ABSTRACT

NANCE, EZRA FRANKLIN. Parametrizing Copositive Polynomials. (Under the direction of Hoon Hong).

In this thesis we parametrize families of copositive polynomials. A copositive polynomial is simply a polynomial which is nonnegative for all nonnegative inputs. These polynomials are not only very natural but are useful to applications from many diverse areas of science and engineering.

Broadly speaking, there are two ways to describe a set: implicit and parametric. Implicit descriptions are good for checking whether an element belongs to the set, and parametric descriptions are good for exploring the set. Much work has been done finding implicit descriptions of copositive sets, but surprisingly little has been done on finding parametric descriptions. Thus this thesis aims to make progress in parametrization.

Parametrizing a copositive set involves identifying a domain for the parameters and a map which sends a domain element to a copositive polynomial. In order for a parametrization to be useful, first the map should be (almost) bijective, and second the domain and map should be “simple" in some sense. The (almost) bijectivity is important because it allows us to explore almost every element of the set and also only once. The simplicity is important because it allows easy exploration of that set. In this thesis we present almost bijective and simple parametrizations for several families of copositive polynomials. Below is a summary of the results in each chapter.

1. In Chapter 1, we introduce the main concepts of copositive polynomials and parametrization. We do this by contrasting them with nonnegative polynomials and implicitization, both of which are highly studied. We then review important results in the areas of nonnegative polynomials, copositive polynomials, implicitization, and parametrization.

2. In Chapter 2, we present a parametrization of the set of copositive univariate polynomials of arbitrary degree d, see Theorem 2.2.1. This parametrization is almost bijective, the domain is simple, namely $\mathbb{R}^d_{\geq 0}$, and the map is a polynomial function.

3. In Chapter 3, we present a parametrization of the set of copositive bivariate polynomials of degree 2 (equivalently, symmetric 3×3 matrices), see Theorem 3.2.1. This parametrization is almost bijective, the domain is simple, namely $\mathbb{R}^4_{\geq 0} \times \Delta_3$ (Δ_3 is the standard 2-dimensional simplex), and the map is a rational function.

4. In Chapter 4, we generalize our ideas to copositive degree 2 polynomials with any number of variables (equivalently, symmetric $n \times n$ matrices). In so doing we characterize the

boundary, and partition it into "faces," see Theorem 4.3.1. We then extend these faces out into full dimensional pieces we call "shards." Finally, we present a parametrization of a particularly important shard, see Theorem 4.2.1. This parametrization is almost bijective, the domain is simple, namely $\mathbb{R}_{\geq 0}^{n-1} \times \mathbb{R}^{\binom{n-1}{2}} \times \mathbb{R}_{\geq 0}^{n-1} \times \mathbb{R}_{\geq 0}$, and the map is a radical function.

5. In Chapter 5, we present some preliminary results for arbitrary copositive polynomials (equivalently, symmetric tensors) in preparation for parametrizing those polynomials.

This work has many possible future directions to go. We could try to parametrize different families of copositive matrices, and eventually we could try to parametrize the entire set of copositive matrices. More ambitiously, we could try to parametrize a natural family of copositive tensors with the grand goal of parametrizing the entire set of copositive tensors.

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Parametrizing Copositive Polynomials

by
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BIOGRAPHY

Ezra Nance was born in the northwest corner of Tennessee. Always enjoying puzzles, math, and science he eventually became an undergraduate engineering student at the University of Tennessee at Martin, graduating in 2013. He then got a job for a crane manufacturing company in Chicago, Illinois and worked with power and logic systems. After spending a couple of years doing this he became disheartened and bored with the work. It was at this time he began independently studying mathematics.

Eventually he decided to go back to the University of Tennessee at Martin to get his undergraduate degree in mathematics with the intention of going to graduate school. While finishing his degree he worked with Dr. Jason Devito and jointly published his first math paper. Dr. Devito had a connection to North Carolina State, and he suggested that Ezra should apply there for graduate school. He was accepted for the 2018 fall semester.

While in Raleigh Ezra suffered several hardships. Not only was the graduate level material difficult, but the world went through the Covid-19 pandemic. On top of that, in the fall of 2020 he suffered a hemorrhagic stroke resulting in the paralysis of his right side. Luckily, through surgery and physical therapy he was able to recover. It was around this time that Ezra began to work with his advisor, Dr. Hoon Hong. Through Dr. Hong's patience and mentorship Ezra is expected to graduate with his PhD in mathematics in 2024.

ACKNOWLEDGEMENTS

First I would like to acknowledge that I wouldn't be in this position without the tremendous help of others. I can't name them all, but I can name a few. First I would like to thank my mother and father, Vicki and Jim, for always supporting me in whatever I wished to pursue. I would like to thank my brother, Kramer, for being a role model in his willingness to create. And I would like to thank the rest of my family for always believing in me, maybe even a little too much.

On the academic side, of course I need to thank my advisor, Dr. Hoon Hong, for being patient, kind, and wise; and for always trying to guide me toward a better path. I truly stand on the shoulders of a giant, both of heart and mind. I would like to thank Dr. Jason Devito for showing me just how vast mathematical research is and for agreeing to work with me as an undergraduate student. I would like to thank my committee member, Dr. Irina Kogan, for being my introduction to graduate level mathematics. While taking her classes in differential geometry she helped nurture and grow my love of the subject. I have my committee member, Dr. Dàvid Papp, to thank for his spectacular classes in Matrix Theory, without which I wouldn't have the appreciation of Linear Algebra that I now have. And finally I would like to thank my committee members, Dr. Martin Helmer and Dr. Zheng Li, for generously sacrificing their time to give me the opportunity to succeed. I sincerely appreciate it. Finally, I would like to thank my entire committee for helping me greatly improve this thesis. Without everyone's willingness to pitch in, my thesis would've been a shadow of what it has become.

While in Raleigh there were several people who helped me on a personal level. First, I would like to thank my roommates, Jack and Joe, for all of the fun nights filled with cooking, drinking, and games. I would like to thank my friend, Ashley, for helping me during a particularly difficult time in my life. For that I am forever in your debt. And finally I would like to thank my dog, Ozzy, for being the best boy. Though he probably didn't appreciate all of the time I spent doing math and not paying attention to him.

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1

INTRODUCTION

In this chapter, we will introduce the problem, provide examples of previous work, and eventually summarize the original contributions reported in the following chapters.

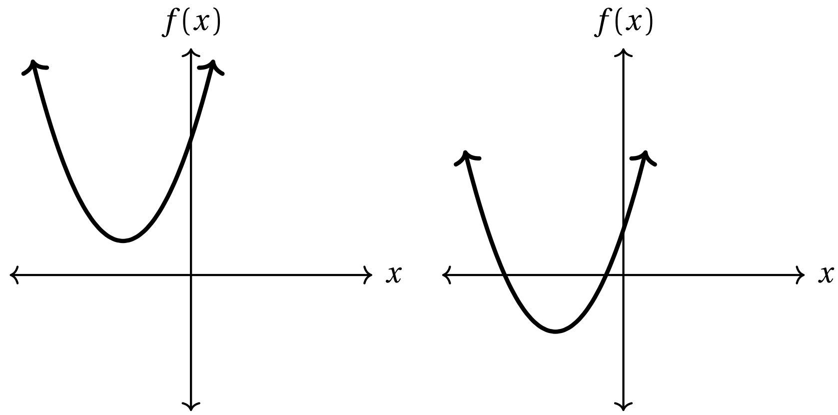
1.1 Problem

In this thesis we aim to make significant progress in parametrizing copositive polynomials. So what are copositive polynomials? What does it mean to parameterize them?

Copositive polynomials

Let us start by explaining what copositive polynomials are and why they are studied. In order to put copositivity in context, we will contrast copositive polynomials with nonnegative polynomials. Below we formally define both copositive and nonnegative polynomials and illustrate them by simple plots:

f is *nonnegative*	f is *copositive*
$f(x) \geq 0$ for all $x \in \mathbb{R}^n$	$f(x) \geq 0$ for all $x \in \mathbb{R}^n_{\geq 0}$

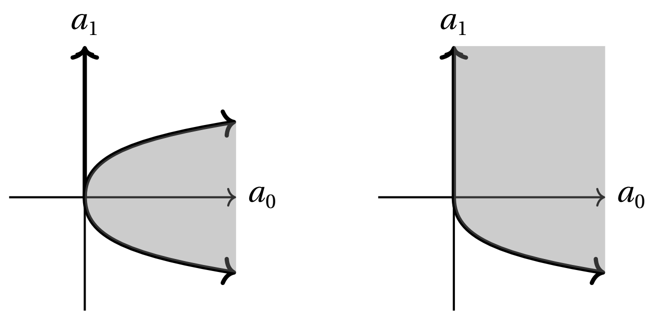


Nonnegativity is a natural requirement. After all, many quantities we encounter in the world don't make sense for negative values, for instance mass, time, area, etc. It was for this very reason that people in the past were slow to adopt negative numbers as legitimate numbers. While we accept them now, in applications we often have to ignore negative solutions. Thus, nonnegativity is often an important property to have.

Copositivity relaxes the nonnegativity requirement slightly to allow for negative outputs when the input is negative. Again, these conditions are quite natural. If we think of nonnegative quantities as being physically realizable, we have polynomials which can take in values that make physical sense and produce values which also make physical sense. Not only that, but by allowing copositivity, instead of nonnegativity, we allow for polynomials of odd degree. Again, one could imagine this being crucial for applications involving something like volume where polynomials of degree three often appear.

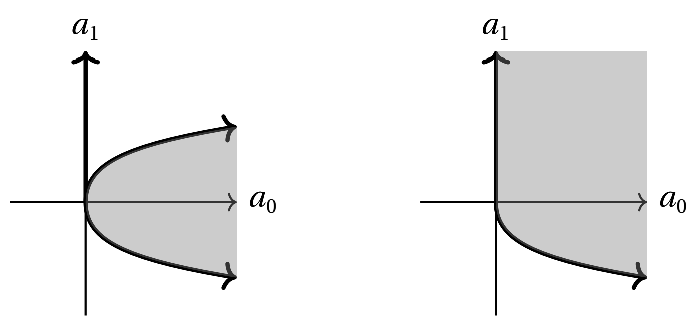
We would like to get a handle on these sets, that is, nonnegative and copositive polynomials. However, it can be quite challenging to think about or to visualize a set which contains an infinite number of polynomials. However, every polynomial is uniquely determined by its coefficients. Therefore, referring to the set of nonnegative or copositive polynomials is identical to referring to the set of coefficients which result in that polynomial being nonnegative or copositive. This means that we can think about these sets of polynomials as simply subsets of the coefficient space. Below we see the sets of nonnegative and copositive monic univariate quadratic polynomials expressed through their coefficients. These are the types of sets we are working with.

For all $x \in \mathbb{R}$	For all $x \in \mathbb{R}_{\geq 0}$
$f(x) = x^2 + a_1 x + a_0 \geq 0$	$f(x) = x^2 + a_1 x + a_0 \geq 0$



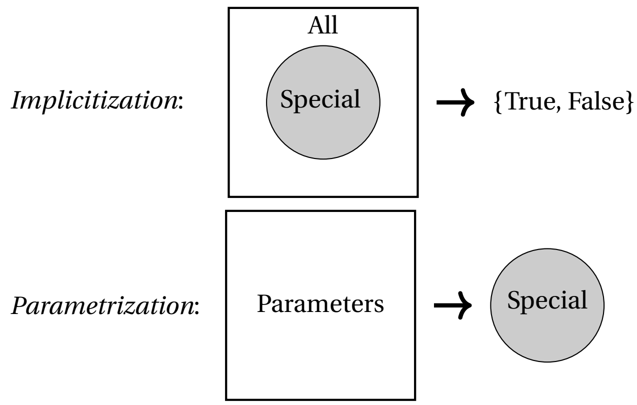
Parametrization

Now we will explain what parametrization is and why it is studied. In order to put everything in context, we will contrast parametrization with implicitization. Both of these methods are used to describe sets, and specifically, we are looking at semialgebraic sets. In short, an implicitization of a semialgebraic set is a conjunction and disjunction of polynomial equations and inequalities that completely determine which points are in the set. On the other hand, a parametrization consist of a domain and a map such that the image of that map is the set being described. We can see examples of an implicitization and a parametrization of the same sets as above.



Implicitization:	$a_1^2 - 4a_0 \leq 0$	$a_1^2 - 4a_0 \leq 0 \vee (a_0 \geq 0 \wedge a_1 \geq 0)$
Parametrization:	$\Phi : \mathbb{R} \times \mathbb{R}_{\geq 0} \to \{\text{Nonnegative}\}$	$\Phi : \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \to \{\text{Copositive}\}$
	$(t_0\ ,\ t_1) \mapsto (a_0, a_1)$	$(t_0\ ,\ t_1) \mapsto (a_0, a_1)$
	$a_0 = t_0^2 + t_1$	$a_0 = t_0^2$
	$a_1 = 2t_0$	$a_1 = t_1 - 2t_0$

We can think about implication and parametrization on a high level schematically:

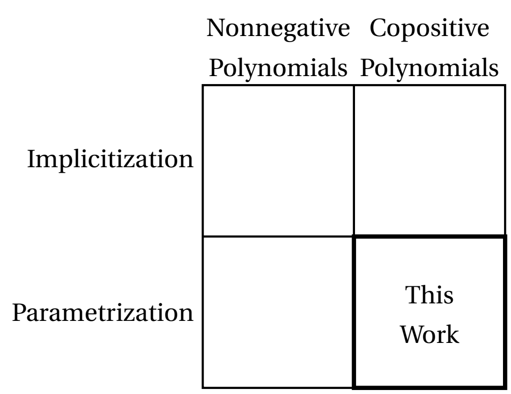


Implicitization is an approach for addressing the fundamental need of checking whether an object has a special property. For this, it generates a boolean expression on the representation of an arbitrary object such that the boolean expression is either true or false, depending on whether the object has that special property or not. One strives to obtain a “simple” boolean expression.

Parametrization is an approach for addressing the fundamental need of exploring all of the special objects economically. For this, one generates a bijective map from a domain of parameters to the set of all special objects. Often “almost” bijectivity is sufficient in practice and thus allowed. One strives to obtain a “simple” domain and a “simple” map.

Parametrization of Copositive polynomials

We can visualize everything discussed so far as a grid. Some quadrants have a huge amount of work associated with them, while others have far less. Now that we can see where this thesis fits into the larger body of work, we will go over previous works in this diagram.



1.2 Previous Works

Here we review previous works and acknowledge some of the people who have contributed to this area. We will begin by covering some results for creating an implicit description of a family of polynomials. Below we have separated these results by the degree of the polynomials as well as the number of variables. Afterwards, we repeat this process for parametrization results.

1.2.1 Implicitization

Implicitization is a well-studied area. We will now provide some context by discussing some of these implicitization results as they apply to copositive and nonnegative polynomials.

Arbitrary degree and Arbitrary number of variables

Based upon our discussions so far we can formalize what we mean by nonnegative and copositive polynomials with quantifiers as follows.

$$\begin{array}{lcl} f \text{ is nonnegative} & : & \underset{x\in\mathbb{R}^n}{\forall} f(x) \geq 0 \\ f \text{ is copositive} & : & \underset{x\in\mathbb{R}^n_{\geq 0}}{\forall} f(x) \geq 0 \end{array} \tag{1.1}$$

Note that these are formulas in the first order theory of a real closed field, that is, they are quantified boolean combinations of polynomial inequalities. The variables in these first order formulas are x and the coefficients of f. The condition is not simple because x is universally quantified. Hence, one would like to eliminate the variables x to arrive at an implicit description for either the nonnegative or copositive polynomials.

Alfred Tarski's celebrated theorem on real closed fields states that every first order formula is equivalent to a quantifier-*free* formula [64], in other words, a boolean combination of polynomial inequalities in the unquantified variables only. Tarski's proof was constructive, that is, the proof provided the first algorithm for eliminating quantifiers [65]. Since then, various alternative or improved algorithms have been developed. To list a just a few: Collins' CAD (cylindrical algebraic decomposition) method and further improvements [14, 1, 41, 31, 32, 16, 33, 42, 15, 43, 45, 44, 48, 46, 5, 47, 13, 9, 17, 12, 8, 59, 60, 61]. Analyzing and improving asymptotic worst case computing bounds [3, 26, 25, 10, 11, 28, 53, 69, 7]. Special family of inputs [67, 40, 68, 34, 23, 24, 35, 37, 36]. Some of them have fully implemented software packages: QEPCAD [32, 16, 6], Reduce in Mathematica [59], RedLog [63], SyNRAC [71], Discoverer [70], RAGlib [55], Regular Chain [13] and so on.

Thus, one might wonder whether we could just run those software on the desired quantified formula above. However, they become practically infeasible as n grows. Hence, there has been intensive research on various special theories and methods which exploits the structure of the above formulas. Below we elaborate on some of them.

Degree 1 and Arbitrary number of variables

If we restrict our attention to polynomials of degree one, then the problem becomes trivial. Let $f \in \mathbb{R}[x_1,\dots,x_n]$ be of the form

$$f(x_1,\dots,x_n) = a_0 + a_1x_1 + \cdots + a_nx_n.$$

Then clearly f is nonnegative if and only if $a_0 \geq 0$ and $a_1 = \cdots = a_n = 0$. Furthermore, f is copositive if and only if $a_0, a_1, \dots, a_n \geq 0$. Thus, the problem is solved for degree 1 polynomials.

Degree 2 and Arbitrary number of variables

Let $f \in \mathbb{R}[x_1,\dots,x_n]$ be of degree 2. Let

$$\bar{f} = x_{n+1}^2 f(x_1/x_{n+1},\dots,x_n/x_{n+1}) \ \in \ \mathbb{R}[x_1,\dots,x_n,x_{n+1}]$$

be the homogenization of f. Then it is easy to show that

$$f \text{ is nonnegative} \quad \Longleftrightarrow \quad \bar{f} \text{ is nonnegative},$$

and

$$f \text{ is copositive} \quad \Longleftrightarrow \quad \bar{f} \text{ is copositive}.$$

Recall that every degree two homogeneous polynomial can be expressed as

$$\bar{f}(x) = x^{\intercal}Ax,$$

where A is a real symmetric matrix. Thus, we can identify the polynomial f with the matrix A. Hence, the polynomial f being nonnegative corresponds to the matrix A being positive semidefinite. This motivates the following definition: a real symmetric matrix, A, is copositive if its corresponding polynomial is copositive. Therefore, from now on, we will present previous works in terms of matrices.

The next two theorems offer implicit descriptions for the set of positive semidefinite matrices and the set of copositive matrices, respectively. The positive semidefinite results are classic and well known. However, the copositive results are newer and less known.

Theorem 1.2.1. *Let $f \in \mathbb{R}[x_1,\dots,x_n]$ be of degree 2 and let A be its associated real symmetric matrix. Then the following are equivalent:*

1. *f is nonnegative, that is, A is positive semidefinite.*
2. *All principal minors of A are nonnegative.*

Example 1.2.1. We will find an implicitization of the set of nonnegative quadratic polynomials of two variables. From our previous discussion we know that these polynomials correspond to 3×3 positive semidefinite matrices. From the above theorem we have that the matrix

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}$$

is positive semidefinite if and only if all of its principal minors are nonnegative. In other words, the following boolean expression needs to be true:

$$\bigwedge \begin{cases} a_{11} \geq 0 \\ a_{22} \geq 0 \\ a_{33} \geq 0 \\ \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix} \geq 0 \\ \begin{vmatrix} a_{11} & a_{13} \\ a_{13} & a_{33} \end{vmatrix} \geq 0 \\ \begin{vmatrix} a_{22} & a_{23} \\ a_{23} & a_{33} \end{vmatrix} \geq 0 \\ \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{vmatrix} \geq 0, \end{cases}$$

where this notation is AND'ing each row together to form one boolean expression.

Theorem 1.2.2 (Väliaho, 1986, [66])**.** *Let $f \in \mathbb{R}[x_1, \ldots, x_n]$ be of degree 2 and let A be its associated real symmetric matrix. Then following are equivalent:*

1. *f is copositive, that is, A is copositive.*
2. *For every principal submatrix D of A such that* $\det(D) < 0$*, the last row of* $\operatorname{adj}(D)$ *contains a negative element.*

Example 1.2.2. We will find an implicitization of the set of copositive quadratic polynomials of two variables. As before, these polynomials correspond to 3×3 copositive matrices. From the above theorem we know that the matrix

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}$$

is copositive if and only if the following boolean expression is true:

$$\bigwedge \begin{cases} a_{11} \geq 0 & \vee & 1 < 0 \\ a_{22} \geq 0 & \vee & 1 < 0 \\ a_{33} \geq 0 & \vee & 1 < 0 \\ \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix} \geq 0 & \vee & -a_{12} < 0 \quad \vee \quad a_{11} > 0 \\ \begin{vmatrix} a_{11} & a_{13} \\ a_{13} & a_{33} \end{vmatrix} \geq 0 & \vee & -a_{13} < 0 \quad \vee \quad a_{11} > 0 \\ \begin{vmatrix} a_{22} & a_{23} \\ a_{23} & a_{33} \end{vmatrix} \geq 0 & \vee & -a_{23} < 0 \quad \vee \quad a_{22} > 0 \\ \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{vmatrix} \geq 0 & \vee & \begin{vmatrix} a_{12} & a_{22} \\ a_{13} & a_{23} \end{vmatrix} < 0 \quad \vee \quad -\begin{vmatrix} a_{11} & a_{12} \\ a_{13} & a_{23} \end{vmatrix} < 0 \quad \vee \quad \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix} < 0. \end{cases}$$

Here we can see that the first column is the same as the condition for being positive semidefinite. However, each row contains a logical OR operator which relaxes the condition. This illustrates how copositivity is a relaxation of nonnegativity.

Arbitrary degree and 1 variable

One way to approach this problem is by counting the number of real roots a polynomial has. However, we begin to run into issues with multiplicity. For instance, a polynomial with a positive real root can still be copositive, as long the root has even multiplicity. Thus, these root counting techniques are better suited for finding implicitizations for polynomials with no positive roots, or no real roots at all. Generally speaking, this is fine since polynomials that are strictly positive make up *most* of the nonnegative polynomials. Similarly, polynomials which have no positive real roots make up *most* of the copositive polynomials. With that in mind we will proceed by counting the number of real roots a polynomials has. This idea has a long history with many results. Here we will name just a few. In order to do this let

$$
\begin{aligned}
p(f) &= \text{the number of positive real roots of } f \text{ (counting multiplicity)}\\
v(f) &= \text{the number of sign variations between consecutive non-zero coefficients.}
\end{aligned}
$$

Theorem 1.2.3 (Descartes, 1637 [19]). *Let $f \in \mathbb{R}[x]$ be nonzero. Then*

1. $p(f) \leq v(f)$.
2. $p(f)$ *and* $v(f)$ *have the same parity.*

Descartes' Rule of Signs can be used to check if some polynomials are nonnegative or copositive. However, it cannot accurately sort all univariate polynomials. Thus, we have to move on. For the following theorems, we define

$$
\begin{aligned}
r_I(f) &= \text{the number of real roots of } f \text{ (counting multiplicity) in the interval } I\\
r_I^*(f) &= \text{the number of distinct real roots of } f \text{ in the interval } I\\
v(S) &= \text{the number of sign variations in the sequence } S
\end{aligned}
$$

Budan and Fourier independently proved a generalization of Descartes' Rule of Signs.

Theorem 1.2.4 (Budan 1807 [18] Fourier 1820 [21]). *Let $f \in \mathbb{R}[x]$ of degree d. Let*

$$S_x = \left\{ f(x), f'(x), \ldots, f^{(d)}(x) \right\}$$

Then for any interval $(a, b]$, we have

1. $r_{(a,b]}(f) \leq v(S_a) - v(S_b)$
2. $v(S_a) - v(S_b) - r_{(a,b]}(f)$ *is a non-negative even integer*

Note that this is still an upper bound of the count of real roots of f and Descartes' Rule of Signs is a special case of the above theorem. Later, Sturm defined a new sequence in order to improve upon this counting technique.

Definition 1.2.1. The Sturm sequence of a polynomial $f \in \mathbb{R}[x]$ is the sequence given by

1. $f_0 = f$
2. $f_1 = f'$ (the derivative of f)
3. $f_{i+1} = -\mathrm{rem}(f_{i-1}, f_i)$

for $i \geq 1$ and where $\mathrm{rem}(f_{i-1}, f_i)$ is the remainder in the Euclidean division of f_{i-1} by f_i.

