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Moment Problems for Jacobi Matrices & Inverse Problems for Systems of Many Coupled Oscillators

by

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Abstract

In this thesis we study a family of inverse problems for finite-dimensional Jacobi matrices. The family of problems arises from the undamped linearized dynamics for a system of many coupled oscillators, and is closely connected to the classical moment problem in analysis and the attendant theory of orthogonal polynomials.

In the physical context one considers a differential equation of the form

$$\ddot{x} + Ax = M^{-1}f,$$

where the constant coefficient matrix A is tridiagonal, M is a diagonal matrix of mass terms, and f is an external force. For each fixed pair of indices (i, j) let $G_{ij}(t)$ denote the displacement $x_j(t)$ of the jth component of the system in response to a unit impulse force $f(t) = \delta(t)e_i$ applied to the ith component. We pose the following inverse problem: Given the function G_{ij}, determine the matrices A and M. In general this problem is nonlinear, the solution is not unique, and the dimension of a solution is not determined or even bounded. This formulation of the family of inverse problems, corresponding to all possible values of i and j, is new and our work extends known results for the special case $i = j = 1$.

The above family of physical inverse problems can be reduced to the following matrix-theoretic statement. Fix a Jacobi matrix J and a pair of indices (i, j). Let m_n denote the (i, j)-entry of the nth power J^n of J. Given the sequence $\{m_n\}_{n\geq 0}$ up to a positive scalar multiple, determine J. The latter problem may be viewed as a variant of the classical moment problem which dates back to the 19th century.

Our objective in this thesis is to describe the manifold of least-dimensional solutions to each inverse problem in the given family. For each specific problem in

the family we define a pair of polynomials, the characteristic polynomial and the composite polynomial, which can be computed from the given data. We show that least-dimensional solutions to the problem correspond to divisors modulo the characteristic polynomial of the composite polynomial. Our description of the solution manifold depends on a detailed analysis of the location of the zeros of the composite polynomial. This analysis is facilitated by formulas we derive by means of the flip transpose. Ultimately, we give an explicit parameterization of the solution manifold over a connected semi-algebraic subset of the vector space of real univariate polynomials.

As a byproduct of this analysis, we obtain general methods to construct orthogonal polynomials, which has allowed us to show for the first time that well-known upper bounds on the number of common zeros between orthogonal polynomials are in fact attained.

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Chapter 1

Introduction

1.1 A brief overview

This thesis studies a family of inverse problems which can be stated in terms of matrices in a very simple way. This matrix formulation, given at the beginning of Chapter 2, shows the problems to be close cousins of the classical moment problem, a key difference being that we study finite-dimensional matrices only. A rather different formulation for the problems comes from a consideration of physical systems of coupled oscillators. In the physical context, discussed in Chapter 4, the inverse problems correspond to a family of simple non-destructive experiments. The physical setting provided the original motivation for the thesis.

Either formulation of the problems boils down to the following. Given spectral data of a specific type, determine all so-called Jacobi matrices whose spectra conform to the data. The spectral data consists of a possibly incomplete list of eigenvalues, with associated weights. Stated this way, a solution to the inverse problems is a

matrix, and one can speak of solutions having minimum dimension. Ultimately, we develop methods to determine the solutions of minimum dimension for the entire family of inverse problems. And for a particular subfamily of problems, we show how to find all solutions.

The main focus of the thesis is on Jacobi matrices. Despite being a narrow class of matrices, with a specialized structure, Jacobi matrices have many important connections. They are significant in their own right as operators, or as the reduced form of an operator. In this connection, see [BG, Gl1, Gl2, Gl3, L] and also Chapter 4. Secondly, Jacobi matrices are connected to probability distributions on the real line and to orthogonal polynomials; see [F,S] and also [G].

We give a brief overview of the thesis as follows. Chapters 2 and 3 are purely mathematical in content. In Chapter 2 we state the matrix formulation of the family of inverse problems, collectively called the "main problem", then establish the context and work out preliminary results which are needed in Chapter 3. Chapter 3 contains the heart of the thesis. There we systematically develop a body of results which allows us to describe in a precise way the set of least-dimensional solutions to the entire family of problems considered.

As already mentioned, Chapter 4 is concerned with applications to systems of coupled oscillators. There we consider physical systems consisting of many coupled oscillators, and we show that a family of associated physical inverse problems coincides exactly with the moment problems for Jacobi matrices considered in the preceding two chapters.

We make no attempt in this thesis to address the numerical and computational aspects of the solution to the main problem. This is a reasonable topic for future

study, now that the theoretical aspects of a solution have been dealt with, at least in part.

1.2 What's new in this thesis

There is a considerable amount of literature relating to the preliminary material presented in Chapter 2. The essential connection between Jacobi matrices, probability distribution functions and orthogonal polynomials dates back to the work of Stieltjes in the 1890's, as well as a succession of other mathematicians, including Chebyshev, Markov and M. Reisz. See [F,S] for an extensive list of references. With respect to the specific reconstruction of a finite-dimensional Jacobi matrix from its associated probability distribution function (or equivalently, discrete inner product), the papers [dG,BG] discuss this in detail, as does the book [Gl1]. But this construction can be viewed as being much older, since it fits into the more general framework of the classical results, where one constructs an infinite Jacobi matrix from a continuous distribution function. The papers [dG,BG] also consider the numerical aspects of the problem, and develop reconstructions based on other types of spectral data not considered in this thesis. With respect to the specific types of oscillating systems treated in Chapter 4, the papers [Gl2,Gl3] are relevant: they treat the simplest special case $i = j = 1$. Both these papers use results given in [dG] and discuss numerical algorithms, in particular the so-called Lanczos algorithm, presented earlier in [BG].

The specific formulation of the main problem presented at the beginning of Chapter 2 is new. And the particular proofs given in that chapter are my own, although they relate to well-known results.

By contrast, all the main results in Chapter 3 are new, starting with Lemma 3.2.1 and Theorem 3.2.2. As evidence of this, the paper [G] is based entirely on Theorem 3.2.2. The definition of the composite polynomial, which plays a central role in Chapter 3, is original as well. Note that the results thought to be most significant are labeled as theorems, or occasionally lemmas. On the other hand, results labeled as propositions serve the role of needed facts.

The main novelty of Chapter 4, lies in the theorem at the end, which connects it to the results in the previous chapter. The formulation of the family of inverse problems for systems of coupled oscillators given in Chapter 4 is new. The proofs given there are my own, but most of them are straightforward and hence not of intrinsic mathematical interest.

Thus in brief, the formulation of the problem given in Chapter 2 is new, but the results in Chapter 2 are known; everything in Chapter 3 is new. The results in Chapter 4 are original as is the formulation of the family of inverse problems, however the main interest of Chapter 4 lies in the theorem which connects it to the earlier parts of the thesis.

Chapter 2

Preliminaries

2.1 Problem Statement

Definition. A *Jacobi matrix* is a symmetric, tridiagonal matrix whose next-to-diagonal entries are strictly negative. The dimension of a Jacobi matrix may be finite or (one-way) infinite. Thus a $d \times d$ Jacobi matrix has the form

$$\begin{pmatrix} a_1 & -b_1 & 0 & \dots & 0 \\ -b_1 & a_2 & -b_2 & \ddots & \vdots \\ 0 & -b_2 & a_3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -b_{d-1} \\ 0 & \dots & 0 & -b_{d-1} & a_d \end{pmatrix}$$

where each $b_n > 0$.

Classically, the main interest lies in infinite Jacobi matrices; see Szegö [S]. By contrast the principal considerations in this thesis involve finite-dimensional Jacobi matrices only.

We use the following non-standard notation in order to avoid cluttered subscripts: $M(i,j)$ denotes the $(i,j)^{\text{th}}$ entry of the matrix M.

This thesis centres on a family of inverse problems which collectively have a very simple formulation in terms of Jacobi matrices. Roughly speaking, *we want to determine a Jacobi matrix J, given—up to a positive scalar multiple—the sequence* $(J^n)(i,j)$ $(n = 0,1,2,\ldots)$.

This problem is complicated by two essential features:

1. it is non-linear;

2. the solution is not unique.[1]

We now give a more formal statement of the main problem.

Notation. Let A, B be objects which admit multiplication by a scalar. We write $A \propto B$ to mean: there exists a real number $r > 0$ such that $A = rB$. In other words, A and B are positively proportional.

Let J be a Jacobi matrix. We write $m(J,i,j)$ to denote the sequence $(m_0, m_1, m_2, \ldots)$ defined by $m_n = (J^n)(i,j)$. (We assume that the obvious requirement $1 \leq i,j \leq \dim J$ is always satisfied.)

In order to avoid writing the statement "J is a finite-dimensional Jacobi matrix" over and over again, we make the convention that whenever the notation $m(J,i,j)$ is used it means that J is a finite-dimensional Jacobi matrix, unless the contrary is explicitly stated.

---

[1] If the indices i and j are also given as part of the problem then there are exceptions to 2. The case $i = j = 1$ has a unique solution, as does the case $i = j = \dim J$.

Main Problem (Version 1). *Given the sequence $m(J,i,j)$, determine all Jacobi matrices $\tilde{J}$ such that for some k,l,*

$$m(\tilde{J},k,l) \propto m(J,i,j). \tag{2.1}$$

We call a matrix $\tilde{J}$ satisfying (2.1) a *solution* to the problem. The set of all solutions is denoted $\mathcal{S}(J,i,j)$. We are mainly interested in a distinguished subset of the solutions: those solutions having least possible dimension. We denote this distinguished subset by $\mathcal{S}_{\min}(J,i,j)$.

Our objective for this thesis is to describe $\mathcal{S}_{\min}(J,i,j)$ as a manifold, for arbitrary J,i,j. (More precisely, we seek a parametrization of $\mathcal{S}_{\min}(J,i,j)$.) Note that if we can solve the main problem, then we can also solve the following somewhat restricted version of the main problem, which may seem more natural.

Restricted Problem (Version 1). *Suppose that indices i,j are known, and that the sequence $m(J,i,j)$ is given. Determine all Jacobi matrices $\tilde{J}$ such that*

$$m(\tilde{J},i,j) \propto m(J,i,j).$$

2.2 Background

Distribution functions

Definition. A *probability distribution function* on the real line $\mathbf{R}$ is a right-continuous, non-decreasing function α on $\mathbf{R}$ such that $\lim_{x\to-\infty}\alpha(x) = 0$ and $\lim_{x\to\infty}\alpha(x) = 1$. The associated differential $d\alpha$ is called a *probability distribution.* More generally, a *distribution function* on the real line $\mathbf{R}$ is a right-continuous function γ of bounded variation such that $\lim_{x\to-\infty}\gamma(x) = 0$. The differential $d\gamma$ associated to γ is called a *distribution.* We abbreviate "probability distribution function" and "distribution function" to p.d.f. and d.f. respectively.

Every distribution function γ can be written in the form $\gamma = a\alpha + b\beta$ where $a, b \in \mathbf{R}$ and α, β are probability distribution functions.

Definition. Let γ be a d.f. on $\mathbf{R}$ and set $t(x)$ to be the total variation of γ on the interval $(-\infty, x]$. Set $\gamma_+(x) = (t(x)+\gamma(x))/2$, and set $\gamma_-(x) = (t(x)-\gamma(x))/2$. Then each of γ_+ and γ_- is non-decreasing, and $\gamma(x) = \gamma_+(x) - \gamma_-(x)$. A *point of increase* of γ is a point $x \in \mathbf{R}$ such that for every $\epsilon > 0$, $\gamma_+(x+\epsilon) > \gamma_+(x-\epsilon)$. A *point of decrease* of γ is a point $x \in \mathbf{R}$ such that for every $\epsilon > 0$, $\gamma_-(x+\epsilon) > \gamma_-(x-\epsilon)$.

In this thesis we consider primarily d.f.s which take on finitely many values, or, in other words, d.f.s whose range is a finite set. A d.f. γ having finite range is necessarily a pure jump function. In this context we call a point $x \in \mathbf{R}$ which is either a point of increase or decrease of γ a *jump point* of γ. Note that for a p.d.f. having finite range, every jump point is a point of increase, and the two terms can be used interchangeably; when speaking of a p.d.f. we will do so.

It is convenient to represent d.f.s having finite range in terms of the Heaviside function. We fix the notation as follows. Let H denote the Heaviside function, defined on the real line as follows:

$$H(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}.$$

Let $\mathcal{H}$ denote the collection of finite linear combinations of translates of H; this is precisely the set of d.f.s having finite range. Thus $\mathcal{H}$ denotes the collection of functions of the form

$$\gamma(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n) \tag{2.2}$$

where $w_1, \ldots, w_d, \lambda_1, \ldots, \lambda_d$ are real, and d is a positive integer. Of course such a representation for γ is not unique. Each non-zero function $\gamma \in \mathcal{H}$ can be expressed in the form (2.2) with d minimal, and in this case $\lambda_1, \ldots, \lambda_d$ are necessarily distinct and each w_n is non-zero. If $\lambda_1, \ldots, \lambda_d$ are distinct then whenever $w_n > 0$, the corresponding value λ_n is a point of increase of γ; whenever $w_n < 0$, the corresponding value λ_n is a point of decrease.

Notation. Let $\mathcal{H}_+$ denote the subset of $\mathcal{H}$ consisting of positive linear combinations of translates of H. That is, $\mathcal{H}_+$ consists of functions γ which can be expressed in the form (2.2) such that $\lambda_1, \ldots, \lambda_d$ are distinct and each $w_n > 0$. If in addition $\sum_{n=1}^{d} w_n = 1$ then γ is a p.d.f. having finite range, and conversely every p.d.f. having finite range has such a representation. We denote the collection of p.d.f.s having finite range by $\mathcal{H}_{+,1}$.

We now come to an important definition, which is particular to this thesis.

Definition. Let $0 \neq \gamma \in \mathcal{H}$. Write

$$\gamma(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n)$$

with d minimal. We call the polynomial

$$p_\gamma(x) = \prod_{n=1}^{d} (\lambda_n - x)$$

the *characteristic polynomial* of γ (reserving the notation p_γ for this purpose). We define the characteristic polynomial of $\gamma = 0$ to be 0. Thus two d.f.s $\beta, \gamma \in \mathcal{H}$ have the same jump points if and only if they have the same characteristic polynomial.

The Lebesgue-Stieltjes integral

The Lebesgue-Stieltjes integral provides a convenient framework for much of the discussion in this thesis. In this subsection we discuss very briefly the Lebesgue-Stieltjes theory so as to fix our notation, and to highlight some facts which are particularly relevant. As a reference for the Lebesgue-Stieltjes theory, we cite Friedman [Fr].

Based on a d.f. γ, the standard Lebesgue-Stieltjes construction yields a signed measure μ_γ and an associated integral $\int \cdot \, d\gamma$. We treat the distribution $d\gamma$ formally as an independent object, as is common practice, but its meaning is tied to the integral $\int \cdot \, d\gamma$. Thus the statement $d\beta = d\gamma$ is shorthand for: $\mu_\beta = \mu_\gamma$, or equivalently, for every x, $\int_{-\infty}^{x} d\beta = \int_{-\infty}^{x} d\gamma$. Now, let $f, g : \mathbf{R} \to \mathbf{R}$ be functions of bounded variation, without any further restriction. Then $df = dg$ if and only if there exists a constant c such that $f(x) = g(x) + c$ a.e. with respect to Lebesgue measure. Thus a single distribution arises from many different functions. There is however a unique distribution function γ (as we have defined the term) such that $df = d\gamma$, namely $\gamma(x) = \int_{-\infty}^{x} df$. (Note: $\int_{-\infty}^{x} df = \int_{-\infty}^{\infty} \chi_{(-\infty,x]} \, df$ is right-continuous—as required by the definition of d.f. By contrast the function $\int_{-\infty}^{\infty} \chi_{(-\infty,x)} \, df$ is left-continuous.) This

bijective correspondence between distributions and d.f.s allows us to pass freely from one to the other, and we will do so whenever it's convenient.

If we base Lebesgue-Stieltjes integration on a p.d.f. α, instead of an arbitrary $d.f.$, then the standard theory gives us an inner product space, namely the Hilbert space $L^2_{d\alpha}$. We review briefly the underlying structure of $L^2_{d\alpha}$. Let $\mathcal{L}^2_{d\alpha}$ denote the vector space of functions $f : \mathbf{R} \to \mathbf{R} \cup \{-\infty, \infty\}$ for which the integral $\int_{-\infty}^{\infty} f^2 d\alpha$ is finite. (Note: if $f, g \in \mathcal{L}^2_{d\alpha}$ then the product fg is integrable, though it need not belong to $\mathcal{L}^2_{d\alpha}$.) The operator $\langle \cdot, \cdot \rangle_{d\alpha}$, defined by $\langle f, g \rangle_{d\alpha} = \int_{-\infty}^{\infty} fg\, d\alpha$, makes $\mathcal{L}^2_{d\alpha}$ into a semi-inner product space.

For $f, g \in \mathcal{L}^2_{d\alpha}$, write $f \sim g$ if $f(x) = g(x)$ μ_α-a.e. Denote the equivalence class of f mod $\sim$ by $\overline{f}$. The quotient space $\mathcal{L}^2_{d\alpha}/\sim$, which is denoted $L^2_{d\alpha}$, is then an inner product space. (Of course much more is true—$L^2_{d\alpha}$ is complete.)

These remarks pertain to an arbitrary d.f. We now turn our attention to the special case of interest in this thesis: d.f.s having finite range. Let $\gamma \in \mathcal{H}$ and write

$$\gamma(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n),$$

where d is minimal. Every extended real-valued function $f : \mathbf{R} \to \mathbf{R} \cup \{-\infty, \infty\}$ is μ_γ-measurable. The Lebesgue-Stieltjes integral engendered by γ is a weighted sum:

$$\int_{-\infty}^{\infty} f\, d\gamma = \sum_{n=1}^{d} w_n f(\lambda_n),$$

and the function f is integrable precisely if the value $f(\lambda_n)$ is finite at each jump point λ_n. If γ is a p.d.f. (i.e. if $\gamma \in \mathcal{H}_{+,1}$) then $\mathcal{L}^2_{d\gamma}$ consists of all integrable functions. The semi-inner product $\langle \cdot, \cdot \rangle_{d\gamma}$ is given by

$$\langle f, g \rangle_{d\gamma} = \sum_{n=1}^{d} w_n f(\lambda_n) g(\lambda_n).$$

The Hilbert space $L^2_{d\gamma}$ is isometrically isomorphic to $\mathbf{R}^d$ with the inner product $\langle \cdot, \cdot \rangle^\gamma$, defined by

$$\langle x, y \rangle^\gamma = \sum_{n=1}^{d} w_n x_n y_n,$$

an explicit isometry being

$$\overline{f} \longmapsto (f(\lambda_1), \ldots, f(\lambda_d)).$$

Let $\beta, \gamma \in \mathcal{H}$. The Lebesgue decomposition of μ_β with respect to μ_γ induces a "Lebesgue decomposition" of β with respect to γ. Explicitly, we say β is *absolutely continuous* with respect to γ, and write $\beta \ll \gamma$, if every jump point of β is a jump point of γ. We say β is *singular* with respect to γ, and write $\beta \perp \gamma$, if β and γ have no common jump point. With this terminology and notation, β decomposes uniquely as $\beta = \beta_0 + \beta_1$, where $\beta_1 \ll \gamma$ and $\beta_0 \perp \gamma$. This corresponds to the usual Lebesgue decomposition, $\mu_\beta = \mu_0 + \mu_1$, of μ_β with respect to μ_γ in the sense that $\mu_0 = \mu_{\beta_0}$ and $\mu_1 = \mu_{\beta_1}$.

The restriction of $\mathcal{L}^2_{d\alpha}$ to polynomials

Polynomials play a fundamental role in the analysis of Jacobi matrices and hence in this thesis. To begin, we fix notation. The symbol $\mathbf{P}$ denotes the vector space of real polynomials in a single variable; $\mathbf{P}_d$ denotes the subspace of $\mathbf{P}$ consisting of polynomials of degree at most d. A p.d.f. α (possibly with infinite range), or the associated distribution $d\alpha$, is said *to have moments* if $\mathbf{P} \subset \mathcal{L}^2_{d\alpha}$. Distribution functions having infinite range and which also have moments are the focus of the classical moment problem, where one objective is to characterize those probability

distributions $d\alpha$ for which $\mathbf{P}$ is dense in $\mathcal{L}^2_{d\alpha}$ (see Freud [F]). In the special case of interest to this thesis, $\alpha \in \mathcal{H}_{+,1}$, the p.d.f. α necessarily has moments, and the question of whether $\mathbf{P}$ is dense in $\mathcal{L}^2_{d\alpha}$ becomes trivial: it is automatically so. This allows us to restrict our considerations exclusively to polynomials.

Let α be a p.d.f. with moments. We denote $\mathbf{P}$, considered as a subspace of $\mathcal{L}^2_{d\alpha}$, by $\mathcal{P}^2_{d\alpha}$. Let p, q be arbitrary elements of $\mathcal{P}^2_{d\alpha}$. Not only is the product pq integrable ($|\int_{-\infty}^{\infty} pq\, d\alpha| < \infty$), but pq is itself a member of $\mathcal{P}^2_{d\alpha}$. (This differs from the situation for $\mathcal{L}^2_{d\alpha}$, where $f, g \in \mathcal{L}^2_{d\alpha}$ does *not* imply that $fg \in \mathcal{L}^2_{d\alpha}$.) Thus $\mathcal{P}^2_{d\alpha}$ is an *algebra*, in addition to being a semi-inner product space. Of course this algebraic structure is inherent in $\mathbf{P}$ and does not depend on $d\alpha$. In the algebraic context, for $p \in \mathbf{P}$, we write $\langle p \rangle$ to denote the principal ideal of $\mathbf{P}$ generated by p.

OBSERVATION 2.2.1 *For $p \in \mathcal{P}^2_{d\alpha}$, $\langle p, p \rangle_{d\alpha} = 0$ if and only if every point of increase of α is a zero of p.*

By this fact it is evident that if α has infinite range (equivalently, has infinitely many points of increase) then $\langle \cdot, \cdot \rangle_{d\alpha}$ is actually an inner product on $\mathbf{P}$, since $\langle p, p \rangle_{d\alpha} = 0$ would imply p has infinitely many zeros and hence that $p = 0$. Thus if the p.d.f. α has infinite range then $\mathcal{P}^2_{d\alpha}$ is an inner product space.

If α has finite range, then we can write

$$\alpha(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n),$$

with d minimal. In this case

$$\begin{aligned} \langle p, p \rangle_{d\alpha} = 0 \quad &\Longleftrightarrow \quad p(\lambda_n) = 0 \quad \text{for each } n \\ &\Longleftrightarrow \quad p_\alpha | p \\ &\Longleftrightarrow \quad p \in \langle p_\alpha \rangle, \end{aligned}$$

where p_α is the characteristic polynomial of α. Thus, letting $\sim$ denote the equivalence relation "equals μ_α-a.e.", we have that $p \sim 0$ if and only if $p \in \langle p_\alpha \rangle$. So the quotient space $\mathcal{P}^2_{d\alpha}/\sim$ coincides with the quotient algebra $\mathbf{P}/\langle p_\alpha \rangle$, and the relation "$p = q$ μ_α-a.e." is identical with the (algebraic) relation "$p = q \bmod p_\alpha$". We write $P^2_{d\alpha}$ to indicate the space $\mathcal{P}^2_{d\alpha}/\sim$, or equivalently, $\mathbf{P}/\langle p_\alpha \rangle$ with the inner product $\langle \cdot, \cdot \rangle_{d\alpha}$. We reserve the notation $P^2_{d\alpha}$ for the case of a p.d.f. α having finite range (i.e. $\alpha \in \mathcal{H}_{+,1}$).

Let $\alpha \in \mathcal{H}_{+,1}$ have d jump points (equivalently, d points of increase). Note that for every $p \in \mathbf{P}$ there is a unique polynomial $q \in \mathbf{P}_{d-1}$ such that $p = q \bmod p_\alpha$. Note also that $\langle \cdot, \cdot \rangle_{d\alpha}$ is an inner product on $\mathbf{P}_{d-1}$. Thus $P^2_{d\alpha}$ is isometrically isomorphic to $\mathbf{P}_{d-1}$, endowed with the inner product $\langle \cdot, \cdot \rangle_{d\alpha}$. Recalling the structure $L^2_{d\alpha}$ and letting $\cong$ denote "isometrically isomorphic" we have

$$L^2_{d\alpha} \cong P^2_{d\alpha} \cong \mathbf{P}_{d-1}.$$

The Gram-Schmidt procedure

The Gram-Schmidt procedure, as it is usually presented, is an algorithm which applies to a sequence of linearly independent vectors in an inner product space. Essentially the same algorithm—with an obvious minor modification—applies just as well to an arbitrary sequence of vectors in a semi-inner product space.

Modified Gram-Schmidt procedure. Let V be a vector space and $\langle \cdot, \cdot \rangle$ a semi-inner product on V. Let $v_0, v_1, v_2, \ldots$ be a sequence of vectors in V, called the *input*. Construct a new sequence of vectors $u_0, u_1, u_2, \ldots$, called the *output*, as follows.

Initial step. If $\langle v_0, v_0 \rangle = 0$ set $u_0 = v_0$. Otherwise set $u_0 = v_0/\langle v_0, v_0 \rangle^{1/2}$.

Continuing step. Suppose that $u_0, \ldots, u_{n-1}$ have been defined. Set

$$\tilde{u}_n = v_n - \sum_{i=0}^{n-1} \langle v_n, u_i \rangle u_i.$$

If $\langle \tilde{u}_n, \tilde{u}_n \rangle = 0$ set $u_n = \tilde{u}_n$. Otherwise set $u_n = \tilde{u}_n / \langle \tilde{u}_n, \tilde{u}_n \rangle^{1/2}$.

The output sequence $u_0, u_1, u_2, \ldots$ evidently has the following properties:

1. for each n, span$\{u_0, \ldots, u_n\}$ =span$\{v_0, \ldots, v_n\}$;
2. $\langle u_i, u_j \rangle = 0$ if $i \neq j$;
3. for each n, $\langle u_n, u_n \rangle = 0$ or 1;
4. for each n, $u_n \propto v_n - \sum_{i=0}^{n-1} \langle v_n, u_i \rangle u_i$.

The usual proofs of Bessel's and Schwarz's inequalities are easily adapted to the present context. The former yields another property of the modified Gram-Schmidt procedure:

5. for each n, $\langle u_n, v_n \rangle \geq 0$.

To see this, note that

$$\begin{aligned} \langle u_n, v_n \rangle &\propto \langle v_n - \sum_{i=0}^{n-1} \langle v_n, u_i \rangle u_i, v_n \rangle \\ &= \langle v_n, v_n \rangle - \sum_{i=0}^{n-1} \langle v_n, u_i \rangle^2 \\ &\geq 0 \qquad \text{(Bessel's inequality)}. \end{aligned}$$

Finally, Schwarz's inequality yields the following fact about semi-inner product spaces generally:

$$\langle v, v \rangle = 0 \Longrightarrow \forall u \in V, \langle u, v \rangle = 0.$$

From this point on, the term "Gram-Schmidt procedure" refers to the modified Gram-Schmidt procedure described above.

Polynomials and orthogonalization

We now present a key definition.

Definition. Let α be a p.d.f. having moments. Working in the semi-inner product space $\mathcal{P}^2_{d\alpha}$, apply the Gram-Schmidt procedure to the sequence of signed moment functions

$$1, -x, x^2, \ldots, (-x)^n, \ldots$$

The resulting output sequence

$$q_0^\alpha, q_1^\alpha, q_2^\alpha, \ldots, q_n^\alpha, \ldots \tag{2.3}$$

is called the sequence of *orthogonal polynomials* determined by α. We fix the notation: q_n^α will henceforth always denote the $(n+1)^{\text{st}}$ term in the sequence of orthogonal polynomials determined by the p.d.f. α.

We examine briefly some properties of the sequence (2.3). General properties of the output of the Gram-Schmidt procedure, listed in the previous subsection, give us the following facts.

1. For each n, $\text{span}\{q_0^\alpha, \ldots, q_n^\alpha\} = \mathbf{P}_n$.

In particular, q_n^α is a polynomial of precise degree n.

2. $\langle q_i^\alpha, q_j^\alpha \rangle_{d\alpha} = 0$ if $i \neq j$.

Therefore if $i < n$, $q_n^\alpha \perp \mathbf{P}_i$ (i.e. for each $p \in \mathbf{P}_i$, $\langle q_n^\alpha, p \rangle_{d\alpha} = 0$).

