Matrix monotone functions

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Chapter 1

Matrix monotone functions – part 0

1.1 Disclaimer

Let's be honest: this master's thesis is not really about matrix monotone functions. What is it about, then? Well, unfortunately the only way I know how to answer that question is to explain what the matrix monotone functions are.[1] Hence the title.

1.2 What are matrix monotone functions?

Definition 1.1. Let $(a, b) \subset \mathbb{R}$ be an open, possibly unbounded interval and n positive integer. We say that $f : (a, b) \to \mathbb{R}$ is **n-monotone** or **matrix monotone** of order n on (a, b), if for any two $n \times n$ Hermitian matrices A and B with spectra in (a, b), such that $B - A$ is positive semidefinite, also $f(B) - f(A)$ positive semidefinite. Here $f(A)$ and $f(B)$ are defined via functional calculus.

Now, it might not be too big of a surprise that, on the surface level at least, the main question of this thesis is the following.

Question 1.2. Fix a positive integer n and an open interval (a, b). Which functions are n-monotone on (a, b)?

If all this makes sense to you, great! Feel free to skip this section. If not, what follows is an attempt to give some kind of handwavy picture of the setup. Alternatively, if you don't like handwaving, you may feel free to visit chapter 2 for rigorous foundations.

Matrix monotonicity is a generalization of standard monotonicity of real functions: now we are just having functions mapping matrices to matrices. Formally, f is **matrix**

[1] Worry not: one need not read beyond this chapter to get some kind of answer to the question.

monotone if for any two matrices A and B such that

$$A \leq B$$

we also have

$$f(A) \leq f(B).$$

This kind of function might be more properly called **matrix increasing** but we will stick to monotonicity for couple of reasons:

- For some reason, that is what people have been doing in the field.
- It doesn't make much difference whether we talk about increasing or decreasing functions, so we might just ignore the latter but try to symmetrize our thinking by the choice of words.
- Somehow I can't satisfactorily fill the following table:

monotonic	monotonicity
increasing	?

  How very inconvenient.

Of course, it's not really obvious how one should make any sense of this "definition". There are essentially two things to understand.

- How should matrices be ordered?
- How should functions act on matrices?

Both of these questions can be certainly answered in many ways, but for both of them there is very natural, in fact tensorial, answer. Instead of comparing matrices we can compare bilinear forms, $(0, 2)$-tensors (bilinear maps $V^2 \to \mathbb{R}$). Similarly we can naturally apply function to linear mappings, $(1, 1)$-tensors (bilinear maps $V^* \times V \to \mathbb{R}$). Here V is a n-dimensional vector space over $\mathbb{R}$.

For matrix (bilinear form) ordering we should first understand which matrices are *positive*, which here, a bit confusingly maybe, means "at least zero". We say that a form is positive if its diagonal is non-negative. This gives a partial order on the space of all bilinear forms.

For matrix functions, i.e. "how to apply function to matrix" the idea is to take a real function, $f : \mathbb{R} \to \mathbb{R}$, and interpret it as function $f : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$, *matrix function.*

Polynomials extend rather naturally, given the ring structure of linear maps themselves. If the argument (a linear map) is diagonalizable, this extension merely applies the function to the eigenvalues. This motivates us to define $f(A)$ for linear map A to be linear map with same eigenspace structure as A but the eigenvalues changed from $\lambda \to f(\lambda)$, respectively. All this works for diagonalizable maps with real eigenvalues, so the domain isn't quite $\mathbb{R}^{n\times n}$. This extension idea is called **functional calculus**.

All this is kind of enough to make sense of matrix monotonicity, but to drastically simplify the setup it is customary to restrict the attention to a special set of diagonalizable matrices, which in this text are called **real maps**. They are exactly the symmetric matrices and they hold special place amidst the set of all matrices.

- They exactly correspond to symmetric bilinear forms.
- They correspond to diagonalizable linear maps with real eigenvalues and orthogonal eigenbasis.

In the second point we are thinking about everything in terms of standard inner product of $\mathbb{R}^n$. So the statement should be corrected to

- If considered as matrix of a linear map with respect to the standard orthonormal basis of $\mathbb{R}^n$ (with the standard inner product), then the linear map is diagonalizable with real eigenvalues and has orthogonal eigenbasis.

Real maps are usually called **Hermitian** or **self-adjoint matrices** and positive matrices **positive semidefinite matrices**. Now the definition of matrix monotinicity 1.1 should make sense. We will call positive matrices **positive maps**.

Whether one should think about real maps as matrices, bilinear forms or linear maps depends on the context. If one does calculations, one might think about matrices. If one thinks about additive structure, bilinear forms are better suited. And of course functional calculus makes only sense with linear maps. We use the (linear) map terminology throughout mainly because it short. Also, it is a constant reminder that there is something tensorial going on.

1.3 ...And why should we care?

It's easy to come up with one family of matrix monotone functions: $x \mapsto \alpha x + \beta$ for $\alpha, \beta \in \mathbb{R}$ with $\alpha \geq 0$. It is n-monotone for every $n \geq 1$ on $(-\infty, \infty)$. This is the only easy example.

But there are lot more.

Matrix monotone functions are truly horrible. All matrix monotone functions are increasing (in the usual sense) but not every increasing function is matrix monotone. They have some obscure regularity properties. Constructing non-trivial matrix monotone functions is a pain. Although usual increasing real functions and matrix monotone functions should be very much interlinked, hardly any of the properties of increasing functions pass on to matrix monotonicity. Generally, if one attacks matrix monotone functions, especially of order $n > 2$, and doesn't use sophisticated weaponry, one will perish. The reader is encouraged to try.

All this is exactly what makes them so interesting. One is driven to ask the question:

Question 1.3. How should one think about matrix monotone functions?

If this sounds like the same question to you, think about increasing functions on $\mathbb{R}^n$. Function $f : \mathbb{R}^n \to \mathbb{R}$ is called n-increasing (this termonology lasts only for next couple of paragraphs) if $f(x_1, x_2, \ldots, x_n) \leq f(y_1, y_2, \ldots, y_n)$ whenever $x_i \leq y_i$ for every $1 \leq i \leq n$. Which functions are n-increasing? I would argue that n-increasing functions are awful, much more so than the usual (1-)increasing functions. The reason is that they don't have good "building blocks".

One might say that "non-negative derivative" property (let's ignore regularity issues for a while) makes increasing functions easy to understand, and while there is certain truth to that, I would argue that what makes them so simple is really the dual property: "increasing functions are sums of increasing step functions". This roughly implies that in order to understand increasing functions, it is enough to understand step functions, or just step functions with one jump upwards.

Note that we are heavily using the fact that increasing functions (of all types introduced before) form a convex cone:

Definition 1.4. Subset C of a vector space V over $\mathbb{R}$ is a convex cone if whenever $v, w \in C$ and $\alpha, \beta \geq 0$, also $\alpha v + \beta w \in C$.

Also, applicability of the "only needing to understand step functions" is somewhat limited: it doesn't really explain smoothness phenomena all too well, for instance. But it is always nice to know that some objects are really sums of other much simpler objects.

There's no such nice dual property for n-increasing functions (for $n > 1$). One can understand them locally with derivatives, but there are no simple decompositions. Same thing could be said about convex functions on $\mathbb{R}^n$.

Much more importantly for us, these is no such nice additive structure for n-monotone functions. This is by no means trivial (as it is not even with n-increasing functions). It is also not even clear what one means by "nice" and whether even increasing functions are that "nice" in the end. These ideas shall however merely work as our guideline, so one should not feel too troubled.

All these issues can be, in a way, avoided by change of perspective: instead of trying to characterize matrix monotone functions by expressing them as sums of something simple, we express the definition itself as a sum of somethings simple. In particular we try to understand the "dual" (or a "predual" to be exact) of matrix monotone functions.

1.4 Dual cones

Let in the following V be a vector space over $\mathbb{R}$ and denote its dual by V^*.

Definition 1.5. For a subset C^* of V^* we define its **dual cone** to be

$$C = \{v \in V | w^* v \geq 0 \text{ for every } w^* \in V^*\} \subset V.$$

One immediately makes the following observation justifying the terminology.