Theorem 1.2.5 (Sturm 1829 [62]). *Let $f \in \mathbb{R}[x]$ and $a < b$ such that $f(a), f(b) \neq 0$. Let S_a be the Sturm sequence for f evaluated at $x = a$. Then*

$$r^*_{(a,b)}(f) = v(S_a) - v(S_b).$$

Sturm's theorem provides an exact count of the number of distinct real roots of a polynomial in a given interval, but it is not easily generalizable to multivariate polynomials. Hermite provided another such exact result, but several definitions are needed first.

Definition 1.2.2. Let $f \in \mathbb{R}[x]$ of degree d and let $f = (x - z_1) \cdots (x - z_d)$, where $z_i \in \mathbb{C}$. Then the discriminant matrix Q of f is defined by $Q = V V^T$ where

$$V = \begin{bmatrix} z_1^0 & \cdots & z_d^0 \\ \vdots & & \vdots \\ z_1^{d-1} & \cdots & z_d^{d-1} \end{bmatrix}.$$

It can be easily shown that Q is a real symmetric matrix. Furthermore, it can be easily computed from the coefficients of the polynomial f.

Definition 1.2.3. Let M be a real symmetric matrix. The signature of M, written as $\sigma(M)$, is the number of positive eigenvalues of M minus the number of negative eigenvalues of M, counting multiplicity.

Once we have the discriminant matrix, we can compute its characteristic polynomial. Since the discriminant matrix is a real symmetric matrix, all of its eigenvalues are real. That is, all of the roots of its characteristic polynomial are real. In this special case Descartes' rule of signs gives an exact count for the number of positive roots. Hence, computing the signature from the characteristic polynomial is easily done. Finally, we have a theorem from Hermite which relates the signature of the discriminant matrix to the number of real roots a polynomial has.

Theorem 1.2.6 (Hermite 1853 [29])**.** *Let $f \in \mathbb{R}[x]$. Then*

$$r_{\mathbb{R}}^*(f) = \sigma(Q)$$

where Q is the discriminant matrix of f and σ is the signature.

1.2.2 Parametrization

Arbitrary degree and Arbitrary number of variables

Currently, there are two general approaches: Cylindrical Algebraic Decomposition (CAD) and Sum Of Squares (SOS).

CAD based approach: As mentioned at the beginning of Section 1.2.1, due to Tarski's theorem [65], one can construct a quantifier-free formula in the coefficients of f which is equivalent to the nonnegativity or copositivity conditions given in (1.1). In 1966, González-López, Recio, and Santos [22] gave an algorithm that can parametrize an arbitrary semialgebraic set represented by a quantifier-free formula. Their algorithm first partitions the semialgebraic set into cylindrical cells using Collins' CAD algorithm [14]. Then it parametrizes each cell by exploiting its cylindrical shape. This results in a parametrization with the following properties:

- The map is bijective.
- The map is piece-wise (one piece per a cell).
- Each piece is a real-semialgebraic function.

It is known that the number of cells in a CAD are at least doubly exponential in the number of variables [14]. Thus the resulting parametrization map consists of numerous pieces. Furthermore it can be time-consuming to evaluate each piece on parameters values since it would often involve solving system of equations and inequalities of polynomials with high degrees. In conclusion, this approach, though providing a bijective map, is not practically useful for exploring the set of nonnegative polynomials or the set of copositive polynomials.

SOS based approach: SOS is usually used as a form of certificate of nonnegativity of a polynomial. However, one could also try to use it for parametrization. Below, we will briefly review a few major results on SOS and then we will discuss how one might use them for parametrization.

SOS research was originally initiated in 1900 by Hilbert in his 17th problem [30]:

> *Given a multivariate polynomial that takes only non-negative values over the reals, can it be represented as a sum of squares of rational functions?*

Of course, when a polynomial is written as a sum of squares then it is obviously nonnegative. Hence, it is called a certificate of nonnegativity. Hilbert's 17th problem inspired intensive research and various generalizations. Here we will highlight results which are relevant, that is, the ones which pertain to nonnegative and copositive polynomials.

In [2] Artin showed that all nonnegative polynomials $f \in \mathbb{R}[x_1, \ldots, x_n]$ can be expressed as a sum of rational functions squared. In other words, there exist polynomials $p_i, q \in \mathbb{R}[x_1, \ldots, x_n]$ such that

$$f = \frac{\sum_i p_i^2}{q^2}.$$

In theory we could use this as a parametrization of nonnegative polynomials where the coefficients of p_i and q are the parameters. If we carried this out we would have a parametrization with the following properties:

- This parametrization is surjective.
- This parametrization is highly non-injective. In [39] an upper bound for the degree of p_i was found to be
$$2^{2^{2^{d^{4^n}}}}$$
where d is the degree of f and n is the number of variables.
- This parametrization has a complicated domain since we must ensure that q^2 divides the sum $\sum_i p_i^2$.

Since this method requires a large number of parameters with complicated conditions on them, this parametrization is not practical. However, this the best completely general result we have for nonnegative polynomials. Now we move to copositive polynomials.

In [50] Pólya showed that $f \in \mathbb{R}[x_1, \dots, x_n]$ being (strictly) copositive implies the existence of a polynomial $p \in \mathbb{R}[x_1, \dots, x_n]$ with nonnegative coefficients and $k \in \mathbb{N}$ such that

$$f = \frac{p}{(x_1 + \dots + x_n + 1)^k}.$$

We could try to create a parametrization of copositive polynomials based on this idea where the parameters are the coefficients of p. However, by looking at the degree bounds for p, which are found in [51], we see that we would need an infinite number of parameters to produce all (strictly) copositive polynomials of a particular degree. Thus, we cannot use this result.

Degree 2 and Arbitrary number of variables

As previously stated, when the polynomial is quadratic we can identify it with a real symmetric matrix. For positive semidefinite matrices we have the well known Cholesky decomposition.

Theorem 1.2.7 (Cholesky)**.** *Let $f \in \mathbb{R}[x_1, \dots, x_n]$ be of degree 2 and let A be its associated real symmetric matrix. Then we have*

$$A = LL^{\intercal},$$

where L is an real lower-triangular matrix with nonnegative diagonal entries.

Example 1.2.3. When considering 3×3 matrices we have the following parametrization for positive semidefinite matrices.

$$A = \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{12} & \ell_{22} & 0 \\ \ell_{13} & \ell_{23} & \ell_{33} \end{bmatrix} \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{12} & \ell_{22} & 0 \\ \ell_{13} & \ell_{23} & \ell_{33} \end{bmatrix}^{\intercal}$$

This decomposition gives us an almost bijective parametrization of positive semidefinite matrices, that is, degree 2 nonnegative polynomials. Unfortunately, things get a bit more complicated if we want to parametrize copositive matrices. The following result is a decomposition into a sum. However, this only holds for small matrices.

Theorem 1.2.8 (Diananda, 1962 [20])**.** *Let A be an $n \times n$ real copositive matrix with $n \leq 4$. Then*

$$A = P + N,$$

where P is an $n \times n$ real positive semidefinite matrix, and N is an $n \times n$ real symmetric matrix with nonnegative entries.

Note that we can use the decomposition described in Theorem 1.2.8, along with the Cholesky decomposition, to parametrize small copositive matrices. However, this parametrization cannot be injective since the dimension of the domain will be too high.

Example 1.2.4. When considering 3×3 matrices we have the following parametrization for copositive matrices.

$$A = \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{12} & \ell_{22} & 0 \\ \ell_{13} & \ell_{23} & \ell_{33} \end{bmatrix} \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{12} & \ell_{22} & 0 \\ \ell_{13} & \ell_{23} & \ell_{33} \end{bmatrix}^{\intercal} + \begin{bmatrix} p_1 & p_2 & p_3 \\ p_2 & p_4 & p_5 \\ p_3 & p_5 & p_6 \end{bmatrix}$$

In this case the domain is $\mathbb{R}^3 \times \mathbb{R}^9_{\geq 0}$, which is 12-dimensional. However, 3×3 matrices, and thus copositive bivariate quadratic polynomials, are determined by only 6 values. So this parametrization has no hope of being injective.

It was initially conjectured that Theorem 1.2.8 would hold for matrices of arbitrary size, though it was only proven for $n \leq 4$. However, soon afterwards, research was done by Hall and Newman [27] to find a counterexample

Example 1.2.5. Here we have the counterexample presented in [27].

$$\begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}$$

This 5×5 copositive matrix cannot be decomposed into a sum of a positive semidefinite and nonnegative matrix.

Arbitrary degree and 1 variable

For the case of nonnegative polynomials, parametrization becomes essentially trivial. We can simply use the complex roots as parameters. For instance, consider the quartic polynomial

$$\begin{aligned} f(x) &= (x-(\alpha_1+\beta_1 i))(x-(\alpha_1-\beta_1 i))(x-(\alpha_2+\beta_2 i))(x-(\alpha_1-\beta_1 i)) \\ &= \left(x^2-(2\alpha_1)x+(\alpha_1^2+\beta_1^2)\right)\left(x^2-(2\alpha_2)x+(\alpha_2^2+\beta_2^2)\right). \end{aligned}$$

Then for all $(\alpha_1,\alpha_2,\beta_1,\beta_2)\in\mathbb{R}^4$, f is nonnegative. This of course generalizes to all nonnegative polynomials. However, for copositive polynomials it is not so simple. We could do something similar if we split the parametrization up in terms of the root structure. This would result in a piecewise parametrization. Unfortunately, the the number of pieces would grow rapidly as the degree got bigger. Thus, we prefer a parametrization with a single piece.

There is a classic result inspired by the SOS research which gives us the following characterization of copositive univariate polynomials.

Theorem 1.2.9 (Brickman and Steinberg, 1962 [4])**.** *Let the polynomial $f(x)$ be copositive. There there exist polynomials $p(x)$ and $q(x)$ such that*

$$f(x)=[p(x)]^2+[q(x)]^2x.$$

Clearly, the converse of this statement is also true. Thus, we can use this to parametrize univariate copositive polynomials. For example, the quadratic univariate copositive polynomials have the parametrization given by

$$\begin{aligned} f(x) &= (a_1x+a_0)^2+(b_0)^2x \\ &= \left(a_1^2\right)x^2+\left(2a_0a_1+b_0^2\right)x+\left(a_0^2\right), \end{aligned}$$

where $(a_0,a_1,b_0)\in\mathbb{R}^3$. However, this is not bijective. We can see this by considering the copositive polynomial

$$f(x)=x^2+4x+1.$$

Note that we can find two different triples, (a_0,a_1,b_0), that result in f. Namely, we have

$$\left(1,1,\sqrt{2}\right)$$

and

$$\left(1,-1,\sqrt{6}\right).$$

We could try to limit the domain of this parametrization to achieve (almost) bijectivity. For instance, forcing $a_1, b_0 \geq 0$ and $a_0 \leq 0$ results in a bijective map. However, as the degree grows the conditions on the parameters to maintain (almost) bijectivity become highly nontrivial. This again results in a complicated domain. Therefore, we will abandon this method and develop a new one in Chapter 2.

1.2.3 Summary

As we can see, not much work has been done on the parametrization of copositive polynomials. Furthermore, no attempts have been made for an almost bijective parametrization with polynomial, rational, or radical functions of one piece. Thus, this is where more work is needed.

1.3 Contributions

In Chapter 2 we limit our scope to parametrizing the set of copositive univariate polynomials. We begin by analyzing the boundary of the set, and we note that the entire set can be recovered from a 1-dimensional extension of a portion of the boundary. We then introduce a method to parametrize that crucial portion of the boundary utilizing the set of copositive polynomials with lower degree. This sets up a recursion, and we build our parametrization based upon this idea. The parametrization map is a polynomial map which is almost everywhere bijective and whose domain is $\mathbb{R}^d_{\geq 0}$. Finally, we illustrate how using a change of coordinates yields an almost everywhere bijective parametrization of polynomials which have no real roots in a given interval $(a, b) \subset \mathbb{R}$.

We then set our sights on multivariate copositive polynomials. We begin by limiting our scope to quadratics, and in Chapter 3 we work through what we consider to be the smallest nontrivial case: copositive bivariate quadratic polynomials, or equivalently, copositive homogeneous quadratic polynomials in three variables. As we have seen, this corresponds to copositive 3×3 matrices. Initially we normalize the set so that we can visualize it. Then by using that visualization we develop a method to parametrize the normalized set, which involves a 1-dimensional extension of a portion of the boundary.

We then work to understand the behavior of polynomials on this boundary. By utilizing particular properties of these boundary polynomials we are able to parametrize them. However, this initial parametrization has some undesirable properties, namely, the domain, while easily described, isn't standard. Furthermore, the parametrization map has singularities which prevent it from being surjective. We then go through a series of reparametrizations to address each of these issues. Afterwards we are left with a bijective map from a standard simplex to the desired boundary. Then we extend this surface out and denormalize the matrices to achieve our almost everywhere bijective rational parametrization of 3×3 copositive matrices.

With this strategy working so well in the 3×3 case, in Chapter 4 we generalize the methods used in Chapter 3 to the case of copositive matrices of any size. In so doing we clarify how to partition the boundary of copositive matrices into pieces which we can analyze separately. We call these pieces *faces*. Furthermore, we generalize the 1-dimensional extension idea to create sets that we call *shards*. These shards partition the set of $n \times n$ copositive matrices. One of these shards seems to be more important than the others, and we call that the *base shard*. We then develop a method to parametrize it with an almost everywhere bijective radical map.

Finally, in Chapter 5 we push the ideas developed in Chapters 3 and 4 to the limit, and we explore how these ideas generalize to the case of copositive polynomials of arbitrary degree with an arbitrary number of variables. In so doing we create a partition of the boundary of copositive polynomials into faces. Furthermore, we conjecture about a method of parametrization for a particular face.

CHAPTER

2

PARAMETRIZING COPOSITIVE UNIVARIATE POLYNOMIALS

In this chapter we will parameterize the set of copositive univariate polynomials. As stated in Chapter 1, González-López, Recio, and Santos [22] show that by using cylindrical algebraic decomposition it is possible obtain a semialgebraic, bijective parametrization of any semialgebraic set. However, this result is very general, and in our particular case that approach would be very difficult to implement. As a result we will take a different approach to solve this problem.

We will begin by formally stating the problem with the relevant definitions. Then we will exhibit the parametrization via Theorem 2.2.1. Afterwards, we will discuss how this result came about, and end the section with a formal proof. Finally, we end the chapter with an application for this parametrization.

2.1 Problem

To begin we will provide some definitions specific to the univariate case so that we may formally state the problem we will be solving.

Definition 2.1.1. We say that $f \in \mathbb{R}[x]$ is *copositive* if $f(x) \geq 0$ for all $x \geq 0$.

Note that the set of copositive polynomials form a closed convex cone. However, this cone is infinite dimensional. Thus, we will consider polynomials of a particular degree. Furthermore, to simplify as much as possible we will only consider monic polynomials. This is illustrated in the following definitions.

Definition 2.1.2. The set of monic univariate polynomials of degree d will be written as

$$F_d = \{f \in \mathbb{R}[x] : \deg(f) = d \text{ and } \operatorname{lc}(f) = 1\}.$$

Definition 2.1.3. The *d-copositive set*, written as $\mathscr{C}_d$, is defined to be the set of all monic univariate copositive polynomials of degree d, that is,

$$\mathscr{C}_d = \left\{f \in F_d : \ f \text{ is copositive}\right\}.$$

Note that in general $\mathscr{C}_d$ is a d-dimensional closed convex cone. Thus, we can only visualize small examples. Below we show the 2-copositive set, $\mathscr{C}_2$. Geometrically, this gives us the set in Figure 2.1.

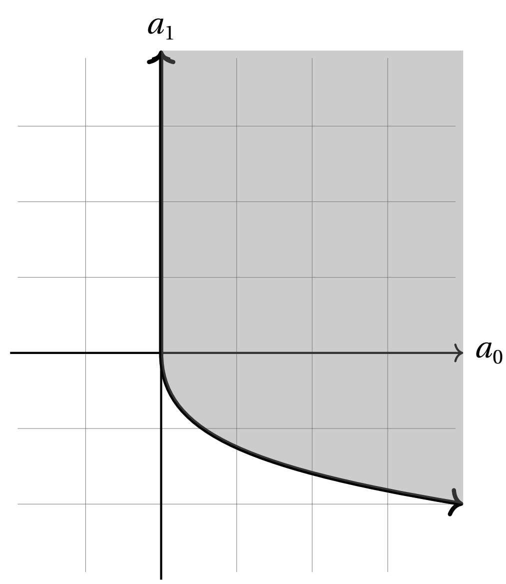


Figure 2.1: The set $\mathscr{C}_2$

Now that we have a description of the sets, we can discuss parametrization. As mentioned in the introduction, on the whole parametrization consists of two main components, the domain and the map, and often the complexity of these two components are inversely related. In other words, if we start with a very complicated domain, we can parametrize a complicated set with a relatively simple map and vice versa. In the extreme case one can bijectively parametrize any set by simply starting with the set itself as the domain and using the identity map. Hopefully everyone can agree that this is not a very satisfying or useful parametrization. A “good" parametrization strikes a balance in the complexity of these two components.

Here we will be quite demanding of both the domain and the map. For the domain we will choose one of the simplest closed convex cones we can think of, that is, $\mathbb{R}^d_{\geq 0}$. For the map we demand that it is also quite simple, meaning *polynomial*. Furthermore, we demand that this map be *almost bijective*.

Definition 2.1.4. A map $\phi : X \to Y$ is *almost bijective* if there exists $U \subset X$ such that

1. $X \setminus U$ is Zariski closed
2. $Y \setminus \operatorname{im}\left(\phi|_U\right)$ is Zariski closed
3. $\phi|_U$ bijects onto its image

Now with these definitions in hand we can state the problem we wish to solve in this chapter.

Problem 2.1.1. Find a parametrization map $\Phi_d : U \to \mathscr{C}_d$ such that

1. The domain U is easily described.
2. The map Φ_d is almost bijective.

2.2 Main Result

Though the conditions of Problem 2.1.1 seem fairly strict, we offer quite a simple solution with the following.

Theorem 2.2.1. *The map* $\Phi_d : \mathbb{R}^d_{\geq 0} \to \mathscr{C}_d$ *recursively defined by*

$$\Phi_d(t_0,\ldots,t_{d-1}) = \begin{cases} 1 & \textit{if} \quad d = 0 \\ x + t_0 & \textit{if} \quad d = 1 \\ (x - t_{d-2})^2 \, \Phi_{d-2}(t_0,\ldots,t_{d-3}) + t_{d-1}x & \textit{if} \quad d \geq 2 \end{cases}$$

is almost bijective.

Example 2.2.1. Here we will parametrize $\mathscr{C}_3$.

$$\begin{aligned}\Phi_3(t_0,t_1,t_2) &= (x-t_1)^2\Phi_1(t_0)+t_2x \\ &= (x^2-2t_1x+t_1^2)(x+t_0)+t_2x \\ &= x^3+(t_0-2t_1)x^2+(t_1^2-2t_0t_1+t_2)x+(t_0t_1^2)\end{aligned}$$

So

$$\mathscr{C}_3=\{x^3+(t_0-2t_1)x^2+(t_1^2-2t_0t_1+t_2)x+(t_0t_1^2): t_0,t_1,t_2\geq 0\}.$$

2.3 Derivation and Proof

In this section we will step through the process of deriving the map described in Theorem 2.2.1. We will begin with the set $\mathscr{C}_2$, as seen in Figure 2.1. We will then find a parametrization for polynomials with nonnegative critical points which relies on lower degree copositive polynomials. This suggests a recursive method for parametrizing $\mathscr{C}_d$. Then by extending these critical polynomials “up," we are able to recover the whole set. Finally, we offer a formal proof for Theorem 2.2.1.

2.3.1 Degree 2 Case

If we look at Figure 2.1 we can start to form a plan for parametrizing $\mathscr{C}_2$. Note that the boundary of the set seems to consist of two pieces: a vertical ray extending up from the origin and half of a parabola. Simply from visual inspection it seems like we can parametrize $\mathscr{C}_2$ if we create copies of the bottom boundary and shift them up, see Figure 2.2.

Now we have to figure out how to parametrize that bottom boundary curve. There are many ways to see this, but without too much effort we can deduce that polynomials on that boundary have a nonnegative critical point. Fortunately, it’s quite easy to parametrize univariate quadratic polynomials with a nonnegative critical point. Note that

$$f(x)=(x-t_0)^2=x^2-2t_0x+t_0^2$$

is the unique polynomial in F_2 which has a critical point at $x=t_0$. Thus, we can use this to retrieve any polynomial on the bottom curved boundary.

Now we simply have to extend the polynomial up in the a_1 direction. In other words, we need to positively grow the linear term without bound. To do this we will simply add a linear

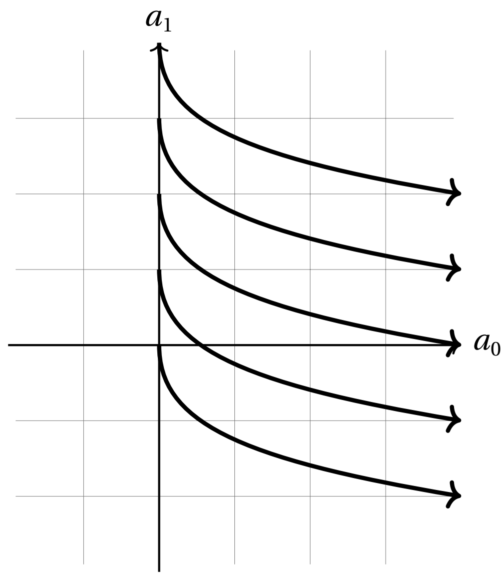


Figure 2.2: Parametrization Plan for $\mathscr{C}_2$

polynomial with nonnegative slope to get

$$f(x) = (x - t_0)^2 + t_1 x = x^2 + (t_1 - 2t_0)x + t_0^2.$$

This bijectively parametrizes $\mathscr{C}_2$ where $(t_0, t_1) \in \mathbb{R}^2_{\geq 0}$. Now the challenge is to extend this idea to polynomials of any degree.

2.3.2 Parametrizing Polynomials with Nonnegative Critical Points

To mirror what occurred in the degree 2 case, we will begin by parametrizing copositive polynomials with a nonnegative critical point. It will be helpful to have notation for this set.

Definition 2.3.1. The set of copositive polynomials of degree d with a nonnegative critical point will be written as

$$\mathscr{B}_d = \{f \in \mathscr{C}_d : f(t) = f'(t) \text{ for some } t \geq 0\}.$$

It will be helpful to have a running example polynomial to work with. So, consider $f \in \mathscr{C}_d$. In terms of its complex roots we have

$$f = (x - z_1)(x - z_2) \cdots (x - z_d).$$

Now if we assume f has a nonnegative critical point, then there is some $t \geq 0$ for which $f(t) = f'(t) = 0$. In this case f takes the form

$$f = (x - z_1)(x - z_2) \cdots (x - z_{d-2})(x - t)^2.$$

Now consider the polynomial

$$g = \frac{f}{(x-t)^2} = (x - z_1)(x - z_2) \cdots (x - z_{d-2}).$$

Note that g must be an element of $\mathscr{C}_{d-2}$.

Now we will use this idea to build $\mathscr{B}_d$ from $\mathscr{C}_{d-2}$. To that end we can consider the following map. Let $d \geq 2$ and define $\psi_d : \mathscr{C}_{d-2} \times \mathbb{R}_{\geq 0} \to \mathscr{B}_d$ such that

$$\psi_d(f, t)(x) = f(x) \cdot (x - t)^2.$$

We will now check the properties of this map.