3. For each n, $\langle q_n^\alpha, q_n^\alpha \rangle_{d\alpha} = 0$ or 1.

4. For each n, $q_n^\alpha \propto (-x)^n - \sum_{i=0}^{n-1} \langle (-x)^n, q_i^\alpha \rangle_{d\alpha} q_i^\alpha$.

This shows that the leading coefficient of q_n^α has sign $(-1)^n$.

5. For each n, $\langle (-x)^n, q_n^\alpha \rangle_{d\alpha} \geq 0$.

Property 3 can be somewhat refined. There is a basic dichotomy depending on whether or not α has finite range. If not then (as noted earlier) $\mathcal{P}_{d\alpha}^2$ is an inner product space and so (2.3) is an orthonormal sequence: for each n, $\langle q_n^\alpha, q_n^\alpha \rangle_{d\alpha} = 1$. If α has finite range, then it has a finite number, d, of jump points. In this case, as noted earlier, $P_{d\alpha}^2$ is isometric to $\mathbf{P}_{d-1}$, where the latter is given the inner product $\langle \cdot, \cdot \rangle_{d\alpha}$. It follows immediately that

$$q_0^\alpha, \ldots, q_{d-1}^\alpha$$

is an orthonormal sequence. Also in this case, for $0 \leq n \leq d-1$, property 5 becomes $\langle (-x)^n, q_n^\alpha \rangle_{d\alpha} > 0$, since $\langle (-x)^n, q_n^\alpha \rangle_{d\alpha} \neq 0$. Furthermore, for each $n \geq d$, there is a unique polynomial $p \in \mathbf{P}_{d-1}$ such that $q_n^\alpha = p \bmod p_\alpha$, and therefore (expanding p in terms of $q_0^\alpha, \ldots, q_{d-1}^\alpha$ and applying property 2) $\langle q_n^\alpha, q_n^\alpha \rangle_{d\alpha} = 0$. In the particular case of $n = d$, we have that: q_d^α has precise degree d; $q_d^\alpha = 0 \bmod p_\alpha$; and the leading coefficient of q_d^α has sign $(-1)^d$. It follows that q_d^α is positively proportional to the characteristic polynomial of α: $q_d^\alpha \propto p_\alpha$. And for $n > d$, q_n^α is a polynomial multiple of p_α. To put this in another way, $q_n^\alpha \in \langle p_\alpha \rangle$ for $n \geq d$.

Note also that in $P_{d\alpha}^2$ Parseval's Theorem is valid, as follows.

6. For any $p \in \mathbf{P}$, $\langle p, p \rangle_{d\alpha} = \sum_{n=0}^{d-1} \langle p, q_n^\alpha \rangle_{d\alpha}^2$.

For later reference, we summarize some of these remarks as propositions.

PROPOSITION 2.2.2 *Let $\alpha \in \mathcal{H}_{+,1}$ have d points of increase. For $0 \leq n \leq d-1$, q_n^α is characterized as being the unique member of $\mathbf{P}$ with the following properties:*

(i) *q_n^α has precise degree n;*

(ii) *$q_n^\alpha \perp \mathbf{P}_{n-1}$ with respect to $\langle \cdot, \cdot \rangle_{d\alpha}$;*

(iii) *$\langle q_n^\alpha, q_n^\alpha \rangle_{d\alpha} = 1$ and the leading coefficient of q_n^α has sign $(-1)^n$.*

Alternatively, we can replace property (iii) with

(iii)$'$ *$\langle q_n^\alpha, q_n^\alpha \rangle_{d\alpha} = 1$ and $\langle q_n^\alpha, (-x)^n \rangle_{d\alpha} > 0$.*

The polynomial q_d^α satisfies $q_d^\alpha \propto p_\alpha$. In the case of a p.d.f. α (with moments) having infinite range, properties (i),(ii),(iii) (or, (i),(ii),(iii)$'$) characterize q_n^α without upper bound on n.

PROPOSITION 2.2.3 *Let $\alpha \in \mathcal{H}_{+,1}$ have d points of increase. Then $\langle x q_n^\alpha, q_{n+1}^\alpha \rangle_{d\alpha} < 0$ for each n in the range $0 \leq n \leq d-2$, and $\langle x q_n^\alpha, q_{n+1}^\alpha \rangle_{d\alpha} = 0$ for $n \geq d-1$. If α is a p.d.f. having moments whose range is infinite, then $\langle x q_n^\alpha, q_{n+1}^\alpha \rangle_{d\alpha} < 0$ holds for all $n \geq 0$. For any p.d.f. α having moments, $\langle x q_i^\alpha, q_j^\alpha \rangle_{d\alpha} = 0$ if $|i-j| \geq 2$.*

Proof. Suppose that $\alpha \in \mathcal{H}_{+,1}$ has d points of increase and $0 \leq n \leq d-2$. Observe that $x q_n^\alpha \propto x(-x)^n + p$ for some $p \in \mathbf{P}_n$. Thus

$$\begin{aligned} \langle x q_n^\alpha, q_{n+1}^\alpha \rangle_{d\alpha} &\propto \langle x(-x)^n, q_{n+1}^\alpha \rangle_{d\alpha} + \langle p, q_{n+1}^\alpha \rangle_{d\alpha} \\ &= -\langle (-x)^{n+1}, q_{n+1}^\alpha \rangle_{d\alpha} \\ &< 0. \end{aligned}$$

The last inequality follows by property 5. We know that for $n \geq d-1$ $\langle q_{n+1}^\alpha, q_{n+1}^\alpha \rangle_{d\alpha} = 0$. It follows that for any $p \in \mathbf{P}$, $\langle p, q_{n+1}^\alpha \rangle_{d\alpha} = 0$, and in particular for $p = x q_n^\alpha$.

If α has infinite range then the same reasoning as in the finite case shows that $\langle xq_n^\alpha, q_{n+1}^\alpha \rangle_{d\alpha} < 0$ holds for all $n \geq 0$. Finally, it follows readily from property 2 that $\langle xq_i^\alpha, q_j^\alpha \rangle_{d\alpha} = 0$ if $|i-j| \geq 2$ for any p.d.f. α having moments. ∎

Oscillation of orthogonal polynomials I

Let $a = (a_1, \ldots, a_d)$ be a real-valued sequence. For l, r satisfying $1 \leq l < r \leq d$, we say that a has a *sign change* from a_l to a_r if: $a_l a_r < 0$, and for any i in the range $l < i < r$, $a_i = 0$. We say that l is the *left index*, and r is the *right index*, of the sign change.

PROPOSITION 2.2.4 *Let $\alpha \in \mathcal{H}_{+,1}$ have d points of increase $\lambda_1 < \ldots < \lambda_d$. Then for every n in the range $0 \leq n \leq d-1$, the sequence*

$$q_n^\alpha(\lambda_1), \ldots, q_n^\alpha(\lambda_d)$$

has precisely n sign changes.

Proof. The sequence $q_n^\alpha(\lambda_1), \ldots, q_n^\alpha(\lambda_d)$ exhibits at most n sign changes since q_n^α has degree n.

Let $l_1 < \ldots < l_j$ and $r_1 < \ldots < r_j$ be the left and right indices respectively corresponding to the sign changes of $q_n^\alpha(\lambda_1), \ldots, q_n^\alpha(\lambda_d)$. Then

$$l_1 < r_1 \leq l_2 < r_2 \leq \ldots \leq l_j < r_j.$$

Now for each i $(1 \leq i \leq j)$, choose x_i such that $l_i < x_i < r_i$ and $x_i \notin \{\lambda_1, \ldots, \lambda_d\}$. Set

$$p(x) = \prod_{i=1}^{j} (x - x_i).$$

Then by construction the sequence $q_n^\alpha(\lambda_1)p(\lambda_1), \ldots, q_n^\alpha(\lambda_d)p(\lambda_d)$ has constant sign. Also, $q_n^\alpha(\lambda_i)p(\lambda_i) = 0$ only if $q_n^\alpha(\lambda_i) = 0$; since $n < d$ this implies that for at least one i, $q_n^\alpha(\lambda_i)p(\lambda_i) \neq 0$. It follows that $\langle q_n^\alpha, p\rangle_{d\alpha} \neq 0$. Recall that $q_n^\alpha \perp P_{n-1}$, so $p \notin P_{n-1}$. That is, the degree j of p is at least n, so q_n^α has at least n sign changes. ∎

Let $p, q \in \mathbf{P}$ each have all real, distinct roots. (Although the roots of p need not be distinct from those of q.) Suppose that p, q have degrees $i < j$ respectively. Let $r_1 < \ldots < r_i$ denote the roots of p. If each of the $i + 1$ open intervals

$$(-\infty, r_1), (r_1, r_2), \ldots, (r_{i-1}, r_i), (r_i, \infty)$$

contains a root of q, then we say that the roots of p *interlace* with the roots of q.

If $\alpha \in \mathcal{H}_{+,1}$ has d points of increase, we have seen already that $q_d^\alpha \propto p_\alpha$, which implies that the roots of q_d^α are real and distinct. It follows immediately from Proposition 2.2.4 that: for $1 \leq n \leq d - 1$, the zeros of q_n^α are real and distinct, and the roots of q_n^α interlace with those of q_d^α.

2.3 Analysis of Jacobi matrices

The matrix generated by a distribution

Let 0_∞ denote the (one-way) infinite zero matrix

$$0_\infty = \begin{pmatrix} 0 & 0 & \cdots \\ 0 & 0 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$

Definition. Let α be a p.d.f. having moments. Set $\tilde{J}_\alpha$ to be the infinite matrix defined by $\tilde{J}_\alpha(i,j) = \langle x q^\alpha_{i-1}, q^\alpha_{j-1} \rangle_{d\alpha}$ for $i,j \geq 1$. (Note the shift in index from the left to the right side of the equation.) Proposition 2.2.3 shows that there are two cases. If α has infinite range then $\tilde{J}_\alpha$ is an infinite Jacobi matrix. In this case set $J_\alpha = \tilde{J}_\alpha$. If α has finite range and hence a finite number, d, of jump points, then $\tilde{J}_\alpha = J \oplus 0_\infty$, where J is a $d \times d$ Jacobi matrix. In this case set $J_\alpha = J$. In either case we define J_α to be the *Jacobi matrix generated by* α. We reserve the notation J_α for this purpose.

Let $\alpha \in \mathcal{H}_{+,1}$ and write $\alpha(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n)$, with d minimal. Set $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$, $W = \mathrm{diag}(w_1, \ldots, w_d)$, and

$$Q = \begin{pmatrix} q^\alpha_0(\lambda_1) & \cdots & q^\alpha_0(\lambda_d) \\ q^\alpha_1(\lambda_1) & \cdots & q^\alpha_1(\lambda_d) \\ \vdots & & \vdots \\ q^\alpha_{d-1}(\lambda_1) & \cdots & q^\alpha_{d-1}(\lambda_d) \end{pmatrix}.$$

Then it follows immediately from the definition that $J_\alpha = Q\Lambda W Q^t$. Now write $W^{1/2}$ for the positive definite square root of W (i.e. $W^{1/2} = \mathrm{diag}(w_1^{1/2}, \ldots, w_d^{1/2})$), and set

$O = QW^{1/2}$. Then, since $q_0^\alpha, \ldots, q_{d-1}^\alpha$ is an orthonormal sequence with respect to $\langle \cdot, \cdot \rangle_{d\alpha}$, O is an orthogonal matrix, and the factorization

$$J_\alpha = O\Lambda O^t \tag{2.4}$$

is an orthogonal diagonalization of J_α. Therefore, for every $n \geq 0$, $J_\alpha^n = O\Lambda^n O^t$, or equivalently, $J_\alpha^n = Q\Lambda^n W Q^t$. The latter formula translates into integral notation to yield

$$J_\alpha^n(i,j) = \int_{-\infty}^{\infty} x^n q_{i-1}^\alpha q_{j-1}^\alpha \, d\alpha \quad (n \geq 0). \tag{2.5}$$

If J_α is non-singular then (2.5) is valid also for negative n; in particular

$$J_\alpha^{-1}(i,j) = \int_{-\infty}^{\infty} x^{-1} q_{i-1}^\alpha q_{j-1}^\alpha \, d\alpha.$$

Note that the factorization (2.4) shows that the eigenvalues of J_α are precisely the jump points of α. In other words, *the characteristic polynomial of J_α is precisely p_α, the characteristic polynomial of α.*

PROPOSITION 2.3.1 *Suppose that two p.d.f.s α, β generate the same finite-dimensional Jacobi matrix. Then $\alpha = \beta$.*

Proof. By hypothesis, $J_\alpha = J_\beta$ is finite-dimensional. Therefore α and β both have finite range, and $p_\alpha = p_\beta$. This implies that α and β have the same jump points; label these as $\lambda_1 < \ldots < \lambda_d$. Write $\alpha(x) = \sum_{n=1}^d v_n H(x - \lambda_n)$ and $\beta(x) = \sum_{n=1}^d w_n H(x - \lambda_n)$. By formula (2.5), for each $n \geq 0$,

$$\int_{-\infty}^{\infty} x^n \, d\alpha = J_\alpha^n(1,1) = J_\beta^n(1,1) = \int_{-\infty}^{\infty} x^n \, d\beta.$$

Thus for any polynomial $p \in \mathbf{P}$, $\int_{-\infty}^{\infty} p\, d\alpha = \int_{-\infty}^{\infty} p\, d\beta$. For $1 \leq n \leq d$, set χ_n to be the unique polynomial of degree $d-1$ such that $\chi_n(\lambda_i) = \delta_{ni}$ $(1 \leq i \leq d)$. Then $v_n = \int_{-\infty}^{\infty} \chi_n\, d\alpha = \int_{-\infty}^{\infty} \chi_n\, d\beta = w_n$ which proves $\alpha = \beta$. ∎

The above proposition says that the p.d.f. which generates a finite dimensional Jacobi matrix is unique, provided it exists.[2] But is every Jacobi matrix realized as the matrix generated by a p.d.f.? The answer is yes, for both finite and infinite dimensional Jacobi matrices. We show this for the case of finite dimensional Jacobi matrices in the next subsection.

Every finite Jacobi matrix comes from a distribution

Let J be an arbitrary finite dimensional Jacobi matrix, to be fixed throughout this subsection. Write

$$J = \begin{pmatrix} a_1 & -b_1 & 0 & \dots & 0 \\ -b_1 & a_2 & -b_2 & \ddots & \vdots \\ 0 & -b_2 & a_3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -b_{d-1} \\ 0 & \dots & 0 & -b_{d-1} & a_d \end{pmatrix}.$$

In order to construct a p.d.f. which generates J, note first that J is orthogonally diagonalizable, since it is symmetric. Thus write $J = O\Lambda O^t$ where $OO^t = I$ and $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_d)$. Let r^n denote the nth row of O, so that $J(i,j) = \langle r^i \Lambda, r^j \rangle$

[2]The corresponding statement fails for infinite dimensional Jacobi matrices, a fact which lies at the heart of the classical moment problem; see Freud [F].

where $\langle \cdot, \cdot \rangle$ denotes the standard inner product on $\mathbf{R}^d$. Set $r^0 = (0, 0, \ldots, 0)$, and, for $1 \leq n \leq d-1$, consider the vector

$$\begin{aligned} v &= -r^n\Lambda + \langle r^n\Lambda, r^n\rangle r^n + \langle r^n\Lambda, r^{n-1}\rangle r^{n-1} \\ &= -r^n\Lambda + a_n r^n - b_{n-1}r^{n-1}. \end{aligned}$$

Using the identity $J = O\Lambda O^t$, straightforward calculation reveals that $\langle v, r^i\rangle = b_n\delta_{n+1,i} = b_n\langle r^{n+1}, r^i\rangle$ for $1 \leq i \leq d$. It follows that $v = b_n r^{n+1}$, since $\{r^1, \ldots, r^d\}$ is an orthonormal basis for $\mathbf{R}^d$ (with the standard inner product). Thus, for $1 \leq n \leq d-1$,

$$b_n r^{n+1} = -r^n\Lambda + a_n r^n - b_{n-1}r^{n-1}. \tag{2.6}$$

Iteration of the recurrence (2.6) shows that if some entry, say the ith, of r^1 is 0, then the ith entry of each successive r^n is 0 also. This cannot be: since $\{r^1, \ldots, r^d\}$ is a linearly independent set, $r^1, \ldots, r^d$ cannot have a common entry be zero. Therefore each entry of r^1 is non-zero, and the matrix $\text{diag}(r^1)$ is invertible.

For each n in the range $0 \leq n \leq d$, set $s^n = r^n(\text{diag}(r^1))^{-1}$. Then $s^0 = (0.0, \ldots, 0)$, $s^1 = (1, 1, \ldots, 1)$, and for $1 \leq n \leq d-1$,

$$b_n s^{n+1} = -s^n\Lambda + a_n s^n - b_{n-1}s^{n-1}. \tag{2.7}$$

Let W denote the matrix $(\text{diag}(r^1))^2$, and write $W = \text{diag}(w_1, \ldots, w_d)$. Observe that

$$\begin{aligned} \langle s^i\Lambda, s^jW\rangle &= \langle r^i\Lambda, r^j\rangle = J(i,j), \\ \langle s^i, s^jW\rangle &= \langle r^i, r^j\rangle = \delta_{ij}, \end{aligned} \tag{2.8}$$

for $1 \leq i, j \leq d$. Set

$$\alpha(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n).$$

Note that α is a p.d.f. since each $w_n > 0$ and $\sum w_n = 1$. To show that α generates J, we first argue that the eigenvalues $\lambda_1, \ldots, \lambda_d$ are distinct. Let D be the number of distinct eigenvalues, so that $\langle \cdot, \cdot \rangle_{d\alpha}$ is an inner product on $\mathbf{P}_{D-1}$. The recurrence (2.7) shows that if two eigenvalues λ_i, λ_j coincide, then the corresponding i^{th} and j^{th} enties of each s^n coincide. Thus for each n, $1 \leq n \leq d$, there is a unique polynomial $q_{n-1} \in \mathbf{P}_{D-1}$ which satisfies: $q_{n-1}(\lambda_i) =$ the ith entry of s^n $(1 \leq i \leq d)$. (Note the shift in index between the left and right sides of this equation.) Set $q_{-1} = 0$. Observe that with this definition,

$$\langle s^i, s^j W \rangle = \langle q_{i-1}, q_{j-1} \rangle_{d\alpha},$$
$$\langle s^i \Lambda, s^j W \rangle = \langle x q_{i-1}, q_{j-1} \rangle_{d\alpha}.$$

Now (2.8) shows that $q_0, \ldots, q_{d-1}$ are orthogonal in $\mathbf{P}_{D-1}$ with respect to $\langle \cdot, \cdot \rangle_{d\alpha}$, so $D = d$ and the eigenvalues of J are distinct. Furthermore $\langle x q_{i-1}, q_{j-1} \rangle_{d\alpha} = J(i, j)$.

It remains to show that $q_n = q_n^\alpha$ before we can conclude that J is the Jacobi matrix generated by α. Note that the polynomials $q_0, \ldots, q_{d-1}$ satisfy the "same" recurrence as $s^1, \ldots, s^d$:

$$b_n q_n = -x q_{n-1} + a_n q_{n-1} - b_{n-1} q_{n-2} \qquad (1 \leq n \leq d-1). \tag{2.9}$$

Iteration of (2.9) shows that each q_n has precise degree n, and the leading coefficient of q_n has sign $(-1)^n$. Since $q_0, \ldots, q_{d-1}$ are orthonormal with respect to $\langle \cdot, \cdot \rangle_{d\alpha}$, this suffices to prove that $q_n = q_n^\alpha$ $(0 \leq n \leq d-1)$, by Proposition 2.2.2. Therefore J is the Jacobi matrix generated by α. To summarize, we have proved the following. (Note that we incorporate the uniqueness result of Proposition 2.3.1.)

PROPOSITION 2.3.2 *Every finite dimensional Jacobi matrix is realized as the Jacobi matrix generated by a unique p.d.f.*

Oscillation of orthogonal polynomials II

Let J be a $d \times d$ Jacobi matrix,

$$J = \begin{pmatrix} a_1 & -b_1 & 0 & \dots & 0 \\ -b_1 & a_2 & -b_2 & \ddots & \vdots \\ 0 & -b_2 & a_3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -b_{d-1} \\ 0 & \dots & 0 & -b_{d-1} & a_d \end{pmatrix}.$$

We write J_n to denote the $n \times n$ leading, principal submatrix of J. Thus $J_1 = a_1$,

$$J_2 = \begin{pmatrix} a_1 & -b_1 \\ -b_1 & a_2 \end{pmatrix},$$

and $J_d = J$. For $1 \leq n \leq d$, set $p_n(x) = \det(J_n - xI)$ to be the characteristic polynomial of J_n. Set $p_{-1} = 0$ and $p_0 = 1$. The Laplace expansion for $\det(J_n - xI)$ along the bottom row of $J_n - xI$ leads immediately to the recurrence

$$p_n = (a_n - x)p_{n-1} - b_{n-1}^2 p_{n-2} \qquad (1 \leq n \leq d-1). \tag{2.10}$$

For n in the range $1 \leq n \leq d-1$, set $q_n = p_n/(b_1 \cdots b_n)$; set $q_{-1} = 0, q_0 = 1$. In terms of the q_n the recurrence (2.10) becomes

$$b_n q_n = -xq_{n-1} + a_n q_{n-1} - b_{n-1} q_{n-2} \qquad (1 \leq n \leq d-1).$$

In the previous section we showed that the polynomials $q_0^\alpha, \dots, q_{d-1}^\alpha$ satisfy precisely this recurrence (see (2.9)) where α is the p.d.f. which generates J.

Given that $q_{-1} = 0$ and $q_0 = 1$, the above recurrence uniquely determines $q_1, \ldots, q_{d-1}$. It follows that

$$q_n^\alpha = \frac{1}{b_1 \cdots b_n} p_n \qquad (1 \leq n \leq d-1).$$

Thus q_n^α *is determined, up to multiplication by a positive scalar, by the submatrix* J_n *of* J, *and determined completely by the submatrix* J_{n+1}.

PROPOSITION 2.3.3 *Let* $\alpha \in \mathcal{H}_{+,1}$ *have* d *points of increase. If* $0 \leq i < j \leq d$ *then the roots of* q_i *interlace with the roots of* q_j. *If* α *is a p.d.f. with infinite range (having moments), then the roots of* q_i *and* q_j *interlace for any* $0 \leq i < j$.

Proof. Consider the leading principal submatrix J_j of J_α. The matrix J_j is generated by a unique distribution function $\beta \in \mathcal{H}_{+,1}$. Proposition 2.2.4 shows that the roots of q_i^β and q_j^β interlace. But $q_i^\alpha = q_i^\beta$, since $(J_\alpha)_{i+1} = (J_j)_{i+1}$. And $q_j^\alpha \propto q_j^\beta$, since $(J_\alpha)_j = J_j$. Therefore the roots of q_i^α interlace with the roots of q_j^α. ∎

A note on infinite Jacobi matrices

We established the formula (2.5) for finite-dimensional Jacobi matrices. In this subsection we show that it is valid also for infinite Jacobi matrices.

LEMMA 2.3.4 *Let* $N \geq 1$, *and let* α, β *be p.d.f.s having moments, with at least* $N+1$ *points of increase. If* $q_n^\alpha = q_n^\beta$ *for every* n *in the range* $0 \leq n \leq N$, *then for any* $p \in \mathbf{P}_{2N}$, $\int_{-\infty}^{\infty} p \, d\alpha = \int_{-\infty}^{\infty} p \, d\beta$.

Proof. For any $q, r \in \mathbf{P}_N$, we can write

$$q = \sum_{n=0}^{N} c_n q_n^\alpha = \sum_{n=0}^{N} c_n q_n^\beta,$$
$$r = \sum_{n=0}^{N} d_n q_n^\alpha = \sum_{n=0}^{N} d_n q_n^\beta,$$

so that $\langle q, r\rangle_{d\alpha} = \sum_{n=0}^{N} c_n d_n = \langle q, r\rangle_{d\beta}$. Now, let $p \in \mathbf{P}_{2N}$ be arbitrary. Note that p can be written in the form $p = x^N p_1 + p_2$ where $p_1, p_2 \in \mathbf{P}_N$. Then

$$\begin{aligned}\int_{-\infty}^{\infty} p\, d\alpha &= \langle x^N, p_1\rangle_{d\alpha} + \langle 1, p_2\rangle_{d\alpha} \\ &= \langle x^N, p_1\rangle_{d\beta} + \langle 1, p_2\rangle_{d\beta} \\ &= \int_{-\infty}^{\infty} p\, d\beta,\end{aligned}$$

as desired. ∎

PROPOSITION 2.3.5 *Let α be a p.d.f. having moments. Then*

$$J_\alpha^n(i,j) = \int_{-\infty}^{\infty} x^n q_{i-1}^\alpha q_{j-1}^\alpha \, d\alpha \qquad (n \geq 0).$$

Proof. Fix i, j, n and choose $N \geq \max\{i, j, (n+i+j)/2\}$ sufficiently large that the entry $J_\alpha^n(i,j)$ is determined by the submatrix $(J_\alpha)_N$ of J_α; i.e. so that $((J_\alpha)_N)^n(i,j) = J_\alpha^n(i,j)$. (It is easy to see that in fact $N = \max\{i,j\}+n-1$ will do.) Let $\beta \in \mathcal{H}_{+,1}$ be the p.d.f. which generates $(J_\alpha)_N$. Then $q_n^\alpha = q_n^\beta$ for $0 \leq n \leq N-1$, so $x^n q_{i-1}^\alpha q_{j-1}^\alpha = x^n q_{i-1}^\beta q_{j-1}^\beta$. Also, $\deg(x^n q_{i-1}^\alpha q_{j-1}^\alpha) \leq 2N$. Thus

$$\begin{aligned}J_\alpha^n(i,j) &= J_\beta^n(i,j) \\ &= \int_{-\infty}^{\infty} x^n q_{i-1}^\beta q_{j-1}^\beta \, d\beta \quad \text{by (2.5)} \\ &= \int_{-\infty}^{\infty} x^n q_{i-1}^\alpha q_{j-1}^\alpha \, d\beta \\ &= \int_{-\infty}^{\infty} x^n q_{i-1}^\alpha q_{j-1}^\alpha \, d\alpha,\end{aligned}$$

the last equality by Lemma 2.3.4. ∎

Let α be an arbitrary p.d.f. having moments, so that J_α is either finite or infinite dimensional. Then Proposition 2.3.5 shows that $m(J, 1, 1) = (m_0, m_1, m_2, \ldots)$ is precisely the so-called *moment sequence of* α; that is, $m_n = \int_{-\infty}^{\infty} x^n \, d\alpha$ for all $n \geq 0$. (Recall that unless J is explicitly allowed to be infinite—as we have done here—the notation $m(J, i, j)$ is restricted to finite dimensional Jacobi matrices J.)

2.4 Revised problem statement

Given $\gamma \in \mathcal{H}$, write $m(d\gamma)$ to denote the *moment sequence* $(m_0, m_1, m_2, \ldots)$ defined by $m_n = \int_{-\infty}^{\infty} x^n \, d\gamma$. We make the convention that whenever the notation $m(d\gamma)$ is used, it means that γ is a d.f. with finite range, unless the contrary is explicitly stated. Observe that, by the formula (2.5), if $\alpha \in \mathcal{H}_{+,1}$ then

$$m(q_{i-1}^{\alpha} q_{j-1}^{\alpha} \, d\alpha) = m(J_\alpha, i, j). \tag{2.11}$$

LEMMA 2.4.1 *Let $\gamma \in \mathcal{H}$. If $q \in \mathbf{P}$ has the property that for every $p \in \langle q \rangle$, $\int_{-\infty}^{\infty} p \, d\gamma = 0$, then $q \in \langle p_\gamma \rangle$.*

Proof. The case $\gamma = 0$ is vacuous; assume $\gamma \neq 0$. We will show that if $q \notin \langle p_\gamma \rangle$ then there exists $p \in \langle q \rangle$ such that $\int_{-\infty}^{\infty} p \, d\gamma \neq 0$. If $q \notin \langle p_\gamma \rangle$ then $q(\lambda_n) \neq 0$ for some jump point λ_n of γ. Set $r(x) = p_\gamma(x)/(\lambda_n - x)$. Then $\int_{-\infty}^{\infty} qr \, d\gamma = w_n q(\lambda_n) r(\lambda_n) \neq 0$, but $qr \in \langle q \rangle$. ∎

PROPOSITION 2.4.2 *Let $\gamma \in \mathcal{H}$. The sequence $m(d\gamma)$ determines γ uniquely.*

Proof. The sequence $m(d\gamma)$ determines the value $\int_{-\infty}^{\infty} p \, d\gamma$ for every $p \in \mathbf{P}$. It follows from Lemma 2.4.1 that $\mathcal{I} = \langle p_\gamma \rangle$ is the unique ideal maximal with respect to the property that for every $p \in \mathcal{I}$, $\int_{-\infty}^{\infty} p \, d\gamma = 0$. Thus $m(d\gamma)$ determines p_γ, and hence the jump points of γ. If $p_\gamma \equiv 1$ then $\gamma = 0$; otherwise we may write

$$\gamma(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n),$$

with d minimal. For each n in the range $1 \leq n \leq d$, consider the polynomial χ_n characterized by: $\chi_n \in \mathbf{P}_{d-1}$; $\chi_n(\lambda_i) = \delta_{ni}$ for $1 \leq i \leq n$. Note that $w_n = \int_{-\infty}^{\infty} \chi_n \, d\gamma$, enabling us to construct γ. ∎

We now give a reformulation of the central problem considered in this thesis. The fact that a p.d.f. $\beta \in \mathcal{H}_{+,1}$ uniquely determines J_β, together with Proposition 2.4.2 and the formula (2.11), show that the following statement is equivalent to the original version, given on page 7.