Theorem 1.6. *Let $C^* \subset V^*$. Then the dual cone of C^* is a convex cone.*

Definition 1.7. Let $C \subset V$. Then C^* is a **predual** of C if C is the dual cone of C^*.

Of course only convex cones have preduals. Easy examples show that preduals are not unique in general (in fact never).

As an example, for an open interval (a, b) consider the set

$$P_1(a, b) := \{\text{Increasing functions } f : (a, b) \to \mathbb{R}\}.$$

This set is a convex cone. If one denotes the evaluation functional or measure at x by δ_x, i.e. $\delta_x(f) = f(x_0)$, then one possible predual of $P_1(a, b)$ if given by

$$\{\delta_y - \delta_x | a < x < y < b\}.$$

I hope the reader agrees that this predual is in many ways much simpler than the set of increasing functions (at least if one looks at objects themselves) and yet it carries the information thereof. As we will see, if chosen suitably, preduals can offer convenient and clean language for talking about the cone itself. And that is what this thesis is really about.

1.5 Contents

As mentioned, one of the aims of this thesis is to answer question 1.2. An answer, if you're curious, is given as theorem 5.1. An obvious follow up question is

Question 1.8. Fix an open interval (a, b). Which functions are n-monotone on (a, b) for any $n \geq 1$?

It turns out that this question has a surprisingly simple answer, given as theorems 5.12 and 5.14.

Aim of the chapters entitled "Matrix monotone functions – part i" for $0 \leq i \leq 3$ is to answer to these questions. Other chapters, ones with even number, offer supplementary information.

The whole theory of matrix monotone functions originates from a 1934 paper by Charles Loewner (then known as Karl Löwner) entitled "Über monotone Matrixfunktionen" [11]. In the paper Loewner asked the questions 1.2 and 1.8, and gave them both answers. Since then the theory has been reworked and expanded by various authors, and many open questions remain. This text is an amalgamation of countless works on the subject. "Notes and references" -sections at the end of each chapter (except this one) are an attempt to give attribution to these ancestors.

Arguments of this thesis are largely elementary, requiring only basic calculus, complex analysis, linear algebra and topology. Many of the underlying ideas and heuristics are however inspired by functional analysis and measure theory, so it pays to have a good understanding of them.

1.6 Notation and conventions

TODO: fix this

w.l.o.g	without loss of generality
t.f.i.f	this follows immediately from
$Lip(f)$	(the best) Lipschitz constant of f
V^*	(continuous) dual of (topological) vector space V
$\mathcal{L}(V)$	linear self-maps over vector space V
$\mathcal{H}(V)$	real maps over inner product space V
$\mathcal{H}_+(V)$	positive maps over inner product space V
$\mathcal{H}_{(a,b)}(V)$	real maps over inner product space V with spectra on (a,b)
$P_n(a,b)$	n-monotone functions on (a,b) (change this?)
$P_\infty(a,b)$	intersection of $P_n(a,b)$ for $n \geq 1$
$P_W = P_{W,V}$	orthogonal projection to $W \subset V$
A^*	adjoint of a map $A \in \mathcal{L}(V)$
f_V	matrix function lift of f to V
$\mathbb{R}_n[x]$	Real polynomials of degree at most n
$\mathbb{C}_n[x]$	Complex polynomial of degree at most n
q^*	for given polynomial q, q^* is a polynomial with $q^*(z) = \overline{q(\overline{z})}$
$N(q)$	qq^*

We also preserve certain letters to have particular meaning.

a, b	extended reals with $-\infty \leq a < b \leq \infty$
n, k	positive integers
V	inner product space over $\mathbb{C}$ (with inner product $\langle \cdot, \cdot \rangle$) of dimension n

TODO:

- When is $\mathcal{P}(X)$ dense in $\mathcal{P}(\mathbb{H}_+)$? Nicolau might imply that this is the case if (and only if?)

$$\sum_{z \in X} \frac{\Im(z)}{|z|^2 + 1} = \infty$$

- Main theorem simplification: note that the rational function is non-negative outside (a, b) just by monotonicity of inverse function. What kind of rational functions will there be?

TODO: check the TODO-lists (in comments).

Chapter 2

Positive maps

2.1 Motivation

2.1.1 The right definition

Throughout this thesis, if not stated otherwise, $V = (V, \langle\cdot,\cdot\rangle)$ denotes an inner product space over $\mathbb{C}$ of dimension n (where n is an arbitrary but fixed positive integer).

Definition 2.1. We say that A is *positive map*, or simply *positive*, and write $A \geq 0$, if for any $v \in V$ we have

$$\langle Av, v\rangle \geq 0.$$

Why is this the right definition for positivity? Do we really need an inner product to define positivity?

While these are both excellent questions (and one should definitely think about them), there is no way to satisfactorily answer them in the scope of this thesis. Instead, this section is an attempt to explain why the definition is pretty damn good.

Note that, contrary to the previous chapter, we snuck in the complex numbers and "general" vector space to the definition (see "Notation and conventions" in the previous chapter). It doesn't make much difference whether we talk about real or complex numbers but the author thinks that some of the arguments are more natural in the complex world. Also, having the general vector space V is mostly just a reminder of the fact that there is something tensorial going on.

Theorem 1.6 immediately implies

Theorem 2.2. *The set*

$$\{A \in \mathcal{L}(V) |\ A \text{ is positive}\}$$

is a convex cone.

We denote this cone of positive maps (of V) by $\mathcal{H}_+(V)$.

In general one should think that the convex cones are models of positive real numbers. Such model need not be very good however: the whole vector space is always a convex cone. To fix this problem one introduces the concept of salient cone.

Definition 2.3. A convex cone $C \subset V$ is **salient cone**, or simply **salient**, if whenever both $v \in C$ and $-v \in C$, then necessarily $v = 0$.

Conveniently enough $\mathcal{H}_+(V)$ is a salient cone, but this is by no means trivial property.

Lemma 2.4. *If $A \in \mathcal{L}(V)$ and $\langle Av, v\rangle = 0$ for any $v \subset V$, then $A = 0$.*

Proof. The idea is that we can recover the inner product from norm. Indeed, if $v, w \in V$, then $\|v + w\|^2 = \|v\|^2 + \|w\|^2 + 2\Re(\langle v, w\rangle)$, so knowing the norm, we at least know the real part of the inner product. Doing the same trick with $\|v + iw\|^2$ we can figure out the imaginary part.

How does this help us? By a similar argument $\langle A(v+w), v+w\rangle = \langle Av, v\rangle + \langle Aw, w\rangle + \langle Av, w\rangle + \langle Aw, v\rangle$, so given that the quadratic form is always zero, we have $\langle Av, w\rangle + \langle Aw, v\rangle = 0$ for any $v, w \in V$. Expanding $\langle A(v + iw), v + iw\rangle$ we see that $-i\langle Av, w\rangle + i\langle Av, w\rangle = 0$, which together with the previous observation implies that $\langle Av, w\rangle = 0$ for any $v, w \in V$. Now setting $w = Av$ this implies that $\|Av\|^2 = 0$ for every $v \in V$ so $A = 0$. $\square$

The idea of recovering the inner product from the norm is called **polarization**.

As V has a topology, the concept of **closed convex cone**, which is defined as one would expect, makes sense. As subset of dual lead to convex cones, subsets of continuous dual lead to closed convex cones.

A closed convex cone that is also salient is, as is somewhat customary, called **proper cone**. We have

Theorem 2.5. *$\mathcal{H}_+(V)$ is a proper cone (with the usual topology).*

Previous arguments carry directly to a much more general setting:

Theorem 2.6. *Let V be a topological vector space (over $\mathbb{R}$ or $\mathbb{C}$) and C^* a subset of its continuous dual. Then*

$$C := \{v \in V | w^*(v) \geq 0 \text{ for every } w^* \in C^*\}$$

is a closed convex cone of V. If also

$$\{v \in V | w^*(v) = 0 \text{ for every } w^* \in C^*\} = \{0\},$$

then C is proper.

In our case the subset of the linear functionals are the mappings of the form $A \mapsto \langle Av, v \rangle$: they are called *quadratic functionals*. For fixed $A \in \mathcal{L}(V)$ the map $v \mapsto \langle Av, v \rangle$ is the *quadratic form* of A.