Lemma 2.3.1. *Let $d \geq 2$. Then $\psi_d : \mathscr{C}_{d-2} \times \mathbb{R}_{\geq 0} \to \mathscr{B}_d$ defined by $(f, t) \mapsto f(x) \cdot (x-t)^2$ is surjective.*

Proof. Let $g \in \mathscr{B}_d$. Then by definition of the base boundary g takes the form

$$g = (x - z_1)(x - z_2) \cdots (x - z_{d-2})(x - t)^2$$

for some $t \geq 0$. Now it suffices to show that $f = (x - z_1) \cdots (x - z_{d-2})$ is an element of $\mathscr{C}_{d-2}$. Clearly f is a monic, degree $d - 2$ polynomial with real coefficients. By means of contradiction assume that $f(y) < 0$ for some $y \geq 0$. Then

$$\begin{aligned} g(y) &= f(y)(y - t)^2 \\ &\leq 0. \end{aligned}$$

If $(y - t)^2 > 0$, then we have our contradiction. So now assume that $(y - t)^2 = 0$. In other words, $t = y$. Since f is continuous there exists some $\varepsilon > 0$ such that $f(y + \varepsilon) < 0$. Then

$$\begin{aligned} g(y + \varepsilon) &= f(y + \varepsilon)(y + \varepsilon - t)^2 \\ &= f(y + \varepsilon)\varepsilon^2 \\ &< 0. \end{aligned}$$

Again, we arrive at a contradiction. □

Lemma 2.3.2. *Let $d \geq 2$. Then $\psi_d : \mathscr{C}_{d-2} \times \mathbb{R}_{\geq 0} \to \mathscr{B}_d$ defined by $(f,t) \mapsto f(x) \cdot (x-t)^2$ is almost injective.*

Proof. Note that $\mathscr{B}_{d-2}$ is part of the boundary of $\mathscr{C}_{d-2}$, and thus it is a measure zero subset. This also means that $\mathscr{B}_{d-2} \times \mathbb{R}_{\geq 0} \subset \mathscr{C}_{d-2} \times \mathbb{R}_{\geq 0}$ is a measure zero subset. We will avoid this subset. By means of contradiction let $f, g \in \mathscr{C}_{d-2} \setminus \mathscr{B}_{d-2}$ and $t, s \in \mathbb{R}_{\geq 0}$ such that $f \neq g$ and $\psi_d(f,t) = \psi_d(g,s)$.

One case is when $t = s$. If this is true, then we have $f(x) \cdot (x-t)^2 = g(x) \cdot (x-s)^2$, which implies $f(x) = g(x)$. This contradicts our assumption. Now we can assume that $t \neq s$. From the fundamental theorem of algebra we know that $\psi_d(f,t)$ and $\psi_d(g,s)$ have the same set of complex roots. Using this along with $t \neq s$ we have

$$\psi_d(f,t) = \psi_d(g,s) = (x-z_1)\cdots(x-z_{d-4})(x-t)^2(x-s)^2.$$

Hence, $g = (x-z_1)\cdots(x-z_{d-4})(x-t)^2$. However, this implies that $g \in \mathscr{B}_{n-2}$ since $g(t) = g'(t) = 0$. Again, this contradicts our assumption. □

Note that we need to go up to $d = 4$ to begin to see injectivity failing. The main issue algebraically is that when $d \geq 4$ a polynomial can have two different critical points which are also non-negative roots. Luckily, as long as the original polynomial doesn't have any roots with multiplicity 2, this issue disappears.

Example 2.3.1. Here we can see injectivity failing.

$$\psi_4\big((x-1)^2, 2\big) = (x-1)^2(x-2)^2 = \psi_4\big((x-2)^2, 1\big)$$

2.3.3 Extending Critical Polynomials Up

In the case of $\mathscr{C}_2$ we had very limited options for directions to extend $\mathscr{B}_2$. By looking at Figure 2.1, we see that the only direction that works is extending $\mathscr{B}_2$ in the direction of the linear term. However, once the degree d grows we start to get many more directions we could go. If we were to take naive guesses at the direction to extend, I believe there are two very natural choices given $\mathscr{C}_2$. We could view the direction we extended $\mathscr{B}_2$ to get $\mathscr{C}_2$ as either the direction of the linear term or as the direction of the term which is one degree less than d. Each of these give us a general approach for any d.

We believe that always using the linear term to extend will yield the simplest parametrization. So that is what we will use. However, there is freedom here to possibly choose a different direction. This idea suggests that we consider the map $\phi_d : \mathscr{B}_d \times \mathbb{R}_{\geq 0} \to \mathscr{C}_d$ defined by

$$\phi_d(f,t)(x) = f(x) + tx.$$

Just as before, we will now check the properties of this map.

Lemma 2.3.3. *Let $d \geq 2$. Then $\phi_d : \mathscr{B}_d \times \mathbb{R}_{\geq 0} \to \mathscr{C}_d$ defined by $(f,t) \mapsto f(x) + tx$ is surjective.*

Proof. Let $g \in \mathscr{C}_d$. Note that ϕ_d is surjective if we can find a $t \in \mathbb{R}_{\geq 0}$ such that $g(x) - tx \in \mathscr{B}_d$. To that end let

$$t = \inf\left\{\frac{g(x)}{x} : x > 0\right\}.$$

Now we must show that $g(x) - tx \in \mathscr{C}_d$ and for some $y \geq 0$ we have $g(y) - ty = g'(y) - t = 0$. Both of these together would give us that $g(x) - tx \in \mathscr{B}_d$.

For the first claim assume that $g(x) - tx \notin \mathscr{C}_d$. Thus, there exists some $y \geq 0$ such that $g(y) - ty < 0$. If $y = 0$, then $g(0) < 0$. This contradicts $g \in \mathscr{C}_d$. So we can assume that $y > 0$. Then by rearranging $g(y) - ty < 0$ we have

$$t > \frac{g(y)}{y}.$$

This contradicts t being the infimum of the set above. So we can conclude that $g(x) - tx \in \mathscr{C}_d$.

The second claim needs to be split into two cases. For the first case assume that $t \in \left\{\frac{g(x)}{x} : x > 0\right\}$. In other words, $t = \min\left\{\frac{g(x)}{x} : x > 0\right\}$. In this case there exists a $y > 0$ such that $t = \frac{g(y)}{y}$. Rearranging this equation gives us $g(y) - ty = 0$. Also, since y minimizes the function $\frac{g(x)}{x}$ over an open set, we must have that y causes the derivative of $\frac{g(x)}{x}$ to vanish. To be explicit,

$$\frac{yg'(y) - g(y)}{y^2} = 0.$$

If we rearrange this equation we get $g'(y) = \frac{g(y)}{y} = t$. In other words, $g'(y) - t = 0$.

Now we must consider the case when the set $\left\{\frac{g(x)}{x} : x > 0\right\}$ has no minimum. In this case we have either

$$t = \lim_{x \to \infty} \frac{g(x)}{x}$$

or

$$t = \lim_{x \to 0} \frac{g(x)}{x}.$$

Since the degree of g is at least 2 the limit in the first option doesn't exist. Thus,

$$t = \lim_{x \to 0} \frac{g(x)}{x}.$$

The only way for this limit to exist is if g factors as $g(x) = x \cdot h(x)$ for some $h \in \mathscr{C}_{d-1}$. Then we have $g(0) - t \cdot 0 = 0 \cdot h(0) - t \cdot 0 = 0$. Also, by applying L'Hôpital's rule we have

$$t = \lim_{x\to 0} \frac{g(x)}{x} = \lim_{x\to 0} (x \cdot h(x))' = \lim_{x\to 0} \big(h(x) + x \cdot h'(x)\big) = h(0).$$

Using this we have $g'(0) - t = h(0) - h(0) = 0$. Thus, we can conclude that $g(x) - tx \in \mathscr{B}_d$. □

Lemma 2.3.4. *Let $d \geq 2$. Then $\phi_d : \mathscr{B}_d \times \mathbb{R}_{\geq 0} \to \mathscr{C}_d$ defined by $(f, t) \mapsto f(x) + tx$ is injective.*

Proof. Let $f, g \in \mathscr{B}_d$ and $t, s \in \mathbb{R}_{\geq 0}$ such that $\phi_d(f, t) = \phi_d(g, s)$. Clearly if $t = s$, then we have $f = g$, and the map is injective. So without loss of generality we will assume that $t > s$ and eventually arrive at a contradiction. Note that we have the equation

$$f(x) - g(x) + (t - s)x = 0 \tag{2.1}$$

which holds for all $x \in \mathbb{R}$. Since $g \in \mathscr{B}_d$ we have some $y \geq 0$ such that $g(y) = g'(y) = 0$. Substituting y into equation (2.1) we have

$$f(y) + (t - s)y = 0.$$

Note that both $f(y)$ and $(t-s)y$ are non-negative. Then we can conclude $f(y) = 0$ and $(t-s)y = 0$. By assumption $t - s > 0$, and so $y = 0$. Now if we differentiate equation (2.1) and evaluate at $x = y = 0$ we get

$$f'(y) - g'(y) + (t - s) = f'(0) + (t - s) = 0.$$

Thus, f is decreasing at $x = 0$. But this along with the fact that $f(0) = 0$ implies that f is not copositive. This contradicts f being an element of $\mathscr{B}_d$. □

2.3.4 Proof

Here we offer an inductive proof for Theorem 2.2.1.

Proof. (Theorem 2.2.1) We will begin with Φ_0 and Φ_1. Technically speaking Φ_0 is not bijective, but we can say that is if we allow ourselves to claim that the "empty element" maps to the only element in the codomain. Regardless, this is a small detail, and it doesn't affect the recursion. Clearly Φ_1 is bijective since it is essentially the identity map.

Now let $d \geq 2$ and consider Φ_d. For a proof by induction assume that Φ_k is surjective and injective almost everywhere for all $k < d$. We will now show that $\Phi_d : (\mathbb{R}_{\geq 0})^d \to \mathscr{C}_d$ is surjective and injective almost everywhere. Note that using the maps ψ_d and ϕ_d defined in Lemmas 2.3.1

and 2.3.3, we can write Φ_d as follows.

$$\Phi_d(t_0,\dots,t_{d-1}) = \phi_d\Big(\ \psi_d\big(\Phi_{d-2}(t_0,\dots,t_{d-3}),\ t_{d-2}\big),\ t_{d-1}\Big)$$

Let $f \in \mathscr{C}_d$. For surjectivity we must now find an element $(t_0,\dots,t_{d-1}) \in (\mathbb{R}_{\geq 0})^d$ which maps to f. From Lemmas 2.3.3 and 2.3.4 we know that ϕ_d is bijective. Thus, there is a pair $(g, t_{d-1}) \in \mathscr{B}_d \times \mathbb{R}_{\geq 0}$ such that $\phi_d(g, t_{d-1}) = f$. From Lemma 2.3.1 we have that ψ_d is surjective. Thus, there exists a pair $(h, t_{d-2}) \in \mathscr{C}_{d-2} \times \mathbb{R}_{\geq 0}$ such that $\psi_d(h, t_{d-2}) = g$. Hence, $f = \phi_d\big(\psi_d(h, t_{d-2}), t_{d-1}\big)$. We have $(t_0,\dots,t_{d-3}) \in (\mathbb{R}_{\geq 0})^{d-2}$ such that $\Phi_{d-2}(t_0,\dots,t_{d-3}) = h$ by the induction hypothesis. This gives us surjectivity.

For injectivity assume that $\Phi_d(t_0,\dots,t_{d-1}) = \Phi_d(t'_0,\dots,t'_{d-1})$. Again, using the maps ϕ_d and ψ_d we have

$$\phi_d\Big(\ \psi_d\big(\Phi_{d-2}(t_0,\dots,t_{d-3}),\ t_{d-2}\big),\ t_{d-1}\Big) = \phi_d\Big(\ \psi_d\big(\Phi_{d-2}(t'_0,\dots,t'_{d-3}),\ t'_{d-2}\big),\ t'_{d-1}\Big).$$

Since ϕ_d is bijective the above equation simplifies to

$$\Big(\psi_d\big(\Phi_{d-2}(t_0,\dots,t_{d-3}),\ t_{d-2}\big),\ t_{d-1}\Big) = \Big(\psi_d\big(\Phi_{d-2}(t'_0,\dots,t'_{d-3}),\ t'_{d-2}\big),\ t'_{d-1}\Big).$$

So, $t_{d-1} = t'_{d-1}$ and $\psi_d\big(\Phi_{d-2}(t_0,\dots,t_{d-3}),\ t_{d-2}\big) = \psi_d\big(\Phi_{d-2}(t'_0,\dots,t'_{d-3}),\ t'_{d-2}\big)$. From Lemma 2.3.2 we have that ψ_d is injective almost everywhere. Therefore we can change $(t_0,\dots,t_{d-1})$ and $(t'_0,\dots,t'_{d-1})$ so that ψ_d has a unique inverse, and we have equality on the ordered pair

$$\big(\Phi_{d-2}(t_0,\dots,t_{d-3}),\ t_{d-2}\big) = \big(\Phi_{d-2}(t'_0,\dots,t'_{d-3}),\ t'_{d-2}\big).$$

Now we have that $t_{d-2} = t'_{d-2}$ and $\Phi_{d-2}(t_0,\dots,t_{d-3}) = \Phi_{d-2}(t'_0,\dots,t'_{d-3})$. Here the induction hypothesis takes over, and we have injectivity almost everywhere. □

2.4 Application

The parametrization developed in this chapter can be used to parametrize other sets of polynomials. For instance, in this section we will parametrize the polynomials which avoid a given interval. Let's fist note that polynomials which avoid a particular interval make a semialgebraic set, and we can use implicitization methods to describe the set. See the following example.

Example 2.4.1. We will use Sturm's Theorem to look at all monic quadratic polynomials which avoid the interval $(1,3)$. To that end let $f(x) = x^2 + ax + b$. Now we will calculate the Sturm sequence:

$$S_0 = f = x^2 + ax + b$$
$$S_1 = f' = 2x + a$$
$$S_2 = -\mathrm{rem}(f, f') = \frac{a^2}{4} - b.$$

Now to use Sturm's Theorem we need to look at the sign variation count of the sequence evaluated at the end points. So we have

$$S\Big|_{x=1} = \left(1 + a + b, 2 + a, \frac{a^2}{4} - b\right)$$
$$S\Big|_{x=3} = \left(9 + 3a + b, 6 + a, \frac{a^2}{4} - b\right).$$

In Figures 2.3 and 2.4 we have shown the regions with a particular sign variation count on an a, b-plane. The blue regions have a sign variation count of zero, the green regions have a sign variation count of one, and the red regions have a sign variation count of two.

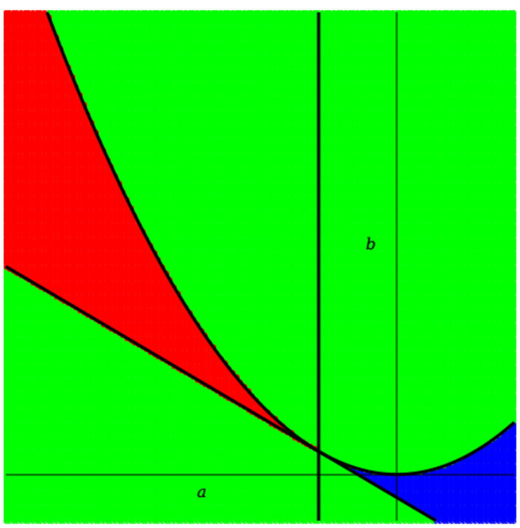


Figure 2.3: Sign Variations at $x = 1$

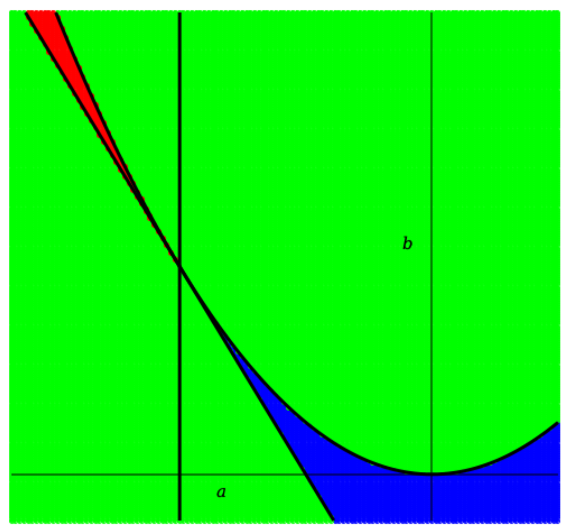


Figure 2.4: Sign Variations at $x = 3$

By comparing these we can map out the region where the difference of sign variation counts is zero. If we do this we get the following regions shown in Figure 2.5.

Note that by using this method, not only can we visualize the set, but we can extract the

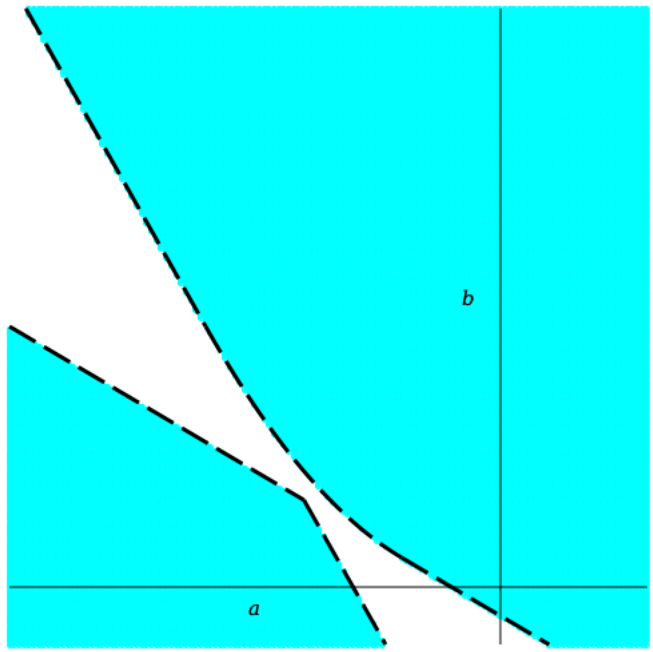


Figure 2.5: Quadratic Polynomials of the form $x^2 + ax + b$ which avoid the interval $(1,3)$

defining inequalities. Thus, we can get an implicitization of the set. However, this doesn't really give us any method for parametrization. Here is where our previous results can help. Let $a < b$ and let $f \in \mathscr{C}_d$ such that $f(-1) \neq 0$. Then via a change of coordinates we have that the polynomial

$$\frac{(-1)^d (x-b)^d}{f(-1)} \cdot f\left(-\frac{x-a}{x-b}\right)$$

has no roots in the interval (a,b). Furthermore, all degree d polynomials which avoid the interval (a,b) can be obtained this way. Applying this to the previous example we get the following rational parametrization of the set in Figure 2.5. For $f(x) = x^2 + ax + b$,

$$a = -\frac{6t_0^2 + 8t_0 - 4t_1 + 2}{t_0^2 + 2t_0 - t_1 + 1}$$
$$b = \frac{9t_0^2 + 6t_0 - 3t_1 + 1}{t_0^2 + 2t_0 - t_1 + 1}$$

with $(t_0, t_1) \in \mathbb{R}^2_{\geq 0}$ will cause f to avoid the interval $(1,3) \subset \mathbb{R}$.

CHAPTER

3

PARAMETRIZING COPOSITIVE BIVARIATE QUADRATIC POLYNOMIALS

Moving on from Chapter 2 with univariate polynomials, naturally we wish to parametrize bivariate polynomials next. As is often the case, jumping from one variable to multiple variables causes several new issues to emerge. In this chapter we parametrize copositive bivariate polynomials of degree two.

One could try to use the classic results developed in [2] to achieve this parametrization. For instance, one could parametrize all nonnegative bivariate degree 4 polynomials as the sum of three squares, each being a quadratic polynomial. Then utilize the fact that a degree 2 polynomial $f(x, y)$ is copositive if and only if the degree 4 polynomial $f(x^2, y^2)$ is nonnegative. This leads to a useful method for certifying copositive bivariate quadratic polynomials. However, if we use this as a parametrization we end up with a map which is non-injective whose domain is defined by several quadratic equations. In other words, the domain becomes complicated. So now we will develop a new approach.

To do this first we switch to the language of linear algebra to state the problem. Then we provide our final parametrization in Theorem 3.2.1. Afterwards we step through the logic of how we created this parametrization while overcoming obstacles as they appear.

3.1 Problem

Quadratic polynomials are often studied through the lens of linear algebra, and we will do the same thing. First, note that

$$f(x,y)=a_{20}x^2+a_{11}xy+a_{02}y^2+a_{10}x+a_{01}y+a_{00}$$

is copositive if and only if its homogenization,

$$\bar{f}(x,y,z)=a_{20}x^2+a_{11}xy+a_{02}y^2+a_{10}xz+a_{01}yz+a_{00}z^2,$$

is copositive. From here we can write $\bar{f}$ as a product of vectors with a symmetric matrix as follows,

$$\bar{f}(x,y,z)=\begin{bmatrix} x & y & z \end{bmatrix}\begin{bmatrix} a_{20} & \frac{1}{2}a_{11} & \frac{1}{2}a_{10} \\ \frac{1}{2}a_{11} & a_{02} & \frac{1}{2}a_{01} \\ \frac{1}{2}a_{10} & \frac{1}{2}a_{01} & a_{00} \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

Thus, in the quadratic case it makes sense to only consider the matrix, since it uniquely defines the polynomial. So for the remainder of this chapter we will discuss 3×3 matrices which result in the associated polynomial being copositive.

Definition 3.1.1. An $n\times n$ symmetric matrix A is *copositive* if $x^\intercal Ax\geq 0$ for all $x\geq 0$.

Definition 3.1.2. Let $\mathrm{CF}_n\subset\mathbb{R}^{\binom{n+1}{2}}$ be the set of $n\times n$ copositive matrices.

With this definition in hand we can state that we will parametrize CF_3 in this chapter. One might wonder why we didn't start with CF_2. Recall that matrices in CF_2 correspond to homogeneous quadratic polynomials of two variables. However, when we dehomogenize we are back in the univariate case. Thus, with a little tweaking we can change our univariate parametrization and obtain

$$\mathrm{CF}_2=\left\{\begin{bmatrix} t_1^2 & -t_1t_2+\lambda \\ -t_1t_2+\lambda & t_2^2 \end{bmatrix}: t_1,t_2,\lambda\geq 0\right\}.$$

So starting at CF_3 really is the next natural step. This brings us to the problem.

Problem 3.1.1. Find a parametrization map $\Phi: U\to\mathrm{CF}_3$ such that

1. The domain U is easily described.

2. The map Φ is almost bijective.

3.2 Main Result

Here we have our almost bijective parametrization. Note that the domain consists of four nonnegative real numbers and the standard 2-dimensional simplex.

Definition 3.2.1. Let $n \in \mathbb{N}$. The standard $(n-1)$-dimensional simplex, written Δ_n, is the set

$$\Delta_n = \left\{ x \in \mathbb{R}^n_{\geq 0} : \sum_i x_i = 1 \right\}.$$

Also, note that the map in our parametrization is rational, not polynomial like in the univariate case. So we are beginning to see more complexity in both the domain and the map.

Theorem 3.2.1. *The map* $\Phi : \mathbb{R}^4_{\geq 0} \times \Delta_3 \to \mathrm{CF}_3$ *defined by*

$$\Phi(s_1, s_2, s_3, \lambda, t_1, t_2, t_3) = \begin{bmatrix} s_1^2 & w_{12} & w_{13} \\ w_{12} & s_2^2 & w_{23} \\ w_{13} & w_{23} & s_3^2 \end{bmatrix}$$

with

$$w_{ij} = (2s_i s_j + \lambda)\frac{(1 - t_i - t_j)^2(1 + t_i)(1 + t_j)}{(t_i^2 + t_i t_j - t_i + 1)(t_j^2 + t_i t_j - t_j + 1)} - s_i s_j$$

is almost bijective.

3.3 Derivation & Proof

Initially we create a plan based on visualizing the geometry of CF_3. Then we parametrize the matrices on the boundary which cause a nonnegative critical point to occur. However, this parametrization has singularities around its boundary. Thus, we go through a series of reparametrizations to get rid of these problematic areas, and eventually we arrive at a bijective parametrization of the portion of the boundary we are concerned with.

From here we extend this boundary out from a point to achieve our parametrization. At which point we have one last issue to address. This parametrization is not surjective, but instead is almost surjective. While this meets our requirements, we perform one last tweak to our parametrization to achieve surjectivity.