Main Problem (Version 2). *Given the d.f. corresponding to the distribution* $q_i^\alpha q_j^\alpha \, d\alpha$, *where* $\alpha \in \mathcal{H}_{+,1}$, *determine all p.d.f.s* $\beta \in \mathcal{H}_{+,1}$ *such that for some* k, l

$$q_k^\beta q_l^\beta \, d\beta \propto q_i^\alpha q_j^\alpha \, d\alpha. \tag{2.12}$$

As with the original version, we call a distribution satisfying (2.12) a *solution* to the given problem, and the set of all solutions is denoted $\mathcal{S}(q_i^\alpha q_j^\alpha \, d\alpha)$.

Definition. Write $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$. We say that a solution β to the above problem is *regular*, if β is absolutely continuous with respect to γ (i.e. if $\beta \ll \gamma$). We denote the set of regular solutions by $\mathcal{S}_{\text{reg}}(d\gamma)$.

It does not follow immediately from this definition that $\mathcal{S}_{\text{reg}}(d\gamma) \neq \emptyset$. We prove later that in general regular solutions do exist, so that $\mathcal{S}_{\text{reg}}(q_i^\alpha q_j^\alpha \, d\alpha)$ corresponds exactly to $\mathcal{S}_{\min}(J_\alpha, i+1, j+1)$, the set of least dimensional solutions to Version 1 of the main problem. Version 2 will serve as our working formulation; *beyond this point, all unqualified references to the main problem refer to Version 2.* Our objective for this thesis is to describe $\mathcal{S}_{\text{reg}}(q_i^\alpha q_j^\alpha \, d\alpha)$ as a manifold, for arbitrary α, i, j.

Chapter 3

The manifold of regular solutions to the main problem

3.1 Integers determined by the given distribution function

The "known data" in the main problem (as stated at the end of the previous chapter) is a d.f. having finite range. This d.f. determines three useful integer quantities which bear directly on the qualitative structure of the manifold of regular solutions, and which make for convenient division of the problem into cases. Let $\gamma \in \mathcal{H}$ denote the d.f. given in the main problem. According to the statement of the problem, γ corresponds to a distribution of the form $q_i^\alpha q_j^\alpha \, d\alpha$, for some $\alpha \in \mathcal{H}_{+,1}$. This means simply that γ satisfies $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$, and of course this defines γ uniquely. Henceforth in this section, γ plays the role of the "known" distribution given in the main problem, and α denotes the associated p.d.f.

The number d of jump points

It is possible for q_i^α or q_j^α to have a root in common with p_α (the characteristic polynomial of α). In this case γ has strictly fewer jump points than α, so that $\alpha \not\ll \gamma$. We write d, or possibly d_γ, for the number of jump points of γ. Note that the value d characterizes a regular solution: a solution β to the main problem is regular precisely if β has d jump points.

The number σ of sign changes in the coefficients

Write

$$\gamma(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n),$$

such that d is minimal and $\lambda_1 < \lambda_2 < \ldots < \lambda_d$. We denote by σ, or possibly σ_γ, the number of sign changes in the sequence $w_1, \ldots, w_d$. Thus, as with d, the value σ can be read off directly from γ.

The degree Δ of orthogonality

In this subsection we refer explicitly to the indices i, j in the representation $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$. To begin, let $n \geq 0$ be less than the number of jump points of the p.d.f. α, and recall that if $p \in \mathbf{P}_n$ has exact degree n then

$$\int_{-\infty}^{\infty} p q_n^\alpha \, d\alpha \neq 0.$$

Also, for every $p \in \mathbf{P}_{n-1}$, $\int_{-\infty}^{\infty} pq_n^\alpha \, d\alpha = 0$. (Here we make the convention that 0 is the unique polynomial of degree -1, and we write $\mathbf{P}_{-1} = \{0\}$.) Now, note that if $p \in \mathbf{P}_{|i-j|}$ has exact degree $|i-j|$, then

$$\int_{-\infty}^{\infty} pq_i^\alpha q_j^\alpha \, d\alpha = \int_{-\infty}^{\infty} p \, d\gamma \neq 0;$$

and if $p \in \mathbf{P}_{|i-j|-1}$ then

$$\int_{-\infty}^{\infty} pq_i^\alpha q_j^\alpha \, d\alpha = \int_{-\infty}^{\infty} p \, d\gamma = 0.$$

Based on these observations we define Δ, or for emphasis Δ_γ, to be the largest integer such that for every $p \in \mathbf{P}_{\Delta-1}$, $\int_{-\infty}^{\infty} p \, d\gamma = 0$. In other words, Δ is the degree of the first non-zero moment of $d\gamma$. We call Δ the *degree of orthogonality* of γ. And by design, $\Delta = |i-j|$. In general it is not possible to determine either i or j, given γ (where, as above, $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$). But it is always possible to determine the difference $|i-j| = \Delta$.

Basic inequalities among these integers

The values d, σ, Δ satisfy the inequalities

$$0 \leq \Delta \leq \sigma < d. \tag{3.1}$$

It follows immediately from the definition that $\Delta = |i-j| \geq 0$. It also follows from the definition that $\sigma < d$, since a sequence $w_1, \ldots, w_d$ of d terms cannot have more than $d-1$ sign changes. Finally, one can easily construct a polynomial p of degree σ such that

$$\int_{-\infty}^{\infty} p \, d\gamma \neq 0$$

(this is done in the proof of Proposition 2.2.4). Therefore $\Delta \leq \sigma$, and the statement (3.1) is proved.

Note that if $\Delta = 0$ then $i = j$ and so $d\gamma$ has the form $d\gamma = (q_i^\alpha)^2\, d\alpha$. It follows that the coefficients $w_1, \ldots, w_d$ in the representation

$$\gamma(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n)$$

are all positive (and hence do not change sign) making $\sigma = 0$. Thus if $\Delta = 0$ then $\sigma = 0$ follows automatically. Moreover, in this case

$$\int_{-\infty}^{\infty} d\gamma = \int_{-\infty}^{\infty} (q_i^\alpha)^2\, d\alpha = 1,$$

(since q_i^α is normalized in $P_{d\alpha}^2$) which shows that γ is a p.d.f.

3.2 General solution for the case $\Delta = 0$

The composite polynomial of a distribution function

In Section 2.2 we defined the characteristic polynomial p_γ of a d.f. $\gamma \in \mathcal{H}$. (Recall that in the special case of a p.d.f. $\alpha \in \mathcal{H}_{+,1}$, the characteristic polynomial p_α of α coincides with the characteristic polynomial—in the usual sense—of the Jacobi matrix generated by α.) A second polynomial associated to γ plays a pivotal role in partially solving the main problem of this thesis.

Definition. Write

$$\gamma(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n)$$

with d minimal. Define $p^\gamma \in \mathbf{P}_{d-1}$ to be the (unique) interpolator of the values $w_n p'_\gamma(\lambda_n)$ at λ_n $(1 \leq n \leq d)$, where p'_γ denotes the derivative of p_γ. We call p^γ the *composite polynomial* of γ, and reserve the notation p^γ for this purpose.[1]

Observe that p^γ has the representation

$$p^\gamma(x) = \sum_{n=1}^{d} w_n p_\gamma(x)/(x - \lambda_n),$$

which is easily verified by evaluating the latter expression at each λ_n.

[1]The reason for the name "composite polynomial" lies in the fact that solutions to the main problem will be seen to come ultimately from divisors of $p^\gamma \pmod{p_\gamma}$.

A technical lemma

The key to solving the case $\Delta = 0$ of the main problem is the following somewhat technical fact.

LEMMA 3.2.1 *Let q be a polynomial of degree n which has no repeated roots, and let $\gamma \in \mathcal{H}$. Then*

$$\int_{-\infty}^{\infty} pq^{-1}\, d\gamma = 0 \text{ for all } p \in \mathbf{P}_{n-1} \tag{3.2}$$

if and only if q divides p^γ.

Proof. It is convenient to consider the space $\mathbf{P}^{\mathbf{C}}$ of complex valued polynomials of a real variable. (As with real valued polynomials, we write $\mathbf{P}_k^{\mathbf{C}}$ to denote the subspace of $\mathbf{P}^{\mathbf{C}}$ consisting of polynomials having degree at most k.) Note that (3.2) is equivalent to

$$\int_{-\infty}^{\infty} pq^{-1}\, d\gamma = 0 \text{ for all } p \in \mathbf{P}_{n-1}^{\mathbf{C}}, \tag{3.3}$$

where the latter integral is complex valued. The given polynomial q can be written in the form

$$q(x) = a \prod_{k=1}^{n} (z_k - x)$$

where $a \neq 0$ is a scalar, and $z_1, \ldots, z_n$ are its distinct (complex) roots. Now, observe that the n distinct polynomials $q_1, \ldots, q_n$, defined by

$$q_k(x) = q(x)/(z_k - x) \quad (1 \leq k \leq n),$$

span $\mathbf{P}_{n-1}^{\mathbf{C}}$. Thus (3.3) is equivalent to

$$\int_{-\infty}^{\infty} q_k q^{-1}\, d\gamma = \int_{-\infty}^{\infty} \frac{d\gamma}{z_k - x} = 0 \text{ for each } k, \text{ where } 1 \leq k \leq n. \tag{3.4}$$

Write $\gamma(x) = \sum_{k=1}^{d} w_k H(x - \lambda_k)$ with d minimal, and let z be an arbitrary complex number. Then

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{d\gamma}{z-x} &= \sum_{k=1}^{d} \frac{w_k}{z-\lambda_k} \\ &= \frac{1}{p_\gamma(z)} \sum_{k=1}^{d} \frac{w_k p_\gamma(z)}{z-\lambda_k} \\ &= p^\gamma(z)/p_\gamma(z).\end{aligned}$$

It follows from the definition of the composite polynomial that $p^\gamma(\lambda_k) \neq 0$ for each k $(1 \leq k \leq d)$, so p^γ and p_γ have no common root, and

$$\int_{-\infty}^{\infty} \frac{d\gamma}{z-x} = 0 \quad \Longleftrightarrow \quad p^\gamma(z) = 0.$$

Thus (3.4) is equivalent to: $p^\gamma(z_k) = 0$ for each root z_k of the polynomial q. ∎

The proof actually shows that Lemma 3.2.1 is valid even if the polynomial q is allowed to be complex valued. We will apply the lemma with q complex valued later, in the proof of Lemma 3.3.2.

The main result

THEOREM 3.2.2 *Let $\gamma \in \mathcal{H}_{+,1}$. A p.d.f. β satisfies $(q_i^\beta)^2\, d\beta = d\gamma$ for some i if and only if*

$$d\beta \propto q^{-2}\, d\gamma + d\beta_0$$

for some monic divisor q of p^γ and some $\beta_0 \in \mathcal{H}_+ \cup \{0\}$ whose jump points occur at roots of q.

Proof. ($\Longrightarrow$) Suppose that $(q_i^\beta)^2\, d\beta = d\gamma$. Write $\beta = \beta_1 + \beta_0$ where $\beta_1 \ll \gamma$ and $\beta_0 \perp \gamma$. Thus the jumps of β_0 occur at zeros of q_i^β and the jumps of β_1 do not, so that

$$q_i^\beta\, d\beta_1 = q_i^\beta\, d\beta$$

and

$$q_i^\beta\, d\beta = (q_i^\beta)^{-1}\, d\gamma.$$

Now, q_i^β has simple zeros and for every $p \in \mathbf{P}_{i-1}$,

$$\int_{-\infty}^{\infty} p q_i^\beta\, d\beta = \int_{-\infty}^{\infty} p (q_i^\beta)^{-1}\, d\gamma = 0,$$

so Lemma 3.2.1 tells us that q_i^β divides p^γ. Furthermore,

$$\begin{aligned} d\beta &= d\beta_1 + d\beta_0 \\ &= (q_i^\beta)^{-2}\, d\gamma + d\beta_0. \end{aligned}$$

Thus $d\beta$ conforms to the second part of the theorem.

($\Longleftarrow$) Suppose conversely that: q is monic of degree i; q divides p^γ; $\beta_0 \in \mathcal{H}_+$ has jump points only at zeros of p^γ; and $d\beta \propto q^{-2}\, d\gamma + d\beta_0$ for some $\beta \in \mathcal{H}_{+,1}$. Note that since $\gamma \in \mathcal{H}_{+,1}$, the zeros of p^γ are real and simple, and therefore so are the zeros of q. Since the jumps of β_0 occur at zeros of q,

$$q\, d\beta_0 = 0$$

and

$$q\, d\beta \propto \pm q^{-1}\, d\gamma.$$

Lemma 3.2.1 implies

$$\int_{-\infty}^{\infty} p q^{-1}\, d\gamma = 0 \quad \text{for all } p \in \mathbf{P}_{i-1}$$

and so

$$\int_{-\infty}^{\infty} pq\, d\beta = 0 \quad \text{for all } p \in \mathbf{P}_{i-1}.$$

Since q has degree i, the latter statement implies $q = rq_i^\beta$ for some real $r \neq 0$. Thus

$$(q_i^\beta)^2\, d\beta \propto d\gamma.$$

But $(q_i^\beta)^2\, d\beta$ is a probability distribution, so in fact $(q_i^\beta)^2\, d\beta = d\gamma$. ∎

There are several comments to be made about this result. Firstly, it is important to note that because $\gamma \in \mathcal{H}_{+,1}$ in the statement of the theorem, p^γ alternates sign at the d_γ jump points of γ and so has exactly $d_\gamma - 1$ simple zeros, one in each open interval determined by the jump points. In the general case (i.e. allowing $\Delta > 0$) the zeros of p^γ are much more difficult to describe. Secondly, the statement of the theorem contains all the information required to actually construct all solutions to the main problem for the case $\Delta = 0$. The construction consists essentially of choosing a subset of the zeros of p^γ (to form the polynomial q), and then choosing an arbitrary non-negative weight for each zero in the subset (to form β_0). Regular solutions to the problem correspond to $\beta_0 = 0$. There are exactly $2^{d_\gamma - 1}$ regular solutions, one for each subset of the zeros of p^γ. Finally, there is a bound on the number of jump points in a singular solution, the maximum possible being $2d_\gamma - 1$. This contrasts with results in control theory; specifically, see Gohberg, Lancaster and Rodman [GLR, Chapter 8] where "dilation" creates solutions (here a matrix, not a d.f.) of unbounded dimension.[2]

[2]Curiously, this bound on the number of jump points that a singular solution can have disappears in the case $\Delta > 0$. See Section 3.7.

An example

In this subsection we choose a particular p.d.f. $\gamma \in \mathcal{H}_{+,1}$, and use Theorem 3.2.2 to calculate explicitly all solutions to the main problem with known data γ. That is, we explicitly calculate the set of all p.d.f.s β such that for some k, $(q_k^\beta)^2\, d\beta \propto d\gamma$.

Set $\gamma(x) = \frac{1}{3}H(x-1) + \frac{1}{3}H(x-2) + \frac{1}{3}H(x-3)$. Then $\Delta_\gamma = 0$ and $\gamma \in \mathcal{H}_{+,1}$. The composite polynomial of γ is easily calculated by hand; it works out to be

$$p^\gamma(x) = -x^2 + 4x - 11/3.$$

The two roots of p^γ are $r_1 = 2 - \frac{1}{\sqrt{3}}$ and $r_2 = 2 + \frac{1}{\sqrt{3}}$. Hence there are four monic divisors of p^γ corresponding to the four subsets of $\{r_1, r_2\}$: $\emptyset, \{r_1\}, \{r_2\}, \{r_1, r_2\}$. Explicitly, we have:

$$q_\emptyset(x) = 1,\ q_{\{r_1\}}(x) = x - r_1,\ q_{\{r_2\}}(x) = x - r_2,\ q_{\{r_1,r_2\}} = -p^\gamma.$$

These four divisors give rise to the four regular solutions to the main problem, by normalizing the d.f.s of the form $q^{-2}\, d\gamma$. Carrying out the calculation yields:

$$\begin{aligned}
\beta_\emptyset &= \gamma, \\
\beta_{\{r_1\}}(x) &= \frac{2+\sqrt{3}}{6}H(x-1) + \frac{1}{3}H(x-2) + \frac{2-\sqrt{3}}{6}H(x-3), \\
\beta_{\{r_2\}}(x) &= \frac{2-\sqrt{3}}{6}H(x-1) + \frac{1}{3}H(x-2) + \frac{2+\sqrt{3}}{6}H(x-3), \\
\beta_{\{r_1,r_2\}}(x) &= \frac{1}{6}H(x-1) + \frac{2}{3}H(x-2) + \frac{1}{6}H(x-3).
\end{aligned}$$

The singular solutions to the main problem are generated by adding to a regular solution an arbitrary d.f. $\beta_0 \in \mathcal{H}_+$ whose jumps are confined to the zeros of the corresponding divisor of p^γ, and then normalizing. Thus there is no singular solution

corresponding to the regular solution $\beta_{\emptyset}$. There is a one parameter family of singular solutions corresponding to $\beta_{\{r_1\}}$; this consists of all p.d.f.s of the form:

$$(1-t)\beta_{\{r_1\}}(x) + tH(x-r_1) \qquad (0 < t < 1).$$

Similarly, there is a one parameter family family of singular solutions corresponding to the regular solution $\beta_{\{r_2\}}$:

$$(1-t)\beta_{\{r_2\}}(x) + tH(x-r_2) \qquad (0 < t < 1).$$

Since $q_{\{r_1,r_2\}}$ has two roots, there is a two parameter family of singular solutions corresponding to $\beta_{\{r_1,r_2\}}$:

$$(1-s-t)\beta_{\{r_1,r_2\}}(x) + sH(x-r_1) + tH(x-r_2) \qquad (0 < s+t < 1, 0 < s, 0 < t).$$

According to Theorem 3.2.2 there are no other solutions; this comprises a complete discription of the set of solutions to the main problem with known data $\gamma(x) = \frac{1}{3}H(x-1) + \frac{1}{3}H(x-2) + \frac{1}{3}H(x-3)$.

3.3 A first look at the case $\Delta > 0$

General approach

Let γ be the "known" d.f. given in the main problem, so that $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$ for some $\alpha \in \mathcal{H}_{+,1}$ and some i, j. If $\alpha \ll \gamma$ then the problem is guaranteed to have a regular solution. But it may happen that a root of either q_i^α or q_j^α coincides with a jump point of α, in which case $\alpha \not\ll \gamma$. In this case how can we be sure that there exists a regular solution to the problem? As a first step in dealing with this question, we establish below a basic strategy to look for solutions. We confine our attention exclusively to regular solutions. As before, γ will continue to play the role of the known d.f. given in the main problem.

Suppose that β is a regular solution to the main problem, so that $q_k^\beta q_l^\beta \, d\beta \propto d\gamma$, for some k, l. We list several straightforward observations:

(i) $q_l^\beta \, d\beta \propto (q_k^\beta)^{-1} \, d\gamma$;

(ii) $q_k^\beta \, d\beta \propto (q_l^\beta)^{-1} \, d\gamma$;

(iii) $d\beta \propto (q_k^\beta q_l^\beta)^{-1} \, d\gamma$;

(iv) $l = k + \Delta_\gamma$.

The statements (i) and (ii), together with Proposition 2.2.2 (on page 18) imply that

$$\begin{aligned} \int_{-\infty}^{\infty} p(q_k^\beta)^{-1} \, d\gamma &= 0 \quad \text{for every } p \in \mathbf{P}_{l-1}, \\ \int_{-\infty}^{\infty} p(q_l^\beta)^{-1} \, d\gamma &= 0 \quad \text{for every } p \in \mathbf{P}_{k-1}. \end{aligned} \tag{3.5}$$

Also, $\beta \in \mathcal{H}_{+,1}$ by assumption. Therefore statement (iii) implies that

$$(q_k^\beta q_l^\beta)^{-1}\, d\gamma \text{ is } \textit{positive.} \tag{3.6}$$

That is, define $\tilde{\beta}$ by $d\tilde{\beta} = (q_k^\beta q_l^\beta)^{-1}\, d\gamma$; then $\tilde{\beta} \in \mathcal{H}_+$.

From these observations comes a simple strategy to find regular solutions to the main problem, roughly as follows. Given γ, "pick" the polynomials q_k^β and q_l^β such that the orthogonality conditions (3.5) and the positivity condition (3.6) are satisfied. Then use (iii) to write the solution β in terms of γ and the chosen polynomials. (This reduces the problem to picking polynomials with the right properties, something we discuss a little later.) The following proposition formalizes, and slightly refines, the strategy just described.

PROPOSITION 3.3.1 *Let $\gamma \in \mathcal{H}$ satisfy $d\gamma = q_i^\alpha q_j^\alpha\, d\alpha$ for some $\alpha \in \mathcal{H}_{+,1}$ and $i \neq j$. Let $q_k \in \mathbf{P}_k$ have degree k and leading coefficient $(-1)^k$, where $0 \leq k < d_\gamma - \Delta_\gamma$. Let $q_l \in \mathbf{P}_l$ have degree $l = k + \Delta_\gamma$ and leading coefficient $(-1)^l$. Suppose that:*

(i) $\int_{-\infty}^{\infty} p q_k^{-1}\, d\gamma = 0$ *for every* $p \in \mathbf{P}_{k-1}$;

(ii) $\int_{-\infty}^{\infty} p q_l^{-1}\, d\gamma = 0$ *for every* $p \in \mathbf{P}_{k-1}$;

(iii) $(q_k q_l)^{-1}\, d\gamma$ *is positive.*

Then the unique p.d.f. $\beta \in \mathcal{H}_{+,1}$ satisfying $d\beta \propto (q_k q_l)^{-1}\, d\gamma$ is a regular solution to the main problem (with given d.f. γ). That is, $q_k^\beta q_l^\beta\, d\beta \propto d\gamma$.

Proof. Let $\beta \in \mathcal{H}_{+,1}$ satisfy $d\beta \propto (q_k q_l)^{-1}\, d\gamma$. Then $q_l^{-1}\, d\gamma \propto q_k\, d\beta$, so in light of (ii) we can apply Proposition 2.2.2 to conclude that $q_k \propto q_k^\beta$. Similarly $q_k^{-1}\, d\gamma \propto q_l\, d\beta$,

but this time the statement (i) is not sufficient to conclude that $q_l \propto q_l^\beta$. Nevertheless we can reach the latter conclusion as follows. Note that the set

$$\mathbf{P}_{k-1} \cup \{q_k, xq_k, x^2q_k, \ldots, x^{\Delta-1}q_k\}$$

spans $\mathbf{P}_{l-1}$. In addition to (i), we have that

$$\int_{-\infty}^{\infty} (x^n q_k) q_k^{-1}\, d\gamma = \int_{-\infty}^{\infty} x^n\, d\gamma = 0$$

for every n in the range $0 \leq n \leq \Delta_\gamma - 1$. Therefore

$$\int_{-\infty}^{\infty} p q_k^{-1}\, d\gamma = 0 \quad \text{for every } p \in \mathbf{P}_{l-1}.$$

Now Proposition 2.2.2 applies to yield $q_l \propto q_l^\beta$ as desired. Thus

$$q_k^\beta q_l^\beta\, d\beta \propto q_k q_l\, d\beta \propto d\gamma,$$

completing the proof. ∎

The problem of how to pick polynomials with the right orthogonality conditions—given γ—has already been partly answered. Lemma 3.2.1 says that the polynomial q_k satisfies property (i) of the above Proposition if and only if it divides p^γ. (Of course it is not at all obvious at this point whether p^γ has any real roots in general.) But how do we pick q_l such that property (ii) of the Proposition is satisfied? In the next subsection we establish a useful analogue of Lemma 3.2.1 to (partly) answer this question.

A key technical lemma

LEMMA 3.3.2 *Let $\gamma \in \mathcal{H}$ have d jump points and fix i, j such that $0 \leq i < j < d$. Let $q \in \mathbf{P}_j$ have exact degree j and no repeated roots. Then*

$$\int_{-\infty}^{\infty} pq^{-1}\, d\gamma = 0 \quad \textit{for every} \quad p \in \mathbf{P}_{i-1} \tag{3.7}$$

if and only if

$$q \textit{ divides a member of the set } p^{\gamma} + p_{\gamma}\mathbf{P}_{j-i-1}. \tag{3.8}$$

Proof. If q has a common divisor with p_γ, it follows easily that neither (3.7) nor (3.8) holds. So assume q has no common divisor with p_γ, and factor q (over $\mathbf{C}$) as $q = ab$ where a has degree $j - i$ and b has degree i. Define $\tilde{\gamma}$ by $d\tilde{\gamma} = a^{-1}\, d\gamma$. Then $p_{\tilde{\gamma}} = p_\gamma$, and the condition

$$\int_{-\infty}^{\infty} pb^{-1}\, d\tilde{\gamma} \quad \text{for every} \quad p \in \mathbf{P}_{i-1} \tag{3.9}$$

is equivalent to (3.7).

Now, suppose (3.7) holds. Then, using (3.9), Lemma 3.2.1 implies that b divides $p^{\tilde{\gamma}}$, and so we may write $p^{\tilde{\gamma}} = br$ where r has degree at most $d - 1 - i$. Observe that

$$\begin{aligned} p^{\tilde{\gamma}} &= p^{\gamma}/a \pmod{p_\gamma} \\ \Longrightarrow \quad ap^{\tilde{\gamma}} &= p^{\gamma} \pmod{p_\gamma} \\ \Longrightarrow \quad abr &= p^{\gamma} \pmod{p_\gamma} \\ \Longrightarrow \quad qr &= p^{\gamma} \pmod{p_\gamma}. \end{aligned}$$

The latter statement implies (3.8), since the degree of r is at most $d - 1 - i$.

Conversely, suppose (3.8) holds. Then $qr = p^\gamma \pmod{p_\gamma}$ for some polynomial r of degree at most $d-1-i$. This implies

$$\begin{aligned} abr &= p^\gamma \pmod{p_\gamma} \\ \Longrightarrow \quad br &= p^\gamma/a \pmod{p_\gamma} \\ \Longrightarrow \quad br &= p^{\tilde{\gamma}} \pmod{p_\gamma}. \end{aligned}$$

Now, the degree of br is at most $d-1$, so in fact $br = p^{\tilde{\gamma}}$ without the restriction mod p_γ. In other words, b divides $p^{\tilde{\gamma}}$ and we may apply Lemma 3.2.1 once more to conclude that (3.9), and hence (3.7), holds. ∎

OBSERVATION 3.3.3 *Referring to the statement of Lemma 3.3.2, the polynomial q cannot divide more than one member of the set $p^\gamma + p_\gamma \mathbf{P}_{j-i-1}$.*

Proof. Suppose a, b are polynomials such that both qa and qb belong to the set $p^\gamma + p_\gamma \mathbf{P}_{j-i-1}$. Then $qa = p^\gamma + p_\gamma r$ and $qb = p^\gamma + p_\gamma s$ for some $r, s \in \mathbf{P}_{j-i-1}$. Note that

$$q(a-b) = p_\gamma(r-s),$$

so that either: $(a-b) = (r-s) = 0$, or p_γ divides $q(a-b)$. But the latter cannot happen, for q has no common divisor with p_γ, and $(a-b)$ has degree at most $d-i-1 < d$, whereas p_γ has degree d. So p_γ does not divide $q(a-b)$, forcing $a = b$ and $r = s$. ∎

Solutions in terms of the composite polynomial

We now bring together Proposition 3.3.1 and Lemmas 3.2.1 and 3.3.2 in a single statement.