As one would hope, map $v \to \alpha v$, i.e. αI is positive, if and only if $\alpha \geq 0$. In particular, in one-dimensional spaces the notion works as expected. Fortunately there are other examples also. Indeed, any orthogonal projection is positive.

Proposition 2.7. *If $A \in \mathcal{L}(V)$ is a orthogonal projection, then $A \geq 0$.*

Proof. As any orthogonal projetion is sum of one-dimensional orthogonal projections, we can assume that the A is one-dimensional in the first place. It follows that $A = \langle \cdot, v \rangle v / \|v\|^2$ for some $v \in V \setminus \{0\}$. Now for every $w \in V$ we have

$$\langle Aw, w \rangle = \langle \langle w, v \rangle v, w \rangle / \|v, v\|^2 = |\langle w, v \rangle|^2 / \|v\|^2 \geq 0,$$

so A is positive. □

We denote the one-dimensional orthogonal projection to the span of $v \in V \setminus \{0\}$, i.e. the map $\langle \cdot, v \rangle v / \|v\|^2$ by P_v. More generally, orthogonal projection to a subspace $W \subset V$ is denoted by P_W.

Taking positive linear combinations of orhogonal projections leads to large number of examples of positive maps.

2.1.2 Real maps and adjoint

Dual cone thinking lets us also lift other important notions.

Definition 2.8. We say that a map $A \in \mathcal{L}(V)$ is *real*, if

$$\langle Av, v \rangle \in \mathbb{R}$$

for any $v \in V$.

Definition 2.9. We say that a map $A \in \mathcal{L}(V)$ is *imaginary*, if

$$\langle Av, v \rangle \in i\mathbb{R}$$

for any $v \in V$.

Definition 2.10. We say that a map $A \in \mathcal{L}(V)$ is *strictly positive*, if

$$\langle Av, v \rangle > 0$$

for any $v \in V \setminus \{0\}$.

Map is strictly positive, if and only if it is positive and invertible, or equivalently: is real and has positive eigenvalues.

Families of real, imaginary and strictly positive maps are usually called Hermitian and Skew-Hermitian and positive definite. Reals maps will have a special role in our discussion. We write $A > 0$ if A is strictly positive. They form a vector space over $\mathbb{R}$, which is denoted by $\mathcal{H}(V)$. Of course, every imaginary map is just i times real map, and we won't preserve any special notation for such maps. Also, they don't really play any role in this thesis anyway.

We can also lift the concept of complex conjugate.

Theorem 2.11. *For any $A \in \mathcal{L}(V)$ there exists unique map $A^* \in \mathcal{L}(V)$, called the adjoint of A, for which for any $v \in V$ we have*

$$\langle A^* v, v\rangle = \overline{\langle Av, v\rangle}$$

Proof. The uniqueness of adjoint is immediate from the lemma 2.4. The map $(\cdot)^* : \mathcal{L}(V) \to \mathcal{L}(V)$ should evidently be conjugate linear, so for existence it suffices to find adjoint for suitable basis elements of $\mathcal{L}(V)$: the maps of the form $A = (x \mapsto \langle x, v\rangle w)$ for $v, w \in V$ will do.

The quadratic form for such map is given by

$$\langle Ax, x\rangle = \langle x, v\rangle\langle w, x\rangle.$$

But if we define $A^* = (x \mapsto \langle x, w\rangle v)$, we have

$$\langle A^* x, x\rangle = \langle x, w\rangle\langle v, x\rangle = \overline{\langle w, x\rangle\langle x, v\rangle} = \overline{\langle Ax, x\rangle}$$

for any $x \in V$, so A^* is indeed the adjoint of A. □

In more common terms: a adjoint of linear map $A \in \mathcal{L}(V)$ is the unique map A^* such that

$$\langle Av, w\rangle = \langle v, A^* w\rangle \tag{2.12}$$

for any $v, w \in V$. This fact is easily verified by a polarization argument.

As real maps are their own adjoints, they are often called appropriately **self-adjoint**.

The previous observation makes many of the basic properties of adjoint, which we collect below, evident.

Theorem 2.13. *For any linear maps A and B, with appropriate domains and codomains, and $\lambda \in \mathbb{C}$ we have* *i)* *Matrix of* A^* *with respect to any orthonormal basis is conjugate transpose of matrix of* A*, i.e.* $A^*_{i,j} = \overline{A_{j,i}}$*.*

ii) $(A^*)^* = A$

iii) $(A + B)^* = A^* + B^*$

iv) $(\lambda I)^* = \overline{\lambda} I$

v) $(AB)^* = B^* A^*$*.*

Using 2.12, adjoint could also be defined between arbitrary two inner product spaces. With this more general definition the maps

$$\begin{aligned} v &: \mathbb{C} \to V & v(x) &= xv \\ v^* &: V \to \mathbb{C} & v^*(w) &= \langle w, v \rangle \end{aligned}$$

will be adjoints of each other. This lets us rewrite one-dimensional projections conveniently in the form

$$P_v = \frac{1}{\|v\|^2} v v^*.$$

More generally, for subspace $W \subset V$ the orthogonal projection $V \to W$ is the adjoint of the inclusion $J_W : W \to V$.

2.1.3 More convincing

Positive maps have many other desirable properties. First of all, eigenvalues of a positive map are non-negative. This fact is a corollary of a more general property.

Definition 2.14. Let $W \subset V$ be a subspace and $A \in \mathcal{L}(V)$. Then the **compression** of A to W, denoted by A_W is the linear map

$$J_W^* A J_W : W \to W.$$

Lemma 2.15. *Let* $W \subset V$ *and* $A \geq 0$*. Then also* $A_W \geq 0$*. In particular all the eigenvalues of* A *are non-negative.*

Proof. Note that quadratic form gives essentially the one-dimensional compressions. Indeed, if $W = (v)$, then

$$A_W x = \frac{\langle Ax, v \rangle}{\langle v, v \rangle} v = \frac{\langle Av, v \rangle}{\langle v, v \rangle} x$$

for any $x \in (v)$. This means that a map is positive, if and only if its compressions to one-dimensional subspaces are.

Now the trick is that nested compressions work nicely: if $W' \subset W \subset V$ and $A \in \mathcal{L}(V)$, then $(A_W)_{W'} = A_{W'}$. Consequently, if every one-dimensional compression A is positive, same is true for all of its compressions.

By compressing to an eigenspace, we see that if A is positive, all its eigenvalues are non-negative. □

In addition, (direct) sum of two positive map is positive.

Lemma 2.16. *Let $A_1 \in \mathcal{L}(V_1)$ and $A_2 \in \mathcal{L}(V_2)$. Then $A_1 \oplus A_2 \in \mathcal{H}_+(V_1 \oplus V_2)$, if and only if $A_1 \in \mathcal{H}_+(V_1)$ and $A_2 \in \mathcal{H}_+(V_2)$.*

Proof. Recall that one defines $\langle (v_1, v_2), (w_1, w_2) \rangle_{V_1 \oplus V_2} = \langle v_1, w_1 \rangle_{V_1} + \langle w_2, w_2 \rangle_{V_2}$. Now clearly

$$\langle (A_1 \oplus A_2)(v_1, v_2), (v_1, v_2) \rangle_{V_1 \oplus V_2} = \langle A_1 v_1, v_1 \rangle_{V_1} + \langle A_2 v_2, v_2 \rangle_{V_2} \geq 0$$

for every $(v_1, v_2) \in V_1 \oplus V_2$, if and only if both $\langle A_1 v_1, v_1 \rangle_{V_1} \geq 0$ for every $v_1 \in V_1$ and $\langle A_2 v_2, v_2 \rangle_{V_2} \geq 0$ for every $v_2 \in V_2$. □

2.2 Spectral theorem

The most important result in the theory of positive and real maps is the spectral theorem.

Theorem 2.17 (Spectral theorem, version 1). *$A \in \mathcal{L}(V)$ is real if and only there exists real numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$ and for pairwise orthogonal vectors $v_1, v_2, \ldots, v_n \in V$ such that*

$$A = \sum_{i=1}^{n} \lambda_i P_{v_i}. \tag{2.18}$$

Proof. We first prove the theorem for the positive maps.

