 6 that $\partial\hat{t}/\partial x$ is in the same direction as $\mathbf{C}^\top(t)v_1(t)$. However, we also know that $(\partial\hat{t}/\partial q) \cdot [\mathbf{C}(t)u_1(t)] = 1$, on γ . by the phase equation that we derived. We have the normalization condition that $v_1(t) \cdot [\mathbf{C}(t)u_1(t)] = 1$. Therefore, we must maintain that $\partial\hat{t}/\partial q = v_1(t)$ on γ .

Let us also state that

$$\frac{\partial\hat{t}}{\partial q} \cdot f(x) = 1, \quad \text{with } \hat{t}(q(x^\gamma(t))) = t \forall t \in [0, T] \quad (3.31)$$

is the PDE (Partial Differential Equation) to solve for \hat{t} . Notice that this equation has almost the same form as the one in the ODE case, with $\partial\hat{t}/\partial x$ replaced by $\partial\hat{t}/\partial q$.

We have outlined and provided explanations above on how to modify our definitions and theorems in Sections 3.1 to 3.3 for the DAE case. The most crucial parts of the modification are that $\partial\hat{t}/\partial q = v_1(t)$, and that we must not forget that $\partial\hat{t}/\partial q$, in the close neighborhood of γ , does not define a hyperplane, with dimension $(M - 1)$, but a subspace with dimension $(m - 1)$, m being the number of Floquet modes with finite Floquet exponents that correspond to the LPTV equation derived from the generic DAE in (2.4).

3.5 Analytical Methods of Computing Isochrons For Simple Systems

Definition 11 for isochrons suggests that we make use of the state transition function, Φ , to compute analytical expressions for isochrons over \mathcal{W} , associated with γ . However, although this is a plausible method, it requires that oscillator equations are analytically solvable. For purposes of demonstration, we choose to analyze an extremely simple example, expressed

in polar coordinates on the plane.

The coupled equations of our simple example read as follows.

$$\dot{r} = 1 - r \quad (3.32)$$

$$\dot{\theta} = r \quad (3.33)$$

The solution for the system in (3.32) and (3.33) are as follows.

$$r(t) = 1 - (1 - r_0)e^{-t} \quad (3.34)$$

$$\theta(t) = t - (1 - r_0)(1 - e^{-t}) + \theta_0 \quad (3.35)$$

Above, $r_0 = r(t = 0)$ and $\theta_0 = \theta(t = 0)$. It is easy to see that as time progresses, $r(t) \rightarrow 1$, and $\theta(t) \rightarrow (t + \theta_0 + r_0 - 1)$. Also if $r_0 = 1$, $r(t) = 1$, and $\theta(t) = t + \theta_0$, $\forall t \geq 0$.

It must be noted here that θ is one of the states for this particular example. In general, the system phase, which happens to be θ in this example, does not have to be a state variable. Therefore, this example is just a contrived one for illustration purposes. Also, we will be showing shortly that θ accounts for the phase on γ only. The expression for phase around γ , actually in the domain of attraction of differs from θ .

$r = 1$ defines the only limit cycle, γ , of this system. \mathcal{W} , the domain of attraction associated with $r = 1$, is the whole plane.

Any periodic solution, whose points constitute γ , happens to have the asymptotically orbital stability property, for any solution, with an initial condition not on γ , approaches $r = 1$, as time progresses.

Also, any periodic solution on γ has asymptotic phase. Let $r(t) = 1$ and $\theta(t) = t$ be a periodic solution on γ . As stated before, a solution, whose initial condition at $t = 0$ is not on γ , will take the form $r(t) \rightarrow 1$ and $\theta(t) \rightarrow (t + \theta_0 + r_0 - 1)$. Therefore, the difference between these expressions and the periodic solution, as time progresses, approaches a constant, for the phase, θ , on γ . This constant is $\theta_0 + r_0 - 1$. This fact ensures asymptotic phase.

The observation about the asymptotic phase associated with $r = 1$, the limit cycle, actually defines the steps to be followed in order to compute the expression for the isochrons, associated with γ , which is $r = 1$ in this system, through Definition 11. Let us formulate the problem of finding an expression for isochrons as follows. The state transition function

of the system in (3.32) and (3.33) is naturally

$$\Phi(t, 0, x(0)) = \begin{pmatrix} 1 - (1 - r_0)e^{-t} \\ t - (1 - r_0)(1 - e^{-t}) + \theta_0 \end{pmatrix}, \quad (3.36)$$

where we have $x(0) = (r_0 \theta_0)^\top$, the initial condition that is not necessarily on γ , $r = 1$. An initial condition on γ would have the form $x^\gamma(0) = (1 \ c)$. We have to spell out

$$\Phi(t, 0, x(0)) - \Phi(t, 0, x^\gamma(0)) = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

and evaluate both sides of this equality as $t \rightarrow \infty$. This is what Definition 11 dictates us to do to figure out an expression for the isochrons of this system.

The expression that we find is $c = \theta_0 + r_0 - 1$. The fact that θ is a state in this example is essential in that we may now call $\theta = c$ the level sets of θ on γ . Fortunately, the angular phase of $r = 1$ is equal to θ , for this example in particular. Therefore, we readily have access to values of the phase on γ . Suppose that $c \in [0, 2\pi)$, so that $(1, c)^\top$ is allowed to be any point on $r = 1$, with no point excluded. Then, through $c = \theta_0 + r_0 - 1$ we deduce that there are points in \mathcal{W} that evaluate to the same value of the level set given by $\theta = c$, for a particular c . These points are declared to reside on the same isochron. This fact makes

$$\eta_c = \left\{ x(0) = \begin{pmatrix} r_0 \\ \theta_0 \end{pmatrix} \middle| \theta_0 + r_0 - 1 = c \right\} \quad (3.37)$$

a single isochron out of the many in \mathcal{W} . Calling ϕ the phase in \mathcal{W} , we have

$$\phi = \theta + r - 1 \quad (3.38)$$

as the expression for ϕ . Notice that $\phi = \theta$ on $r = 1$. We stated before that the phase in \mathcal{W} differs from θ for this example. In fact, ϕ in (3.38) generally depends on r as well in \mathcal{W} . Brown et al. in [2] draw attention to this phenomenon.

Notice that we have called the phase of our system ϕ , but not \hat{t} . We reach \hat{t} from ϕ through a simple normalization. The angular frequency of this system in \mathcal{W} is given by $\omega_0 = 2\pi/T = 1$, for $T = 2\pi$. Using the relation that $\phi = \omega_0 \hat{t}$, we find out ϕ yields the same value as \hat{t} numerically, for this solution.

Now let us compute the gradient expression of (3.38) as in

$$\nabla \phi = \begin{pmatrix} \frac{\partial \hat{t}}{\partial r} \\ \frac{\partial \hat{t}}{\partial \theta} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

The scalar product of this gradient and the velocity vector yields

$$(\nabla\phi)^\top \begin{pmatrix} 1-r \\ r \end{pmatrix} = w_0 = 1,$$

as expected. We are justified once more that ϕ is the same as \hat{t} numerically for this example.

Again, to figure out the structure of isochrons in \mathcal{W} , we have to let $\phi = \theta + r - 1$ take constant values in the interval $[0, T) = [0, 2\pi)$. Each such separate equation will obviously yield the equation for a single isochron. $\phi_0 = \theta + r - 1$ for example is the level set, i.e. isochron, of ϕ , whose elements are in phase with $(1 \ \phi_0)^\top$.

Noting the method outlined above as the first procedure in figuring out expressions for isochrons in simple two-dimensional systems, we proceed to explain the second method, for which we refer to Winfree [19]. This second method is superior to the first one in that it does not require an analytical state transition function to exist. Winfree exploits the polar symmetry in systems like the one in (3.32) and (3.33).

For the second method, we repeat that the angular frequency of our system is $\dot{\phi} = \omega_0 = 1$. Again, ϕ is the phase of our system in radians. Winfree in [19] guesses that ϕ must have polar symmetry, so that it is of the form given in $\phi = \theta - h(r)$, where h is a function of r . Notice that this formulation for ϕ is only valid for systems expressed in polar coordinates and whose limit cycles are circles with the origin as their centers. We have

$$\frac{d\phi}{dt} = 1 = \frac{d\theta}{dt} - \frac{dh}{dr} \frac{dr}{dt},$$

and

$$\frac{dh}{dr} = \frac{\dot{\theta} - 1}{\dot{r}} = \frac{r - 1}{1 - r} = -1.$$

Notice that $h(r) = -r + c$, where c is some integration constant. Then, $\phi = \theta - h(r) = \theta + r - c$. Setting $\phi = \theta$, with $r = 1$, since the familiar system phase on γ is θ , we have again the expression for the system phase in \mathcal{W} as $\phi = \theta + r - 1$. The isochrons of the system are the level sets of the phase.

Before moving on, let us note an interesting observation, again pointed out in [19]. If we modify the system in our example as

$$\dot{r} = 1 - r \tag{3.39}$$

$$\dot{\theta} = 1 \tag{3.40}$$

the phase of this modified system turns out to be $\phi = \theta$, i.e. the phase is a function of only θ all over \mathcal{W} . Winfree's method directly conveys this fact. With again $\phi = \theta - h(r)$, accounting for polar symmetry, we have

$$\frac{dh}{dr} = \frac{\dot{\theta} - 1}{\dot{r}} = 0.$$

Then, $h(r) = 0$, just a constant that turns out to be zero, to have $\phi = \theta$. This is an exceptional case where we have radial isochrons.

Let us also analyze isochron behaviour on γ , for the modified system in (3.39) and (3.40). Recall that $u_1(t)$ is a periodic solution of the linear equation to be derived from these equations, and $v_1(t)$ is a periodic solution of the adjoint linear equation. We have always employed the normalization condition in $v_1^T(t)u_1(t) = 1$. For this modified system, we have to be able to show the validity of this normalization condition, since we have numerically \hat{t} as the same as ϕ , for again $T = 2\pi$. Numerically speaking,

$$v_1(t) = \nabla \hat{t} = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

at every point on γ . We also have

$$u_1(t) = \frac{d}{dt} \begin{pmatrix} r \\ \theta \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

on γ . The normalization condition is naturally satisfied, but we observe a more conspicuous bit of information that $v_1(t) = u_1(t)$ at every point on γ . Systems like these are called self-adjoint. They are significant in that once we have figured out $u_1(t)$, we have figured out $v_1(t)$ as well. $u_1(t)$ is just the derivative of the steady-state periodic solution on γ , $x^\gamma(t)$. We observe through this example that in self-adjoint systems, the velocity vector on γ , $u_1(t_0)$, is orthogonal to the isochron η_{t_0} , at $x^\gamma(t_0)$, for all $t_0 \in [0, T)$.

We must again note that these analytical methods can be used only in very simple two-dimensional systems. In this section, we frequently pointed out that we are figuring out expressions for isochrons, over the whole domain of attraction, \mathcal{W} , associated with γ , the limit cycle. This is because we most of the time assume that there is only a single limit cycle of interest. However, when there are more limit cycles associated with the simple system we are working on, these methods, if they can, are capable of conveying the isochron portrait in the whole domain, in which the states vector, x , is defined.

3.6 Comments on Numerical Methods

We outline in here a very simple numerical method, to print the isochron portrait, associated with an oscillator, with a two-dimensional state. However, we have to note one particular aspect of the method we are about to explain. In view of our last comment at the end of the previous section, the following numerical methods can compute the structure of isochrons around a single limit cycle of the oscillator at hand, as opposed to the analytical methods of the previous section, which were able to compute isochron portraits over the whole domain, in which the states of the oscillator are defined. Although this aspect is a limitation, this numerical method are always more plausible, since neither an analytical state transition function nor polar symmetry on the plane is required.

Solving the PDE in (3.25) for \hat{t} and then printing the level sets of \hat{t} in \mathcal{W} naturally yields the isochrons in \mathcal{W} . However, this is not a plausible method. The method to be outlined instead, provided by Izhikevich as an exercise in [9], overcomes most of the stated difficulties, associated with the first numerical method. We still prefer to work on oscillators with two-dimensional state vectors. In [9], for the purpose of displaying isochron layout around γ , the PDE we have derived in (3.25) is not needed. Izhikevich makes use of only the generic ODE in (2.1).

For the second method, again the steady-state periodic solution, $x^\gamma(t)$, is required. For demonstration purposes, we pick two points that are very close to a single point on γ . Let us pick two solutions of (2.1) and call these $x^1(t)$ and $x^2(t)$. Let $x^1(0)$ and $x^2(0)$ be the first and the second point respectively, which we have chosen to be very close to a point on γ . A time reversal operation is carried out to numerically integrate backward, starting with initial condition $x^1(0)$, and then the same integration task is accomplished with initial condition $x^2(0)$. The essence is that $x^1(0)$ and $x^2(0)$ are assumed to be on the same isochron, for they are chosen to be so close to each other and to a point on γ that we will call, for simplicity, $x^\gamma(0)$. So $x^1(0)$, $x^2(0)$, and $x^\gamma(0)$ are on the isochron called η_0 .

It happens that at any time $-t_0$, which is a negative time value for we solve (2.1) backwards in time, $x^1(-t_0)$ and $x^2(-t_0)$ still are instantaneously on the same isochron, but not the isochron they were at $t = 0$. The isochron these two solutions are on, at $t = -t_0$, is η_{-t_0} , on which also $x^\gamma(-t_0)$ resides. Let us again note that $x^\gamma(-t_0) = x^\gamma(-t_0 + nT)$ and η_{-t_0} is the same set as $\eta_{-t_0 + nT}$, for integer n . Therefore, on the plane, the line segment drawn

between $x^1(-t_0)$ and $x^2(-t_0)$ can be assumed to consist of points that are all enclosed by η_{-t_0} . This line segment approximates η_{-t_0} between $x^1(-t_0)$ and $x^2(-t_0)$. The essence of Izhikevich's approximate method revolves around this little piece of information. So this method is able to disclose the structure of isochrons very near γ [9].

To accomplish time reversal, the velocity vector, associated with (2.1) must be reversed, to write $\dot{x} = -f(x)$, and then forward integration must be performed on this new system [9]. To see why $x^1(-t_0)$ and $x^2(-t_0)$ must be on the same isochron, we refer back to Theorem 2.

As can be clearly admired, Izhikevich's method is intuitive and applicable to simple oscillatory systems. In two-dimensional systems, this method is the one to use to plot isochron portraits, if an acceptable level of accuracy is required.

3.7 Summary

In this chapter, we have made use of Winfree's intuition [22, 19] and relied on Guckenheimer's justified statements [7] to define isochrons and review some of their basic properties. It is perceived that the intuition leading to the discovery of isochrons is based on the notion of asymptotic phase.

The isochron definition through the state transition function of the generic ODE in (2.1), declared in Section 3.1, is crucial, for we could prove that the isochron gradient at $x^\gamma(t_0)$, a point on γ , is in the same direction as $v_1(t_0)$, and that a solution $x^0(t)$, with its initial condition $x^0(0) \in \mathcal{W}$, hits the same isochron after subsequent intervals of length T . These proofs were given in Section 3.2. Then, in Section 3.3, we utilized these results to define \hat{t} , the phase in units of time, associated with $x^\gamma(t)$ in particular. We also established that $\partial\hat{t}/\partial x^\gamma = v_1(t)$ on γ . In Section 3.5, we focused primarily on Winfree's method [19] of figuring out expressions for isochrons in simple two dimensional systems. Then, in Section 3.6, we explained Izhikevich's method of numerically computing the structure of isochrons around γ , for again simple two dimensional systems. We needed to modify some definitions and proofs of Sections 3.1 to 3.3 to accommodate DAEs as well, and what we did in Section 3.4 was to primarily show that $\partial\hat{t}/\partial q = v_1(t)$ on γ . We established this and that $v_1(t)$ defines a subspace rather than a hyperplane generally, in DAEs, i.e. the linearized form of an isochron, in the close neighborhood of γ , is not a hyperplane but a subspace [3].

We have to note that all the derivations and explanations provided in this chapter cover unperturbed oscillators. In the next chapter we explore how the phase of an oscillator is affected when perturbations are afflicted on these systems. It happens that the study of isochrons and these derivations prove to be most helpful while analyzing perturbed oscillators.

Chapter 4

OSCILLATOR PHASE ANALYSIS WITH PERTURBATIONS

In this chapter, we develop the theory that is needed to carry out oscillator phase analysis in the presence of perturbations. Perturbations cause a phase drift together with orbital deviation. Our aim is to derive a phase equation for the generic ODE in (2.1), along with the DAE in (2.4). The concern is not only perturbations afflicted on states, but also parameters. In developing the theory needed, we refer to [1], [2], [5], and [3].

4.1 Phase Equation for the Generic ODE System

The perturbed ODE system may be written as

$$\frac{dx}{dt} = f(x) + g(x, t), \text{ with } x(0) = x^\gamma(0). \quad (4.1)$$

where $g(x, t)$ is the perturbations vector. Notice that $g(x, t)$ depends on both the states vector x and time t . When $g = 0$, this equation is the same as the generic ODE in (2.1). However, in here we especially consider the case when $g \neq 0$. Also note that since isochrons are the level sets of \hat{t} , by Theorem 3, $x(0), x^\gamma(0) \in \eta_0$. Without loss of generality, we can impose the initial condition $x(0) = x^\gamma(0)$ on the perturbed ODE in (4.1). We will first be noting a few substantial observations.

Let $x^0(t)$ be a solution of the unperturbed equation in (2.1). Then, we know that $\hat{t}(x^0(t)) = t, \forall t \geq 0$, provided that $x^0(0) \in \eta_0$. η_0 , by our convention, is such that it passes through $x^\gamma(0)$, a point on γ . Note that, again by our convention, $\hat{t}(x^\gamma(0)) = 0$.

In turn, let $x(t)$ be a solution of the perturbed equation in (4.1). We have already required that the initial condition, $x(0)$, be on the isochron η_0 . In fact, $x(0) = x^\gamma(0)$. Then, the initial condition for \hat{t} is zero, i.e. $\hat{t}(x(0)) = 0$.

We have just noted that $\hat{t}(x^0(0)) = 0$ and $\hat{t}(x(0)) = 0$. Moreover, that $\hat{t}(x^0(t)) = t$ is true. However, we cannot right away declare that $\hat{t}(x(t)) = t$. Most probably, $\hat{t}(x(t)) \neq t$, because in (4.1) there is g present. g may affect $\hat{t}(x(t))$ such that $\hat{t}(x(t))$ may deviate from the delicately computed t .

The following sections focus on the derivation and proof of the accuracy, of a differential equation describing $\hat{t}(x(t))$, phase of the solution $x(t)$ of the generic perturbed ODE in (4.1). We have already set the initial condition, $\hat{t}(x(0)) = 0$, for this new differential equation, which we will from this point on call the *Phase Equation*.

4.1.1 Derivation of the Phase Equation

As the first step in deriving the phase equation, we proceed as follows. Noting that \hat{t} is a function of the states vector, x , we write

$$\frac{d\hat{t}(x)}{dt} = \left[\frac{\partial \hat{t}(x)}{\partial x} \right]^T \frac{dx}{dt}.$$

In view of (4.1), we continue to write

$$\frac{d\hat{t}(x)}{dt} = \left[\frac{\partial \hat{t}(x)}{\partial x} \right]^T [f(x) + g(x, t)]. \quad (4.2)$$

Note that the equation above is derived through substitutions only, and therefore it is exact.

There is a further simplification which can be carried out, sustaining the exactness of (4.2). The expression for \hat{t} is not explicitly known, but the gradient of \hat{t} is known to satisfy

$$\left[\frac{\partial \hat{t}(x)}{\partial x} \right]^T f(x) = 1. \quad (4.3)$$

Recalling the discussion in Section 3.3, \hat{t} is introduced in Definition 16 as $\hat{t} = \hat{t}(x^0(t^*))$, provided that $x^0(t)$ is a solution of the unperturbed ODE in (2.1), such that $x^0(0) \in \mathcal{W}$. Then, $x^0(t^*) \in \mathcal{W}$, $\forall t^* > 0$. In Section 3.3, the only requirement to satisfy

$$\left[\frac{\partial \hat{t}(x^0(t^*))}{\partial x^0(t^*)} \right]^T \frac{dx^0(t^*)}{dt} = 1$$

is that $x^0(t^*) \in \mathcal{W}$. We assume that by adding the perturbations vector g to (2.1) and obtaining (4.1), the isochron structure in \mathcal{W} , and \mathcal{W} and γ themselves are not altered, which brings about the condition on g that the magnitude of g must be small. Also we know that $f(x)$ is still a function of x . Therefore, (4.3) is valid for the solution $x(t)$ of (4.1) as well.

This observation leads to a simplified and still exact form,

$$\frac{d\hat{t}(x)}{dt} = 1 + \left[\frac{\partial \hat{t}(x)}{\partial x} \right]^T g(x, t), \quad (4.4)$$

of (4.2). The next step will be to derive an approximate form of (4.4) to facilitate numerical computations.

4.1.2 Solution of Perturbed Oscillating Systems

An approximate form of (4.4) can be derived if we choose to expand

$$\left[\frac{\partial \hat{t}(x(t))}{\partial x(t)} \right]^\top g(x(t), t) \quad (4.5)$$

around some point $x^\gamma(t^*)$. We know by Corollary 3 of Theorem 3, both that $x^\gamma(\hat{t}(x(t)))$ and $x(t)$ are on the same isochron and that the phases of these two points are the same, i.e. $\hat{t}(x^\gamma(\hat{t}(x(t)))) = \hat{t}(x(t))$. In fact, that $x(t)$ is the solution of the perturbed ODE in (4.1) does not matter, because \hat{t} is a function of the states vector in \mathcal{W} . For this reason, we choose $x^\gamma(t^*) = x^\gamma(\hat{t}(x(t)))$ as the point on γ , around which to expand (4.5).

Also, by Theorem 5, $\partial \hat{t}(x^\gamma(\hat{t}(x(t)))) / \partial x^\gamma(\hat{t}(x(t))) = v_1(\hat{t}(x(t)))$. We then have

$$\frac{d\hat{t}(x(t))}{dt} = 1 + v_1^\top(\hat{t}(x(t))) g(x^\gamma(\hat{t}(x(t))), t), \text{ with } \hat{t}(x(0)) = 0, \quad (4.6)$$

as the approximate form of the phase equation in (4.4). Naturally, at $t = 0$, $\hat{t}(x(0)) = 0$, because of the initial condition imposed on (4.1). Our aim was to derive the phase equation in (4.6). The rest of this section focuses on proving the accuracy and pointing out the significance of (4.6).

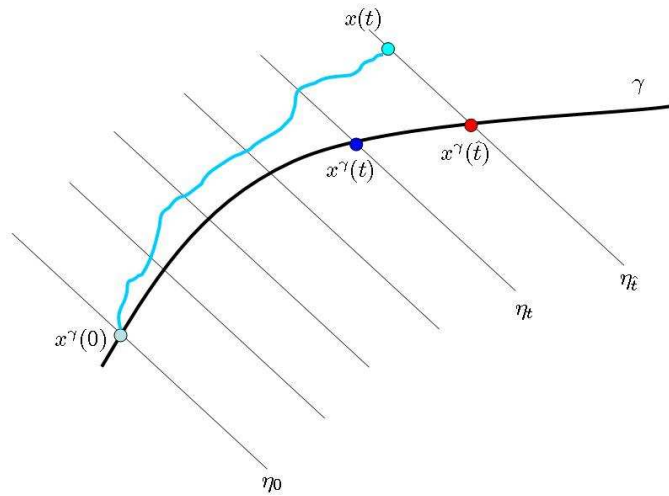


Figure 4.1: Comparison of the phases of perturbed and unperturbed equations.

Notice that since $x^\gamma(\hat{t})$ and $x(t)$ are on the same isochron, $\eta_{\hat{t}}$, where $\hat{t} = \hat{t}(x(t))$, if $x^\gamma(\hat{t})$ and $x(t)$ are sufficiently close together, we have

$$x(t) = x^\gamma(\hat{t}) + \sum_{i=2}^M c_i u_i(\hat{t}). \quad (4.7)$$

The decomposition in (4.7) holds, for $\{u_2(\hat{t}), \dots, u_M(\hat{t})\}$ span the linearized form of $\eta_{\hat{t}}$ at $x^\gamma(\hat{t})$. We assume that $x^\gamma(\hat{t})$ and $x(t)$ are so close together that this linearization is accurate. For simplicity, let us call

$$y(\hat{t}) = \sum_{i=2}^M c_i u_i(\hat{t}). \quad (4.8)$$

Then we have $x(t) = x^\gamma(\hat{t}) + y(\hat{t})$. Figure 4.1 depicts the perturbed solution $x(t)$ and the unperturbed solution $x^\gamma(t)$, and shows that the two solutions at t are very close to each other but different.

Lemma 1 *The following equality is valid.*

$$\frac{d}{dt}x^\gamma(\hat{t}) = f(x^\gamma(\hat{t})) + [v_1^\top(\hat{t}) g(x^\gamma(\hat{t}), t)] u_1(\hat{t}) \quad (4.9)$$

$\hat{t} = \hat{t}(x(t))$. $x(t)$ is the solution of (4.1), such that $x(0) = x^\gamma(0)$.

Proof: Observe the obvious equalities in

$$\frac{dx^\gamma(\hat{t})}{d\hat{t}} = u_1(\hat{t}) = f(x^\gamma(\hat{t})). \quad (4.10)$$

Making use of (4.10) and the approximate phase equation in (4.6), we obtain

$$\begin{aligned} \frac{dx^\gamma(\hat{t})}{d\hat{t}} \left\{ \frac{d\hat{t}}{dt} \right\} &= u_1(\hat{t}) \{1 + v_1^\top(\hat{t}) g(x^\gamma(\hat{t}), t)\} \\ \frac{d}{dt}x^\gamma(\hat{t}) &= f(x^\gamma(\hat{t})) + [v_1^\top(\hat{t}) g(x^\gamma(\hat{t}), t)] u_1(\hat{t}), \end{aligned} \quad (4.11)$$

which is the claim. ■

Theorem 8 *The following equation is valid.*

$$\frac{d}{dt}y(\hat{t}) = \frac{\partial f(x^\gamma(\hat{t}))}{\partial x^\gamma(\hat{t})} y(\hat{t}) + \sum_{i=2}^M [v_i^\top(\hat{t}) g(x^\gamma(\hat{t}), t)] u_i(\hat{t}) \quad (4.12)$$

$\hat{t} = \hat{t}(x(t))$. $x(t)$ is the solution of (4.1), such that $x(0) = x^\gamma(0)$.

Proof: In view of (4.7) and (4.8), (4.1) can be written as

$$\begin{aligned} \frac{d}{dt} [x^\gamma(\hat{t}) + y(\hat{t})] &= f(x^\gamma(\hat{t}) + y(\hat{t})) + g(x^\gamma(\hat{t}) + y(\hat{t}), t) \\ \frac{d}{dt} x^\gamma(\hat{t}) + \frac{d}{dt} y(\hat{t}) &\approx f(x^\gamma(\hat{t})) + \frac{\partial f(x^\gamma(\hat{t}))}{\partial x^\gamma(\hat{t})} y(\hat{t}) + g(x^\gamma(\hat{t}), t), \end{aligned} \quad (4.13)$$

Taylor-expanding both sides. Notice that we have employed the zeroth order approximation for g , since we assume that the magnitude of g is bounded.

Notice that $\{u_1(\hat{t}), \dots, u_M(\hat{t})\}$ span \mathfrak{R}^M . Therefore,

$$g(x^\gamma(\hat{t}), t) = \sum_{i=1}^M [v_i^\top(\hat{t})g(x^\gamma(\hat{t}), t)] u_i(\hat{t}). \quad (4.14)$$

We have used the biorthogonality property to write the decomposition in (4.14).

Subtracting (4.9) from (4.13),

$$\frac{d}{dt} y(\hat{t}) = \frac{\partial f(x^\gamma(\hat{t}))}{\partial x^\gamma(\hat{t})} y(\hat{t}) + \sum_{i=2}^M [v_i^\top(\hat{t})g(x^\gamma(\hat{t}), t)] u_i(\hat{t}). \quad (4.15)$$

which is exactly the same as (4.12). While obtaining (4.15), we have utilized the decomposition in (4.14).

It remains to show that $y(\hat{t})$ in (4.8) actually satisfies (4.15). For this purpose, an approximation should be employed. Basically,

$$\begin{aligned} \frac{d}{dt} y(\hat{t}) &= \frac{dy(\hat{t})}{d\hat{t}} \frac{d\hat{t}}{dt} \\ &= \frac{dy(\hat{t})}{d\hat{t}} [1 + v_1^\top(\hat{t})g(x^\gamma(\hat{t}), t)] \\ &\approx \frac{dy(\hat{t})}{d\hat{t}}. \end{aligned} \quad (4.16)$$

Now we obtain, from (4.15) and the approximation in (4.16),

$$\frac{d}{dt} y(\hat{t}) = \frac{\partial f(x^\gamma(\hat{t}))}{\partial x^\gamma(\hat{t})} y(\hat{t}) + \sum_{i=2}^M [v_i^\top(\hat{t})g(x^\gamma(\hat{t}), t)] u_i(\hat{t}). \quad (4.17)$$

In order to show that $y(\hat{t})$ in (4.8) solves (4.17), we must proceed as follows. Recall that $\exp(\mu_i t)u_i(t)$ was shown to satisfy

$$\frac{d}{dt} [\exp(\mu_i t)u_i(t)] = \frac{\partial f(x^\gamma(t))}{\partial x^\gamma(t)} [\exp(\mu_i t)u_i(t)], \quad (4.18)$$

in Section 2.2.3. Manipulating (4.18), we obtain

$$\frac{d}{dt} u_i(t) = \frac{\partial f(x^\gamma(t))}{\partial x^\gamma(t)} - \mu_i u_i(t). \quad (4.19)$$

Then, through (4.8) and (4.19), we get

$$\frac{d}{d\hat{t}}y(\hat{t}) = \frac{\partial f(x^\gamma(\hat{t}))}{\partial x^\gamma(\hat{t})}y(\hat{t}) - \sum_{i=2}^M c_i \mu_i u_i(\hat{t}). \quad (4.20)$$

Substituting (4.20) in (4.17) and cancelling terms,

$$-\sum_{i=2}^M c_i \mu_i u_i(\hat{t}) = \sum_{i=2}^M [v_i^\top(\hat{t})g(x^\gamma(\hat{t}), t)] u_i(\hat{t}). \quad (4.21)$$

Defining

$$\mathbf{U}_{2,M} = (u_2(\hat{t}) \cdots u_M(\hat{t})), \quad (4.22)$$

an $(M \times (M - 1))$ -sized matrix,

$$c = (c_2 \cdots c_M)^\top, \quad (4.23)$$

an $((M - 1) \times 1)$ -sized vector, and

$$b = \sum_{i=2}^M [v_i^\top(\hat{t})g(x^\gamma(\hat{t}), t)] u_i(\hat{t}), \quad (4.24)$$

another $((M - 1) \times 1)$ -sized vector, we may express (4.21) in compact form as

$$\mathbf{U}_{2,M}c = b. \quad (4.25)$$

We will now draw attention to several facts about the system in (4.25). (4.25) is an over-determined full-rank system. Therefore, if there is a solution c , then it must be unique. There is no doubt that b in (4.24) is in the column space of $\mathbf{U}_{2,M}$ in (4.22). Then, (4.25) has a solution c , and c is unique. Indeed,

$$c_i = -\frac{v_i^\top(\hat{t})g(x^\gamma(\hat{t}), t)}{\mu_i}. \quad (4.26)$$

This proves that $y(\hat{t})$ in (4.8) satisfies (4.17) exactly, and that $y(\hat{t})$ satisfies (4.15) after approximations. ■

The form of the phase equation remains the same as in (4.6) for the DAE case. Noting that $\partial \hat{t}(q(x^\gamma(\hat{t}))) / \partial q(x^\gamma(\hat{t})) = v_1(\hat{t})$ for a DAE, (4.6) can again be easily derived. This derivation is presented in detail in [3].

4.2 Incorporation of Parameter Perturbations into Oscillator Phase Analysis

Up to this point, we had the need to orient our derivations to analyze our generic oscillators, in the presence of perturbations appended to the system states that reside on the limit cycle, γ . However, in the generic system of equations, describing an oscillator in ODE form, as in (2.1) for example, there exist usually a set of parameters, which we are obliged to consider, to fully describe the system. In some applications, one is required to analyze oscillator phase when time-dependent perturbations are appended to these parameters.

The generic set of equations are given as $\dot{x} = f(x)$, for an ODE. The assumption is that we have M states, i.e. the states vector, x , has M entries. In addition to x , f is usually a function of p , a parameters vector that we assume has L entries. Therefore, we have $f = f(x, p)$.

Note that the actual number of parameters incorporated in f might be more than L , so p usually is not required to consist of all the possible parameters we could include in it. The essence is to comprise p of those parameters that we could wish to perturb in a time-dependent manner. The other parameters, which we might deem ineligible for perturbations, could just be regarded as constants.

Also note that, although the values of x on γ vary in time, the values of p on γ are strictly constants. The perturbations appended on p will, on the other hand, naturally be time-dependent.

Little work has been done in the relevant literature, to analyze oscillator phase drift in the presence of parameter perturbations. Most of the contributions seem to accumulate in a single paper. In [6], some basic theory is borrowed from [10], in order to bear the ground for oscillator phase analysis when parameter perturbations exist. However, neither in [10], nor in [6], association of the developed theory with the familiar Floquet theory is established. We have, in this work, after defining the phase of an oscillator in ODE form, namely \hat{t} , shown that $\partial\hat{t}/\partial x^\gamma(t) = v_1(t)$. Also we have stated that the phase referred to in [10] is again our \hat{t} . We have shown that the numerical scheme, given in [10], to compute the gradient of \hat{t} with respect to the states of an oscillator on γ , again computes precisely $v_1(t)$.

The aim now is to utilize our knowledge of Floquet and sensitivity theories to bind a link between the theory developed in [6] and $v_1(t)$. The first task will be to express the parameters vector, p , in our system of equations, such that the entries of p also become the

states of our generic ODE system, given in (2.1).

4.2.1 Augmenting the Generic ODE for Parameter Perturbations

We now have to derive a new representation for the generic ODE system in (2.1), which is simply $\dot{x} = f(x)$. We have already stated that $f = f(x, p)$, where x has M entries and p has L . We would like to convert this generic system, in which p will be explicitly available as if its entries were also the states of the system.

Let us define a new vector w . In w , we concatenate the entries of x and p , as in

$$w = (x_1 \cdots x_M p_1 \cdots p_L)^\top. \quad (4.27)$$

Then, we may declare that $f = f(w)$. Noting that $w_j = x_j$ for $1 \leq j \leq M$, the generic ODE in (2.1), is simply modified as

$$\dot{w}_j = f_j(w) \quad \forall j \in \{1, \dots, M\}. \quad (4.28)$$

Notice that, above, we have M equations, but the argument of every f_j , which is w , has $(M + L)$ entries.