THEOREM 3.3.4 *Let $\gamma \in \mathcal{H}$ satisfy $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$ for some $\alpha \in \mathcal{H}_{+,1}$ and $i \neq j$. Let $q_k \in \mathbf{P}_k$ have degree k and leading coefficient $(-1)^k$, where $0 \leq k < d_\gamma - \Delta_\gamma$. Let $q_l \in \mathbf{P}_l$ have degree $l = k + \Delta_\gamma$ and leading coefficient $(-1)^l$. Suppose that:*

(i) *q_k divides p^γ;*

(ii) *q_l divides a (necessarily unique) member of the set $p^\gamma + p_\gamma \mathbf{P}_{\Delta_\gamma - 1}$;*

(iii) *$(q_k q_l)^{-1} \, d\gamma$ is positive.*

Then the p.d.f. $\beta \in \mathcal{H}_{+,1}$ satisfying $d\beta \propto (q_k q_l)^{-1} \, d\gamma$ is a regular solution to the main problem with given d.f. γ. That is, $q_k^\beta q_l^\beta \, d\beta \propto d\gamma$. Moreover, every regular solution can be realized in this way.

Proof. The only part of the theorem which hasn't already been proved is the fact that every regular solution can be realized in the way described, and this is easy. Suppose β is a regular solution to the main problem with given d.f. γ, so that $q_k^\beta q_l^\beta \, d\beta \propto d\gamma$ for some $k \leq l$. Note that $l - k = \Delta_\gamma$ necessarily holds. Now, $(q_k^\beta)^{-1} \, d\gamma \propto q_l^\beta \, d\beta$, so

$$\int_{-\infty}^{\infty} p(q_k^\beta)^{-1} \, d\gamma = 0 \quad \text{for every } p \in \mathbf{P}_{l-1}.$$

In particular, since $k \leq l$,

$$\int_{-\infty}^{\infty} p(q_k^\beta)^{-1} \, d\gamma = 0 \quad \text{for every } p \in \mathbf{P}_{k-1}.$$

Therefore q_k^β divides p^γ by Lemma 3.2.1. Similarly, $(q_l^\beta)^{-1} \, d\gamma \propto q_k^\beta \, d\beta$, so

$$\int_{-\infty}^{\infty} p(q_l^\beta)^{-1} \, d\gamma = 0 \quad \text{for every } p \in \mathbf{P}_{k-1}.$$

Therefore q_l^β divides a member of the set $p^\gamma + p_\gamma \mathbf{P}_{\Delta - 1}$ by Lemma 3.3.2. Finally $\beta \in \mathcal{H}_{+,1}$, so $(q_k^\beta q_l^\beta)^{-1} \, d\gamma \propto d\beta$ is positive. ∎

Thus we have tied regular solutions of the main problem directly to divisors, and divisors mod p_γ, of the composite polynomial p^γ. But at this point it is unclear whether p^γ even has real roots, not to mention precisely how many. Before we can advance any further along these lines, it is therefore necessary to get precise information about the roots of the composite polynomial. As it turned out, the only way I was able to shed light on the nature and location of the roots of the composite polynomial, was indirectly, by an investigation into certain symmetry considerations. This is the subject of the next section.

3.4 The flip transpose

Definition of the flip transpose

Definition. [3] Given a $d \times d$ matrix M, we call the $d \times d$ matrix M^f defined by

$$M^f(i,j) = M(d+1-j, d+1-i)$$

the *flip transpose* of M. We refer collectively to the entries $M(i,j)$ whose indices satisfy $i+j = d+1$ as the *antidiagonal* of M. Thus the matrix M^f is obtained by "flipping" M about its antidiagonal.

Note that flip transposition commutes with ordinary transposition ($M \mapsto M^t$). The composition of these two operations is a permutation, as follows. Set F to be the $d \times d$ permutation matrix

$$F = \begin{pmatrix} 0 & \cdots & 0 & 0 & 0 & 1 \\ 0 & \cdots & 0 & 0 & 1 & 0 \\ 0 & \cdots & 0 & 1 & 0 & 0 \\ \vdots & & & & & \vdots \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 & 0 \end{pmatrix}.$$

Then $F^2 = I$, and $M^{ft} = FMF$. The relevance of this permutation to the present thesis is expressed in the following (straightforward) result.

PROPOSITION 3.4.1 *Apart from the identity, the only permutation that leaves invariant the class of $d \times d$ Jacobi matrices is the map $J \mapsto FJF$.*

[3] We use the same terminology as Lamoureux in [L,p.48].

Now, a (finite dimensional) Jacobi matrix J is symmetric, so that $J^{ft} = J^f$, and $J^f = FJF$. In other words, for Jacobi matrices the flip transpose on its own acts like a permutation.

Definition. Let $\alpha \in \mathcal{H}_{+,1}$. We define $\alpha^f \in \mathcal{H}_{+,1}$ to be the (unique) generator of the Jacobi matrix $(J_\alpha)^f$. Note that since J_α and $(J_\alpha)^f$ are similar, $p_\alpha = p_{\alpha^f}$.

This definition prompts a basic question: is there a more direct relationship between α and α^f, expressible without referring to their associated Jacobi matrices? We explore this at the end of the next subsection, after establishing some needed technical results.

Formulas arising from the flip transpose

The flip transpose allows us to establish several useful identities. Among other things, these identities give essential information about the roots of the composite polynomial p^γ of a d.f. γ.[4]

Let J be a $d \times d$ Jacobi matrix. To begin, note that for any $n \geq 0$ we have $(J^f)^n = (J^n)^f$, since $J^f = FJF$ and $F^2 = I$. Now, for $1 \leq i, j \leq d$,

$$\begin{aligned} (J^n)^f(i,j) &= J^n(d+1-j, d+1-i) \qquad \text{(by definition of the flip transpose)} \\ &= \int_{-\infty}^{\infty} x^n q^\alpha_{d-j} q^\alpha_{d-i}\, d\alpha \qquad \text{(by formula (2.5) on page 22).} \end{aligned}$$

[4]These identities are (apparently) new. De Boor and Golub mention the flip transpose (although they do not use this term) in their paper [dG], but their use of it is confined to defining a "persymmetric" matrix $J = J^f$.

Applying the same formula (2.5) to $(J^f)^n$, we get

$$(J^f)^n(i,j) = \int_{-\infty}^{\infty} x^n q_{i-1}^{\alpha^f} q_{j-1}^{\alpha^f} \, d\alpha^f.$$

Thus for every $n \geq 0$ and i, j in the (shifted!) range $0 \leq i, j \leq d-1$, we have

$$\int_{-\infty}^{\infty} x^n q_{d-1-j}^{\alpha} q_{d-1-i}^{\alpha} \, d\alpha = \int_{-\infty}^{\infty} x^n q_i^{\alpha^f} q_j^{\alpha^f} \, d\alpha^f.$$

Since $(\alpha^f)^f = \alpha$ (i.e. the flip transpose is an involution), we can rewrite the above statement with α and α^f interchanged, giving

$$\int_{-\infty}^{\infty} x^n q_i^{\alpha} q_j^{\alpha} \, d\alpha = \int_{-\infty}^{\infty} x^n q_{d-1-j}^{\alpha^f} q_{d-1-i}^{\alpha^f} \, d\alpha^f \qquad (n \geq 0 \text{ and } 0 \leq i, j \leq d-1).$$

It follows that

$$q_i^{\alpha} q_j^{\alpha} \, d\alpha = q_{d-1-j}^{\alpha^f} q_{d-1-i}^{\alpha^f} \, d\alpha^f \qquad (0 \leq i, j \leq d-1). \tag{3.10}$$

In the special case $i = j = 0$ we get

$$(q_0^{\alpha})^2 \, d\alpha = \, d\alpha = (q_{d-1}^{\alpha^f})^2 \, d\alpha^f. \tag{3.11}$$

Rewriting this as

$$d\alpha^f = (q_{d-1}^{\alpha^f})^{-2} \, d\alpha + 0,$$

Theorem 3.2.2 applies (with α^f, α in the roles of β, γ respectively, and $\beta_0 = 0$). The theorem says that $q_{d-1}^{\alpha^f}$ divides p^{α}. But p^{α} and $q_{d-1}^{\alpha^f}$ have the same degree, therefore

$$q_{d-1}^{\alpha^f} \propto \pm \, p^{\alpha}.$$

An examination of the definition of p^{α} easily reveals that in fact

$$q_{d-1}^{\alpha^f} \propto \, -p^{\alpha}. \tag{3.12}$$

We are now in a position to prove some needed technical results.

LEMMA 3.4.2 *Let $\alpha \in \mathcal{H}_{+,1}$ have d points of increase. For n in the range $0 \le n < d$,*

$$q_n^\alpha p^\alpha \propto -q_{d-1-n}^{\alpha^f} \quad (mod\ p_\alpha).$$

Proof. The identity (3.10) with $i = n$ and $j = 0$ yields

$$q_n^\alpha \, d\alpha = q_{d-1-n}^{\alpha^f} q_{d-1}^{\alpha^f} \, d\alpha^f.$$

By (3.11) we can replace $d\alpha$ by $(q_{d-1}^{\alpha^f})^2 \, d\alpha^f$, giving

$$\begin{aligned} q_n^\alpha (q_{d-1}^{\alpha^f})^2 \, d\alpha^f &= q_{d-1-n}^{\alpha^f} q_{d-1}^{\alpha^f} \, d\alpha^f \\ \Longrightarrow \quad q_n^\alpha q_{d-1}^{\alpha^f} &= q_{d-1-n}^{\alpha^f} \pmod{p_{\alpha^f}, \text{ or equivalently, mod } p_\alpha}. \end{aligned}$$

Finally, apply the relation (3.12) to yield

$$q_n^\alpha (-p^\alpha) \propto q_{d-1-n}^{\alpha^f} \pmod{p_\alpha},$$

which is equivalent to the conclusion of the lemma. ∎

LEMMA 3.4.3 *Let $\alpha \in \mathcal{H}_{+,1}$ have d points of increase $\lambda_1 < \lambda_2 < \ldots < \lambda_d$. Fix $0 \le i < d$. The locations of the roots of q_i^α and $q_{d-1-i}^{\alpha^f}$ are related as follows.*

(i) For each n, $q_i^\alpha(\lambda_n) = 0$ if and only if $q_{d-1-i}^{\alpha^f}(\lambda_n) = 0$.

(ii) For each $n \le d-1$, the polynomial q_i^α has a root in the open interval $(\lambda_n, \lambda_{n+1})$ if and only if $q_{d-1-i}^{\alpha^f}$ has no root in the closed interval $[\lambda_n, \lambda_{n+1}]$.

Proof. Proposition 2.2.4 (on page 19) states that the sequence

$$q_{d-1}^{\alpha^f}(\lambda_1), q_{d-1}^{\alpha^f}(\lambda_2), \ldots, q_{d-1}^{\alpha^f}(\lambda_d)$$

has $d-1$ sign changes, the maximum possible. In particular, $q_{d-1}^{\alpha^f}(\lambda_n) \neq 0$ for each n. Now, consider the identity (3.10) with $j = 0$: $q_i^\alpha \, d\alpha = q_{d-1}^{\alpha^f} q_{d-1-i}^{\alpha^f} \, d\alpha^f$. Thus

$q_i^\alpha(\lambda_n) = 0$ if and only if $q_{d-1}^{\alpha^f}(\lambda_n)q_{d-1-i}^{\alpha^f}(\lambda_n) = 0$ if and only if $q_{d-1-i}^{\alpha^f}(\lambda_n) = 0$, proving part (i) of the lemma. Moreover, for each n, $q_i^\alpha(\lambda_n)$ and $q_{d-1}^{\alpha^f}(\lambda_n)q_{d-1-i}^{\alpha^f}(\lambda_n)$ have the same sign. Note in addition that, since the roots of q_i^α, and also the roots of $q_{d-1-i}^{\alpha^f}$, interlace with $\lambda_1, \ldots, \lambda_d$ (which are the roots of $p_\alpha = p_{\alpha^f}$), each of q_i^α and $q_{d-1-i}^{\alpha^f}$ has at most one root (necessarily simple) in an interval of the form $[\lambda_n, \lambda_{n+1}]$. Thus the sequence $q_i^\alpha(\lambda_1), \ldots, q_i^\alpha(\lambda_d)$ has a sign change from λ_n to λ_{n+1} if and only if the sequence $q_{d-1-i}^{\alpha^f}(\lambda_1), \ldots, q_{d-1-i}^{\alpha^f}(\lambda_d)$ has the same sign at λ_n as at λ_{n+1}. Part (ii) of the lemma follows. ∎

THEOREM 3.4.4 *Let $\alpha \in \mathcal{H}_{+,1}$ have d points of increase. Fix indices i, j such that $0 \le i \le j < d$, and define $\gamma \in \mathcal{H}$ by $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$. There are two cases.*

(i) If $\alpha \ll \gamma$, or equivalently if $p_\alpha = p_\gamma$, then:

(a) $p^\gamma \propto -q_i^\alpha q_{d-1-j}^{\alpha^f}$;

(b) $p^\gamma \propto -q_j^\alpha q_{d-1-i}^{\alpha^f}$ (mod p_γ).

(ii) If $\alpha \not\ll \gamma$, write $\alpha = \alpha_1 + \alpha_0$ where $\alpha_1 \ll \gamma$ and $\alpha_0 \perp \gamma$. Then p_{α_0} divides both $q_i^\alpha q_{d-1-j}^{\alpha^f}$ and $q_j^\alpha q_{d-1-i}^{\alpha^f}$, and:

(a) $p^\gamma \propto -q_i^\alpha q_{d-1-j}^{\alpha^f}/p_{\alpha_0}$;

(b) $p^\gamma \propto -q_j^\alpha q_{d-1-i}^{\alpha^f}/p_{\alpha_0}$ (mod p_γ).

Proof. We can prove parts (i) and (ii) at the same time with the following convention. If $\alpha \ll \gamma$ we write $\alpha = \alpha_1 + \alpha_0$ where $\alpha_1 = \alpha$ and $\alpha_0 = 0$, and in this case we agree to set $p_{\alpha_0} = 1$. Otherwise we have the decomposition $\alpha = \alpha_1 + \alpha_0$ given in the hypothesis of part (ii). Thus in terms of characteristic polynomials we have (in both cases): $p_\gamma = p_{\alpha_1}$ and $p_\alpha = p_{\alpha_1}p_{\alpha_0} = p_\gamma p_{\alpha_0}$. Note that $d = d_\alpha$ according to the statement of the theorem and the notation used for the number of jump points of a d.f.

In terms of the numbers of jump points (equivalently, degrees of the characteristic polynomials) we have: $d_\gamma = d_{\alpha_1}$ and $d_\alpha = d_{\alpha_1} + d_{\alpha_0} = d_\gamma + d_{\alpha_0}$.

Now, write

$$\alpha(x) = \sum_{n=1}^{d_\alpha} w_n H(x - \lambda_n).$$

Then by definition,

$$\gamma(x) = \sum_{n=1}^{d_\alpha} q_i^\alpha(\lambda_n) q_j^\alpha(\lambda_n) w_n H(x - \lambda_n).$$

The jump points of α_0 are precisely the jump points λ_n of α at which $q_i^\alpha(\lambda_n)q_j^\alpha(\lambda_n) = 0$. Thus p_{α_0} divides $q_i^\alpha q_j^\alpha$. By part (i) of Lemma 3.4.3, p_{α_0} therefore also divides each of $q_i^\alpha q_{d-1-j}^{\alpha^f}$ and $q_j^\alpha q_{d-1-i}^{\alpha^f}$.

Observe that $p'_\gamma/p'_\alpha = p'_\gamma/(p'_\gamma p_{\alpha_0} + p_\gamma p'_{\alpha_0})$, so that at each jump point λ_n of γ (equivalently, root of p_γ), $p'_\gamma(\lambda_n)/p'_\alpha(\lambda_n) = 1/p_{\alpha_0}(\lambda_n)$. Consider now the value $p^\gamma(\lambda_n)$ of the composite polynomial p^γ at each jump point λ_n of γ. At each such point λ_n,

$$\begin{aligned} p^\gamma(\lambda_n) &= q_i^\alpha(\lambda_n) q_j^\alpha(\lambda) w_n p'_\gamma(\lambda_n) \\ &= q_i^\alpha(\lambda_n) q_j^\alpha(\lambda_n) w_n p'_\alpha(\lambda_n) p'_\gamma(\lambda_n)/p'_\alpha(\lambda_n) \\ &= q_i^\alpha(\lambda_n) q_j^\alpha(\lambda_n) w_n p'_\alpha(\lambda_n)/p_{\alpha_0}(\lambda_n) \\ &= q_i^\alpha(\lambda_n) q_j^\alpha(\lambda_n) p^\alpha(\lambda_n)/p_{\alpha_0}(\lambda_n). \end{aligned}$$

Thus

$$p^\gamma = q_i^\alpha q_j^\alpha p^\alpha / p_{\alpha_0} \pmod{p_\gamma}.$$

Now, Lemma 3.4.2 says that $q_j^\alpha p^\alpha \propto -q_{d-1-j}^{\alpha^f} \pmod{p_\alpha}$, and the same is true mod p_γ (since p_γ divides p_α). Thus

$$p^\gamma \propto -q_i^\alpha q_{d-1-j}^{\alpha^f} / p_{\alpha_0} \pmod{p_\gamma}. \tag{3.13}$$

And similarly, interchanging the roles of i and j,

$$p^\gamma \propto -q_j^\alpha q_{d-1-i}^{\alpha^f}/p_{\alpha_0} \pmod{p_\gamma}. \tag{3.14}$$

Note that by assumption $i \leq j$. Therefore the degree of the right-hand side of (3.13) is

$$d_\alpha - 1 - \Delta_\gamma - d_{\alpha_0} = d_\gamma - 1 - \Delta_\gamma,$$

and $p^\gamma \in \mathbf{P}_{d_\gamma - 1}$ is the unique interpolator of the values taken by the right-hand side at the jump points of γ. It follows that (3.13) holds *without* the restriction mod p_γ. On the other hand, the right-hand side of (3.14) has degree

$$d_\alpha - 1 + \Delta_\gamma - d_{\alpha_0} = d_\gamma - 1 + \Delta_\gamma,$$

so the proportionality is in general only valid mod p_γ. ∎

To close out the present section, we return briefly to the relationship between α and α^f. Interchanging the roles of α and α^f in (3.11) yields

$$d\alpha^f = (q_{d-1}^\alpha)^2 \, d\alpha,$$

which allows one to compute α^f directly, given α. In terms of the composite polynomials p^α and p^{α^f}, the relationship between α and α^f takes a particularly simple form: up to multiplication by a positive scalar, p^α and p^{α^f} are reciprocals of one another, mod p_α $(= p_{\alpha^f})$. We state this formally as follows.

PROPOSITION 3.4.5 *For $\alpha \in \mathcal{H}_{+,1}$, $p^\alpha p^{\alpha^f} \propto 1$ (mod p_α, or equivalently, mod p_{α^f}).*

Proof. Write $\alpha(x) = \sum_{n=1}^d w_n H(x - \lambda_n)$ with d minimal, and write $\alpha^f(x) = \sum_{n=1}^d w_n^f H(x - \lambda_n)$. Combining the identities (3.11) and (3.12) yields the identity

$$d\alpha \propto (p^\alpha)^2 \, d\alpha^f.$$

That is, for some scalar $r > 0$,

$$r\, d\alpha = (p^\alpha)^2\, d\alpha^f.$$

Thus for each n $(1 \leq n \leq d)$,

$$\begin{aligned} rw_n &= (p^\alpha(\lambda_n))^2 w_n^f \\ &= p^\alpha(\lambda_n)(w_n p'_\alpha(\lambda_n))w_n^f \\ &= p^\alpha(\lambda_n)(w_n p'_{\alpha^f}(\lambda_n))w_n^f \\ \iff \quad r &= p^\alpha(\lambda_n)(p'_{\alpha^f}(\lambda_n)w_n^f) \\ &= p^\alpha(\lambda_n)p^{\alpha^f}(\lambda_n). \end{aligned}$$

Therefore $p^\alpha p^{\alpha^f} \propto 1 \pmod{p_\alpha}$, as desired. ∎

3.5 Existence of regular solutions

Realizable patterns of roots

The following notation is to be fixed throughout the present section. Let $\alpha \in \mathcal{H}_{+,1}$ and fix i, j such that $0 \leq i < j < d_\alpha$. Define $\gamma \in \mathcal{H}$ by $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$. Let $\lambda_1 < \ldots < \lambda_{d_\alpha}$ be the jump points of α and let $\lambda'_1 < \ldots < \lambda'_{d_\gamma}$ be those of γ. Thus $\lambda'_1, \ldots, \lambda'_{d_\gamma}$ is the subsequence of $\lambda_1, \ldots, \lambda_{d_\alpha}$ obtained by deleting the points λ_n at which $q_i^\alpha(\lambda_n) q_j^\alpha(\lambda_n) = 0$. Writing $\alpha(x) = \sum_{n=1}^{d_\alpha} w_n H(x - \lambda_n)$, we have

$$\begin{aligned} \gamma(x) &= \sum_{n=1}^{d_\alpha} q_i^\alpha(\lambda_n) q_j^\alpha(\lambda_n) w_n H(x - \lambda_n) \\ &= \sum_{n=1}^{d_\gamma} q_i^\alpha(\lambda'_n) q_j^\alpha(\lambda'_n) w_n H(x - \lambda'_n). \end{aligned}$$

We explore the arrangement of the roots of $q_i^\alpha q_j^\alpha$ in an open interval of the form $(\lambda'_n, \lambda'_{n+1})$. The result on interlacing of zeros of orthogonal polynomials deriving from Proposition 2.2.4 on page 19 (and stated explicitly in the discussion following its proof) narrowly restricts the possibilities.

PROPOSITION 3.5.1 *Suppose that $q_i^\alpha q_j^\alpha$ has a multiple root r in the interval $(\lambda'_n, \lambda'_{n+1})$. Then the multiplicity of r is exactly 2, and $q_i^\alpha q_j^\alpha$ has no root in $(\lambda'_n, \lambda'_{n+1})$ distinct from r.*

Proof. That the multiplicity of r is 2 follows immediately from the fact that q_i and q_j each have simple roots. Now, suppose that $q_i^\alpha q_j^\alpha$ has a root in $(\lambda'_n, \lambda'_{n+1})$ distinct from r, and let $s \neq r$ be the root of $q_i^\alpha q_j^\alpha$ in $(\lambda'_n, \lambda'_{n+1})$ closest to r. Then s is a root of either q_i^α or q_j^α. In either case, it follows from Proposition 2.2.4 that there is a

jump point λ_m of α strictly between r and s. But this implies that λ_m is not a jump point of γ (since λ'_n and λ'_{n+1} are consecutive jump points of γ, and λ_m is between them). Therefore $q_i^\alpha(\lambda_m)q_j^\alpha(\lambda_m) = 0$. Yet λ_m is closer to r than s is, contradicting the fact that s is the closest root of $q_i^\alpha q_j^\alpha$ to r. ∎

PROPOSITION 3.5.2 *Suppose that $q_i^\alpha q_j^\alpha$ has at least two distinct roots in the interval $(\lambda'_n, \lambda'_{n+1})$, and list all such roots as $r_1 < \ldots < r_k$. Then each of the roots is simple, and in the sequence $r_1, \ldots, r_k$, roots of q_i^α alternate with roots of q_j^α (i.e. there are never two consecutive roots of either q_i^α or q_j^α). Moreover, for each m in the range $2 \leq m \leq k-1$, the root r_m is a jump point of α.*

Proof. That the roots are simple follows immediately from the preceding Proposition 3.5.1. Suppose that for some m, r_m and r_{m+1} are both roots of q_i^α. Then by Proposition 2.2.4. the open interval (r_m, r_{m+1}) contains a jump point of α, which is necessarily a root of $q_i^\alpha q_j^\alpha$, a contradiction. Exactly the same reasoning shows that r_m and r_{m+1} are not both roots of q_j^α. Therefore, roots of q_i^α and q_j^α alternate in the sequence $r_1, \ldots, r_k$, as desired.

Now, if m is in the range $2 \leq m \leq k-1$, then r_{m-1} and r_{m+1} are both roots of q_i^α or both roots of q_j^α. Therefore, by Proposition 2.2.4, the open interval (r_{m-1}, r_{m+1}) contains a jump point of α. This jump point has to be a root of $q_i^\alpha q_j^\alpha$. The only possibility is r_m, so r_m is a jump point of α. ∎

Notation. Let R_i, R_j denote the number of roots of q_i^α, q_j^α respectively in the interval $(\lambda'_n, \lambda'_{n+1})$.

COROLLARY 3.5.3 *If $q_i^\alpha q_j^\alpha$ has an odd number of roots (counting multiplicity) in $(\lambda'_n, \lambda'_{n+1})$ then $|R_i - R_j| = 1$. On the other hand, if $q_i^\alpha q_j^\alpha$ has an even number of*

roots (counting multiplicity) in $(\lambda'_n, \lambda'_{n+1})$ *then* $R_i = R_j$.

The above corollary shows that there are only 3 possibilities for the interval $(\lambda'_n, \lambda'_{n+1})$: $R_i = R_j$, $R_i = R_j + 1$, or $R_j = R_i + 1$. This leads immediately to a classification of the intervals $(\lambda'_n, \lambda'_{n+1})$ $(0 \leq n \leq d_\gamma - 1)$ according to which possibility is realized. We formalize this classification as follows.

Definition. We call $(\lambda'_n, \lambda'_{n+1})$ an interval of *constant sign* if $R_i = R_j$. If $R_i = R_j + 1$, we call $(\lambda'_n, \lambda'_{n+1})$ a *lower degree* interval; if $R_j = R_i + 1$, we call $(\lambda'_n, \lambda'_{n+1})$ a *higher degree* interval.

A crucial consideration in the construction of solutions to the main problem is the sign sequence of the coefficients of γ. To simplify notation, write

$$\gamma(x) = \sum_{n=1}^{d_\gamma} w'_n H(x - \lambda'_n),$$

so that $w'_n = q_i^\alpha(\lambda'_n) q_j^\alpha(\lambda'_n) w_n$ for each n. Then the sequence $w'_1, \ldots, w'_{d_\gamma}$ has a sign change from w'_n to w'_{n+1} if and only if $q_i^\alpha q_j^\alpha$ has an odd number of roots in the interval $(\lambda'_n, \lambda'_{n+1})$. This happens if and only if $(\lambda'_n, \lambda'_{n+1})$ is either a lower degree or a higher degree interval. On the other hand, w'_n and w'_{n+1} have the same sign if and only if $(\lambda'_n, \lambda'_{n+1})$ is an interval of constant sign—hence the name.

Now, consider the $d_\gamma - 1$ intervals

$$(\lambda'_1, \lambda'_2), \ldots, (\lambda'_{d_\gamma - 1}, \lambda'_{d_\gamma}).$$

Of these, let C denote the number of intervals of constant sign, L the number of lower degree intervals, and H the number of higher degree intervals (not to be confused with the Heaviside function which shares the same symbol). Then $C + L + H = d_\gamma - 1$ and $L + H = \sigma_\gamma$. Note also that $H - L = \Delta_\gamma$, since straightforward counting shows

$H - L = j - i$. These facts lead easily to the following observation, which we record for later reference.

OBSERVATION 3.5.4 *With C, L, H being the integers defined above, we have that $C = d_\gamma - 1 - \sigma_\gamma$, $L = (\sigma_\gamma - \Delta_\gamma)/2$ and $H = (\sigma_\gamma + \Delta_\gamma)/2$.*

We now present the next key technical result. Let $\alpha = \alpha_1 + \alpha_0$ where $\alpha_1 \ll \gamma$ and $\alpha_0 \perp \gamma$. We allow the possibility $\alpha_0 = 0$ (if $\alpha \ll \gamma$) in which case we set $p_{\alpha_0} = 1$. To reduce the use of double subscripts, set $d = d_\alpha$ which is of course different from d_γ (unless $\alpha \ll \gamma$).

LEMMA 3.5.5 *The chart below indicates the precise number of roots that each of the polynomials p^γ and $q_j^\alpha q_{d-1-i}^\alpha / p_{\alpha_0}$ has in the interval $(\lambda'_n, \lambda'_{n+1})$, according to the interval's type.*

interval type \ *polynomial*	p^γ	$q_j^\alpha q_{d-1-i}^{\alpha\prime} / p_{\alpha_0}$
constant sign $(R_i = R_j)$	*1*	*1*
lower degree $(R_i = R_j + 1)$	*2*	*0*
higher degree $(R_j = R_i + 1)$	*0*	*2*

Proof. We show first that the polynomials have at least the stated number of roots in intervals of each type. This takes up most of the proof. To begin, suppose that $q_i^\alpha q_j^\alpha$ has at least 3 roots in $(\lambda'_n, \lambda'_{n+1})$ and list these (using Proposition 3.5.2) as

$$r_1 < r_2 < \ldots < r_k.$$

(We will deal afterward with the cases where $q_i^\alpha q_j^\alpha$ has two or fewer roots in the given interval.) By Proposition 3.5.2 all of these roots, except possibly r_1 and r_k, are jump points of α and hence roots of p_{α_0}.