3.3.1 Visualizing CF_3

In order the visualize $\mathrm{CF}_3 \subset \mathbb{R}^6$, we will need to take a 3-dimensional slice. However, we would like lose minimal information with this slice. When studying copositive matrices it is quite common to scale the diagonal elements of the matrix to be 1 since

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \in \mathrm{CF}_3 \iff \begin{bmatrix} 1 & \frac{a_{12}}{\sqrt{a_{11}a_{22}}} & \frac{a_{13}}{\sqrt{a_{11}a_{33}}} \\ \frac{a_{12}}{\sqrt{a_{11}a_{22}}} & 1 & \frac{a_{23}}{\sqrt{a_{22}a_{33}}} \\ \frac{a_{13}}{\sqrt{a_{11}a_{33}}} & \frac{a_{23}}{\sqrt{a_{22}a_{33}}} & 1 \end{bmatrix} \in \mathrm{CF}_3 \,.$$

This works as long as no $a_{ii} = 0$. In other words, this almost always works. With this property in mind we now will define a particular slice of CF_3.

Definition 3.3.1. Let $\widehat{\mathrm{CF}}_3$ be the subset of CF_3 consisting of matrices whose diagonal elements equal 1, that is,

$$\widehat{\mathrm{CF}}_3 = \left\{ A \in \mathrm{CF}_3 : A = \begin{bmatrix} 1 & a_{12} & a_{13} \\ a_{12} & 1 & a_{23} \\ a_{13} & a_{23} & 1 \end{bmatrix} \right\}.$$

Note that $\widehat{\mathrm{CF}}_3$ is a 3-dimensional, closed, convex set. Thus, we can visualize it. In Figure 3.1 we can see the result of sampling the set.

From visual inspection we can pick out a few notable features:

1. The boundary of $\widehat{\mathrm{CF}}_3$ seems to be comprised of 4 discrete pieces: 3 flat pieces and 1 curved piece.

2. The set appears to be bounded by the planes formed by the inequalities $a_{ij} \geq -1$ for all $i \neq j$.

3. The curved side looks like it is bounded by the boundary of a 2-dimensional simplex.

These observations are much clearer in Figures 3.2 and 3.3 where we have color coded the parts of the boundary. The red, blue, and green portions are the flat pieces, and the gray portion is the curved 2-dimensional simplex. It should be noted that the gaps between these pieces are not really there. They are a result of using software to plot the boundary. We can confirm observation 2 in the following lemma.

Lemma 3.3.1. *Let $A \in \widehat{\mathrm{CF}}_3$. Then $a_{12}, a_{13}, a_{23} \geq -1$.*

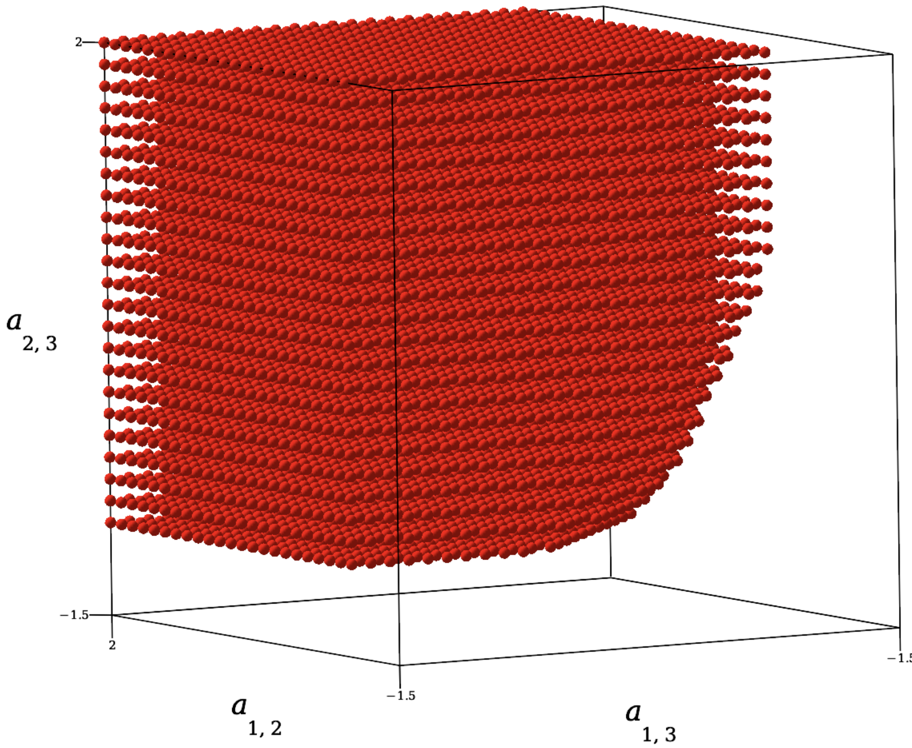


Figure 3.1: Sampled Points from $\widehat{\mathrm{CF}}_3$

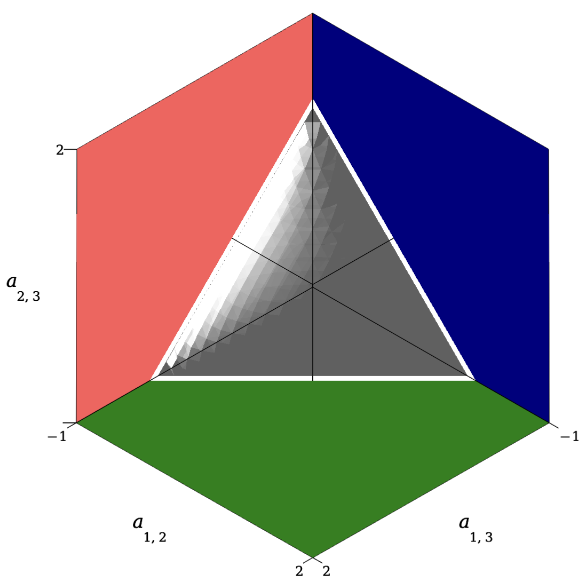


Figure 3.2: Boundary of $\widehat{\mathrm{CF}}_3$

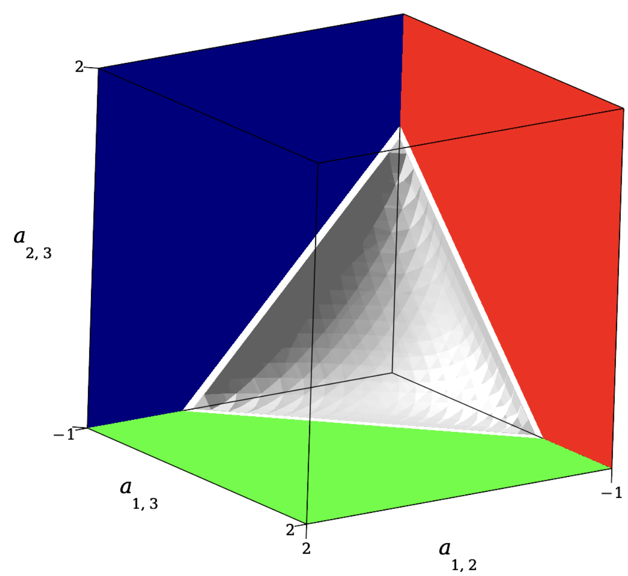


Figure 3.3: Boundary of $\widehat{\mathrm{CF}}_3$

Proof. Let $A \in \widehat{\mathrm{CF}}_3$. By way of contradiction assume that $a_{12} < -1$. Thus, $a_{12} = -1 - \varepsilon$ for some

$\varepsilon > 0$. Then the associated quadratic form is

$$x_1^2 + x_2^2 + x_3^2 + 2a_{12}x_1x_2 + 2a_{13}x_1x_3 + 2a_{23}x_2x_3 = x_1^2 + x_2^2 + x_3^2 + -2(1+\varepsilon)x_1x_2 + 2a_{13}x_1x_3 + 2a_{23}x_2x_3$$
$$= (x_1 - x_2)^2 + x_3^2 - 2\varepsilon x_1x_2 + 2a_{13}x_1x_3 + 2a_{23}x_2x_3.$$

Evaluating this polynomial at $x = (1,1,0)$ gives us $-2\varepsilon < 0$. Therefore, $A \notin \widehat{\mathrm{CF}}_3$, which is a contradiction. By symmetry we also have that $a_{13} \geq -1$ and $a_{23} \geq -1$. □

Lemma 3.3.1 as well as looking at pictures like Figures 3.2 and 3.3 suggests a method for parametrizing this set. We can take a portion of $\widehat{\mathrm{CF}}_3$ and project it out from the point $(-1,-1,-1)$. This should result in obtaining all of $\widehat{\mathrm{CF}}_3$, see Figure 3.4.

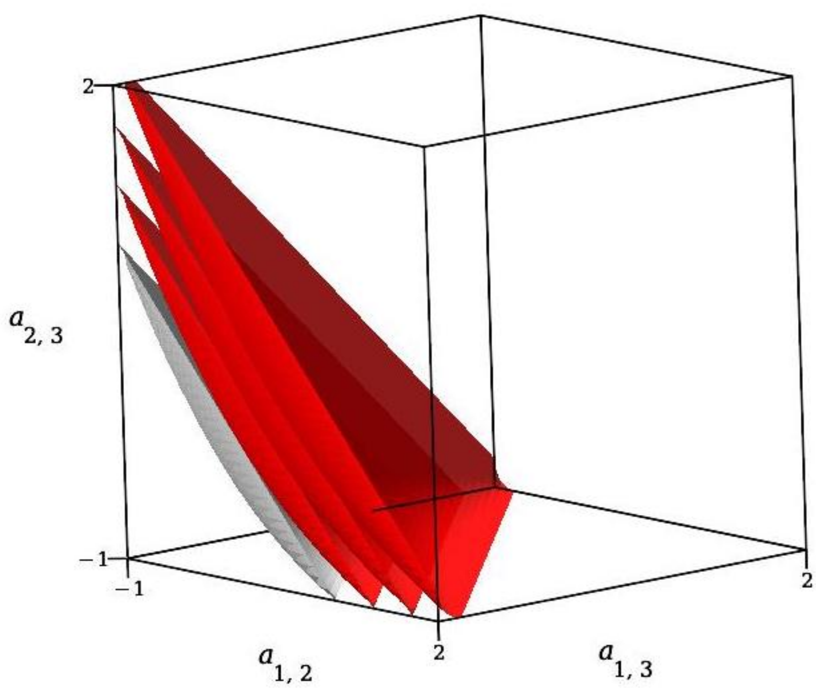


Figure 3.4: Projection of the curved boundary of $\widehat{\mathrm{CF}}_3$

Thus, we have our plan of action. First we will parametrize this curved portion of the boundary of $\widehat{\mathrm{CF}}_3$. Next we will project it out from the point $(-1,-1,-1)$ to get the entirety of $\widehat{\mathrm{CF}}_3$. Finally we will scale the diagonal elements to be any nonnegative number to form CF_3.

3.3.2 Parametrizing the Curved Boundary of $\widehat{\mathrm{CF}}_3$

Note that for a matrix to be on the boundary of $\widehat{\mathrm{CF}}_3$, its quadratic form must evaluate to 0 on some non-negative vector. With that in mind, we will begin by trying to figure out what the defining property is for being in this curved boundary. Looking at this set we can pull out a couple of examples.

$$A = \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix} \qquad B = \begin{bmatrix} 1 & -1/2 & -1/2 \\ -1/2 & 1 & -1/2 \\ -1/2 & -1/2 & 1 \end{bmatrix}$$

We will contrast these with a matrix which is on the boundary but not the curved portion.

$$C = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

One can check that all three of these matrices are on the boundary of $\widehat{\mathrm{CF}}_3$, but one difference is that $|A| = |B| = 0$, whereas $|C| \neq 0$. However, being copositive and singular isn't quite enough. Note that the matrix

$$\begin{bmatrix} 1 & 1/2 & 1/2 \\ 1/2 & 1 & 1/2 \\ 1/2 & 1/2 & 1 \end{bmatrix}$$

is singular and copositive but is in the interior of $\widehat{\mathrm{CF}}_3$. Analyzing these matrices a little more we can see that not only are A and B singular, but they have a null vector which has non-negative components. This gives us the following lemma.

Notation 3.3.1. We will use the convention ∂A to denote the *boundary* of a set A.

Lemma 3.3.2. *Let $A \in \partial \widehat{\mathrm{CF}}_3$ with $a_{12} + a_{13} + a_{23} \leq -1$. Then A is singular and has a null vector with non-negative components.*

Proof. Since $A \in \partial \widehat{\mathrm{CF}}_3$, we have $y^\intercal A y = 0$ for some $y \in \mathbb{R}_{\geq 0} \setminus \{0\}$. First we will consider what happens when a component of y is zero. So without loss of generality assume that $y_1 = 0$. Then we have

$$\begin{aligned} y^\intercal A y &= y_2^2 + 2a_{23} y_2 y_3 + y_3^2 \\ &= (y_2 - y_3)^2 + 2(a_{23} + 1) y_2 y_3. \end{aligned}$$

Note that if y_2 or y_3 is zero, then we get a contradiction with $y = 0$. Thus, y_2 and y_3 are both non-zero, and we can solve for a_{23}.

$$a_{23} = -\frac{(y_2 - y_3)^2}{2y_2 y_3} - 1$$

From this we can see that $a_{23} \leq -1$, but from Lemma 3.3.1 we see that $a_{23} \geq -1$. Hence, a_{23} must equal -1. To achieve this we must have have $y_2 = y_3 = t > 0$. Furthermore, the condition $a_{12} + a_{13} + a_{23} \leq -1$ becomes the condition $a_{12} + a_{13} \leq 0$. With these in mind we arrive at

$$Ay = \begin{bmatrix} a_{12}y_2 + a_{13}y_3 \\ y_2 - y_3 \\ -y_2 + y_3 \end{bmatrix} = t \begin{bmatrix} a_{12} + a_{13} \\ 0 \\ 0 \end{bmatrix}.$$

From here we will rule out the possibility of $a_{12} + a_{13} < 0$. To see this we will consider the quadratic form on a general x and get

$$x_1^2 + (x_2 - x_3)^2 + 2a_{12}x_1x_2 + 2a_{13}x_1x_3.$$

Evaluating this on $x = \left(1, -\frac{1}{a_{12}+a_{13}}, -\frac{1}{a_{12}+a_{13}}\right)$ we get the value $1 - 2 = -1 < 0$. This contradicts A being copositive, and we finish the first case. When $y_1 = 0$, A is singular with a null vector of $(0, t, t) \in \mathbb{R}_{\geq 0} \setminus \{0\}$. We will have symmetric arguments if a different component of y is zero.

For the next case assume that $y \in \mathbb{R}_{>0}$. Here we will show that $y^\intercal Ay = 0$ implies that $Ay = 0$. To proceed we will assume that $y^\intercal Ay = 0$ and $Ay \neq 0$, and we will arrive at a contradiction. Since $Ay \neq 0$ there exists some $i \in \{1, 2, 3\}$ such that the ith component of the vector (Ay) is non-zero. Here we have to split into two cases.

Assume that $(Ay)_i > 0$. Let $\varepsilon \in \mathbb{R}$ be such that $0 < \varepsilon < \min\{2(Ay)_i, y_i\}$. With this setup we have two valuable properties. We have $\varepsilon - 2(Ay)_i < 0$, which implies $\varepsilon^2 - 2\varepsilon(Ay)_i < 0$. Also, we have $y - \varepsilon e_i \in \mathbb{R}_{>0}$. With these in mind we have

$$\begin{aligned}(y - \varepsilon e_i)^\intercal A(y - \varepsilon e_i) &= y^\intercal Ay - \varepsilon e_i^\intercal Ay - \varepsilon y^\intercal Ae_i + \varepsilon^2 e_i^\intercal Ae_i \\ &= -\varepsilon(Ay)_i - \varepsilon(Ay)_i + \varepsilon^2 \\ &< 0.\end{aligned}$$

This contradicts A being copositive.

For the last case assume that $(Ay)_i < 0$. Let $\varepsilon \in \mathbb{R}$ be such that $0 < \varepsilon < \min\{-2(Ay)_i, y_i\}$. Similar to the last case now we have $\varepsilon^2 + 2\varepsilon(Ay)_i < 0$ and $y + \varepsilon e_i \in \mathbb{R}_{>0}$. Now we calculate the quadratic form

$$\begin{aligned}(y+\varepsilon e_i)^\intercal A(y+\varepsilon e_i) &= y^\intercal Ay+\varepsilon e_i^\intercal Ay+\varepsilon y^\intercal Ae_i+\varepsilon^2 e_i^\intercal Ae_i\\ &= \varepsilon(Ay)_i+\varepsilon(Ay)_i+\varepsilon^2\\ &< 0,\end{aligned}$$

and we arrive at our contradiction. □

This leads us to an idea. Since all of the matrices on this curved surface have a non-negative null vector, we can use the coordinates of that null vector as our parameters. If we assume that $p \geq 0$ is a null vector, then we have the following system.

$$\begin{bmatrix} 1 & a_{12} & a_{13}\\ a_{12} & 1 & a_{23}\\ a_{13} & a_{23} & 1\end{bmatrix}\begin{bmatrix}p_1\\p_2\\p_3\end{bmatrix}=\begin{bmatrix}0\\0\\0\end{bmatrix}$$

Luckily, we can uniquely solve this system for a_{ij} as long as $p>0$. This leads to the following lemma.

Lemma 3.3.3. *Let $p \in \mathbb{R}^3_{>0}$ and A be a 3×3 real symmetric matrix with 1's along the diagonal. Then $Ap = 0$ if and only if*

$$a_{12}=\frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2},\qquad a_{13}=\frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3},\qquad a_{23}=\frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3}.$$

Proof. We have

$$A=\begin{bmatrix} 1 & a_{12} & a_{13}\\ a_{12} & 1 & a_{23}\\ a_{13} & a_{23} & 1\end{bmatrix}.$$

Note that $Ap = 0$ if and only if

$$Ap=\begin{bmatrix}p_1+a_{12}p_2+a_{13}p_3\\ a_{12}p_1+p_2+a_{23}p_3\\ a_{13}p_1+a_{23}p_2+p_3\end{bmatrix}=\begin{bmatrix}0\\0\\0\end{bmatrix}.$$

Thus, we have the system

$$\begin{bmatrix}p_2 & p_3 & 0\\ p_1 & 0 & p_3\\ 0 & p_1 & p_2\end{bmatrix}\begin{bmatrix}a_{12}\\a_{13}\\a_{23}\end{bmatrix}=-\begin{bmatrix}p_1\\p_2\\p_3\end{bmatrix}.$$

Since $p \in \mathbb{R}^3_{>0}$ the system has a unique solution, which is

$$a_{12} = \frac{p_3^2 - (p_1^2 + p_2^2)}{2p_1 p_2}, \qquad a_{13} = \frac{p_2^2 - (p_1^2 + p_3^2)}{2p_1 p_3}, \qquad a_{23} = \frac{p_1^2 - (p_2^2 + p_3^2)}{2p_2 p_3}.$$

□

Given Lemma 3.3.3 we have a parametrization for 3×3 real symmetric matrices with 1's along the diagonal with a positive null vector:

$$\begin{bmatrix} 1 & \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} \\ \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & 1 & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} \\ \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} & 1 \end{bmatrix}.$$

However, it's possible that not all of these matrices are copositive. In order to check this, we need a sufficient condition for copositivity. Luckily, we don't need a sufficient condition for a general 3×3 to be copositive, but we only have to worry about singular matrices with a positive null vector. Under these constraints we have a nice way to check copositivity.

Lemma 3.3.4. *Let A be a real symmetric matrix such that $Ap = 0$ for some $p \in \mathbb{R}^n_{>0}$. Then $A \in \mathrm{CF}_n$ if and only if A is positive semi-definite.*

Proof. If A is positive semi-definite, then $x^\intercal Ax \geq 0$. Thus, $A \in \mathrm{CF}_n$. For the other direction assume that A is not positive semi-definite. Then there exists some $q \in \mathbb{R}^3$ such that $q^\intercal Aq < 0$. Note that there exists some $\varepsilon > 0$ such that $p + \varepsilon q \in \mathbb{R}^3_{>0}$. Then we have

$$\begin{aligned}(p+\varepsilon q)^\intercal A(p+\varepsilon q) &= p^\intercal Ap + \varepsilon p^\intercal Aq + \varepsilon q^\intercal Ap + \varepsilon^2 q^\intercal Aq \\ &= \varepsilon^2 q^\intercal Aq \\ &< 0.\end{aligned}$$

Hence A is not copositive. □

So in this special case checking copositivity is the same as checking if the matrix is positive semi-definite. Thus, we can check all of the principal minors. Note that by construction the determinant of the whole matrix is 0, and all of the 1×1 principal minors are 1. Therefore, we really only need to check the 2×2 principal minors. Doing so gives us the following.

$$\begin{vmatrix} 1 & \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} \\ \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & 1 \end{vmatrix} = -\frac{1}{4p_1^2p_2^2}(p_1+p_2+p_3)(p_1-p_2+p_3)(p_1+p_2-p_3)(p_1-p_2-p_3)$$
$$\begin{vmatrix} 1 & \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} \\ \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} & 1 \end{vmatrix} = -\frac{1}{4p_1^2p_3^2}(p_1+p_2+p_3)(p_1-p_2+p_3)(p_1+p_2-p_3)(p_1-p_2-p_3)$$
$$\begin{vmatrix} 1 & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} \\ \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} & 1 \end{vmatrix} = -\frac{1}{4p_2^2p_3^2}(p_1+p_2+p_3)(p_1-p_2+p_3)(p_1+p_2-p_3)(p_1-p_2-p_3)$$

The sign of each of these minors is determined by signs of the factors $(p_1+p_2+p_3)$, $(p_1-p_2+p_3)$, $(p_1+p_2-p_3)$, and $(p_1-p_2-p_3)$. Note that $(p_1+p_2+p_3)>0$ for all $p>0$. So we arrive at a result. Namely, the singular matrices we have parametrized are copositive if and only if $(p_1-p_2+p_3)(p_1+p_2-p_3)(p_1-p_2-p_3)\leq 0$. This is what we must answer now, which leads into the next lemma.

Lemma 3.3.5. *Let A be a 3×3 real symmetric matrix with 1's along the diagonal, and let p be a positive null vector of A. Then $A\in\widehat{\mathrm{CF}}_3$ if and only if*

$$p\in\operatorname{cone}\{e_1+e_2, e_1+e_3, e_2+e_3\}\setminus(\operatorname{span}\{e_1+e_2\}\cup\operatorname{span}\{e_1+e_3\}\cup\operatorname{span}\{e_2+e_3\}).$$

Proof. From the discussion above we know that $A\in\widehat{\mathrm{CF}}_3$ if and only if

$$(p_1-p_2+p_3)(p_1+p_2-p_3)(p_1-p_2-p_3)\leq 0.$$

So we must consider the signs of the following expressions.

$$(p_1-p_2-p_3) \tag{3.1}$$
$$(p_1-p_2+p_3) \tag{3.2}$$
$$(p_1+p_2-p_3) \tag{3.3}$$

We now have cases.

1. Assuming that expression (3.1), (3.2), or (3.3) is equal to zero gives us $p_1=p_2+p_3$, $p_2=p_1+p_3$, or $p_3=p_1+p_2$ respectively. In all three of these cases

$$p\in\operatorname{cone}\{e_1+e_2, e_1+e_3, e_2+e_3\}\setminus(\operatorname{span}\{e_1+e_2\}\cup\operatorname{span}\{e_1+e_3\}\cup\operatorname{span}\{e_2+e_3\}).$$

2. Assume that expressions (3.1), (3.2), and (3.3) are all less than zero. Then adding the

inequalities formed by (3.2) and (3.3) gives us $2p_1 < 0$, which is a contradiction.

3. Assume that expression (3.3) is less than zero while expressions (3.1) and (3.2) are greater than zero. Then negating inequality (3.2) and adding it to (3.3) gives us $2p_2 < 0$, a contradiction.

4. Assume that expression (3.2) is less than zero while expressions (3.1) and (3.3) are greater than zero. Then negating inequality (3.1) and adding it to (3.2) gives us $2p_3 < 0$, a contradiction.

5. Assume that expression (3.1) is less than zero while expressions (3.2) and (3.3) are greater than zero. These inequalities imply that $p \in \text{cone}\{e_1+e_2, e_1+e_3, e_2+e_3\}$. However, p being strictly positive implies that $p \notin \text{span}\{e_1+e_2\} \cup \text{span}\{e_1+e_3\} \cup \text{span}\{e_2+e_3\}$.