There is no doubt that (4.28) is an under-determined system. We have to append L many equations to the system given in (4.28). Here is how we proceed. On the limit cycle, the parameters vector, p , does not vary with time. Every entry of p has a nominal constant value. Let us call these nominal values p_i^{nom} for $1 \leq i \leq L$. The L more equations we need are

$$0 = p_i^{nom} - w_{M+i} \quad \forall i \in \{1, \dots, L\}, \quad (4.29)$$

noting that $w_{M+i} = p_i$ for $1 \leq i \leq L$.

In all, we have

$$\begin{aligned} \dot{w}_j &= f_j(w) & \forall j \in \{1, \dots, M\} \\ 0 &= p_i^{nom} - w_{M+i} & \forall i \in \{1, \dots, L\} \end{aligned} \quad (4.30)$$

from (4.28) and (4.29), as the modified and augmented system. The next step is to try and write (4.30) in compact form. Let us define a vector q , as

$$q = (w_1 \cdots w_M \underbrace{0 \cdots 0}_{L \text{ many}})^\top. \quad (4.31)$$

Defining also

$$i = (f_1(w) \cdots f_M(w) h_1(w) \cdots h_L(w))^\top, \quad (4.32)$$

where $h_i(w) = p_i^{nom} - w_{M+i}$ for $1 \leq i \leq L$. Then, (4.30) is written in compact form as

$$\frac{dq(w)}{dt} = i(w). \quad (4.33)$$

Comparing this compact form with (2.4), we observe that (4.33) is a DAE.

In the forthcoming derivations, we will also need the explicit forms of the Jacobians of q and i , with respect to w . Examining q in (4.31) and w in (4.27), we have

$$\frac{\partial q}{\partial w} = \begin{pmatrix} \mathbf{I}_M & \mathbf{0}_{M \times L} \\ \mathbf{0}_{L \times M} & \mathbf{0}_{L \times L} \end{pmatrix}, \quad (4.34)$$

where \mathbf{I}_M is the identity matrix of size $(M \times M)$, and the others are zero matrices of the subscripted sizes. Similarly, examining i in (4.32) and w in (4.27), we have

$$\frac{\partial i}{\partial w} = \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial p} \\ \mathbf{0}_{L \times M} & -\mathbf{I}_L \end{pmatrix}. \quad (4.35)$$

Above, $\partial f / \partial p$ is evaluated by substituting the values for x and the nominals for p , after considering p as a variable and figuring out the expression for the partial differential.

Having figured out the compact DAE form in (4.33), the matter now is how to append time-varying perturbations to the nominal parameter values. The solution is very simple. Let us define a perturbations vector

$$s(t) = (s_1(t) \cdots s_L(t))^T, \quad (4.36)$$

and a perturbation modulation matrix

$$\mathbf{B} = \begin{pmatrix} \mathbf{0}_{M \times L} \\ \mathbf{I}_L \end{pmatrix}. \quad (4.37)$$

In view of (4.36) and (4.37), we incorporate the compact form in (4.33) with the parameter perturbations functionality, as in

$$\frac{dq(w)}{dt} = i(w) + \mathbf{B}s(t). \quad (4.38)$$

The time-dependent perturbations vector, $s(t)$ above, directly modifies the nominal value of the perturbations vector, p .

In order to be able to monitor the effects of parameter perturbations on the phase of our generic ODE system in (2.1), we first modified the M -sized original system into

the $(M + L)$ -sized system of (4.33). Then, we spelt out (4.38), in which p also became a perturbation-prone part of the augmented state variable w , along with the old states vector, x . We focus on only parameters in our analysis, so we needed to define $s(t)$ and \mathbf{B} , through which only the nominal values in p have become vulnerable.

We have already associated $v_1(t)$ with the generic ODE in (2.1), and repeated this reservation many times. The new augmented compact system in (4.33) also has a similar vector function, which we will call $v_1^{aug}(t)$. Although (4.33) is a DAE, it has been derived from (2.1). Therefore, $v_1^{aug}(t)$ is related to $v_1(t)$ through a very simple expression. We will be deriving this relation, but we need to explain first the theory developed in [6]. $v_1^{aug}(t)$ will surface naturally through the methods crafted in [6].

4.2.2 Augmenting the Generic DAE for Parameter Perturbations

We now describe how to modify the generic DAE in (2.4) to be able to carry parameter perturbation analysis. This procedure proves to be very similar to the scheme that we described in Section 4.2.1.

We do not redefine the augmented vector w , already defined in (4.27). Let us simply state that $w = (x^T p^T)^T$, where x is the $(M \times 1)$ -sized states vector, and p the $(L \times 1)$ -sized parameters vector. Let us note again that p_i^{nom} , for $1 \leq i \leq L$, are the constant nominal values for the parameters, defined on γ .

The nonlinear functions q and f in (2.4) actually share the entries in p . Recall that we do not dump into p , all the available parameters to be used in expressing q and f . Some parameters may be ineligible for perturbation, and we treat these parameters merely as constants. These parameters are not among the entries of p . p consists of the parameters that are eligible for parameter perturbation analysis. Some entries in p may belong to only q , another set of entries may belong to only f , and then there may be a third set that belongs to both q and f .

In the following derivations, we regard the nonlinear functions as $f = f(x, p)$ and $q = q(x, p)$. We have already introduced the augmented vector w , so we have indeed $f(w)$ and $q(w)$.

We now repeat what we did in the ODE case as follows.

$$\begin{aligned}\dot{q}_j(w) &= f_j(w) & \forall j \in \{1, \dots, M\} \\ 0 &= p_i^{nom} - w_{M+i} & \forall i \in \{1, \dots, L\}\end{aligned}\quad (4.39)$$

In the ODE case, the ODE that we have, in the form of (2.1), is converted into a DAE, in the form of (2.4). The DAE derived from an ODE is of the form $\dot{q}(w) = i(w)$. However, we are now trying to derive another DAE from an original DAE, so let us have the new DAE in the form given by $\dot{Q}(w) = I(w)$. Q and I are to be defined as

$$Q = (q_1 \cdots q_M \underbrace{0 \cdots 0}_{L \text{ many}})^\top \quad (4.40)$$

and

$$I = (f_1 \cdots f_M \ h_1 \cdots h_L)^\top \quad (4.41)$$

respectively. Note that $h_i = p_i^{nom} - p_i = p_i^{nom} - w_{M+i}$, for $1 \leq i \leq L$.

In solving $\dot{Q}(w) = I(w)$, we need

$$\frac{\partial Q}{\partial w} = \begin{pmatrix} \frac{\partial q}{\partial x} & \frac{\partial q}{\partial p} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \quad (4.42)$$

and

$$\frac{\partial I}{\partial w} = \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial p} \\ \mathbf{0} & -\mathbf{I}_L \end{pmatrix}. \quad (4.43)$$

Both matrices above are $(M+L) \times (M+L)$. \mathbf{I}_L is the $(L \times L)$ -sized identity matrix. The zero matrices are of the appropriate sizes.

We may again write

$$\frac{dQ(w)}{dt} = I(w) + \mathbf{B}s(t), \quad (4.44)$$

in order to append actual perturbations to the parameters only. \mathbf{B} , the perturbation modulation matrix, is defined in (4.37), and $s(t)$, the vector of appended perturbations, is defined in (4.36).

We assume that $v_1(t)$ is a periodic solution of the adjoint LPTV equation, derived from the generic DAE in (2.4). Let us now assume that $v_1^{aug}(t)$ is a periodic solution of the adjoint equation derived from the augmented DAE, $\dot{Q}(w) = I(w)$.

Chapter 5

RELATIONSHIP WITH PREVIOUS WORK

Previous work on oscillator phase analysis has much in common with the theory developed in the last chapter. In this chapter, we review some methods to compute $v_1(t)$, although in most references oscillator phase analysis has not been pointed out as related to Floquet theory. We show through rigorous derivations that all the theory developed for oscillator phase analysis in the presence of state and parameter perturbations indeed aim to compute $v_1(t)$ first.

5.1 ISF (Impulse Sensitivity Function)

It happens that if we set the perturbation vector to be an impulse, shifted in time, \hat{t} computed through the phase equation turns out to be a single sample of $v_1(t)$. Therefore, exciting the perturbed system by impulses, each of the coupled equations at all timepoints along a period, waiting long enough so that the system again returns to steady-state, and then measuring the phase difference with an unperturbed system that was initially in-phase with the perturbed system, we can theoretically compute $v_1(t)$. This approach was first introduced by Winfree in 1967 [19], [9]. Later in 1998, Hajimiri et al. [8], utilized the same method for electronic oscillators, possibly unaware of Winfree's innovation.

5.2 PPV (Perturbation Projection Vector)

In the electronic domain, particularly Kaertner in [21], foresaw $u_1(t)$ as the vector function, on which perturbations appended to a system of the generic ODE form in (2.1) must be projected, in order to compute the phase drift that plagues such oscillators. Thereon, it is easier to guess that perturbations along the other functions, $u_i(t)$ for $2 \leq i \leq M$, contribute to orbital deviation. However, provided that the states vector, x , never leaves the close neighborhood of γ , the appended orbital deviation dies out in time, for oscillators possessing the asymptotically orbital stability property. This latter property is maintained

if, again, we assume that the first Floquet exponent is zero, i.e. $\mu_1 = 0$, and all the other exponents are negative, i.e. $\mu_i < 0$ for $2 \leq i \leq M$ [17].

Remembering Floquet theory, $u_i(t)$, for $1 \leq i \leq M$, and $v_j(t)$, for $1 \leq j \leq M$, are biorthogonal sets at any $t = t_0$. Therefore, supposing we have an arbitrary vector a which may be written as

$$a = \sum_{i=1}^M a_i u_i(t_0),$$

we may compute coefficient a_1 , through $a_1 = v_1(t_0) \cdot a$. a_1 is the coefficient of component along $u_1(t_0)$. This simple projection demonstrates why we need to compute $v_1(t)$, i.e. in order to figure out the perturbation component along $u_1(t)$.

It was Kaertner's intuitive approach in [21] to compute first $v_1(t)$, in order to figure out the phase drift afflicting oscillators. Later, Demir et al. in [5] derived a phase equation, bearing the ground of their work on Kaertner's intuition and particularly the biorthogonality property dictated by Floquet theory. Demir et al. in [5] assume $u_1(t)$ to be the only persistent mode, again referring to the basic assumption that $\mu_1 = 0$ and all other Floquet exponents are negative, which is what we have assumed right from the outset. Since they adopt Kaertner's exclusive intuition in [21] to project perturbations over $u_1(t)$, Demir et al. rightfully call $v_1(t)$, the *Perturbation Projection Vector* (PPV) [5].

5.3 Phase Gradient Computation for ODEs

In Chapter 3, we stated several findings relating Floquet Theory to the concept of isochrons. That we have established $\partial \hat{t} / \partial x = v_1(t)$ is theoretically valuable information, but practically we still do not know how to compute $v_1(t)$. When explaining numerical methods, it will be clear how we compute $v_1(t)$. However, we are now going to introduce a simpler numerical method, based on an intuitive understanding of phase, that is aimed to compute the phase gradient, i.e. $v_1(t)$, the vector function we need. When this method was introduced in an earlier work, no relation to Floquet theory was established. We are going to prove that this proposed numerical method computes exactly $v_1(t)$. This proof will consolidate the comprehension of Floquet theory and will publicly declare its power.

Kramer et al. in [10] develop a numerical method to compute the partial derivative, $\partial \hat{t} / \partial x$, when x is on γ , the limit cycle of interest. Through the derivations given in [10],

the notion of phase is shown to originate from a more familiar sensitivity expression, in particular $\partial x_j^\gamma(\tau)/\partial x_i^\gamma(t)$. This expression can be translated into simpler language as the sensitivity of the j^{th} entry of $x^\gamma(\tau)$ with respect to the i^{th} entry of $x^\gamma(t)$. The reservation adhered to in [10] is that if a perturbation is appended to $x_i^\gamma(t)$, i.e. to the i^{th} entry of $x^\gamma(t)$, the effect of this perturbation on the j^{th} entry can be observed only when the oscillator returns to the limit cycle, γ . The oscillators we are concerned with are assumed to have the asymptotically orbital stability property. Therefore, our oscillator is not expected to return to γ before a long enough time has passed. It naturally follows that

$$\lim_{\tau \rightarrow \infty} \frac{\partial x_j^\gamma(\tau)}{\partial x_i^\gamma(t)} \quad (5.1)$$

must be analyzed.

Kramer et al. in [10] split the previous partial differential expression into two factors in order to develop their notion of phase, as in

$$\lim_{\tau \rightarrow \infty} \frac{\partial x_j^\gamma(\tau)}{\partial x_i^\gamma(t)} = \lim_{\tau \rightarrow \infty} \frac{dx_j^\gamma(\tau)}{dt} \frac{\partial \hat{t}}{\partial x_i^\gamma(t)}. \quad (5.2)$$

Notice that above \hat{t} emerges suddenly, and therefore it is not for certain that \hat{t} is the phase of the generic ODE in (2.1), as defined in Chapter 3. We will assume for now that \hat{t} in (5.2) is the \hat{t} of Definition 15 in Chapter 3. $dx_j^\gamma(\tau)/dt$ is a derivative expression evaluated at time τ . $\partial \hat{t}/\partial x_i^\gamma(t)$ is then the i^{th} entry of the gradient expression we are looking for, evaluated at t . Algebraically, there is no doubt whether $\partial \hat{t}/\partial x_i^\gamma(t)$ should have been scaled by a coefficient, because \hat{t} is the phase in units of time, and the derivation carried out in [10] leaves the familiar t intact. There is no need to scale the gradient to be computed.

Since $\partial \hat{t}/\partial x_i^\gamma(t)$ is not a function of τ , the following is automatically written.

$$\frac{\partial \hat{t}}{\partial x_i^\gamma(t)} = \lim_{\tau \rightarrow \infty} \frac{\partial x_j^\gamma(\tau)}{\partial x_i^\gamma(t)} \bigg/ \frac{dx_j^\gamma(\tau)}{dt} \quad (5.3)$$

is the expression to compute the i^{th} entry of the isochron gradient at $x^\gamma(t)$, which is a point on γ .

Some facts must be noted about the expression in (5.3). First of all, it is clear that (5.3) can be used as a numerical method to compute the phase gradient. So far, we have not derived any numerical methods to compute this gradient, and (5.3) is, as of now, the only available and reliable numerical method for this purpose. However, we may readily

list three problems that afflict the scheme of (5.3). Evaluation of the limit at infinity is not possible, and practically there is no hint suggesting how big τ must be chosen. Also (5.3) is able to compute only a single entry of the isochron gradient, at a single shot. We are going to spell out more accurate and systematic schemes in the numerical methods chapter, to compute not only a single entry, but the entries of this gradient, all together.

The second fact that must be noted about (5.3) is that this expression does not seem to depend on the choice of j . In [10], it is stated that the phase, \hat{t} , is a property of the whole oscillator. Therefore, the claim that the choice of j can be arbitrary is stated without justification. Shortly, we are going to prove that j can indeed be arbitrary.

The third fact about (5.3) is we have already noted that $v_1(t) = \partial\hat{t}/\partial x^\gamma(t)$. However, in (5.3), this equality is not at first obvious. The theorem and its proof that we are shortly to present will establish clearly that the gradient expression computed through (5.3) is exactly $v_1(t)$.

Again, the scheme in (5.3) and the problems that are stated about this scheme hold if \hat{t} in (5.3) is actually the \hat{t} introduced in Definition 15.

Theorem 9 *Let the phase, associated with the generic ODE in (2.1), be \hat{t} . The i^{th} entry of the gradient of \hat{t} , evaluated at $x^\gamma(t)$, which is a point on γ , the limit cycle of interest, can be computed through*

$$\frac{\partial\hat{t}}{\partial x_i^\gamma(t)} = \lim_{\tau \rightarrow \infty} \frac{\partial x_j^\gamma(\tau)}{\partial x_i^\gamma(t)} \bigg/ \frac{dx_j^\gamma(\tau)}{dt},$$

the same expression as in (5.3). The gradient expression in (5.3) is exactly equal to the i^{th} entry of $v_1(t)$, i.e.

$$\partial\hat{t}/\partial x_i^\gamma(t) = v_{1,i}(t)$$

Also, the choice of j in (5.3) is arbitrary.

Proof: Let us first recall that if we linearize the generic ODE equation around γ , we get an equation of the form, $\dot{y} = \mathbf{G}(t)y$, where dot denotes derivative with respect to time. $u_1(t)$ is a periodic solution of this equation. Again, $\mathbf{G}(t) = \partial f/\partial x$, evaluated at $x^\gamma(t)$. This linear differential equation has a state transition function that is written in a straightforward manner as $\mathbf{odK}(\tau, t) = \partial x^\gamma(\tau)/\partial x^\gamma(t)$, for $\tau > t$. Regard τ as a dummy variable. The adjoint of this linear equation is then written as $\dot{z} = -\mathbf{G}^\top(t)z$. $v_1(t)$ is a periodic

solution of this adjoint equation. The state transition function of the adjoint form is the transpose of the original, i.e. $\mathbf{odK}^\top(t, \tau)$.

Let us now express $\mathbf{odK}(\tau, t)$ in explicit form as

$$\mathbf{odK}(\tau, t) = \begin{pmatrix} \frac{\partial x_1^\gamma(\tau)}{\partial x_1^\gamma(t)} & \cdots & \frac{\partial x_1^\gamma(\tau)}{\partial x_M^\gamma(t)} \\ \vdots & \ddots & \vdots \\ \frac{\partial x_M^\gamma(\tau)}{\partial x_1^\gamma(t)} & \cdots & \frac{\partial x_M^\gamma(\tau)}{\partial x_M^\gamma(t)} \end{pmatrix}.$$

It is then possible to express the entries of $\mathbf{odK}^\top(t, \tau)$ as in

$$(\mathbf{odK}^\top(t, \tau))_{ij} = \frac{\partial x_j^\gamma(\tau)}{\partial x_i^\gamma(t)}. \quad (5.4)$$

Through Floquet theory, $\mathbf{odK}(\tau, t)$ is known to be

$$\mathbf{odK}(\tau, t) = \sum_{i=1}^M e^{\mu_i(\tau-t)} u_i(\tau) v_i^\top(t).$$

Recalling our basic assumption that $\mu_1 = 0$ and $\mu_i < 0$ for $2 \leq i \leq M$, and that we have to let $\tau \gg t$, we have

$$\mathbf{odK}(\tau, t) = u_1(\tau) v_1^\top(t).$$

Then, we may express the expanded form

$$\mathbf{odK}^\top(t, \tau) = \begin{pmatrix} v_{1,1}(t) \\ \vdots \\ v_{1,M}(t) \end{pmatrix} \begin{pmatrix} u_{1,1}(\tau) & \cdots & u_{1,M}(\tau) \end{pmatrix}.$$

Spelling out a single row,

$$(\mathbf{odK}^\top(t, \tau))_{i*} = \begin{pmatrix} v_{1,i}(t) u_{1,1}(\tau) & \cdots & v_{1,i}(t) u_{1,M}(\tau) \end{pmatrix}.$$

The previous equality together with (5.4) justify

$$(\mathbf{odK}^\top(t, \tau))_{ij} = \frac{\partial x_j^\gamma(\tau)}{\partial x_i^\gamma(t)} = v_{1,i}(t) u_{1,j}(\tau), \quad (5.5)$$

for $\tau \gg t$.

We have figured out an expression for the numerator in (5.3), which is true in the limit. Let us now examine the denominator term. $dx^\gamma(\tau)/dt$ is the time derivative of x^γ , evaluated at τ . $u_1(t)$ is in the same direction as the time derivative of x^γ , and one of assumptions is to have $dx^\gamma(t)/dt = u_1(t)$.

In all, we have the means to simplify (5.3), as in

$$\frac{\partial \hat{t}}{\partial x_i^\gamma(t)} = \frac{v_{1,i}(t)u_{1,j}(\tau)}{u_{1,j}(\tau)} = v_{1,i}(t), \quad (5.6)$$

where the limit notifier is omitted for convenience. Recall that the equality is true for $\tau \gg t$.

(5.6) establishes that the gradient of the level sets of \hat{t} , which we have called isochrons, on γ , the limit cycle, is $v_1(t)$, the vector function, which is the solution of the adjoint linear equation derived from the generic ODE in (2.1).

Another obvious significance, examining (5.6), is that the claim in [10] that the computation in (5.3) does not depend on the choice of j is now justified, for the terms depending on j cancel in (5.6). ■

5.4 Phase Response to Parametric Perturbations

5.4.1 Parameter Sensitivity Equation for an ODE

The theory developed in [6] requires the sensitivity equation to be derived. We will be spelling out the differential equation whose solution is $\partial x/\partial p$ on γ . We will also be solving this equation and giving the explicit form of the solution.

Kramer et al. in [10] derive the sensitivity equation for a generic ODE, as given in (2.1). They show that this equation is an inhomogeneous version of the LPTV equation, derived from (2.1). Therefore, as it can be easily deduced, the solution of the sensitivity equation involves a convolution expression with $\mathbf{odK}(t, 0)$, the state transition function of the LPTV equation, $\dot{y} = \mathbf{G}(t)y$, with $\mathbf{G}(t) = \partial f/\partial x$ computed on γ . Taylor et al. in [6] borrow this formulation and use the explicit form of the solution for the sensitivity equation to conduct a part of their derivations. However, neither in [10], nor in [6], Floquet theory for spelling out $\mathbf{odK}(t, 0)$ is exploited.

Larter in [11] explores sensitivity based on Floquet theory. However, this approach is not generalizable, since Larter assumes that the solutions of the LPTV equation, which we write as $\exp(\mu_i t)u_i(t)$, for $i \leq i \leq M$, not only span the column space of $\mathbf{odK}(t, 0)$, but are the actual columns of $\mathbf{odK}(t, 0)$. Then, it is awfully difficult to deduce the benefits of biorthogonality and projections based on this feature. Larter distinguishes between a single persistent mode and the others, i.e. implicitly assumes that the first Floquet exponent is zero, $\mu_1 = 0$ and that the others are less than zero. However, without spelling out

the explicit form of $\mathbf{odK}(t, 0)$ through Floquet theory, it is not possible to benefit from the biorthogonality property that we extensively exploit in this work. As a consequence, Larter is able to apply this approach only to specific, simple chemical oscillator models of low dimension, and these analyses cannot cover the generic oscillator of the form in (2.1), because the approach in [11] consists of and is hampered by the difficulty of figuring out the column space of $\mathbf{odK}(t, 0)$, associated with the LPTV equation derived from (2.1).

In this section, we again derive the sensitivity equation for the ODE case, as carried out in [10]. We spell out the solution in terms of $\mathbf{odK}(t, 0)$ and make use of the explicit of this solution, derived with the help of Floquet theory, in the next section.

In 2.1.3, we stated that the nonlinear multi-dimensional function, f , of the generic ODE equation in (2.1), is actually a function of both the states vector, x , and the parameters vector, p , i.e. $f = f(x, p)$. x , in turn, is naturally a function of both time, t , and also the parameters, vector, p . Therefore, it would be most accurate to express f as $f = f(x(t, p), p)$.

For our purposes, we would like to compute, numerically, the sensitivity of the states vector, x , with respect to the parameters vector, p , i.e. $\partial x / \partial p$. The sensitivities around the limit cycle, γ , will suffice. Therefore, we will again be able to make use of the notion of linearization around the limit cycle.

Now, let us evaluate the partial derivative of both sides of (2.1), with respect to p , as in

$$\frac{\partial}{\partial p} \left(\frac{dx(t, p)}{dt} \right) = \frac{\partial}{\partial p} (f(x(t, p), p)).$$

Using the chain rule of partial derivatives and evaluating x on the limit cycle, γ , we obtain

$$\begin{aligned} \frac{d}{dt} \left\{ \frac{\partial x^\gamma(t, p)}{\partial p} \right\} &= \frac{\partial f(x^\gamma(t, p), p)}{\partial x^\gamma(t, p)} \left\{ \frac{\partial x^\gamma(t, p)}{\partial p} \right\} \\ &+ \frac{\partial f(x^\gamma(t, p), p)}{\partial p}. \end{aligned} \quad (5.7)$$

We must note that the second expression on the right-hand side of the equation above is the partial derivative of f with respect to the second argument of f , which is p . The expression in set brackets is the sensitivity we are trying to compute. (5.7) is a linear ordinary differential equation. We can make use of this equation and the initial condition,

$$\left. \frac{\partial x^\gamma(t, p)}{\partial p} \right|_{t=0} = 0, \quad (5.8)$$

to compute the sensitivity, $\partial x^\gamma / \partial p$, with the arguments of x^γ omitted for convenience, for all $t \geq 0$.

(5.7) is actually an inhomogeneous equation. Its homogeneous form reads

$$\frac{d}{dt} \left\{ \frac{\partial x^\gamma(t, p)}{\partial p} \right\} = \frac{\partial f(x^\gamma(t, p), p)}{\partial x^\gamma(t, p)} \left\{ \frac{\partial x^\gamma(t, p)}{\partial p} \right\}.$$

We may recall that the equation above is the linearized form of the generic ODE equation in (2.1). The linearization has been done around γ . Also, through Floquet theory, we have established that the state transition function of the homogeneous equation above is $\mathbf{odK}(t, 0)$. As this section is just a brief restatement of sensitivity computations, we will not again spell out the explicit form of $\mathbf{odK}(t, 0)$, but this explicit form will be needed in the derivations to come.

From linear systems theory, we know that solutions of inhomogeneous equations like (5.7) are of a certain form. These solutions consist of homogeneous and inhomogeneous parts. In this case, let us call the homogeneous part, S_{hom} , and the inhomogeneous part, S_{inh} . Then, we may express the solution to (5.7) as

$$\frac{\partial x^\gamma}{\partial p}(t) = S_{hom} + S_{inh}. \quad (5.9)$$

We know, again through linear systems theory, that to express the explicit forms of S_{hom} and S_{inh} , we need to make use of the state transition function, $\mathbf{odK}(t, 0)$.

In (5.9), S_{hom} is to be expressed explicitly as

$$S_{hom} = \mathbf{odK}(t, 0) \frac{\partial x^\gamma}{\partial p}(0). \quad (5.10)$$

However, through (5.8), $S_{hom} = 0$. Therefore, we only need the inhomogeneous part of the solution, S_{inh} .

S_{inh} in (5.9) is expressed explicitly as

$$S_{inh} = \int_0^t \mathbf{odK}(t, \tau) \frac{\partial f}{\partial p}(\tau) d\tau. \quad (5.11)$$

The arguments of the nonlinear function, f , were omitted for convenience. (5.11) is actually a convolution expression.

In summary, the solution of the linear inhomogeneous differential equation, with the initial condition of (5.8), is

$$\frac{\partial x^\gamma}{\partial p}(t) = \int_0^t \mathbf{odK}(t, \tau) \frac{\partial f}{\partial p}(\tau) d\tau. \quad (5.12)$$

We must note that we mean, by the abbreviated notations,

$$\frac{\partial x^\gamma}{\partial p}(t) = \frac{\partial x^\gamma(t, p)}{\partial p},$$

and

$$\frac{\partial f}{\partial p}(\tau) = \frac{\partial f(x^\gamma(\tau, p), p)}{\partial p}.$$

We again note that the second expression is the partial derivative of f with respect to the second argument of f , which is p .

In order to compute the sensitivity of the states vector, x , with respect to p , we need to fix p to its nominal value, around the limit cycle, γ . The nominal values of the parameters are constant on γ . This is the reason why we do not need a time tag for p , as in $p(t)$.

Having derived the sensitivity equation and having spelt out its solution, we now move on to analyzing the contribution in [6], with the help of this equation and Floquet theory.

5.4.2 Phase Sensitivity with Respect to the Parameters of an ODE System

Taylor et al. in [6] refer to the work of Kramer et al. in [10], in order to develop a reliable numerical method that computes oscillator phase changes when parameter perturbations do exist.

We showed earlier that $\partial \hat{t} / \partial x^\gamma(t)$, the partial differential expression, for which Kramer et al. in [10] devise a numerical method to compute, is exactly $v_1(t)$. $v_1(t)$ is a periodic solution of the adjoint linear equation, $\dot{z} = -\mathbf{G}^T(t)z$, associated with generic ODE equation in (2.1).

Taylor et al. in [6] focus on a single parameter p_j out of the L entries of the parameters vector p . Having defined the same \hat{t} in our work, which satisfies $d\hat{t}/dt = 1$, in the absence of perturbations, so that their notion of phase is again in units of time, they venture to spell out

$$\frac{\partial \hat{t}}{\partial p_j} = \sum_{i=1}^M \frac{\partial \hat{t}}{\partial x_i^\gamma} \frac{\partial x_i^\gamma}{\partial p_j}, \quad (5.13)$$

which is a simple consequence of the chain rule of partial differentiation. Both terms in the summation above are functions of time, so any argument notifier is omitted for convenience. Then, Taylor et al. derive the time derivative of the expression in (5.13) through what may

be called a lengthy proof. The derived expression reads

$$\frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) = \sum_{i=1}^M \frac{\partial \hat{t}}{\partial x_i^\gamma} \frac{\partial f_i}{\partial p_j}, \quad (5.14)$$

where again both terms in the summation are functions of time [6].

Examining (5.14), we observe that both terms in the summation are periodic with T . This makes the whole expression in (5.14) periodic with T . Then it is easy to deduce that the expression in (5.13) is not necessarily periodic, because it is the time integral of (5.14).

Taylor et al. in [6] make use of $\partial \hat{t} / \partial x^\gamma(t)$ to compute the phase deviation of oscillators when state perturbations are present. However, when it is the parameters that are perturbed, they do not resort to $\partial \hat{t} / \partial p_j$ in (5.13), to utilize in the same manner as they handle $\partial \hat{t} / \partial x^\gamma(t)$. The time derivative expression in (5.14) seems to be the counterpart of $\partial \hat{t} / \partial x^\gamma(t)$, when they switch from state perturbations to parameter perturbations. This counterparts relation is not well justified in [6], although the proof enabling the derivation of (5.14) from (5.13) is correct. In fact, this proof is the major contribution of [6].

We will next show that the time derivative expression in (5.14) is related to $v_1^{aug}(t)$, associated with the DAE system that we derived in the previous section. There, we maintained that $v_1(t)$ is associated with the generic ODE system in (2.1), and similarly $v_1^{aug}(t)$ is associated with $\dot{q}(w) = i(w)$, the augmented system with w accounting for the states vector, x , and the parameters vector, p , of (2.1). Then, we will provide a very simple and short proof for the transition from (5.13) to (5.14), with the help of Floquet theory.

Theorem 10 *In 4.2.1, we modified the generic ODE in (2.1) into (4.33), concatenating x and p in w . We also let $v_1^{aug}(t)$ be a periodic solution of the adjoint linear equation, associated with this augmented nonlinear equation, i.e. $\dot{q}(w) = i(w)$. Our claim is that*

$$v_{1,M+j}^{aug}(t) = \frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right), \quad (5.15)$$

where the explicit form of the right-hand side expression is given in (5.14).

Proof: As stated before, we take for granted the transition from (5.13) to (5.14), for the moment. We will be providing the proof of this transition as the justification of a following lemma.

Let us first figure out the differential equation representation of the LPTV system derived from $\dot{q}(w) = i(w)$. We get

$$\left(\begin{array}{cc} \mathbf{I}_M & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{array} \right) \Big|_{\gamma} \frac{d}{dt} y^{aug} = \left(\begin{array}{cc} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial p} \\ \mathbf{0} & -\mathbf{I}_L \end{array} \right) \Big|_{\gamma} y^{aug},$$

where both matrices are evaluated on γ , i.e. $x^\gamma(t)$ and p^{nom} are substituted for evaluation. recall that the nominal values for the parameters, p^{nom} , are everywhere constant on γ . \mathbf{I}_M is the identity matrix of size $(M \times M)$. $\partial f/\partial x$ on γ is the familiar $\mathbf{G}(t)$. $\partial f/\partial p$ is the partial differential expression of $f(x, p)$ with respect to its second argument. Remembering that this linear system is of size $(M + L)$, the zeros matrices must be regarded as being of appropriate sizes so as to make both matrices square. Also, $y^{aug} = (y_1^\top y_2^\top)^\top$, where y_1 and y_2 are $(M \times 1)$ - and $(L \times 1)$ -sized vectors, respectively.

The linear adjoint equation, associated with $\dot{q}(w) = i(w)$, is then

$$\left(\begin{array}{cc} \mathbf{I}_M & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{array} \right) \Big|_{\gamma} \frac{d}{dt} z^{aug} = - \left(\begin{array}{cc} \left(\frac{\partial f}{\partial x} \right)^\top & \mathbf{0} \\ \left(\frac{\partial f}{\partial p} \right)^\top & -\mathbf{I}_L \end{array} \right) \Big|_{\gamma} z^{aug}, \quad (5.16)$$

where clearly $z^{aug} = (z_1^\top z_2^\top)^\top$, where z_1 and z_2 are $(M \times 1)$ - and $(L \times 1)$ -sized vectors, respectively. (5.16) can be written as two sets of coupled equations.

$$\frac{dz_1}{dt} = -\mathbf{G}^\top(t) z_1 \quad (5.17)$$

$$\left(\frac{\partial f}{\partial p} \Big|_{\gamma} \right)^\top z_1 = z_2 \quad (5.18)$$

It is no surprise that the first equation above is the adjoint equation, associated with the original generic ODE in (2.1). Then, $z_1 = v_1(t)$ is a periodic solution for (5.17). Obviously, if we set $z_1 = v_1(t)$ and then compute z_2 with the help of (5.18), The concatenation of z_1 and z_2 will be $z^{aug} = v_1^{aug}(t)$, associated with the augmented adjoint equation in (5.16).

Let us focus on the j^{th} component of both vectors on each side of (5.18). We naturally substitute $z_1 = v_1(t) = \partial \hat{t}/\partial x^\gamma(t)$, to get

$$\sum_{i=1}^M \frac{\partial \hat{t}}{\partial x_i^\gamma} \frac{\partial f_i}{\partial p_j} = z_{2,j}.$$

However, $z_{2,j}$ becomes, with our substituting $z_1 = v_1(t)$,

$$z_{2,j} = v_{1,M+j}^{aug}.$$

As a result, considering (5.14), we have (5.15). ■

The previous proof is significant in that once we figure out a reliable and accurate numerical scheme to compute $v_1(t)$, associated with the generic ODE in (2.1), and $v_1^{aug}(t)$, associated with $\dot{q}(w) = i(w)$, which is derived very simply from (2.1), we will not need the numerical schemes for $\partial\hat{t}/\partial x_i^\gamma(t)$ in (5.3) and $\partial\hat{t}/\partial p_j$ in (5.14). If we spell out a scheme to compute $v_1(t)$ for the generic ODE in (2.1) and the generic DAE in (2.4), then the sensitivity of \hat{t} , the phase of a generic ODE, with respect to both its states and parameters, on γ , can be calculated very easily.

We now provide the justification of the transition from (5.13) to (5.14).