Case 1: $(\lambda'_n, \lambda'_{n+1})$ is an interval of constant sign. Then k is even and one of r_1, r_k is a root of q_i^α while the other is a root of q_j^α. For definiteness, suppose that r_1 is a root of q_i^α and r_k is a root of q_j^α. We appeal to Theorem 3.4.4 and consider $q_i^\alpha q_{d-1-j}^\alpha / p_{\alpha_0}$ in place of p^γ. If r_1 is not a jump point of α then r_1 is a root of q_i^α and not of p_{α_0}, so r_1 is a root of p^γ. If r_1 is a jump point of α, then q_j^α has no root in the closed interval $[\lambda'_n, r_1]$ and so by Lemma 3.4.3, part (ii), $q_{d-1-j}^{\alpha f}$ has a root in (λ'_n, r_1) (which is not a root of p_{α_0}), so p^γ has a root in (λ'_n, r_1). Thus p^γ has at least 1 root in $(\lambda'_n, \lambda'_{n+1})$. To see that $q_j^\alpha q_{d-1-i}^{\alpha f} / p_{\alpha_0}$ has at least one root in $(\lambda'_n, \lambda'_{n+1})$, repeat the above argument using the interval (r_k, λ'_{n+1}) in place of (λ'_n, r_1) with the roles of i and j interchanged.

Case 2: $(\lambda'_n, \lambda'_{n+1})$ is a lower degree interval. Then k is odd and both r_1 and r_k are roots of q_i^α, by Proposition 3.5.2. As in Case 1, we consider $q_i^\alpha q_{d-1-j}^\alpha / p_{\alpha_0}$ in place of p^γ. If r_1 is not a jump point of α, then r_1 is a root of q_i^α and not of p_{α_0}, so r_1 is a root of p^γ. If r_1 is a jump pont of α, then q_j^α has no root in $[\lambda'_n, r_1]$, so by Lemma 3.4.3 $q_{d-1-j}^{\alpha f}$ has a root in (λ'_n, r_1) (which is not a root of p_{α_0}), so p^γ has a root in (λ'_n, r_1). In either case p^γ has a root in $(\lambda'_n, r_1]$. The same argument shows that p^γ also has a root in $[r_k, \lambda'_{n+1})$. Since $r_1 < r_k$, this shows p^γ has at least two roots in $(\lambda'_n, \lambda'_{n+1})$.

Case 3: $(\lambda'_n, \lambda'_{n+1})$ is a higher degree interval. Then k is odd and both r_1 and r_k are roots of q_j^α, by Proposition 3.5.2. Interchanging the roles of i and j in the argument given for Case 2 shows that $q_j^\alpha q_{d-1-i}^{\alpha f} / p_{\alpha_0}$ has at least two roots in $(\lambda'_n, \lambda'_{n+1})$.

It remains to consider the cases where $q_i^\alpha q_j^\alpha$ has 0, 1 or 2 roots in $(\lambda'_n, \lambda'_{n+1})$. We deal with each of these in turn.

If $q_i^\alpha q_j^\alpha$ has no root in $(\lambda'_n, \lambda'_{n+1})$, then $(\lambda'_n, \lambda'_{n+1})$ is an interval of constant sign. In this case none of q_i^α, q_j^α or p_{α_0} has a root in $[\lambda'_n, \lambda'_{n+1}]$. Therefore by Lemma 3.4.3,

part (ii), both $q^{\alpha f}_{d-1-i}$ and $q^{\alpha f}_{d-1-j}$ have a root in $(\lambda'_n, \lambda'_{n+1})$, and it follows that p^γ and $q^\alpha_j q^{\alpha f}_{d-1-i}/p_{\alpha_0}$ each has at least one root in $(\lambda'_n, \lambda'_{n+1})$.

Next suppose that $q^\alpha_i q^\alpha_j$ has just one root r in $(\lambda'_n, \lambda'_{n+1})$. If r is a root of q^α_i then $(\lambda'_n, \lambda'_{n+1})$ is a lower degree interval. If in addition r is a jump point of α, then neither $[\lambda'_n, r]$ nor $[r, \lambda'_{n+1}]$ contains a root of q^α_j, so $q^{\alpha f}_{d-1-j}$ has a root in (λ'_n, r) and a root in (r, λ'_{n+1}), whence p^γ has at least two roots in $(\lambda'_n, \lambda'_{n+1})$. If r is a root of q^α_i and *not* a jump point of α, then $[\lambda'_n, \lambda'_{n+1}]$ contains no root of q^α_j (or of p_{α_0}). Therefore $q^{\alpha f}_{d-1-j}$ has a root s in $(\lambda'_n, \lambda'_{n+1})$. Thus $q^\alpha_i q^{\alpha f}_{d-1-j}/p_{\alpha_0}$, and hence p^γ, has at least two roots, r and s, in $(\lambda'_n, \lambda'_{n+1})$. (Note: it is conceivable that $r = s$ is a multiple root; this creates no difficulty.) If r is a root of q^α_j, then $(\lambda'_n, \lambda'_{n+1})$ is a higher degree interval, and the same argument shows that $q^\alpha_j q^{\alpha f}_{d-1-i}/p_{\alpha_0}$ has at least two roots in $(\lambda'_n, \lambda'_{n+1})$.

Lastly, suppose that $q^\alpha_i q^\alpha_j$ has exactly 2 roots $r_1 \leq r_2$ in $(\lambda'_n, \lambda'_{n+1})$. Then $(\lambda'_n, \lambda'_{n-1})$ is an interval of constant sign. Exactly the same argument as given for Case 2 works here. The only difference is that here we allow the possibility $r_1 = r_2 (= r_k)$, but this contingency has no effect on the argument.

Thus we have proven that p^γ and $q^\alpha_j q^{\alpha f}_{d-1-i}/p_{\alpha_0}$ have at least the stated number of roots in an interval of each of the three possible types. We now argue that each polynomial has exactly the stated number of roots in each type of interval. First consider p^γ. We have shown that p^γ has at least 2 roots in each lower degree interval and at least 1 root in each interval of constant sign. Using Observation 3.5.4 this accounts for

$$2L + C = 2(\sigma_\gamma - \Delta_\gamma)/2 + d_\gamma - 1 - \sigma_\gamma = d_\gamma - 1 - \Delta_\gamma$$

roots in all. But p^γ has exact degree $d_\gamma - 1 - \Delta_\gamma$ (see the proof of Theorem 3.4.4), so these are *all* the roots of p^γ.

Similarly, we have accounted for

$$2H + C = 2(\sigma_\gamma + \Delta_\gamma)/2 + d_\gamma - 1 - \sigma_\gamma = d_\gamma - 1 + \Delta_\gamma$$

roots of $q_j^\alpha q_{d-1-i}^{\alpha^f}/p_{\alpha_0}$. But the latter polynomial has exact degree $d_\gamma - 1 + \Delta_\gamma$ (again this is given explicitly in the proof of Theorem 3.4.4), so $q_j^\alpha q_{d-1-i}^{\alpha^f}/p_{\alpha_0}$ has no roots extra to this minimum number. ∎

Note that if one knows the d.f. γ, there is not enough information to determine the polynomial $q_j^\alpha q_{d-1-i}^{\alpha^f}/p_{\alpha_0}$. On the other hand the composite polynomial p^γ is completely determined by γ and can be written explicitly if one knows γ. Moreover the classification of the intervals between successive jump points of γ into the three types (constant sign, lower degree and higher degree) can also be carried out if one knows γ. For example, it follows from the above lemma that a lower degree interval $(\lambda'_n, \lambda'_{n+1})$ can be characterized as follows: the coefficients w'_n and w'_{n+1} of γ have opposite sign, and p^γ has a root (in fact 2 roots) in $(\lambda'_n, \lambda'_{n+1})$. An interval of constant sign corresponds to successive coefficients of γ that have the same sign. Finally, a higher degree interval is an interval which is neither of the other two types. *Note: this classification of the intervals determined by γ will be used repeatedly in Section 3.6.*

The existence theorem

We are now in a position to prove the existence in general of a regular solution to the main problem. Recall that such a result is made necessary by the fact that the

"known data" γ in the main problem may come from a singular solution, meaning that $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$ where $q_i^\alpha q_j^\alpha$ has common roots with p_α, so that γ has fewer jump points than the underlying p.d.f. α. In this case it is not clear a priori whether there exists a regular solution to the problem.

THEOREM 3.5.6 *Let $\gamma \in \mathcal{H}$ satisfy $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$ for some $\alpha \in \mathcal{H}_{+,1}$ and $i \neq j$. Then there exists a p.d.f. $\beta \ll \gamma$ and k, l such that $q_k^\beta q_l^\beta \, d\beta \propto d\gamma$. In other words, there exists a regular solution to the main problem.*

Proof. If $\alpha \ll \gamma$ then there is nothing to prove, so suppose $\alpha \not\ll \gamma$ and set $\alpha = \alpha_1 + \alpha_0$ where $\alpha_1 \ll \gamma$ and $\alpha_0 \perp \gamma$. By Observation 3.5.4, the number of lower degree intervals determined by γ is $(\sigma_\gamma - \Delta_\gamma)/2$. Set $k = (\sigma_\gamma - \Delta_\gamma)/2$ and choose k roots $r_1, \ldots, r_k$ of p^γ, one in each lower degree interval determined by γ. Lemma 3.5.5 guarantees that such a choice is possible. (More precisely there are 2^k such choices of roots.) Set

$$q_k(x) = \prod_{n=1}^{k} (r_n - x),$$

so that q_k divides p^γ.

Next consider the polynomial $q = -q_j^\alpha q_{d-1-i}^{\alpha^f} / p_{\alpha_0}$ where $d = d_\alpha (\neq d_\gamma)$. By Theorem 3.4.4, $q \propto p^\gamma \pmod{p_\gamma}$. The degree of q is exactly $d_\gamma - 1 + \Delta_\gamma$, and it follows that $q \propto \tilde{q}$ for some $\tilde{q} \in p^\gamma + p_\gamma \mathbf{P}_{\Delta_\gamma - 1}$. Set $l = (\sigma_\gamma + \Delta_\gamma)/2$, the number of higher degree intervals determined by γ (see Observation 3.5.4). Lemma 3.5.5 states that q has 2 roots in each of these higher degree intervals. Thus let $s_1, \ldots, s_l$ be a collection of l roots of q, one in each of the higher degree intervals determined by γ (again, there are precisely 2^l such collections of roots of q), and set

$$q_l(x) = \prod_{n=1}^{l} (s_n - x).$$

Then evidently q_l divides $\tilde{q} \in p^\gamma + p_\gamma \mathbf{P}_{\Delta_\gamma - 1}$.

Note that q_k and q_l satisfy conditions (i) and (ii) of Theorem 3.3.4. Now consider the d.f. $\tilde{\beta}$ defined by

$$d\tilde{\beta} = (q_k q_l)^{-1} \, d\gamma.$$

By construction, $q_k q_l$ has precisely one root in each interval corresponding to a sign change in the coefficients of γ (i.e. in the lower degree and higher degree intervals taken together). And $q_k q_l$ has no root outside these intervals. Therefore the coefficients of $\tilde{\beta}$ have constant sign. In fact the coefficients of $\tilde{\beta}$ are positive, since $q_k q_l$ is positive at $-\infty$ (by construction), and so condition (iii) of Theorem 3.3.4 is satisfied. It follows that the p.d.f. $\beta \in \mathcal{H}_{+,1}$ determined by the condition $\beta \propto \tilde{\beta}$ satisfies $q_k^\beta q_l^\beta \, d\beta \propto d\gamma$ and is thus a regular solution to the main problem. ∎

The proof of the above theorem made essential use of Lemma 3.5.5 in combination with Theorems 3.4.4 and 3.3.4. A more careful argument along the same lines serves as the basis for a description of the manifold of *all* regular solutions. This is the subject of the next section. The main virtue of the above theorem, is that we may henceforth assume without loss of generality that the known d.f. γ given in the statement of the main problem comes from a *regular* solution. That is, $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$ where $\alpha \ll \gamma$. This puts us in case (i) of Theorem 3.4.4 and makes it unnecessary to regard the jump points of γ as a subset of the jump points of α, which simplifies the exposition.

The results obtained so far have been achieved by means of mainly algebraic considerations. Specifically, we tied solutions of the main problem (with known d.f. γ) to divisors, and divisors mod p_γ, of p^γ. Then we used the flip transpose to extract detailed information about the roots of p^γ, and this enabled us to prove

the existence of the required divisors and hence of regular solutions. In the next section, we take a more geometric view, making use of what has been established thus far, and in particular Lemma 3.5.5. We continue to pursue the basic strategy embodied in Theorem 3.3.4. That is, we construct a regular solution by choosing a divisor q_k of p^γ and a divisor q_l of some member of the set $p^\gamma + p_\gamma \mathbf{P}_{\Delta-1}$ such that $(q_k q_l)^{-1} d\gamma \geq 0$. The essential obstacle to describing the manifold of regular solutions is: *precisely which members of* $p^\gamma + p_\gamma \mathbf{P}_{\Delta-1}$ *have a divisor* q_l *such that* $(q_k q_l)^{-1} d\gamma \geq 0$ *for some divisor* q_k *of* p^γ*?* In other words, precisely which part of $p^\gamma + p_\gamma \mathbf{P}_{\Delta-1}$ actually corresponds to solutions to the main problem?

3.6 The manifold of regular solutions for $\Delta > 0$

Introduction

This is the longest and most technically involved section in the thesis, so we begin with an overview. Our goal is to describe the set $\mathcal{S}_{\text{reg}}(d\gamma)$ of regular solutions to the main problem, viewed as a manifold in $\mathbf{R}^d$. We follow the terminology in Milnor [M] for the theory of differentiable manifolds. In particular we adopt that book's convention that all manifolds are subsets of some euclidean space $\mathbf{R}^m$. To describe $\mathcal{S}_{\text{reg}}(d\gamma)$ we construct an explicit parameterization of $\mathcal{S}_{\text{reg}}(d\gamma)$ over a Δ-dimensional set $\mathcal{C}$ of polynomials, which we call the coordinate base of $\mathcal{S}_{\text{reg}}(d\gamma)$. Since the structure of $\mathcal{S}_{\text{reg}}(d\gamma)$ is tied to that of $\mathcal{C}$, we go to some lengths to describe the basic geometric properties of $\mathcal{C}$. Ultimately, we show that $\mathcal{S}_{\text{reg}}(d\gamma)$ consists of 2^{d-1} "sheets", each of which is diffeomorphic to $\mathcal{C}$. The chain of argument leading up to this result proceeds as follows.

1. We define $\mathcal{C}$ in terms of the known d.f. γ, and prove that each regular solution corresponds to a unique member of $\mathcal{C}$.

2. We show that $\mathcal{C}$ is a semi-algebraic set, and therefore a finite union of real analytic manifolds.

3. We construct explicitly a connected 1-dimensional manifold sitting in the interior of $\mathcal{C}$. This explicitly constructed set is used in later proofs, and we call its construction our "key lemma".

4. We prove that $\mathcal{C}$ is connected.

5. We prove that $\mathcal{C}$ has dimension Δ.

6. We show that every member of $\mathcal{C}$ corresponds to at most 2^{d-1} different members of $\mathcal{S}_{\text{reg}}(d\gamma)$.

7. We construct a surjective map $\theta : \mathcal{C} \times (\text{a discrete set of size } 2^{d-1}) \longrightarrow \mathcal{S}_{\text{reg}}(d\gamma)$, and show that for each fixed s in the discrete set, θ is a diffeomorphism almost everywhere on $\mathcal{C} \times \{s\}$.

Definition of the coordinate base

We fix notation for the present section as follows. Let γ be a d.f. defined by $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$ for some $\alpha \in \mathcal{H}_{+,1}$ and $i < j$, where $\alpha \ll \gamma$. Set $\Delta = \Delta_\gamma$ and $\sigma = \sigma_\gamma$. Let $\lambda_1 < \ldots < \lambda_d$ denote the jump points of γ (equivalently of α). We use the notation I_n for each open interval of the form

$$I_n = (\lambda_n, \lambda_{n+1}) \quad \text{where } 1 \leq n \leq d-1.$$

As before, we divide the intervals I_n into three classes: intervals of constant sign, higher degree intervals and lower degree intervals. Thus set:

$$\begin{aligned} \mathbf{c} &= \text{the set of intervals of constant sign determined by } \gamma; \\ \mathbf{h} &= \text{the set of higher degree intervals determined by } \gamma; \\ \mathbf{l} &= \text{the set of lower degree intervals determined by } \gamma. \end{aligned}$$

The map which carries a tuple of roots to its associated polynomial plays a role in the present section. We formalize the notation for this map and the domain of interest as follows.

Definition. For each $k \geq 1$, define the map $\Psi_k : \mathbf{R}^k \longrightarrow \mathbf{P}_k$ by

$$\Psi_k(a_1, \ldots, a_k) = -\prod_{n=1}^{k}(a_n - x).$$

(The choice of sign is made for technical convenience in proofs to be given later in this section.) Note that the map Ψ_k is multilinear. Next we define a "triangle" T_n in $\mathbf{R}^2$ for each interval $I_n \in \mathbf{h}$ as follows. Set

$$T_n = \{(a, b) \in I_n \times I_n \,\big|\, a \leq b\}.$$

Note that T_n is neither open nor closed in $\mathbf{R}^2$. Rather, T_n contains the part of its boundary corresponding to the diagonal of the open square $I_n \times I_n$. In symbols,

$$\partial T_n \cap T_n = \{(a, a) \,\big|\, a \in I_n\}.$$

Lemma 3.5.5 gives the number and location of the roots of the polynomial $q_j^a q_{d-1-i}^{a^f}$ in terms of the intervals $I_1, \ldots, I_{d-1}$ determined by γ. We want to consider the set of all polynomials (whose leading coefficient has the right sign) having the same number of roots in precisely the same intervals as $q_j^a q_{d-1-i}^{a^f}$. *Warning: we use the symbol $\prod$ to denote the Cartesian product of a collection of intervals. The same symbol is used, for example, to denote a product of monomials. It should be clear from context which use is intended.*

Definition. Set

$$\mathcal{R} = (\prod_{I_n \in \mathbf{h}} T_n) \times (\prod_{I_n \in \mathbf{c}} I_n).$$

Observe that the interior of $\mathcal{R} \subseteq \mathbf{R}^{d-1+\Delta}$ is an open convex polytope, and for every $a = (a_1, \ldots, a_{d-1+\Delta}) \in \text{int}\mathcal{R}$, the entries of a are all distinct. Put another way, if $a = (a_1, \ldots, a_{d-1+\Delta}) \in \mathcal{R}$ and $a_m = a_n$ for some $m \neq n$, then $a \in \partial\mathcal{R}$.

PROPOSITION 3.6.1 *The map $\Psi_{d-1+\Delta}$ is 1-1 and continuous on $\mathcal{R}$, and a diffeomorphism on int$\mathcal{R}$.*

Proof. That $\Psi_{d-1+\Delta}$ is 1-1 and continuous on $\mathcal{R}$ follows easily from the definitions. We will argue that $\Psi_{d-1+\Delta}$ is a diffeomorphism on int$\mathcal{R}$. Let $H \subseteq \mathbf{P}_{d-1+\Delta}$ denote the hyperplane consisting of polynomials whose coefficient of $x^{d-1+\Delta}$ is $(-1)^{d+\Delta}$. The choice of sign in the definition of $\Psi_{d-1+\Delta}$ is such that $\Psi_{d-1+\Delta}[\mathcal{R}] \subseteq H$. Coordinatize H in terms of lower order coefficients. That is, let the tuple $(b_0, \ldots, b_{d-2+\Delta})$ represent the polynomial $(-1)^{d+\Delta}x^{d-1+\Delta} + \sum b_n x^n \in H$. Let π_n denote projection onto the nth coordinate. In terms of the given coordinates, each $\pi_n \circ \Psi_{d-1+\Delta}$ is an elementary symmetric polynomial (or the negative of one) and hence infinitely differentiable. Straightforward calculation shows that the matrix M of partial derivatives of $\Psi_{d-1+\Delta}$ at the point $a = (a_1, \ldots, a_{d-1+\Delta}) \in \mathcal{R}$ has the following structure. Setting $D = d - 1 + \Delta$,

$$M(i,j) = \sum_{\substack{k_1 < \cdots < k_{D-j} \\ k_n \neq i}} \prod_{n=1}^{D-j} a_{k_n}$$

for $1 \leq i \leq D-1$ and $1 \leq j \leq D$; and $M(D,j) = 1$ for each j. Thus the determinant of M is a polynomial in $a_1, \ldots, a_D$ of degree $\binom{D}{2}$. If any two entries of a agree, then M has two identical columns and $\det M = 0$. Thus the polynomial $p_a = \prod_{1 \leq i < j \leq D} (a_i - a_j)$ divides $\det M$. But p_a has degree $\binom{D}{2}$, so $\det M$ is a multiple of p_a. If $\det M$ is identically zero, then the dimension of $\Psi_{d-1+\Delta}[\mathcal{R}]$ has to be less than that of $\mathcal{R}$. Using the fact that $\Psi_{d-1+\Delta}$ is multilinear, it is straightforward to see that there are $d - 1 + \Delta$ linearly independent directions within the interior of $\Psi_{d-1+\Delta}[\mathcal{R}]$, so the latter has dimension $d - 1 + \Delta$, the same as $\mathcal{R}$. Thus $\det M$ is a non-zero multiple of p_a, which shows that the Jacobian of $\Psi_{d-1+\Delta}$ is non-zero provided a has no repeated

entries. And this is indeed the case for $a \in \text{int}\mathcal{R}$. Thus $\Psi_{d-1+\Delta}$ is a diffeomorphism on $\text{int}\mathcal{R}$. ∎

We define $\mathcal{P} \subseteq \mathbf{P}_{d-1+\Delta}$ to be the positive cone over $\Psi_{d-1+\Delta}[\mathcal{R}]$. That is,

$$\mathcal{P} = \{a_0 \Psi_{d-1+\Delta}(a) \,\big|\, a_0 > 0 \text{ and } a \in \mathcal{R}\}.$$

Thus $\mathcal{P}$ consists of the set of polynomials $p \in \mathbf{P}_{d-1+\Delta}$ such that: (i) the leading coefficient of p has sign $(-1)^{d+\Delta}$; (ii) p has precisely two roots in each interval $I_n \in \mathbf{h}$ and precisely one root in each interval $I_n \in \mathbf{c}$. Note that $\partial\mathcal{P} \cap \mathcal{P}$ consists of those polynomials $p \in \mathcal{P}$ having a double root in at least one $I_n \in \mathbf{h}$.

Set $\mathcal{A} = p^\gamma + p_\gamma \mathbf{P}_{\Delta-1}$. (This is the set we have been dealing with all along.) Note that $\mathcal{A}$ is a Δ-dimensional affine subspace of $P_{d-1+\Delta}$. The following definition is of central importance, as will be seen by the proposition which comes afterward.

Definition. We call the set $\mathcal{C} = \mathcal{P} \cap \mathcal{A}$ the *coordinate base* for the manifold of regular solutions to the main problem.

PROPOSITION 3.6.2 *Let β be a regular solution to the main problem, so that $q_k^\beta q_l^\beta \, d\beta \propto d\gamma$ for some $k < l$. Then q_l^β divides a unique member of the coordinate base $\mathcal{C}$. Conversely, for every $q \in \mathcal{C}$, there exist a divisor q_l of q and a divisor q_k of p^γ such that $(q_k q_l)^{-1} \, d\gamma \geq 0$, whence q_k, q_l engender a regular solution to the main problem.*

Proof. Evidently q_l^β divides the polynomial $q = -q_l^\beta q_{d-1-k}^{\beta\prime}$. Since $d\gamma \propto q_k^\beta q_l^\beta \, d\beta$, we can replace α with β in the statement of Lemma 3.5.5 (and replace p_{α_0} with 1, since $\beta \ll \gamma$), and conclude that $q \in \mathcal{P}$. Also, part (i)(a) of Theorem 3.4.4 (again replacing α with β) states that $q \propto p^\gamma \pmod{p_\gamma}$. Since q has exact degree $d - 1 + \Delta$, it follows that $q \propto p^\gamma + p_\gamma r$ for some $r \in \mathbf{P}_{\Delta-1}$. I.e. $cq \in \mathcal{A}$ for some scalar $c > 0$.

Thus $cq \in \mathcal{P} \cap \mathcal{A} = \mathcal{C}$. This shows that q_l^β divides a member, cq, of $\mathcal{C}$. That cq is unique in this respect follows from Observation 3.3.3 on page 47.

Conversely, let $q \in \mathcal{C}$ be arbitrary. To construct a regular solution based on a divisor of q we proceed exactly as in the proof of Theorem 3.5.6 (using q in the same role as it occurs there). The fact that $q \in \mathcal{P}$ ensures that it has all the necessary roots. ∎

In the above proof, we showed that for each $\beta \in \mathcal{S}_{\text{reg}}(d\gamma)$ (the set of regular solutions to the main problem), there corresponds a unique scalar $c > 0$ such that the polynomial $-cq_l^\beta q_{d-1-k}^{\beta^f}$ is in $\mathcal{C}$. Thus the map

$$\beta \mapsto -cq_l^\beta q_{d-1-k}^{\beta^f}$$

is a surjection from $\mathcal{S}_{\text{reg}}(d\gamma)$ onto $\mathcal{C}$.

The coordinate base $\mathcal{C}$ is a semi-algebraic set

A subset S of $\mathbf{R}^n$ is said to be real semi-algebraic if it is the solution to a finite system of real polynomial inequalities in n variables, or more generally, if it is a finite union of such solutions. If each system of inequalities reduces to a system of polynomial equations, then the set S is said to be algebraic. In this connection see Benedetti and Risler [BR]. It follows from the definition that the class of semi-algebraic sets in $\mathbf{R}^n$ is closed under finite unions and intersections. Two deeper facts about semi-algebraic sets will be needed in what follows.

1. The image of a semi-algebraic set by a map, each of whose coordinates is a polynomial, is again a semi-algebraic set. This is a special case of the so-called

Tarski-Seidenberg theorem (see [BR,p.60]).

2. Every semi-algebraic set in $\mathbf{R}^n$ is a finite union of real-analytic submanifolds of $\mathbf{R}^n$. See [BR,p.75 Proposition 2.5.1].