□

With Lemma 3.3.5 in hand we can cut down our domain to come from the specified to domain to arrive at a parametrization of the curved boundary. Furthermore, since each expression for a_{ij} is homogeneous and quadratic in the numerator and denominator, the length of the positive null vector chosen has no effect on the copositive matrix generated. Thus, we can assume that the null vector is from a simplex to simplify our domain even further.

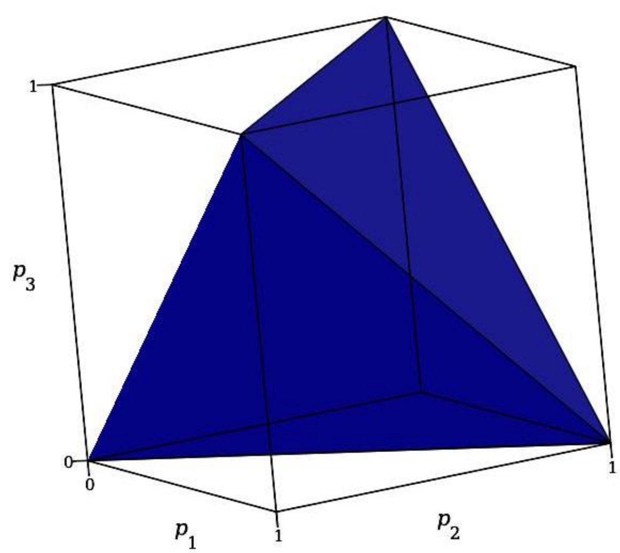


Figure 3.5: Possible null vectors for $\widehat{\text{CF}}_3$

Since our domain now is a portion of a simplex. We will do a change of variables so that it is just a simplex. We will do the change of variables:

$$p_1 = t_2 + t_3, \quad p_2 = t_1 + t_3, \quad p_3 = t_1 + t_2,$$

and now our domain is the standard simplex, Δ_3, without its corners. Following this change of variables through gives us matrices of the following form.

$$\begin{bmatrix} 1 & \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} \\ \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & 1 & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} \\ \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} & 1 \end{bmatrix} \mapsto \begin{bmatrix} 1 & \frac{2t_1t_2}{(1-t_1)(1-t_2)}-1 & \frac{2t_1t_3}{(1-t_1)(1-t_3)}-1 \\ \frac{2t_1t_2}{(1-t_1)(1-t_2)}-1 & 1 & \frac{2t_2t_3}{(1-t_2)(1-t_3)}-1 \\ \frac{2t_1t_3}{(1-t_1)(1-t_3)}-1 & \frac{2t_2t_3}{(1-t_2)(1-t_3)}-1 & 1 \end{bmatrix}$$

We can formalize this in the following theorem.

Theorem 3.3.1. *The map* $\Psi : \operatorname{int}(\Delta_3) \to \{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} < -1\}$ *defined by*

$$(t_1, t_2, t_3) \mapsto \begin{bmatrix} 1 & \frac{2t_1t_2}{(1-t_1)(1-t_2)}-1 & \frac{2t_1t_3}{(1-t_1)(1-t_3)}-1 \\ \frac{2t_1t_2}{(1-t_1)(1-t_2)}-1 & 1 & \frac{2t_2t_3}{(1-t_2)(1-t_3)}-1 \\ \frac{2t_1t_3}{(1-t_1)(1-t_3)}-1 & \frac{2t_2t_3}{(1-t_2)(1-t_3)}-1 & 1 \end{bmatrix}$$

is Ψ *bijective.*

Proof. As discussed above, Ψ is a composition. Namely, $\Psi = f \circ g$, where

$$g : \operatorname{int}(\Delta_3) \to \operatorname{int}(\operatorname{conv}\{e_1 + e_2, e_1 + e_2, e_2 + e_3\})$$

is defined by $g(t_1, t_2, t_3) = (t_2 + t_3, t_1 + t_3, t_1 + t_2)$, and

$$f : \operatorname{int}(\operatorname{conv}\{e_1 + e_2, e_1 + e_2, e_2 + e_3\}) \to \{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} < -1\}$$

is defined by

$$f(p_1, p_2, p_3) = \begin{bmatrix} 1 & \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} \\ \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & 1 & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} \\ \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} & 1 \end{bmatrix}.$$

It can be easily checked that the linear map g is bijective. Now we will check that f is bijective, completing the proof. Note that f is bijective if all matrices in $\{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} < -1\}$ can be uniquely determined by a single null vector. We will begin by checking the rank of matrices in the image of f. This map f was specifically chosen so that $|f(p)| = 0$. So clearly the rank of $f(p)$ is either 1 or 2. For now let us assume that the rank is 1. Then by following the discussion in the proof of Lemma 3.3.5 we see that at least one of the following equations must be true to force the 2×2 minors to be 0.

$$p_1 - p_2 - p_3 = 0$$
$$p_1 - p_2 + p_3 = 0$$
$$p_1 + p_2 - p_3 = 0$$

This implies $p_1 = p_2 + p_3$, $p_2 = p_1 + p_3$, or $p_3 = p_1 + p_2$. All of these conditions occur on the boundary of $\text{conv}\{e_1+e_2, e_1+e_3, e_2+e_3\}$, which is not in the domain of f. Hence, $f(p)$ is rank 2 for all p in the domain.

This is actually all we need. If $f(p) = f(p')$ with $p \neq p'$. Then because of our choice of domain, p and p' are linearly independent. Hence, $f(p)$ has at least a 2 dimensional null space, but this contradicts $f(p)$ being rank 2. Thus, f is injective. Based on Lemma 3.3.5 we know that if the domain of f is expanded to be $\text{conv}\{e_1+e_2, e_1+e_3, e_2+e_3\}\setminus\{e_1+e_2, e_1+e_3, e_2+e_3\}$, then its image would be a superset of $\{A \in \partial\widehat{\text{CF}}_3 : a_{12}+a_{13}+a_{23} < -1\}$. So to check surjectivity we will show that all of the points left out of the domain of f do not map to points in the codomain. From symmetry we only need to see where f maps points which satisfy $p_1 = p_2 + p_3$. If we make this substitution we see that

$$f(p_2+p_3, p_2, p_3) = \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix},$$

which does not satisfy the condition that $a_{12}+a_{13}+a_{23} < -1$. Thus, f is surjective.

□

3.3.3 Resolving Singularities in the Boundary Parametrization

The parametrization in Theorem 3.3.1 works for almost all points on this curved boundary. Unfortunately, we miss out on most of its limit points. For instance, we cannot obtain the matrix

$$\begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Furthermore, the domain in Theorem 3.3.1 is slightly awkward. In this section we will fix both of these issues. We will change our map so that it is defined everywhere on Δ_3, and in doing so we will pick up the desired limit points so that we will be parametrizing the closed set $\{A \in \partial\widehat{\text{CF}}_3 : a_{12}+a_{13}+a_{23} \leq -1\}$. To do this we will dive a little deeper into the limit points of our parametrization

$$\Phi : \operatorname{conv}\{e_1+e_2, e_1+e_3, e_2+e_3\} \setminus \{e_1+e_2, e_1+e_3, e_2+e_3\} \longrightarrow \{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12}+a_{13}+a_{23} \le -1\}$$

$$(p_1,p_2,p_3) \mapsto \begin{bmatrix} 1 & \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} \\ \frac{p_3^2-(p_1^2+p_2^2)}{2p_1p_2} & 1 & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} \\ \frac{p_2^2-(p_1^2+p_3^2)}{2p_1p_3} & \frac{p_1^2-(p_2^2+p_3^2)}{2p_2p_3} & 1 \end{bmatrix}.$$

As we saw in Theorem 3.3.1, this map is nicely behaved when we restrict the domain to be just the interior of $\operatorname{conv}\{e_1+e_2, e_1+e_3, e_2+e_3\}$, that is, when the matrix has a null vector with strictly positive components. So now let us consider matrices in $\widehat{\mathrm{CF}}_3$ with null vectors which have 0 components. So we will assume $A \in \widehat{\mathrm{CF}}_3$ and that $Ap = 0$ for some $p \in \mathbb{R}^3_{\ge 0} \setminus \{0\}$. Note that p cannot have two components being 0. So we will arbitrarily choose p_1 to be 0 and see the results. In order for p to be a null vector we have

$$\begin{bmatrix} 1 & a_{12} & a_{13} \\ a_{12} & 1 & a_{23} \\ a_{13} & a_{23} & 1 \end{bmatrix} \begin{bmatrix} 0 \\ p_2 \\ p_3 \end{bmatrix} = \begin{bmatrix} a_{12}p_2 + a_{13}p_3 \\ p_2 + a_{23}p_3 \\ a_{23}p_2 + p_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

From the last two equations we have that $a_{23} = -1$ and $p_2 = p_3 = 1$. Now from the first equation we get $a_{12} + a_{13} = 0$. Also, from Lemma 3.3.1 we know that $a_{12}, a_{13} \ge -1$. Putting this all together we now have

$$A = \begin{bmatrix} 1 & t & -t \\ t & 1 & -1 \\ -t & -1 & 1 \end{bmatrix}$$

for some $-1 \le t \le 1$. In other words, requiring the null vector to be $(0,1,1)$ doesn't give us just one matrix in $\{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12}+a_{13}+a_{23} \le -1\}$. Instead, we obtain a 1-dimensional set. This is the important idea. Here we see a single point "splitting" into infinitely many points. And by symmetry we get similar results if we require a different component of the null vector to be 0. These results are summarized in Figure 3.6.

Let's continue to see what happens if we consider other points on the boundary of the domain. So now we will assume that the null vector, p, has components $(1, t, 1-t)$ for $0 < t < 1$. In other words p is strictly in between the points $(1,1,0)$ and $(1,0,1)$. Here we get

$$\begin{bmatrix} 1 & a_{12} & a_{13} \\ a_{12} & 1 & a_{23} \\ a_{13} & a_{23} & 1 \end{bmatrix} \begin{bmatrix} 1 \\ t \\ 1-t \end{bmatrix} = \begin{bmatrix} (1+a_{13})+(a_{12}-a_{13})t \\ (a_{12}+a_{23})+(1-a_{23})t \\ (1+a_{13})-(1-a_{23})t \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

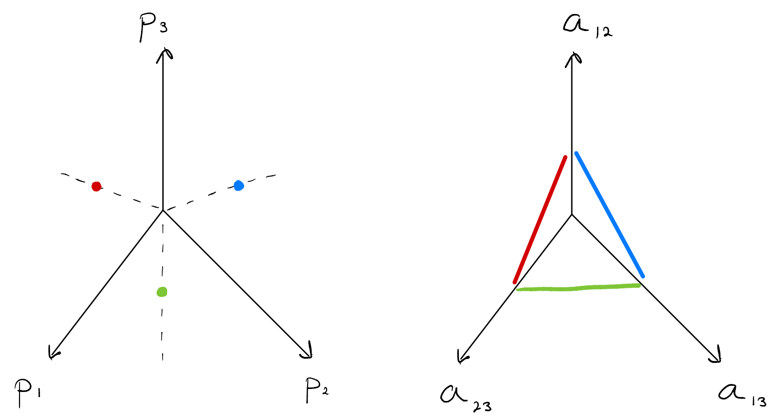


Figure 3.6: Null vector (left) and corresponding matrices in $\widehat{\mathrm{CF}}_3$ (right)

Since t is not 0 or 1, we only get a single solution for this system, namely, $(a_{12}, a_{13}, a_{23}) = (-1, -1, 1)$. So here we kind of have the opposite behavior of what we saw before. Now we have infinitely many points "collapsing" to a single point. Again, by symmetry we have similar behavior for a permutation of the null vector. We can summarize this in Figure 3.7.

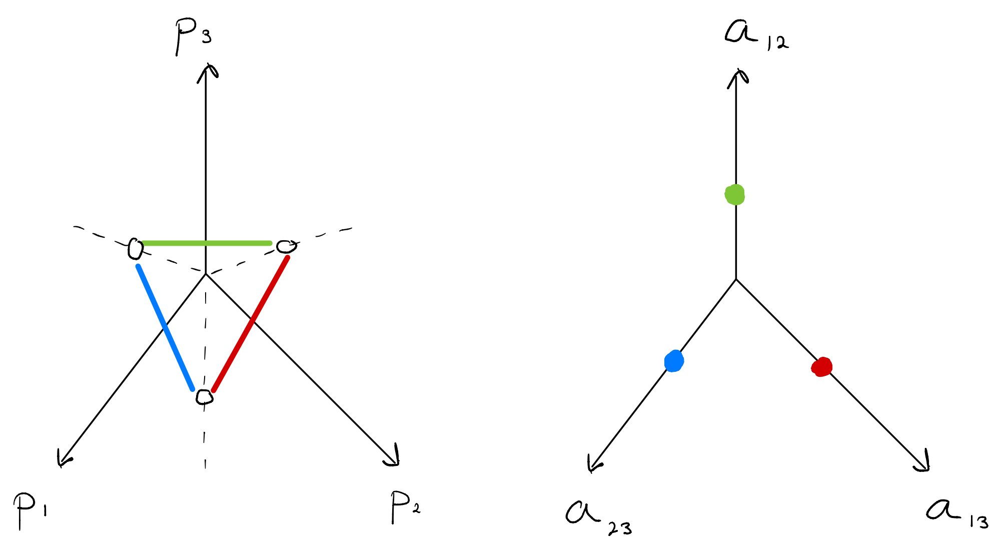


Figure 3.7: Null vector (left) and corresponding matrix in $\widehat{\mathrm{CF}}_3$ (right)

Now that we see the issues we can require our change of coordinates to address them. Not only do we want to do a change of coordinates so that our domain is Δ_3, but we also want this change of coordinates to have singularities which will "counter act" the behaviors we see in our parametrization. So now we have the problem. Find a map $\psi : \Delta_3 \to \text{conv}\{e_1+e_2, e_1+e_3, e_2+e_3\}$ such that ψ applied to a corner point is singular, and ψ applied to an edge gives us a corner point.

This required some searching, but eventually we found the map $\psi : \Delta_3 \setminus \{e_1, e_2, e_3\} \to \text{conv}\{e_1+e_2, e_1+e_3, e_2+e_3\}$ defined by

$$\psi(t) = \left(\frac{t_3(1-t_1t_2)}{(1-t_1)(1-t_2)}, \frac{t_2(1-t_1t_3)}{(1-t_1)(1-t_3)}, \frac{t_1(1-t_2t_3)}{(1-t_2)(1-t_3)} \right).$$

This map has all of the desired properties. However, we don't have a good explanation of how to construct this map. We simply looked for one which has the outlined properties. This of course leads to questions like, is this the best way to change our coordinates to cancel out the singularities? Is this the only way to change coordinates to achieve this? We don't have the answers to these questions.

With the ultimate goal of having a bijective or almost bijective map in the end we will now check this in the following lemma.

Lemma 3.3.6. *The map* $\psi : \text{int}(\Delta_3) \to \text{int}(\text{conv}\{e_1+e_2, e_1+e_3, e_2+e_3\})$ *defined by*

$$\psi(t) = \left(\frac{t_3(1-t_1t_2)}{(1-t_1)(1-t_2)}, \frac{t_2(1-t_1t_3)}{(1-t_1)(1-t_3)}, \frac{t_1(1-t_2t_3)}{(1-t_2)(1-t_3)} \right)$$

is bijective.

Proof. We will start with injectivity. Assume $\psi(t) = \psi(r)$ for $t, r \in \text{int}(\Delta_3)$. Writing out this condition gives us

$$\begin{aligned}
\frac{t_3(1-t_1t_2)}{(1-t_1)(1-t_2)} - \frac{r_3(1-r_1r_2)}{(1-r_1)(1-r_2)} &= 0\\
\frac{t_2(1-t_1t_3)}{(1-t_1)(1-t_3)} - \frac{r_2(1-r_1r_3)}{(1-r_1)(1-r_3)} &= 0\\
\frac{t_1(1-t_2t_3)}{(1-t_2)(1-t_3)} - \frac{r_1(1-r_2r_3)}{(1-r_2)(1-r_3)} &= 0.
\end{aligned}$$

Now if we combine these fractions, set the numerators equal to zero, and reduce the equations using the conditions that $t_1+t_2+t_3-1=0$ and $r_1+r_2+r_3-1=0$, we get the incredibly long equations

$$
\begin{aligned}
&r_2^2 r_3 t_2^2 + r_2^2 r_3 t_2 t_3 - r_2^2 t_2^2 t_3 - r_2^2 t_2 t_3^2 + r_2 r_3^2 t_2^2 + r_2 r_3^2 t_2 t_3 - r_2 r_3 t_2^2 t_3 - r_2 r_3 t_2 t_3^2 - \\
&r_2^2 r_3 t_2 - r_2^2 r_3 t_3 + r_2^2 t_2 t_3 - r_2 r_3^2 t_2 - r_2 r_3^2 t_3 - r_2 r_3 t_2^2 + r_2 t_2^2 t_3 + r_2 t_2 t_3^2 + r_3 t_2^2 t_3 + \\
&\qquad r_3 t_2 t_3^2 - r_2^2 t_3 + r_2 r_3 t_2 - r_2 t_2 t_3 + r_3 t_2^2 + r_2 t_3 - r_3 t_2 = 0 \\
&r_2^2 r_3 t_2 t_3 + r_2^2 r_3 t_3^2 + r_2 r_3^2 t_2 t_3 + r_2 r_3^2 t_3^2 - r_2 r_3 t_2^2 t_3 - r_2 r_3 t_2 t_3^2 - r_3^2 t_2^2 t_3 - r_3^2 t_2 t_3^2 - \\
&r_2^2 r_3 t_2 - r_2^2 r_3 t_3 - r_2 r_3^2 t_2 - r_2 r_3^2 t_3 - r_2 r_3 t_3^2 + r_2 t_2^2 t_3 + r_2 t_2 t_3^2 + r_3^2 t_2 t_3 + r_3 t_2^2 t_3 + \\
&\qquad r_3 t_2 t_3^2 + r_2 r_3 t_3 + r_2 t_3^2 - r_3^2 t_2 - r_3 t_2 t_3 - r_2 t_3 + r_3 t_2 = 0 \\
&r_2^2 r_3 t_2 t_3 - r_2 r_3^2 t_2 t_3 + r_2 r_3 t_2^2 t_3 + r_2 r_3 t_2 t_3^2 + r_2^2 r_3 t_2 + r_2^2 r_3 t_3 + r_2 r_3^2 t_2 + r_2 r_3^2 t_3 - \\
&\qquad r_2 t_2^2 t_3 - r_2 t_2 t_3^2 - r_3 t_2^2 t_3 - r_3 t_2 t_3^2 - r_2^2 r_3 - r_2 r_3^2 - \\
&\qquad 2 r_2 r_3 t_2 - 2 r_2 r_3 t_3 + 2 r_2 t_2 t_3 + 2 r_3 t_2 t_3 + t_2^2 t_3 + t_2 t_3^2 + 2 r_2 r_3 - 2 t_2 t_3 = 0.
\end{aligned}
$$

Using a computer algebra system we get that the solutions to this system are either $(t_1, t_2, t_3) = (r_1, r_2, r_3)$ or t_1 is free and t_2 is a root of

$$
\begin{aligned}
&\Big(r_2^4 r_3^2 + 2 r_2^3 r_3^3 + r_2^2 r_3^4 - r_2^4 r_3 - 3 r_2^3 r_3^2 - 2 r_2^2 r_3^3 + r_2^3 + 2 r_2^2 r_3 + r_2 r_3^2 - r_2^2 - 2 r_2 r_3 - r_3^2 + r_2 + r_3\Big) z^3 + \\
&\Big(-r_2^4 r_3^2 - 2 r_2^3 r_3^3 - r_2^2 r_3^4 + r_2^4 r_3 + 3 r_2^3 r_3^2 + 2 r_2^2 r_3^3 - 3 r_2^3 r_3 - 3 r_2^2 r_3^2 - 2 r_2 r_3^2 + 2 r_2^2 + 5 r_2 r_3 + 3 r_3^2 - r_2 - 3 r_3\Big) z^2 + \\
&\Big(-r_2^4 r_3^2 - 2 r_2^3 r_3^3 - r_2^2 r_3^4 - r_2^4 r_3 + r_2^3 r_3^2 + 2 r_2^2 r_3^3 + 3 r_2^3 r_3 + r_2^2 r_3^2 - r_2^2 r_3 + r_2 r_3^2 + r_2^2 - r_2 r_3 - 2 r_2\Big) z + \\
&\Big(r_2^4 r_3^2 + 2 r_2^3 r_3^3 + r_2^2 r_3^4 + r_2^4 r_3 - r_2^3 r_3^2 - 2 r_2^2 r_3^3 - 2 r_2^3 r_3 + r_2^3 + r_2^2 r_3 - 2 r_2^2\Big).
\end{aligned}
$$

Again, using a computer algebra system tells us that when $r \in \Delta_3$, the only root that can happen on the interval $[0,1]$ is a root precisely at zero. This tells us if t_1 is free, then $t_2 = 0$. But this implies t is on the boundary of Δ_3. Hence, ψ is injective.

Now for surjectivity. Let $r \in \operatorname{int}(\operatorname{conv}\{e_1 + e_2, e_1 + e_3, e_2 + e_3\})$. Then $r = s_1(e_2 + e_3) + s_2(e_1 + e_3) + s_3(e_1 + e_2)$ for some $s \in \operatorname{int}(\Delta_3)$. Now we must find $t \in \operatorname{int}(\Delta_3)$ such that $\psi(t) = r$. So we get the following system.

$$
\begin{aligned}
\frac{t_3(1 - t_1 t_2)}{(1 - t_1)(1 - t_2)} &= s_1 + s_2 \\
\frac{t_2(1 - t_1 t_3)}{(1 - t_1)(1 - t_3)} &= s_1 + s_3 \\
\frac{t_1(1 - t_2 t_3)}{(1 - t_2)(1 - t_3)} &= s_2 + s_3.
\end{aligned}
$$

Again, we can use a computer algebra system to show that this system has a solution for all $s \in \operatorname{int}(\Delta_3)$. □

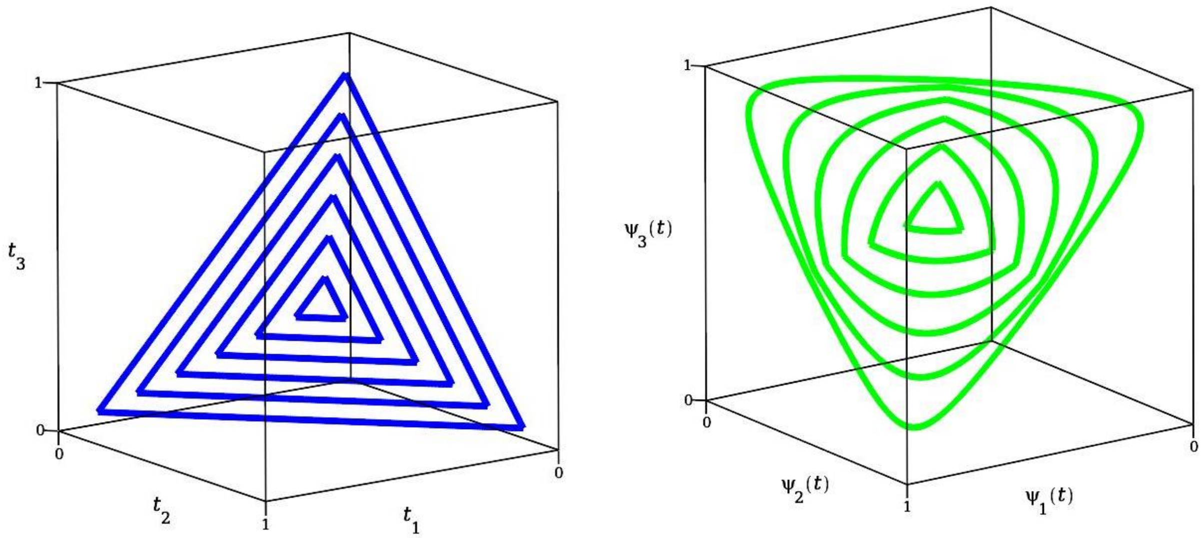


Figure 3.8: Standard simplex (left) and ψ evaluated on those curves (right)

We can visualize this change of coordinates in Figure 3.8. Now if we compose this change of coordinates map with our parametrization map, we get the following map $\Psi : \Delta_3 \to \{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} \leq -1\}$, which leads to the following theorem.