Lemma 2 *The time derivative of the expression in*

$$\frac{\partial\hat{t}}{\partial p_j} = \sum_{i=1}^M \frac{\partial\hat{t}}{\partial x_i^\gamma} \frac{\partial x_i^\gamma}{\partial p_j},$$

where both terms in the summation are functions of t , is given by

$$\frac{d}{dt} \left(\frac{\partial\hat{t}}{\partial p_j} \right) = \sum_{i=1}^M \frac{\partial\hat{t}}{\partial x_i^\gamma} \frac{\partial f_i}{\partial p_j}.$$

Above, $x^\gamma(t)$ is the steady-state periodic solution on γ , p is the parameters vector, associated with the generic ODE in (2.1), and f is the nonlinear functions vector in (2.1).

Proof: Let us conduct this proof with not the extrics of vectors but with vectors themselves.

We know that $\partial\hat{t}/\partial x^\gamma(t) = v_1(t)$. Also, we know the explicit expression for $\partial x^\gamma/\partial p$, through the analysis given in 5.4.1. All we need to do is to substitute the expression for $\mathbf{odK}(t, \tau)$, the state transition function of the LPTV equation, derived from (2.1). We have

$$\begin{aligned} \frac{\partial x^\gamma}{\partial p_j} &= \int_0^t \mathbf{odK}(t, \tau) \frac{\partial f}{\partial p_j}(\tau) d\tau \\ &= \int_0^t \left[\sum_{i=1}^M e^{\mu_i(t-\tau)} u_i(t) v_i^\top(\tau) \right] \frac{\partial f}{\partial p_j}(\tau) d\tau \\ &= \sum_{i=1}^M e^{\mu_i t} u_i(t) \int_0^t e^{-\mu_i \tau} v_i^\top(\tau) \frac{\partial f}{\partial p_j}(\tau) d\tau. \end{aligned} \quad (5.19)$$

Let us define for convenience

$$S_i(t) = \int_0^t e^{-\mu_i \tau} v_i^\top(\tau) \frac{\partial f}{\partial p_j}(\tau) d\tau. \quad (5.20)$$

Then, we proceed as in

$$\begin{aligned}
\frac{\partial \hat{t}}{\partial p_j} &= \sum_{i=1}^M e^{\mu_i t} \underbrace{v_1^\top(t) u_i(t)}_{\delta_{1i}} S_i(t) \\
&= S_1(t) \\
&= \int_0^t v_1^\top(\tau) \frac{\partial f}{\partial p_j}(\tau) d\tau.
\end{aligned} \tag{5.21}$$

Let us not forget our assumption that $\mu_1 = 0$, and $\mu_i < 0$ for $2 \leq i \leq M$.

By the fundamental theorem of calculus, we get

$$\frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) = v_1^\top(t) \frac{\partial f}{\partial p_j}(t),$$

which is the same as the expression in (5.14). ■

The proof above is much simpler than the one provided in [6]. Considering that the justification of Lemma (2) is the main contribution of [6], the proof above, making use of the results of Floquet theory, is significant.

We have shown that the time derivative of $\partial \hat{t} / \partial p_j = v_{1, M+j}^{aug}(t)$, where this augmented vector is associated with the augmented system given as $\dot{q}(w) = i(w)$, derived from the generic ODE in (2.1). A reliable numerical scheme to compute vector function $v_1(t)$, associated with either an ODE, as in (2.1), or a DAE, as in (2.4), would suffice in replacing all the related theory developed in [10] and [6]. Particularly, two such numerical procedures will be presented in the numerical methods section.

The question remains as to whether we may also modify originally a generic DAE in order to incorporate our analysis with the capability of exploring into parameter perturbations afflicting DAEs. The answer is in the affirmative, and this is what we try to show next.

5.4.3 Parameter Sensitivity Equation for a DAE

The technique in deriving the sensitivity equation in the DAE case is very similar to that exercised in the ODE case, of Section 5.4.1. The forms of the generic solutions in the two cases are not that similar.

(2.4) has the form $\dot{q}(x) = f(x)$. Recalling that q and f depend on both x and p and that x is a function of both t and p , we have $q = q(x(t, p), p)$ and $f = f(x(t, p), p)$. We take the partial derivative of both sides of (2.4) with respect to p .

$$\frac{d}{dt} \left(\frac{\partial}{\partial p} [q(x(t, p), p)] \right) = \frac{\partial}{\partial p} [f(x(t, p), p)]$$

x is the first argument of both q and f . p is the second argument of both q and f . So let us call $arg_1 = x$ and $arg_2 = p$. We proceed as follows.

$$\begin{aligned} & \frac{d}{dt} \left(\frac{\partial q}{\partial arg_1} \frac{\partial arg_1}{\partial p} + \frac{\partial q}{\partial arg_2} \frac{\partial arg_2}{\partial p} \right) \\ &= \frac{\partial f}{\partial arg_1} \frac{\partial arg_1}{\partial p} + \frac{\partial f}{\partial arg_2} \frac{\partial arg_2}{\partial p} \end{aligned}$$

Notice that

$$\frac{\partial arg_2}{\partial p} = \frac{\partial p}{\partial p} = 1,$$

and then in compact form we have

$$\frac{d}{dt} \left(\frac{\partial q}{\partial x} \frac{\partial x}{\partial p} + \frac{\partial q}{\partial p} \right) = \frac{\partial f}{\partial x} \frac{\partial x}{\partial p} + \frac{\partial f}{\partial p}.$$

All our evaluations are on γ . Invoking the definitions $\mathbf{C}(t) = \partial q / \partial x$ and $\mathbf{G}(t) = \partial f / \partial x$, which hold on γ , and rearranging,

$$\begin{aligned} \frac{d}{dt} \left(\mathbf{C}(t) \left\{ \frac{\partial x^\gamma}{\partial p} \right\} \right) &= \mathbf{G}(t) \left\{ \frac{\partial x^\gamma}{\partial p} \right\} \\ &+ \left[\frac{\partial f}{\partial p} - \frac{d}{dt} \left(\frac{\partial q}{\partial p} \right) \right]. \end{aligned} \quad (5.22)$$

Above is the very sensitivity equation we have been seeking. We know that $\mathbf{C}(t)$ and $\mathbf{G}(t)$ are T -periodic. $\partial q / \partial p$ and $\partial f / \partial p$ are also T -periodic. The time derivative of $\partial q / \partial p$ is again T -periodic. Therefore, (5.22) is a T -periodic LPTV system, excited with an input of the same period, T .

Let us call $y = \partial x^\gamma / \partial p$ and

$$b(t) = \frac{\partial f}{\partial p} - \frac{d}{dt} \left(\frac{\partial q}{\partial p} \right).$$

Then, we have

$$\frac{d}{dt} (\mathbf{C}(t)y) = \mathbf{G}(t)y + b(t). \quad (5.23)$$

It is clear that the equation above is the inhomogeneous form of the LPTV equation, derived from the generic DAE in (2.4). Demir in [3] shows that the solution of the equation in (5.23) is the sum of a homogeneous part, $S_{hom}(t)$, and an inhomogeneous part, $S_{inh}(t)$, i.e. $y(t) = S_{hom}(t) + S_{inh}(t)$.

In [3], the generic forms given by

$$\begin{aligned} S_{hom}(t) &= \mathbf{K}(t, 0)y(0) \\ &= \sum_{i=1}^m \exp(\mu_i t) u_i(t) v_i^\top(0) \mathbf{C}(0)y(0) \end{aligned} \quad (5.24)$$

and

$$\begin{aligned}
S_{inh}(t) &= \int_0^t \mathbf{odK}(t, \tau) b(\tau) d\tau + F(t) b(t) \\
&= \sum_{i=1}^m u_i(t) \int_0^t \exp(\mu_i(t - \tau)) v_i^\top(\tau) b(\tau) d\tau \\
&\quad + F(t) b(t)
\end{aligned} \tag{5.25}$$

are proposed and justified. Above,

$$\mathbf{K}(t, \tau) = \sum_{i=1}^m \exp(\mu_i(t - \tau)) u_i(t) v_i^\top(\tau) \mathbf{C}(\tau)$$

is the state transition function of the LPTV equation given by $d/dt(\mathbf{C}(t)y) = \mathbf{G}(t)y$, the equation derived from (2.4).

$$\mathbf{odK}(t, \tau) = \sum_{i=1}^m u_i(t) \exp(\mu_i(t - \tau)) v_i^\top(\tau)$$

is in the form of the state transition function of the LPTV equation derived from the generic ODE in (2.1), but the Floquet exponents and functions, the Floquet components overall, belong to the forward and adjoint LPTV equations derived from the generic DAE in (2.4).

Notice that in (5.24) and (5.25), the upper limit of both summations is not M , the dimension of our generic system, but $m \leq M$. The reason for this is that there may be some modes, belonging to the LPTV equation $d/dt(\mathbf{C}(t)y) = \mathbf{G}(t)y$, that are in the nullspace of $\mathbf{C}(t)$. We have, therefore,

$$\mathbf{C}(t) [u_{m+1}(t), \dots, u_M(t)] = 0.$$

These modes, $u_i(t)$ for $(m+1) \leq i \leq M$, are nullified instantly by $\mathbf{K}(t, 0)$, so $\mu_i = -\infty$, for $(m+1) \leq i \leq M$ [3]. Therefore, examining $S_{hom}(t)$ in (5.24), whether or not $y(0)$ has components along $u_i(0)$, for $(m+1) \leq i \leq M$, $S_{hom}(t)$ will not have components along $u_i(t)$, for $t > 0$.

By the biorthogonality conditions proved in [3], we have the following.

$$\begin{aligned}
v_j^\top(t) \mathbf{C}(t) u_i(t) &= \delta_{ij}, \quad 1 \leq i, j \leq m \\
v_j^\top(t) \mathbf{C}(t) u_i(t) &= 0, \quad 1 \leq i \leq m, (m+1) \leq j \leq M \\
v_j^\top(t) \mathbf{G}(t) u_i(t) &= 0, \quad (m+1) \leq i \leq M, 1 \leq j \leq m
\end{aligned}$$

In [3], it is shown through these conditions that

$$\{ \mathbf{C}(t)u_1(t), \dots, \mathbf{C}(t)u_m(t), \mathbf{G}(t)u_{m+1}(t), \dots, \mathbf{G}(t)u_M(t) \}$$

is a legitimate basis set for \mathfrak{R}^M , for any $t \geq 0$. Therefore, $b(t)$ in (5.23) can be written as a linear combination of the basis functions in this set at any t .

$F(t)$ in $S_{inh}(t)$ of (5.25) has the following property [3].

$$F(t) [\mathbf{C}(t)u_1(t), \dots, \mathbf{C}(t)u_m(t)] = 0$$

Therefore, $\mathbf{C}(t)u_i(t)$, for $1 \leq i \leq m$, reside in the nullspace of $F(t)$. Also, the following is true.

$$F^\top(t) [\mathbf{C}^\top(t)v_1(t), \dots, \mathbf{C}^\top(t)v_m(t)] = 0$$

$\mathbf{C}^\top(t)v_i(t)$, for $1 \leq i \leq m$, span the left nullspace of $F(t)$.

In all, we have the following. Let us have $b(t) = b_1(t) + b_2(t)$, where

$$b_1(t) = \sum_{i=1}^m c_i \mathbf{C}(t)u_i(t)$$

and

$$b_2(t) = \sum_{j=m+1}^M c_j \mathbf{G}(t)u_j(t).$$

We get through the contributions provided by [3], that

$$\int_0^t \mathbf{odK}(t, \tau) b_2(\tau) d\tau = 0$$

and

$$F(t)b_1(t) = 0.$$

In addition,

$$\int_0^t \mathbf{odK}(t, \tau) b_1(\tau) d\tau \neq 0$$

and

$$F(t)b_2(t) \neq 0,$$

if not all of c_i 's are zero, for $1 \leq i \leq M$. Therefore, if $b(t)$ has components in the subspace spanned by $\mathbf{C}(t)u_i(t)$, for $1 \leq i \leq m$, then these components show up in $y(t)$ through the convolution expression in $S_{inh}(t)$ of (5.25). If $b(t)$, on the other hand, has components in

the subspace spanned by $\mathbf{G}(t)u_i(t)$, $(m+1) \leq i \leq M$, these components show up in $y(t)$ through the expression containing $F(t)$ in $S_{inh}(t)$ [3].

This review of Demir's work in [3] was necessary, for we will make use of the explicit form of $S_{inh}(t)$ in (5.25). Particularly, we will utilize the information about the vector functions spanning the left nullspace of $F(t)$, in addition to the explicit form of the convolution expression in $S_{inh}(t)$.

The homogeneous part of the solution, $S_{hom}(t)$ in (5.24), is not necessary, since we assume that

$$y(0) = \frac{\partial x^\gamma}{\partial p}(0) = 0.$$

This initial condition follows from the assumption that changes in p start affecting $x^\gamma(t)$ at $t = 0$. Also, $x^\gamma(0^-)$ should be strictly on the limit cycle, γ , which is naturally true.

We proceed now to mathematically relate the drift in \hat{t} , the phase, due to parameter perturbations, to $v_1^{aug}(t)$. $v_1^{aug}(t)$ is associated with the adjoint LPTV system, to be derived from $\dot{Q}(w) = I(w)$. $\dot{Q}(w) = I(w)$ is the new augmented system we derived from the generic DAE in (2.4), through augmenting the states vector x with p , the parameters vector, to get $w = (x^\top p^\top)^\top$.

5.4.4 Phase Sensitivity with Respect to the Parameters of a DAE System

In Section (2.1), we showed that

$$\frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) = v_{1, M+j}^{aug}(t),$$

where \hat{t} is the phase of the generic ODE in (2.1), p_j is the j^{th} entry of the parameters vector, p , associated with the nonlinear functions vector, f in (2.1). $v_1(t)$ is a periodic solution of the adjoint LPTV equation derived from (2.1). We augmented (2.1) by assigning the entries of p as states, in Section 4.2.1, and obtained $\dot{q}(w) = i(w)$, the augmented system, with x and p concatenated in w . In Section (2.1), what we did was to find the periodic solution of the adjoint LPTV equation, derived from $\dot{q}(w) = i(w)$ and call it $v_1^{aug}(t)$. The work of Taylor et al. in [6] was referred to as crucial in showing that

$$\frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) = \frac{\partial \hat{t}}{\partial x^\gamma} \cdot \frac{\partial f}{\partial p_j},$$

but we also provided our own proof for justifying this equality. Then, with the tools of Floquet theory, we related $\partial \hat{t} / \partial p_j$ to $v_1^{aug}(t)$ as above.

We are now exploring the DAE case, and we are again induced to define $\partial\hat{t}/\partial p_j$ and its time derivative. The definition will be different compared to the ODE case. However, the essence of our derivations is the same as those presented in Section 5.4.2. First, we will define $\partial\hat{t}/\partial p_j$. We will naturally face $\partial x^\gamma/\partial p_j$, through this definition, but fortunately we know how to solve for $\partial x^\gamma/\partial p_j$, considering the contributions of Demir's work in [3], which we reviewed in the last section. Second, we will compute the time derivative of $\partial\hat{t}/\partial p_j$ and will obtain an expression. Third, we will figure out the form of the adjoint LPTV equation, to be derived from $\dot{Q}(w) = I(w)$, which is the augmented system we acquired through our derivation in Section 4.2.2. There, we assigned the entries of the parameters vector, p , as states, and augmented the generic DAE system in (2.4), to get $\dot{Q}(w) = I(w)$. And the last but not the least, we will figure out the periodic solution of the adjoint equation obtained from $\dot{Q}(w) = I(w)$, and calling it $v_1^{aug}(t)$, we will finally relate $v_1^{aug}(t)$ to the time derivative of $\partial\hat{t}/\partial p_j$, computed in the second step. The series of derivations in this section will once more establish the vitality of $v_1(t)$, associated with any oscillatory system, whether ODE or DAE, if we concerned with analyzing the phase of such systems in the close neighborhood of γ .

Let us define the following partial differential expression through the chain rule.

$$\frac{\partial\hat{t}}{\partial p_j} = \frac{\partial\hat{t}}{\partial q} \cdot \frac{\partial q}{\partial p_j} \quad (5.26)$$

We define $\partial\hat{t}/\partial p_j$ as such since we have already established $\partial\hat{t}/\partial q = v_1(t)$ on γ . Let us review briefly how we figured out this finding. Note that the trivial differential equation given by $d\hat{t}/dt = 1$, with $\hat{t}(0) = 0$, is correct for a DAE, as in (2.4), as well. We showed that

$$\frac{d\hat{t}}{dt} = \frac{\partial\hat{t}}{\partial q} \cdot \frac{dq}{dt} = 1$$

is true over the whole domain of attraction, \mathcal{W} , associated with γ , the limit cycle of interest, for γ is assumed to have asymptotic orbital stability and asymptotic phase. Then, on γ ,

$$\frac{\partial\hat{t}}{\partial q} \cdot \frac{dq}{dt} = \frac{\partial\hat{t}}{\partial q(x^\gamma(t))} \cdot \left[\frac{\partial q(x^\gamma(t))}{\partial x^\gamma(t)} \frac{dx^\gamma}{dt} \right] = 1.$$

Invoking the usual notations $\partial q/\partial x = \mathbf{C}(t)$ on γ and $dx^\gamma/dt = u_1(t)$, we had

$$\frac{\partial\hat{t}}{\partial q(x^\gamma(t))} \cdot (\mathbf{C}(t)u_1(t)) = 1.$$

After showing that $\partial\hat{t}/\partial q$ is in the same direction as $v_1(t)$, we had to recall the biorthogonality relation for DAEs, given as $v_1^\top \mathbf{C}(t)u_1(t) = 1$. Then, this discussion led us to deduce that $\partial\hat{t}/\partial q = v_1(t)$ on γ .

We now return to the current discussion to process the definition of $\partial\hat{t}/\partial p_j$, in (5.26) as

$$\frac{\partial\hat{t}}{\partial p_j} = v_1(t) \cdot \frac{\partial q}{\partial p_j}, \quad (5.27)$$

on γ . We now have to prove the following lemma to figure out what the time derivative of $\partial\hat{t}/\partial p_j$ is.

Lemma 3 *Let \hat{t} be the phase of the generic DAE in (2.4) and p be the vector of parameters that are eligible for perturbation and take place in the analytic expressions constituting the nonlinear functions q and f in (2.4). Having defined $\partial\hat{t}/\partial p_j$ as in (5.27), the time derivative of this expression is given as*

$$\frac{d}{dt} \left(\frac{\partial\hat{t}}{\partial p_j} \right) = \frac{dv_1}{dt} \cdot \frac{\partial q}{\partial p_j} + v_1(t) \cdot \frac{\partial f}{\partial p_j}. \quad (5.28)$$

Proof: We start by noting that q in (2.4) is a function of both x and p , and in turn, x is a function of both time t and p . Therefore, we have $q = q(x(t, p), p)$ and we compute $\partial q/\partial p_j$ on γ as

$$\frac{\partial q}{\partial p_j} = \frac{\partial q(x^\gamma(t))}{\partial x^\gamma(t)} \frac{\partial x^\gamma}{\partial p_j} + \frac{\partial q}{\partial p_j} = \mathbf{C}(t) \frac{\partial x^\gamma}{\partial p_j} + \frac{\partial q}{\partial p_j}.$$

We stated through the contributions in [3] that $\partial x^\gamma/\partial p_j = S_{inh}(t)$ with $S_{inh}(t)$ given in (5.25), with now

$$b(t) = \frac{\partial f}{\partial p_j} - \frac{d}{dt} \left(\frac{\partial q}{\partial p_j} \right).$$

Simply substituting, we have

$$\begin{aligned} \frac{\partial\hat{t}}{\partial p_j} &= \sum_{i=1}^m \underbrace{v_1^\top(t) \mathbf{C}(t) u_i(t)}_{\delta_{1i}} \int_0^t \exp(\mu_i(t - \tau)) v_i^\top(\tau) b(\tau) d\tau \\ &+ v_1^\top(t) \mathbf{C}(t) F(t) b(t) \\ &+ v_1(t) \cdot \frac{\partial q}{\partial p_j}. \end{aligned}$$

Notice that above in the first expression on the right-hand side, the biorthogonality relation holds because the upper limit of the summation is m , not M . m is the number of Floquet modes, to which correspond finite Floquet multipliers, i.e. $u_i(t)$, for $1 \leq i \leq m$, are not in the nullspace of $\mathbf{C}(t)$, whereas $u_i(t)$, for $(m + 1) \leq i \leq M$, are in the nullspace of $\mathbf{C}(t)$.

Also, $\mathbf{C}^\top(t)v_1(t)$ is in the left nullspace of $F(t)$ [3], so the second term on the right-hand side vanishes. We have, therefore,

$$\begin{aligned} \frac{\partial \hat{t}}{\partial p_j} &= \int_0^t v_1^\top(\tau)b(\tau)d\tau \\ &+ v_1(t) \cdot \frac{\partial q}{\partial p_j}, \end{aligned}$$

noting our assumption that $\mu_1 = 0$. Taking the time derivative of both sides,

$$\frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) = v_1(t) \cdot b(t) + \frac{d}{dt} \left(v_1(t) \cdot \frac{\partial q}{\partial p_j} \right),$$

through the fundamental theorem of calculus. Now it is time to substitute the expression for $b(t)$ and invoke the differentiation rule for products of functions, as in

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) &= v_1(t) \cdot \frac{\partial f}{\partial p_j} \\ &- \left\{ v_1(t) \cdot \frac{d}{dt} \left(\frac{\partial q}{\partial p_j} \right) \right\} \\ &+ \frac{d}{dt} \left(v_1(t) \cdot \frac{\partial q}{\partial p_j} \right) \\ &= v_1(t) \cdot \frac{\partial f}{\partial p_j} \\ &- \left\{ \frac{d}{dt} \left(v_1(t) \cdot \frac{\partial q}{\partial p_j} \right) - \frac{dv_1}{dt} \cdot \frac{\partial q}{\partial p_j} \right\} \\ &+ \frac{d}{dt} \left(v_1(t) \cdot \frac{\partial q}{\partial p_j} \right). \end{aligned}$$

After the obvious cancellation, we have

$$\frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) = v_1(t) \cdot \frac{\partial f}{\partial p_j} + \frac{dv_1}{dt} \cdot \frac{\partial q}{\partial p_j},$$

which is the same result as in (5.28). ■

We are now going to use the lemma above to relate the time derivative of $\partial \hat{t}/\partial p_j$ to the periodic solution of the adjoint LPTV system, derived from $\dot{Q}(w) = I(w)$.

Theorem 11 $\dot{Q}(w) = I(w)$ is the augmented DAE system derived from the generic DAE in (2.4), $w = (x^\top p^\top)^\top$. Let $v_1^{aug}(t)$ be the periodic solution of the adjoint LPTV equation, derived from $\dot{Q}(w) = I(w)$. Then,

$$v_{1,M+j}^{aug} = \frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right), \quad (5.29)$$

i.e. the $(M+j)^{th}$ entry of $v_1^{aug}(t)$ is the same as the expression in (5.28).

Proof: The LPTV equation that is derived from $\dot{Q}(w) = I(w)$ is

$$\frac{d}{dt} \left(\left. \frac{\partial Q}{\partial w} \right|_{\gamma} y^{aug} \right) = \left. \frac{\partial I}{\partial w} \right|_{\gamma} y^{aug}.$$

Note that the dimension of this system is $(M + L)$, so $y^{aug}(t)$ is an $((M + L) \times 1)$ -sized vector function. The explicit form of this LPTV equation is written as

$$\frac{d}{dt} \left[\left(\left. \begin{pmatrix} \frac{\partial q}{\partial x} & \frac{\partial q}{\partial p} \\ 0 & 0 \end{pmatrix} \right|_{\gamma} y^{aug} \right) \right] = \left(\left. \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial p} \\ 0 & -\mathbf{I}_L \end{pmatrix} \right|_{\gamma} y^{aug} \right).$$

The adjoint equation can then be written as

$$\left(\left. \begin{pmatrix} \left(\frac{\partial q}{\partial x} \right)^{\top} & 0 \\ \left(\frac{\partial q}{\partial p} \right)^{\top} & 0 \end{pmatrix} \right|_{\gamma} \frac{dz^{aug}}{dt} \right) = - \left(\left. \begin{pmatrix} \left(\frac{\partial f}{\partial x} \right)^{\top} & 0 \\ \left(\frac{\partial f}{\partial p} \right)^{\top} & -\mathbf{I}_L \end{pmatrix} \right|_{\gamma} z^{aug} \right). \quad (5.30)$$

Let us assume $z^{aug}(t) = v_1^{aug}(t)$ is a periodic solution of this adjoint equation. Also let us denote $z^{aug}(t)$ as a concatenated vector function as in $z^{aug}(t) = (z_1^{\top}(t) z_2^{\top}(t))^{\top}$, where $z_1(t)$ is $(M \times 1)$ -sized and $z_2(t)$ is $(L \times 1)$ -sized.

We can now write a set of coupled equations, originating from the adjoint equation.

$$\begin{aligned} \left(\frac{\partial q}{\partial x^{\gamma}} \right)^{\top} \frac{dz_1}{dt} &= - \left(\frac{\partial f}{\partial x^{\gamma}} \right)^{\top} z_1 \\ \left(\frac{\partial q}{\partial p} \right)^{\top} \frac{dz_1}{dt} &= - \left(\frac{\partial f}{\partial p} \right)^{\top} z_1 + z_2 \end{aligned}$$

The first equation above, when expressed in the form of $\mathbf{C}(t)\dot{z} = -\mathbf{G}(t)z$, strikes us as the adjoint LPTV equation derived from the original DAE in (2.4). $v_1(t)$ is a periodic solution of this adjoint form. When we set $z_1(t) = v_1(t)$ in the second equation above, we get

$$z_2 = \left(\frac{\partial q}{\partial p} \right)^{\top} \frac{dv_1}{dt} + \left(\frac{\partial f}{\partial p} \right)^{\top} v_1(t). \quad (5.31)$$

There is no doubt that $z^{aug}(t) = (z_1^{\top}(t) z_2^{\top}(t))^{\top}$, when we set $z_1(t) = v_1(t)$, will be a periodic solution of the augmented adjoint form in (5.30) above. We deduce that $v_1^{aug}(t)$ is the periodic solution we have been seeking.

The j^{th} entry of z_2 in (5.31) can be written as

$$z_{2,j} = \frac{dv_1}{dt} \cdot \frac{\partial q}{\partial p_j} + v_1(t) \cdot \frac{\partial f}{\partial p_j}.$$

Notice that $z_{2,j} = v_{1,M+j}^{aug}(t)$ in this case. Examining (5.28), we have the result, (5.29). ■

Through our derivations we have established the following. $v_1(t)$ is the periodic solution of $\mathbf{C}^\top(t)\dot{z} = -\mathbf{G}^\top(t)z$, the adjoint LPTV equation derived from the generic DAE in (2.4). In fact, any multiple of $v_1(t)$ is a periodic solution, but with the normalization condition given by $v_1^\top(t)\mathbf{C}(t)u_1(t) = 1$, with $u_1(t) = dx^\gamma/dt$, $v_1(t)$ becomes unique. $v_1^{aug}(t)$, on the other hand, is the periodic solution of the adjoint LPTV equation to be derived from $\dot{Q}(w) = I(w)$, the augmented nonlinear system. $v_1^{aug}(t)$ accounts for both $\partial\hat{t}/\partial q = v_1(t)$ and $d/dt(\partial\hat{t}/\partial p_j)$, on γ .

If we had a reliable and accurate numerical scheme to compute $v_1(t)$, associated with any DAE system, as given in (2.4), then we could apply this scheme on the adjoint forms of both (2.4) and $\dot{Q}(w) = I(w)$, and then we could calculate the effects of both state and parameter perturbations on a system in DAE form, through the phase equation for DAEs.

Chapter 6

NUMERICAL METHODS

6.1 Numerical Solution of Linear Equation Systems

A linear system of equations is of the form

$$\mathbf{A}x = b, \quad (6.1)$$

where \mathbf{A} is a square matrix of size $(M \times M)$, and x and b are $(M \times 1)$ -sized vectors. x is the solution of the problem in (6.1).

Generally, two methods of solving linear equation systems are used. Gaussian Elimination computes an exact solution and therefore requires that \mathbf{A} in (6.1) is full-rank. Krylov Subspace Methods, on the other hand, are iterative schemes. A convergence check may be employed to decide whether an iterate is as accurate as desired. Also, Krylov Methods do not require that \mathbf{A} in (6.1) be full-rank.

6.2 Newton's Method for Solving Nonlinear Algebraic Equation Systems

Newton's method is devised to solve nonlinear algebraic equations of the form

$$h(x) = 0, \quad (6.2)$$

where h is a nonlinear function of x , and $h : \Re^M \rightarrow \Re^M$.

In order to solve (6.2), an iterative scheme is employed through Newton [14]. Letting the k^{th} iterate of x , the solution, be x^k , the following system of linear equations are solved at iteration k .

$$\frac{\partial h(x^k)}{\partial x^k} [x^{k+1} - x^k] = -h(x^k) \quad (6.3)$$

Above, $\mathbf{J}^k = \partial h(x^k)/\partial x^k$ is called the Jacobian of h at iteration k . \mathbf{J}^k is an $(M \times M)$ -sized matrix. Also in (6.3), we may define

$$\Delta x^k = x^{k+1} - x^k \quad (6.4)$$

to be the update that enables the computation of the next iterate x^{k+1} . Obviously, $x^{k+1} = x^k + \Delta x^k$.

Since Newton's method is iterative, a convergence check is needed to decide whether x^k is as accurate as desired to be declared as a solution. Both convergence checks in

$$\left| h(x^k) \right| < \epsilon_h \quad (6.5)$$

$$\left| \Delta x^k \right| < \epsilon_a + \epsilon_r x^{k+1} \quad (6.6)$$

are necessary at iteration k . (6.5) is needed for the actual function value needs to be small, considering (6.2). (6.6) ensures that the update Δx^k does not perturb x^k to some value x^{k+1} that is far away. Subscripted ϵ values are arranged according to specifications and absolute values of the vectors involved.

Newton's method is proved to converge quadratically provided that a guess, close enough to the actual solution x , is initially supplied as x^1 . In order to facilitate convergence, in the case of initial guesses that are far away, continuation schemes may be employed [14].

6.3 Multistep Methods for Differential Equations

Multistep discretization is one of the methods that facilitates the numerical solution of differential equations. In this section, we are going to focus on solving the generic DAE in (2.4) through multistep discretization and Newton's method.

Let $x(t_0)$ be the initial condition provided for solving the generic DAE in (2.4). Then, the solution of (2.4) for $t > t_0$ is required. Through numerical methods, the values of the solution $x(t)$ for discrete values of time can be calculated. In other words, we are required to compute the elements of

$$\chi = \{x(t_0), x(t_1), x(t_2), \dots, x(t_N)\}, \quad (6.7)$$

through numerical methods, supposing that (2.4) is to be solved from $t = t_0$ until $t = t_N$.

Before presenting the discretized form of (2.4), we define the set

$$\mathcal{H} = \{h_i, \dots, h_{i-r+1}\}, \quad (6.8)$$

where we know that $h_j = t_j - t_{j-1}$, for $1 \leq j \leq N$. \mathcal{H} is a set with r elements, these r elements being the lengths of the intervals between consecutive timepoints. We are going to need this set when spelling out the discretized form below.

The discretized form of (2.4) reads

$$\sum_{j=0}^r \hat{\alpha}_j(\mathcal{H})q(x(t_{i-j})) = \sum_{j=0}^r \hat{\beta}_j(\mathcal{H})f(x(t_{i-j})), \quad (6.9)$$

$\hat{\alpha}_j(\mathcal{H})$ and $\hat{\beta}_j(\mathcal{H})$, for $0 \leq j \leq r$, above are the multistep coefficients. These coefficients are numerical values that implicitly depend on all the elements of \mathcal{H} .

Note that the discretization method given in (6.9) is designed to accommodate variable timesteps, i.e. all elements of \mathcal{H} are allowed to be different from each other. This multi-step discretized form is presented as an r -step method, i.e. we are computing sample $x(t_i)$, but in doing that we make use of the r samples before $x(t_i)$, which are $x(t_{i-j})$ for $1 \leq j \leq r$. The discretized form in (6.9) might be thought of as having an r -deep memory.

Note also that we, by no means, imply that r in (6.9) is constant. r can be a function of i , as in $r = r(i)$. This means the depth of memory that the discretization method exploits may change according to which sample is computed. In this aspect, we accommodate, through (6.9), variable order schemes as well.

Remark 2 *There are simpler multistep discretization schemes that we can utilize. For example, note the first element in \mathcal{H} , $h_i = t_i - t_{i-1}$. There are $(r - 1)$ other elements in \mathcal{H} . Let us set $h_{i-j} = h_i$ for $1 \leq j \leq r - 1$. Then, all elements in \mathcal{H} will be equal to h_i . This means we will have $\mathcal{H} = \{h_i\}$, i.e. \mathcal{H} will consist of only one element. In addition to this modification, in simpler schemes, we have different forms for $\hat{\alpha}_j(\mathcal{H})$ and $\hat{\beta}_j(\mathcal{H})$, as in $\hat{\alpha}_j(h_i) = \alpha_j/h_i$ and $\hat{\beta}_j(h_i) = \beta_j$, for $0 \leq j \leq r$. α_j and β_j are constant predetermined coefficients, calculated according to the multistep method employed. Then, the scheme in (6.9) is simplified into*

$$\frac{1}{h_i} \sum_{j=0}^r \alpha_j q(x(t_{i-j})) = \sum_{j=0}^r \beta_j f(x(t_{i-j})). \quad (6.10)$$

Notice that the discretization scheme in (6.9) is used to solve for $x(t_i)$ through Newton's method. (6.9) can be solved for $x(t_i)$, provided that $x(t_{i-j})$, for $1 \leq j \leq r$, are known. Note the manipulation of (6.9) into the following.

$$\begin{aligned} h(x(t_i)) &= \left[\hat{\alpha}_0(\mathcal{H})q(x(t_i)) - \hat{\beta}_0(\mathcal{H})f(x(t_i)) \right] \\ &+ \sum_{j=1}^r \left[\hat{\alpha}_j(\mathcal{H})q(x(t_{i-j})) - \hat{\beta}_j(\mathcal{H})f(x(t_{i-j})) \right] \\ &= 0 \end{aligned} \quad (6.11)$$

(6.11) is in the form that is convenient for the application of Newton's method, i.e. a nonlinear function of a vector variable, equated to zero. In short, (6.11) could be written as $h(x(t_i)) = 0$, where h is the nonlinear function in (6.11).