Based on 2., the dimension of a semi-algebraic set is defined to be the dimension of its highest-dimensional component manifold. We now set up notation for the coming proposition. For each set of intervals $\mathbf{h}_m \subseteq \mathbf{h}$, set

$$\mathcal{R}_m = (\prod_{I_n \in \mathbf{h}_m} \partial T_n \cap T_n) \times (\prod_{I_n \in \mathbf{h} \setminus \mathbf{h}_m} \mathrm{int} T_n) \times (\prod_{I_n \in \mathbf{c}} I_n).$$

(For the cases $\mathbf{h}_m = \emptyset$ and $\mathbf{h}_m = \mathbf{h}$ we simply delete the term corresponding to a Cartesian product over the empty set.) Thus in total there are $2^{(\sigma+\Delta)/2}$ such sets $\mathcal{R}_m$ (noting that $\mathbf{h}$ contains $(\sigma + \Delta)/2$ intervals). Each $\mathcal{R}_m$ is a convex polytope, open relative to its affine hull. In terms of the $\mathcal{R}_m$, $\mathcal{R}$ decomposes as a finite disjoint union,

$$\mathcal{R} = \bigcup_{m=1}^{2^{(\sigma+\Delta)/2}} \mathcal{R}_m.$$

Note that for $\mathbf{h}_m = \emptyset$, $\mathcal{R}_m = \mathrm{int}\mathcal{R}$. The above decomposition of $\mathcal{R}$ results in a corresponding decomposition of $\mathcal{P}$ by setting

$$\mathcal{P}_m = \left\{ a_0 \Psi_{d-1+\Delta}(a) \,\middle|\, a_0 > 0 \text{ and } a \in \mathcal{R}_m \right\}.$$

Thus $\mathcal{P}$ can be written as a disjoint union of the $\mathcal{P}_m$,

$$\mathcal{P} = \bigcup_{m=1}^{2^{(\sigma+\Delta)/2}} \mathcal{P}_m.$$

PROPOSITION 3.6.3 *The set $\mathcal{P}_m \cap \mathcal{A}$ is semi-algebraic for each m.*

Proof. Coordinatize $\mathbf{P}_{d-1+\Delta}$ in terms of coefficients. That is, let the tuple $(b_0, \ldots, b_{d-1+\Delta})$ represent the polynomial $\sum b_n x^n \in \mathbf{P}_{d-1+\Delta}$. In terms of these coordinates, the map $\phi : (0,\infty) \times \mathcal{R} \longrightarrow \mathcal{P} \subseteq \mathbf{P}_{d-1+\Delta}$, defined by $\phi(a_0, a) = a_0 \Psi_{d-1+\Delta}(a)$, is 1-1. And, letting π_n denote projection onto the nth coordinate, each $\pi_n \circ \phi$ has the form $a_0 f_n$ where f_n is an elementary symmetric polynomial in $a_1, \ldots, a_{d-1+\Delta}$. Each set $(0,\infty) \times \mathcal{R}_m \subseteq (0,\infty) \times \mathcal{R}$ is an open convex polyhedron, and hence a semi-algebraic set. Therefore each $\mathcal{P}_m = \phi[(0,\infty) \times \mathcal{R}_m]$ is a semi-algebraic set. Finally, $\mathcal{P}_m \cap \mathcal{A}$ is semi-algebraic, since the affine subspace $\mathcal{A} \subseteq \mathbf{P}_{d-1+\Delta}$ is a semi-algebraic set. ∎

COROLLARY 3.6.4 *Each of $\mathcal{C}$ and $\mathcal{C} \cap \partial\mathcal{P}$ is a semi-algebraic set.*

Proof. Both $\mathcal{C}$ and $\mathcal{C} \cap \partial\mathcal{P}$ are unions of sets of the form $\mathcal{P}_m \cap \mathcal{A}$. ∎

A key lemma

Our objective for this subsection is to explicitly construct a set of polynomials which corresponds to a line segment in $\mathcal{C} \cap \text{int}\mathcal{P}$. (By a line segment, or a segment, we mean the affine image in $\mathbf{P}_{d-1+\Delta}$ of an interval in $\mathbf{R}^1$.) The basic idea of the construction is as follows. We choose a particular "vertex" q_0 of $\Psi_{d-1+\Delta}[\mathcal{R}]$ (i.e. q_0 is the image by $\Psi_{d-1+\Delta}$ of a vertex of $\mathcal{R}$) having the special form $q_0 = p_\gamma r_0$. Then we show that every sufficiently small perturbation of q_0, $q_0 + \varepsilon p^\gamma$, in the direction of p^γ, carries the vertex q_0 into the interior of $\Psi_{d-1+\Delta}[\mathcal{R}]$. Normalizing $q_0 + \varepsilon p^\gamma$ to the form $p^\gamma + \varepsilon^{-1} q_0$, we obtain a segment of points $p^\gamma + \varepsilon^{-1} q_0$ both in $\text{int}\mathcal{P}$ (since they are in the positive cone over $\text{int}\Psi_{d-1+\Delta}[\mathcal{R}]$) and in $\mathcal{A}$ (since they have the form $p^\gamma + \varepsilon^{-1} p_\gamma r_0$). The

actual proof that the perturbation $q_0 + \varepsilon p^\gamma$ moves q_0 to the interior of $\Psi_{d-1+\Delta}[\mathcal{R}]$ requires a very detailed (and rather tedious) analysis of sign patterns, which takes up much of the present subsection.

To facilitate proving the main result of this subsection, we further refine our division of intervals I_n into the sets $\mathbf{c}, \mathbf{h}, \mathbf{l}$. Thus set:

$$\begin{aligned} \mathbf{c}^* &= \text{the set of } I_k \in \mathbf{c} \text{ such that } I_n \in \mathbf{h} \;\&\; n > k \Rightarrow \exists I_m \in \mathbf{l} \text{ where } k < m < n; \\ \mathbf{h}' &= \text{the set of } I_k \in \mathbf{h} \text{ such that } \exists I_n \in \mathbf{h}, n > k \text{ such that } k < m < n \Rightarrow I_m \in \mathbf{c}. \end{aligned}$$

In words, $\mathbf{c}^*$ is the set of intervals I_n of constant sign such that: either every interval to the right of I_n has constant sign; or, the left-most non-constant interval to the right of I_n has lower degree. And $\mathbf{h}'$ is the set of higher degree intervals I_n such that there is a non-constant interval to the right of I_n, and the left-most such interval has higher degree. Recall that each interval $I_n \in \mathbf{c}$ contains either no root of $q_i^\alpha q_j^\alpha$, or one root each of q_i^α and q_j^α. Each interval $I_n \in \mathbf{h}$ contains one root of q_j^α and none of q_i^α. And each interval $I_n \in \mathbf{l}$ contains one root of q_i^α and no root of q_j^α. Recall also (from the definition of p^γ) that $p^\gamma(\lambda_1), \ldots, p^\gamma(\lambda_d)$ has precisely the opposite sign sequence to the coefficients $w'_1, \ldots, w'_d$ of γ (writing $\gamma(x) = \sum_{n=1}^d w'_n H(x - \lambda_n)$). Thus the former sequence has a sign change precisely where the latter sequence does not.

OBSERVATION 3.6.5 *The left-most and right-most intervals not in* $\mathbf{c}$ *are both in* $\mathbf{h}$. *And for every* $I_k, I_n \in \mathbf{l}, k < n$, *there exist* $I_m \in \mathbf{h}, k < m < n$.

Proof. This follows from Proposition 2.3.3. ∎

OBSERVATION 3.6.6 *The set* $\mathbf{h}'$ *contains exactly* $\Delta - 1$ *intervals.*

Proof. Given Observation 3.6.5, this is straightforward counting. ∎

Definition. Set $r_0(x) = -\prod_{I_n \in \mathbf{h}'} (\lambda_{n+1} - x)$. Thus the roots of r_0 are the right endpoints of the higher degree intervals in $\mathbf{h}'$, and the degree of r_0 is $\Delta - 1$. Set $q_0 = p_\gamma r_0$. Then q_0 has degree $d - 1 + \Delta$, and the sign of q_0 is such that $q_0(x) < 0$ for $x < \lambda_1$.

Notation. For each interval $I_n = (\lambda_n, \lambda_{n+1})$, set

$$\lambda_n^* = \begin{cases} \lambda_{n+1} \text{ if } I_n \in \mathbf{c}^* \\ \lambda_n \text{ otherwise} \end{cases}.$$

Set $\mu_n = (\lambda_n + \lambda_{n+1})/2$.

PROPOSITION 3.6.7 *$q_0(\mu_n)q_0(\mu_{n+1}) > 0$ if and only if $I_n \in \mathbf{h}'$.*

Proof. By construction, the polynomial q_0 has either a single or a double root at each jump point λ_n of γ. In particular, q_0 has a double root at λ_{n+1} if and only if $I_n \in \mathbf{h}'$. The proposition then follows from the fact that $q_0(\mu_n)q_0(\mu_{n+1}) > 0$ if and only if λ_{n+1} is a double root of q_0. ∎

PROPOSITION 3.6.8 *$p^\gamma(\lambda_n^*)p^\gamma(\lambda_{n+1}^*) > 0$ if and only if $I_n \notin \mathbf{c} \setminus \mathbf{c}^*$ and $I_{n+1} \notin \mathbf{c}^*$.*

Proof. ($\Longrightarrow$) Suppose that $I_n \in \mathbf{c} \setminus \mathbf{c}^*$ or $I_{n+1} \in \mathbf{c}^*$. (We will show that $p^\gamma(\lambda_n^*)p^\gamma(\lambda_{n+1}^*) < 0$ follows.) In the former case I_{n+1} cannot be in $\mathbf{c}^*$, by definition of $\mathbf{c}^*$. Thus $\lambda_n^* = \lambda_n$, $\lambda_{n+1}^* = \lambda_{n+1}$ and $p^\gamma(\lambda_n)p^\gamma(\lambda_{n+1}) < 0$ since $I_n \in \mathbf{c}$. On the other hand, if $I_{n+1} \in \mathbf{c}^*$ then $\lambda_{n+1}^* = \lambda_{n+2}$ and $I_n \notin \mathbf{c} \setminus \mathbf{c}^*$. So either I_n is a non-constant interval—in which case $\lambda_n^* = \lambda_n$ and $p^\gamma(\lambda_n)$ has the same sign as $p^\gamma(\lambda_{n+1})$—or $I_n \in \mathbf{c}^*$, in which case $\lambda_n^* = \lambda_{n+1}$. In both cases $p^\gamma(\lambda_n^*)p^\gamma(\lambda_{n+2})$ has the same sign as $p^\gamma(\lambda_{n+1})p^\gamma(\lambda_{n+2}) < 0$, since $I_{n+1} \in \mathbf{c}$.

($\Longleftarrow$) Conversely suppose that $I_n \notin \mathbf{c} \setminus \mathbf{c}^*$ and $I_{n+1} \notin \mathbf{c}^*$. Since $I_{n+1} \notin \mathbf{c}^*$, $\lambda^*_{n+1} = \lambda_{n+1}$. Now, either $I_n \in \mathbf{c}^*$, in which case $\lambda^*_n = \lambda_{n+1}$ and $p^\gamma(\lambda^*_n)p^\gamma(\lambda^*_{n+1}) = p^\gamma(\lambda_{n+1})^2 > 0$, or $I_n \notin \mathbf{c}$. In the latter case $\lambda^*_n = \lambda_n$ and I_n is a non-constant interval, so $p^\gamma(\lambda^*_n)p^\gamma(\lambda^*_{n+1}) = p^\gamma(\lambda_n)p^\gamma(\lambda_{n+1}) > 0$. ∎

PROPOSITION 3.6.9 *If $I_n \in \mathbf{l}$ then $p^\gamma(\lambda^*_n)q_0(\mu_n) > 0$. Otherwise $p^\gamma(\lambda^*_n)q_0(\mu_n) < 0$.*

Proof. We argue by considering the intervals I_n from left to right. To begin, consider I_1. By Observation 3.6.5 $I_1 \notin \mathbf{l} \cup \mathbf{c}^*$, so $\lambda^*_1 = \lambda_1$. Note that q_0 has a single root at λ_1 and $q_0(x) < 0$ for $x < \lambda_1$, so $q_0(\mu_1) > 0$. Now, by definition of p^γ, $p^\gamma(\lambda_1) < 0$. Thus $p^\gamma(\lambda^*_1)q_0(\mu_1) < 0$, i.e. the proposition is valid for $n = 1$.

Next, note that the expression $p^\gamma(\lambda^*_n)q_0(\mu_n)$ changes sign from n to $n+1$ if and only if one of $p^\gamma(\lambda^*_n)p^\gamma(\lambda^*_{n+1})$ and $q_0(\mu_n)q_0(\mu_{n+1})$ is negative and the other is positive. Propositions 3.6.7 and 3.6.8 tell us precisely when this happens: either (i) $I_n \in \mathbf{h}'$ and $I_{n+1} \in \mathbf{c}^*$, or (ii) $I_n \notin \mathbf{h}'$, $I_n \notin \mathbf{c} \setminus \mathbf{c}^*$ and $I_{n+1} \notin \mathbf{c}^*$. The situation (i) is self-contradictory (by the definitions of $\mathbf{h}'$ and $\mathbf{c}^*$). On the other hand, systematic checking of cases reveals that the configurations consistent with (ii) are precisely the following: 1. $I_n \in \mathbf{l}$ and $I_{n+1} \in \mathbf{h} \cup \mathbf{c}$; 2. $I_n \in \mathbf{h} \cup \mathbf{c}$ and $I_{n+1} \in \mathbf{l}$. (Recall that Observation 3.6.5 prohibits $I_n, I_{n+1} \in \mathbf{l}$.) Thus if the proposition is true for I_n, it continues to be true for I_{n+1}. Since the proposition holds for I_1, the result for all $n \leq d-1$ follows by induction. ∎

Notation. Set $M = \min_{1 \leq n \leq d-1} \{|q_0(\mu_n)/p^\gamma(\mu_n)|\}$. (Note that $M > 0$.) Given $\varepsilon > 0$, set

$$q_\varepsilon = p^\gamma + \varepsilon^{-1} q_0.$$

LEMMA 3.6.10 *(i) For every ε in the range $0 < \varepsilon < M$, $q_\varepsilon \in \mathcal{C} \cap \text{int}\mathcal{P}$.*
(ii) (roots of q_ε) $\longrightarrow$ (roots of q_0) as $\varepsilon \longrightarrow 0$.

Proof. Note that q_ε has the same roots as $\varepsilon p^\gamma + q_0$, from which (ii) is immediate. We now consider part (i) of the lemma. First note that for ε in the given range and any n, $q_\varepsilon(\mu_n)$ has the same sign as $q_0(\mu_n)$ since

$$|\varepsilon^{-1} q_0(\mu_n)| > |M^{-1} q_0(\mu_n)| \geq |p^\gamma(\mu_n)|.$$

Also, $q_\varepsilon(\lambda_n^*) = p^\gamma(\lambda_n^*)$ since $q_0(\lambda_n^*) = 0$. Thus $q_\varepsilon(\lambda_n^*) q_\varepsilon(\mu_n)$ has the same sign as $p^\gamma(\lambda_n^*) q_0(\mu_n)$, and Proposition 3.6.9 implies that $q_\varepsilon(\lambda_n^*) q_\varepsilon(\mu_n) > 0$ if and only if $I_n \in \mathbf{l}$. Therefore, if $I_n \in \mathbf{c} \cup \mathbf{h}$ then q_ε has a root strictly between μ_n and λ_n^*. Moreover we claim that if $I_n \in \mathbf{h}$—in which case $\lambda_n^* = \lambda_n$—then q_ε also has a root strictly between μ_n and λ_{n+1}. To see this, note that for $I_n \in \mathbf{h}$, $p^\gamma(\lambda_n) p^\gamma(\lambda_{n+1}) > 0$. Therefore $p^\gamma(\lambda_n) q_0(\mu_n) < 0$ implies $p^\gamma(\lambda_{n+1}) q_0(\mu_n) < 0$. Arguing as before, it follows that $q_\varepsilon(\lambda_{n+1}) q_\varepsilon(\mu_n) < 0$, forcing a root strictly between μ_n and λ_{n+1}. To summarize, we have shown that: if $I_n \in \mathbf{h}$ then q_ε has a root in each of (λ_n, μ_n) and (μ_n, λ_{n+1}); if $I_n \in \mathbf{c}$ then q_ε has a root strictly between λ_n^* and μ_n. This accounts for

$$2(\sigma + \Delta)/2 + d - 1 - \sigma = d - 1 + \Delta$$

roots of q_ε. But q_ε has degree $d - 1 + \Delta$, so these are all the roots of q_ε. It follows that $q_\varepsilon \in \text{int}\mathcal{P}$. Finally, the representation $q_\varepsilon = p^\gamma + \varepsilon^{-1} p_\gamma r_0$ shows q_ε to be in $\mathcal{A}$, and so $q_\varepsilon \in \mathcal{C} \cap \text{int}\mathcal{P}$ as desired. ∎

The above lemma helps us to demonstrate some basic geometric properties of the coordinate base $\mathcal{C}$: it is connected and has dimension Δ.

The coordinate base C is connected

To begin, we need some additional facts about the map $\Psi_k : \mathbf{R}^k \longrightarrow \mathbf{P}_k$. The following notation is to be fixed throughout the present subsection. Let $l_1, \ldots, l_m$ and $r_1, \ldots, r_m$ be ordered such that

$$l_1 < r_1 \leq l_2 < r_2 \leq \ldots \leq l_m < r_m,$$

and write K_n for each closed interval of the form $K_n = [l_n, r_n]$.

PROPOSITION 3.6.11 *Let $h \in \mathbf{P}_m$ have exact degree m, and suppose that the leading coefficient of h has sign $(-1)^{m+1}$. Then the following conditions are equivalent:*
(i) for each n $(1 \leq n \leq m)$, $(-1)^n h(l_n) \geq 0$ and $(-1)^n h(r_n) \leq 0$;
(ii) h has m real roots $s_1 \leq \ldots \leq s_m$ such that $s_n \in K_n$ for each n.

Proof. The equivalence of the following slightly modified conditions is straightforward: (i') for each n $(1 \leq n \leq m)$, $(-1)^n h(l_n) > 0$ and $(-1)^n h(r_n) < 0$; (ii') h has m real roots $s_1 \leq \ldots \leq s_m$ such that each s_n is in the interior of K_n. The equivalence of the statements (i) and (ii) then follows by considering degree m perturbations of h and taking limits. (Or, one can prove the latter equivalency directly by a rather tedious counting of sign changes and roots.) ∎

The next result requires some further notation, as follows. We call a polynomial

$$p \in \Psi_m \left[\prod_{n=1}^{m} K_n \right]$$

a *vertex* of $\Psi_m \left[\prod_{n=1}^m K_n\right]$ if $p = \Psi(a_1, \ldots, a_m)$ for some $(a_1, \ldots, a_m) \in \prod_{n=1}^m K_n$ where

$$\{a_1, \ldots, a_m\} \subseteq \{l_1, \ldots, l_m, r_1, \ldots, r_m\}.$$

Write V_m for the set of all vertices of $\Psi_m[\prod_{n=1}^m K_n]$.

LEMMA 3.6.12 *$\Psi_m[\prod_{n=1}^m K_n]$ is a closed convex polytope in $\mathbf{P}_m$. Specifically, $\Psi_m[\prod_{n=1}^m K_n]$ is the convex hull of the finite set V_m.*

Proof. Let V denote the convex hull of V_m. We show first that $V \subseteq \Psi_m[\prod_{n=1}^m K_n]$. Let $\sum t_n v_n \in V$ be an arbitrary convex combination of vertices $v_n \in V_m$. Note that each vertex v_n satisfies condition (ii) of Proposition 3.6.11 (with $h = v_n$) and hence condition (i) also. But condition (i) is easily seen to be invariant under positive combinations. That is, if condition (i) holds for $h = f$ and $h = g$, then condition (i) holds also for $h = sf + tg$ for any scalars $s, t > 0$. Thus $h = \sum t_n v_n$ satisfies condition (i) and hence condition (ii) of Proposition 3.6.11. But condition (ii), together with the observation that the leading coefficient of $\sum t_n v_n$ is $(-1)^{k+2}$, implies that $\sum t_n v_n = \Psi_m(a)$ for some $a \in \prod_{n=1}^m K_n$.

We now argue the reverse inclusion $\Psi_m[\prod_{n=1}^m K_n] \subseteq V$. We proceed by induction on m. If $m = 1$ then Ψ_m is linear and the inclusion is obvious. So assume $k \geq 1$ and the desired inclusion holds for $m \leq k$. We will show that it holds for $m = k+1$ also. Let $a = (a_1, \ldots, a_{k+1}) \in \prod_{n=1}^{k+1} K_n$ be arbitrary. Then $a_{k+1} \in K_{k+1}$, so we may express a_{k+1} as a convex combination of l_{k+1} and r_{k+1}, say $a_{k+1} = (1-t)l_{k+1} + tr_{k+1}$. Also, $(a_1, \ldots, a_k) \in \prod_{n=1}^k K_n$, so by the inductive assumption, $\Psi_k(a_1, \ldots, a_k) = \sum t_n v_n$ for some convex combination of vertices $v_n \in V_k$. Thus,

$$\begin{aligned}
\Psi_{k+1}(a_1, \ldots, a_{k+1}) &= \Psi_{k+1}(a_1, \ldots, a_k, (1-t)l_{k+1} + tr_{k+1}) \\
&= (1-t)\Psi_{k+1}(a_1, \ldots, a_k, l_{k+1}) + t\Psi_{k+1}(a_1, \ldots, a_k, r_{k+1}) \\
&= (1-t)(l_{k+1} - x)\Psi_k(a_1, \ldots, a_k) + t(r_{k+1} - x)\Psi_k(a_1, \ldots, a_k) \\
&= (1-t)(l_{k+1} - x)(\textstyle\sum t_n v_n) + t(r_{k+1} - x)(\sum t_n v_n)
\end{aligned}$$

$$= \sum((1-t)t_n(l_{k+1}-x)v_n + tt_n(r_{k+1}-x)v_n).$$

The latter is a convex combination of vertices $(l_{k+1}-x)v_n$ and $(r_{k+1}-x)v_n$ in V_{k+1}. Thus $\Psi_{k+1}\left[\prod_{n=1}^{k+1} K_n\right]$ is contained in the convex hull of V_{k+1} as desired. ∎

It is essential in the above lemma that the intervals $K_1, \ldots, K_m$ do not overlap, except possibly at their endpoints. With overlapping intervals the lemma is false. For example, the Bezier patch $\Psi_2[K_1 \times K_1]$ is not convex—it has a parabolic bounding curve.[5]

THEOREM 3.6.13 *The coordinate base $\mathcal{C}$ is arcwise connected.*

Proof. Let $q \in \mathcal{C}$ be arbitrary. Recall that the intervals $I_n = (\lambda_n, \lambda_{n+1})$ are defined to be open, and that since $q \in \mathcal{P}$, q has two roots in each interval $I_n \in \mathbf{h}$ and one root in each interval $I_n \in \mathbf{c}$. For each interval $I_n \in \mathbf{h}$, let μ_n denote the midpoint of the two roots of q in I_n. (These roots may coincide; this creates no difficulty.) Now consider the collection of numbers

$$\{\lambda_n \,\big|\, I_n \in \mathbf{h} \cup \mathbf{c}\} \cup \{\mu_n \,\big|\, I_n \in \mathbf{h}\}.$$

List these in order as $l_1 < l_2 < \ldots < l_{d-1+\Delta}$. Next list the set of numbers

$$\{\lambda_{n+1} \,\big|\, I_n \in \mathbf{h} \cup \mathbf{c}\} \cup \{\mu_n \,\big|\, I_n \in \mathbf{h}\}$$

in order as $r_1 < r_2 < \ldots < r_{d-1+\Delta}$. Observe that the l_n and r_n defined this way interlace, since they are left and right endpoints of non-overlapping intervals. That is,

$$l_1 < r_1 \leq l_2 < r_2 \leq \ldots \leq l_{d-1+\Delta} < r_{d-1+\Delta}.$$

[5]See Farin [Fa] for a discussion of Bezier patches. It seems as though the set $\mathcal{P}$ itself can be described as a "polytope" with quadratic "facets"—such a detailed description will require further investigation.

Now, set $K_n = [l_n, r_n]$ for each n. We know that $\Psi_{d-1+\Delta}\left[\prod_{n=1}^{d-1+\Delta} K_n\right]$ is a convex polytope by Lemma 3.6.12. Set $\mathcal{K}$ to be the positive cone over $\Psi_{d-1+\Delta}\left[\prod_{n=1}^{d-1+\Delta} K_n\right]$ in $\mathbf{P}_{d-1+\Delta}$. Thus $\mathcal{K}$ and $\text{int}\mathcal{K}$ are both convex as well. Observe that $\text{int}\mathcal{K} \subseteq \text{int}\mathcal{P}$, and that $q \in \mathcal{K}$.

We now appeal to Lemma 3.6.10 which allows us (by part (ii)) to choose $\varepsilon > 0$ sufficiently small that $q_\varepsilon \in \text{int}\mathcal{K}$ and also $q_\varepsilon \in \mathcal{C} \cap \text{int}\mathcal{P}$. (To get $q_\varepsilon \in \text{int}\mathcal{K}$, we need to ensure that the two roots of q_ε sitting in each $I_n \in \mathbf{h}$ lie on either side of μ_n. This is always possible, since these two roots tend to opposite endpoints of I_n as $\varepsilon \longrightarrow 0$.) Now consider the closed segment $\overline{s}$ in $\mathbf{P}_{d-1+\Delta}$ with endpoints q and q_ε. Since $\mathcal{K}$ is convex, $\overline{s} \subseteq \mathcal{K}$.

Moreover, we claim that, except possibly for q, $\overline{s} \subseteq \text{int}\mathcal{K}$. This is immediate if $q \in \text{int}\mathcal{K}$, since $\text{int}\mathcal{K}$ is convex. Consider the case where $q \in \partial\mathcal{K}$. Then q has a root at some l_n or r_n; since $q \in \mathcal{P}$ the only possibility is that q has a (double) root at some μ_n. (q cannot have a root at any λ_n and be in $\mathcal{P}$.) Again using that $\text{int}\mathcal{K}$ is convex, partition $\overline{s}$ into disjoint segments $\overline{s}_\partial \subseteq \partial\mathcal{K}$ and $\overline{s}_{\text{int}} \subseteq \text{int}\mathcal{K}$, so that $\overline{s} = \overline{s}_\partial \cup \overline{s}_{\text{int}}$. Suppose that $\overline{s}_\partial$ contains a point other than q and hence has positive length. Observe that every $q_1 \in \overline{s}_\partial$ sufficiently close to q is non-zero at each endpoint l_n or r_n where q is non-zero. Thus to be in $\partial\mathcal{K}$, each such q_1 must have a root μ_n in common with q. On the other hand, each such $q_1 \neq q$ can be written as a proper convex combination $q_1 = (1-t)q + tq_\varepsilon$ of q and q_ε. Since $q_\varepsilon(\mu_n) \neq 0$ (by choice) it follows that $q_1(\mu_n) \neq 0$, a contradiction. So $\overline{s}_\partial$ contains no point other than q, proving the claim.

Since $\overline{s} \setminus \{q\} \subseteq \text{int}\mathcal{K}$ and $\text{int}\mathcal{K} \subseteq \text{int}\mathcal{P}$, it follows that $\overline{s} \subseteq \mathcal{P}$ (including q). Note that $\mathcal{A}$, being affine, is convex. Both q, q_ε are in $\mathcal{A}$, so $\overline{s} \subseteq \mathcal{A}$. Thus $\overline{s} \subseteq \mathcal{C}$.

Lemma 3.6.10 states that the open segment $\overline{s}_0 \subseteq \mathbf{P}_{d-1+\Delta}$ consisting of the polynomials q_ε, for all ε in the range $0 < \varepsilon < M$, is contained in $\mathcal{C}$. We have shown that for an arbitrary polynomial $q \in \mathcal{C}$, there is a closed segment $\overline{s}$ in $\mathcal{C}$ connecting q to $\overline{s}_0$. It follows that $\mathcal{C}$ is arcwise connected. ∎

Based on the above proof, we might say that $\mathcal{C}$ has the geometric attribute of being "almost" star-shaped.[6] The following consequence of the proof will be needed later.

COROLLARY 3.6.14 *The coordinate base $\mathcal{C}$ is contained in the closure of $\mathcal{C} \cap int\mathcal{P}$.*

Proof. Consider $q \in \mathcal{C} \cap \partial\mathcal{P}$. We showed in the proof of Theorem 3.6.13 that q is the endpoint of a line segment $\overline{s}$ where $\overline{s} \setminus \{q\} \subseteq \mathcal{C} \cap \text{int}\mathcal{P}$. Therefore q is contained in the closure of $\mathcal{C} \cap \text{int}\mathcal{P}$. ∎

The coordinate base $\mathcal{C}$ has dimension Δ

Since $\mathcal{C}$ is contained in the Δ-dimensional affine space $\mathcal{A}$, the dimension of $\mathcal{C}$ cannot exceed Δ. On the other hand, one can imagine a "degenerate" situation where $\mathcal{C} = \mathcal{P} \cap \mathcal{A}$ lies entirely in the boundary of $\mathcal{P}$ in such a way as to have dimension less than Δ. In fact Lemma 3.6.10 precludes such a degenerate configuration, as will be demonstrated below.

[6] A set S in a vector space is star-shaped if there is a point p_0 in S such that for every $p \in S$, the segment from p to p_0 lies entirely in S. In the case of $\mathcal{C}$ an open segment $\overline{s}_0$ plays the role of the point p_0. Note that we could replace $\overline{s}_0$ with an arbitrarily small segment corresponding to ε in the range $0 < \varepsilon < N$ where $N < M$.

Definition. We say that a point $p \in \mathcal{C}$ is in the *relative interior* of $\mathcal{C}$ if p has a neighbourhood N in $\mathbf{P}_{d-1+\Delta}$ such that $N \cap \mathcal{A} \subseteq \mathcal{C}$.

THEOREM 3.6.15 *The relative interior of $\mathcal{C}$ is a non-empty, connected, open subset of $\mathcal{A}$, and hence has dimension Δ.*

Proof. It follows from the above definition that the relative interior of $\mathcal{C}$ contains $\mathcal{C} \cap \text{int}\mathcal{P}$ (noting that $\text{int}\mathcal{P}$ is an open subset of $\mathbf{P}_{d-1+\Delta}$). Consequently, the proof that the relative interior of $\mathcal{C}$ is connected, is exactly the same as the proof that $\mathcal{C}$ is connected. It also follows from the above definition that the relative interior of $\mathcal{C}$ is open in $\mathcal{A}$ and Δ-dimensional, since the affine space $\mathcal{A}$ has dimension Δ. Lastly, Lemma 3.6.10 shows that $\mathcal{C} \cap \text{int}\mathcal{P}$ is non-empty, and so the relative interior of $\mathcal{C}$ is non-empty. ∎

We will use $\mathcal{C}$ to parameterize the set of all regular solutions to the main problem. We explicitly assign euclidean coordinates to $\mathcal{A}$ as follows. Each point $p \in \mathcal{A}$ can be written uniquely as $p^\gamma + p_\gamma r$ for some $r \in \mathbf{P}_{\Delta-1}$. We let the Δ coefficients of r serve as coordinates for p, and in this way we identify $\mathcal{A}$ with $\mathbf{R}^\Delta$.