Theorem 3.3.2. *The map* $\Psi : \Delta_3 \to \{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} \leq -1\}$ *defined by*

$$\Psi(t) = \begin{bmatrix} 1 & \frac{2t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} - 1 & \frac{2t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} - 1 \\ \frac{2t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} - 1 & 1 & \frac{2t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - 1 \\ \frac{2t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} - 1 & \frac{2t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - 1 & 1 \end{bmatrix}.$$

is bijective.

Proof. Based on Theorem 3.3.1 and Lemma 3.3.6 we already have that Ψ restricted to the interior of Δ_3 is injective. Furthermore, the image of this restricted map is the interior of the codomain. Thus, this restriction of Ψ is bijective. Now we must see where the boundaries of the domain get mapped. To see this let us consider an edge of the domain where $t = (s, 1-s, 0)$. Then we get

$$\Psi(t) = \begin{bmatrix} 1 & -1 & \frac{(2s-1)(s^2-s-1)}{s^2-s+1} \\ -1 & 1 & -\frac{(2s-1)(s^2-s-1)}{s^2-s+1} \\ \frac{(2s-1)(s^2-s-1)}{s^2-s+1} & -\frac{(2s-1)(s^2-s-1)}{s^2-s+1} & 1 \end{bmatrix}.$$

Note that in this case $a_{12} + a_{13} + a_{23} = -1$. Furthermore, this expression

$$\frac{(2s-1)(s^2-s-1)}{s^2-s+1}$$

bijectively maps the interval $[0,1]$ to the interval $[-1,1]$. So we have bijectively mapped one edge of the domain to one edge of the codomain. Now by symmetry we can argue that the others behave the same. $\square$

3.3.4 Projecting to Parametrize $\widehat{\mathrm{CF}}_3$

Now that we have a nice parametrization for the set $\{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} \leq -1\}$, we can extend this set to recover all of $\widehat{\mathrm{CF}}_3$. As we described before we will do this by projecting the curved boundary from the point $(a_{12}, a_{13}, a_{23}) = (-1,-1,-1)$. We can see a 2-dimensional version of this idea in Figure 3.9. This leads to the following lemma.

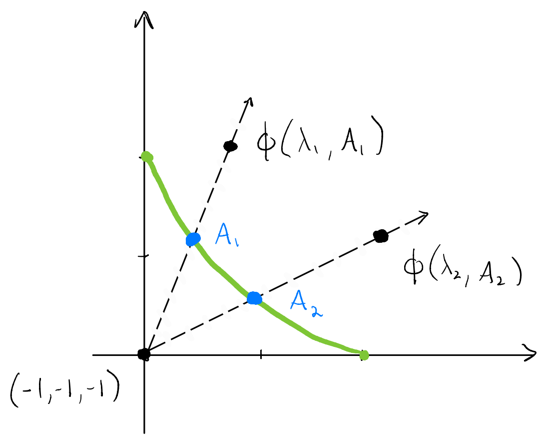


Figure 3.9: Projecting the boundary to the whole set

Lemma 3.3.7. *The map* $\Phi : \mathbb{R}_{\geq 0} \times \left\{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} \leq -1\right\} \to \widehat{\mathrm{CF}}_3$ *defined by*

$$\Phi(\lambda, A) = A + \lambda\left(A - \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}\right) = \begin{bmatrix} 1 & (1+\lambda)a_{12}+\lambda & (1+\lambda)a_{13}+\lambda \\ (1+\lambda)a_{12}+\lambda & 1 & (1+\lambda)a_{23}+\lambda \\ (1+\lambda)a_{13}+\lambda & (1+\lambda)a_{23}+\lambda & 1 \end{bmatrix}$$

is a bijection.

Proof. Note that Φ is injective since there is no way for two distinct rays from $(a_{12}, a_{13}, a_{23}) = (-1,-1,-1)$ to intersect $\left\{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} \leq -1\right\}$ in two different points and eventually meet up. Also, Φ is surjective since every point in $\widehat{\mathrm{CF}}_3$ can be traced back to a point in $\left\{A \in \partial\widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} \leq -1\right\}$ when following a line back towards $(-1,-1,-1)$. $\square$

3.3.5 Scaling to Parametrize CF_3

Now that we have a good parametrization for $\widehat{\mathrm{CF}}_3$, we can scale the diagonal to obtain all of CF_3. In other words we can extend our chosen slice of CF_3 to *almost* the whole set with the following method. Let $A \in \widehat{\mathrm{CF}}_3$, then we can scale A to have whatever diagonal we wish via the map

$$\left(\begin{bmatrix} s_1 \\ s_2 \\ s_3 \end{bmatrix}, \begin{bmatrix} 1 & a_{12} & a_{13} \\ a_{12} & 1 & a_{23} \\ a_{13} & a_{23} & 1 \end{bmatrix} \right) \mapsto \begin{bmatrix} s_1^2 & s_1 s_2 a_{12} & s_1 s_3 a_{13} \\ s_1 s_2 a_{12} & s_2^2 & s_2 s_3 a_{23} \\ s_1 s_3 a_{13} & s_2 s_3 a_{23} & s_3^2 \end{bmatrix},$$

where $s \in \mathbb{R}^3_{\geq 0}$. This will work for all but a measure zero set in CF_3. So if we wanted to we could stop here. However, we will try to dive a little deeper to examine the problem and see if we can fix it.

Just like some of our other issues while developing this parametrization, we run into difficulties when zeros occur, but this time we are concerned with zeros in the diagonal. To highlight the problem let's look at the matrices

$$A = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \qquad \text{and} \qquad B = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

Clearly both A and B are copositive, but with the current method of scaling the diagonal we can only obtain B. This is happening because when we scale a diagonal element, we have to scale an entire row and column as well. This is an issue.

On the road to fixing this problem let's try to reverse the order of scaling and extending. In other words, right now we are parametrizing a portion of the boundary of $\widehat{\mathrm{CF}}_3$, extending that to all of $\widehat{\mathrm{CF}}_3$, and then scaling the diagonal to get CF_3. Instead let's try to take the curved portion of the boundary of $\widehat{\mathrm{CF}}_3$, scale the diagonal, and then extend the set to get CF_3. Algebraically nothing changes when we do this, we still end up with the map $\Phi : \mathbb{R}^4_{\geq 0} \times \left\{ A \in \partial \widehat{\mathrm{CF}}_3 : a_{12} + a_{13} + a_{23} \leq -1 \right\} \to \mathrm{CF}_3$

$$(s_1, s_2, s_3, \lambda, A) \mapsto \begin{bmatrix} s_1^2 & s_1 s_2 (1+\lambda) a_{12} + s_1 s_2 \lambda & s_1 s_3 (1+\lambda) a_{13} + s_1 s_3 \lambda \\ s_1 s_2 (1+\lambda) a_{12} + s_1 s_2 \lambda & s_2^2 & s_2 s_3 (1+\lambda) a_{23} + s_2 s_3 \lambda \\ s_1 s_3 (1+\lambda) a_{13} + s_1 s_3 \lambda & s_2 s_3 (1+\lambda) a_{23} + s_2 s_3 \lambda & s_3^2 \end{bmatrix}.$$

However, thinking about the process in this order will help us fix some of the issues. Namely, the issue that this map is not surjective.

To try to visualize the problem, we will set $s_2 = s_3 = 1$, but we will allow s_1 to decrease

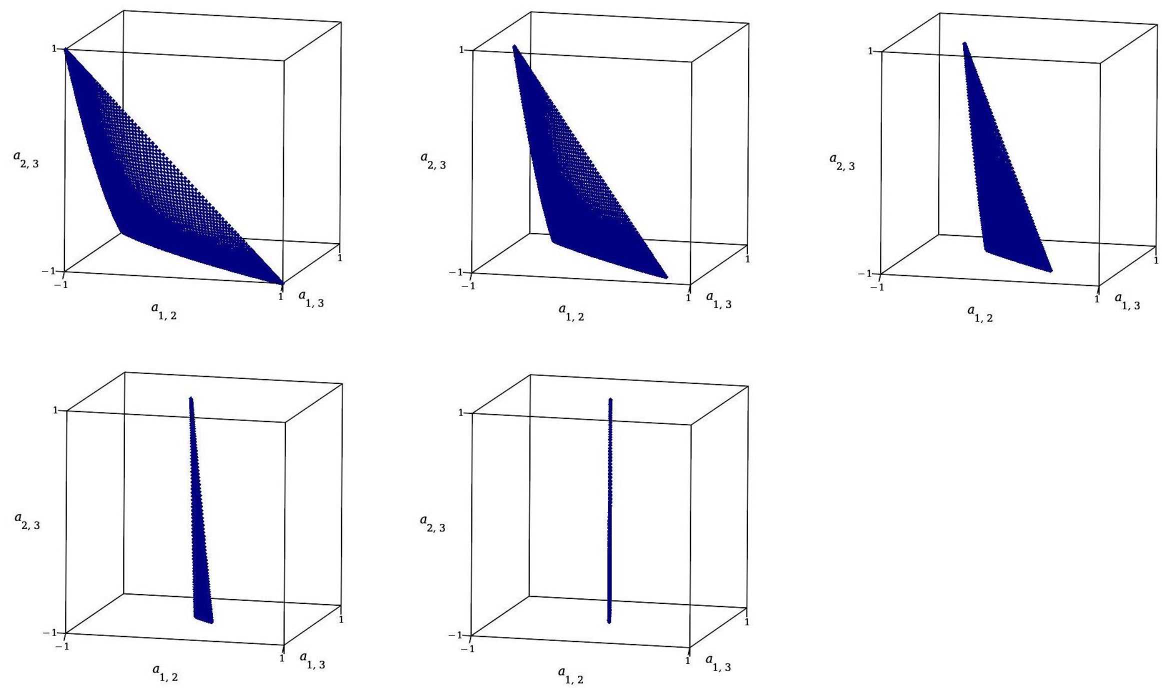


Figure 3.10: The off-diagonal elements as a diagonal element changes from 1 to 0

from 1 to 0. See Figure 3.10. There are two big issues here. One is that when $s[1] = 0$ this boundary collapses into a 1-dimensional object, and so we lose injectivity. Unfortunately, we can't do much about this issue. The second problem is that the point we need to project from, $(-s_1 s_2, -s_1 s_3, -s_2 s_3)$, lies directly under this vertical line when $s_1 = 0$. So projecting will only give us a vertical line, when the copositive set here is everything in a non-negative direction from this line. This issue we can address, and we will do so by projecting a ray *towards* a non-negative direction instead of *from* a point.

To achieve this we will take the curved simplex that we already have which has vertices at $(s_1 s_2, -s_1 s_3, -s_2 s_3)$, $(-s_1 s_2, s_1 s_3, -s_2 s_3)$, and $(-s_1 s_2, -s_1 s_3, s_2 s_3)$, and we will project towards one with vertices at $(s_1 s_2 + 1, -s_1 s_3, -s_2 s_3)$, $(-s_1 s_2, s_1 s_3 + 1, -s_2 s_3)$, $(-s_1 s_2, -s_1 s_3, s_2 s_3 + 1)$. We can do this without introducing any new parameters since this surface we are projecting towards solely depends on the boundary that we've already parametrized. This surface is given by

$$a_{12} = (2s_1s_2+1)\frac{t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} - s_1s_2$$
$$a_{13} = (2s_1s_3+1)\frac{t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} - s_1s_3$$
$$a_{23} = (2s_2s_3+1)\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - s_2s_3.$$

Projecting towards this surface gives us our final version of the parametrization: $\Phi : \mathbb{R}^4_{\geq 0} \times \Delta_3 \to \mathrm{CF}_3$, where $(s_1, s_2, s_3, \lambda, t_1, t_2, t_3)$ gets mapped to the matrix

$$\begin{bmatrix} s_1^2 & (2s_1s_2+\lambda)\frac{t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} - s_1s_2 & (2s_1s_3+\lambda)\frac{t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} - s_1s_3 \\ (2s_1s_2+\lambda)\frac{t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} - s_1s_2 & s_2^2 & (2s_2s_3+\lambda)\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - s_2s_3 \\ (2s_1s_3+\lambda)\frac{t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} - s_1s_3 & (2s_2s_3+\lambda)\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - s_2s_3 & s_3^2 \end{bmatrix}.$$

Theorem 3.3.3. *This map $\Phi : \mathbb{R}^4_{\geq 0} \times \Delta_3 \to \mathrm{CF}_3$ is surjective and almost injective.*

Proof. Let $A \in \mathrm{CF}_3$. The diagonal of A uniquely determines s_1, s_2, and s_3. Let's first consider the case where all $s_i > 0$. In this case the problem simplifies to considering the map $\widehat{\Phi} : \mathbb{R}_{\geq 0} \times \Delta_3 \to \widehat{\mathrm{CF}}_3$, where (λ, t_1, t_2, t_3) maps to

$$\begin{bmatrix} 1 & (2+\frac{\lambda}{s_1s_2})\frac{t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} - 1 & (2+\frac{\lambda}{s_1s_3})\frac{t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} - 1 \\ (2+\frac{\lambda}{s_1s_2})\frac{t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} - 1 & 1 & (2+\frac{\lambda}{s_2s_3})\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - 1 \\ (2+\frac{\lambda}{s_1s_3})\frac{t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} - 1 & (2+\frac{\lambda}{s_2s_3})\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - 1 & 1 \end{bmatrix}.$$

Note that λ separates the image of $\widehat{\Phi}$ into distinct layers. Thus, λ is uniquely determined by A as well. For each λ we have a map which is essentially the same as the bijective map in Theorem 3.3.2. The only difference is that it is a curved simplex with corner points at $(1+\frac{\lambda}{s_1s_1}, -1, -1)$, $(-1, 1+\frac{\lambda}{s_1s_3}, -1)$, and $(-1, -1, 1+\frac{\lambda}{s_2s_3})$ instead of at $(1, -1, -1)$, $(-1, 1, -1)$, and $(-1, -1, 1)$. Hence, each layer is a bijection, and we have achieved surjectivity. Also, this means that our original map Φ is injective as long as we avoid the measure-zero set of $s_1 = 0$, $s_2 = 0$, or $s_3 = 0$.

Now we will consider the case when $s_1 = 0$. This leads to A having the form

$$\begin{bmatrix} 0 & \lambda\frac{t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} & \lambda\frac{t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} \\ \lambda\frac{t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)} & s_2^2 & (2s_2s_3+\lambda)\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - s_2s_3 \\ \lambda\frac{t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)} & (2s_2s_3+\lambda)\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - s_2s_3 & s_3^2 \end{bmatrix}.$$

Here we lose injectivity. Since $\lambda = 0$ causes the first row and columns to be zero regardless of what (t_1, t_2, t_3) is. However, this map still surjects onto matrices in CF_3 with their top-right entry being 0. Notice that the 2×2 bottom-right corner is

$$\begin{bmatrix} s_2^2 & (2s_2s_3+\lambda)\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - s_2s_3 \\ (2s_2s_3+\lambda)\frac{t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)} - s_2s_3 & s_3^2 \end{bmatrix} = \begin{bmatrix} s_2^2 & -s_2s_3+\gamma \\ -s_2s_3+\gamma & s_3^2 \end{bmatrix},$$

where $\gamma \in [0,\infty)$. This matches our description of matrices in CF_2. Now for the $(1,2)$ and $(1,3)$ entries, they can be any non-negative numbers. And note, that's exactly what we have here. We can think of t as choosing a non-negative direction, and λ extends that direction to achieve any non-negative numbers we wish. By symmetry we can extend this argument, and we have surjectivity in this case. □

CHAPTER

4

PARAMETRIZING COPOSITIVE QUADRATIC POLYNOMIALS

So far we have parametrized copositive univariate polynomials of arbitrary degree in Chapter 2 and copositive bivariate quadratic polynomials in Chapter 3. Naturally, in this chapter we will move on to degree 2 polynomials with an arbitrary number of variables.

4.1 Problem

In Chapter 3 we parametrized a special portion of the boundary and extended it out from a point to recover all of CF_3. We wish to generalize this idea to arbitrary copositive quadratic polynomials. Using what was established in Chapter 3, this means we have to generalize the ideas we applied to 3×3 matrices to matrices of arbitrary size. This generalization will consist of three parts.

Problem 4.1.1. For CF_n, generalize:

- The notion of the “curved boundary."
- The method of extending from a point.

- Parametrize these extensions.

4.2 Main Results

Here we have generalized the pieces of the boundary into *faces*, the extension of these faces into *shards*, and we offer an almost bijective parametrization of the shard associated with our generalized notion of “curved boundary."

Definition 4.2.1. Let $I \subset \{1,\ldots,n\}$ be nonempty. The I-Face, S_n^I, of CF_n is defined as follows.

$$S_n^I = \{A \in \mathrm{CF}_n : \text{there exists a nonzero } x \geq 0 \text{ such that } A_I x = 0\},$$

where A_I is the submatrix of A consisting of the rows and columns indexed by I.

Definition 4.2.2. Let $A \in \mathrm{CF}_n$. The center, $C(A)$, of A is defined by

$$C(A) = \begin{bmatrix} \sqrt{A_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{A_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{A_{nn}} \end{bmatrix} \begin{bmatrix} 1 & -1 & \cdots & -1 \\ -1 & 1 & \cdots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} \sqrt{A_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{A_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{A_{nn}} \end{bmatrix}$$

Definition 4.2.3. Let $I \subset \{1,\ldots,n\}$. The I-shard, $\tilde{S}_n^I$, of CF_n is defined by

$$\tilde{S}_n^I = \left\{A \in \mathrm{CF}_n : \text{there exists a } B \in S_n^I \text{ such that } A, B, C(A) \text{ are collinear}\right\}$$

Theorem 4.2.1. *The map* $\Phi : \mathbb{R}_{\geq 0}^{n-1} \times \mathbb{R}^{\binom{n-1}{2}} \times \mathbb{R}_{\geq 0}^{n-1} \times \mathbb{R}_{\geq 0} \to \tilde{S}_n^{[n]}$ *defined by*

$$\Phi(d,\ell,c,\lambda) = (1+\lambda)B - \lambda C(B)$$

where $B = \begin{bmatrix} A & -Ac \\ -c^{\intercal}A & c^{\intercal}Ac \end{bmatrix}$ *and*

$$A = \begin{bmatrix} d_1 & 0 & 0 & \cdots & 0 \\ \ell_{12} & d_2 & 0 & \cdots & 0 \\ \ell_{13} & \ell_{23} & d_3 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ \ell_{1(n-1)} & \cdots & \cdots & \ell_{(n-2)(n-1)} & d_{n-1} \end{bmatrix} \begin{bmatrix} d_1 & 0 & 0 & \cdots & 0 \\ \ell_{12} & d_2 & 0 & \cdots & 0 \\ \ell_{13} & \ell_{23} & d_3 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ \ell_{1(n-1)} & \cdots & \cdots & \ell_{(n-2)(n-1)} & d_{n-1} \end{bmatrix}^{\intercal}$$

is almost bijective.

4.3 Derivation and Proof

We will begin by generalizing our descriptions of the boundary pieces that have appeared in the copositive sets. Further, we give an implicitization for each of these pieces. This gives us a very natural generalization of what we described as the “curved boundary" in Chapter 3. Next we generalize the extension idea that we saw in Chapter 3, which amounts to creating an equivalence on CF_n based on the diagonal elements. This will create what we call shards.

With these ideas fully generalized we are ready to parametrize this special extension of a face. So naturally, we have to start by parametrizing the face itself. Then by using the ideas we've developed in this chapter we can easily extend this face and retrieve our parametrization of the shard.

4.3.1 General Characterization of Boundary

We begin by understanding the structure of boundary matrices in CF_n. In Chapters 2 and 3 we saw that the boundary seems to be partitioned into distinct pieces. In fact, some of these pieces proved to be much more useful than others for parametrization.

Here we will generalize this notion of the boundary pieces into that of “faces." In so doing we will give an implicit description of them. Ultimately, in Theorem 4.3.1 we show that these faces actually do cover the entire boundary.

Because we are discussing the boundary so much in this section, we will again adopt the convention that $\partial\,\mathrm{CF}_n$ refers to the boundary of CF_n. With that in mind we need to find some kind of algebraic description of $\partial\,\mathrm{CF}_n$. To do this let us recall the definition of a copositive matrix, namely,

$$\mathrm{CF}_n = \left\{ A \in \mathbb{R}^{\binom{n+1}{2}} : A \text{ is symmetric and } x^{\mathsf{T}} A x \geq 0 \text{ for all } x \in \mathbb{R}^n_{\geq 0} \right\}.$$

Note that $x^{\mathsf{T}}Ax$ always equals zero when x is the zero vector. So really we don't have to consider that case. Now by looking at this definition and using continuity it's not hard to show that

$$\partial\,\mathrm{CF}_n = \left\{ A \in \mathrm{CF}_n : \text{there exists } x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x^{\mathsf{T}} A x = 0 \right\}.$$

In other words, the matrices on the boundary are those whose associated homogeneous polynomial have a zero with nonnegative components. However, this gives us a very natural way to split up the boundary. All we have to do is keep track of which components of x are equal to zero. To represent this idea more easily we will introduce some notation.

Notation 4.3.1. Let $x \in \mathbb{R}^n_{\geq 0}$ and A be a real symmetric matrix.

- $[n] = \{1, \ldots, n\}$
- x_I is the subvector consisting of the components of x indexed by I, where $I \subset [n]$ with $I \neq \emptyset$.
- A_I is the submatrix consisting of the rows and columns of A indexed by I, where $I \subset [n]$ with $I \neq \emptyset$.

With this we can rewrite the condition for being in the boundary as follows,

$$\partial \operatorname{CF}_n = \left\{A \in \operatorname{CF}_n : \exists \text{ nonempty } I \subset [n] \text{ and } x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x_I > 0 \text{ and } x_I^\intercal A_I x_I = 0\right\}.$$

Now we can split this up,

$$\partial \operatorname{CF}_n = \bigcup_{\substack{I \subset [n] \\ I \neq \emptyset}} \left\{A \in \operatorname{CF}_n : \exists x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x_I > 0 \text{ and } x_I^\intercal A_I x_I = 0\right\}.$$

This is looking good, but it isn't quite matching what we observing in the 3×3 case. In that case the faces seemed to be associated to critical points, not just zeros. We can actually connect these ideas with the following lemma.

Lemma 4.3.1. *Let F be a copositive homogeneous polynomial of degree greater than one, and let $x \in \mathbb{R}^n_{>0}$. Then we have $F(x) = 0$ if and only if $(\nabla F)(x) = 0$.*

Proof. Since we can write F in terms of its partial derivatives via Euler's homogeneous function theorem, clearly $(\nabla F)(x) = 0$ implies $F(x) = 0$. To see that $F(x) = 0$ implies that $(\nabla F)(x) = 0$, note that $(\nabla F)(x) \geq 0$ since F is copositive. Now consider the directional derivative at x in the direction of x, which is $(\nabla F)(x) \cdot \frac{x}{\|x\|} = 0$. Since the components of x are nonzero, this implies that $(\nabla F)(x) = 0$. □

Since the associated homogeneous polynomials take the form $f(x) = x^\intercal A x$, then the gradient vector is given by $\nabla f(x) = 2Ax$. Now by Lemma 4.3.1, if $x > 0$ and $x^\intercal A x = 0$, then $2Ax = 0$. Thus, we can rewrite our partition of the boundary again as follows,

$$\partial \operatorname{CF}_n = \bigcup_{\substack{I \subset [n] \\ I \neq \emptyset}} \left\{A \in \operatorname{CF}_n : \exists x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x_I > 0 \text{ and } A_I x_I = 0\right\}.$$

This is very close to what we saw in Chapter 3. The main difference is that this partition splits the boundary into pieces which don't contain their boundary, but as we saw in the 3×3 case, we want these pieces to be closed sets. So with one tweak, we can close these sets and arrive at our definition of face. That is,

$$S_n^I = \left\{A \in \mathrm{CF}_n : \exists x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x_I \geq 0 \text{ and } A_I x_I = 0\right\}.$$

Then we immediately get the following theorem.