In order to solve (6.11) for $x(t_i)$, we proceed as follows. Let us introduce the auxiliary notation, at iteration l of Newton's method,

$$\mathbf{J}_{i,j}^l = \frac{\partial h(x^l(t_{i-j}))}{\partial x^l(t_{i-j})} = \hat{\alpha}_j(\mathcal{H}) \frac{\partial q(x^l(t_{i-j}))}{\partial x^l(t_{i,j})} - \hat{\beta}_j(\mathcal{H}) \frac{\partial f(x^l(t_{i,j}))}{\partial x^l(t_{i,j})}. \quad (6.12)$$

Note that the l^{th} iterate for $x(t_i)$ is $x^l(t_i)$. Then, the linear system of equations to solve at iteration l is, making use of the definition notation in (6.12),

$$\begin{aligned} \frac{\partial h(x^l(t_i))}{\partial x^l(t_i)} [x^{l+1}(t_i) - x^l(t_i)] &= \mathbf{J}_{i,0}^l \Delta x^l(t_i) \\ &= -h(x^l(t_i)). \end{aligned} \quad (6.13)$$

In (6.13), we solve for $\Delta x^l(t_i) = x^{l+1}(t_i) - x^l(t_i)$. The Jacobian $\mathbf{J}_{i,0}^l = \partial h(x^l(t_i))/\partial x^l(t_i)$ above is a sparse full-rank matrix. Therefore, (6.13) may be solved through computing the LU factors of $\mathbf{J}_{i,0}^l$, i.e $\mathbf{J}_{i,0}^l = \mathbf{L}_{i,0}^l \mathbf{U}_{i,0}^l$, and calculating $x^l(t_i)$ through

$$\Delta x^l(t_i) = \left(\mathbf{U}_{i,0}^l\right)^{-1} \left(\mathbf{L}_{i,0}^l\right)^{-1} \left(-h(x^l(t_i))\right). \quad (6.14)$$

Note that $x^1(t_i) = x(t_{i-1})$ is a legitimate initial guess for solving $x(t_i)$ through Newton's method, because solutions of (2.4) are assumed to be smooth and continuous. When Newton's method converges, we call the computed solution $x(t_i)$, the i^{th} timepoint in χ of (6.7).

In addition, we may make a note of the Jacobian and its LU factors at the last iteration of Newton's method. We have, dropping the l notifier,

$$\begin{aligned} \mathbf{J}_{i,0} &= \mathbf{L}_{i,0} \mathbf{U}_{i,0} \\ &= \hat{\alpha}_0(\mathcal{H}) \mathbf{C}(t_i) - \hat{\beta}_0(\mathcal{H}) \mathbf{G}(t_i), \end{aligned} \quad (6.15)$$

with $\mathbf{C}(t_i) = \partial q(x(t_i))/\partial x(t_i)$ and $\mathbf{G}(t_i) = \partial f(x(t_i))/\partial x(t_i)$. The LU factors of $\mathbf{J}_{i,0}$ will have to be stored when running particularly one of the steady-state periodic solution algorithms in Section 6.4, along with other factors.

Remark 3 Notice that in this section, we utilize Newton's method of Section 6.2, for computing each timepoint of a solution $x(t)$ of the generic DAE in (2.4). In turn, each iteration

of Newton's method must make use of the linear system of equation solutions, explained in Section 6.1. The particular linear system solution technique employed here is Gaussian Elimination, for we compute LU factors. In all, considering differential equation solutions through multistep methods, we make use of, in descending order of hierarchy,

1. Multistep discretization for each timepoint as in (6.11)
2. Newton's method to solve (6.11) for $x(t_i)$
3. Gaussian Elimination to solve the linear equation in (6.13) for $\Delta x^l(t_i) = x^{l+1}(t_i) - x^l(t_i)$ at each iteration l of Newton's method

One of the steady-state periodic solution methods in Section 6.4 will again be designed as an iterative technique, and each iteration of that method will exploit the encapsulated hierarchy noted in this remark, i.e. this particular method in Section 6.4 will top the above list, considering the new hierarchy formed.

6.4 Steady-State Periodic Solutions

We have maintained throughout our derivations that we call a particular steady-state periodic solution on γ , the limit cycle of interest, $x^\gamma(t)$. Most of our derivations rely on $x^\gamma(t)$, since, for our purposes, we see it fit to employ linearizations around γ . However, up to this point, we have not been concerned about how $x^\gamma(t)$ may actually be computed numerically. Our only former statement that can be regarded as related to the numerical computation of $x^\gamma(t)$ is that we are to obtain a discretized form of $x^\gamma(t)$ and that the number of samples over a single period of length T , we set as N .

Definition 19 (Timepoints on γ) *In this section of our work, whenever we refer to $x^\gamma(t)$, the particular steady-state periodic solution on γ , we mean the N samples of $x^\gamma(t)$ over a single period of length T . Set*

$$\chi = \{x^\gamma(t_i) \text{ for } 0 \leq i \leq N - 1\} \quad (6.16)$$

includes these N samples as necessary. Let us have $0 \leq i, j \leq N - 1$. Naturally, $t_i = t_j$ if and only if $i = j$. Also, if $j > i$, then $t_j > t_i$. We also have the convention that if we are

to employ t_N in our discussions, that $t_N - t_0 = T$ is tacitly conceded beforehand. Then, naturally $x^\gamma(t_N) = x^\gamma(t_0)$, and $x^\gamma(t_0)$ and $x^\gamma(t_N)$ are indeed treated as the same sample.

Definition 20 (Timepoint Intervals) *The lengths of the intervals between consecutive timepoints are defined as*

$$h_i = t_i - t_{i-1}, \quad (6.17)$$

for $1 \leq i \leq N$. Naturally, $t_N = t_{N-1} + h_N$.

Remark 4 *Observe that we have called the first time tag t_0 , but for all practical purposes, we may accept to use the convention that $t_0 = 0$. However, in the forthcoming derivations, it would be confusing to have the first time tag as zero and the others as t_i for $1 \leq i \leq N - 1$. Therefore, we let t_0 remain as it is but recall that setting $t_0 = 0$ is perfectly legitimate. What is important is the value of sample $x^\gamma(t_0)$, not its time tag.*

Remark 5 *The distribution of the timepoints along the interval of length T depends on the numerical method to be used. It is most convenient to have frequent samples when $x^\gamma(t)$ is changing at a high rate. When $x^\gamma(t)$ stagnates, however, we can have sparse samples along the particular interval. Some numerical methods do not allow this suitable timepoint distribution to be utilized. In those cases, we are to take*

$$h_i = t_i - t_{i-1} = \frac{T}{N} \quad \text{for } 1 \leq i \leq N, \quad (6.18)$$

so that our samples are uniformly spaced along the interval of length T .

Having defined the timepoints and their distribution along a single period, we still wonder how the samples in set χ of (6.16) are to be computed numerically. A feasible method could be outlined as follows.

Let $x^0(t)$ be a solution of, for example, the generic ODE in (2.1), and let $x^0(0) \in \mathcal{W}$, where \mathcal{W} is the domain of attraction associated with γ , the limit cycle of interest. We know $x^0(t)$, as time progresses, will approach γ , through our assumption that γ has the asymptotically orbital stability property. Therefore, we intuitively guess that $x^0(\tau)$ for some $\tau \gg 0$ will almost be on γ . Whether $x^0(\tau)$ is as close to γ as desired is numerically distinguishable through the following procedure.

One of the M signals in $x^0(t)$ could be monitored through time. A minimum or maximum in the waveform of this signal could be watched, as the value of this critical point on

watch would, in time, seem to settle to a stable equilibrium. Then, after deciding that the simulation had run long enough to achieve this equilibrium, we would measure the length of the time interval between two consecutive instances, where the signal of choice would have crossed the equilibrium value, and we would call this length the period, T , of $x^\gamma(t)$. The discrete points together with their time tags in between these two instances would define $x^\gamma(t)$ as follows. We would shift our time scale so as to call the time tag of the first instance, $t = 0$, and the time tag of the second instance, $t = T$. In between and including times $t = 0$ and $t = T$, we would have a number of time points. We would call this number, $N + 1$. Then, we would throw out the time point with tag $t = T$, because $x^\gamma(t)$ would take the same value at $t = 0$ and $t = T$. Therefore, at the end of this scheme, we would have figured out T and the set of discrete points defining $x^\gamma(t)$, together with their time tags.

The problem with the crude method outlined above is that it is not accurate enough, and the computation takes a very long time to complete. Although this brute-force scheme would require only the oscillator model and a differential equation solver, the stated caveats on accuracy and computational complexity would outdo this minor advantage.

In the schemes called shooting, explained in Section 6.4.1, and harmonic balance, of Section 6.4.2, we are forced to modify differential equation solvers or implement procedures outside the scope of such solvers. However, we maintain that the computational complexity is reduced and a tractable measure of accuracy can be achieved through these methods.

As a final note before proceeding to explain shooting, regard our convention to outline these methods for only DAEs, as in the equations given by (2.4), in this part of our work. The simplifications to incorporate the similar theory with the ability to encompass ODEs as well, as given in (2.1), can be found in the appendices.

6.4.1 Shooting Method

The key property of γ , the limit cycle, and $x^\gamma(t)$, the solution on γ , is periodicity. We have called the period of $x^\gamma(t)$ simply T . Periodic signals are expected to return to the same state after subsequent intervals of their period as the length. Therefore, we know that if we start simulating from a point on γ , $x^\gamma(t_0)$ for example, we are going to return to the same state after T units of time. Mathematically speaking, we have $x^\gamma(t_0 + T) = x^\gamma(t_0)$. Let us write

this as

$$\Upsilon(t_0 + T, t_0, x^\gamma(t_0)) - x^\gamma(t_0) = 0, \quad (6.19)$$

where Υ is the state transition function associated with (2.4). We are going to be explaining the related theory for DAEs, but the simplifications regarding ODEs can be found in the appendices.

(6.19) is the main equation that the shooting method is based on [14]. Basically, we aim to solve for $x^\gamma(t_0)$, provided with an initial guess for this vector. An iterative solution scheme, particularly Newton's method, is employed in this case, for (6.19) is a nonlinear equation, with its right-hand side zero.

Another key aspect of steady-state solution computations, as can be obviously noted, is that we do not have previous information about the period of the signal to be figured out. Therefore, in (6.19), T , the period of $x^\gamma(t)$, is also an unknown. We have got to have an initial guess on T as well, before embarking on numerical computations.

Although the intuition leading to shooting is simple enough, the computations require rigorous theory to be developed. In the following section, we derive which components are to be rigorously computed, in relation to the shooting method.

Required Computational Components

Recall once more that we are going to employ Newton's method, an iterative scheme to solve (6.19). In this section, we are to define the setup at iteration number k . The transition from iteration k to $k + 1$ can be accomplished through the scheme we are about to outline.

Let us denote the fact that we are spelling out computational components for iteration k by superscripting our related variables with k . The steady-state periodic solution is given by $x^k(t)$. Let us denote our timepoints at iteration k , by t_i^k for $0 \leq i \leq N$. Notice that we employ t_N^k as well, but we also concede that $t_N^k - t_0^k = T^k$, T^k being the proposed solution for T , at iteration k . Also, we denote the length of the time intervals between consecutive timepoints by $h_i^k = t_i^k - t_{i-1}^k$ for $0 \leq i \leq N$.

In all, the samples we have at iteration k are given in set

$$\chi^k = \left\{ x^k(t_i^k) \text{ for } 0 \leq i \leq N \right\},$$

and we have T^k as the proposed solution for T . Again, notice that we need $x^k(t_N^k)$ as well.

Now let us return to the basic equation of the shooting method in (6.19). If we write this equation with the corresponding computational components at iteration k , we are going to have

$$F_{sh}^k = \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k)) - x^k(t_0^k), \quad (6.20)$$

where F_{sh}^k might be regarded as a residual. This residual is not exactly equal to zero, for $x^k(t_0^k)$ is not exactly on γ . In the equation above, we are going to treat $x^k(t_0^k)$ as a variable, and the expression with Υ as a function of $x^k(t_0^k)$, to complete some parts of our derivations. However, the numerical value of F_{sh}^k is also known, and it is given by $F_{sh}^k = x^k(t_N^k) - x^k(t_0^k)$.

Newton's method for solving nonlinear equations of the form in (6.19) requires that we compute the Jacobian of the residual at iteration k , with respect to the proposed solution vector, again at iteration k . In our case, we call this necessary Jacobian, $\mathbf{J}_{sh}^k = \partial F_{sh}^k / \partial x^k(t_0^k)$. The expression for \mathbf{J}_{sh}^k is yet to be derived, but there we are going to make use of the symbolic expression in (6.20). As to how we utilize F_{sh}^k and \mathbf{J}_{sh}^k , we have to define

$$\Delta x^k(t_0^k) = x^{k+1}(t_0^{k+1}) - x^k(t_0^k). \quad (6.21)$$

Our aim through the computation we are now to present is to figure out $x^{k+1}(t_0^{k+1})$, the proposed solution vector at iteration $k + 1$. The linear system of equations given by

$$\mathbf{J}_{sh}^k \Delta x^k(t_0^k) = -F_{sh}^k, \quad (6.22)$$

is solved for $\Delta x^k(t_0^k)$, and we figure out $x^{k+1}(t_0^{k+1})$ through (6.21).

If all we needed to do were to figure out $x^{k+1}(t_0^{k+1})$ for use in the next iteration, we would be done. However, recall that T , the period, is also an unknown in (6.19). Remember that $x^\gamma(t_0)$ is an $(M \times 1)$ -dimensional vector, and there is also T . Therefore, we have $M + 1$ unknowns in (6.19), but only M equations. (6.19) is an under-determined system. We need another equation to append to the system in (6.19), to have a fully determined system.

We now proceed to provide the intuitive explanation as to why we need an extra condition, in addition to (6.19), to obtain a fully determined system. γ , the limit cycle, consists of infinitely many points. Each of these points is a candidate for $x^\gamma(t_0)$. If there is no condition fixing $x^\gamma(t_0)$, any point on γ will satisfy the condition in (6.19).

The extra condition to fix $x^\gamma(t_0)$ may be figured out follows. Newton's method needs an initial guess for the solution, in order to operate iteratively to find a solution. This

initial guess must be close enough to the actual solution for Newton's method to converge quadratically. Otherwise, this method may not converge. Our initial guess for $x^\gamma(t_0)$ is simply $x^1(t_0^1)$, the proposed solution at the first iteration. We suppose that $x^1(t_0^1)$ is very close to some point that is exactly on γ , so that Newton's method may converge. However, $x^1(t_0^1)$ is not expected to be exactly on γ . We may suppose that an entry in $x^1(t_0^1)$, one of the M entries in this vector, will not change very much by the time Newton's method converges. So we are encouraged to fix a single entry of $x^\gamma(t_0)$ to the value contained in $x^1(t_0^1)$. Mathematically speaking, let us have vector e_l , with l fixed. e_l is one of the standard basis vectors, and its l^{th} entry is one while its other entries are zero. Then, we write

$$e_l^\top x^\gamma(t_0) - x_l^1(t_0^1) = 0, \quad (6.23)$$

as the appended condition alongside (6.19). The residual at iteration k , corresponding to (6.23) is

$$G_{sh}^k = e_l^\top x^k(t_0^k) - x_l^1(t_0^1), \quad (6.24)$$

which is again not expected to be sufficiently close to zero before convergence.

Since we now have another unknown T , we need another update equation as well. The proposed solution for T at iteration k is T^k . We have to define another update as in

$$\Delta T^k = T^{k+1} - T^k. \quad (6.25)$$

Notice that T^{k+1} is the proposed solution for T at iteration $k+1$.

(6.22) would be all that would be needed at iteration k to solve for $x^{k+1}(t_0^{k+1})$ if $x^k(t_0^k)$ were the only unknown. However, T is also an unknown. Therefore, we declare that F_{sh}^k and G_{sh}^k are functions of both $x^k(t_0^k)$ and T^k . The coupled linear equations to be solved at iteration k become

$$\frac{\partial F_{sh}^k}{\partial x^k(t_0^k)} \Delta x^k(t_0^k) + \frac{\partial F_{sh}^k}{\partial T^k} \Delta T^k = -F_{sh}^k \quad (6.26)$$

$$\frac{\partial G_{sh}^k}{\partial x^k(t_0^k)} \Delta x^k(t_0^k) + \frac{\partial G_{sh}^k}{\partial T^k} \Delta T^k = -G_{sh}^k \quad (6.27)$$

instead of (6.22). Above, we have already called $\partial F_{sh}^k / \partial x^k(t_0^k) = \mathbf{J}_{sh}^k$, and we need to figure out a systematic method to compute \mathbf{J}_{sh}^k . Simply, $\partial G_{sh}^k / \partial x^k(t_0^k) = e_l^\top$ and $\partial G_{sh}^k / \partial T^k = 0$. However, $\partial F_{sh}^k / \partial T^k$ is another vector whose calculation requires a systematically derived method. We will call $\partial F_{sh}^k / \partial T^k = \mathbf{J} T_{sh}^k$.

We now need to summarize the discussion above to spell out the problem definition of shooting. The task after that will be to figure out iterative methods to compute \mathbf{J}_{sh}^k and JT_{sh}^k .

Shooting Problem Definition

Let Υ be the state transition function of the generic DAE in (2.4). The shooting problem is to solve the following set of nonlinear equations for $x^\gamma(t_0)$ and T .

$$\Upsilon(t_0 + T, t_0, x^\gamma(t_0)) - x^\gamma(t_0) = 0 \quad (6.28)$$

$$e_l^\top x^\gamma(t_0) - x_l^1(t_0^1) = 0 \quad (6.29)$$

$x^1(t_0^1)$ and T^1 are our initial guesses for $x^\gamma(t_0)$, an initial point on γ , and T , the period on γ , respectively. l in e_l above is a fixed value such that $1 \leq l \leq M$. The shooting problem is solved using Newton's method. Then, the linear set of equations to be solved at iteration k can be spelt out as

$$\begin{pmatrix} \mathbf{J}_{sh}^k & JT_{sh}^k \\ e_l^\top & 0 \end{pmatrix} \begin{pmatrix} \Delta x^k(t_0^k) \\ \Delta T^k \end{pmatrix} = - \begin{pmatrix} F_{sh}^k \\ G_{sh}^k \end{pmatrix}. \quad (6.30)$$

Above, we have to note the following.

- $\Delta x^k(t_0^k)$, the state update at iteration k , is as given in (6.21).
- ΔT^k , the period update at iteration k , is as given in (6.25).
- F_{sh}^k is the numerical value for the expression in (6.20).
- G_{sh}^k is the numerical value for the expression in (6.24).
- $\mathbf{J}_{sh}^k = \partial F_{sh}^k / \partial x^k(t_0^k)$. We may refer to \mathbf{J}_{sh}^k as the shooting Jacobian.
- $JT_{sh}^k = \partial F_{sh}^k / \partial T^k$.
- $e_l^\top = \partial G_{sh}^k / \partial x^k(t_0^k)$.

With close enough initial guesses $x^1(t_0^1)$ and T^1 , Newton's method can converge quadratically. The next sections focus on the systematic computation of \mathbf{J}_{sh}^k and JT_{sh}^k .

Shooting Jacobian Calculation

We proceed to explore \mathbf{J}_{sh}^k , the shooting Jacobian. Let us first write, in a straight-forward manner,

$$\begin{aligned}\mathbf{J}_{sh}^k &= \frac{\partial F_{sh}^k}{\partial x^k(t_0^k)} \\ &= \frac{\partial \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k))}{\partial x^k(t_0^k)} - \frac{\partial x^k(t_0^k)}{\partial x^k(t_0^k)} \\ &= \frac{\partial \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k))}{\partial x^k(t_0^k)} - \mathbf{I}_M,\end{aligned}\tag{6.31}$$

where \mathbf{I}_M is the identity matrix of size $(M \times M)$. The challenge here is to figure out the first expression in (6.31), with Υ , the state transition function of (2.4). We know and have stated before $t_N^k = t_0^k + T^k$. Therefore, that $x^k(t_N^k) = \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k))$ is true. In all, we have to compute $\partial x^k(t_N^k)/\partial x^k(t_0^k)$.

For simplicity, let us introduce the notation in

$$\mathbf{S}_i^k = \frac{\partial x^k(t_i^k)}{\partial x^k(t_0^k)},\tag{6.32}$$

which is actually a sensitivity matrix. Note that $\mathbf{S}_N^k = \partial x^k(t_N^k)/\partial x^k(t_0^k)$. Shortly, we will also need

$$\mathbf{G}(t_j^k) = \frac{\partial f(x^k(t_j^k))}{\partial x^k(t_j^k)}\tag{6.33}$$

and

$$\mathbf{C}(t_j^k) = \frac{\partial q(x^k(t_j^k))}{\partial x^k(t_j^k)},\tag{6.34}$$

in order to spell out our iterative method.

Let us now return to the discretized form of (2.4) in (6.9) and compute

$$\begin{aligned}&\frac{\partial}{\partial x^k(t_0^k)} \left(\sum_{j=0}^r \hat{\alpha}_j(\mathcal{H}) q(x^k(t_{i-j}^k)) \right) \\ &= \frac{\partial}{\partial x^k(t_0^k)} \left(\sum_{j=0}^r \hat{\beta}_j(\mathcal{H}) f(x^k(t_{i-j}^k)) \right).\end{aligned}$$

We then have

$$\begin{aligned}&\sum_{j=0}^r \hat{\alpha}_j(\mathcal{H}) \frac{\partial q(x^k(t_{i-j}^k))}{\partial x^k(t_{i-j}^k)} \frac{\partial x^k(t_{i-j}^k)}{\partial x^k(t_0^k)} \\ &= \sum_{j=0}^r \hat{\beta}_j(\mathcal{H}) \frac{\partial f(x^k(t_{i-j}^k))}{\partial x^k(t_{i-j}^k)} \frac{\partial x^k(t_{i-j}^k)}{\partial x^k(t_0^k)}.\end{aligned}$$

Then, using our definitions, we obtain a simpler form as in

$$\sum_{j=0}^r \hat{\alpha}_j(\mathcal{H})\mathbf{C}(t_{i-j}^k)\mathbf{S}_{i-j}^k = \sum_{j=0}^r \hat{\beta}_j(\mathcal{H})\mathbf{G}(t_{i-j}^k)\mathbf{S}_{i-j}^k.$$

Let us now collect the terms corresponding to $j = 0$ on the left-hand side and the others on the right-hand side to get

$$\begin{aligned} & \left[\hat{\alpha}_0(\mathcal{H})\mathbf{C}(t_i^k) - \hat{\beta}_0(\mathcal{H})\mathbf{G}(t_i^k) \right] \mathbf{S}_i^k \\ &= - \sum_{j=1}^r \left[\hat{\alpha}_j(\mathcal{H})\mathbf{C}(t_{i-j}^k) - \hat{\beta}_j(\mathcal{H})\mathbf{G}(t_{i-j}^k) \right] \mathbf{S}_{i-j}^k. \end{aligned}$$

Now let us define

$$\mathbf{J}_{i,j}^k = \left[\hat{\alpha}_j(\mathcal{H})\mathbf{C}(t_{i-j}^k) - \hat{\beta}_j(\mathcal{H})\mathbf{G}(t_{i-j}^k) \right], \quad (6.35)$$

to obtain finally

$$\mathbf{J}_{i,0}^k \mathbf{S}_i^k = - \sum_{j=1}^r \mathbf{J}_{i,j}^k \mathbf{S}_{i-j}^k. \quad (6.36)$$

Note that

$$\mathbf{S}_0^k = \frac{\partial x^k(t_0^k)}{\partial x^k(t_0^k)} = \mathbf{I}_M,$$

and this is the initial condition to use when utilizing (6.36) in order to calculate $\mathbf{S}_i^k = \partial x^k(t_i^k)/\partial x^k(t_0^k)$. Our final objective is to calculate

$$\mathbf{S}_N^k = \frac{\partial x^k(t_N^k)}{\partial t_0^k} = \frac{\partial \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k))}{\partial x^k(t_0^k)}.$$

Of course, we compute the shooting Jacobian, through $\mathbf{J}_{sh}^k = \mathbf{S}_N^k - \mathbf{I}_M$.

Notice that \mathbf{S}_i^k , for $0 \leq i \leq N$, are generally dense matrices. On the other hand, $\mathbf{G}(t_i^k)$ and $\mathbf{C}(t_i^k)$, for $0 \leq i \leq N$, are sparse matrices in most applications. Therefore, numerically we would not like to compute and store \mathbf{S}_i^k at each time point, t_i^k , for $0 \leq i \leq N$. Instead, we would like to exploit the sparsity of $\mathbf{G}(t_{i-j}^k)$ and $\mathbf{C}(t_{i-j}^k)$, which lend $\mathbf{J}_{i,j}^k$ in (6.35) the same graceful property.

The part of the shooting Jacobian that is tricky to compute, \mathbf{S}_N^k , can be stored in sparse factors, instead of storing all dense \mathbf{S}_i^k . Examining the recursive scheme defined by (6.36), we deduce that the sparse LU factors of $\mathbf{J}_{i,0}^k$ can be stored, along with $\mathbf{J}_{i,j}^k$, for $1 \leq j \leq r$, themselves, at each time point t_i^k , for $0 \leq i \leq N$.

Notice again that these components to be stored can be assembled from the by-products of the inner Newton's method, used to solve the discretized equation in (6.9), for $x^k(t_i^k)$.

At iteration k of the shooting method, we make use of a differential equation solver to solve for $x^k(t_i^k)$, for $1 \leq i \leq N$. $x^k(t_0^k)$ is already available at the beginning of iteration k . The differential equation solver employs Newton's method, to solve for $x^k(t_i^k)$. At each timepoint t_i^k , for $0 \leq i \leq N$, we have some auxiliary computational components that this inner Newton's method uses to generate $x^k(t_i^k)$. These components, which may be regarded as the by-products of the differential equation solver, can then be manipulated to assemble the necessary factors to generate \mathbf{J}_{sh}^k , the shooting Jacobian.

Recall that we are to use not Gaussian Elimination but Krylov Subspace Methods to compute the update in (6.30), which is the linear equation to solve at each iteration of Newton's method. There we will be required to compute the product of the shooting Jacobian, \mathbf{J}_{sh}^k , with vectors. It happens that the sparse factors of \mathbf{S}_N^k that we store facilitate the computation of these matrix vector products.

For example, let b_0 be some vector that will be multiplied with \mathbf{S}_N^k . Observe that the computation goes simply as $\mathbf{S}_0^k b_0 = \mathbf{I}_M b_0 = b_0$, at time point t_0^k . Let $b_j = \mathbf{S}_j^k b_0$, for convenience. By the time we reach time point t_i^k in our recursive scheme of (6.36), b_j , for $(i-r) \leq j \leq (i-1)$, will already have been calculated, and then our task will be to compute $b_i = \mathbf{S}_i^k b_0$. Letting \mathbf{L}_i and \mathbf{U}_i be the L and U factors of $\mathbf{J}_{i,0}^k$, respectively, in (6.36). Then,

$$b_i = -\mathbf{U}_i^{-1} \mathbf{L}_i^{-1} \left(\sum_{j=1}^r \mathbf{J}_{i,j}^k b_{i-j} \right)$$

and we will finally compute $b_N = \mathbf{S}_N^k b_0$, at time point t_N^k .

Remark 6 *If we require set \mathcal{H} to consist of only h_i^k , as stated in Remark 2, and so employ $\hat{\alpha}_j(\mathcal{H}) = \alpha_j$ and $\hat{\beta}_j(\mathcal{H}) = h_i^k \beta_j$, then the auxiliary Jacobian, $\mathbf{J}_{i,j}^k$, can be written as*

$$\mathbf{J}_{i,j}^k = \left[\alpha_j \mathbf{C}(t_{i-j}^k) - h_i^k \beta_j \mathbf{G}(t_{i-j}^k) \right], \quad (6.37)$$

instead of (6.35). This is a minor simplification of the recursive scheme in (6.36).

For this part of our work, involving the shooting Jacobian calculation, we have referred to [14].

Derivative with Respect to the Period

We now explain how to compute $JT_{sh}^k = \partial F_{sh}^k / \partial T^k$. We have

$$\begin{aligned} JT_{sh}^k &= \frac{\partial \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k))}{\partial T^k} - \frac{\partial x^k(t_0^k)}{\partial T^k} \\ &= \frac{\partial \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k))}{\partial T^k}, \end{aligned} \quad (6.38)$$

where we assume $\partial x^k(t_0^k) / \partial T^k = 0$. Notice again that $x^k(t_N^k) = \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k))$, and so we have to compute $JT_{sh}^k = \partial x^k(t_N^k) / \partial T^k$.

Let us take the discretized form in (6.9) and compute

$$\begin{aligned} &\frac{\partial}{\partial T^k} \left(\sum_{j=0}^r \hat{\alpha}_j(\mathcal{H}) q(x^k(t_{i-j}^k)) \right) \\ &= \frac{\partial}{\partial T^k} \left(\sum_{j=0}^r \hat{\beta}_j(\mathcal{H}) f(x^k(t_{i-j}^k)) \right). \end{aligned}$$

We explicitly express the left- and right-hand sides of the equation above, as in *LHS* and *RHS*, respectively.

$$\begin{aligned} LHS &= \sum_{j=0}^r \hat{\alpha}_j(\mathcal{H}) \frac{\partial q(x^k(t_{i-j}^k))}{\partial x^k(t_{i-j}^k)} \frac{\partial x^k(t_{i-j}^k)}{\partial T^k} \\ &\quad + \sum_{j=0}^r \left(\sum_{m=0}^{r-1} \frac{\partial \hat{\alpha}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} \right) q(x^k(t_{i-j}^k)) \\ RHS &= \sum_{j=0}^r \hat{\beta}_j(\mathcal{H}) \frac{\partial f(x^k(t_{i-j}^k))}{\partial x^k(t_{i-j}^k)} \frac{\partial x^k(t_{i-j}^k)}{\partial T^k} \\ &\quad + \sum_{j=0}^r \left(\sum_{m=0}^{r-1} \frac{\partial \hat{\beta}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} \right) f(x^k(t_{i-j}^k)) \end{aligned}$$

We have used the fact that set \mathcal{H} , defined in (6.8), consists of r interval lengths. Therefore, we needed the chain rule of partial differentiation.

Now, let us define, for simplicity,

$$\Psi_i^k = \frac{\partial x^k(t_i^k)}{\partial T^k}. \quad (6.39)$$

Note that

$$\Psi_N^k = \frac{\partial x^k(t_N^k)}{\partial T^k} = \frac{\partial \Upsilon(t_0^k + T^k, t_0^k, x^k(t_0^k))}{\partial T^k} = JT_{sh}^k.$$

Invoking (6.33) and (6.34), we may carry out the following simplifications in notation.

$$\begin{aligned}
LHS &= \sum_{j=0}^r \hat{\alpha}_j(\mathcal{H}) \mathbf{C}(t_{i-j}^k) \Psi_{i-j}^k \\
&\quad + \sum_{j=0}^r \left(\sum_{m=0}^{r-1} \frac{\partial \hat{\alpha}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} \right) q(x^k(t_{i-j}^k)) \\
RHS &= \sum_{j=0}^r \hat{\beta}_j(\mathcal{H}) \mathbf{G}(t_{i-j}^k) \Psi_{i-j}^k \\
&\quad + \sum_{j=0}^r \left(\sum_{m=0}^{r-1} \frac{\partial \hat{\beta}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} \right) f(x^k(t_{i-j}^k))
\end{aligned}$$

Now let us group some terms and exploit the fact that $LHS = RHS$ to write the following.

$$\begin{aligned}
&\left[\hat{\alpha}_0(\mathcal{H}) \mathbf{C}(t_i^k) - \hat{\beta}_0(\mathcal{H}) \mathbf{G}(t_i^k) \right] \Psi_i^k \\
&= - \sum_{j=1}^r \left[\hat{\alpha}_j(\mathcal{H}) \mathbf{C}(t_{i-j}^k) - \hat{\beta}_j(\mathcal{H}) \mathbf{G}(t_{i-j}^k) \right] \Psi_{i-j}^k \\
&\quad - \sum_{j=0}^r \left(\sum_{m=0}^{r-1} \frac{\partial \hat{\alpha}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} \right) q(x^k(t_{i-j}^k)) \\
&\quad + \sum_{j=0}^r \left(\sum_{m=0}^{r-1} \frac{\partial \hat{\beta}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} \right) f(x^k(t_{i-j}^k))
\end{aligned}$$

Finally, through the definition of the auxiliary Jacobian, $\mathbf{J}_{i,j}^k$, in (6.35),

$$\begin{aligned}
\mathbf{J}_{i,0}^k \Psi_i^k &= - \sum_{j=1}^r \mathbf{J}_{i,j}^k \Psi_{i-j}^k \\
&\quad - \sum_{j=0}^r \left(\sum_{m=0}^{r-1} \frac{\partial \hat{\alpha}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} \right) q(x^k(t_{i-j}^k)) \\
&\quad + \sum_{j=0}^r \left(\sum_{m=0}^{r-1} \frac{\partial \hat{\beta}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} \right) f(x^k(t_{i-j}^k)). \tag{6.40}
\end{aligned}$$

The previous equation is used to compute $\Psi_i^k = \partial x^k(t_i^k) / \partial T^k$, at timepoint t_i^k . Our final objective is again to figure out $\Psi_N^k = JT_{sh}^k$. We assume $\Psi_0^k = 0$.

In (6.40), everything except $\partial h_j^k / \partial T^k$, for $1 \leq j \leq N$, is known. It happens that we have to decide on the values of $\partial h_j^k / \partial T^k$ before we start executing the shooting method.

One of the two methods in [18] is to set these ratios as

$$\frac{h_j^k}{T^k} = \frac{h_j^1}{T^1},$$

for $1 \leq j \leq N$, and $k > 1$. h_j^1 and T^1 are our initial guesses for interval lengths between consecutive timepoints and the period, respectively. These values are obtained through simulating the system in a differential equation solver. As the proposed solution for the period, T , changes through iterations of Newton's method, h_j^k/T^k ratios remain the same. This means that the ratios of the changes in these variables remain the same. Therefore, we have

$$\frac{h_j^k}{T^k} = \frac{\partial h_j^k}{\partial T^k} = \frac{h_j^1}{T^1},$$

for $1 \leq j \leq N$, and $k > 1$. This method is more plausible than having the first $N - 1$ interval lengths the same, throughout the execution of shooting, and having the last interval length, h_N^k , change, since the latter method would at times require backward integration [18].

Note again that Newton's method is used to solve the shooting problem. At each iteration of Newton's method, we have to solve a linear system of equations, in order to compute the updates, for the states vector, $x^\gamma(t_0)$, and the period, T . The linear system to be solved at iteration k , for example, is given in (6.30). We have stated that we are going to solve this linear system by Krylov Subspace Methods, not Gaussian Elimination. For this purpose, we have explained how matrix vector products, involving \mathbf{J}_{sh}^k , the shooting Jacobian, may be facilitated via storing the sparse factors of \mathbf{J}_{sh}^k .

Examining (6.30), we observe that in the required matrix vector products scheme of Krylov methods concerning this linear system, we have to calculate $JT_{sh}^k = \Psi_N^k$ multiplied with a scalar factor. This is easily managed by calculating Ψ_N^k first. The recursive scheme in (6.40) tells us that by the time Ψ_i^k is to be calculated, Ψ_{i-j}^k for $1 \leq j \leq r$ will already have been computed. Then, again calling the L and U factors of $\mathbf{J}_{i,0}^k$, \mathbf{L}_i and \mathbf{U}_i , respectively, and naming the right-hand side of (6.40) ς_i , for convenience, we have $\Psi_i^k = \mathbf{U}_i^{-1} \mathbf{L}_i^{-1} \varsigma_i$.