We already proved one direction: every map of the previous form is positive.

The other direction is tricky. The idea is to somehow find the vectors v_i. The problem is that such representation is by no means unique. If A is any projection for instance, we could let v_i's be any orthonormal basis of the corresponding subspace (and λ_i's be all equal to one). There's no vector one has to choose.

But we can think in reverse: there could be many vectors we cannot choose, depending on the map A. If A is any non-identity projection to subspace W, say, we can only choose v_i's in W itself. Indeed, if $x \in W^{\perp}$, we have $Ax = 0$, and hence $\langle Ax, x \rangle = 0$. By comparing the quadratic form it follows $\langle P_{v_i}x, x\rangle = |\langle v_i, x\rangle|^2$ for any $1 \leq i \leq m$. But this means that $v_i \perp W^\perp$ and hence $v_i \in W$.

More generally, if it so happens that for some $v \in V$ we have $\langle Av, v\rangle = 0$, we must have $v_i \perp v$ for any $1 \leq i \leq m$. But this means that were there such representation, we should have the following.

Lemma 2.19. *If $A \in \mathcal{H}_+(V)$ and $\langle Av, v\rangle = 0$ for some $v \in V$, then $Av = 0$ and $Aw \perp v$ for any $w \in v$.*

Before proving the Lemma, we complete the proof given the Lemma.

Proof is by induction on n, the dimension of the space. If $n = 0$, the claim is evident. For induction step assume first that there exists $v \in V$ such that $\langle Av, v\rangle = 0$. Then by the lemma for any $w \in v^\perp$ we have $Aw \in (v)^\perp =: W$. But this means that $A = A_W \oplus 0$. Now A_W is also positive, and $\dim(W) < n$, so by the induction assumption we have numbers λ_i and vectors $v_i \in V$ for the map A_W. Such representation for A_W immediately gives one also for A.

We just have to get rid of the extra assumption on the existence of such v. But for this, note that if $\lambda = \inf_{|v|=1}\langle Av, v\rangle$, one may consider $B = A - \lambda I$. Now $\inf_{|v|=1}\langle Bv, v\rangle = 0$, and B is hence positive. Also, by compactness, the infimum is attained at some point v, so B satisfies our assumptions. Representation for B easily gives one for A.

Note that the previous trick also covers the case of a general real map. $\square$

Proof of lemma 2.19. Take any $w \in V$. By assumption for any $c \in \mathbb{C}$ we have

$$\langle A(cv + w), cv + w\rangle = c\langle Av, w\rangle + \overline{c}\langle Aw, v\rangle + \langle Aw, w\rangle \geq 0$$

But this easily implies that $\langle Av, w\rangle = 0 = \langle Aw, v\rangle$ for any $w \in V$. The first equality implies that $Av = 0$ and the second that $Aw \perp v$ for any $w \in V$. $\square$

In the representation 2.18 the numbers λ_i are evidently the eigenvalues of A and vectors v_i the corresponding eigenvectors; this is why we call it the *Spectral representation.* While the representation is not unique, there is a way to make it unique. For this we have to change v_i to corresponding eigenspaces.

Theorem 2.20 (Spectral theorem, version 2)**.** *Let $A \in \mathcal{H}(V)$. Then there exists unique non-negative integer m, distinct real numbers $\lambda_1, \lambda_2, \ldots, \lambda_m$ and (non-trivial) subspaces of V, $E_{\lambda_1}, E_{\lambda_2}, \ldots E_{\lambda_m}$ with $V = \bigoplus_{i=1}^m E_i$, such that*

$$A = \sum_{i=1}^{m} \lambda_i P_{E_{\lambda_i}}. \tag{2.21}$$

Moreover, this representation is unique.

Proof. Existence of such representation immediately follows from the previous form of Spectral theorem. For uniqueness, note that λ_i's are necessarily the eigenvalues of A and E_{λ_i}'s the corresponding eigenspaces. $\square$

Although the latter version is definitely of theoretical importance, we will mostly stick the former as it only contains one-dimensional projections. Let's denote the eigenvalues of real map A by $\lambda_1(A) \geq \lambda_2(A) \geq \ldots \geq \lambda_n(A)$. One may interpret that the spectral theorem is saying that 2.16 is essentially the only way to build real maps from identity.

Spectral representation makes many of the properties of real maps obvious. For instance, any power of a real map is real: indeed, if $A = \sum_{1\leq i\leq n} \lambda_i P_{v_i}$, then

$$A^2 = \left(\sum_{i=1} \lambda_i P_{v_i}\right)\left(\sum_{j=1} \lambda_j P_{v_j}\right) = \sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j P_{v_i}P_{v_j} = \sum_{i=1}^{n} \lambda_i^2 P_{v_i},$$

since $P_v P_w = 0$ for $v \perp w$. By induction one can extend the previous to higher powers. In other words: eigenspaces are preserved under powers, and eigenvalues are the ones to get powered up. From the original definition of a real map this is not all that clear. One could even extend to polynomials. If $p(x) = c_n x^n + c_{n-1}x^{n-1} + \ldots c_1 x + c_0$, with $c_i \in \mathbb{R}$, we should write

$$p(A) = c_n A^n + c_{n-1}A^{n-1} + \ldots c_1 A + c_0 = \sum_{1\leq i\leq n} p(\lambda_i)P_{v_i}.$$

This implies that if p is the characteristic polynomial of A, then $p(A) = 0$: the special case of Cayley Hamilton theorem. Moreover, the minimal polynomial of A is the polynomial with the eigenvalues of A as single roots.

But even better, if p is polynomial with all except one, say λ_i, of the eigenvalues of A as roots, then $p(A) = p(\lambda_i)P_{E_{\lambda_i}}$. In particular, the projections to eigenspaces of A are actually polynomials of A.

Fix $A \in \mathcal{H}(V)$ with eigenbasis $(v_i)_{i=1}^n$. For any $v \in V$ we have $Av = \sum_{1\leq i\leq n} \lambda_i \langle v, v_i\rangle v_i$, so for instance

- $\langle Av, v\rangle = \sum_{1\leq i\leq n} \lambda_i |\langle v, v_i\rangle|^2$: the quadratic form is just a positive linear combination of eigenvalues.

- $\|Av\|^2 = \sum_{1\leq i\leq n} \lambda_i^2 |\langle v, v_i\rangle|^2 \leq (\max_{1\leq i\leq n} \lambda_i^2)\, \|v\|^2$. Hence $\|A\| = \max_{1\leq i\leq n} |\lambda_i|$.

2.3 Matrix functions

2.3.1 Functional calculus

Given the spectral theorem, it is rather clear how one should define general matrix functions. We denote by $\mathcal{H}_{(a,b)}$ elements of $\mathcal{H}$ spectra of which lie in (a, b).

Definition 2.22. For any $-\infty \leq a < b \leq \infty$ $f : (a, b) \to \mathbb{R}$ the associated matrix function on V is the map $f_V : \mathcal{H}_{(a,b)}(V) \to \mathcal{H}(V)$ given by

$$f_V(A) = \sum_{\lambda \in \operatorname{spec}(A)} f(\lambda) P_{E_\lambda}$$

if $A = \sum_{\lambda \in \operatorname{spec}(A)} \lambda P_{E_\lambda}$.

Note that as the spectral representation is unique this definition makes sense. Matrix functions enjoy many natural and useful properties.

Proposition 2.23. *Let $f : (a, b) \to \mathbb{R}$ and $A \in \mathcal{H}_{(a,b)}$*

1. *If $f[(a, b)] \subset (c, d)$ then $f_V(A) \in \mathcal{H}_{(c,d)}$.*
2. *If also $g : (a, b) \to \mathbb{R}$ then $(f + g)_V = f_V + g_V$ and $(fg)_V = f_V g_V$.*
3. *$f_{V_1 \oplus V_2} = f_{V_1} \oplus f_{V_2}$.*
4. *If $g : (a, b) \to \mathbb{R}$ and f and g agree on spectrum of A, then $f(A) = g(A)$.*
5. *If $f[(a, b)] \subset (c, d)$ and $g : (c, d) \to \mathbb{R}$ then $(g \circ f)_V = g_V \circ f_V$.*
6. *If $f_n : (a, b) \to \mathbb{R}$ converge pointwise to f, then the same holds true for $(f_n)_V$'s. In other words, the map $f \mapsto f_V$ is continuous.*

These properties make it clear that such definition is natural. We will drop the subscript V and identify f with its matrix function f_V if there is no fear of confusion.