PROPOSITION 3.6.16 *The semi-algebraic set $\mathcal{C} \cap int\mathcal{P}$ has dimension strictly less than Δ. Thus $\mathcal{C} \cap int\mathcal{P}$ has Lebesgue measure zero in $\mathcal{A}$ (identified with $\mathbf{R}^\Delta$).*

Proof. Evidently $\mathcal{C} = (\mathcal{C} \cap \text{int}\mathcal{P}) \cup (\mathcal{C} \cap \partial\mathcal{P})$. It follows from Corollary 3.6.14 that $\mathcal{C} \cap \partial\mathcal{P}$ has empty interior. Since $\mathcal{C} \cap \partial\mathcal{P}$ is a semi-algebraic set, its dimension must be strictly less than Δ, for otherwise it would have interior points in $\mathcal{A}$. Any smooth manifold in $\mathcal{A}$ of dimension less than Δ has Lebesgue measure zero. (See Milnor [M,p.10].) ∎

The Lebesgue measure (in $\mathcal{A}$) of $\mathcal{C}$ is of course positive (possibly infinite), since $\mathcal{C}$ has dimension Δ.

The number of regular solutions associated to a point in $\mathcal{C}$

Recall that in the proof of Proposition 3.6.2 we established a map, call it ϕ, from the set $\mathcal{S}_{reg}(d\gamma)$ of regular solutions onto the coordinate base $\mathcal{C}$. This map had the explicit form

$$\beta \overset{\phi}{\mapsto} -cq_l^{\beta} q_{d-1-k}^{\beta^f},$$

where $c > 0$ is a uniquely determined scalar. The corresponding inverse map ϕ^{-1} is many-valued; in order to parameterize $\mathcal{S}_{\mathrm{reg}}(d\gamma)$ we have to count precisely how many values it takes. To do so we look back at our original strategy for constructing a regular solution to the main problem. Our strategy consists of choosing a divisor q_k of p^γ, and a divisor q_l of some $q \in \mathcal{C}$ such that $(q_k q_l)^{-1}\, d\gamma \geq 0$. The solution β is then constructed by scaling $(q_k q_l)^{-1}\, d\gamma \geq 0$. Note that in this construction, the resultant solution β is completely determined by the roots of $q_k q_l$. The proposition below allows us to count the total number of possible choices for roots of $q_k q_l$, given a fixed $q \in \mathcal{C}$.

PROPOSITION 3.6.17 *Let q_k divide p^γ and q_l divide some $q \in \mathcal{C}$, and suppose that the leading coefficients of q_k and q_l are $(-1)^k$ and $(-1)^l$ respectively, where k and l are the respective degrees of q_k and q_l. Then $(q_k q_l)^{-1}\, d\gamma \geq 0$ if and only if each of the following conditions holds. (i) For each $I_n \in \mathbf{c}$, either q_k, q_l both have a root in*

I_n, or neither q_k or q_l has a root in I_n. (ii) For each $I_n \in \mathbf{h}$, q_l has one (simple) root in I_n. (iii) For each $I_n \in \mathbf{l}$, q_k has one (simple) root in I_n.

Proof. Observe that $q_k q_l$ has to have an even number of roots in each interval $I_n \in \mathbf{c}$, because the coefficients of γ do not change sign in any such interval. Also, $q_k q_l$ has to have an odd number of roots in each $I_n \in \mathbf{h} \cup \mathbf{l}$, since the coefficients of γ go through a sign change in each such interval. By Lemma 3.5.5 and the definition of $\mathcal{C}$, the only way to satisfy these requirements is that each of the conditions (i),(ii) and (iii) be satisfied. Conversely, if each of (i),(ii) and (iii) is satisfied, then the coefficients of $\tilde{\beta}$, defined by $d\tilde{\beta} = (q_k q_l)^{-1}\, d\gamma$, have constant sign. Since $q_k q_l$ has leading coefficient $(-1)^{k+l}$ and degree $k+l$, $q_k(\lambda_1) q_l(\lambda_1) > 0$ and the sign is positive. ∎

Let $q \in \mathcal{C}$ be fixed, and consider an interval $I_n \in \mathbf{c}$. We know each of p^γ and q has precisely one root in I_n. By Proposition 3.6.17, we must choose either both these roots to be roots of $q_k q_l$ or neither. Thus there are exactly two choices associated with each $I_n \in \mathbf{c}$: BOTH or NEITHER. Next consider an interval $I_n \in \mathbf{l}$. We know that p^γ has exactly two roots in I_n, and q has no roots in I_n. By Proposition 3.6.17, we must choose one of these two roots of p^γ as a root of q_k, and hence as a root of $q_k q_l$. If we label the two roots LEFT and RIGHT according to their relative position, then we have exactly two possible choices associated with each $I_n \in \mathbf{l}$: LEFT or RIGHT. Similarly for an interval $I_n \in \mathbf{h}$, we know q has two roots in I_n, p^γ has none, and by Proposition 3.6.17 we must choose one or the other of the two roots of q. Labeling the roots as before, we thus have exactly two choices associated with each $I_n \in \mathbf{h}$: LEFT or RIGHT. In summary, for each of the $d-1$ intervals I_n, there are exactly two alternative choices in selecting the roots of $q_k q_l$, making 2^{d-1} possible choices in all. In other words there is a total of 2^{d-1} different polynomials $q_k q_l$ associated with

a given $q \in \mathcal{C}$. The only possible degeneracy is if LEFT=RIGHT for some $I_n \in \mathbf{h} \cup \mathbf{l}$. This corresponds to p^γ or q having a double root. Note that $q \in \mathcal{C}$ has a double root if and only if $q \in \mathcal{C} \cap \partial\mathcal{P}$.

Notation. We define the set $\mathcal{D}$ of "choices" determined by γ as follows. Set $\mathcal{D}$ to be the collection of sequences $(s_1, \ldots, s_{d-1})$ where

$$s_n \in \begin{cases} \{\text{BOTH,NEITHER}\} \text{ if } I_n \in \mathbf{c} \\ \{\text{LEFT,RIGHT}\} \text{ if } I_n \in \mathbf{h} \cup \mathbf{l} \end{cases}.$$

Each $s = (s_1, \ldots, s_{d-1}) \in \mathcal{D}$ will be called a *choice vector.*

Thus each pair $(q, s) \in \mathcal{C} \times \mathcal{D}$ determines a unique polynomial $q_k q_l$ satisfying $(q_k q_l)^{-1}\, d\gamma \geq 0$ and hence a unique $\beta \in \mathcal{S}_{\text{reg}}(d\gamma)$ determined by the condition $d\beta \propto (q_k q_l)^{-1}\, d\gamma$. And conversely each solution $\beta \in \mathcal{S}_{\text{reg}}(d\gamma)$ corresponds to a pair $(q, s) \in \mathcal{C} \times \mathcal{D}$.

Parametrization of the set of regular solutions over the coordinate base

By definition a regular solution β to the main problem has precisely the same jump points $\lambda_1, \ldots, \lambda_d$ as the known d.f. γ. Writing $\beta(x) = \sum_{n=1}^{d} v_n H(x - \lambda_n)$, we can thus represent $\beta \in \mathcal{S}_{\text{reg}}(d\gamma)$ by its coefficients, that is, by the tuple $v = (v_1, \ldots, v_d) \in \mathbf{R}^d$. Note that, since $\beta \in \mathcal{H}_{+,1}$, v is in the open $(d-1)$-dimensional simplex determined by the equations $\sum v_n = 1$ and $v_n > 0$ (each n). In the present subsection we will identify $\mathcal{S}_{\text{reg}}(d\gamma)$ with the corresponding subset of $\mathbf{R}^d$. We will thus talk of a p.d.f. $\beta \in \mathbf{R}^d$, and refer to the coefficients $v_1, \ldots, v_d$ of β as the coordinates of β, writing $\beta = (v_1, \ldots, v_d)$.

We know that to each pair $(q, s) \in \mathcal{C} \times \mathcal{D}$ there corresponds a unique solution $\beta \in \mathcal{S}_{\text{reg}}(d\gamma)$. Let

$$\theta : \mathcal{C} \times \mathcal{D} \longrightarrow \mathbf{R}^d$$

denote the corresponding map. For each fixed choice vector $s \in \mathcal{D}$, define

$$\theta_s : \mathcal{C} \longrightarrow \mathbf{R}^d$$

by $\theta_s(q) = \theta(q, s)$.

THEOREM 3.6.18 *For each fixed $s \in \mathcal{D}$, the map $\theta : \mathcal{C} \longrightarrow \mathbf{R}^d$ is continuous and 1-1 on $\mathcal{C}$, and a diffeomorphism on $\mathcal{C} \cap int\mathcal{P}$.*

Proof. Note that the choice vector s fixes the degrees $k < l$ of the divisors q_k of p^γ and q_l of $q \in \mathcal{C}$ to be chosen in constructing $\theta_s(q)$. In fact s determines q_k completely. Note also that $l = k + \Delta$, so that we are guaranteed $l \geq \Delta$. We first show that θ_s is

1-1. Suppose $\beta = \theta_s(q) = \theta_s(\tilde{q})$, so that $q_k^\beta q_l^\beta \, d\beta \propto d\gamma$. Then q_l^β divides both q and $\tilde{q}$. By Observation 3.3.3, q_l^β divides at most one member of $\mathcal{C}$, so $q = \tilde{q}$.

To show that θ_s is continuous on $\mathcal{C}$ and a diffeomorphism on $\mathcal{C} \cap \text{int}\mathcal{P}$, we factor θ_s into "steps", each of which corresponds to a map which is continuous on its respective domain and a diffeomorphism on the part of its domain that is the image of $\mathcal{C} \cap \text{int}\mathcal{P}$ by the preceding steps.

Step 1. Radial projection of $\mathcal{C}$ onto the hyperplane $H = \Psi_{d-1+\Delta}[\mathbf{R}^{d-1+\Delta}] \subseteq \mathbf{P}_{d-1+\Delta}$. That is $q \mapsto ((-1)^{d+\Delta}/b_{d-1+\Delta})q$, where $b_{d-1+\Delta}$ is the coefficient of $x^{d-1+\Delta}$ in q. To see that this map has the desired properies, it suffices to note that each $q \in \mathcal{C}$ has degree $d - 1 + \Delta$, and that no two distinct members of $\mathcal{C}$ (or of $\mathcal{A}$, for that matter) are proportional.

Step 2. Mapping $q \in H$ to the divisor q_l of q determined by the choice vector s. Note that the map $q \mapsto q_l$ corresponds in $\mathcal{R}$ to taking the projection π_s (determined by s) onto a fixed set of l coordinates. In other words, this step corresponds to the map

$$\Psi_l \circ \pi_s \circ \Psi_{d-1+\Delta}^{-1}.$$

The first factor $\Psi_{d-1+\Delta}^{-1}$ is a diffeomorphism by Proposition 3.6.1. Since $l \geq \Delta$, the projection π_s is guaranteed to have a derivative of rank Δ at each point in the relative interior of the image of Step 1. Finally, the proof of Proposition 3.6.1 shows also that Ψ_l is a diffeomorphism.

Step 3. Write $\gamma(x) = \sum_{n=1}^{d} w_n H(x - \lambda_n)$ and map each q_l to the tuple $(u_1, \ldots, u_d)$, defined by

$$u_n = q_l(\lambda_n)^{-1} q_k(\lambda_n)^{-1} w_n.$$

This map is well-behaved since $q_l(\lambda_n) \neq 0$ for each n, for every $q \in \mathcal{C}$. (Recall that

q_k is fixed, since it is predetermined by the choice vector s.)

Step 4. Normalize. That is, map $u = (u_1, \ldots, u_d)$ to

$$\beta = \frac{1}{\sum u_n}(u_1, \ldots, u_d).$$

By construction each $u_n > 0$, and no two members of the domain are proportional (since θ_s is 1-1), so this map is continuous on the image of Step 3, and a diffeomorphism on the image of $\mathcal{C} \cap \text{int}\mathcal{P}$ by Steps 1-3. ∎

For each k in the range $\frac{\sigma-\Delta}{2} \leq k \leq d-1-\frac{\sigma+\Delta}{2}$, let $\mathcal{D}_k \subseteq \mathcal{D}$ denote the set of choice vectors s for which the corresponding divisor of p^γ has degree k (and hence for which the corresponding divisor of $q \in \mathcal{C}$ has degree $l = k + \Delta$). This establishes a partition of $\mathcal{D}$ into $d - \sigma$ sets:

$$\mathcal{D} = \mathcal{D}_{(\sigma-\Delta)/2} \cup \ldots \cup \mathcal{D}_{d-1-(\sigma+\Delta)/2}.$$

The set $\mathcal{D}_k$ is easily seen to contain $2^\sigma \binom{d-1-\sigma}{k-(\sigma-\Delta)/2}$ different choice vectors. For each $q \in \mathcal{C}$ define $\theta^q : \mathcal{D} \longrightarrow \mathbf{R}^d$ by $\theta^q(s) = \theta(q, s)$.

THEOREM 3.6.19 *Suppose that p^γ has no double roots, and let k be in the range $\frac{\sigma-\Delta}{2} \leq k \leq d-1-\frac{\sigma+\Delta}{2}$. Then, except for $q \in \mathcal{C} \cap \partial\mathcal{P}$, θ^q maps $\mathcal{D}_k$ onto a discrete set of size $2^\sigma \binom{d-1-\sigma}{k-(\sigma-\Delta)/2}$. Thus the map θ^q is 1-1 on $\mathcal{D}_k$ for almost every $q \in \mathcal{C}$.*

Proof. If $q \in \mathcal{C} \cap \text{int}\mathcal{P}$ then q does not have a double root, and by assumption p^γ has no double root. In this case, distinct choice vectors give rise to distinct sets of roots. Now, let $s, \tilde{s} \in \mathcal{D}_k$ and suppose that $\beta = \theta^q(s) = \theta^q(\tilde{s})$. Then $q_k \propto q_k^\beta$ and $\tilde{q}_k \propto q_k^\beta$; also $q_l \propto q_l^\beta$ and $\tilde{q}_l \propto q_l^\beta$. Therefore $q_k q_l$ has the same set of roots as $\tilde{q}_k \tilde{q}_l$ (in fact $q_k q_l = \tilde{q}_k \tilde{q}_l$), and this implies $s = \tilde{s}$. Thus θ^q is 1-1 on $\mathcal{D}_k$. ∎

More generally, if p^γ has D double roots, then θ^q maps $\mathcal{D}_k$ onto a discrete set of size $2^{\sigma-D}\binom{d-1-\sigma}{k-(\sigma-\Delta)/2}$ for almost every $q \in \mathcal{C}$. We close out the present section with an illustration of the map θ.

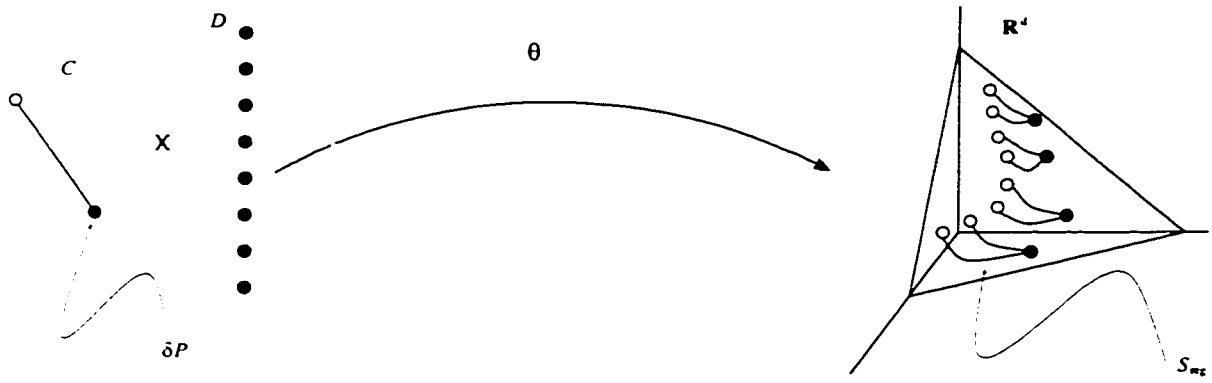

Figure 3.1: The parameterization of $\mathcal{S}_{\text{reg}}(d\gamma)$

3.7 A note on singular solutions for the case $\Delta > 0$

With Theorems 3.6.18 and 3.6.19 we have attained our principal objective for this thesis, which was to describe $\mathcal{S}_{reg}(q_i^\alpha q_j^\alpha \, d\alpha)$ as a manifold, for arbitrary $\alpha \in \mathcal{H}_{+,1}$ and arbitrary indices i, j. Recall that in Section 3.2 we described the singular solutions as well as the regular solutions for the case $\Delta = 0$. The singular solutions had up to $2d - 1$ jump points, d being the number of jump points of the given data. At this point it is natural to inquire as to the structure of the set of singular solutions to the main problem in the case $\Delta > 0$. As yet we do not have complete results, however a preliminary investigation has revealed the following fact: If $\Delta > 0$ then the number of jump points in a singular solution is no longer bounded. Below we give an example exhibiting this behaviour, omitting the derivation and proof; these will be given in future work, once more complete results have been obtained.

For each integer $d \geq 2$, define the p.d.f. $\beta_d \in \mathcal{H}_{+,1}$ as follows:

$$\begin{aligned} \beta_d(x) \quad \propto \quad & \frac{1}{(d-1)!} H(x-1) + \frac{1}{d!} H(x-2) \\ & + \sum_{n=1}^{(d-2)/2} \left\{ \frac{(d+1)(d-2n)}{(2n)!(d+1-2n)!} H\left(x - \frac{d+1+2n}{d+1}\right) \right. \\ & \left. + \frac{2n(d+1)(d-2n-1)^2}{d(2n+1)!(d-2n)!} H\left(x - \frac{d+2+2n}{d+1}\right) \right\}. \end{aligned}$$

PROPOSITION 3.7.1 *Set* $d\gamma = q_0^{\beta_2} q_1^{\beta_2} \, d\beta_2$. *Then for each even* $d \geq 2$

$$q_{(d-2)/2}^{\beta_d} q_{d/2}^{\beta_d} \, d\beta_d \propto d\gamma.$$

Hence $\mathcal{S}(d\gamma)$ *contains p.d.f.s having arbitrarily many jump points.*

In the next chapter we discuss systems of coupled oscillators, which provided the original motivation for this thesis.

Chapter 4

Systems of coupled oscillators

4.1 Statement of the inverse problem

Mathematical model of a system of coupled pendulums

A system of coupled pendulums is a mechanical apparatus like the one pictured in Figure 4.1. It consists of several pendulum bobs $B_1, \ldots, B_d$ suspended by wires and interconnected by springs. Based on this physical system we describe below a particular mathematical model, consisting of a list of parameters and corresponding equations of motion. Properly speaking, the object of study in this thesis is the mathematical model, rather than the underlying physical system. Nevertheless the physical system serves as the original motivation. Here we make some brief comments concerning the connection between the physical system and mathematical model, before shifting attention exclusively to the mathematical model.

Definition. To get around the awkward phrase "system of coupled pendulums",

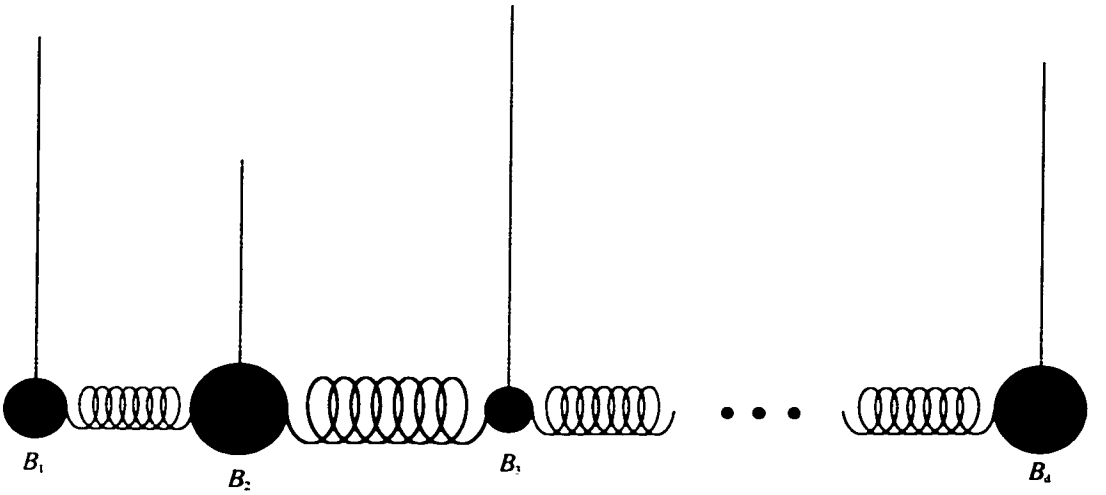

Figure 4.1: A system of coupled pendulums

we define a *c-pendulum* to be a system of coupled pendulums.

Firstly, our mathematical model is based on the linearized dynamics of the c-pendulum and is therefore applicable only for small displacements of the system from equilibrium. Secondly, restricting our attention to linearized dynamics means that from the physical point of view we do not distinguish between two (possibly different) c-pendulums provided they have the same linearized dynamics. Finally, the mathematical model is more general than the physical system of the c-pendulum, in that other mechanical systems also give rise to the same linearized dynamics, so that the inverse theory we develop applies more or less directly to these other types of mechanical systems as well.

Now to a precise description of our mathematical model for the c-pendulum. Our model is designed to capture the linearized dynamics of the c-pendulum, without friction or damping. (Thus for our purposes, each B_i moves within a line.) We

consider in particular the response of the c-pendulum to external forces from an initial state at equilibrium. We employ the following notation:

$$\begin{aligned} x_i(t) &= \text{the displacement from equilibrium of } B_i \text{ at time } t; \\ m_i &= \text{mass of } B_i; \\ k_i &= \text{spring constant for the } i^{\text{th}} \text{ spring}; \\ l_i &= \text{pendulum constant for the } i^{\text{th}} \text{ pendulum}; \\ f_i(t) &= \text{external force applied to } B_i \text{ at time } t. \end{aligned}$$

For each i, x_i and f_i are real-valued functions. To capture the situation of initial equilibrium, and for the technical reason that we need later on to convolve f_i with a bounded function, we restrict f_i to the family of functions $L^1(\mathbf{R}^+)$. We define the pendulum constant l_i to be inversely proportional to the length of the kth pendulum:

$$l_i = m_i \frac{\text{gravitational const.}}{\text{length of the } i^{\text{th}} \text{ pendulum}}.$$

(With this formalism, pendulum forces and spring forces act in the same way.) The linearized equations of motion are

$$m_i \ddot{x}_i = -l_i x_i + k_{i-1}(x_{i-1} - x_i) + k_i(x_{i+1} - x_i) + f_i, \tag{4.1}$$

where $k_0 = k_d = 0$ and $x_i(0) = \dot{x}_i(0) = 0$.

For a vector $v = (v_1, \ldots, v_d)$, we write $v \gg 0$ or $v^t \gg 0$ to indicate that for each i, $v_i > 0$. We write $v > 0$ or $v^t > 0$ to indicate that for each i, $v_i \geq 0$ and for some i, $1 \leq i \leq d$, $v_i > 0$.

Based on the equations of motion (4.1), a c-pendulum is characterized entirely by a list of its parameters m_i, l_i, k_i.

DEFINITION 4.1.1 A *system* is an array of the form

$$S = \begin{pmatrix} m \\ l \\ k \end{pmatrix} = \begin{pmatrix} m_1, \ldots, m_d \\ l_1, \ldots, l_d \\ k_1, \ldots, k_{d-1} \end{pmatrix},$$

where d is a positive integer, $m \gg 0$, $k \gg 0$ and $l > 0$. We refer to d as the *dimension* of the system. The collection of all systems is denoted $\mathcal{S}$.

The equations of motion in matrix form are

$$\ddot{x} + Ax = M^{-1}f, \quad x(0) = \dot{x}(0) = 0, \tag{4.2}$$

where: $f = (f_1, \ldots, f_d)^t$; A is the tridiagonal matrix

$$A = \begin{pmatrix} \frac{l_1+k_1}{m_1} & -\frac{k_1}{m_1} & & & & & \\ -\frac{k_1}{m_2} & \frac{l_2+k_1+k_2}{m_2} & -\frac{k_2}{m_2} & & & & \\ & -\frac{k_2}{m_3} & \frac{l_3+k_2+k_3}{m_3} & -\frac{k_3}{m_3} & & & \\ & & & \ddots & & & \\ & & & & & -\frac{k_{d-1}}{m_{d-1}} & \\ & & & & -\frac{k_d}{m_d} & \frac{l_d+k_{d-1}}{m_d} & \end{pmatrix}; \tag{4.3}$$

and M =diag$(m_1, \ldots, m_d)$. Given a system $S = \begin{pmatrix} m \\ l \\ k \end{pmatrix}$, of dimension d, we write

M =diag(m), L =diag(l), and

$$K = \begin{pmatrix} k_1 & -k_1 & & & & & \\ -k_1 & k_1+k_2 & -k_2 & & & & \\ & -k_2 & k_2+k_3 & -k_3 & & & \\ & & & \ddots & & & \\ & & & & & -k_{d-1} & \\ & & & & -k_{d-1} & k_{d-1} & \end{pmatrix}.$$

With this notation,

$$A = M^{-1}(K + L).$$

To emphasize the dependence of these various matrices on the system S, we write M_S, A_S and so on. We also write d_S to indicate the dimension of the system S.

Classes of experiments

For a fixed system S and external force f, the equation of motion (4.2) (where $A = A_S$) has a unique solution which we denote

$$x(t; S, f).$$

The associated velocity is denoted $\dot{x}(t; S, f)$, with components $\dot{x}_i(t; S, f)$ where $1 \leq i \leq d_S$. An *experiment* on a system S is a pair

$$(f, r),$$

where intuitively f represents an external force and r represents the response to f of part of the system.

Definition. Let $S \in \mathcal{S}$ and let $e_1, \ldots, e_d$ denote the standard basis vectors in $\mathbf{R}^d$, where $d = d_S$. For i, j in the range $1 \leq i, j \leq d_S$, we write $\mathcal{E}_{ij}(S)$ to denote the set of all pairs (f, r) where:

1. $f = \varphi e_i$ for some $\varphi \in L^1(\mathbf{R}^+)$;
2. $r(t) = \dot{x}_j(t; S, f)$.

We call $\mathcal{E}_{ij}(S)$ a *class* of experiments. Note: for convenience we make the condition $1 \leq i, j \leq d_S$ implicit in the notation $\mathcal{E}_{ij}(S)$.

Note that in the above definition the response $r(t)$ was defined in terms of the velocity of the jth body and not the displacement. In fact the displacement and velocity functions contain precisely the same information; it just happens that the formal expression for velocity is slightly simpler.

The inverse problem induced by a class of experiments

We are now in a position to state precisely the main problem of this chapter.

Main Problem. *Given the class of experiments $\mathcal{E}_{ij}(S)$, determine all systems $\widetilde{S}$ such that for some k, l*

$$\mathcal{E}_{kl}(\widetilde{S}) = \mathcal{E}_{ij}(S) \tag{4.4}$$

We call a system $\widetilde{S}$ satisfying (4.4) a *solution* to the main problem. The set of all solutions is denoted $\mathcal{S}(S, i, j)$. For the present thesis we focus mainly on a distinguished subset of $\mathcal{S}(S, i, j)$, namely the set $\mathcal{S}_{\min}(S, i, j)$ of minimum-dimensional solutions to the main problem. Thus our objective for the present chapter is to

parameterize $\mathcal{S}_{\min}(S, i, j)$ in terms of the "known data" $\mathcal{E}_{ij}(S)$. We do this by reducing the above main problem to the main problem of Chapters 2 and 3, and then appealing to the results obtained there. Note that if we can solve the main problem of the present chapter, then we can also solve the following restricted version, which corresponds to knowing the indices i, j.

Restricted Problem. *Given the class of experiments $\mathcal{E}_{ij}(S)$, and the indices i, j, determine all systems $\tilde{S}$ such that*

$$\mathcal{E}_{ij}(\tilde{S}) = \mathcal{E}_{ij}(S).$$

Intuitively, the main problem corresponds to the following physical situation. Imagine having "access" to two pendulum bobs B_i, B_j in a particular c-pendulum C_0, such that one can apply an arbitrary known force to B_i, and measure the response at B_j. Given only that C_0 is a c-pendulum, the problem is to determine as much as possible about C_0 using the limited experiment available. Of course, the best one can do in this respect is to describe the set of all c-pendulums consistent with the experimental data.