In order to solve for \mathbf{J}_{sh}^k , the shooting Jacobian, we have to store, at each t_i^k , for $1 \leq i \leq N$, the LU factors of $\mathbf{J}_{i,0}^k$, which we call \mathbf{L}_i and \mathbf{U}_i , and $\mathbf{J}_{i,j}^k$, for $1 \leq j \leq r$, themselves. As we stated before, these components can be generated from the by-products of the inner Newton's method that the differential equation solver employs. At each iteration k of the shooting method, which we may also call the shooting Newton, we utilize a differential equation solver to generate $x^k(t_i^k)$, for $1 \leq i \leq N$. At each t_i^k , $x^k(t_i^k)$ is calculated through this inner Newton's method. The by-products of this method, then, may be used to assemble the components above.

In addition to the components needed for \mathbf{J}_{sh}^k , the shooting Jacobian, we have to obtain $f(x^k(t_i^k))$ and $q(x^k(t_i^k))$ for $0 \leq i \leq N$, in order to solve for Ψ_i^k through (6.40). The partial derivatives of multi-step coefficients with respect to timepoint intervals are also necessary. It happens that all these other components can be acquired from the by-products of the inner Newton's method. The timepoint intervals over the period ratios are determined again by the differential equation solver, prior to the shooting Newton.

Remark 7 *If we require as in Remark (2) that $\mathcal{H} = \{h_i^k\}$ and so $\hat{\alpha}_j(\mathcal{H}) = \alpha_j$ and $\hat{\beta}_j(\mathcal{H}) = h_i^k \beta_j$, then we will obtain several simplifications in the recursive scheme of (6.40). First, we will have*

$$\sum_{m=0}^{r-1} \frac{\partial \hat{\alpha}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} = \frac{\partial \alpha_j}{\partial h_i^k} \frac{\partial h_i^k}{\partial T^k} = 0,$$

since α_j is a constant. Second, we will have

$$\sum_{m=0}^{r-1} \frac{\partial \hat{\beta}_j(\mathcal{H})}{\partial h_{i-m}^k} \frac{\partial h_{i-m}^k}{\partial T^k} = \frac{\partial (h_i^k \beta_j)}{\partial h_i^k} \frac{\partial h_i^k}{\partial T^k} = \beta_j \frac{\partial h_i^k}{\partial T^k}.$$

In all, the recursive scheme will be modified as follows.

$$\begin{aligned} \mathbf{J}_{i,0}^k \Psi_i^k &= - \sum_{j=1}^r \mathbf{J}_{i,j}^k \Psi_{i-j}^k \\ &+ \frac{\partial h_i^k}{\partial T^k} \sum_{j=0}^r \beta_j f(x^k(t_{i-j}^k)) \end{aligned} \quad (6.41)$$

Above, $\mathbf{J}_{i,j}^k$ is as defined in (6.37).

In this section, we have elaborated on the method stated in [18].

A Simple Walkthrough and Summary

We now present a simple walkthrough, defining in order the steps of the shooting method.

1. Generate an initial guess, through a differential equation solver, for $x^\gamma(t_0)$, a point on γ , and T , the period on γ , and call them $x^1(t_0^1)$ and T^1 , respectively, so that these values are used in the first iteration of shooting. Make sure that these are guesses, close enough to the actual solution. A multistep discretization scheme, employed in the differential equation solver, is required. Make sure that the computation of $x^1(t_1^1)$ from $x^1(t_0^1)$ is accomplished through the Backward Euler scheme. The reason will be clear when explaining the persistent mode calculation based on shooting.

2. Fix an integer l such that $1 \leq l \leq M$. Store the l^{th} entry of $x^1(t_0^1)$, i.e. $x_l^1(t_0^1)$. At iteration k , $e_l^\top x^k(t_0^k) - x_l^1(t_0^1) = x_l^k(t_0^k) - x_l^1(t_0^1)$ must be computed, since this measure will be one of the two conditions to decide on convergence.
3. After generating the initial guesses for the timepoints, call $h_j^1 = t_j^1 - t_{j-1}^1$, for $1 \leq j \leq N$. h_j^1 are the lengths of the intervals between consecutive timepoints. The ratios h_j^1/T^1 must be stored for $1 \leq j \leq N$. At iteration k of shooting, the guess for T will be called T^k , however, for our purposes, the h_j^k/T^k ratios will have been determined a priori. We will set $h_j^k/T^k = h_j^1/T^1$.
4. At the beginning of iteration k , $x^k(t_0^k)$ and T^k will be available, as initial guesses for $x^\gamma(t_0)$ and T , respectively. Using these guesses and employing again a differential equation solver, compute $x^k(t_N^k) = x^k(t_0^k + T^k)$. Again, the timepoints along the interval of length T^k must be distributed such that $h_j^k/T^k = h_j^1/T^1$, for $1 \leq j \leq N$. Also, remember to generate $x^k(t_1^k)$ from $x^k(t_0^k)$, through Backward Euler.
5. While solving for $x^k(t_0^k + T^k)$, some by-products of the differential equation solver must be stored such that \mathbf{J}_{sh}^k , the shooting Jacobian at iteration k , and JT_{sh}^k , the derivative with respect to the period again at iteration k , can be easily computed afterwards. Since matrix-vector products constitute the essence of Krylov Subspace Methods for solving linear systems of equations, it will be advantageous to store only the sparse factors of \mathbf{J}_{sh}^k and JT_{sh}^k , for use in a matrix-vector product computation procedure.
6. Since there will be access to the numerical values $F_{sh}^k = x^k(t_N^k) - x^k(t_0^k)$, $G_{sh}^k = e_l^\top x^k(t_0^k) - x_l^1(t_0^1)$, \mathbf{J}_{sh}^k , JT_{sh}^k , and e_l^\top , the linear system at iteration k , spelt in (6.30), can be solved through Krylov Subspace Methods. Using the updates that are the solutions of (6.30), $x^{k+1}(t_0^{k+1})$ and T^{k+1} can be computed.
7. At this point, a check for convergence is necessary, since the algorithm might generate a result without running the next iteration of shooting. Checking the norms of F_{sh}^k and G_{sh}^k to be small and also making sure that the norms of the updates, i.e. the solutions of the linear system of equations in (6.30), are small enough is enough justification to

end shooting and yield a solution for $x^\gamma(t_0)$ and T . Otherwise, go back to step 4, for iteration $k + 1$.

For close enough initial guesses $x^1(t_0^1)$ and T^1 , the algorithm outlined above should converge quadratically. A continuation scheme might be necessary to incorporate into the procedure above, in order to enhance performance.

The Finite Differences Formulation

Note that the differential equation solver that we employ in shooting is able to compute the timepoints one by one. It can be arranged such that we figure out all timepoints at any iteration of the shooting method, at once. For this purpose, we will have to formulate the finite differences approach. However, the essence is that we would not like to make use of finite differences to compute the steady-state periodic solution of an oscillator. Rather, persistent mode calculation, i.e. figuring out $v_1(t)$, through finite differences, is facilitated, utilizing the samples of $x^\gamma(t)$, along with other useful ingredients, computed via shooting. We will be investigating more into this scheme in Section 6.5.3.

6.4.2 Harmonic Balance

In steady-state periodic solution computations, the problem is to compute N samples of $x^\gamma(t)$ along a single period. We observe that the shooting method, at any iteration during its runtime, computes the candidates for these N samples one by one, through a differential equation solver. It should be possible, however, to compute these N candidates altogether, at any iteration. In this section, we review and devise a method that accomplishes the required task in the stated manner.

Let us work again on the generic DAE in (2.4). We will be introducing several notations to facilitate the current presentation.

Definition 21 (Concatenated Timepoints) *Recalling that $x^\gamma(t_i)$, for $1 \leq i \leq (N - 1)$, are the timepoints to be computed, we define*

$$\bar{x}^\gamma = \left((x^\gamma(t_0))^\top \cdots (x^\gamma(t_{N-1}))^\top \right)^\top \quad (6.42)$$

as the concatenated timepoints vector. We will not be needing timepoint $x^\gamma(t_N) = x^\gamma(t_0)$

for the particular numerical method we are to derive in this section. This information is already embedded in the method.

We may proceed to generalize f and q in (2.4), in the same manner.

Definition 22 (Concatenated Nonlinear Functions) *Following the notation in Definition 21, let us define $\bar{f}(\bar{x}^\gamma)$ and $\bar{q}(\bar{x}^\gamma)$ as*

$$\bar{f}(\bar{x}^\gamma) = \left((f(x^\gamma(t_0)))^\top \cdots (f(x^\gamma(t_{N-1})))^\top \right)^\top \quad (6.43)$$

and

$$\bar{q}(\bar{x}^\gamma) = \left((q(x^\gamma(t_0)))^\top \cdots (q(x^\gamma(t_{N-1})))^\top \right)^\top, \quad (6.44)$$

respectively.

Notice that \bar{x}^γ , $\bar{f}(\bar{x}^\gamma)$, and $\bar{q}(\bar{x}^\gamma)$ are all defined in the time domain. We may need transformation functions to switch back and forth between the time domain and another domain, where numerical computation might be facilitated. In harmonic balance, this other domain is the frequency domain. Thus, the basis to switch to is the Fourier basis.

The transformation into the frequency domain has several advantages. When we operate on discrete samples in time, the switch to the frequency domain means, in the case of harmonic balance particularly, computing the Fourier coefficients associated with the discrete samples in time. Fourier basis functions computed over a single fundamental frequency are inherently periodic and these functions inherently form an orthogonal set. These properties of Fourier bases deem the transformations between the time and frequency domains computationally less expensive, compared to the cases where other types of bases are employed.

Another advantage of switching to the frequency domain is that with a Fourier basis employed, the counterpart, in the frequency domain, of differentiation with respect to time, in the time domain, is multiplication with a diagonal matrix only. This differentiation scheme is also numerically more accurate, compared to the multi-step discretization scheme, carried out in the time domain.

The disadvantage of resorting to harmonic balance is that we lose the ability to vary the time intervals between consecutive timepoints. The time intervals, provided that N is the number of samples along a single period, are given by

$$h_i = t_i - t_{i-1} = \frac{T}{N}, \quad \text{for } 1 \leq i \leq N, \quad (6.45)$$

i.e. consecutive timepoints are separated by uniform intervals. This is the only scheme in which Fourier transforms do work.

In addition to the disadvantage stated above we are required to solve larger linear systems at each iteration of harmonic balance. In shooting, the dimension of the linear systems was only M . However, in harmonic balance, we aim to compute all timepoints via a linear system solution, at each iteration, i.e. the dimension of this linear system is the product of the number of signals, M , and the number of timepoints, N .

We have stated several items in comparing the two steady-state periodic solution finding algorithms that we have. In all, harmonic balance is shown to be numerically more accurate than shooting. However, the size of the linear systems to solve and the loss of variable timestep utilization through harmonic balance may still render shooting more desirable.

We go on to introduce the computational components that we need to solve for, in the harmonic balance method. The next steps will be to define the harmonic balance problem and figuring out numerical procedures to calculate the required components. We will be primarily referring to [13] in the forthcoming sections about harmonic balance.

Computational Components

Note first that we will denote the DFT (Discrete Fourier Transform) matrix by Γ and the inverse of Γ is given by Γ^{-1} . Let us start by defining the states vector in the frequency domain.

Definition 23 (Concatenated Harmonics) *We choose to let the states vector in the frequency domain have an odd number of harmonics. The total number of harmonics is, of course, N , the number of samples along an interval of length T . Therefore, $N = 2K + 1$, for some integer K . Then, we let \bar{X}^γ , the concatenated harmonics vector, alias the states vector in the frequency domain, be*

$$\bar{X}^\gamma = ((X_{-K}^\gamma)^* \cdots (X_K^\gamma)^*)^*, \quad (6.46)$$

with X_i^γ being the i^{th} harmonic, i.e. X_i^γ is the Fourier coefficient that corresponds to $(i\omega_0^\gamma)$, an integer multiple of the fundamental angular frequency on γ , ω_0^γ . We can, by all means, adopt the convention to use the generalized angular frequency notation, ω_0 , due to the fact that periodicity exists in the domain of attraction, \mathcal{W} , associated with γ , and we will do so.

Note that we naturally have

$$\bar{X}^\gamma = \Gamma \bar{x}^\gamma \quad \text{and} \quad \bar{x}^\gamma = \Gamma^{-1} \bar{X}^\gamma, \quad (6.47)$$

where \bar{x}^γ is the concatenated timepoints vector, introduced in Definition 21.

We also have to define the differentiation operator in the frequency domain.

Definition 24 *The differentiation operator in the frequency domain will be denoted by $j\Omega^\gamma$, where j is the imaginary number notifier with $j^2 = -1$. We have*

$$j\Omega^\gamma = j \begin{pmatrix} \omega_0(-K)\mathbf{I}_M & & \\ & \ddots & \\ & & \omega_0(+K)\mathbf{I}_M \end{pmatrix}, \quad (6.48)$$

defining this operator that depends on ω_0 . $j\Omega^\gamma$ is a block diagonal matrix with N -many ($M \times M$)- sized diagonal blocks.

We have the tools ready to spell out the basic equation of the harmonic balance problem.

$$j\Omega^\gamma \Gamma \bar{q}(\bar{x}^\gamma) - \Gamma \bar{f}(\bar{x}^\gamma) = 0 \quad (6.49)$$

Notice that unlike shooting, we do not need a differential equation solver this time. We have to solve (6.49) through Newton's method. At iteration k of Newton the proposed solution for \bar{x}^γ will be denoted by \bar{x}^k . The Fourier transform of \bar{x}^k will be given by $\bar{X}^k = \Gamma \bar{x}^k$. We do not know the exact the period either, so let us denote the proposed solution for ω_0 , the angular frequency, by ω_0^k , at again iteration k . $j\Omega^\gamma$, the differentiation operator, depends on ω_0 , therefore we will also need $j\Omega^k$. We may now define a residual at iteration k as

$$F_{hb}^k = j\Omega^k \Gamma \bar{q}(\bar{x}^k) - \Gamma \bar{f}(\bar{x}^k), \quad (6.50)$$

which may not be sufficiently close to zero at iteration k . The objective is to reduce the norm of F_{hb}^k through the iterations of Newton's method.

In (6.49) we have actually \bar{X}^γ , the state harmonics defined in the frequency domain, as the unknown. Therefore, we can actually modify (6.49) as

$$j\Omega^\gamma \Gamma \bar{q}(\Gamma^{-1} \bar{X}^\gamma) - \Gamma \bar{f}(\Gamma^{-1} \bar{X}^\gamma) = 0.$$

Notice F_{hb}^k in (6.50) is a vector in the frequency domain, and we may visualize F_{hb}^k as the concatenation of $N = 2K + 1$ harmonics, as in

$$F_{hb}^k = \left(\left(F_{hb,-K}^k \right)^* \cdots \left(F_{hb,+K}^k \right)^* \right)^*$$

with $F_{hb,i}^k$ as the i^{th} harmonic of F_{hb}^k , which corresponds to $i\omega_0$, an integral multiple of the fundamental angular frequency, ω_0 . In harmonic balance, our aim is to reduce the norms of all these residual harmonics. Indeed, this is the objective of collocation methods, as opposed to Galerkin schemes. In Galerkin schemes, the essence is to make the residual, F_{hb}^k , orthogonal to the Fourier basis functions in the range given by $-K \leq i \leq K$, with the fundamental frequency chosen as ω_0 , i.e. in Galerkin schemes, we seek to make $\Gamma^{-1}F_{hb}^k$, the residual transformed into the time domain, orthogonal to the Fourier basis functions given by $\exp(j\omega_0 i)$, for $-K \leq i \leq K$. $\Gamma^{-1}F_{hb}^k$ in this case will be spanned by $\exp(j\omega_0 i)$, with $|i| > K$.

The scheme we use to solve the harmonic balance problem is called, in view of the last paragraph, the *pseudo-spectral collocation method*.

In solving (6.49) through Newton's method, we have to define the following update at iteration k , after introducing the residual in (6.50).

$$\Delta \bar{X}^k = \bar{X}^{k+1} - \bar{X}^k \quad (6.51)$$

If we treat F_{hb}^k as a function of \bar{X}^k only, as in $F_{hb}^k = F_{hb}^k(\bar{X}^k)$, the linear system to solve at iteration k becomes

$$\frac{\partial F_{hb}^k}{\partial \bar{X}^k} \Delta \bar{X}^k = -F_{hb}^k. \quad (6.52)$$

Let us call $\mathbf{J}_{hb}^k = \partial F_{hb}^k / \partial \bar{X}^k$ the harmonic balance Jacobian. We do not yet explain how to numerically compute \mathbf{J}_{hb}^k but note it as a computational component necessary to be calculated to fully implement the harmonic balance method.

As in shooting and as we stated before in this section, we do not have prior knowledge about the period of oscillation on γ . All we have is an initial guess for the angular frequency, which we call ω_0^1 , the guess for ω_0 at the first iteration of Newton's method. Therefore, we need to figure out a solution for ω_0 as well. F_{hb}^k is a function not only of \bar{X}^k but also of ω_0^k , i.e. $F_{hb}^k = F_{hb}^k(\bar{X}^k, \omega_0^k)$. That means the nonlinear system of equations in (6.49) is an under-determined system. We have $(NM + 1)$ unknowns, \bar{X}^γ and ω_0 , but only NM equations. We need another condition to fully determine the system.

The answer to the question as to why we need another condition to exactly specify this system of equations is very similar to the answer given in the shooting problem discussion. Any time-shifted version of \bar{x}^k is a legitimate solution to (6.49), provided the exact frequency, ω_0 , is given. We have to be able to pick a single solution out of the infinitely many. The extra condition to append to the system in (6.49) will be designed to accomplish this task.

The extra condition is described in [12]. The facts that \bar{x}^k is a real multi-dimensional signal and $\bar{X}^k = \Gamma \bar{x}^k$ are exploited therein. If we pick a single signal out of the M that we have, and call its index sig , we know that $\bar{X}_{sig,+i}^k$, the i^{th} harmonic of \bar{x}_{sig}^k , will be the complex conjugate of $\bar{X}_{sig,-i}^k$, i.e. $\bar{X}_{sig,+i}^k = \left(\bar{X}_{sig,-i}^k\right)^*$. This is true because \bar{x}^k is a real signal. It can also be proved that via shifting \bar{x}^k by a particular length in time, the imaginary part of $\bar{X}_{sig,+i}^k$ can be set to zero. It follows naturally that $\left(\mathbf{Im}(\bar{X}_{sig,+i}^k) = 0\right) \Rightarrow \left(\mathbf{Im}(\bar{X}_{sig,-i}^k) = 0\right)$. Then, the extra condition to append to (6.49) becomes

$$s_{sig}^\top \bar{X}^\gamma = 0. \quad (6.53)$$

s_{sig} is used here to extract a multiple of $\mathbf{Im}(\bar{X}_{sig,1}^k)$. Recalling that \bar{X}^k is a concatenated harmonics vector, the harmonics being in the order given by $-K \leq i \leq K$, we set s_{sig} as follows. Let the entry with index $(M(K-1) + sig)$, of s_{sig} , be -1 , and let the entry with index $(M(K+1) + sig)$, of s_{sig} , be 1 . Then, (6.53) is the condition to set the imaginary part of $\bar{X}_{sig,1}^k$ to zero.

The condition given in (6.53) requires us to augment the residual vector, F_{hb}^k in (6.50). We define

$$G_{hb}^k = s_{sig}^\top \bar{X}^k. \quad (6.54)$$

We may treat G_{hb}^k as $G_{hb}^k = G_{hb}^k(\bar{X}^k, \omega_0^k)$.

We have set the condition in (6.53), for ω_0 is another unknown in the system of equations given by (6.49). Then, we also need to define the update for ω_0^k , at iteration k of Newton's method, as

$$\Delta\omega_0^k = \omega_0^{k+1} - \omega_0^k. \quad (6.55)$$

We can now modify the linear system to be solved at iteration k .

We have both $F_{hb}^k = F_{hb}^k(\bar{X}^k, \omega_0^k)$ and $G_{hb}^k = G_{hb}^k(\bar{X}^k, \omega_0^k)$. The linear system of equations to solve at iteration k must be modified as

$$\frac{\partial F_{hb}^k}{\partial \bar{X}^k} \Delta \bar{X}^k + \frac{\partial F_{hb}^k}{\partial \omega_0^k} \Delta \omega_0^k = -F_{hb}^k, \quad (6.56)$$

$$\frac{\partial G_{hb}^k}{\partial \bar{X}^k} \Delta \bar{X}^k + \frac{\partial G_{hb}^k}{\partial \omega_0^k} \Delta \omega_0^k = -G_{hb}^k, \quad (6.57)$$

instead of (6.52). We have already called $\mathbf{J}_{hb}^k = \partial F_{hb}^k / \partial \bar{X}^k$ the harmonic balance Jacobian. Let us call $J\omega_{hb}^k = \partial F_{hb}^k / \partial \omega_0^k$. We simply know that $\partial F_{hb}^k / \partial \omega_0^k = s_{sig}^\top$ and $\partial G_{hb}^k / \partial \omega_0^k = 0$.

After stating the problem definition of harmonic balance in the next section, the following task will be to figure out numerical methods for calculating \mathbf{J}_{hb}^k and $J\omega_{hb}^k$.

Harmonic Balance Problem Definition

The following equations form a nonlinear set, for whose solution we require the use of the harmonic balance method. Harmonic balance is one of the methods of figuring out the steady-state periodic solution of interest, of the generic DAE in (2.4).

$$j\Omega^\gamma \Gamma \bar{q}(\bar{x}^\gamma) - \Gamma \bar{f}(\bar{x}^\gamma) = 0 \quad (6.58)$$

$$s_{sig}^\top \bar{X}^\gamma = 0 \quad (6.59)$$

Note \bar{x}^γ in Definition 21, $\bar{X}^\gamma = \Gamma \bar{x}^\gamma$ in Definition 23, $\bar{f}(\bar{x}^\gamma)$ and $\bar{q}(\bar{x}^\gamma)$ in Definition 22, $j\Omega^\gamma$, the differentiation operator in Definition 24, and Γ , the DFT (Discrete Fourier Transform) operator.

Newton's method is used to solve the system in (6.58) and (6.59). The linear system of equations to solve at iteration k of Newton's method reads as follows.

$$\begin{pmatrix} \mathbf{J}_{hb}^k & J\omega_{hb}^k \\ s_{sig}^\top & 0 \end{pmatrix} \begin{pmatrix} \Delta \bar{X}^k \\ \Delta \omega_0^k \end{pmatrix} = - \begin{pmatrix} F_{hb}^k \\ G_{hb}^k \end{pmatrix} \quad (6.60)$$

We must note the following items about (6.60)

- $\Delta \bar{X}^k$ is the harmonics update vector as given in (6.51).
- $\Delta \omega_0^k$ is the frequency update vector as given in (6.55).
- F_{hb}^k is the numerical value of the residual defined in (6.50).

- G_{hb}^k is the numerical value of the residual defined in (6.54).
- \mathbf{J}_{hb}^k is called the harmonic balance Jacobian and it is defined as $\mathbf{J}_{hb}^k = \partial F_{hb}^k / \partial \bar{X}^k$.
- $J\omega_{hb}^k = \partial F_{hb}^k / \partial \omega_0^k$.
- $s_{sig}^\top = \partial G_{hb}^k / \partial \bar{X}^k$.

The related items in (6.60) have been superscripted with k , in order to notify that these values are valid during only iteration k of Newton's method.

The task now is to figure out numerical methods to compute \mathbf{J}_{hb}^k , the harmonic balance Jacobian, and $J\omega_{hb}^k$.

Harmonic Balance Jacobian

We explain here the method to compute $\mathbf{J}_{hb}^k = \partial F_{hb}^k / \partial \bar{X}^k$, the harmonic balance Jacobian. The computation is straight-forward, but we have to introduce some more notation for convenience.

Let us define

$$\begin{aligned} \bar{\mathbf{G}}(\bar{x}^k) &= \frac{\partial \bar{f}(\bar{x}^k)}{\partial \bar{x}^k} \\ &= \begin{pmatrix} \mathbf{G}(t_0^k) & & \\ & \ddots & \\ & & \mathbf{G}(t_{N-1}^k) \end{pmatrix} \end{aligned} \quad (6.61)$$

and

$$\begin{aligned} \bar{\mathbf{C}}(\bar{x}^k) &= \frac{\partial \bar{q}(\bar{x}^k)}{\partial \bar{x}^k} \\ &= \begin{pmatrix} \mathbf{C}(t_0^k) & & \\ & \ddots & \\ & & \mathbf{C}(t_{N-1}^k) \end{pmatrix}, \end{aligned} \quad (6.62)$$

where

$$\mathbf{G}(t_i^k) = \left. \frac{\partial f}{\partial x} \right|_{x^k(t_i^k)}, \text{ and } \mathbf{C}(t_i^k) = \left. \frac{\partial q}{\partial x} \right|_{x^k(t_i^k)},$$

for $0 \leq i \leq N - 1$. $\bar{\mathbf{G}}(\bar{x}^k)$ and $\bar{\mathbf{C}}(\bar{x}^k)$ are $(NM \times NM)$ -sized block diagonal matrices. The diagonal blocks are obviously $(M \times M)$ -sized and there are N -many such blocks in each of $\bar{\mathbf{G}}(\bar{x}^k)$ and $\bar{\mathbf{C}}(\bar{x}^k)$.

We have to make use of the chain of partial differentiation to write

$$\begin{aligned} \frac{\partial \bar{f}(\bar{x}^k)}{\partial \bar{X}^k} &= \frac{\partial \bar{f}(\bar{x}^k)}{\partial \bar{x}^k} \frac{\partial \bar{x}^k}{\partial \bar{X}^k} \\ &= \bar{\mathbf{G}}(\bar{x}^k) \Gamma^{-1} \end{aligned}$$

and

$$\begin{aligned} \frac{\partial \bar{q}(\bar{x}^k)}{\partial \bar{X}^k} &= \frac{\partial \bar{q}(\bar{x}^k)}{\partial \bar{x}^k} \frac{\partial \bar{x}^k}{\partial \bar{X}^k} \\ &= \bar{\mathbf{C}}(\bar{x}^k) \Gamma^{-1}. \end{aligned}$$

We use the fact that $\bar{x}^k = \Gamma^{-1} \bar{X}^k$. Then, we compute \mathbf{J}_{hb}^k , the harmonic balance Jacobian, as in

$$\begin{aligned} \mathbf{J}_{hb}^k &= \frac{\partial F_{hb}^k}{\partial \bar{X}^k} \\ &= j\Omega^k \Gamma \frac{\partial \bar{q}(\bar{x}^k)}{\partial \bar{X}^k} - \Gamma \frac{\partial \bar{f}(\bar{x}^k)}{\partial \bar{X}^k} \\ \mathbf{J}_{hb}^k &= j\Omega^k \Gamma \bar{\mathbf{C}}(\bar{x}^k) \Gamma^{-1} - \Gamma \bar{\mathbf{G}}(\bar{x}^k) \Gamma^{-1}. \end{aligned} \tag{6.63}$$

Above, the fact that $j\Omega^k$ is a linear operator is implicitly necessary to use. In deriving \mathbf{J}_{hb}^k , we have referred to [13] and [14].

Note that \mathbf{J}_{hb}^k in (6.63) does not itself turn out to be a sparse matrix. However, all factors of \mathbf{J}_{hb}^k are sparse, except Γ , the DFT operator, and Γ^{-1} , its inverse, but computing the Fourier transform of a vector is computationally less costly through FFT (Fast Fourier Transform) than through straight-forward matrix vector multiplication. Therefore, \mathbf{J}_{hb}^k times a vector can be calculated via exploitation of the sparse factors structure in (6.63).

We draw attention to the observations in the last paragraph, because the linear systems at each iteration of Newton's method, as given in (6.60), will not be solved through Gaussian Elimination. These systems are to be solved through Krylov Subspace Methods, which benefit from computationally inexpensive matrix vector product computations to solve linear systems.

Derivative with Respect to the Frequency

We now move on to the numerical computation of $J\omega_{hb}^k = \partial F_{hb}^k / \partial \omega_0^k$. There is only one term in F_{hb}^k that depends on ω_0^k , and that is the term with $j\Omega^k$, the differentiation operator. This observation allows us to write

$$\begin{aligned} J\omega_{hb}^k &= \frac{\partial F_{hb}^k}{\partial \omega_0^k} \\ &= \frac{\partial(j\Omega^k)}{\partial \omega_0^k} \Gamma \bar{q}(\bar{x}^k). \end{aligned} \quad (6.64)$$

The partial differential term above can easily be spelt out as

$$\frac{\partial(j\Omega^k)}{\partial \omega_0^k} = \begin{pmatrix} (-K)\mathbf{I}_M & & \\ & \ddots & \\ & & (+K)\mathbf{I}_M \end{pmatrix}. \quad (6.65)$$

Authors of [12] are credited for this particular contribution.

6.5 Computing Floquet Modes of LPTV Systems

6.5.1 Eigenvalue Problems in Floquet Theory

We are to explain how to numerically compute the persistent Floquet mode through harmonic balance. After the steady-state periodic solution computation is accomplished through harmonic balance, we gain access to the harmonic balance Jacobian after convergence, \mathbf{J}_{hb} with the iteration k notifier dropped, which will facilitate the computation of $v_1(t)$, the persistent mode. Before making use of \mathbf{J}_{hb} , however, we have to introduce the auxiliary topic of eigenvalue problems in Floquet theory. This reservation will enable us to derive the components of a theory that will help in numerically computing not only the persistent mode, but all Floquet modes, $v_1(t)$ through $v_M(t)$.

Our discussion again focuses on the more general DAE case. Remember from [3] that in the DAE case, some modes are in the nullspace of $\mathbf{C}(t) = \partial q / \partial x^\gamma$. We have $\mathbf{C}(t)u_i(t) = 0$, for $(m+1) \leq i \leq M$, with $m < M$. Therefore, the biorthogonality condition $v_j^\top(t)\mathbf{C}(t)u_i(t) = \delta_{ij}$ holds only for $1 \leq i \leq m$ and $1 \leq j \leq m$.

Also, let us assume that the Floquet exponents, μ_k for $1 \leq k \leq M$, are real, for simplicity.

LPTV Equation

In this case, we explore, first, how the eigenfunction $u_k(t)$, for any $k \in \{1, \dots, m\}$, at $t = 0$, namely $u_k(0)$, is transformed by means of the state transition function, \mathbf{K} . We call the transformed solution $y_k(t)$.

$$\begin{aligned}
 y_k(t) &= \mathbf{K}(t, 0) u_k(0) \\
 &= \sum_{i=1}^m e^{\mu_i t} u_i(t) \underbrace{v_i^\top(0) \mathbf{C}(0) u_k(0)}_{\delta_{ik}} \\
 &= e^{\mu_k t} u_k(t)
 \end{aligned} \tag{6.66}$$

Recall that

$$\mathbf{G}(t) = \left. \frac{\partial f}{\partial x} \right|_{x^\gamma(t)}, \quad \mathbf{C}(t) = \left. \frac{\partial q}{\partial x} \right|_{x^\gamma(t)}.$$

Notice that we have not yet taken into account the modes that happen to reside in the nullspace of $\mathbf{C}(t)$. Let us see how $u_k(t)$, for $(m+1) \leq k \leq M$, are transformed. We have simply

$$\begin{aligned}
 y_k(t) &= \mathbf{K}(t, 0) u_k(0) \\
 &= \sum_{i=1}^m e^{\mu_i t} u_i(t) \underbrace{v_i^\top(0) \mathbf{C}(0) u_k(0)}_0 \\
 &= 0.
 \end{aligned} \tag{6.67}$$

These modes are killed instantly by the state transition function. However, we can still write these trivial solutions in the form given in (6.66), if we consider that $e^{\mu_k t} u_k(t) = 0$, with $\mu_k = -\infty$ for $(m+1) \leq k \leq M$. Therefore, the Floquet exponent that corresponds to each of these modes is $-\infty$. This Floquet exponent has $(M - m)$ multiplicity.

In all, we have

$$y_k(t) = \mathbf{K}(t, 0) u_k(0) = e^{\mu_k t} u_k(t), \tag{6.68}$$

considering both cases, $1 \leq k \leq m$ and $(m+1) \leq k \leq M$, with $\mu_k = -\infty$ for $(m+1) \leq k \leq M$.

Second, we substitute the expression for $y_k(t)$, since we have explicitly made use of the state transition function, \mathbf{K} , to calculate $y_k(t)$, and we know that it will satisfy the LPTV

equation for the DAE case.

$$\begin{aligned}\frac{d}{dt} [\mathbf{C}(t) \{e^{\mu_k t} u_k(t)\}] &= \mathbf{G}(t) \{e^{\mu_k t} u_k(t)\} \\ \frac{d}{dt} (\mathbf{C}(t) u_k(t)) - \mathbf{G}(t) u_k(t) &= -\mu_k \mathbf{C}(t) u_k(t)\end{aligned}\quad (6.69)$$

Remark 8 We must note that (6.69) is an instance of a generalized eigenvalue problem. Finding the eigenpairs, i.e. the negated Floquet exponents, $-\mu_k$, and the eigenfunctions, $u_k(t)$, for $1 \leq k \leq M$, requires sophisticated numerical methods. We can represent the eigenvalue problem in (6.69), through matrices, in the time or frequency domain, and then apply numerical methods to solve it. We will shortly relate this eigenvalue problem statement to the finite differences formulation and the harmonic balance method.

Adjoint LPTV Equation

In the same manner as in the previous section, we now present the eigenvalue problem, which may be used to figure out the eigenfunctions $v_k(t)$, for $1 \leq k \leq m$. We, first, need to explore how the state transition function, \mathbf{L} , of the adjoint LPTV equation transforms $v_k(t)$. We call the transformed solution $z_k(t)$, for $t < 0$, with $v_k(0)$ as the initial condition.

$$\begin{aligned}z_k(t) &= \mathbf{L}(t, 0) v_k(0) \\ &= \sum_{i=1}^m e^{-\mu_i t} v_i(t) \underbrace{u_i^T(0) \mathbf{C}^T(0) v_k(0)}_{\delta_{ik}} \\ &= e^{-\mu_k t} v_k(t)\end{aligned}\quad (6.70)$$

Again, we have to consider $v_k(t)$, for $(m+1) \leq k \leq M$. Just as $u_k(t)$, for $(m+1) \leq k \leq M$, span the nullspace of $\mathbf{C}(t)$, $v_k(t)$, for $(m+1) \leq k \leq M$, span the nullspace of $\mathbf{C}^T(t)$ [3]. Therefore, we have for $(m+1) \leq k \leq M$,

$$\begin{aligned}z_k(t) &= \mathbf{L}(t, 0) v_k(0) \\ &= \sum_{i=1}^m e^{-\mu_i t} v_i(t) \underbrace{u_i^T(0) \mathbf{C}^T(0) v_k(0)}_0 \\ &= 0.\end{aligned}\quad (6.71)$$

We have already assigned $\mu_k = -\infty$ to these modes. Recalling that computation of the adjoint equation is stable only backward in time, i.e. $t < 0$, we have $z_k(t) = e^{-\mu_k t} v_k(t) = 0$, for $(m+1) \leq k \leq M$. We can indeed keep the same form as in (6.70).