Theorem 4.3.1. *We have*

$$\partial\, \mathrm{CF}_n = \bigcup_{\substack{I \subset [n] \\ I \neq \emptyset}} S_n^I.$$

Since CF_n is a convex set, it makes sense to study it through its boundary, and this gives us a way to split that work up. Now we only have to study finitely many faces of the boundary to understand it. In Appendix A we go through an in-depth study of the facial structure of CF_3. However, as we saw in Chapter 3 only one of the faces really contributed to our parametrization, and that was the face

$$S_3^{[3]} = \left\{A \in \mathrm{CF}_3 : \exists x \in \mathbb{R}^3_{\geq 0} \setminus \{0\} \text{ such that } Ax = 0\right\},$$

using our new terminology. Since this face is the *base* of our parametrization we will give it a special name.

Definition 4.3.1. We will refer to the face $S_n^{[n]}$, where $[n] = \{1, \ldots, n\}$, as the *base face*.

4.3.2 Extend Boundary Faces

Now that we have a solid definition for the base face. We need to determine how to extend it out, and in general how to extend out any face. To do this we will first analyze what we did in the 3×3 case. Recall that in Chapter 3 we began by parametrizing $S_3^{[3]}$, however, we had normalized the diagonal first. So really we parametrized

$$S_3^{[3]} \cap \left\{A \in \mathbb{R}^{n \times n} : A \text{ is symmetric and } A_{ii} = 1\right\}.$$

When we did this we saw that we could extend rays out from a *central* point where all non-diagonal elements were negative one. In other words, we extended rays from the matrix

$$\begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}$$

in nonnegative directions in such a way that the diagonal didn't change. We confirmed that this was a reasonable thing to do since all non-diagonal elements had to be greater than or equal to negative one to be copositive. We can see this by looking at the polynomial

$$x^2+y^2+z^2+2a_{12}xy+2a_{13}xz+2a_{23}yz$$

and determining the minimum that any a_{ij} can be. Now if we scale all of the variables we can create any nonnegative diagonal that we wish. This results in the following lemma.

Lemma 4.3.2. *Let $A \in \mathrm{CF}_n$. Then $A_{ij} \geq -\sqrt{A_{ii}A_{jj}}$ for all $i<j$.*

Proof. Let A be copositive and assume that $A_{ij} < -\sqrt{A_{ii}A_{jj}}$ for some $i<j$. Then $A_{ij} = -\sqrt{A_{ii}A_{jj}}-\varepsilon$ for some $\varepsilon>0$. Now consider

$$\begin{aligned}(x_ie_i^\intercal+x_je_j^\intercal)A(x_ie_i+x_je_j) &= x_i^2e_i^\intercal Ae_i+x_jx_ie_j^\intercal Ae_i+x_ix_je_i^\intercal Ae_j+x_j^2e_j^\intercal Ae_j\\ &= A_{ii}x_i^2+2A_{ij}x_ix_j+A_{jj}x_j^2\\ &= A_{ii}x_i^2-2\left(\sqrt{A_{ii}A_{jj}}+\varepsilon\right)x_ix_j+A_{jj}x_j^2\\ &= \left(x_i\sqrt{A_{ii}}-x_j\sqrt{A_{jj}}\right)^2-2\varepsilon x_ix_j.\end{aligned}$$

If $A_{ii}=A_{jj}=0$, then evaluating this polynomial at $x_i=x_j=1$ results in a negative value. Without loss of generality, if $A_{ii}=0$ and $A_{jj}\neq 0$, then evaluating this polynomial at $x_i=\frac{\sqrt{A_{jj}}}{\varepsilon}$ and $x_j=\frac{1}{\sqrt{A_{jj}}}$ results in a negative value. Finally, if both A_{ii} and A_{jj} are nonzero, then evaluating the polynomial at $x_i=\sqrt{A_{jj}}$ and $x_j=\sqrt{A_{ii}}$ results in a negative value. This contradicts A being copositive. □

This means that for all copositive matrices $A\in\mathrm{CF}_n$, we have

$$A=\begin{bmatrix} A_{11} & -\sqrt{A_{11}A_{22}} & \cdots & -\sqrt{A_{11}A_{nn}}\\ -\sqrt{A_{11}A_{22}} & A_{22} & \cdots & -\sqrt{A_{22}A_{nn}}\\ \vdots & \vdots & \ddots & \vdots\\ -\sqrt{A_{11}A_{nn}} & -\sqrt{A_{22}A_{nn}} & \cdots & A_{nn}\end{bmatrix}+\begin{bmatrix} 0 & \lambda_{12} & \cdots & \lambda_{1n}\\ \lambda_{12} & 0 & \cdots & \lambda_{2n}\\ \vdots & \vdots & \ddots & \vdots\\ \lambda_{1n} & \lambda_{2n} & \cdots & 0\end{bmatrix},$$

where all $\lambda_{ij}\geq 0$. This suggests that if we extend any copositive matrix A in a nonnegative direction while maintaining the diagonal, we should get similar behavior to what we achieved in Chapter 3. Thus, we have our definition for what we call the *center* matrix, based on the diagonal,

$$C(A) = \begin{bmatrix} \sqrt{A_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{A_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{A_{nn}} \end{bmatrix} \begin{bmatrix} 1 & -1 & \cdots & -1 \\ -1 & 1 & \cdots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} \sqrt{A_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{A_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{A_{nn}} \end{bmatrix}.$$

With this center matrix idea we can now use it to extend any face out. Essentially we are choosing any element in a face, using its diagonal to find the center, and then projecting a ray out from the center to the chosen face element, see Figure 4.1. This leads to the definition above for the shard built from the face S_n^I,

$$\tilde{S}_n^I = \left\{ A \in \mathrm{CF}_n : \underset{B \in S_n^I}{\exists} A, B, C(A) \text{ are collinear} \right\}.$$

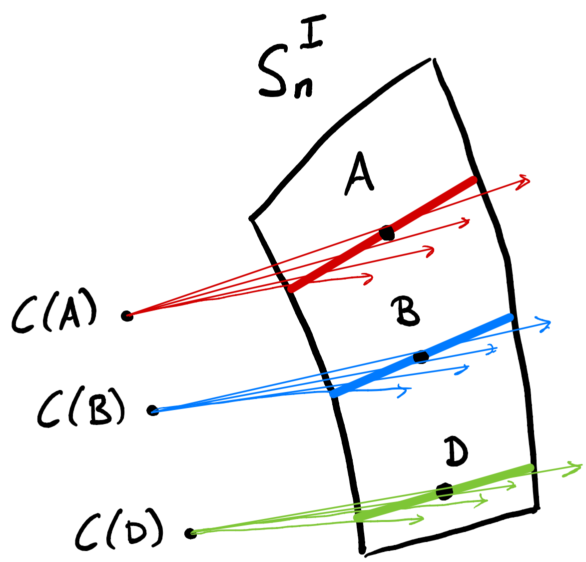


Figure 4.1: Extending a face into a shard

Now we immediately get a partition of CF_n into shards.

Theorem 4.3.2. *We have*

$$\mathrm{CF}_n = \bigcup_{\substack{I \subset [n] \\ I \neq \emptyset}} \tilde{S}_n^I.$$

Again, based on what we saw in Chapter 3, extending the base face out seemed to yield the most in terms of a parametrization. Thus, we will give the shard built from the base face a special name.

Definition 4.3.2. We will refer to the shard $\tilde{S}_n^{[n]}$, where $[n] = \{1, \ldots, n\}$, as the *base shard*.

This is what we will work to parametrize.

4.3.3 Parametrization of Base Shard

As we've seen, parametrizing a shard really comes down to parametrizing a face. Using the center idea to extend the face out isn't very difficult. Thus, we will begin by parametrizing the base face in order to produce the base shard.

Matrices in the base face are copositive and have a nonnegative critical point. However, these polynomials are degree 2. Thus, at least intuitively, this critical point should be a minimum for the overall function. Hence, it makes sense to conjecture that these matrices in the base face are not only copositive, but also positive semidefinite. This is good news because we can almost bijectively parametrize positive semidefinite matrices using the classic Cholesky decomposition. However, we run into issues because utilizing this method doesn't give us control over any critical points.

So we will do what we've been doing throughout this thesis, and we will use the critical point as parameters. Now in order to use the components of the critical point as parameters we will have to give up control over some of the entries of the matrix. For instance, we can split up a matrix into blocks,

$$A = \begin{bmatrix} A_{[n-1]} & b \\ b^\intercal & d \end{bmatrix},$$

where $A_{[n-1]}$ is the upper-left $(n-1) \times (n-1)$ block, b is a length $n-1$ vector, and d is a single scalar value. Now we can force this matrix to have a critical point by giving up control over b and d. Since the length of the critical point is irrelevant, we will scale the last component to be one. Then we have

$$\begin{bmatrix} A_{[n-1]} & b \\ b^\intercal & d \end{bmatrix} \begin{bmatrix} c \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

We can now solve this for b and d to get $b = -A_{[n-1]}c$ and $d = c^\intercal A_{[n-1]}c$. This leaves us with the block matrix

$$A = \begin{bmatrix} A_{[n-1]} & -A_{[n-1]}c \\ -c^\intercal A_{[n-1]} & c^\intercal A_{[n-1]}c \end{bmatrix},$$

where c is the critical point. Now we want this matrix to be copositive, and as we mentioned before, it makes sense to believe this matrix will also be positive semidefinite. If that's the case, then $A_{[n-1]}$ must also be positive semidefinite. We can straighten all this out in the following lemma.

Notation 4.3.2. Let $\mathbb{S}^k$ be the set of positive semi-definite matrices of size $k \times k$.

Lemma 4.3.3. *Let A be an $n \times n$ real symmetric matrix such that $Ax = 0$ for some $x \in \mathbb{R}^n_{>0}$. Then the following are equivalent.*

1. $A \in \mathrm{CF}_n$
2. $A \in \mathbb{S}^n$
3. $A_{[n-1]} \in \mathbb{S}^{n-1}$

Proof. For (1) to (2) assume that $A \in \mathrm{CF}_n$ and $A \notin \mathbb{S}^n$. Then there exists some $y \in \mathbb{R}^n \setminus \{0\}$ such that $y^\intercal A y < 0$. Let $\varepsilon \neq 0$ be such that $x + \varepsilon y \in \mathbb{R}^n_{>0}$. Then we have

$$\begin{aligned}(x^\intercal + \varepsilon y^\intercal)A(x + \varepsilon y) &= x^\intercal A x + \varepsilon x^\intercal A y + \varepsilon y^\intercal A x + \varepsilon^2 y^\intercal A y \\ &= \varepsilon^2 y^\intercal A y \\ &< 0.\end{aligned}$$

This contradicts $A \in \mathrm{CF}_n$.

For (2) to (3) is clear since a matrix being positive semi-definite implies all of its principal minors are positive semidefinite. Now we must show that (3) implies (1). Let $x \in \mathbb{R}^n_{>0}$ be such that $Ax = 0$, and note

$$\begin{aligned}Ax &= \begin{bmatrix} A_{[n-1]} & b \\ b^\intercal & c \end{bmatrix} \begin{bmatrix} x_{[n-1]} \\ x_n \end{bmatrix} \\ &= \begin{bmatrix} A_{[n-1]} x_{[n-1]} + x_n b \\ b^\intercal x_{[n-1]} + c\, x_n \end{bmatrix} \\ &= \begin{bmatrix} 0 \\ 0 \end{bmatrix}.\end{aligned}$$

This forces the structure of A to be

$$A = \begin{bmatrix} A_{[n-1]} & -\frac{1}{x_n} A_{[n-1]} x_{[n-1]} \\ -\frac{1}{x_n} x_{[n-1]}^\intercal A_{[n-1]}^\intercal & \frac{1}{x_n^2} x_{[n-1]}^\intercal A_{[n-1]} x_{[n-1]} \end{bmatrix}.$$

Now let $y \in \mathbb{R}^n_{\geq 0}$, and consider the quadratic form, $y^\intercal A y$, then we have

$$\begin{aligned} y^\intercal A y &= \begin{bmatrix} y_{[n-1]}^\intercal & y_n \end{bmatrix} \begin{bmatrix} A_{[n-1]} & -\frac{1}{x_n} A_{[n-1]} x_{[n-1]} \\ -\frac{1}{x_n} x_{[n-1]}^\intercal A_{[n-1]}^\intercal & \frac{1}{x_n^2} x_{[n-1]}^\intercal A_{[n-1]} x_{[n-1]} \end{bmatrix} \begin{bmatrix} y_{[n-1]} \\ y_n \end{bmatrix} \\ &= y_{[n-1]}^\intercal A_{[n-1]} y_{[n-1]} - \frac{2y_n}{x_n} \left(y_{[n-1]}^\intercal A_{[n-1]} x_{[n-1]} \right) + \left(\frac{y_n}{x_n} \right)^2 x_{[n-1]}^\intercal A_{[n-1]} x_{[n-1]} \\ &= \left(y_{[n-1]}^\intercal - \frac{y_n}{x_n} x_{[n-1]}^\intercal \right) A_{[n-1]} \left(y_{[n-1]} - \frac{y_n}{x_n} x_{[n-1]} \right) \\ &\geq 0. \end{aligned}$$

Thus, $A \in \mathrm{CF}_n$. □

Lemma 4.3.3 tells us that as long as the upper-left block is positive semidefinite, the whole matrix is copositive. Thus, we have our parametrization of the base face.

Lemma 4.3.4. *The map* $\Psi : \mathbb{S}^{n-1} \times \mathbb{R}^{n-1}_{\geq 0} \to S_n^{[n]}$ *defined by*

$$\Psi(A, c) = \begin{bmatrix} A & -Ac \\ -c^\intercal A & c^\intercal A c \end{bmatrix}$$

is almost bijective.

Proof. Note that the image of Ψ is a subset of $\mathbb{S}_n^{[n]}$ from Lemma 4.3.3. For injectivity assume that $\Psi(A, c) = \Psi(B, d)$. Then

$$\begin{bmatrix} A & -Ac \\ -c^\intercal A & c^\intercal A c \end{bmatrix} = \begin{bmatrix} B & -Bd \\ -d^\intercal B & d^\intercal B d \end{bmatrix}.$$

So clearly $A = B$, and thus $Ac = Ad$. Almost always A is invertible, and so we also have that $c = d$. Now to show surjectivity assume that $M \in S_n^{[n]}$. Note that we can write

$$M = \begin{bmatrix} M_{[n-1]} & -M_{[n-1]} c \\ -c^\intercal M_{[n-1]} & c^\intercal M_{[n-1]} c \end{bmatrix},$$

where $M \begin{bmatrix} c \\ 1 \end{bmatrix} = 0$. Note that if $M_{[n-1]}$ were singular then the rank of M would be too low. Thus, $M_{[n-1]} \in \mathbb{S}^{n-1}$, and we have $\Psi(M_{[n-1]}, c) = M$. □

Now we can easily extend this to the map we have in Theorem 4.2.1 by parametrizing the upper-left block with the Cholesky decomposition. For completeness we offer the following proof.

Proof. (Theorem 4.2.1) From Lemma 4.3.4 we have that the map $\Psi : \mathbb{S}^{n-1} \times \mathbb{R}^{n-1}_{\geq 0} \longrightarrow S^{[n]}_n$ defined by

$$\Psi(A, c) = \begin{bmatrix} A & -Ac \\ -c^\intercal A & c^\intercal Ac \end{bmatrix}$$

is almost bijective. Now since $A \in \mathbb{S}^{n-1}$, we can almost bijectively parametrize it via the Cholesky decomposition, namely,

$$A = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ \ell_{12} & 1 & 0 & \cdots & 0 \\ \ell_{13} & \ell_{23} & 1 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ \ell_{1(n-1)} & \cdots & \cdots & \ell_{(n-2)(n-1)} & 1 \end{bmatrix} \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & 0 & d_{n-1} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ \ell_{12} & 1 & 0 & \cdots & 0 \\ \ell_{13} & \ell_{23} & 1 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ \ell_{1(n-1)} & \cdots & \cdots & \ell_{(n-2)(n-1)} & 1 \end{bmatrix}^\intercal .$$

Let B denote $\Psi(A, c)$. We can extend B from its center, $C(B)$, obtaining the following map

$$\Phi \, : \, \mathbb{R}^{n-1}_{\geq 0} \times \mathbb{R}^{\binom{n-1}{2}} \times \mathbb{R}^{n-1}_{\geq 0} \times \mathbb{R}_{\geq 0} \, \longrightarrow \, \tilde{S}^{[n]}_n$$

where

$$\Phi(d, \ell, c, \lambda) \, = \, (1+\lambda)B - \lambda C(B).$$

By construction the resulting map, Φ, is almost bijective. $\square$

CHAPTER

5

PREPARATION FOR PARAMETRIZING COPOSITIVE POLYNOMIALS

In this chapter we carry out a preliminary study on the structure of copositive polynomials of any degree with any number of variables. We will begin by considering the homogeneous version of the problem. Afterwards, we extend our definition of face so that it applies in this general case. Then we offer a result similar to Lemma 4.3.3 with the long-term goal that we can use these results to parametrize the base face.

5.1 Setup

We will begin by considering an arbitrary polynomial $f \in \mathbb{R}[x_1, \dots, x_n]$ of degree d. As we've done before, we can homogenize f to be

$$\bar{f} = x_{n+1}^d \cdot f(x_1/x_{n+1}, \dots, x_n/x_{n+1}).$$

Again, it's not difficult to show that f is copositive if and only if $\bar{f}$ is copositive. Thus, we really only need to consider the homogeneous case. Often while considering copositive matrices we had to look at submatrices. In order to translate this to general homogeneous polynomials, we will have “subpolynomials." Below we formalize all of the notation.

Notation 5.1.1.

- $\mathrm{F}_{n,d}$ is the set of homogeneous polynomial in n variables of degree d.
- $\mathrm{PF}_{n,d} = \left\{ f \in \mathrm{F}_{n,d} : f(x) \geq 0 \text{ for all } x \in \mathbb{R}^n \right\}$.
- $\mathrm{CF}_{n,d} = \left\{ f \in \mathrm{F}_{n,d} : f(x) \geq 0 \text{ for all } x \in \mathbb{R}^n_{\geq 0} \right\}$.
- $[n] = \{1, 2, \ldots, n\}$
- $x = \{x_1, x_2, \ldots, x_n\}$
- $x_I = \{x_i : i \in I\}$, where $I \subset [n]$ with $I \neq \emptyset$.
- $f_I = f\big|_{x_{I'}=0} \in \mathbb{R}[x_I]$, where I' is the complement of $I \subset [n]$ with $I \neq \emptyset$.

Example 5.1.1. Let $f \in \mathrm{F}_{3,3}$ be the polynomial

$$f(x_1, x_2, x_3) = 4x_1x_2^2 - x_1x_2x_3 + 3x_2^3 + x_1x_3^2.$$

Then for $I = \{1, 2\}$ we have

$$\begin{aligned} f_I &= f(x_1, x_2, 0) \\ &= 4x_1x_2^2 + 3x_2^3. \end{aligned}$$

Now we will explore the structure of the boundary of $\mathrm{CF}_{n,d}$, as we did in previous chapters.

5.2 Boundary Structure

We will try to match the structure that was derived in Chapter 4. To that end let's consider the set of homogeneous copositive polynomials,

$$\mathrm{CF}_{n,d} = \left\{ f \in \mathrm{F}_{n,d} : f(x) \geq 0 \text{ for all } x \in \mathbb{R}^n_{\geq 0} \right\}.$$

It is not difficult to show that

$$\partial\, \mathrm{CF}_{n,d} = \left\{ f \in \mathrm{CF}_{n,d} : f(x) = 0 \text{ for some } x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \right\},$$

where $\partial\,\mathrm{CF}_{n,d}$ is the boundary of $\mathrm{CF}_{n,d}$. Now we will do the same thing as before to partition this set based upon which entries of x are zero. Then we get

$$\partial\,\mathrm{CF}_{n,d} = \left\{ f \in \mathrm{CF}_{n,d} : \exists \text{ nonempty } I \subset [n] \text{ and } x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x_I > 0 \text{ and } f_I(x_I) = 0 \right\}.$$

Now we will write this as a union to get

$$\partial\,\mathrm{CF}_{n,d} = \bigcup_{\substack{I \subset [n] \\ I \neq \emptyset}} \left\{ f \in \mathrm{CF}_{n,d} : \exists x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x_I > 0 \text{ and } f_I(x_I) = 0 \right\}.$$

Note that if f is copositive and homogeneous, then f_I is also copositive and homogeneous. Thus, by using Lemma 4.3.1 we get the following partition.

$$\partial\,\mathrm{CF}_{n,d} = \bigcup_{\substack{I \subset [n] \\ I \neq \emptyset}} \left\{ f \in \mathrm{CF}_{n,d} : \exists x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x_I > 0 \text{ and } \nabla f_I(x_I) = 0 \right\},$$

where ∇f_I is the gradient of f_I with respect to *only* the variables indexed by I. Now again, these sets do not contain their boundary. So we will close them and arrive at our generalization.

Definition 5.2.1. Let $I \subseteq [n]$ with $I \neq \emptyset$. Define the I-face, $S^I_{n,d}$, of $\mathrm{CF}_{n,d}$ to be the set

$$S^I_{n,d} = \left\{ f \in \mathrm{CF}_{n,d} : \exists x \in \mathbb{R}^n_{\geq 0} \setminus \{0\} \text{ such that } x_I \geq 0 \text{ and } \nabla f_I(x_I) = 0 \right\}.$$

This immediately gives us the following theorem.

Theorem 5.2.1. *We have*

$$\partial\,\mathrm{CF}_{n,d} = \bigcup_{\substack{I \subset [n] \\ I \neq \emptyset}} S^I_{n,d}.$$

So again, we can understand the boundary by understanding the faces. Further, we can understand the whole set by understanding the boundary. We can solidify this idea with the following theorem.

Theorem 5.2.2. *Let $n > 1$. Then*

$$\mathrm{CF}_{n,d} = \mathrm{conv}\left(\partial\,\mathrm{CF}_{n,d}\right)$$

Proof. Clearly $\mathrm{CF}_{n,d} \supseteq \mathrm{conv}\left(\partial\,\mathrm{CF}_{n,d}\right)$ since $\mathrm{CF}_{n,d}$ is convex. Now to show $\mathrm{CF}_{n,d} \subseteq \mathrm{conv}\left(\partial\,\mathrm{CF}_{n,d}\right)$, let $f \in \mathrm{CF}_{n,d}$. If $f \in \partial\,\mathrm{CF}_{n,d}$, then we are done. Thus, we will assume that $f \in \mathrm{int}(\mathrm{CF}_{n,d})$. Let

$i, j \in [n]$ with $i \neq j$, and note that

$$\underset{\lambda>0}{\exists}[f + \lambda(x_i^d - x_j^d)] \in \partial\, \mathrm{CF}_{n,d}\,.$$

Similarly,

$$\underset{\mu>0}{\exists}[f + \mu(x_j^d - x_i^d)] \in \partial\, \mathrm{CF}_{n,d}\,.$$

Then we have $[f + \lambda(x_i^d - x_j^d)] \in S_{n,d}^I$ and $[f + \mu(x_j^d - x_i^d)] \in S_{n,d}^J$ for some subsets I and J. Note that

$$\frac{\mu}{\lambda+\mu}[f + \lambda(x_i^d - x_j^d)] + \frac{\lambda}{\lambda+\mu}[f + \mu(x_j^d - x_i^d)] = f.$$

Thus, $f \in \mathrm{conv}\left(\bigcup_{I\subseteq[n]} S_{n,d}^I\right)$. □

5.3 Base Face

Following Chapter 4, the next task is to define the base face. This isn't too difficult. There is really only one way to extend this definition and remain consistent.

Definition 5.3.1. The *base face*, denoted $S_{n,d}^{[n]}$, is the set

$$S_{n,d}^{[n]} = \left\{ f \in \mathrm{CF}_{n,d} : \exists x \in \mathbb{R}_{\geq 0}^n \text{ such that } x \geq 0 \text{ and } \nabla f(x) = 0 \right\}.$$

Now we can try to do something similar to Lemma 4.3.3. In other words, we can try to partition the polynomial into an "upper-left" block while keeping the rest free to insert a critical point. The following conjecture is our attempt to do so.

Conjecture 5.3.1. *Let $f \in \mathrm{F}_{n,d}$ and let $t > 0$ be such that all $(d-1)$-order derivatives of f vanish on t. Then the following are equivalent.*

1. $f \in \mathrm{CF}_{n,d}$
2. $f \in \mathrm{PF}_{n,d}$
3. $f_{[n-1]} \in \mathrm{PF}_{n-1,d}$ *and* $\mathrm{coeff}(f, x_n^d) \geq 0$.