There is one more property which is not all that trivial.

Proposition 2.24. *If $f : (a, b) \to \mathbb{R}$ is continuous, then so is f_V.*

Ultimately this is a statement about eigenvalue dynamics: if two real maps are close to each other, so are their eigenvalues.

Lemma 2.25. *For any $A, H \in \mathcal{H}$ we have* $\operatorname{spec}(A + H) \subset \operatorname{spec}(A) + [-\|H\|, \|H\|]$.

Proof. We prove a claim evidently equivalent: if all eigenvalues of A are greater than $\|H\|$ in absolute value, then $A + H$ is invertible. Note that in this case the eigenvalues of A^{-1} are less than $\|H\|^{-1}$ in absolute value and hence $\|A^{-1}H\| \leq \|A^{-1}\|\|H\| < 1$. This means that all eigenvalues $A^{-1}H$ are less than 1 in absolute value, so $I + A^{-1}H$ is invertible: hence is also $A(I + A^{-1}H) = A + H$. □

Note that the previous lemma implies that $\mathcal{H}_{(a,b)}$ or more generally $\mathcal{H}_U$ is an open set (in $\mathcal{H}$) for any open $U \subset \mathbb{R}$, where $\mathcal{H}_U$ is defined as one would expect.

Proof of proposition 2.24. By lemma 2.25 f_V is clearly continuous at $A \in \mathcal{H}_{(a,b)}$ at least if $f(A) = 0$. But if this is not the case, we may interpolate f_V by polynomial: find a polynomial p with $p(\lambda) = f(\lambda)$ for $\lambda \in \operatorname{spec}(A)$ and write $f = p + g$. Now g_V is continuous at A. Also, as

$$(A + H)^k = A^k + O(\|H\|)$$

for any $k \geq 0$, so is p_V and hence also f_V. □

Previous argument also implies a bit more general claim: f_V is continuous at A, if and only if f is continuous at $\operatorname{spec}(A)$.

2.3.2 Holomorphic functional calculus

If f is entire, there's another way to appoach the concept of matrix functions. Since f can be written as

$$f(z) = \sum_{n=0}^{\infty} a_n z^n,$$

power series convergent for any $z \in \mathbb{C}$, we should have

$$f_V(A) = \sum_{n=0}^{\infty} a_n A^n.$$

This matrix power series indeed converges as $\|A^n\| \leq \|A\|^n$. Also, this definition coincides with the spectral one. Indeed, if one writes $f_n : z \mapsto \sum_{k=0}^{n} a_n z^n$, we have

$$\sum_{n=0}^{\infty} a_n A^n = \lim_{n\to\infty} [(f_n)_V(A)] = f_V(A)$$

by part (6) of proposition (2.23).

Note that the power series definition makes perfect sense even if $a_n \notin \mathbb{R}$ or if A is not real.

If f is not entire, the power series might not converge every $A \in \mathcal{H}_{(a,b)}$. Instead, we can use Cauchy's integral formula for matrix functions.

$$f_V(A) = \frac{1}{2\pi i} \int_\gamma (zI - A)^{-1} f(z) dz,$$

where γ is simple closed curve enclosing the spectrum of A (contained in the domain of f). This formula is immediate when viewed in a eigenbasis of A and again, the formula makes perfect sense even if A is not real.

2.4 Real maps and composition

2.4.1 Commuting real maps

Warning! Composition of positive maps need not be positive!

Since for any $A, B \in \mathcal{H}(V)$ we have $(AB)^* = B^* A^* = BA$, product of two real maps is real, if and only if the maps commute. So: when do two real maps commute?

It turns out that real maps commute, if and only if they are **simultaneously diagonalizable**, i.e. if there exists vectors $v_1, v_2, \ldots, v_n$ and numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$ and $\lambda'_1, \lambda'_2, \ldots, \lambda'_n$ such that

$$A = \sum_{1 \le i \le n} \lambda_i P_{v_i} \text{ and } B = \sum_{1 \le i \le n} \lambda'_i P_{v_i}.$$

A similar statement holds for arbitrary families of commuting real maps.

Theorem 2.26. *Let $\mathcal{A} = (A_j)_{j \in J}$ be an arbitrary family of commuting real maps. Then there exists $m \ge 1$ and a decomposition $V = \bigoplus_{i=1}^m E_i$, such that*

$$\mathcal{A} \subset \operatorname{span}\{P_{E_i} | 1 \le i \le m\}.$$

Proof. As with the spectral theorem, the main difficulty is finding the "eigenspaces" E_i. TODO Let $\mathcal{A}' \subset \mathcal{L}(V)$ be the smallest (unital) algebra containing $\mathcal{A}$. Note that $\mathcal{A}'$ is commutative and elements of it are real maps. As $\mathcal{H}(V)$ is finite dimensional and closed under taking polynomials, $\mathcal{A}'$ is spanned by projections to a finite set of subspaces of V. Let $\{E_i\}_{i=1}^m$ be such set of subspaces minimizing $\sum \dim(E_i)$. If we manage to prove that the subspaces E_i are orthogonal we are done, as the respective projections span I and the family $\mathcal{A}$.

Note that for any $1 \leq i < j \leq m$ the map $A := P_{E_i} P_{E_j}$ is a projection, as it is real (P_{E_i} and P_{E_j} commute) and $A^2 = P_{E_i} P_{E_j} P_{E_i} P_{E_j} = P_{E_i}^2 P_{E_j}^2 = P_{E_i} P_{E_j} = A$. But as $\operatorname{im}(A) \subset E_i, E_j$, the maps $P_{E_0} := A, P_{E_i'} := P_{E_i} - A$ and $P_{E_j'} := P_{E_j} - A$, are projections in $\mathcal{A}'$ spanning P_{E_i} and P_{E_j}. Since $\dim(E_0) + \dim(E_i') + \dim(E_j') = \dim(E_i) + \dim(E_j) - \dim(E_0)$, by the minimality of $(E_i)_{i=1}^m$ we must have $\dim(E_0) = 0$. Indeed, otherwise we could replace E_i and E_j by E_0, E_i' and E_j'. Consequently $P_{E_i} P_{E_j} = 0$, and hence $E_i \perp E_j$. $\square$

It is not very hard to see that decomposition with minimal $m \geq 1$ is unique and attained by the previous construction.

The message is: if one wants products to preserve positivity, everything degenerates to $\mathbb{R}^m$, i.e. diagonal maps.

Philosophy 2.27. Commutativity kills the exciting phenomena.

Conversely, if one wants exciting things to happen, one should make things very non-commutative.

As a corollary to theorem 2.26 we have

Corollary 2.28. *If $A, B \geq 0$ and A and B commute, then $AB \geq 0$.*

2.4.2 Symmetric product

As normal product doesn't quite work with positivity, next attempt might be symmetrized product

$$S(A, B) = AB + BA,$$

(or maybe with normalizing constant $\frac{1}{2}$ in the front), instead of the usual one. It turns out that even this doesn't fix positivity.

For one dimesional projections things go as badly as they possibly can.

Proposition 2.29. *If $v, w \in V \setminus \{0\}$, then*

$$P_v P_w + P_w P_v \geq 0,$$

if and only if v and w are parallel or orthogonal, i.e. if and only if P_v and P_w commute.