Note that the experiment described, forcing B_i and observing B_j, is essentially the most elementary type of dynamical, non-destructive test one could perform on C_0. Knowing the solution to the problem for this elementary case enables one to handle any more complicated test built up from elementary ones (e.g. forcing several pendulums and observing the response of several pendulums). Thus we are dealing with the most general situation we can.

4.2 Analysis of the coefficient matrix A_S

Definition of the Jacobi matrix J_S associated to a system

Definition. Let A_S be the coefficient matrix corresponding to the system S given in (4.3). Thus A_S has the form $A_S = M_S^{-1}(K_S + L_S)$. Set

$$J_S = M_S^{1/2} A_S M_S^{-1/2},$$

where $M_S^{1/2}$ denotes the positive definite square root of M_S. Observe that J_S is a Jacobi matrix.

PROPOSITION 4.2.1 *J_S is positive definite.*

Proof. From the definition,

$$J_S = M_S^{-1/2}(K_S + L_S)M_S^{-1/2}.$$

Note that K_S, L_S have quadratic forms

$$f(y) = \sum_{i=1}^{d-1} k_i(y_i + y_{i+1})^2, \quad g(y) = \sum_{i=1}^{d} l_i y_i^2,$$

respectively. Observe that $f(y) \geq 0$, and $f(y) = 0$ only if

$$y = (y_1, \ldots, y_n) = a(-1, 1, -1, \ldots, (-1)^d)$$

for some $a \in \mathbf{R}$. Also, $g(y) \geq 0$, and $g(y) = 0$ only if at least one $y_i = 0$. The quadratic form for the symmetric matrix $K_S + L_S$ is $q(y) = f(y) + g(y)$. We have that $q(y) \geq 0$, and $q(y) = 0$ only if

$$y = a(-1, 1, -1, \ldots, (-1)^d)$$

and at least one $y_i = 0$, that is, only if $y = 0$. Thus $K_S + L_S$ is positive definite. It follows that J_S, being congruent to $K_S + L_S$, is positive definite also. ∎

The relation of J_S to the system S

PROPOSITION 4.2.2 *The pair (M_S, J_S) determines the system S completely.*

Proof. For the present proof S is fixed, so we drop it as a subscript. As in the previous proof, we use the representation $J = M^{-1/2}(K + L)M^{-1/2}$, which follows from the definition of $J = J_S$. Let u denote the d-dimensional row vector all of whose entries are 1's, and note that $uK = 0$. This leads immediately to the formulas,

$$\begin{aligned} L &= \operatorname{diag}(uM^{1/2}JM^{1/2}) \\ K &= M^{1/2}JM^{1/2} - L. \end{aligned}$$

Thus M, L and K can all be written in terms of the pair (M, J). ∎

Definition. We say that a pair (M, J) is *physical* if there exists a system S such that $(M, J) = (M_S, J_S)$.

Definition. Given a finite set V in $\mathbf{R}^d$, we define the *convex cone* over V to be the positive cone over the closed, convex hull of V.

LEMMA 4.2.3 *Let J be a positive definite $d \times d$ Jacobi matrix. A d-dimensional row vector v satisfies both inequalities $vJ > 0$ and $v \gg 0$, if and only if v is in the convex cone over the rows of J^{-1}.*

Proof. Suppose $vJ > 0$ and $v \gg 0$. Then $v = (vJ)J^{-1}$ and since $vJ > 0$ this expresses v as a non-negative, non-zero combination of the rows of J^{-1}, which says exactly that v is in the convex cone over the rows of J^{-1}. Conversely, suppose v is in the convex cone over the rows of J^{-1}. Then $v = wJ^{-1}$ for some row vector $w > 0$.

Since J is positive definite, its sign pattern makes it a so-called Stieltjes matrix. (See Varga [V,p.85].) This class of matrices is inverse positive, i.e. each entry of J^{-1} is strictly positive. Since $w > 0$ this yields $v \gg 0$, and also $w = vJ > 0$. ∎

PROPOSITION 4.2.4 *The pair (M, J) is physical if and only if J is a positive definite Jacobi matrix and $M = (diag(\widetilde{m}))^2$ for some $\widetilde{m}$ in the convex cone over the rows of J^{-1}.*

Proof. Suppose $(M, J) = (M_S, J_S)$ is physical, and write $M^{1/2} = \text{diag}(\widetilde{m})$. By Proposition 4.2.1, J is positive definite. We know $L_S = \text{diag}(l)$ for some $l > 0$. By the proof of Proposition 4.2.2,

$$L_S = \text{diag}(uM^{1/2}JM^{1/2}).$$

Therefore

$$\begin{aligned} 0 < uM^{1/2}JM^{1/2} &= \widetilde{m}JM^{1/2} \\ &\Longrightarrow \widetilde{m}J > 0 \end{aligned}$$

Thus $\widetilde{m} = (\widetilde{m}J)J^{-1}$ where $\widetilde{m}J > 0$, and this shows that $\widetilde{m}$ is in the convex cone over the rows of J^{-1}.

Conversely, suppose that J is a positive definite Jacobi matrix and $M = (\text{diag}(\widetilde{m}))^2$ for some $\widetilde{m}$ in the convex cone over the rows of J^{-1}. (We will use M and J to construct matrices L and K such that M, L, K correspond to a system S.) Since J is a Stieltjes matrix, J^{-1} has all positive entries. By assumption $\widetilde{m} = vJ^{-1}$ for some $v > 0$, so $\widetilde{m} \gg 0$ and $\widetilde{m}J = (vJ^{-1})J = v > 0$. Note that $uM = \widetilde{m}$ (where u is the row vector all of whose entries are 1's) and so

$$uM^{1/2}JM^{1/2} = \widetilde{m}JM > 0,$$

since $\widetilde{m}J > 0$. Define

$$\begin{aligned} L &= \operatorname{diag}(uM^{1/2}JM^{1/2}) \\ K &= M^{1/2}JM^{1/2} - L. \end{aligned}$$

Observe that K is a Jacobi matrix, and furthermore

$$\begin{aligned} uK &= uM^{1/2}JM^{1/2} - uL \\ &= uM^{1/2}JM^{1/2} - uM^{1/2}JM^{1/2} \\ &= 0. \end{aligned}$$

Therefore K has the form

$$K = \begin{pmatrix} k_1 & -k_1 & & & & & \\ -k_1 & k_1+k_2 & -k_2 & & & & \\ & -k_2 & k_2+k_3 & -k_3 & & & \\ & & & \ddots & & & \\ & & & & & -k_{n-1} & \\ & & & & -k_{n-1} & k_{n-1} & \end{pmatrix},$$

for some $(k_1, \ldots, k_{d-1}) \gg 0$. It follows that $(M, J) = (M_S, J_S)$ where S is the system whose parameters come from M, K, L. ∎

4.3 Solution to the main problem

Solution to the equation of motion

Let S be a system and $\mathcal{E}_{ij}(S)$ be a class of experiments, to be held fixed throughout the present section. In terms of the matrices $(M, J) = (M_S, J_S)$, the equation of motion (4.2) becomes

$$\ddot{x} + M^{-1/2} J M^{1/2} x = M^{-1} f, \quad x(0) = \dot{x}(0) = 0.$$

The solution can be written formally as

$$x = (M^{-1/2} J^{-1/2} \sin(tJ^{1/2}) M^{-1/2}) * f; \tag{4.5}$$

$$\dot{x} = (M^{-1/2} \cos(tJ^{1/2}) M^{-1/2}) * f. \tag{4.6}$$

The definition of $\mathcal{E}_{ij}(S)$ involves $\dot{x}$ rather than x, so we focus on the solution for $\dot{x}$. An element of $\mathcal{E}_{ij}(S)$ has the form (f, r) where $f = \varphi e_i$ for some $\varphi \in L^1(\mathbf{R}^+)$, and $r(t) = \dot{x}_j(t; S, f)$. In terms of (4.6),

$$\begin{aligned} r &= (e_j^t M^{-1/2} \cos(tJ^{1/2}) M^{-1/2} e_i) * \varphi \\ &= ((m_i m_j)^{-1/2} e_j^t \cos(tJ^{1/2}) e_i) * \varphi, \end{aligned} \tag{4.7}$$

where m_i, m_j are the ith and j^{th} mass terms in S. Let $\alpha \in \mathcal{H}_{+,1}$ denote the p.d.f. which generates J (see Proposition 2.3.2), and write $\alpha(\xi) = \sum_{n=1}^{d} w_n H(\xi - \lambda_n)$. Recall the orthogonal diagonalization of $J = J_\alpha$ given on page 21 as follows.

$$J = (QW^{1/2}) \Lambda (QW^{1/2})^t,$$

where W =diag$(w_1, \ldots, w_d)$, Λ =diag$(\lambda_1, \ldots, \lambda_d)$, and

$$Q = \begin{pmatrix} q_0^\alpha(\lambda_1) & \cdots & q_0^\alpha(\lambda_d) \\ q_1^\alpha(\lambda_1) & \cdots & q_1^\alpha(\lambda_d) \\ \vdots & & \vdots \\ q_{d-1}^\alpha(\lambda_1) & \cdots & q_{d-1}^\alpha(\lambda_d) \end{pmatrix}.$$

In terms of this diagonalization, (4.7) becomes

$$r = \left((m_i m_j)^{-1/2} \sum_{n=1}^{d} q_{i-1}^\alpha(\lambda_n) q_{j-1}^\alpha(\lambda_n) w_n \cos(t\sqrt{\lambda_n}) \right) * \varphi \tag{4.8}$$

$$= \left((m_i m_j)^{-1/2} \int_{-\infty}^{\infty} \cos(t\sqrt{\xi}) d\gamma(\xi) \right) * \varphi, \tag{4.9}$$

where $d\gamma = q_{i-1}^\alpha q_{j-1}^\alpha \, d\alpha$.

Definition. Set $G_S(t) = (m_i m_j)^{-1/2} \sum_{n=1}^{d} q_{i-1}^\alpha(\lambda_n) q_{j-1}^\alpha(\lambda_n) w_n \cos(t\sqrt{\lambda_n})$.

Note that by (4.9), G_S can be viewed as the cosine transform of $d\gamma$ in the sense of distributions. (But we will not treat it on this level.)

Step 1: deconvolution and frequency transform

PROPOSITION 4.3.1 *$\mathcal{E}_{ij}(S)$ determines the function G_S.*

Proof. Note that $G_S \in C_{\text{ucb}}(\mathbf{R}^+)$ (the space of uniformly continuous, bounded functions) and that $L^1(\mathbf{R}^+)$ contains an approximate identity $\{\varphi_n\}$ with respect to $C_{\text{ucb}}(\mathbf{R}^+)$, for which $r_n = G_S * \varphi_n \longrightarrow G_S$ uniformly, as $n \longrightarrow \infty$. Thus the subset $\{(\varphi_n, r_n)\}$ of $\mathcal{E}_{ij}(S)$ determines G_S uniquely. ∎

Recall that α denotes the p.d.f. which generates J.

PROPOSITION 4.3.2 *G_S uniquely determines the d.f. $(m_i m_j)^{-1/2}\gamma$, where γ is defined by $d\gamma = q^{\alpha}_{i-1} q^{\alpha}_{j-1}\, d\alpha$.*

Proof. G_S is an almost periodic function in the sense of Bohr [B]. Thus G_S has an associated Fourier (cosine) series which gives one the frequencies $\sqrt{\lambda_n}$ for which $(m_i m_j)^{-1/2} q^{\alpha}_{i-1}(\lambda_n) q^{\alpha}_{j-1}(\lambda_n) w_n$ is non-zero, as well as the corresponding amplitude $(m_i m_j)^{-1/2} q^{\alpha}_{i-1}(\lambda_n) q^{\alpha}_{j-1}(\lambda_n) w_n$. (See [B,p.47].) From this data we can write down $(m_i m_j)^{-1/2}\gamma$. ∎

Step 2: parameterization of the solution set

From Step 1 we know that $\mathcal{E}_{ij}(S)$ determines the d.f. γ defined by $d\gamma = q^{\alpha}_{i-1} q^{\alpha}_{j-1}\, d\alpha$, up to a positive scalar multiple $(m_i m_j)^{-1/2}$ (where $\alpha \in \mathcal{H}_{+,1}$ is the generator of $J = J_S$). In this section we will not explicitly determine $\mathcal{S}(S, i, j)$. Rather, we will reduce the determination of $\mathcal{S}(S, i, j)$ to solving the main problem of Chapters 2 and 3, as follows.

THEOREM 4.3.3

$$\left\{ J_{\widetilde{S}} \,\middle|\, \widetilde{S} \in \mathcal{S}(S, i, j) \right\} = \left\{ J_{\beta} \,\middle|\, \beta \in \mathcal{S}(d\gamma) \right\}.$$

Proof. Suppose $\widetilde{S} \in \mathcal{S}(S, i, j)$ so that $\mathcal{E}_{kl}(\widetilde{S}) = \mathcal{E}_{ij}(S)$. Then by Step 1, $G_{\widetilde{S}} = G_S$ and so

$$q^{\beta}_{k-1} q^{\beta}_{l-1}\, d\beta \propto d\gamma,$$

where $\beta \in \mathcal{H}_{+,1}$ is the generator of $J_{\widetilde{S}}$. But this is exactly the condition for β to be in the set $\mathcal{S}(d\gamma)$.

Conversely suppose $\beta \in \mathcal{S}(d\gamma)$, so that $q^{\beta}_{k-1} q^{\beta}_{l-1}\, d\beta \propto d\gamma$, for some k, l. Choose $\widetilde{m}$ in the convex hull of the rows of J_{β}^{-1}. (Note that J_β is positive definite, since the jump points of γ are all positive.) Choose the scalar $a > 0$ such that

$$(a\widetilde{m}_k a\widetilde{m}_l)^{-1/2} q^{\beta}_{k-1} q^{\beta}_{l-1}\, d\beta = (m_i m_j)^{-1/2}\, d\gamma. \tag{4.10}$$

Then set $M_\beta = (\mathrm{diag}(a\widetilde{m}))^2$. Observe that the pair (M_β, J_β) is physical, by Proposition 4.2.4. Let $\tilde{S}$ denote the system determined by (M_β, J_β). By (4.10), $G_{\tilde{S}} = G_S$, and therefore $\mathcal{E}_{kl}(\tilde{S}) = \mathcal{E}_{ij}(S)$. So $J_\beta = J_{\tilde{S}}$ and $\tilde{S} \in \mathcal{S}(S, i, j)$. ∎

COROLLARY 4.3.4

$$\left\{ J_{\tilde{S}} \,\middle|\, \tilde{S} \in \mathcal{S}_{\min}(S, i, j) \right\} = \left\{ J_\beta \,\middle|\, \beta \in \mathcal{S}_{\mathrm{reg}}(d\gamma) \right\}.$$

Thus we have shown that our stated goal for the present chapter, determining $\mathcal{S}_{\min}(S, i, j)$, is equivalent to determining the manifold of regular solutions to the main problem stated at the end of Chapter 2 and treated in detail in Chapter 3. The only extra point to be made is that there are many $\tilde{S} \in \mathcal{S}(S, i, j)$ corresponding to each $\beta \in \mathcal{S}(d\gamma)$. We can easily make this correspondence precise by returning to the proof of Theorem 4.3.3, and noting that to construct $\tilde{S}$ given β, we chose an arbitrary $\widetilde{m}$ in the convex hull of the rows of J_{β}^{-1}. If β has d jump points, this corresponds to a $(d-1)$-dimensional "simplex" of possible solutions $\tilde{S}$ corresponding to each $\beta \in \mathcal{S}(d\gamma)$.

4.4 General remarks

Other types of oscillating systems

The main problem of this chapter was stated in terms of c-pendulums, but most of the analysis is valid for a range of system types, not just c-pendulums. We could just as easily have based the definition of "system" on either of the configurations of coupled oscillators depicted below (as well as others). These give rise to slightly

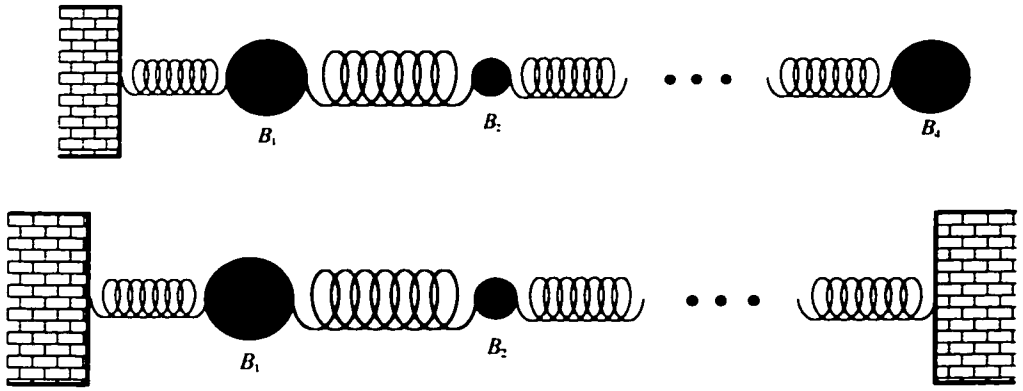

Figure 4.2: Other systems of coupled oscillators

different (and simpler) decompositions of the tridiagonal coefficient matrix which appears in the equations of motion, but there is still a correspondence with Jacobi matrices giving precisely the same flavour of results as for the c-pendulum.

Implementation

If the inverse theory developed in this thesis were to be implemented for some physical application, then one would have to consider the numerical and computational aspects of the problem, which we have intentionally left aside. On the basis of the results in Chapter 3, it seems as if the geometric structure of $\mathcal{S}_{\text{reg}}$ may be sufficiently complicated in the general case to make computation impractical, but this requires further investigation. On the other hand we see that some very important geometric information, such as the dimension Δ of the manifold of solutions, might be quite reasonably estimated on the basis of measured data. And without some theoretical analysis, it might not be obvious that the "degree of orthogonality" Δ is an important thing to calculate. In any case the results in this thesis are a first step, which gives a view to many possible avenues for interesting future research.

Chapter 5

Conclusion

In this chapter we discuss briefly the main accomplishments of the thesis, and sketch the interrelationships among the main results. Physical considerations for systems of coupled oscillators provided the original motivation for this thesis, so we begin with a summary of the implications of the thesis for such systems.

Systems of coupled oscillators

If one carries out force-response experiments between two pendulum bobs B_i, B_j in a particular c-pendulum C_0, what can one infer about C_0? And what sequence of computations should be carried out in order to obtain this information? These questions were asked in Chapter 4, and answered in part by appealing to the earlier results in the thesis. Let S be the system, or list of parameters, representing C_0. In the following paragraph we summarize results obtained in the thesis by sketching the sequence of steps involved in computation of the solution manifold $\mathcal{S}_{\mathsf{min}}(S, i, j)$.

First, the best choice for an input force applied to B_i is an approximation to a Dirac delta function. Then the output response at B_j will be approximately G_S (Proposition 4.3.1). The Fourier cosine transform of the almost periodic function G_S allows one to compute the d.f. $\tilde{\gamma} = (m_i m_j)^{-1/2}\gamma$ where γ has the structure $d\gamma = q_i^\alpha q_j^\alpha \, d\alpha$ with $\alpha \in \mathcal{H}_{+,1}$ being an unknown p.d.f. The relationship of α to S is that α generates the Jacobi matrix J_S. The next step is to compute the polynomials $p_{\tilde{\gamma}}$ and $p^{\tilde{\gamma}}$, and then to compute the roots of $p^{\tilde{\gamma}}$. Note that $p_{\tilde{\gamma}} = p_\gamma$ and $p^{\tilde{\gamma}} \propto p^\gamma$. The number of roots of $p^{\tilde{\gamma}}$ in each interval determined by the jump points of $\tilde{\gamma}$ dictates that intervals type: one root means constant sign; no root means higher degree; two roots means lower degree (Lemma 3.5.5). Using this classification of intervals together with $p^{\tilde{\gamma}}$, construct the coordinate base $\mathcal{C}$ (Section 3.6). Then $\mathcal{S}_{\text{reg}}(d\tilde{\gamma})$ is the image of $\mathcal{C}$ by the map θ whose explicit evaluation is detailed in the proof of Theorem 3.6.18. Finally, each point $\beta \in \mathcal{S}_{\text{reg}}(d\tilde{\gamma})$ generates a family of systems in $\mathcal{S}_{\text{min}}(S, i, j)$ as follows. Note that β carries with it associated indices k, l. Choose any $\widetilde{m}$ in the closed convex hull of the rows of J_β^{-1}. Choose $r > 0$ such that

$$r^{-1}(\widetilde{m}_k \widetilde{m}_l)^{-1} q_k^\beta q_l^\beta \, d\beta = d\tilde{\gamma}.$$

Set $M = r(\text{diag}(\widetilde{m}))^2$. Then (M, J_β) is a physical pair which determines a system $\tilde{S}$ in $\mathcal{S}_{\text{min}}(S, i, j)$. Every member of $\mathcal{S}_{\text{min}}(S, i, j)$ is realized in this way.

Overview of Chapter 3

Chapter 3 contains the core technical arguments in this thesis. Here we highlight the main results of Chapter 3 and sketch the key interdependencies of these results. The

main objective in Chapter 3 is to describe $\mathcal{S}_{\text{reg}}(d\gamma)$ in the general case. If it happens that $\Delta > 0$ then the problem is much more difficult. Consequently the case $\Delta > 0$ takes up most of Chapter 3; we confine the present discussion to that case.

The essential idea behind Chapter 3 is to realize $\mathcal{S}_{\text{reg}}(d\gamma)$ as the image of a set $\mathcal{C}$ of polynomials by a many-valued function. Each polynomial in $\mathcal{C}$ gives rise to several divisors, and each of these corresponds to a member of $\mathcal{S}_{\text{reg}}(d\gamma)$. The main results of Sections 3.1-3.5 build up to an explicit determination of the coordinate base $\mathcal{C}$. These results and their mutual dependencies are illustrated in Figure 5.1, which includes Proposition 3.6.2 from Section 3.6.

The remainder of Section 3.6 after Proposition 3.6.2 consists roughly of two parts. The first part is an analysis of the structure of $\mathcal{C}$, which essentially consists of the three results depicted in Figure 5.2.

The second part of Section 3.6 is an analysis of the structure of $\mathcal{S}_{\text{reg}}(d\gamma)$ relative to that of $\mathcal{C}$. Specifically, in Theorem 3.6.18 we show that $\mathcal{S}_{\text{reg}}(d\gamma)$ consists of a finite union of "sheets", each of which is diffeomorphic to $\mathcal{C}$. In Theorem 3.6.19 we show that the sheets corresponding to divisors having a fixed degree intersect on a set of measure zero.

Main accomplishments of the thesis

With respect to systems of coupled oscillators the main accomplishment of this thesis is to provide a solution to the stated family of inverse problems. This greatly extends the previously known results concerning the special case $i = j = 1$. From a conceptual standpoint, a key insight underpinning the thesis is the connection between

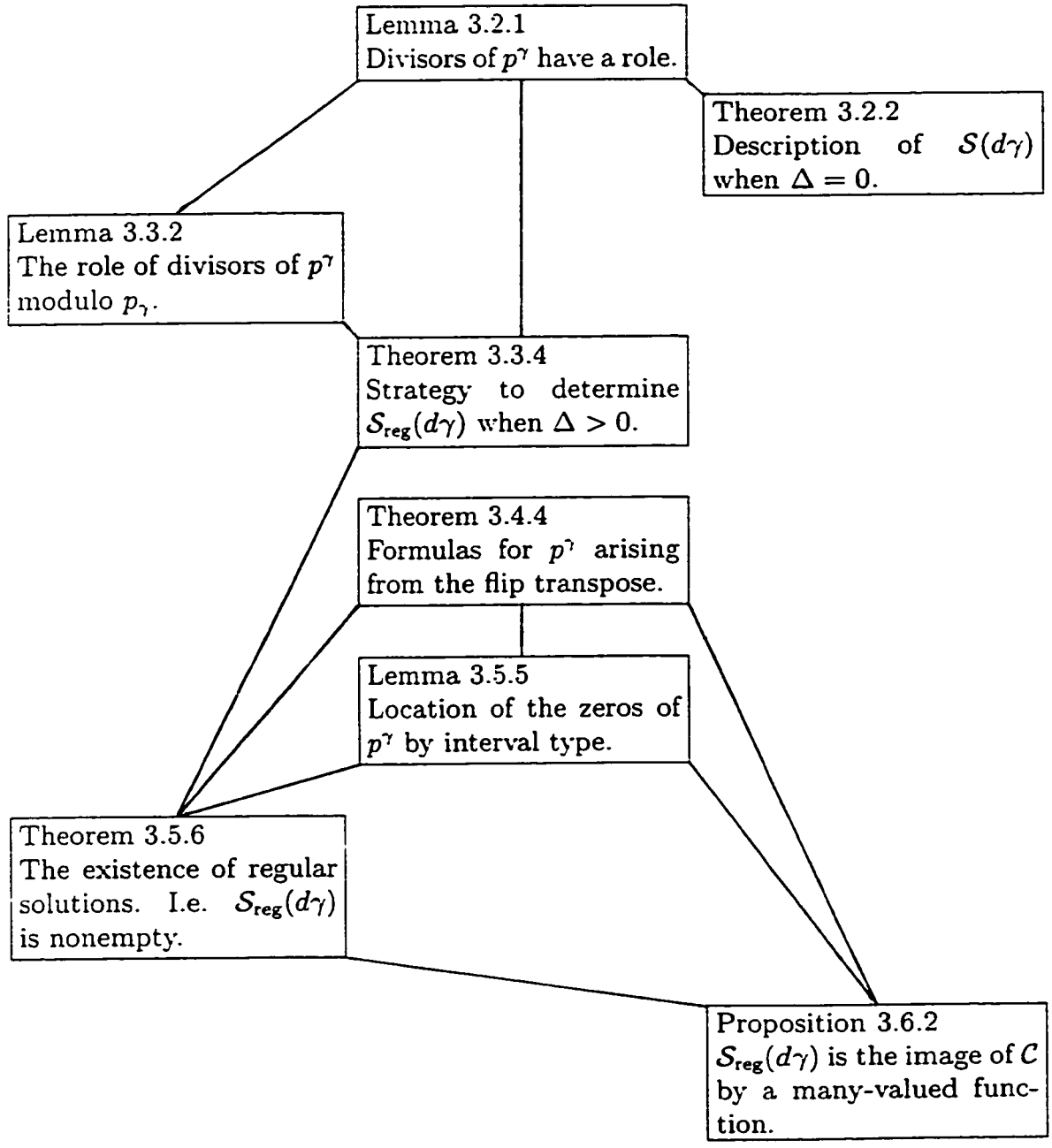

Figure 5.1: The first part of Chapter 3

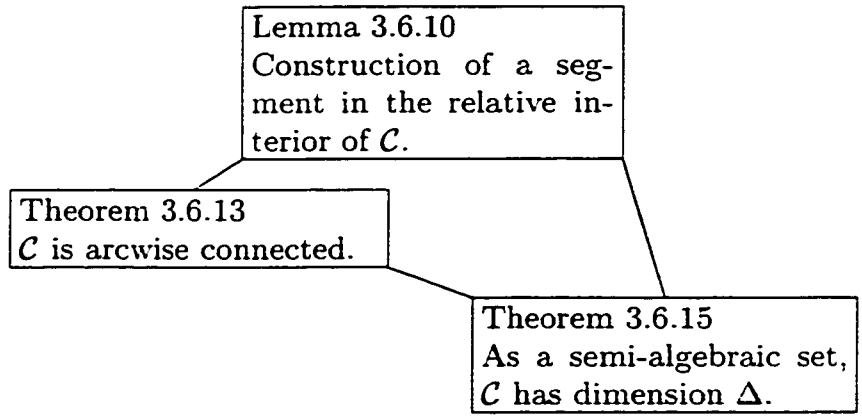

Figure 5.2: Section 3.6

inverse problems for coupled oscillators and the classical moment problem. The fundamental role which orthogonal polynomials play in the moment problem carries over, providing a useful tool. The arguments comprising Chapter 3 involve several technical obstacles. From the technical point of view the following are principal accomplishments of this thesis.

- The composite polynomial plays an important role. Specifically, solutions to the inverse problem are determined by divisors modulo the characteristic polynomial of the composite polynomial.
- The flip transpose yields explicit formulas for the composite polynomial.
- The solution manifold can be parameterized over a semi-algebraic set $\mathcal{C}$ which is determined by the composite polynomial.
- The parameterization of the solution manifold over $\mathcal{C}$ is reasonably well-behaved.

This concludes our look back at the main results of the thesis.

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