In all, we have

$$z_k(t) = \mathbf{L}(t, 0)v_k(0) = e^{-\mu_k t}v_k(t), \quad (6.72)$$

considering both cases, $1 \leq k \leq m$ and $(m+1) \leq k \leq M$, with $\mu_k = -\infty$ for $(m+1) \leq k \leq M$.

We know that $z_k(t)$ satisfies the adjoint LPTV equation, for the DAE case, since we have used \mathbf{L} , the corresponding state transition function. Therefore, all we need to do is substitute.

$$\begin{aligned} \mathbf{C}^\top(t) \frac{d}{dt} \{e^{-\mu_k t}v_k(t)\} &= -\mathbf{G}^\top(t) \{e^{-\mu_k t}v_k(t)\} \\ -\mathbf{C}^\top(t) \frac{dv_k}{dt} - \mathbf{G}^\top(t)v_k(t) &= -\mu_k \mathbf{C}^\top(t)v_k(t) \end{aligned} \quad (6.73)$$

Remark 9 *The equation in (6.73) defines another instance of generalized eigenvalue problems. The eigenvalues are the same as those of the problem in (6.69), the negated Floquet exponents, $-\mu_k$, for $1 \leq k \leq M$. However, the eigenfunctions that correspond to these values are, for the adjoint case, $v_k(t)$. We again have to resort to numerical linear algebra to solve this eigenvalue problem. The finite differences formulation and harmonic balance are two media facilitating this computation.*

Other Eigenpairs

In (6.69), we have presented an eigenvalue problem, where $-\mu_k$ is the eigenvalue, and $u_k(t)$ is the corresponding eigenfunction, for $1 \leq k \leq M$. We now propose that eigenvalues of the form $-(\mu_k - jH)$ and eigenfunctions $e^{jHt}u_k(t)$ are also solutions of the problem in (6.69), for some jH .

Let us modify the problem in (6.69) and try to figure out a condition on jH .

$$\begin{aligned} \frac{d}{dt} [\mathbf{C}(t) \{e^{jHt}u_k(t)\}] &- \\ \mathbf{G}(t) \{e^{jHt}u_k(t)\} &= -(\mu_k - jH)\mathbf{C}(t) \{e^{jHt}u_k(t)\} \end{aligned}$$

After simplifications and grouping we get the following.

$$\begin{aligned}
 jHe^{jHt}\mathbf{C}(t)u_k(t) & - \\
 jHe^{jHt}\mathbf{C}(t)u_k(t) & = -e^{jHt}\frac{d}{dt}(\mathbf{C}(t)u_k(t)) \\
 & + e^{jHt}\mathbf{G}(t)u_k(t) \\
 & - \mu_k e^{jHt}\mathbf{C}(t)u_k(t)
 \end{aligned}$$

The left-hand side of the equation above is obviously zero, and the right-hand side is zero by (6.69). Therefore, we get no constraint on jH , through the eigenpair we have proposed. However, since we are interested in only periodic eigenfunctions, we can figure out discrete values for jH . e^{jHt} must be of the same period with $u_k(t)$, with T being the period. This is possible if $jH = j2\pi/Tn$, for an integral values of n . Therefore, the eigenpairs that solve the problem in (6.69) are the eigenvalues, $-(\mu_k - j2\pi/Tn)$, and the *periodic* eigenfunctions, $e^{j2\pi/Tnt}u_k(t)$, for $1 \leq k \leq M$ and integral values of n .

We must check if the set of eigenvalues we have proposed satisfy (6.73), the eigenvalue problem in the adjoint case. In this case, we will have $-(\mu_k + jH)$ as the eigenvalues, and $e^{jHt}v_k(t)$ as the corresponding eigenfunctions. Again, $jH = j2\pi/Tn$, for integral values of n , will hold, to have T -periodic eigenfunctions.

Let us reformulate the eigenvalue problem in the same manner as for the LPTV case.

$$\begin{aligned}
 -\mathbf{C}^\top(t)\frac{d}{dt}\{e^{jHt}v_k(t)\} & - \\
 \mathbf{G}^\top(t)\{e^{jHt}v_k(t)\} & = -(\mu_k + jH)\{e^{jHt}v_k(t)\}
 \end{aligned}$$

After evaluations and grouping terms, we get the following.

$$\begin{aligned}
 jHe^{jHt}\mathbf{C}^\top(t)v_k(t) & - \\
 jHe^{jHt}\mathbf{C}^\top(t)v_k(t) & = e^{jHt}\mathbf{C}^\top(t)\frac{dv_k(t)}{dt} \\
 & + e^{jHt}\mathbf{G}^\top(t)v_k(t) \\
 & - \mu_k e^{jHt}\mathbf{C}^\top(t)v_k(t)
 \end{aligned}$$

The left-hand side of the equation above is zero. The right-hand side is identically equal to zero by (6.73). Other than the particular choice $jH = j2\pi/Tn$, for integral values of n , to make the eigenfunctions, $e^{jHt}v_k(t)$, T -periodic, there is again no constraint on n .

We may now express the generalized eigenvalue problems, associated with the LPTV and adjoint LPTV equations in the DAE case. Furthermore, we can spell out the general forms of the solutions to these problems, the eigenvalues and the corresponding periodic eigenfunctions.

All Eigenvalues and Periodic Eigenfunctions

Below is the generic form of the eigenvalue problem for the DAE LPTV case.

$$\frac{d}{dt}(\mathbf{C}(t)y_{kn}(t)) - \mathbf{G}(t)y_{kn}(t) = \lambda_{kn}\mathbf{C}(t)y_{kn}(t) \quad (6.74)$$

λ_{kn} is the generic eigenvalue, and $y_{kn}(t)$ is the corresponding eigenfunction. For the adjoint LPTV case, we have the following formulation.

$$-\mathbf{C}^\top(t)\frac{dz_{kn}}{dt} - \mathbf{G}^\top(t)z_{kn}(t) = \lambda_{kn}^*\mathbf{C}^\top(t)z_{kn}(t) \quad (6.75)$$

The complex conjugate of λ_{kn} , as in (6.74), is the eigenvalue, whereas we have $z_{kn}(t)$ as the corresponding eigenfunction.

We have figured out that λ_{kn} is of the form

$$\lambda_{kn} = -(\mu_k - j2\pi/Tn). \quad (6.76)$$

μ_k is the k^{th} Floquet exponent, T is the period on the limit cycle, γ . n is an integer. For fixed values of k and n , λ_{kn} is an eigenvalue for (6.74), and λ_{kn}^* is an eigenvalue for (6.75).

The corresponding eigenfunctions, $y_{kn}(t)$ and $z_{kn}(t)$, are given as follows.

$y_{kn}(t)$ has the form

$$y_{kn}(t) = e^{j2\pi/Tnt}u_k(t), \quad (6.77)$$

where $u_k(t)$ is the k^{th} Floquet eigenfunction of the forward LPTV equation.

$z_{kn}(t)$ has the form

$$z_{kn}(t) = e^{j2\pi/Tnt}v_k(t), \quad (6.78)$$

where $v_k(t)$ is the k^{th} Floquet eigenfunction, corresponding to the adjoint case.

Notice that throughout the derivations in this section, we have assumed that the Floquet exponents μ_k , for $1 \leq k \leq M$, are real. Our derivations still remain intact when μ_k are complex numbers. $\mathbf{K}(t, 0)$ in this case becomes

$$\mathbf{K}(t, 0) = \sum_{i=1}^m \exp(\mu_i t) u_i(t) v_i^*(0) \mathbf{C}(0).$$

Then, $\mathbf{L}(t, 0)$, the state transition function of the adjoint form, becomes

$$\mathbf{L}(t, 0) = \sum_{i=1}^m \exp(-\mu_i^* t) v_i(t) u_i^*(0) \mathbf{C}^\top(0).$$

We replace $^\top$, the transpose operator, with the Hermitian transpose operator, * . Also we have to use the complex conjugate of μ_i for the expression of $\mathbf{L}(t, 0)$. These changes bring about $\lambda_{kn}^* = -(\mu_k^* + j2\pi/Tnt)$ in (6.75).

In the next sections, we aim to show the relation of these derivations to the finite difference formulations and the harmonic balance Jacobian after convergence, \mathbf{J}_{hb} .

6.5.2 Computation Through Shooting

In order to compute Floquet modes through shooting, the steps to be taken are listed as follows. Let us only concentrate on $v_i(t)$, for $1 \leq i \leq m$, in the DAE case.

1. Solve for $\mathbf{L}(-T, 0)$ through $\mathbf{C}^\top(t)\dot{z} = -\mathbf{G}^\top(t)z$ with $\mathbf{L}(0, 0) = \mathbf{I}_M$.
2. Eigen-decompose $\mathbf{L}(-T, 0)$ and compute those eigenvectors not in the nullspace.
3. Associate $e^{\mu_i T}$ with $v_i(T) = v_i(0)$, i.e. the eigenvalues with the eigenvectors respectively.
4. Solve $\mathbf{C}^\top(t)\dot{z} = -\mathbf{G}^\top(t)z$ for $e^{-\mu_i t} v_i(t)$ backwards in time, for $0 \geq t \geq -T$. Scale $e^{-\mu_i t} v_i(t)$ with $e^{\mu_i t}$ to get $v_i(t)$ for all t .

6.5.3 Computation Through Finite Differences

It happens that we can manipulate the multistep discretization scheme in (6.9) to formulate a finite differences approach as given below.

Let us derive the finite differences scheme over the data computed through the shooting method, i.e. after shooting converges, we may write the scheme in (6.9) with the k notifier dropped. In view of this remark, we have

$$\sum_{j=0}^r \hat{\alpha}_j(\mathcal{H}) q(x^\gamma(t_{i-j})) = \sum_{j=0}^r \hat{\beta}_j(\mathcal{H}) f(x^\gamma(t_{i-j})), \quad (6.79)$$

where $\hat{\alpha}_j(\mathcal{H})$ and $\hat{\beta}_j(\mathcal{H})$, for $0 \leq j \leq r$, are multistep coefficients that depend on the r elements of $\mathcal{H} = \{h_i, \dots, h_{i-r+1}\}$. Recall that (6.79) is a scheme that states the relation

of essentially $x^\gamma(t_i)$ to the other samples along the interval of length T . (6.79) is an r -step discretization scheme, i.e. the memory of (6.79) is r -deep, and (6.79) applies to the sample given by $x^\gamma(t_i)$ only. That means r can actually change with respect to i , i.e. $r = r(i)$, the depth of the memory, allocated for a sample, depends on the particular sample. Numerical concerns involving truncation errors determine this depth of the memory incorporated. In all, we accommodate variable order schemes through (6.79).

Since we have N samples, $x^\gamma(t_i)$ for $0 \leq i \leq (N - 1)$, along a period of length T , let us assume for simplicity that the memory of our discretization is $(N - 1)$ -deep for all samples. We will make use of the simple notations $\hat{\alpha}_j^i$ and $\hat{\beta}_j^i$, the j^{th} multistep coefficients for the i^{th} sample. $\hat{\alpha}_j^i$ and $\hat{\beta}_j^i$ depend on $\mathcal{H} = \{h_i, h_{i-N+2}\}$. Notice that the interval lengths between consecutive timepoints exhibit periodicity with period N , i.e. $h_{i+nN} = h_i$, where n is an integer. Note the matrix formulation in

$$\hat{\aleph} = \begin{pmatrix} \hat{\alpha}_0^0 & \hat{\alpha}_{N-1}^0 & \cdots & \hat{\alpha}_2^0 & \hat{\alpha}_1^0 \\ \hat{\alpha}_1^1 & \hat{\alpha}_0^1 & \hat{\alpha}_{N-1}^1 & \cdots & \hat{\alpha}_2^1 \\ & \ddots & \ddots & \ddots & \\ \hat{\alpha}_{N-1}^{N-1} & \hat{\alpha}_{N-2}^{N-1} & \cdots & \hat{\alpha}_1^{N-1} & \hat{\alpha}_0^{N-1} \end{pmatrix} \otimes \mathbf{I}_M \quad (6.80)$$

and

$$\hat{\beth} = \begin{pmatrix} \hat{\beta}_0^0 & \hat{\beta}_{N-1}^0 & \cdots & \hat{\beta}_2^0 & \hat{\beta}_1^0 \\ \hat{\beta}_1^1 & \hat{\beta}_0^1 & \hat{\beta}_{N-1}^1 & \cdots & \hat{\beta}_2^1 \\ & \ddots & \ddots & \ddots & \\ \hat{\beta}_{N-1}^{N-1} & \hat{\beta}_{N-2}^{N-1} & \cdots & \hat{\beta}_1^{N-1} & \hat{\beta}_0^{N-1} \end{pmatrix} \otimes \mathbf{I}_M. \quad (6.81)$$

\otimes denotes Kronecker product, and $\hat{\aleph}$ and $\hat{\beth}$ are block matrices. We may then locate the relations in the form of (6.79) for all timepoints along a single period, noting that after shooting converges, we have $x^\gamma(t_N = t_0 + T) = x^\gamma(t_0)$. This compact form reads

$$\hat{\aleph} \begin{pmatrix} q(x^\gamma(t_0)) \\ q(x^\gamma(t_1)) \\ \vdots \\ q(x^\gamma(t_{N-1})) \end{pmatrix} = \hat{\beth} \begin{pmatrix} f(x^\gamma(t_0)) \\ f(x^\gamma(t_1)) \\ \vdots \\ f(x^\gamma(t_{N-1})) \end{pmatrix}. \quad (6.82)$$

(6.82) is called the finite difference scheme of discretizing the generic DAE in (2.4). Notice that in (6.82), we have put in q and f evaluated at the samples on γ , i.e. we have formulated

the finite differences scheme over the samples along a single period, obtained through the convergence of shooting. We have a point in doing that, because our purpose is not spelling out another scheme for figuring out the steady-state solution on γ . Rather, we would like to use (6.82) for computing the persistent mode of the adjoint LPTV equation, associated with (2.4), after shooting converges.

We have to make sure the left-hand side of (6.82) performs discrete differentiation. For this purpose we will have to define

$$\Lambda = \begin{pmatrix} \hat{h}_N & & & & \\ & \hat{h}_1 & & & \\ & & \ddots & & \\ & & & \hat{h}_{N-2} & \\ & & & & \hat{h}_{N-1} \end{pmatrix} \otimes \mathbf{I}_M, \quad (6.83)$$

where it may be such that $\hat{h}_i \neq h_i = (t_i - t_{i-1})$, for $1 \leq i \leq N$. The values of \hat{h}_i depend on the multi-step coefficients, and the reason behind this reservation is again to ensure that the scaling is correct so that the left-hand side of

$$\aleph \begin{pmatrix} q(x^\gamma(t_0)) \\ q(x^\gamma(t_1)) \\ \vdots \\ q(x^\gamma(t_{N-1})) \end{pmatrix} = \beth \begin{pmatrix} f(x^\gamma(t_0)) \\ f(x^\gamma(t_1)) \\ \vdots \\ f(x^\gamma(t_{N-1})) \end{pmatrix}, \quad (6.84)$$

is a numerically correct measure of the time derivatives of the nonlinear q functions concatenated. Note that $\aleph = \Lambda^{-1}\hat{\aleph}$ and $\beth = \Lambda^{-1}\hat{\beth}$.

The procedure for figuring out $v_1(t)$ through finite differences is yet to follow. Let us for now just spell out the forward and adjoint LPTV equations, obtained from (6.84).

The forward LPTV equation reads

$$\aleph \bar{\mathbf{C}}(\bar{x}^\gamma) \bar{y} = \beth \bar{\mathbf{G}}(\bar{x}^\gamma) \bar{y}. \quad (6.85)$$

And the adjoint LPTV reads

$$\bar{\mathbf{C}}^\top(\bar{x}^\gamma) \aleph^\top \bar{z} = -\bar{\mathbf{G}}^\top(\bar{x}^\gamma) \beth^\top \bar{z}. \quad (6.86)$$

Note that above we have

$$\bar{\mathbf{C}}(\bar{x}^\gamma) = \begin{pmatrix} \mathbf{C}(t_0) & & \\ & \ddots & \\ & & \mathbf{C}(t_{N-1}) \end{pmatrix}$$

and

$$\bar{\mathbf{G}}(\bar{x}^\gamma) = \begin{pmatrix} \mathbf{G}(t_0) & & \\ & \ddots & \\ & & \mathbf{G}(t_{N-1}) \end{pmatrix},$$

where $\mathbf{C}(t_i) = \partial q(x^\gamma(t_i))/\partial x^\gamma(t_i)$ and $\mathbf{G}(t_i) = \partial f(x^\gamma(t_i))/\partial x^\gamma(t_i)$. Also

$$\bar{x}^\gamma = \left((x^\gamma(t_0))^\top \cdots (x^\gamma(t_{N-1}))^\top \right)^\top,$$

$$\bar{y} = \left((y(t_0))^\top \cdots (y(t_{N-1}))^\top \right)^\top,$$

and

$$\bar{z} = \left((z(t_0))^\top \cdots (z(t_{N-1}))^\top \right)^\top.$$

We will make use of the adjoint equation in (6.86) to numerically figure out $v_1(t)$.

Note that \aleph and \beth need not be dense matrices, in terms of their block structure, because the multistep discretization scheme for each sample needs not have $(N - 1)$ -deep memory. As stated before, the depth of this memory can vary over samples. However, the block sparsity structures of \aleph and \beth are the same in any case.

Now, we proceed to numerically figure out $v_1(t)$ through the finite differences formulation. In fact, this formulation can be utilized to compute all modes, as will be clear shortly.

Referring to the findings of the previous section, we may spell out the eigenvalue problem, derived from the forward LPTV equation in (6.85), as

$$[\aleph \bar{\mathbf{C}}(\bar{x}^\gamma) - \beth \bar{\mathbf{G}}(\bar{x}^\gamma)] \{\bar{\vartheta}\} = \lambda \bar{\mathbf{C}}(\bar{x}^\gamma) \{\bar{\vartheta}\}, \quad (6.87)$$

where the solutions are of the form

$$\lambda = \lambda_{kn} = -(\mu_k - j2\pi/Tn), \quad (6.88)$$

for the eigenvalues, and

$$\bar{\vartheta} = \left((e^{j\omega_0 t_0} u_k(t_0))^* \cdots (e^{j\omega_0 t_{N-1}} u_k(t_{N-1}))^* \right)^*, \quad (6.89)$$

for the eigenfunctions.

Fortunately, we need only $u_1(t)$, so the $(-\mu_1 = 0, u_1(t))$ eigenpair will suffice. However, we have already set $u_1(t) = dx^\gamma/dt$, i.e. $u_1(t)$ can be readily computed through the discrete differentiation of $x^\gamma(t)$, the samples of $x^\gamma(t)$ having been found via the shooting method.

Note that to satisfy the normalization condition in $v_1^\top(t)\mathbf{C}(t)u_1(t) = 1$, we need to have access to $\mathbf{C}(t)u_1(t)$, and we can easily verify, again, that $dq(x^\gamma)/dt = \mathbf{C}(t)u_1(t) = f(x^\gamma)$. We will shortly spell out the normalization condition, spelt via the finite differences formulation, but the discrete samples for $v_1(t)$ have to be computed first.

Let us derive the eigenvalue problem through the adjoint equation in (6.86) as

$$[-\bar{\mathbf{C}}^\top(\bar{x}^\gamma)\aleph^\top - \bar{\mathbf{G}}^\top(\bar{x}^\gamma)\beth^\top] \{\bar{q}\} = \lambda^* \bar{\mathbf{C}}^\top \{\bar{q}\}, \quad (6.90)$$

whose solutions are

$$\lambda^* = \lambda_{kn}^* = -(\mu_k + j2\pi/Tn) \quad (6.91)$$

for the eigenvalues, and

$$\bar{q} = \left((e^{j\omega_0 n t_0} v_k(t_0))^* \dots (e^{j\omega_0 n t_{N-1}} v_k(t_{N-1}))^* \right)^* \quad (6.92)$$

for the eigenfunctions. Also, we are able to solve for all the modes, all we need is the $(-\mu_1 = 0, v_1(t))$ eigenpair. We resort to the methods of numerical linear algebra to figure out this eigenpair. Numerically, the eigenvalue is not exactly to be zero. Therefore, we seek the eigenfunction that corresponds to the smallest absolute eigenvalue.

Having computed the samples for $v_1(t)$, the next task is to make sure $v_1(t)$ is normalized. Following our previous discussion, we have $v_1^\top(t)f(x^\gamma(t)) = 1$ as a legitimate normalization condition. The finite differences formulation allows us to write

$$\aleph \bar{q}(\bar{x}^\gamma) = \beth \bar{f}(\bar{x}^\gamma),$$

which helps us to spell the normalization condition as

$$\bar{v}_1^\top \beth \bar{f}(\bar{x}^\gamma) = N, \quad (6.93)$$

considering that we have N timepoints. Note that we have

$$\bar{f}(\bar{x}^\gamma) = \left((f(x^\gamma(t_0)))^\top \dots (f(x^\gamma(t_{N-1})))^\top \right)^\top$$

and

$$\bar{v}_1 = \left((v_1(t_0))^T \cdots (v_1(t_{N-1}))^T \right)^T.$$

Let us now summarize the computation of $v_1(t)$ through the finite differences formulation.

1. Compute the samples for $x^\gamma(t)$ through shooting. Store such factors as $\mathbf{C}(t)$, $\mathbf{G}(t)$, $q(x^\gamma(t))$, $f(x^\gamma(t))$, and the multistep coefficients used for computing each timepoint. These factors are necessary for having available $\bar{\mathbf{C}}(\bar{x}^\gamma)$, $\bar{\mathbf{G}}(\bar{x}^\gamma)$, $\bar{q}(\bar{x}^\gamma)$, $\bar{f}(\bar{x}^\gamma)$, \aleph , and \beth .
2. Compute \bar{v}_1 , the samples of $v_1(t)$ concatenated, through solving the eigenvalue problem in (6.90), which is derived from the adjoint equation in (6.86).
3. Normalize \bar{v}_1 through the normalization condition in (6.93).

The finite differences method for figuring out $v_1(t)$, i.e. solving for all the samples of $v_1(t)$ along an interval of length T , is proved to be numerically more accurate compared to the procedure outlined in Section 6.5.2. Also, we still retain the capability to adjust the time intervals between the samples, as desired. Indeed, the same interval lengths between the consecutive samples of $x^\gamma(t)$ are naturally used to compute the samples of $v_1(t)$.

For the sake of obtaining more accuracy and retaining the feature of computing all the samples of $v_1(t)$ at once, we are going to explain the persistent mode computation through harmonic balance. However, we are to lose the adjustable interval lengths feature through this calculation, because DFT (Discrete Fourier Transform) requires uniform interval lengths between consecutive samples.

6.5.4 Computation Through Harmonic Balance

The method of harmonic balance also facilitates the computation of the persistent Floquet mode. Our assumption that there is a single persistent mode again holds. However, unlike the shooting method, we are induced to make note of the inferred assumption that there is a single Floquet exponent that is zero and that all other Floquet exponents are negative, i.e. $\mu_1 = 0$, by our convention, and $\mu_i < 0$, for $2 \leq i \leq M$. Recall that this inferred assumption, in view of the original assumption that there is a single persistent mode, is equivalent to

the condition that there is a single Floquet multiplier that is equal to 1 and that all other Floquet multipliers are between zero and 1, i.e. $\lambda_1 = 1$, by our convention, and $\lambda_i < 1$, for $2 \leq i \leq M$.

There is an obvious link between the notion of eigenvalue problems, derived through Floquet theory in 6.5.1, and persistent Floquet mode computation through harmonic balance. We herein explore further into this link to figure out a numerical scheme to compute $u_1(t)$ and $v_1(t)$.

Eigenpairs through the Forward LPTV Equation

We aim to numerically solve the eigenvalue problem derived as (6.74), through frequency transformation methods. The DFT of both sides in

$$\frac{d}{dt} (\mathbf{C}(t)\vartheta(t)) - \mathbf{G}(t)\vartheta(t) = \lambda\mathbf{C}(t)\vartheta(t)$$

can be written as

$$\begin{aligned} & [j\Omega^\gamma \Gamma \bar{\mathbf{C}}(\bar{x}^\gamma) \Gamma^{-1} - \Gamma \bar{\mathbf{G}}(\bar{x}^\gamma) \Gamma^{-1}] \{\Gamma \bar{\vartheta}\} \\ &= \lambda \Gamma \bar{\mathbf{C}}(\bar{x}^\gamma) \Gamma^{-1} \{\Gamma \bar{\vartheta}\}, \end{aligned} \quad (6.94)$$

with

$$\bar{\vartheta} = \left((\vartheta(t_0))^\top \cdots (\vartheta(t_{N-1}))^\top \right)^\top.$$

t_i are the timepoints calculated through the harmonic balance method. They are the same timepoints as used in the definition of \bar{x}^γ . Recall that t_i are separated by uniform intervals.

Notice that (6.94) can actually be written in compact form as

$$\mathbf{J}_{hb} \{\Gamma \bar{\vartheta}\} = \lambda \Gamma \bar{\mathbf{C}}(\bar{x}^\gamma) \Gamma^{-1} \{\Gamma \bar{\vartheta}\}, \quad (6.95)$$

where \mathbf{J}_{hb} is the harmonic balance Jacobian after convergence.

Fortunately, we already know the eigenpair solutions of (6.95). For fixed k and n , we have

$$\lambda = \lambda_{kn} = -(\mu_k - j2\pi/Tn) \quad (6.96)$$

and

$$\bar{\vartheta} = \left((e^{j\omega_0 n t_0} u_k(t_0))^* \cdots (e^{j\omega_0 n t_{N-1}} u_k(t_{N-1}))^* \right)^*. \quad (6.97)$$

Therefore, we have transformed the eigenvalue problem in (6.74) into the frequency domain, and we can utilize the methods of numerical linear algebra to solve (6.94), or in more compact form (6.95). The solutions are theoretically given by (6.96), as the eigenvalues, and (6.97) as the eigenfunctions in the time domain.

Above we know that $1 \leq k \leq M$, however, one may still wonder what the range for n is. Since we have an odd number, $N = 2K + 1$, of timepoints in \bar{x}^γ , we have the same number N of harmonics in \bar{X}^γ . We stated before that naturally the range of the harmonics in \bar{X}^γ is $-K \leq i \leq +K$, with i a dummy variable. Note that the range for n is $-K \leq n \leq +K$.

Through the eigenvalue problem stated as (6.95), we can solve for all the eigenpairs. \mathbf{J}_{hb} , the harmonic balance Jacobian after convergence, is thus indispensable. However, we indeed need only the $(-\mu_1 = 0, u_1(t))$ pair. Then, it is really not necessary to solve (6.95), because we have already set $u_1(t) = dx^\gamma/dt$. In the frequency domain, we have $\Gamma \bar{u}_1 = j\Omega^\gamma \bar{X}^\gamma = j\Omega^\gamma \Gamma \bar{x}^\gamma$. \bar{u}_1 is naturally the timepoints of $u_1(t)$ concatenated into a single vector, in the same manner as in \bar{x}^γ . \bar{X}^γ is supposed to be figured out by the time the harmonic balance method converges, so it is no trouble computing $\bar{u}_1 = \Gamma^{-1} j\Omega^\gamma \bar{X}^\gamma$.

Note also that

$$\bar{\mathbf{C}}(\bar{x}^\gamma) \bar{u}_1 = \bar{f}(\bar{x}^\gamma) \quad (6.98)$$

is a natural consequence of the fact that

$$\left. \frac{dq}{dt} \right|_\gamma = \mathbf{C}(t) \frac{dx^\gamma}{dt} = \mathbf{C}(t) u_1(t) = f(x^\gamma(t)).$$

This note will be necessary when normalizing $v_1(t)$, which is to be computed as follows.

Eigenpairs through the Adjoint LPTV Equation

The task is now to numerically solve the eigenvalue problem in (6.75). Let us spell the DFT of both sides of

$$-\mathbf{C}^\top(t) \frac{d\varrho(t)}{dt} - \mathbf{G}^\top(t) \varrho(t) = \lambda^* \mathbf{C}^\top(t) \varrho(t)$$

as

$$\begin{aligned} & -\Gamma \bar{\mathbf{C}}^\top(\bar{x}^\gamma) \Gamma^{-1} j\Omega^\gamma \{\Gamma \bar{\varrho}\} - \Gamma \bar{\mathbf{G}}^\top(\bar{x}^\gamma) \Gamma^{-1} \{\Gamma \bar{\varrho}\} \\ = & \lambda^* \Gamma \bar{\mathbf{C}}^\top(\bar{x}^\gamma) \Gamma^{-1} \{\Gamma \bar{\varrho}\}. \end{aligned} \quad (6.99)$$

Note again that

$$\bar{\varrho} = \left((\varrho(t_0))^T \cdots (\varrho(t_{N-1}))^T \right)^T.$$

t_i are the timepoints, the intervals between which have been calculated through harmonic balance.

(6.99) in compact form is

$$\mathbf{J}_{hb}^* \{\Gamma \bar{\varrho}\} = \lambda^* \Gamma \bar{\mathbf{C}}^T(\bar{x}^\gamma) \Gamma^{-1} \{\Gamma \bar{\varrho}\}, \quad (6.100)$$

where \mathbf{J}_{hb} is the harmonic balance Jacobian after convergence.

The eigenpair solutions for (6.100) are, for fixed k and n ,

$$\lambda^* = \lambda_{kn}^* = -(\mu_k + j2\pi/Tn) \quad (6.101)$$

and

$$\bar{\varrho} = \left((e^{j\omega_0 n t_0} v_k(t_0))^* \cdots (e^{j\omega_0 n t_{N-1}} v_k(t_{N-1}))^* \right)^*. \quad (6.102)$$

We can employ the methods of numerical linear algebra to solve the eigenvalue problem in (6.99), or in more compact form (6.100). The solutions are theoretically given by (6.101) as the eigenvalues and (6.102) as the corresponding eigenfunctions.

We have outlined a technique to figure out all eigenpairs, associated with the adjoint LPTV equation. In fact, all we need is to find the $(-\mu_1 = 0, v_1(t))$ pair. After making use of numerical techniques to figure out \bar{v}_1 , i.e. $v_1(t)$ with all timepoints concatenated into a single vector, we have to make sure to satisfy the biorthonormality relation $v_1^T(t) \mathbf{C}(t) u_1(t) = 1$. Recalling that we have N timepoints, the normalization condition can be written as any of

$$\begin{aligned} \bar{v}_1 \cdot \{\bar{\mathbf{C}}(\bar{x}^\gamma) \bar{u}_1\} &= N \\ \bar{v}_1 \cdot \bar{f}(\bar{x}^\gamma) &= N \end{aligned} \quad (6.103)$$

$$\{\Gamma \bar{v}_1\} \cdot \{\Gamma \bar{f}(\bar{x}^\gamma)\} = N \quad (6.104)$$

$$\begin{aligned} \{\Gamma \bar{v}_1\} \cdot \{[\Gamma \bar{\mathbf{C}}(\bar{x}^\gamma) \Gamma^{-1}] [\Gamma \bar{u}_1]\} &= N \\ \{\Gamma \bar{v}_1\} \cdot \{[\Gamma \bar{\mathbf{C}}(\bar{x}^\gamma) \Gamma^{-1}] [j\Omega^\gamma \bar{X}^\gamma]\} &= N \end{aligned} \quad (6.105)$$

Notice that the harmonic balance method we described operates in the frequency domain. Therefore, harmonic balance figures out $\bar{X}^\gamma = \Gamma \bar{x}^\gamma$. Following the formulations in this section, through numerical methods, we find not \bar{v}_1 but $\Gamma \bar{v}_1$, again a frequency transformed

variable. Above, (6.105) is the most straight-forward method to carry out the necessary normalization, but it is not the simplest.

In (6.105), we calculate $j\Omega^\gamma \bar{X}^\gamma$, after harmonic balance yields \bar{X}^γ , the concatenated harmonic balance vector. $j\Omega^\gamma \bar{X}^\gamma$ is the DFT of $d\bar{x}^\gamma/dt$. If we store $\bar{\mathbf{C}}(\bar{x}^k)$ at each iteration k of harmonic balance, then after convergence we will have access to $\bar{\mathbf{C}}(\bar{x}^\gamma)$. After numerically computing a vector in the direction of $\Gamma\bar{v}_1$, we can readily normalize $\Gamma\bar{v}_1$ according to (6.105).

Consider now (6.103) and (6.104). We know that $d\bar{q}(\bar{x}^\gamma)/dt = \bar{\mathbf{C}}(\bar{x}^\gamma)\bar{u}_1$, on the limit cycle γ . This is why (6.103) works. However, since we carry out harmonic balance in the frequency domain, the normalization scheme of (6.104) is more plausible than (6.103). We just need to store $\bar{f}(\bar{x}^k)$ at each iteration k of harmonic balance. Then, we will have $\bar{f}(\bar{x}^\gamma)$ ready after convergence. Through (6.104), we omit the differentiation via $j\Omega^\gamma$ that is necessary in (6.105).

After obtaining a normalized $\Gamma\bar{v}_1$ through (6.104), we can use inverse DFT to get \bar{v}_1 , which is the concatenated form of $v_1(t_i)$ for $0 \leq i \leq (N-1)$. Note that we may make use of either $\Gamma\bar{v}_1$ or \bar{v}_1 as required by the application.

Summary

Let us briefly summarize how to calculate $v_1(t)$ after harmonic balance converges.

1. We make sure to store $\bar{\mathbf{C}}(\bar{x}^k)$, $\bar{\mathbf{G}}(\bar{x}^k)$, and $\bar{f}(\bar{x}^k)$ at each iteration k of harmonic balance. This way we will readily have access to $\bar{\mathbf{C}}(\bar{x}^\gamma)$, $\bar{\mathbf{G}}(\bar{x}^\gamma)$ and $\bar{f}(\bar{x}^\gamma)$ after the harmonic balance method converges.
2. We spell out in (6.99) and also in (6.100), the generalized eigenvalue problem that emerges from the adjoint LPTV equation, associated with the generic DAE in (2.4). We have, after harmonic balance converges, the sparse factors of \mathbf{J}_{hb}^* , the Hermitian conjugate of the harmonic balance Jacobian. ω_0 to construct $j\Omega^\gamma$, along with $\bar{\mathbf{C}}(\bar{x}^k)$ and $\bar{\mathbf{G}}(\bar{x}^k)$ are the necessary sparse factors.
3. We solve the generalized eigenvalue problem in (6.100) for the eigenpair that is theoretically stated as $(-\mu_1 = 0, \Gamma\bar{v}_1)$. Full eigen-decomposition is a valid choice. Notice that because of numerical errors, an eigenvalue of exactly zero is unexpected. We there-

fore seek the eigenfunction that corresponds to the real eigenvalue with the smallest absolute value.