Proof. Since everything is happening in a (at most) two dimensional subspace of V, we may assume that V is two dimensional in the first place. Note that

$$P_v P_w + P_w P_v = (P_v + P_w)^2 - P_v^2 - P_w^2 = (P_v + P_w)^2 - P_v - P_w = A^2 - A = A(A - I),$$

where $A := P_v + P_w$. This is positive, if and only if the eigenvalues of A lie outside the interval $(0, 1)$. But since $\operatorname{tr}(A) = 2$ and $A \geq 0$, the only way this can happen is that either A has double eigenvalue 1 or A has eigenvalues 0 and 2. To conclude the claim itself, we are left to do two reality checks:

Lemma 2.30. *If $A = P_v + P_w = I$, then v and w are orthogonal.*

Proof. Note that $\langle v, v\rangle = \langle Av, v\rangle = \langle P_v v, v\rangle + \langle P_w v, v\rangle = \langle v, v\rangle + |\langle v, w\rangle|^2/\langle v, v\rangle$, so $\langle v, w\rangle = 0$. ☐

Lemma 2.31. *If $A = P_v + P_w = 2P_u$ for some $u \in V$, then v, w and u are all parallel.*

Proof. Take $u' \in (u)^\perp$. Since $0 = \langle 2P_u u', u'\rangle = \langle P_v u', u'\rangle + \langle P_w u', u'\rangle = |\langle v, u'\rangle|^2/\langle v, v\rangle + |\langle w, u'\rangle|^2/\langle w, w\rangle \geq 0$, we have $\langle v, u'\rangle = 0 = \langle w, u'\rangle$. Consequently $v, u \in ((u)^\perp)^\perp = (u)$. ☐

☐

For more general positive maps things aren't much better. One could for instance prove that

Proposition 2.32. *Let $A \in \mathcal{H}$ such that $AB + BA \geq 0$ for any $B \geq 0$. Then $A = \alpha I$ for some $\alpha \geq 0$.*

2.4.3 $*$-conjugation

Despite all the negative news, there's one non-trivial non-commutative way to produce positive maps from others, called $*$-conjugation. Given any two positive maps A and B, their composition need not be positive, but the map BAB is. First of all, it is real as $(BAB)^* = B^*A^*B^* = BAB$. Also $\langle BABv, v\rangle = \langle A(Bv), (Bv)\rangle \geq 0$ for any $v \in V$. An identical argument shows that one may replace B by an arbitrary $C \in \mathcal{L}(V)$ in the following sense.

Definition 2.33. Let $A, B \in \mathcal{H}$. We say that B is **$*$-conjugate** of A if for some $C \in \mathcal{L}(V)$ we have $B = C^*AC$.

Proposition 2.34. *If $A \geq 0$ and B is $*$-conjugate of A, then also $B \geq 0$.*

2.5 Loewner order

Definition 2.35. If $A, B \in \mathcal{H}(V)$, we write that $A \leq B$ if $B - A \geq 0$. If $B - A > 0$, we write $A < B$.

Proposition 2.5 tells us that $\leq$, is indeed a partial order on the $\mathbb{R}$-vector space of real maps: this partial order is called **Loewner order**. More explicitly, we have the following properties:

Proposition 2.36. *(i) If $A \leq B$ then $\alpha A \leq \alpha B$ for any $\alpha \geq 0$.*

(ii) If $A \leq B$ and $B \leq C$ then $A \leq C$.

(iii) If $A \leq B$ and $B \leq A$ then $A = B$.

(iv) $\lambda I \leq A$, if and only if all the eigenvalues of A are at least λ. Similarly $A \leq \lambda I$, if and only if all the eigenvalues of A are at most λ.

Example 2.37. If $W_1, W_2 \subset V$ are two subspaces of V we have $P_{W_1} \leq P_{W_2}$ if and only if $W_1 \subset W_2$. Indeed if $W_1 \subset W_2$ then $W_2 = W_1 + W_3$ for some $W_3 \perp W_1$ and hence $P_{W_2} = P_{W_1} + P_{W_3} \geq P_{W_1}$. Converse follows as soon as one notes that by 2.19 for any $W \subset V$ we have

$$\{v \in V | \langle P_W v, v\rangle = 0\} = W^{\perp}.$$

$\triangle$

Key thing here is to note that multiplication by positive map doesn't preserve Loewner order. This is the reason why many standard arguments don't work for general real maps.

For example if $0 < a \leq b$, with real numbers one could multiply the inequality by the positive number $(ab)^{-1}$ to get $0 < b^{-1} \leq a^{-1}$. This doesn't quite work with linear maps anymore.

$*$-conjugation is a way to partially fix this deficiency: it works almost like multiplying by a positive number.

Proposition 2.38. *If $A \leq B$, then for any $C \in \mathcal{L}(V)$ we have $C^*AC \leq C^*BC$.*

Using the previous observation one can salvage the above argument.

Theorem 2.39. *If $0 < A \leq B$, then $B^{-1} \leq A^{-1}$.*

Proof. As mentioned, we can't really multiply by $(AB)^{-1}$, as it does not preserve the order and doesn't even need to be positive. We can almost multiply by A^{-1} though: $*$-conjugate by $A^{-\frac{1}{2}}$. This preserves the order, and we get

$$I \leq A^{-\frac{1}{2}} B A^{-\frac{1}{2}}.$$

Now, one would want to multiply by B^{-1}, that is $*$-conjugate by $B^{-\frac{1}{2}}$, but B is in the middle, so that doesn't seem be too helpful. But we can continue with the original strategy instead: since $I \leq X := A^{-\frac{1}{2}} B A^{-\frac{1}{2}}$ we have $X^{-1} \leq I$ (by 2.36 (*iv*)), that is

$$A^{\frac{1}{2}} B^{-1} A^{\frac{1}{2}} \leq I.$$

Now simply $*$-conjugate by $A^{-\frac{1}{2}}$. $\square$

Remark 2.40. Alternatively, as the middle step we could conjugate both sides by $X^{-\frac{1}{2}}$. By doing this we have only used $*$-conjugation in the proof: actually we have $*$-conjugated altogether with

$$A^{-\frac{1}{2}}(A^{-\frac{1}{2}}BA^{-\frac{1}{2}})^{-\frac{1}{2}}A^{-\frac{1}{2}} = (A^{\frac{1}{2}}(A^{-\frac{1}{2}}BA^{-\frac{1}{2}})^{\frac{1}{2}}A^{\frac{1}{2}})^{-1}.$$

The map $A^{\frac{1}{2}}(A^{-\frac{1}{2}}BA^{-\frac{1}{2}})^{\frac{1}{2}}A^{\frac{1}{2}}$, which is real, is usually called the geometric mean of A and B. The point is: somewhat curiously we can almost do the original proof: just replace multiplication by $*$-conjugation by square root, and replace square root of the product by geometric mean. $\triangle$

2.6 Notes and references

All results in this chapter are classic and can be found in numerous books on linear algebra, for instance in [4] and [3] (?). Proof of the spectral theorem is due to (Who?). Proof of 2.26 is from (Where?).

Chapter 3

Matrix monotone functions – part 1

Definition 3.1. We say that $f : (a, b) \to \mathbb{R}$ is n-monotone or matrix monotone of order n, if for any ($n \times n$ matrices) $A, B \in \mathcal{H}_{(a,b)}$, such that $A \leq B$ we have $f(A) \leq f(B)$.

We will denote the space of n-monotone functions on open interval (a, b) by $P_n(a, b)$. We will also denote

$$P_\infty(a, b) = \bigcap_{n \geq 1} P_n(a, b).$$

By 2.6 we have

Proposition 3.2. *The sets $P_n(a, b)$ and $P_\infty(a, b)$ are closed convex cones.*

Note that in the notation $P_n(a, b)$ we don't specify the space V; it doesn't matter.

Proposition 3.3. *If $\dim(V) = \dim(V')$, then f is n-monotone in V, if and only if it is n-monotone in V'.*

Proof. The reason is rather clear: inner product spaces of same dimension are isometric. □

3.1 Examples

Proposition 3.4. *If $\alpha \geq 0$ and $\beta \in \mathbb{R}$ we have $(x \mapsto \alpha x + \beta) \in P_n(a, b)$.*

Proof. Assume that for $A, B \in \mathcal{H}_{(a,b)}$ we have $A \leq B$. Now

$$f(B) - f(A) = (\alpha B + \beta I) - (\alpha A + \beta I) = \alpha(B - A).$$

Since by assumption $B - A \geq$ and $\alpha \geq 0$, also $\alpha(B - A) \geq 0$, so by definition $f(B) \geq f(A)$. This is exactly what we wanted. □

Proposition 3.5. *If* $0 \notin (a,b)$, *we have* $(x \mapsto -x^{-1}) \in P_n(a,b)$.