Note that for this conjecture we had to assume that the f had more than a positive critical point. Instead of the first derivative vanishing, we are requiring that the $(d-1)$st derivative vanishes. Unfortunately, we have not yet been able to prove this conjecture. However, if the conjecture is true, and if we have a parametrization method for $\mathrm{PF}_{n,d}$, then we should be able to parametrize the base face.

This is as far as we could push our results. We have looked into generalizing the idea of finding a center point from which we can extend each face into a shard, but as the degree increases the complexity also seems to increase. Thus, while we couldn't venture too far into the world of completely generic copositive polynomials, we still believe that these first steps could be important.

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APPENDIX

APPENDIX

A

COMPLETE FACIAL STRUCTURE OF CF_3

Here we give parametrizations for every face of CF_3 as well as parametrizations for every intersection of the faces. We obtained the faces from specializing our parametrization of CF_3 from Theorem 3.2.1. Then we carried out all possible intersections as preparation for future study on the combinatorics of the faces, that is, how they are joined together.

A.1 Faces

We have $\dim(\partial\, CF_3) = 5$ and is the union of these 7 faces. We will use a shorthand: $F_I = S_3^I$.

1. F_1

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & a_{1,3} \\ a_{1,2} & a_{2,2}^2 & \lambda - a_{2,2}a_{3,3} \\ a_{1,3} & \lambda - a_{2,2}a_{3,3} & a_{3,3}^2 \end{bmatrix} : a_{1,2}, a_{1,3}, a_{2,2}, a_{3,3}, \lambda \geq 0 \right\}$$

2. F_2

$$\left\{ \begin{bmatrix} a_{1,1}^2 & a_{1,2} & \lambda - a_{1,1}a_{3,3} \\ a_{1,2} & 0 & a_{2,3} \\ \lambda - a_{1,1}a_{3,3} & a_{2,3} & a_{3,3}^2 \end{bmatrix} : a_{1,2}, a_{2,3}, a_{1,1}, a_{3,3}, \lambda \geq 0 \right\}$$

3. F_3

$$\left\{ \begin{bmatrix} a_{1,1}^2 & \lambda - a_{1,1}a_{2,2} & a_{1,3} \\ \lambda - a_{1,1}a_{2,2} & a_{2,2}^2 & a_{2,3} \\ a_{1,3} & a_{2,3} & 0 \end{bmatrix} : a_{1,3}, a_{2,3}, a_{1,1}, a_{2,2}, \lambda \geq 0 \right\}$$

4. F_{12}

$$\left\{ \begin{bmatrix} a_{1,1}^2 & -a_{1,1}a_{2,2} & (2t_1-1)a_{1,1}a_{3,3}+\lambda t_1 \\ -a_{1,1}a_{2,2} & a_{2,2}^2 & (2t_2-1)a_{2,2}a_{3,3}+\lambda t_2 \\ (2t_1-1)a_{1,1}a_{3,3}+\lambda t_1 & (2t_2-1)a_{2,2}a_{3,3}+\lambda t_2 & a_{3,3}^2 \end{bmatrix} : \begin{matrix} a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \\ \lambda \geq 0 \\ t \in \Delta_2 \end{matrix} \right\}$$

5. F_{13}

$$\left\{ \begin{bmatrix} a_{1,1}^2 & (2t_1-1)a_{1,1}a_{2,2}+\lambda t_1 & -a_{1,1}a_{3,3} \\ (2t_1-1)a_{1,1}a_{2,2}+\lambda t_1 & a_{2,2}^2 & (2t_2-1)a_{2,2}a_{3,3}+\lambda t_2 \\ -a_{1,1}a_{3,3} & (2t_2-1)a_{2,2}a_{3,3}+\lambda t_2 & a_{3,3}^2 \end{bmatrix} : \begin{matrix} a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \\ \lambda \geq 0 \\ t \in \Delta_2 \end{matrix} \right\}$$

6. F_{23}

$$\left\{ \begin{bmatrix} a_{1,1}^2 & (2t_1-1)a_{1,1}a_{2,2}+\lambda t_1 & (2t_2-1)a_{1,1}a_{3,3}+\lambda t_2 \\ (2t_1-1)a_{1,1}a_{2,2}+\lambda t_1 & a_{2,2}^2 & -a_{1,1}a_{3,3} \\ (2t_2-1)a_{1,1}a_{3,3}+\lambda t_2 & -a_{1,1}a_{3,3} & a_{3,3}^2 \end{bmatrix} : \begin{matrix} a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \\ \lambda \geq 0 \\ t \in \Delta_2 \end{matrix} \right\}$$

7. F_{123}

$$\left\{ \begin{bmatrix} a_{1,1}^2 & a_{1,1}a_{2,2}\left(\frac{2t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)}-1\right) & a_{1,1}a_{3,3}\left(\frac{2t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)}-1\right) \\ a_{1,1}a_{2,2}\left(\frac{2t_3^2(1+t_1)(1+t_2)}{(1-t_1t_3)(1-t_2t_3)}-1\right) & a_{2,2}^2 & a_{2,2}a_{3,3}\left(\frac{2t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)}-1\right) \\ a_{1,1}a_{3,3}\left(\frac{2t_2^2(1+t_1)(1+t_3)}{(1-t_1t_2)(1-t_2t_3)}-1\right) & a_{2,2}a_{3,3}\left(\frac{2t_1^2(1+t_2)(1+t_3)}{(1-t_1t_2)(1-t_1t_3)}-1\right) & a_{3,3}^2 \end{bmatrix} : \begin{matrix} a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \\ t \in \Delta_3 \end{matrix} \right\}$$

A.2 4-dimensional intersections of faces

1. $F_1 \cap F_2$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & a_{1,3} \\ a_{1,2} & 0 & a_{2,3} \\ a_{1,3} & a_{2,3} & a_{3,3} \end{bmatrix} : a_{1,2}, a_{1,3}, a_{2,3}, a_{3,3} \geq 0 \right\}$$

2. $F_1 \cap F_3$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & a_{1,3} \\ a_{1,2} & a_{2,2} & a_{2,3} \\ a_{1,3} & a_{2,3} & 0 \end{bmatrix} : a_{1,2}, a_{1,3}, a_{2,3}, a_{2,2} \geq 0 \right\}$$

3. $F_2 \cap F_3$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{1,2} & 0 & a_{2,3} \\ a_{1,3} & a_{2,3} & 0 \end{bmatrix} : a_{1,2}, a_{1,3}, a_{2,3}, a_{1,1} \geq 0 \right\}$$

4. $F_1 \cap F_{12}$

$$\left\{ \begin{bmatrix} 0 & 0 & a_{1,3} \\ 0 & a_{2,2} & a_{2,3} \\ a_{1,3} & a_{2,3} & a_{3,3} \end{bmatrix} : a_{1,3}, a_{2,3}, a_{2,2}, a_{3,3} \geq 0 \right\}$$

5. $F_1 \cap F_{13}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & 0 \\ a_{1,2} & a_{2,2} & a_{2,3} \\ 0 & a_{2,3} & a_{3,3} \end{bmatrix} : a_{1,2}, a_{2,3}, a_{2,2}, a_{3,3} \geq 0 \right\}$$

6. $F_1 \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & a_{1,3} \\ a_{1,2} & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ a_{1,3} & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,2}, a_{1,3}, a_{2,2}, a_{3,3} \geq 0 \right\}$$

7. $F_2 \cap F_{12}$

$$\left\{ \begin{bmatrix} a_{1,1} & 0 & a_{1,3} \\ 0 & 0 & a_{2,3} \\ a_{1,3} & a_{2,3} & a_{3,3} \end{bmatrix} : a_{1,3}, a_{2,3}, a_{1,1}, a_{3,3} \geq 0 \right\}$$

8. $F_2 \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & -\sqrt{a_{1,1}a_{3,3}} \\ a_{1,2} & 0 & a_{2,3} \\ -\sqrt{a_{1,1}a_{3,3}} & a_{2,3} & a_{3,3} \end{bmatrix} : a_{1,2}, a_{2,3}, a_{1,1}, a_{3,3} \geq 0 \right\}$$

9. $F_2 \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{1,2} & 0 & 0 \\ a_{1,3} & 0 & a_{3,3} \end{bmatrix} : a_{1,2}, a_{1,3}, a_{1,1}, a_{3,3} \geq 0 \right\}$$

10. $F_3 \cap F_{12}$

$$\left\{ \begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & a_{1,3} \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & a_{2,3} \\ a_{1,3} & a_{2,3} & 0 \end{bmatrix} : a_{1,3}, a_{2,3}, a_{1,1}, a_{2,2} \geq 0 \right\}$$

11. $F_3 \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & 0 \\ a_{1,2} & a_{2,2} & a_{2,3} \\ 0 & a_{2,3} & 0 \end{bmatrix} : a_{1,2}, a_{2,3}, a_{1,1}, a_{2,2} \geq 0 \right\}$$

12. $F_3 \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{1,2} & a_{2,2} & 0 \\ a_{1,3} & 0 & 0 \end{bmatrix} : a_{1,2}, a_{1,3}, a_{1,1}, a_{2,2} \geq 0 \right\}$$

13. $F_{12} \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & -\sqrt{a_{1,1}a_{3,3}} \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & \lambda + \sqrt{a_{2,2}a_{3,3}} \\ -\sqrt{a_{1,1}a_{3,3}} & \lambda + \sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,1}, a_{2,2}, a_{3,3}, \lambda \geq 0 \right\}$$

14. $F_{12} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & \lambda + \sqrt{a_{1,1}a_{3,3}} \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ \lambda + \sqrt{a_{1,1}a_{3,3}} & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,1}, a_{2,2}, a_{3,3}, \lambda \geq 0 \right\}$$

15. $F_{13} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & \lambda + \sqrt{a_{1,1}a_{2,2}} & -\sqrt{a_{1,1}a_{3,3}} \\ \lambda + \sqrt{a_{1,1}a_{2,2}} & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ -\sqrt{a_{1,1}a_{3,3}} & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,1}, a_{2,2}, a_{3,3}, \lambda \geq 0 \right\}$$

16. $F_{123} \cap F_{12}$

$$\left\{ \begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & (2t_1 - 1)\sqrt{a_{1,1}a_{3,3}} \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & (2t_2 - 1)\sqrt{a_{2,2}a_{3,3}} \\ (2t_1 - 1)\sqrt{a_{1,1}a_{3,3}} & (2t_2 - 1)\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : \begin{matrix} a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \\ t \in \Delta_2 \end{matrix} \right\}$$

17. $F_{123} \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & (2t_1-1)\sqrt{a_{1,1}a_{2,2}} & -\sqrt{a_{1,1}a_{3,3}} \\ (2t_1-1)\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & (2t_2-1)\sqrt{a_{2,2}a_{3,3}} \\ -\sqrt{a_{1,1}a_{3,3}} & (2t_2-1)\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : \begin{array}{c} a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \\ t \in \Delta_2 \end{array} \right\}$$

18. $F_{123} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & (2t_1-1)\sqrt{a_{1,1}a_{2,2}} & (2t_2-1)\sqrt{a_{1,1}a_{3,3}} \\ (2t_1-1)\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ (2t_2-1)\sqrt{a_{1,1}a_{3,3}} & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : \begin{array}{c} a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \\ t \in \Delta_2 \end{array} \right\}$$

A.3 3-dimensional intersections of faces

1. $F_1 \cap F_2 \cap F_3$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & a_{1,3} \\ a_{1,2} & 0 & a_{2,3} \\ a_{1,3} & a_{2,3} & 0 \end{bmatrix} : a_{1,2}, a_{1,3}, a_{2,3} \geq 0 \right\}$$

2. $F_1 \cap F_2 \cap F_{12}$

$$\left\{ \begin{bmatrix} 0 & 0 & a_{1,3} \\ 0 & 0 & a_{2,3} \\ a_{1,3} & a_{2,3} & a_{3,3} \end{bmatrix} : a_{1,3}, a_{2,3}, a_{3,3} \geq 0 \right\}$$

3. $F_1 \cap F_2 \cap F_{13}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & 0 \\ a_{1,2} & 0 & a_{2,3} \\ 0 & a_{2,3} & a_{3,3} \end{bmatrix} : a_{1,2}, a_{2,3}, a_{3,3} \geq 0 \right\}$$

4. $F_1 \cap F_2 \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & a_{1,3} \\ a_{1,2} & 0 & 0 \\ a_{1,3} & 0 & a_{3,3} \end{bmatrix} : a_{1,2}, a_{1,3}, a_{3,3} \geq 0 \right\}$$

5. $F_1 \cap F_3 \cap F_{12}$

$$\left\{ \begin{bmatrix} 0 & 0 & a_{1,3} \\ 0 & a_{2,2} & a_{2,3} \\ a_{1,3} & a_{2,3} & 0 \end{bmatrix} : a_{1,3}, a_{2,3}, a_{2,2} \geq 0 \right\}$$

6. $F_1 \cap F_3 \cap F_{13}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & 0 \\ a_{1,2} & a_{2,2} & a_{2,3} \\ 0 & a_{2,3} & 0 \end{bmatrix} : a_{1,2}, a_{2,3}, a_{2,2} \geq 0 \right\}$$

7. $F_1 \cap F_3 \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & a_{1,3} \\ a_{1,2} & a_{2,2} & 0 \\ a_{1,3} & 0 & 0 \end{bmatrix} : a_{1,2}, a_{1,3}, a_{2,2} \geq 0 \right\}$$

8. $F_2 \cap F_3 \cap F_{12}$

$$\left\{ \begin{bmatrix} a_{1,1} & 0 & a_{1,3} \\ 0 & 0 & a_{2,3} \\ a_{1,3} & a_{2,3} & 0 \end{bmatrix} : a_{1,3}, a_{2,3}, a_{1,1} \geq 0 \right\}$$

9. $F_2 \cap F_3 \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & 0 \\ a_{1,2} & 0 & a_{2,3} \\ 0 & a_{2,3} & 0 \end{bmatrix} : a_{1,2}, a_{2,3}, a_{1,1} \geq 0 \right\}$$

10. $F_2 \cap F_3 \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{1,2} & 0 & 0 \\ a_{1,3} & 0 & 0 \end{bmatrix} : a_{1,2}, a_{1,3}, a_{1,1} \geq 0 \right\}$$

11. $F_1 \cap F_{12} \cap F_{13} = F_1 \cap F_{123} \cong \mathrm{CF}_2$

$$\left\{ \begin{bmatrix} 0 & 0 & 0 \\ 0 & a_{2,2} & \lambda - \sqrt{a_{2,2}a_{3,3}} \\ 0 & \lambda - \sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{2,2}, a_{3,3}, \lambda \geq 0 \right\}$$

12. $F_2 \cap F_{12} \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & 0 & -\sqrt{a_{1,1}a_{3,3}} \\ 0 & 0 & a_{2,3} \\ -\sqrt{a_{1,1}a_{3,3}} & a_{2,3} & a_{3,3} \end{bmatrix} : a_{2,3}, a_{1,1}, a_{3,3} \geq 0 \right\}$$

13. $F_3 \cap F_{12} \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & 0 \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & a_{2,3} \\ 0 & a_{2,3} & 0 \end{bmatrix} : a_{2,3}, a_{1,1}, a_{2,2} \geq 0 \right\}$$

14. $F_1 \cap F_{12} \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & 0 & a_{1,3} \\ 0 & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ a_{1,3} & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,3}, a_{2,2}, a_{3,3} \geq 0 \right\}$$

15. $F_2 \cap F_{12} \cap F_{23} = F_2 \cap F_{123} \cong \mathrm{CF}_2$

$$\left\{ \begin{bmatrix} a_{1,1} & 0 & \lambda - \sqrt{a_{1,1}a_{3,3}} \\ 0 & 0 & 0 \\ \lambda - \sqrt{a_{1,1}a_{3,3}} & 0 & a_{3,3} \end{bmatrix} : a_{1,1}, a_{3,3}, \lambda \geq 0 \right\}$$

16. $F_3 \cap F_{12} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & a_{1,3} \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & 0 \\ a_{1,3} & 0 & 0 \end{bmatrix} : a_{1,3}, a_{1,1}, a_{2,2} \geq 0 \right\}$$

17. $F_1 \cap F_{13} \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & 0 \\ a_{1,2} & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ 0 & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,2}, a_{2,2}, a_{3,3} \geq 0 \right\}$$

18. $F_2 \cap F_{13} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & -\sqrt{a_{1,1}a_{3,3}} \\ a_{1,2} & 0 & 0 \\ -\sqrt{a_{1,1}a_{3,3}} & 0 & a_{3,3} \end{bmatrix} : a_{1,2}, a_{1,1}, a_{3,3} \geq 0 \right\}$$

19. $F_3 \cap F_{13} \cap F_{23} = F_3 \cap F_{123} \cong \mathrm{CF}_2$

$$\left\{ \begin{bmatrix} a_{1,1} & \lambda - \sqrt{a_{1,1}a_{2,2}} & 0 \\ \lambda - \sqrt{a_{1,1}a_{2,2}} & a_{2,2} & 0 \\ 0 & 0 & 0 \end{bmatrix} : a_{1,1}, a_{2,2}, \lambda \geq 0 \right\}$$

20. $F_{123} \cap F_{12} \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & -\sqrt{a_{1,1}a_{3,3}} \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & \sqrt{a_{2,2}a_{3,3}} \\ -\sqrt{a_{1,1}a_{3,3}} & \sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \right\}$$

21. $F_{123} \cap F_{12} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & \sqrt{a_{1,1}a_{3,3}} \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ \sqrt{a_{1,1}a_{3,3}} & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \right\}$$

22. $F_{123} \cap F_{13} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & \sqrt{a_{1,1}a_{2,2}} & -\sqrt{a_{1,1}a_{3,3}} \\ \sqrt{a_{1,1}a_{2,2}} & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ -\sqrt{a_{1,1}a_{3,3}} & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{1,1}, a_{2,2}, a_{3,3} \geq 0 \right\}$$

A.4 2-dimensional intersections of faces

1. $F_1 \cap F_2 \cap F_3 \cap F_{12}$

$$\left\{ \begin{bmatrix} 0 & 0 & a_{1,3} \\ 0 & 0 & a_{2,3} \\ a_{1,3} & a_{2,3} & 0 \end{bmatrix} : a_{1,3}, a_{2,3} \geq 0 \right\}$$

2. $F_1 \cap F_2 \cap F_3 \cap F_{13}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & 0 \\ a_{1,2} & 0 & a_{2,3} \\ 0 & a_{2,3} & 0 \end{bmatrix} : a_{1,2}, a_{2,3} \geq 0 \right\}$$

3. $F_1 \cap F_2 \cap F_3 \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & a_{1,3} \\ a_{1,2} & 0 & 0 \\ a_{1,3} & 0 & 0 \end{bmatrix} : a_{1,2}, a_{1,3} \geq 0 \right\}$$

4. $F_1 \cap F_2 \cap F_{12} \cap F_{13}$

$$\left\{ \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & a_{2,3} \\ 0 & a_{2,3} & a_{3,3} \end{bmatrix} : a_{2,3}, a_{3,3} \geq 0 \right\}$$

5. $F_1 \cap F_2 \cap F_{12} \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & 0 & a_{1,3} \\ 0 & 0 & 0 \\ a_{1,3} & 0 & a_{3,3} \end{bmatrix} : a_{1,3}, a_{3,3} \geq 0 \right\}$$

6. $F_1 \cap F_2 \cap F_{13} \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & 0 \\ a_{1,2} & 0 & 0 \\ 0 & 0 & a_{3,3} \end{bmatrix} : a_{1,2}, a_{3,3} \geq 0 \right\}$$

7. $F_1 \cap F_3 \cap F_{12} \cap F_{13}$

$$\left\{ \begin{bmatrix} 0 & 0 & 0 \\ 0 & a_{2,2} & a_{2,3} \\ 0 & a_{2,3} & 0 \end{bmatrix} : a_{2,3}, a_{2,2} \geq 0 \right\}$$

8. $F_1 \cap F_3 \cap F_{12} \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & 0 & a_{1,3} \\ 0 & a_{2,2} & 0 \\ a_{1,3} & 0 & 0 \end{bmatrix} : a_{1,3}, a_{2,2} \geq 0 \right\}$$

9. $F_1 \cap F_3 \cap F_{13} \cap F_{23}$

$$\left\{ \begin{bmatrix} 0 & a_{1,2} & 0 \\ a_{1,2} & a_{2,2} & 0 \\ 0 & 0 & 0 \end{bmatrix} : a_{1,2}, a_{2,2} \geq 0 \right\}$$

10. $F_2 \cap F_3 \cap F_{12} \cap F_{13}$

$$\left\{ \begin{bmatrix} a_{1,1} & 0 & 0 \\ 0 & 0 & a_{2,3} \\ 0 & a_{2,3} & 0 \end{bmatrix} : a_{2,3}, a_{1,1} \geq 0 \right\}$$

11. $F_2 \cap F_3 \cap F_{12} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & 0 & a_{1,3} \\ 0 & 0 & 0 \\ a_{1,3} & 0 & 0 \end{bmatrix} : a_{1,3}, a_{1,1} \geq 0 \right\}$$

12. $F_2 \cap F_3 \cap F_{13} \cap F_{23}$

$$\left\{ \begin{bmatrix} a_{1,1} & a_{1,2} & 0 \\ a_{1,2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} : a_{1,2}, a_{1,1} \geq 0 \right\}$$

13. $F_2 \cap F_{12} \cap F_{13} \cap F_{123}$

$$\left\{ \begin{bmatrix} a_{1,1} & 0 & -\sqrt{a_{1,1}a_{3,3}} \\ 0 & 0 & 0 \\ -\sqrt{a_{1,1}a_{3,3}} & 0 & a_{3,3} \end{bmatrix} : a_{1,1}, a_{3,3} \geq 0 \right\}$$

14. $F_3 \cap F_{12} \cap F_{13} \cap F_{123}$

$$\left\{\begin{bmatrix} a_{1,1} & -\sqrt{a_{1,1}a_{2,2}} & 0 \\ -\sqrt{a_{1,1}a_{2,2}} & a_{2,2} & 0 \\ 0 & 0 & 0 \end{bmatrix} : a_{1,1}, a_{2,2} \geq 0\right\}$$

15. $F_1 \cap F_{12} \cap F_{23} \cap F_{123}$

$$\left\{\begin{bmatrix} 0 & 0 & 0 \\ 0 & a_{2,2} & -\sqrt{a_{2,2}a_{3,3}} \\ 0 & -\sqrt{a_{2,2}a_{3,3}} & a_{3,3} \end{bmatrix} : a_{2,2}, a_{3,3} \geq 0\right\}$$

A.5 1-dimensional intersections of faces

1. $F_1 \cap F_2 \cap F_3 \cap F_{12} \cap F_{13}$

$$\left\{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & a_{2,3} \\ 0 & a_{2,3} & 0 \end{bmatrix} : a_{2,3} \geq 0\right\}$$

2. $F_1 \cap F_2 \cap F_3 \cap F_{12} \cap F_{23}$

$$\left\{\begin{bmatrix} 0 & 0 & a_{1,3} \\ 0 & 0 & 0 \\ a_{1,3} & 0 & 0 \end{bmatrix} : a_{1,3} \geq 0\right\}$$

3. $F_1 \cap F_2 \cap F_3 \cap F_{13} \cap F_{23}$

$$\left\{\begin{bmatrix} 0 & a_{1,2} & 0 \\ a_{1,2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} : a_{1,2} \geq 0\right\}$$

4. $F_1 \cap F_2 \cap F_{13} \cap F_{23} \cap F_{123}$

$$\left\{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & a_{33} \end{bmatrix} : a_{3,3} \geq 0\right\}$$

5. $F_1 \cap F_3 \cap F_{12} \cap F_{23} \cap F_{123}$

$$\left\{\begin{bmatrix} 0 & 0 & 0 \\ 0 & a_{2,2} & 0 \\ 0 & 0 & 0 \end{bmatrix} : a_{2,2} \geq 0\right\}$$

6. $F_2 \cap F_3 \cap F_{12} \cap F_{13} \cap F_{123}$

$$\left\{ \begin{bmatrix} a_{1,1} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} : a_{1,1} \geq 0 \right\}$$