4. After computing a vector in the direction of $\Gamma \bar{v}_1$, the normalization scheme in (6.104) must be employed, with $\bar{f}(\bar{x}^\gamma)$ readily available.
5. Inverse DFT is necessary to return to the time domain, i.e. to get \bar{v}_1 , the concatenated form of $v_1(t_i)$ for $0 \leq i \leq (N - 1)$.

As can be observed, the method outlined above involves solving a larger sparse eigenvalue problem, in order to solve $v_1(t)$, at all timepoints $\{t_0, \dots, t_{N-1}\}$, at once.

6.6 Numerical Methods for Solving the Phase Equation

The phase equation reads

$$\frac{d\hat{t}}{dt} = 1 + v_1^T(\hat{t}) g(x^\gamma(\hat{t}), t),$$

where g is the perturbations vector. In many applications we need to solve for \hat{t} , when deterministic perturbations are present. In this case, a discretization scheme may be applied to this equation, and a solution may be sought step by step, at each timepoint. However, notice that we have access to $v_1(t_i)$, for $0 \leq i \leq (N - 1)$, i.e. only some discrete values are available, of $v_1(t)$ along a single period of length T , although the values of $v_1(t)$ at instances other than these timepoints might needed as well. Therefore, interpolation methods are employed to generate approximations over virtually the whole period. This aspect deems the phase computation ad hoc.

There is the method contributed in [23] that makes use of again systematic techniques to calculate \hat{t} through again the phase equation. In [23], \hat{t} is computed through an improved harmonic balance method, when the perturbations vector that is present is a periodic signal. It is proved that in this case, \hat{t} happens to be the sum of a monotonously increasing ramp function and a periodic wave. Then, this knowledge is exploited to compute \hat{t} through harmonic balance. However, again note that this method is valid only in the case of periodic perturbations.

Chapter 7

RESULTS

We present some results obtained with the Matlab toolbox that we have developed.

7.1 Van der Pol Oscillator

Van der Pol oscillator has two states and one parameter. We consider only state perturbations for this oscillator. The steady-state periodic solution has been computed through shooting and harmonic balance. We present plots of $u_1(t)$ computed through shooting, finite differences, harmonic balance. Also $v_1(t)$ has been computed through harmonic balance.

Figure 7.8 is an indication of the relative accuracy of the computed period versus the number of timepoints employed. As the number of timepoints is increased, the relative accuracy is reduced by several orders, as expected.

Figure 7.1 compares $u_1(t)$, a periodic solution of the forward LPTV equation obtained from the Van der Pol oscillator, computed through shooting and finite differences. The data obtained through the steady-state solution calculation in shooting has been utilized to formulate the finite differences system. As seen in Figure 7.1 the two solutions are in agreement. Also Figure 7.5 provides a shifted version of the same $u_1(t)$, this time obtained through harmonic balance. The solutions through all three methods are in agreement.

Figure 7.2 is a plot of the finite differences matrix eigenvalues on the complex plane. Since the derivative computation is not exact as in harmonic balance, we expect to observe detached sets of eigenvalues for each Floquet exponent. In Figure 7.2, we see two sets constituting circles, whose left-most points are occupied by the Floquet exponents associated with the system. On the other hand, as seen in Figures 7.3 and 7.4, the detached sets of eigenvalues are on straight vertical segments, for the harmonic balance Jacobian. This complies with the theory presented through generalized eigenvalue problems, although for higher harmonics we have some eigenvalues off the expected trail, perhaps due to aliasing. The eigenvalues of the harmonic balance Jacobian in Figure 7.3 and its Jacobian in Figure

7.4 are naturally the same.

In Figure 7.6, $v_1(t)$ computed through harmonic balance is presented. Figure 7.7 compares three methods of normalization for Floquet vectors obtained through harmonic balance. The crude method employs $v_1^\top(t_0)\mathbf{C}(t_0)u_1(t_0) = 1$ at the first timepoint, and then at all other timepoints, the scaling factor that is obtained at t_0 is used. The better method is to make use of $\bar{v}_1^\top \bar{\mathbf{C}} \bar{u}_1 = N$, for all timepoints at once. The best method is as stated before $\bar{v}_1^\top \bar{f}(\bar{x}^\gamma) = N$. There is no difference in accuracy between the better and best method, and they both beat the crude method. The better method requires a differentiation in the frequency domain and a sparse matrix-vector multiplication, along with an inverse FFT, in excess of the best method.

7.2 Circadian Oscillator

We analyze the circadian oscillator whose equations and parameters are presented in [6]. The harmonic balance Jacobian has seven distinct sets of eigenvalues as shown in Figure 7.9, which means that all seven Floquet exponents of this system are real.

The analysis that we carry out is plotting PRCs (Phase Resetting Curves) for this system. After $v_1(t)$ is computed, it is used to solve the phase equation repeatedly for different perturbations. In Figure 7.10, we present these PRCs. The perturbations are pulses of amplitude L and duration d . Each such perturbation is shifted along the period by a predetermined interval in time, for each instance of the computation, and then the phase equation is solved with the perturbation set as the shifted pulse. A PRC for a set L and a d is the continuous curve of the computed phases, plotted on the same graph, after the pulse is finally shifted through the whole period.

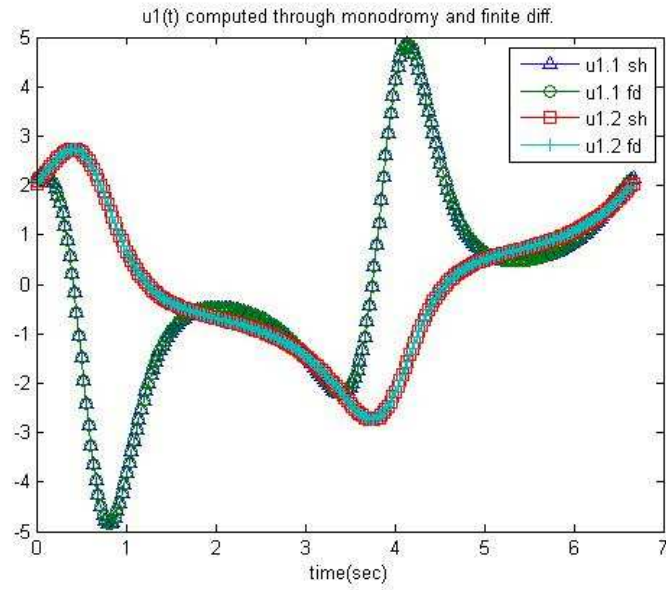


Figure 7.1: $u_1(t)$ computed through shooting and finite differences.

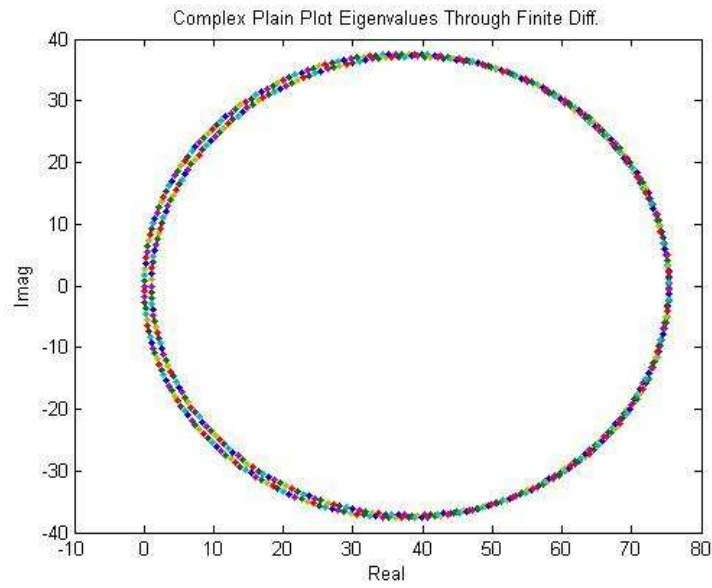


Figure 7.2: Eigenvalues of the finite differences Jacobian, plotted on the complex plane.

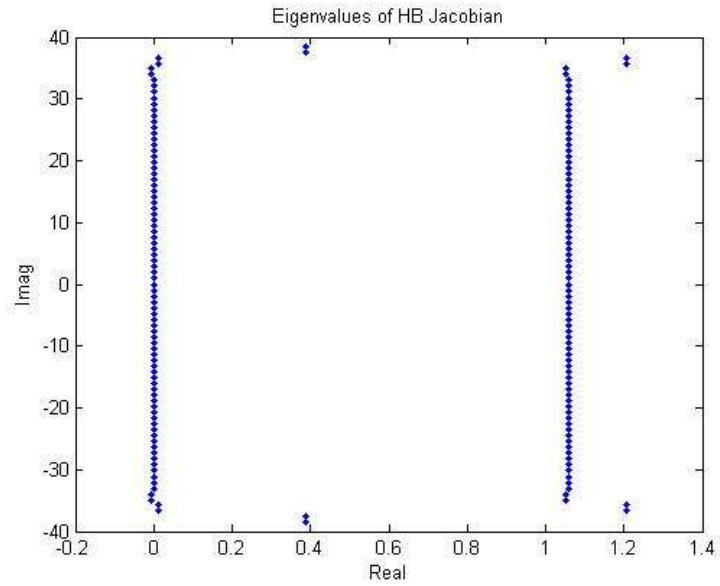


Figure 7.3: Eigenvalues of the harmonic balance Jacobian.

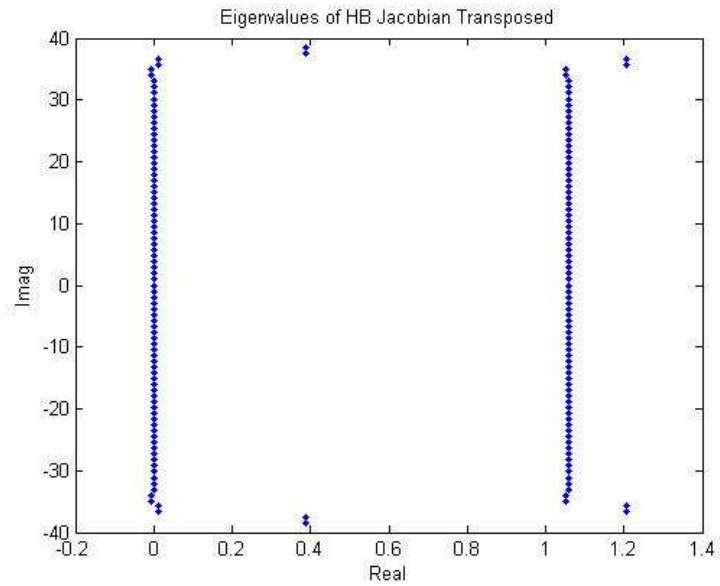
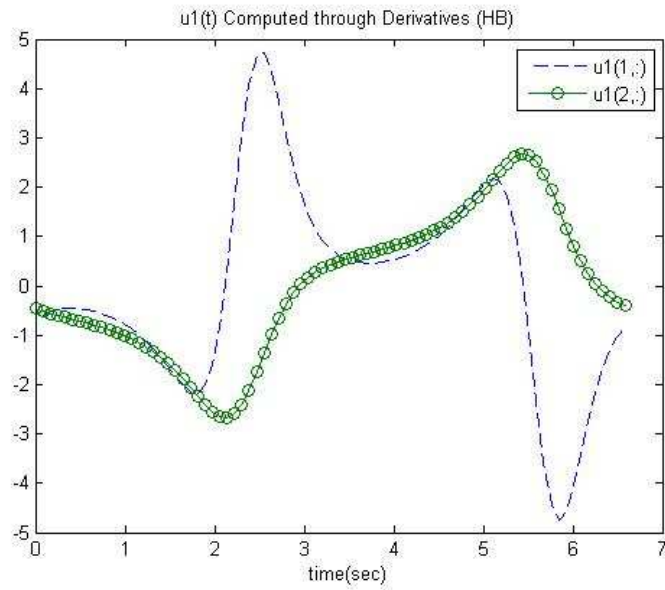
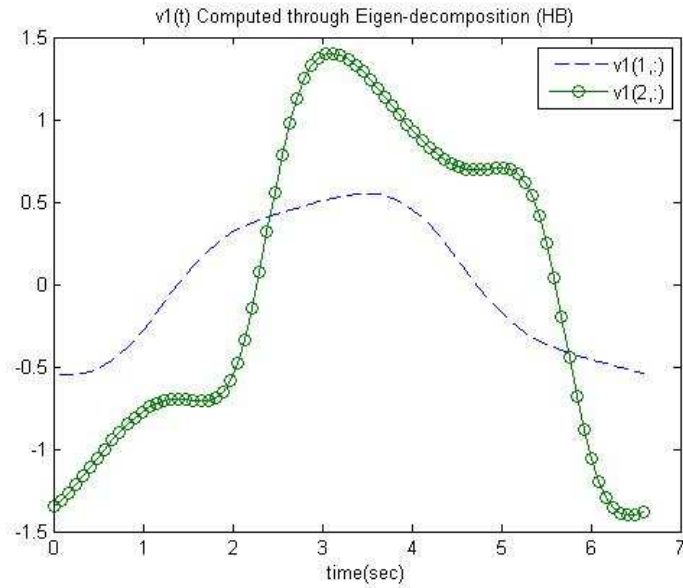


Figure 7.4: Eigenvalues of the Hermitian transpose of the harmonic balance Jacobian.

Figure 7.5: $u_1(t)$ computed through harmonic balance.Figure 7.6: $v_1(t)$ computed through harmonic balance.

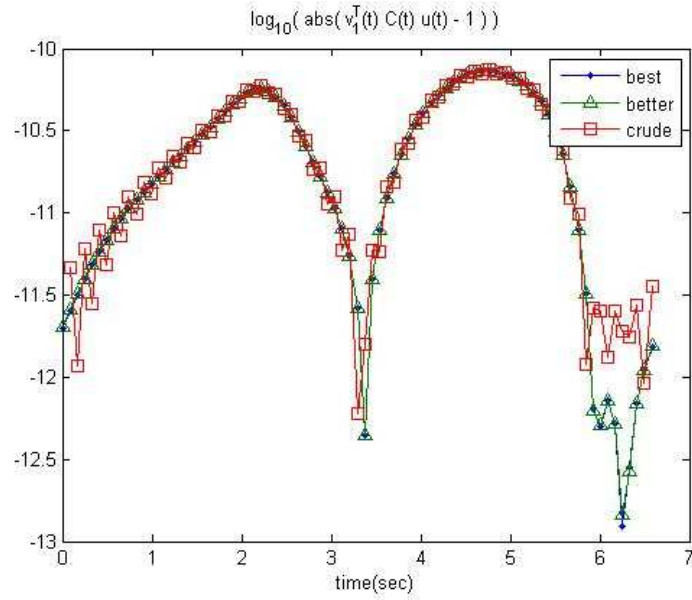


Figure 7.7: Normalization in harmonic balance, through three particular schemes.

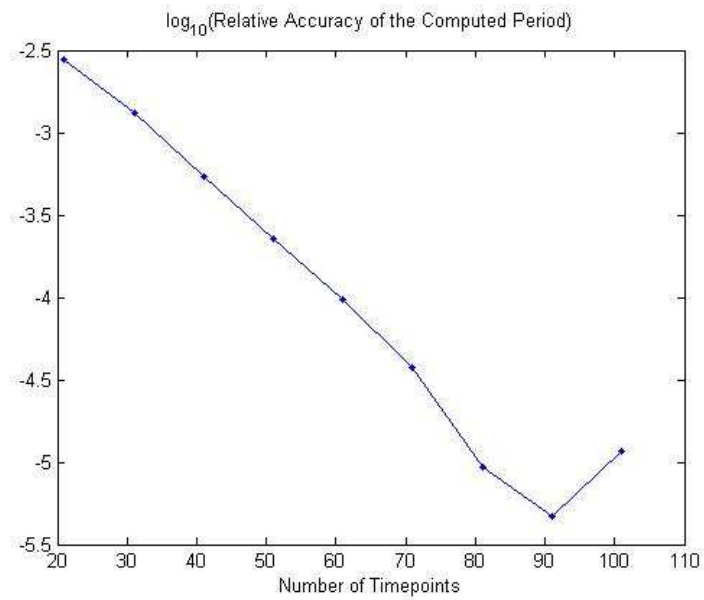


Figure 7.8: Relative accuracy of the computed period.

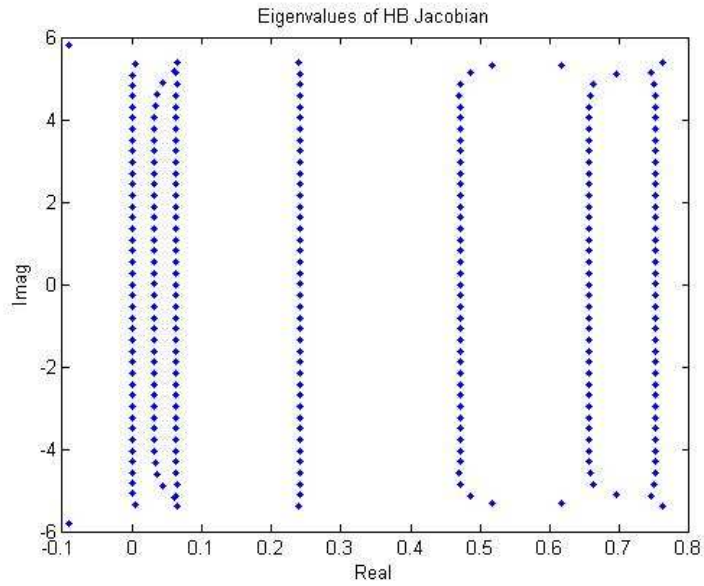


Figure 7.9: Eigenvalues of the harmonic balance Jacobian, for the circadian oscillator.

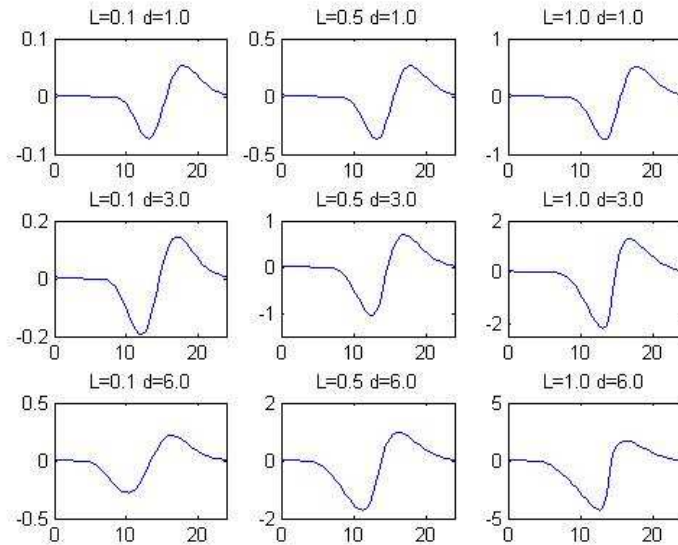


Figure 7.10: PRC (Phase Response or Resetting Curve) plots for the circadian oscillator.

Chapter 8

CONCLUSION

The first achievement in this thesis is to define the phase of an oscillator with the help of isochrons. This has already been accomplished in the biological domain. We thoroughly present the necessary derivations that lead to the definition of oscillator phase. Then, the phase equation for perturbed solutions of oscillators is derived. The phase equation has been known in the biological and electronic domains for decades, although the related work has progressed independently. We also point out the significance of the phase equation, with the help of Floquet theory, while proving the accuracy of this equation. Through this evaluation, a certain component of perturbations is shown to contribute to phase, whereas the other components are proved to cause orbital deviation. In all, in this thesis, we unify the approaches to defining the phase of an oscillator.

The second achievement is the development of a unified approach to oscillator noise analysis in the presence of both state and parameter perturbations. This is possible through system augmentation and use of the phase equation, for the DAE case in general.

There has already been contributions targeting state and parameter perturbation-based phase drift, in both biological and electronic domains. The third major contribution of this thesis is to rigorously prove that all these approaches boil down to the computation of $v_1(t)$.

For the numerical computation of $v_1(t)$, we observe that the methods in biology are indeed ad hoc, so we refer to the methods in electronics. Steady-state periodic solution techniques, shooting and harmonic balance in particular, are rederived. As a fourth contribution, we introduce the generalized eigenvalue problems derived through Floquet theory and adjoint equations, to formulate systematic and accurate methods for the computation of $v_1(t)$. Shooting, finite differences and harmonic balance methods are shown to aid in Floquet mode computation, through the generalized eigenvalue problem formulation.

Appendix A

LOSS OF THE ASYMPTOTIC PHASE PROPERTY

In Section 3.5, we presented an example for illustration purposes of computing the isochron layout associated with the limit cycles of simple oscillators. We now move on to another simple example, which is more interesting than the previous one. The example that we have already presented only had one limit cycle, the unit circle. Also the previous oscillator possessed the asymptotic phase property. We were able to analytically figure out the state transition function for the previous system of differential equations, and then we made use of this state transition function to spell out an expression for the level sets of the phase, associated with that oscillator. These level sets are, as stated before, called the isochrons.

The current oscillator example is again expressed in polar coordinates. It has not one but three limit cycles. The first of these limit cycles is degenerate, only a single point located at the origin. The second limit cycle does not have a domain of attraction, except the set of points that constitute this particular limit cycle, i.e. when we start simulating from a point not on this second limit cycle, the trajectory traversed by the current system never approaches this particular limit cycle, as time progresses. The third limit cycle is again the unit circle.

The aspects stated above are not the only ones that make the current example more interesting than the first. A parameter employed within the model that describes this oscillator may be utilized to change the structure of isochrons on the plane, which are associated with this oscillator. We are going to be exploring how isochrons herald the loss of the asymptotic phase property.

The oscillator model is a modified version of an example, presented by Winfree [19]. The model we aim to analyze is expressed through the following equations. (r, θ) are again the

polar coordinate notifiers, on the plane. Dot denotes derivative with respect to time.

$$\dot{r} = (1-r)(r-p_v)r \quad (\text{A.1})$$

$$\dot{\theta} = 1 + \epsilon(1-r) \quad (\text{A.2})$$

Above, p_v is the variable parameter, which we are going to use to restructure the isochrons associated with the system. ϵ serves as a parameter, again restructuring the isochrons, but p_v is the main parameter that we are going to focus on. We are going to assume that $\epsilon \neq 0$, because otherwise, changes in p_v cannot produce different isochron loci on the plane, i.e. the choice, $\epsilon = 0$, produces a degenerate, not very interesting case.

The closed form solution of the system of equations in (A.1) and (A.2) is not available, so we do not have access to the analytical form of the state transition function, associated with this system. We will have to resort to computations with limits to figure out the limit cycles and their domains of attraction.

Analyzing (A.1), we figure out that all three elements of set

$$\gamma_s = \{r = 1, r = p_v, r = 0\} \quad (\text{A.3})$$

are limit cycles of the system in (A.1) and (A.2), because these choices nullify the change in r with respect to time.

We will maintain the choice that $0 < p_v < 1$. Let us define the vector solution to (A.1) and (A.2) as $x(t) = (r(t) \theta(t))^T$. In order to figure out the domain of attraction, associated with each of the limit cycles in γ_s , we have to analyze for which choices of $x(0)$, the initial condition provided, the system produces a trajectory approaching a particular element in set γ_s , as time progresses.

The system in (A.1) and (A.2) does not have an analytical state transition function, but we are free to try our best with analytical methods when analyzing this system. When we organize and integrate the equation in (A.1), we get

$$\begin{aligned} -t + c &= \left(\frac{1}{1-p_v} \right) \ln(1-r) \\ &- \left(\frac{1}{p_v(1-p_v)} \right) \ln(r-p_v) \\ &+ \left(\frac{1}{p_v} \right) \ln r, \end{aligned}$$

where c is an integration constant given by

$$\begin{aligned} c &= \left(\frac{1}{1-p_v} \right) \ln(1-r_0) \\ &\quad - \left(\frac{1}{p_v(1-p_v)} \right) \ln(r_0-p_v) \\ &\quad + \left(\frac{1}{p_v} \right) \ln r_0. \end{aligned}$$

Notice that the argument of the natural logarithm function should be strictly positive. We then have

$$e^{-t} = \frac{\left(\frac{1-r}{1-r_0} \right)^{\frac{1}{1-p_v}} \left(\frac{r}{r_0} \right)^{\frac{1}{p}}}{\left(\frac{r-p_v}{r_0-p_v} \right)^{\frac{1}{p_v(1-p_v)}}}. \quad (\text{A.4})$$

As $t \rightarrow \infty$ above, both sides of the equality should approach zero. Let us $r = r_s$ the steady-state value of r . Obviously, r_s different for different values of r_0 . We will examine, first, two cases. In each of these cases, one of the bases in the numerator will have to equate to zero, as time progresses, i.e. the value of r_s will make one these bases zero.

Recall once more that all three bases in the numerator and denominator of (A.4) were the arguments of separate natural logarithm functions. So these bases still have to remain positive. Let us examine the first case with $p_v < r_0$. The base in the denominator tells us that $(p_v < r_0) \Rightarrow (p_v < r_s)$. Looking at the second base in the numerator we have $(p_v < r_s) \Rightarrow (0 < r_s)$. Therefore, this second base can never equate to zero. The only choice that will make the whole right-hand side zero is $r_s = 1$. Therefore, $(p_v < r_0) \Rightarrow (r_s = 1)$.

For the second case, let us assume $p_v > r_0$. Looking at the base in the denominator of (A.4), we have $(p_v > r_0) \Rightarrow (p_v > r_s)$. However, we also have the assumption that $0 < p_v < 1$. We can never equate the first base in the numerator zero, so we have $(p_v > r_0) \Rightarrow (r_s = 0)$.

In all, we have $(p_v < r_0) \Rightarrow (r_s = 1)$ and $(p_v > r_0) \Rightarrow (r_s = 0)$, but there is also the case that $r_0 = p_v$. $r = p_v$ is a stable limit cycle of this system. So $(r_0 = p_v) \Rightarrow (r_s = p_v)$. It follows that the domain of attraction, associated with $r = 0$, $\mathcal{W}_{r=1} = \{r > p_v\}$. Similarly, $\mathcal{W}_{r=0} = \{r < p_v\}$ and $\mathcal{W}_{r=p_v} = \{r = p_v\}$. So $r = p_v$ has no domain of attraction associated with it, except the points that constitute itself.

Before proceeding, let us set $p_v = 1$ and carry out a similar analysis. However, we are to examine what happens to the limit cycles, their domains of attraction, and the structure

of isochrons when $p_v = 1$ exactly. Setting $p_v = 1$, we have the following

$$\dot{r} = -(1-r)^2 r \quad (\text{A.5})$$

$$\dot{\theta} = 1 + \epsilon(1-r) \quad (\text{A.6})$$

This system has two limit cycles $r = 1$ and $r = 0$. We cannot solve (A.5) analytically, but let us at least try to integrate to write

$$e^{-t} = \frac{\left(\frac{r}{r_0}\right) e^{\frac{1}{1-r}}}{\left(\frac{1-r}{1-r_0}\right) e^{\frac{1}{1-r_0}}}, \quad (\text{A.7})$$

where $r_0 = r(t = 0)$. The bases in parentheses in both the numerator and denominator should remain positive, since they were the arguments of separate natural logarithm functions after analytical integration. As $t \rightarrow \infty$, we expect both sides of (A.7) to approach zero. Let us again call r_s the steady-state value of r .

We have to examine two cases, $r_0 < 1$ and $r_0 > 1$, to figure out the domains of attraction associated with the limit cycles of (A.5) and (A.6). r_s will change according to r_0 . $r_0 < 1$ is the simpler case. $(r_0 < 1) \Rightarrow (r_s < 1)$, for $(1-r)/(1-r_0)$ must remain positive. If we then choose $r_s = 1 - \Delta$ for diminishing positive values of Δ , the exponential term in the denominator will explode. $r_s = 0$ is a legitimate choice, looking at the first base in the numerator. Therefore, $(r_0 < 1) \Rightarrow (r_s = 0)$.

The second case is a little more tricky. Since $(1-r)/(1-r_0)$ must remain positive, $(r_0 > 1) \Rightarrow (r_s > 1)$. The first base in the numerator can never equate to zero. We guess that $r_s = 1$, but we write this proposition in the form given by $r_s = 1 + \Delta$, as $\Delta \rightarrow 0^+$. In (A.7), we plug in $r = 1 + \Delta$, to evaluate

$$\lim_{\Delta \rightarrow 0^+} \frac{e^{-\frac{1}{\Delta}}}{-\Delta}.$$

We must simply define $C = 1/\Delta$ to write

$$\lim_{C \rightarrow +\infty} -\frac{C}{e^C} = \lim_{C \rightarrow +\infty} -\frac{1}{e^C} = 0,$$

by L'Hôpital's rule after the first equality sign. Therefore, $(r_0 > 1) \Rightarrow (r_s = 1)$.

For the system in (A.5) and (A.6), we have now figured out the domains of attraction as $\mathcal{W}_{r=1} = \{r \geq 1\}$ and $\mathcal{W}_{r=0} = \{r < 1\}$. Both limit cycles have the asymptotically orbital stability property. We are going to make use of these results shortly.

Since the state transition function of the system in (A.1) and (A.2) is not analytically available, we are not able to figure out the analytical expression for the isochrons through the first method described when analyzing the first simple example. Let us use Winfree's method in [19] to figure out an expression for the isochrons of the system in (A.1) and (A.2), assuming that these isochrons exhibit polar symmetry around the origin.

A.1 Vanishing Isochrons

In this example, we do not know beforehand where the isochrons are defined. We have figured out the domain of attraction associated with each of the three limit cycles, but isochrons are defined in the domain of attraction, associated with a limit cycle if that limit cycle has the asymptotic phase property. In this particular case, we will have to make an educated guess on which domain of attraction bears the isochrons. $r = p_v$ does not have a domain of attraction except the points on itself. Therefore, it cannot have the asymptotically orbital stability property, and it does not have asymptotic phase. $r = 0$ is a degenerate limit cycle, and the period on $r = 0$ is not defined. Crossing out two of the limit cycles and their domains of attraction, we pick $r = 1$ as a promising limit cycle, whose domain of attraction might yield the isochrons we are looking for. So we guess that the isochrons, associated with the system in (A.1) and (A.2), foliate $r > p_v$. Then, we also have to compute the angular frequency in $r > p_v$. $\omega_0 = 1$ on $r = 1$, and due to our assumption that $r > p_v$ bears the isochrons of this system, we guess that $\omega_0 = 1$ in $r > p_v$.

Applying Winfree's method to (A.1) and (A.2), we set $d\phi/dt = \omega_0 = 1$, where ϕ is the angular phase of this system, following the discussion in the preceding paragraph. Guessing that the isochron structure has polar symmetry, we have $\phi = \theta - h(r)$, h is a function of r , and we are figure out what $h(r)$ is. Reformulating,

$$\frac{dh}{dr} = \frac{\dot{\theta} - 1}{\dot{r}} = \frac{\epsilon}{r(r - p_v)}.$$

$h(r)$ becomes

$$h(r) = \frac{\epsilon}{p_v} \ln \left(1 - \frac{p_v}{r} \right) + c,$$

where c is an integration constant. Setting $\phi = \theta$ on $r = 1$, since ϕ , the phase in the domain of attraction, is equal to θ , the familiar phase of a system defined in polar coordinates, on

the limit cycle, we have

$$\phi = \theta - \frac{\epsilon}{p_v} \ln \left(\frac{r - p_v}{r(1 - p_v)} \right), \quad (\text{A.8})$$

as the expression describing the isochrons of this system. Since we have assumed from the beginning that $0 < p_v < 1$, (A.8) is defined in $r > p_v$. This is what we had proposed as an educated guess in our discussion above. Let us also check that

$$\begin{pmatrix} \frac{\partial \phi}{\partial r} \\ \frac{\partial \phi}{\partial \theta} \end{pmatrix} \cdot \begin{pmatrix} \dot{r} \\ \dot{\theta} \end{pmatrix} = \omega_0 = 1.$$

This requires a tedious but simple calculation, and it turns out to be true. Since

$$\begin{aligned} \frac{\partial \phi}{\partial r} &= -\frac{\epsilon}{p_v} \left(\frac{1}{r - p_v} - \frac{1}{r} \right) = \frac{-\epsilon}{r(r - p_v)} \text{ and } \frac{\partial \phi}{\partial \theta} = 1, \\ \frac{\partial \phi}{\partial r} \frac{dr}{dt} &= \frac{-\epsilon}{r(r - p_v)} (1 - r)(r - p_v)r = -\epsilon(1 - r), \end{aligned}$$

and the result follows that $\omega_0 = 1$.

Examining the isochron expression in (A.8), we repeat that isochrons may only exist in and foliate $r > p_v$, the domain of attraction associated with $r = 1$. Therefore, we maintain that $r = 1$, one of the three stable limit cycles of this system, has the asymptotic phase property. The structure of isochrons in this example is such that $r = p_v$ can be described as a vortex, with the isochrons asymptotically approaching $r = p_v$ in a revolving manner. The isochrons, of course, can never intersect $r = p_v$.

Notice that when a particular limit cycle has the asymptotic phase property, each point on this limit cycle can be associated with a single isochron in its domain of attraction. If an isochron intersected more than two points on the limit cycle, the phase of a point on this isochron would have to be indeterminate, and then this limit cycle would not possess asymptotic phase.

Proceeding with our intuitive discussion, recall that we have chosen p_v as a variable parameter in this example, such that $0 < p_v < 1$. $p_v \rightarrow 0$ is not interesting, but $p_v \rightarrow 1$ is, as we will convey right now. There is no asymptotic phase for $r = p_v$, and the isochrons of the system in (A.1) and (A.2) approach $r = p_v$, as if this limit cycle were a vortex. Each isochron becomes parallel to $r = p_v$, in the limit as $r \rightarrow p_v^+$. Each isochron has to foot infinitely many cycles around $r = p_v$, before intersecting it. This behavior is as explained for all values in $0 < p_v < 1$. When p_v is changed, the structure of isochrons in $r > p_v$ changes.

As $p_v \rightarrow 1^-$, each isochron will still be associated with a unique point on $r = 1$, but also each isochron has to geometrically whirl around $r = p_v$, infinitely many times. This means each isochron will have all points constituting itself very near $r = 1$, since each isochron is confined in $p_v < r < 1$. In this region, the isochrons should not intersect each other, they should not intersect $r = p_v$. Also they must foliate $r > p_v$, i.e. each point in $r > p_v$ must be contained by a unique isochron.

The description above help us deduce that the isochrons for this system must be re-structured when $p_v = 1$, such that no asymptotic phase for $r = 1$ exists, in this case. In the limit as $p_v \rightarrow 1^-$, each isochron is forced to intersect all points on $r = 1$, following the discussion in the paragraph above. This phenomenon, as stated before, harbingers the loss of asymptotic phase for $r = 1$.

We will again resort to Winfree's method in [19], to figure out the structure of isochrons in the system given by (A.5) and (A.6), since there is no access to the analytical form of the state transition function. Through our discussion above, we maintain that $r = 1$ does not have asymptotic phase for the system in (A.5) and (A.6). $r = 0$ is a degenerate limit cycle, with no period defined on it, so we cannot define phase based on period in its domain of attraction. Then, we intuitively guess that there are no isochrons on the plane for any limit cycle of the system in (A.5) and (A.6).