Proof. The result follows immediately from theorem 2.39. $\square$

By the previous proposition also $(x \mapsto (\lambda - x)^{-1} \in P_n(a,b)$ for any $\lambda \notin (a,b)$, so by the cone property

$$x \mapsto \alpha x + \beta + \sum_{i=1}^{m} \frac{t_i}{\lambda_i - x} \in P_n(a,b) \tag{3.6}$$

for any $\alpha, t_1, t_2, \ldots, t_m \geq 0$ and $\beta, \lambda_1, \lambda_2, \ldots, \lambda_m$ where $\lambda_1, \lambda_2, \ldots, \lambda_m \notin (a,b)$.

3.2 Basic properties

Below we collect many natural properties of the cones $P_n(a,b)$.

Proposition 3.7. *Let* $f : (a,b) \to \mathbb{R}$. *Then the following are equivalent:*

(i) f *is increasing.*

(ii) $f \in P_1(a,b)$.

(iii) For any positive integer n *and commuting* $A, B \in \mathcal{H}_{(a,b)}$ *such that* $A \leq B$ *we have* $f(A) \leq f(B)$.

Proof. *(ii)* $\Rightarrow$ *(i)*: Take any $a < x \leq y < b$. Now for $xI, yI \in \mathcal{H}_{(a,b)}$ we have $xI \leq yI$ so by definition

$$f(x)I = f(xI) \leq f(yI) = f(y)I,$$

from which it follows that $f(x) \leq f(y)$.

(iii) $\Rightarrow$ *(ii)*: All 1×1 matrices commute.

(i) $\Rightarrow$ *(iii)*: If $A \leq B$ and A and B commute, by theorem 2.26 we may write $A = \sum_{i=1}^{n} a_i P_{v_i}$ and $B = \sum_{i=1}^{n} b_i P_{v_i}$ for some $\lambda_1, \ldots, \lambda_n, \lambda'_1, \ldots, \lambda'_n \in \mathbb{R}$ and $v_1, v_2, \ldots, v_n$, orthonormal basis of V, with $\lambda_i \leq \lambda'_i$. But now $f(A) = \sum_{i=1}^{n} f(\lambda_i) P_{v_i}$ and $f(B) = \sum_{i=1}^{n} f(\lambda'_i) P_{v_i}$ so

$$f(B) - f(A) = \sum_{i=1}^{n} (f(\lambda'_i) - f(\lambda_i)) P_{v_i}.$$

But this is positive, since, as f is increasing, the numbers $f(\lambda'_i) - f(\lambda_i)$ is non-negative. $\square$

Proposition 3.8. *If $f : (a, b) \to (c, d)$ and $g : (c, d) \to \mathbb{R}$ are n-monotone, so is $g \circ f : (a, b) \to \mathbb{R}$.*

Proof. Fix any $A, B \in \mathcal{H}_{(a,b)}$ with $A \leq B$. By assumption $f(A) \leq f(B)$ and $f(A), f(B) \in \mathcal{H}_{(c,d)}$ so again by assumption, $g(f(A)) \leq g(f(B))$, our claim. $\square$

Proposition 3.9. *We have $P_{n+1}(a, b) \subset P_n(a, b)$.*

Proof. Take $A, B \in \mathcal{H}_{(a,b)}(V)$ with $A \leq B$. For any $c \in (a, b)$ we have $(A \oplus c), (B \oplus c) \in \mathcal{H}(V \oplus \mathbb{C})$ and $(A \oplus c) \leq (B \oplus c)$. Consequently, if $f \in P_{n+1}(a, b)$, we have

$$f_V(A) \oplus f(c) = f_{V \oplus \mathbb{C}}(A \oplus c) \leq f_{V \oplus \mathbb{C}}(B \oplus c) = f_V(B) \oplus f(c),$$

which implies that $f(A) \leq f(B)$. $\square$

It turns out that these inclusions are strict, as long as our interval is not the whole $\mathbb{R}$.

There are also more trivial inclusions: $P_n(a, b) \subset P_n(c, d)$ for any $(a, b) \supset (c, d)$. Bigger interval, more matrices, more restrictions, fewer functions. To be precise, one should say that if $(a, b) \supset (c, d)$ and $f \in P_n(a, b)$, then also $f\big|_{(c,d)} \in P_n(c, d)$.

3.3 Failures

Most of the common monotone functions fail to be matrix monotone. Let's try some non-examples.

Proposition 3.10. *Function $(x \mapsto x^2)$ is not n-monotone for any $n \geq 2$ on $(0, \infty)$.*

Proof. Let us first think what goes wrong with the standard proof for the case $n = 1$.

Note that if $A \leq B$,

$$B^2 - A^2 = (B - A)(B + A)$$

is positive as a product of two positive matrices (real numbers).

There are two fatal flaws here when $n > 1$.

- $(B - A)(B + A) = B^2 - A^2 + (BA - AB)$, not $B^2 - A^2$.
- Product of two positive matrices need not be positive.

Note that both of these objections result from the non-commutativity and indeed, both would be fixed should A and B commute.

Let's write $B = A + H$ ($H \geq 0$). Now we are to investigate

$$(A+H)^2 - A^2 = AH + HA + H^2.$$

While $H^2 \geq 0$, as we have noticed in proposition 2.29, $AH + HA$ need not be positive! Also, if H is small enough, H^2 is negligible compared to $AH + HA$. So simply pick $A, H \geq 0$ such that $AH + HA \ngeq 0$: for small enough $t > 0$ we have $(A + tH)^2 - A^2 \ngeq 0$. To be entirely honest, we only gave examples of such A and H with $\mathrm{rank}(A) = 1$, so $A \notin \mathcal{H}_{(0,\infty)}$. This deficit is however easily fixed by looking at $A_\varepsilon = A + \varepsilon I$ for $\varepsilon > 0$. $\square$

By a bit more careful arguments one could show that $(x \mapsto x^2)$ is not n-monotone for any $n \geq 2$ on any open interval.

As a corollary with get

Corollary 3.11. *The function $\chi_{(0,\infty)}$ is not n-monotone for any $n \geq 2$.*

Proof. If $\chi_{x>0}$ were n-monotone so would be

$$x^2 = \int_0^\infty 2t\chi_{(t,\infty)}(x)dt.$$

$\square$

The function $\chi_{(0,\infty)}$ is in some sense canonical counterexample: every increasing function is more or less positive linear combination of its tranlates, so if monotone functions are not all matrix monotone, the reason is that it is not matrix monotone. For this reason we should really understand why it is not n-monotone for any $n > 1$.

The idea is the following: we are going to take $n = 2$ and construct $A, B \in \mathcal{H}(V)$ with the following properties:

1. $A \leq B$
2. A and B have both exactly one positive eigenvalue
3. A and B don't commute

If we can do this, A and B work as counterexamples. Indeed then $\chi_{(0,\infty)}(A) = P_{v_1}$ and $\chi_{(0,\infty)}(B) = P_{w_1}$ where eigenvectors v_1 and w_1 are eigenvectors of A and B corresponding to positive eigenvalues. But $\chi_{(0,\infty)}(A) \nleq \chi_{(0,\infty)}(B)$ by 2.37.

Constructing such pair is very easy: just take A with eigenvalues -1 and 1 and consider B of the form $A + tH$ for some $H \geq 0$, $t > 0$ and such that A and H do not commute. For small enough H all of the conditions are easily satisfied.

As we saw with the square function example, product of two n-monotone functions need not be n-monotone in general, even if they are both positive functions. Similarly, taking maximums doesn't preserve monotonicity.

Proposition 3.12. *Maximum of two n-monotone functions need not be n-monotone for $n \geq 2$.*

Proof. Again, let's think what goes wrong with the standard proof for $n = 1$.

Take $n \geq 2$, $f, g \in P_n(a, b)$ and $A, B \in \mathcal{H}_{(a,b)}$ with $A \leq B$. We have $f(A) \leq f(B) \leq \max(f, g)(B)$ and $f(A) \leq f(B) \leq \max(f, g)(B)$. It follows that

$$\max(f, g)(A) = \max(f(A), g(A)) \leq \max(f, g)(B),$$

as we wanted.