The period on $r = 1$ is again $T = 2\pi$. We guess that there is periodicity in the domain of attraction, $r \geq 1$, associated with $r = 1$. Through this assumption, $\omega_0 = 2\pi/T = 1$ in $r \geq 1$. We then again define the angular phase in $r \geq 1$ as in $\dot{\phi} = 1$. We again guess that the isochrons in $r \geq 1$ exhibit polar symmetry, i.e. $\phi = \theta - h(r)$. Then, after tedious calculations, we have

$$\frac{dh}{dr} = \frac{\dot{\theta} - 1}{\dot{r}} = -\frac{\epsilon}{r(1-r)},$$

and

$$\phi = \theta + \epsilon \ln \left(\frac{r}{1-r} \right) + c,$$

for some integration constant c . It happens that above, we cannot set $r = 1$ to have $\phi = \theta$ on the limit cycle of interest, which is again $r = 1$. Tentatively speaking, this test might have turned out inconclusive. We cannot right away state that the system in (A.5) and (A.6) has no isochrons, depending on this test. However, we do not have another example, in which we come across the same consequence, the inability to figure out c , the integration constant,

whereas isochrons indeed do exist, unlike this example. Therefore, we do not have enough evidence to call this test inconclusive, in similar cases. We had intuitively guessed that the asymptotic phase property is lost as a result of the parameter change as in $p_v \rightarrow 1^-$. Above is what may be called a candidate for the algebraic justification for our educated intuition.

A.2 Loss of Biorthogonality

As to what happens to the phase of the system in (A.1) and (A.2) as $p_v \rightarrow 1^-$, in the close neighborhood of $r = 1$, we have to linearize this system and apply Floquet theory. However, let us first guess what to expect. As $p_v \rightarrow 1^-$, the isochrons of the system are confined in the tight region defined by $(1 - \Delta) < r \leq 1$, with Δ as an infinitesimal value. The isochrons should not intersect each other, or else there will be no asymptotic phase for $r = 1$. Also each isochron has to swirl infinitely many times around $r = p_v$. These conclusions were drawn simply through Winfree's analytic method of figuring out expressions for isochrons [19].

Let us recall several important definitions. Defining $x(t) = (r(t) \theta(t))^T$, we let $x^\gamma(t)$ be the particular steady-state solution on $r = 1$, by our convention. The intercept of η_{t_0} on $r = 1$ is again accepted as $x^\gamma(t_0)$. The gradient of η_{t_0} at $x^\gamma(t_0)$ is again $v_1(t_0)$, and $\dot{x}^\gamma(t_0) = u_1(t_0)$, with the normalization condition in $v_1(t_0) \cdot u_1(t_0) = 1$. These statements are true for $0 \leq t_0 < T = 2\pi$. Under the circumstances reviewed above, the isochrons of this system are expected to reside very close to the steady-state periodic trajectory, $r = 1$. This phenomenon should cause $v_1(t_0)$, the isochron gradient at $x^\gamma(t_0)$, to become orthogonal to the steady-state periodic trajectory, $r = 1$. However, $u_1(t_0)$ is tangent to the trajectory. Therefore, it should be such that $v_1(t_0) \cdot u_1(t_0) = 0$. This rules out the very normalization condition we have relied on so far. Biorthogonality is lost as $p_v \rightarrow 1^-$. Therefore, the system given by (A.5) and (A.6), with $p_v = 1$, not only does not have isochrons in the domain of attraction that belongs to $r = 1$, but also $v_1(t)$ and $u_1(t)$ are orthogonal on $r = 1$. This is no more than intuitive thinking, but the following calculations justify our claim.

In addition to $x(t) = (r(t) \theta(t))^T$, let us also define $f(x) = (\dot{r}(t) \dot{\theta}(t))^T$. We aim to linearize the system in (A.1) and (A.2) to derive

$$\frac{dy}{dt} = \frac{\partial f}{\partial x} \Big|_\gamma y,$$

where $\gamma = \{r = 1\}$. Simple calculations yield

$$\frac{dy}{dt} = \begin{pmatrix} 1 - p_v & 0 \\ -\epsilon & 0 \end{pmatrix} y. \quad (\text{A.9})$$

Suspensions may arise as to why (A.9) does not seem to be LPTV (Linear Periodically Time-Variant). In fact, the system described by (A.9) is LPTV, but the initial choice of the coordinate system facilitates computations by transforming the system at hand into one of the form in (A.9). The solution of this equation can be obtained through stright-forward linear algebra and matrix functions methods. We have to eigen-decompose the matrix in this equation to get

$$\left. \frac{\partial f}{\partial x} \right|_{\gamma} = \begin{pmatrix} 0 & 1 - p_v \\ 1 & \epsilon \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & p_v - 1 \end{pmatrix} \begin{pmatrix} \frac{-\epsilon}{1-p_v} & 1 \\ \frac{1}{1-p_v} & 0 \end{pmatrix},$$

since the eigenvalues are $\{0, p_v - 1\}$. We aim to compute $u_1(t)$ and $v_1(t)$ in particular.

However, let us note that the solution of (A.9) is $y(t) = \mathbf{U}(t) \exp(\Lambda t) \mathbf{V}^{\top}(0) y(0)$, with

$$\mathbf{U}(t) = \begin{pmatrix} 0 & 1 - p_v \\ 1 & \epsilon \end{pmatrix}, \quad \mathbf{V}^{\top}(t) = \begin{pmatrix} \frac{-\epsilon}{1-p_v} & 1 \\ \frac{1}{1-p_v} & 0 \end{pmatrix}.$$

and

$$e^{\Lambda t} = \begin{pmatrix} 1 & 0 \\ 0 & e^{(p_v-1)t} \end{pmatrix}.$$

It happens that we have already found $u_i(t)$ and $v_i(t)$ for $1 \leq i \leq 2$. Let us define sets

$$\mathcal{U} = \{u_1(t), u_2(t)\} = \left\{ \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 - p_v \\ \epsilon \end{pmatrix} \right\}$$

and

$$\mathcal{V} = \{v_1(t), v_2(t)\} = \left\{ \begin{pmatrix} \frac{-\epsilon}{1-p_v} \\ 1 \end{pmatrix}, \begin{pmatrix} \frac{1}{1-p_v} \\ 0 \end{pmatrix} \right\}.$$

In particular, we have chosen $u_1(t)$ as such because $\dot{x}^{\gamma}(t) = f(x^{\gamma}) = (0 \ 1)^{\top}$. We can easily check that $v_1(t) \cdot u_1(t) = 1$, $v_2(t) \cdot u_2(t) = 1$, $v_1(t) \cdot u_2(t) = 0$, and $v_2(t) \cdot u_1(t) = 0$. However, observe the form of $v_1(t)$ above. As $p_v \rightarrow 1^-$, the magnitude of the first entry of $v_1(t)$, $v_{1,1}(t)$, grows unbounded with respect to $v_{1,2}(t)$. This consequence is physically not possible, $v_{1,2}(t)$ is zero with respect to the magnitude of $v_{1,1}(t)$. Examining the tangential velocity vector, $u_1(t)$, on $r = 1$, we deduce that as $p_v \rightarrow 1^-$, $v_1(t) \cdot u_1(t) \rightarrow 0$. So biorthogonality is lost, and this is the mathematical justification of our intuitive claim above.

A.3 Loss of Asymptotic Phase

We may also attempt on analyzing the effect of having no asymptotic phase, on θ , in the close neighborhood of $r = 1$, for the system in (A.5) and (A.6), where $p_v = 1$. Let us again resort to linearizations. We have

$$\begin{aligned} \frac{dy}{dt} &= \left. \frac{\partial f}{\partial x} \right|_{\gamma} y \\ &= \begin{pmatrix} 0 & 0 \\ -\epsilon & 0 \end{pmatrix} y \end{aligned} \quad (\text{A.10})$$

and

$$\left. \frac{\partial f}{\partial x} \right|_{\gamma} = \begin{pmatrix} 0 & -\frac{1}{\epsilon} \\ 1 & \beth \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \epsilon \beth & 1 \\ -\epsilon & 0 \end{pmatrix}, \quad (\text{A.11})$$

which is of the form in $\mathbf{U}(t)\Lambda\mathbf{W}^T(t)$. \beth is an arbitrary constant. Let us define sets \mathcal{U} and \mathcal{W} as

$$\mathcal{U} = \{u_1(t), u_2(t)\} = \left\{ \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} -\frac{1}{\epsilon} \\ \beth \end{pmatrix} \right\}$$

and

$$\mathcal{W} = \{w_1(t), w_2(t)\} = \left\{ \begin{pmatrix} \epsilon \beth \\ 1 \end{pmatrix}, \begin{pmatrix} -\epsilon \\ 0 \end{pmatrix} \right\}.$$

We may check that $u_1(t) \cdot w_1(t) = 1$, $u_2(t) \cdot w_2(t) = 1$, $u_1(t) \cdot w_2(t) = 0$, and $u_2(t) \cdot w_1(t) = 0$. The solution to (A.10), derived from (A.5) and (A.6), is given as $y(t) = \mathbf{U}(t)\exp(\Lambda t)\mathbf{W}^T(0)y(0)$.

Now we have to consider that (A.11) is in Jordan Canonical Form. $\partial f/\partial x^\gamma$ has two eigenvalues of zero, but it has only one eigenvector, which is $u_1(t)$. Eigenvalue zero of $\partial f/\partial x^\gamma$ is said to have algebraic multiplicity of two but geometric multiplicity of one. The trick is to decompose $\partial f/\partial x^\gamma$ as we did in (A.11), in such situations.

Let us note that the state transition function of (A.10) is given by $\mathbf{odK}(t, 0) = \mathbf{U}(t)\exp(\Lambda t)\mathbf{W}^T(0)$. We can easily compute the explicit form of this function through

$$\exp(\Lambda t) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & t \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix},$$

since the square of Λ is the matrix of all zeros. Then, we have

$$\mathbf{odK}(t, 0) = \begin{pmatrix} u_1(t) & u_2(t) \end{pmatrix} \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} \begin{pmatrix} w_1^T(0) \\ w_2^T(0) \end{pmatrix}. \quad (\text{A.12})$$

We must now compute $y(t)$ in (A.10), through $y(t) = \mathbf{odK}(t,0)y(0)$, for different values of $y(0)$.

Recall that $u_1(t) = (0 \ 1)^\top$ for all t , but this is the representation that is true in polar coordinates only. At every point on $r = 1$, this expression for $u_1(t)$ is true in polar coordinates. $u_1(t_1)$ and $u_1(t_2)$ are the same vector when t_1 and t_2 are separated by an integer multiple of the period on $r = 1$. Otherwise, $u_1(t_1)$ and $u_1(t_2)$ are not the same vector. However, the representation of $u_1(t)$ in polar coordinates is always $u_1(t) = (0 \ 1)^\top$.

Let us pick an arbitrary $y(0)$ vector, and represent it as

$$y(0) = a_1 u_1(0) + a_2 u_2(0).$$

a_1 and a_2 are arbitrary constants, not both of which are zero. Considering the form of $\mathbf{odK}(t,0)$ above, $y(t) = \mathbf{odK}(t,0)y(0) = a_1 u_1(t)$, if we let $a_2 = 0$. On the other hand, if we let $a_1 = 0$, we have $y(t) = a_2 t u_1(t) + a_2 u_2(t)$. Notice that $y(t)$, in this case, has a component that grows linearly with time. t multiplies $u_1(t) = (0 \ 1)^\top$. Remember that the second entry, $y_2(t) = \dot{\theta}(t)$. Therefore, through $t u_1(t)$, the growth in $\dot{\theta}(t)$ is linear in t . We have crafted this simple analysis, in order to show that when we pick an initial condition, $x(0)$, not on $r = 1$, but very close to this limit cycle, provided that $r(t=0) > 1$, the growth in the time derivative of $\theta(t)$ is linear in t . Therefore, the system in (A.5) and (A.6) cannot have asymptotic phase in the intersection of the close neighborhood of $r = 1$ and $r \geq 1$, the domain of attraction of $r = 1$.

A.4 A Published Example

We now present another example, in which we again observe the loss of asymptotic phase through a parameter change. The system to be analyzed this time is very similar to the one we have elaborated on since the beginning of this section. The system in polar coordinates is

$$\dot{r} = (1 - r)^3 \tag{A.13}$$

$$\dot{\theta} = r \tag{A.14}$$

and the properties of this set of equations were analyzed in [4].

It is fortunate that the solution is analytically available, and is given as follows.

$$r(t) = 1 - \frac{(1 - r_0)}{\sqrt{1 + 2(1 - r_0)^2 t}} \quad (\text{A.15})$$

$$\theta(t) = \theta_0 + t + \frac{\sqrt{1 + 2(1 - r_0)^2 t}}{1 - r_0} \quad (\text{A.16})$$

Again $r_0 = r(t = 0)$ and $\theta_0 = \theta(t = 0)$. We can easily conclude that this system has a single limit cycle, $r = 1$. $r = 1$ has asymptotic orbital stability, and the domain of attraction associated with $r = 1$ is the whole plane.

We would have also deduced that $r = 1$ had the asymptotic phase property, had the fractional term in (A.16) been such that it died away as time progressed. However, this fractional term grows with time, and $r = 1$ does not have asymptotic phase.

It is difficult to analyze the system in (A.13) and (A.14) as it is, but we introduce as an auxiliary

$$\dot{r} = (p_v - r)^2(1 - r) \quad (\text{A.17})$$

$$\dot{\theta} = r \quad (\text{A.18})$$

where $0 < p_v < 1$ is a parameter whose value is going to be altered to help analyze the properties of the system in (A.13) and (A.14). Obviously, when $p_v = 1$, (A.17) and (A.18) are the same as (A.13) and (A.14), respectively.

Let us first determine the limit cycles and the domains of attraction for the system in (A.17) and (A.18). Obviously, one limit cycle is $r = 1$ and the other is $r = p_v$. In order to figure out the domains of attraction, we proceed as follows.

We are going to try solve for r through (A.17), but again the solution is not analytically available. Through simple integration we get

$$e^{-t} = \frac{\left(\frac{1-r}{1-r_0}\right)^{\frac{1}{(1-p_v)^2}} \exp\left(\frac{1}{1-p_v} \frac{1}{p_v-r_0}\right)}{\left(\frac{p_v-r}{p_v-r_0}\right)^{\frac{1}{(1-p_v)^2}} \exp\left(\frac{1}{1-p_v} \frac{1}{p_v-r}\right)}. \quad (\text{A.19})$$

$(1 - r)/(1 - r_0)$ and $(p_v - r)/(p_v - r_0)$ are allowed to be positive only, since they become the arguments of separate natural logarithm functions after integration. The exponent of both these bases is a positive finite number, since $p_v < 1$.

In order to figure out a steady-state value for r , which we call r_s , we have to let r_0 take a different value in each case. We assume that as time progresses, both sides of (A.19) approach zero. The computed value for r_s should satisfy this condition in each case.

The natural exponent expression in the numerator of (A.19) is a constant, for each different set of values for p_v and r_0 . Therefore, we do not take this expression into account when carrying out our analysis through limits. The two cases for r_0 are $r_0 > p_v$ and $r_0 < p_v$.

The $r_0 > p_v$ case is easy. We deduce that $(r_0 > p_v) \Rightarrow (r > p_v)$, for $(p_v - r)/(p_v - r_0) > 0$. We have to choose one of the two cases, $r_s = p_v$ or $r_s = 1$. Notice that the $r_s = p_v$ choice with $r > p_v$ in time lets the denominator go to zero, so the right-hand side of (A.19) explodes. The choice that makes this right-hand side zero is $r_s = 1$. Therefore, $(r_0 > p_v) \Rightarrow (r_s = 1)$.

Analyzing the second case is a little more tricky. We have $(r_0 < p_v) \Rightarrow (r < p_v)$, and naturally $(r_0 < p_v) \Rightarrow (r < 1)$. Therefore, $(1 - r)/(1 - r_0)$ in the numerator is neither infinite nor zero for all time. We are induced to guess that $r_s = p_v$, but this needs to be proved. Through our guess, we have $r = p_v - \Delta$, in time, where Δ is a small positive number. In this case, we take into account neither $(1 - r)/(1 - r_0)$ nor the natural exponent expression in the numerator. With the remaining terms in the right-hand side of (A.19), and substituting $r = p_v - \Delta$, we have to check the value of the limit given by

$$\lim_{\Delta \rightarrow 0^+} \frac{\exp(-1/\Delta)}{\Delta}.$$

For convenience, we define again $C = 1/\Delta$ and write

$$\lim_{C \rightarrow +\infty} \frac{C}{e^C} = \lim_{C \rightarrow +\infty} \frac{1}{e^C} = 0,$$

where we have used L'Hôpital's rule. This proves that $(r_0 < p_v) \Rightarrow (r_s = p_v)$.

The domain of attraction associated with $r = 1$ is therefore $\mathcal{W}_{r=1} = \{r | r > p_v\}$, and $\mathcal{W}_{r=p_v} = \{r | r \leq p_v\}$. We will now apply the methods of our analyses to the model in (A.17) and (A.18).

Let us make use of Winfree's method [19] to figure out an expression for the isochrons over the whole plane. We have two regions, which the isochrons of this system may foliate. $r = p_v$ has $r \leq p_v$ as the domain of attraction. Simulations starting from a point in $r > p_v$ do not approach $r = p_v$. We guess that the isochrons foliating $r > p_v$ intersect $r = p_v$ only after traversing infinitely many cycles around $r = p_v$, while approaching this particular limit cycle. Therefore, we guess that $r = 1$ has asymptotic phase, whereas $r = p_v$ does not, so the period on $r = 1$ is equal to the generalized period over the whole domain of attraction, $r > p_v$. Denoting this period by $T = 2\pi$, the generalized angular frequency in $r > p_v$ becomes $\omega_0 = 2\pi/T = 1$.

By Winfree's method [19], we define ϕ , the angular phase in $r > p_v$, through the differential equation $d\phi/dt = \omega_0 = 1$, with $\phi(0) = 0$. Then, assuming that the isochrons in $r > p_v$ exhibit polar symmetry, ϕ must have the form $\phi = \theta - h(r)$, where h is a function of r . Simple computation yields

$$\frac{dh}{dr} = \frac{r-1}{(p_v-r)^2(1-r)} = \frac{-1}{(p_v-r)^2}.$$

Integrating the expression above and invoking the initial condition that $\phi = \theta$ when $r = 1$, we have

$$\phi = \theta + \frac{1}{p_v-r} - \frac{1}{p_v-1}, \quad (\text{A.20})$$

as the expression for the phase in $r > p_v$. Recall that isochrons are the level sets of ϕ . For example, for a single $\phi_0 \in [0, 2\pi)$, $\phi_0 = \theta + \frac{1}{p_v-r} - \frac{1}{p_v-1}$ is the expression for a single isochron.

We observe through (A.20) that the isochrons foliating $r > p_v$ revolve infinitely many times around $r = p_v$ before intersecting this limit cycle. However, it is clear that each isochron must intersect $r = 1$ at a single point. This observation proves that our educated guess was correct.

Geometrically speaking, as $p_v \rightarrow 1^-$, each isochron tends to lie very close to the limit cycle $r = 1$. These isochrons must not intersect each other, must not intersect $r = p_v$, and each must intersect $r = 1$ at a single point still, as $p_v \rightarrow 1^-$. Satisfying all these conditions become impossible for $p_v = 1$, so isochrons vanish for the system in (A.17) and (A.18).

Let us now examine the biorthogonality relation as $p_v \rightarrow 1^-$. Let us linearize the system in (A.17) and (A.18) into

$$\frac{dy}{dt} = \begin{pmatrix} -(p_v-1)^2 & 0 \\ 1 & 0 \end{pmatrix} y,$$

where y is a two dimensional column vector. Calling the square matrix in the equation above, \mathbf{A} , we have

$$\mathbf{A} = \begin{pmatrix} 0 & (p_v-1)^2 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & -(p_v-1)^2 \end{pmatrix} \begin{pmatrix} 1/(p_v-1)^2 & 1 \\ 1/(p_v-1)^2 & 0 \end{pmatrix}$$

as the eigen-decomposition of \mathbf{A} . Employing polar coordinates, we have obtained a time-invariant expression, although our linearized system is indeed LPTV, so \mathbf{A} is a matrix with constant coefficients.

Recall that $u_1(t)$ is the persistent mode of the forward LPTV equation, and $v_1(t)$ is the persistent mode of the adjoint LPTV equation. Let us denote $u_1(t)$ as u_1 in this case, to benefit from the time-invariant form. Similarly, let us denote $v_1(t)$ as v_1 . We deduce from the eigen-decomposition of \mathbf{A} above that

$$u_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ and } v_1 = \begin{pmatrix} 1/(p_v - 1)^2 \\ 1 \end{pmatrix}.$$

Observe that $v_1 \cdot u_1 = 1$, satisfying the normalization condition. However, as $p_v \rightarrow 1^-$, the first entry of v_1 , i.e. $v_{1,1} \rightarrow +\infty$. Therefore, as $p_v \rightarrow 1^-$, $v_{1,1}/v_{1,2} \rightarrow 0$. This means as $p_v \rightarrow 1^-$, $v_1 \cdot u_1 \rightarrow 0$, i.e. biorthogonality is lost.

As a note, observe that the gradient of ϕ in (A.20),

$$\begin{pmatrix} \frac{\partial \phi}{\partial r} \\ \frac{\partial \phi}{\partial \theta} \end{pmatrix} = \begin{pmatrix} 1/(p_v - r)^2 \\ 1 \end{pmatrix},$$

is numerically equal to v_1 on the limit cycle $r = 1$. Normally, we would have obtained $\omega_0 v_1$ as the gradient of ϕ on $r = 1$, but remember that $\omega_0 = 1$ on $r = 1$.

Lastly in this series of analyses, let us examine the loss of asymptotic phase from the linearization point of view. We set $p_v = 1$, and obtain the system in (A.13) and (A.14). The linearized equation takes the following time-invariant form in polar coordinates.

$$\frac{dy}{dt} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} y$$

Calling the square matrix \mathbf{E} above, we have

$$\mathbf{E} = \begin{pmatrix} 0 & 1 \\ 1 & \beth \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} -\beth & 1 \\ 1 & 0 \end{pmatrix},$$

as the Jordan canonical form. \beth is an arbitrary number. $y(t)$, the solution of the linearized system, is given as

$$y(t) = \begin{pmatrix} 0 & 1 \\ 1 & \beth \end{pmatrix} \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -\beth & 1 \\ 1 & 0 \end{pmatrix} y(0).$$

Note that we may express $y(t)$ as

$$y(t) = \begin{pmatrix} u_1 & u_2 \end{pmatrix} \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} \begin{pmatrix} w_1^\top \\ w_2^\top \end{pmatrix} y(0).$$

Obviously, $w_1 \cdot u_1 = 1$, $w_2 \cdot u_1 = 0$, $w_1 \cdot u_2 = 0$, and $w_2 \cdot u_2 = 0$. Observe that u_1 and u_2 constitute a linearly independent set. For a set of coefficients $\{a_1, a_2\}$, we have $y(0) = a_1 u_1 + a_2 u_2$. For $a_2 = 0$, observe that $y(t) = a_1 u_1$. However, when $a_1 = 0$, $y(t) = a_2 t u_1 + a_2 u_2$. In this case, there is time t multiplying u_1 . However, $u_{1,2}$ contributes to $\dot{\theta}(t)$. For the unperturbed system in (A.13) and (A.14), the growth in $\dot{\theta}(t)$, with an initial condition not on but in the close neighborhood of $r = 1$, is linear in t . Therefore, $r = 1$ cannot have asymptotic phase.

The published example is indeed very similar to the earlier example we presented, in order to show the gradual loss of asymptotic phase, as a parameter p_v is altered. We tried intuitively and rigorously, in these examples, to portray the vanishing isochrons, the loss of biorthogonality, and the loss of asymptotic phase through the analysis employing the LPTV equation derived from the original system.

A.5 Summary

Both examples in this section, the system in (A.5) and (A.6), and the system in (A.13) and (A.14), which we borrowed from [4], are plagued by the same phenomenon. In both examples, there is a limit cycle, given by $r = p_v$ in particular, which does not have asymptotic phase. The isochrons around $r = 1$, the limit cycle that does have asymptotic phase, for both examples, have to revolve infinitely many times around $r = p_v$, before actually intersecting $r = p_v$. Then, as p_v is changed, the structure of the isochrons, foliating $r > p_v$, changes. As $p_v \rightarrow 1^-$, the isochrons are confined in $p_v < r \leq 1$, each isochron intersecting $r = 1$ at a single point and revolving infinitely many times around $r = p_v$. We have adopted an intuitive approach to deduce that in such a case, the isochrons are forced to vanish. Then, we have mathematically shown that $u_1(t)$ and $v_1(t)$, the persistent modes of the forward and adjoint LPTV equations, respectively, derived from the original system at hand, become orthogonal on $r = 1$, obviating the biorthogonality relation. The last observation was that the asymptotic phase property, in the close neighborhood of $r = 1$, is lost through this parameter change.

Appendix B

PARAMETER SENSITIVITY - LENGTHIER PROOF

We stated before that the proof of Lemma 2 in 5.4.2 is the justification of the major contribution of Taylor et al. in [6]. Also, we noted that our proof is quite simple and comprehensible. We will now conduct a more intuitive but also more tedious proof of the same Lemma. This time, we will resort to the eigenvalue problems, originating through Floquet theory, explained in 6.5.1, along with sensitivity theory.

The problem is again to figure out an expression for the time derivative of

$$\frac{\partial \hat{t}}{\partial p_j} = \sum_{i=1}^M \frac{\partial \hat{t}}{\partial x_i^\gamma} \frac{\partial x_i^\gamma}{\partial p_j}.$$

We derived in 5.4.2 that

$$\frac{\partial x^\gamma}{\partial p_j} = \sum_{i=1}^M e^{\mu_i t} u_i(t) \int_0^t e^{-\mu_i \tau} v_i^\top(\tau) \frac{\partial f}{\partial p_j}(\tau) d\tau.$$

Let us redefine, for convenience,

$$S_i(t) = \int_0^t e^{-\mu_i \tau} v_i^\top(\tau) \frac{\partial f}{\partial p_j}(\tau) d\tau.$$

We also know by now that $\partial \hat{t} / \partial x^\gamma(t) = v_1(t)$, by the discussion provided in 5.3.

Let us now note that

$$\frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) = \left(\frac{dv_1}{dt} \right)^\top \frac{\partial x^\gamma}{\partial p_j} + v_1^\top(t) \frac{d}{dt} \left(\frac{\partial x^\gamma}{\partial p_j} \right).$$

We proceed to compute

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial x^\gamma}{\partial p_j} \right) &= \sum_{i=1}^M \mu_i e^{\mu_i t} u_i(t) S_i(t) \\ &+ \sum_{i=1}^M e^{\mu_i t} \frac{du_i}{dt} S_i(t) \\ &+ \sum_{i=1}^M e^{\mu_i t} u_i(t) \frac{dS_i}{dt}. \end{aligned} \tag{B.1}$$

The first term at the right-hand side is easy enough to compute. For the second term, we must note that $\dot{u}_i = \mathbf{G}(t)u_i(t) - \mu_i u_i(t)$, by the derivations in 6.5.1, where $\mathbf{G}(t) = \partial f / \partial x$, evaluated on γ . Finally, for the third term, we recall the fundamental theorem of calculus to spell out, in all,

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial x^\gamma}{\partial p_j} \right) &= \sum_{i=1}^M e^{\mu_i t} \mathbf{G}(t) u_i(t) S_i(t) \\ &+ \sum_{i=1}^M u_i(t) v_i^\top(t) \frac{\partial f}{\partial p_j}(t). \end{aligned} \quad (\text{B.2})$$

We must now consider

$$\begin{aligned} v_1^\top(t) \frac{d}{dt} \left(\frac{\partial x^\gamma}{\partial p_j} \right) &= \sum_{i=1}^M v_1^\top(t) e^{\mu_i t} \mathbf{G}(t) u_i(t) S_i(t) \\ &+ v_1^\top(t) \frac{\partial f}{\partial p_j}(t), \end{aligned} \quad (\text{B.3})$$

and proceed to the next step.

The next step requires the evaluation of the time derivative of $v_1(t)$. This is simple enough, because $v_1(t)$ is a periodic solution of $\dot{z} = -\mathbf{G}^\top(t)z$, the adjoint equation associated with (2.1). We then have $\dot{v}_1^\top(t) = -v_1^\top(t)\mathbf{G}(t)$. We get

$$\left(\frac{dv_1}{dt} \right)^\top \frac{\partial x^\gamma}{\partial p_j} = - \sum_{i=1}^M v_1^\top(t) e^{\mu_i t} \mathbf{G}(t) u_i(t) S_i(t). \quad (\text{B.4})$$

Considering the sum of the terms in (B.3) and (B.4), we have

$$\frac{d}{dt} \left(\frac{\partial \hat{t}}{\partial p_j} \right) = v_1^\top(t) \frac{\partial f}{\partial p_j}(t),$$

which is what we wanted to prove in Lemma 2.

Appendix C

SIMPLIFICATIONS IN COMPUTATION PERTAINING TO ODE SYSTEMS

C.1 Eigenpairs Associated with LPTV Systems

The eigenvalue problem, derived for the generic ODE in (2.1), reads

$$\frac{dy_{kn}(t)}{dt} - \mathbf{G}(t)y_{kn}(t) = \lambda_{kn}y_{kn}(t) \quad (\text{C.1})$$

in the forward LPTV case and

$$-\frac{dz_{kn}}{dt} - \mathbf{G}^\top(t)z_{kn}(t) = \lambda_{kn}^*z_{kn}(t) \quad (\text{C.2})$$

in the adjoint LPTV case. Notice that neither of the statements above are generalized eigenvalue problems. In the ODE case, we are to solve simple eigenvalue problems. We again know the theoretical forms of the solutions to the problems above.

For the problem in (C.1), which is derived from the forward LPTV equation, we have

$$\lambda_{kn} = -(\mu_k - j2\pi/Tn) \quad (\text{C.3})$$

as the eigenvalues and

$$y_{kn}(t) = e^{j2\pi/Tnt}u_k(t) \quad (\text{C.4})$$

as the corresponding eigenfunctions. n is an integer and $1 \leq k \leq M$.

Similarly, for the problem in (C.2), which is derived from the adjoint LPTV equation, we have

$$\lambda_{kn}^* = -(\mu_k + j2\pi/Tn) \quad (\text{C.5})$$

as the eigenvalues and

$$z_{kn}(t) = e^{j2\pi/Tnt}v_k(t) \quad (\text{C.6})$$

as the eigenfunctions.

To numerically solve (C.1) and (C.2), we have to switch to the frequency domain. Again, this computation is facilitated through \mathbf{odJ}_{hb} , the harmonic balance Jacobian after convergence, in the ODE case.

C.2 Persistent Mode Computation Through Harmonic Balance

We are now going to outline the eigenvalue problem solution scheme, through the aid of the harmonic balance Jacobian, \mathbf{odJ}_{hb} in the ODE case. Recall that a variable name with a bar above denotes the concatenated timepoints vector corresponding to that variable.

We may transform the problem in (C.1) to the frequency domain as in

$$[j\Omega^\gamma - \Gamma\bar{\mathbf{G}}(\bar{x}^\gamma)\Gamma^{-1}] \{\Gamma\bar{\vartheta}\} = \lambda \{\Gamma\bar{\vartheta}\}, \quad (\text{C.7})$$

which, in more compact form, is

$$\mathbf{odJ}_{hb} \{\Gamma\bar{\vartheta}\} = \lambda \{\Gamma\bar{\vartheta}\}. \quad (\text{C.8})$$

The solution to the transformed problem above is given by the eigenpair

$$\lambda = \lambda_{kn} = -(\mu_k - j2\pi/Tn) \quad (\text{C.9})$$

and

$$\bar{\vartheta} = \left((e^{j\omega_0 n t_0} u_k(t_0))^* \dots (e^{j\omega_0 n t_{N-1}} u_k(t_{N-1}))^* \right)^*. \quad (\text{C.10})$$

Although the statement above is designed to help in finding all the eigenpairs associated, all we need for our purposes is the $(-\mu_1 = 0, u_1(t))$ pair. However, we have set $u_1(t) = dx^\gamma/dt$, so $\Gamma\bar{u}_1 = j\Omega^\gamma\Gamma\bar{x}^\gamma = j\Omega^\gamma\bar{X}^\gamma$. Therefore, we do not need to solve (C.8).

Transforming (C.2) into the frequency domain, we get

$$-j\Omega^\gamma \{\Gamma\bar{\varrho}\} - \Gamma\bar{\mathbf{G}}^\top(\bar{x}^\gamma)\Gamma^{-1} \{\Gamma\bar{\varrho}\} = \lambda^* \{\Gamma\bar{\varrho}\}. \quad (\text{C.11})$$

In more compact form, we have

$$\mathbf{odJ}_{hb}^* \{\Gamma\bar{\varrho}\} = \lambda^* \{\Gamma\bar{\varrho}\}. \quad (\text{C.12})$$

The solution to the transformed problem above is given by the eigenpair

$$\lambda^* = \lambda_{kn}^* = -(\mu_k + j2\pi/Tn) \quad (\text{C.13})$$

and

$$\bar{\varrho} = \left((e^{j\omega_0 n t_0} v_k(t_0))^* \dots (e^{j\omega_0 n t_{N-1}} v_k(t_{N-1}))^* \right)^*. \quad (\text{C.14})$$

Although the formulation above helps in figuring out all the eigenpairs, we seek the pair $(-\mu_1 = 0, \bar{v}_1)$ for our purposes. One may resort to the methods of numerical linear algebra

to solve (C.12). Numerically, the eigenfunction that corresponds to the real eigenvalue with the smallest absolute value is the eigenfunction that we would like to obtain.

After acquiring a vector in the direction of $\Gamma\bar{v}_1$, the next task is to normalize this vector. All of the normalization conditions below, considering that we have N timepoints, are legitimate.

$$\bar{v}_1 \cdot \bar{u}_1 = N$$

$$\bar{v}_1 \cdot \bar{f}(\bar{x}^\gamma) = N \tag{C.15}$$

$$\{\Gamma\bar{v}_1\} \cdot \{\Gamma\bar{f}(\bar{x}^\gamma)\} = N \tag{C.16}$$

$$\{\Gamma\bar{v}_1\} \cdot \{\Gamma\bar{u}_1\} = N$$

$$\{\Gamma\bar{v}_1\} \cdot \{j\Omega^\gamma \bar{X}^\gamma\} = N \tag{C.17}$$

As we are working in the frequency domain throughout harmonic balance, (C.17) is the most natural choice for the normalization condition, but we can furthermore omit the time derivative computation in the frequency domain, through $j\Omega^\gamma$, by choosing (C.16) for normalization. (C.16) is the simplest method, provided we have $\bar{f}(\bar{x}^k)$ stored at each iteration k of harmonic balance, so that we $\bar{f}(\bar{x}^\gamma)$ ready after convergence.

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VITA

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