Here the flaw is in the expression $\max(f(A), g(A))$: what is maximum of two matrices? It turns out that however one tries to define it, the above inequality doesn't work.

For counterexamples take $f \equiv 0$ and $g = \mathrm{id}$: it's easy to see that we can take same pair as with $\chi_{(0,\infty)}$ as our counterexample. □

The maximum problem is not too bad and maybe it's more of a pleasent surprise anyway that it holds for increasing functions. But there is a very fundamental problem hidden in the square example.

Proposition 3.13. *Let $n \geq 2$. Then there exists no $\alpha > 0$, and no open interval $(a, b) \subset \mathbb{R}$ such that $\alpha x + x^2 \in P_n(a, b)$.*

Proof. Adding linear term means just translating domain and codomain, which is not going to help: $x^2 + \alpha x = (x + \frac{\alpha}{2})^2 - \frac{\alpha^2}{4}$. □

Why is this bad? If $f : (a, b) \to \mathbb{R}$ is not too bad (say Lipschitz), for large enough α the function defined by $g(x) = f(x) + \alpha x$ is increasing. But we can't necessarily do the same thing in the matrix setting even for smooth or analytic functions. Although this might not be such a big surprise or a bad thing in the first place, it is worthwhile to investigate the underlying reason.

Let $f(x) = \alpha x + x^2$ and take $A, H \geq 0$. As observed earlier, we have

$$\begin{aligned}\lim_{t \to 0} \frac{f(A + tH) - f(A))}{t} &= \alpha H \\ &+ HA + AH\end{aligned}$$

In the real setting we could just increase α to make the previous expression positive. In the matrix setting there is a problem: note that if H is of rank 1, increasing α means "increasing the right-hand side only to one direction". Now, if the right-hand side is not positive map in the first place, it might be non-positive in a big subspace, so rank

1 machinery is not going to save the day. Note also that even if we let $A \to 0$ (look at matrix function at 0), the situation isn't a priori better.

On the other hand if $n = 2$, for instance, there is not too much room for things to go south. We still, a priori, can't guarantee positivity with α, but adding also something extra, say βx^3 for some $\beta > 0$ might work. In the end, there isn't too much space in the 2-dimensional space.

When n gets larger we have more and more space to worry about, so we should start worrying about more and more Taylor coefficients.

This leads us to expect two things:

1. Larger the dimension n, the more Taylor coefficients should be under some kind of control.

2. For fixed n we can (at least locally) guarantee n-monotonicity by controlling certain number of first coefficients.

3.4 Heuristics

3.4.1 Taylor coefficients

Let us try to push the ideas of the previous section further. Take entire $f(x) = \sum_{k=0}^{\infty} a_k x^k$ and assume that $0 \in (a, b)$. Note that as for any $k > 0$

$$(A+B)^k = \sum_{i=0}^{k} \sum_{\substack{j_0,\ldots,j_i \geq 0 \\ j_0+\ldots+j_i=k-i}} A^{j_0} B A^{j_1} B \cdots B A^{j_k},$$

we have

$$\lim_{t \to 0} \frac{f(A+tH) - f(A))}{t} = \sum_{i=1}^{\infty} a_i \sum_{j=0}^{i-1} A^j B A^{i-1-j}.$$

If $f \in P_\infty(a, b)$, this expression should be positive for $A \in \mathcal{H}_{(a,b)}$ and $H \geq 0$. Let us denote

$$Df_A(H) := \lim_{t \to 0} \frac{f(A+tH) - f(A))}{t},$$

derivative of a matrix function at A in the direction H. As the derivative is linear in H, it suffices to consider the case $\mathrm{rank}(H) = 1$. Let's say $H = vv^*$ for some $v \in V$ and take any $w \in V$. Now we should have

$$\begin{aligned}
\langle Df_A(H)w, w\rangle &= \sum_{i=1}^{\infty} a_i \sum_{j=0}^{i-1} \langle A^j H A^{i-1-j} w, w\rangle \\
&= \sum_{i=1}^{\infty} a_i \sum_{j=0}^{i-1} \langle A^{i-1-j} w, v\rangle \langle A^j v, w\rangle \\
&\geq 0
\end{aligned}$$

for any $v, w \in V$. Write $c_j = \langle A^j w, v\rangle$ and observe that $\langle A^j w, v\rangle = \overline{\langle A^j w, v\rangle} = \overline{c_j}$. It follows that

$$\sum_{i=1}^{\infty} a_i \sum_{j=0}^{i-1} \overline{c_{i-1-j}} c_j = \sum_{i,j\geq 0} a_{i+j+1} c_i \overline{c_j} \geq 0$$

for some kind of sequences $(c_i)_{i=1}^{\infty}$. This implies that if the infinite matrix $(a_{i+j+1})_{i,j\geq 0}$ is positive, then f is matrix monotone. What about the converse?

It is not very hard to see that

$$c_j = \sum_{i=1}^{n} t_i \lambda_i(A)^j$$

for some $t_1, t_2, \ldots, t_n \in \mathbb{C}$. Conversely, if the eigenvalues of A are simple, we can control first n terms of $(c_i)_{i=1}^{\infty}$ by choice of v and w. This implies the following:

Proposition 3.14. *If f is a polynomial with $2 \leq \deg(f) \leq n$, then $f \notin P_n(a, b)$.*

If f is not polynomial such conclusions are harder to make, as we can only control first c_i's. Nevertheless, also the converse holds.

Theorem 3.15. *$f \in P_\infty(a, b)$, if and only if f is analytic and the infinite matrix $(a_{i+j-1})_{i,j\geq 1}$, where $a_k = f^{(k)}(x)/k!$ and $x \in (a, b)$, is positive for any $x \in (a, b)$.*

As one would hope, there's corresponding result for the classes $P_n(a, b)$.

Theorem 3.16. *$f \in P_n(a, b)$, if and only if $(a_{i+j-1})_{1\leq i,j\leq n}$, where $a_k = f^{(k)}(x)/k!$ and $x \in (a, b)$, is positive for any $x \in (a, b)$.*

Only now there's a problem: it turns out that function in $P_n(a, b)$ need not be analytic, or even $(2n - 1)$ times differentiable, so the condition should be understood in the distributional sense.

3.4.2 Main argument

Let us try to prove the "only if" -directions of these results modulo regularity issues.

Proof "sketch" of the "only if" of 3.16. Denote the matrix in question by $M(= M_n(x, f))$. We may w.l.o.g. take $x = 0 \in (a, b)$. The idea is the following: we know that $\langle Df_A(H)w, w\rangle$ is positive for any $A \in \mathcal{H}_{(a,b)}, H \geq 0$ and $w \in V$ and should prove that $\langle Mv, v\rangle \geq 0$ for any $v \in \mathbb{C}^n$. Best we could hope for is that

$$\lim_{\varepsilon\to 0}\langle Df_{A_\varepsilon}(H_\varepsilon)w_\varepsilon, w_\varepsilon\rangle = \langle Mv, v\rangle$$

for some $H_\varepsilon \geq 0$, $w_\varepsilon \in V$, $A_\varepsilon \in \mathcal{H}_{(a,b)}$, with $\lim_{\varepsilon\to 0} A_\varepsilon = 0$. This works.

To find $H_\varepsilon, w_\varepsilon, A_\varepsilon$, we change the point of view. Recall that if f is entire we have

$$f(A) = \frac{1}{2\pi i}\int_\gamma (zI - A)^{-1} f(z)dz.$$

Now we can write

$$\begin{aligned}\frac{f(A + tH) - f(A)}{t} &= \frac{1}{2\pi i}\int_\gamma \frac{(zI - A - tH)^{-1} - (zI - A)^{-1}}{t} f(z)dz \\ &= \frac{1}{2\pi i}\int_\gamma (zI - A - tH)^{-1} H (zI - A)^{-1} f(z)dz.\end{aligned}$$

Taking $t \to 0$, we find that

$$Df_A(H) = \frac{1}{2\pi i}\int_\gamma (zI - A)^{-1} H (zI - A)^{-1} f(z)dz.$$

Next, take $H = vv^*$ for $v \in V$ and pick $w \in V$: we have

$$\begin{aligned}\langle Df_A(H)w, w\rangle &= \frac{1}{2\pi i}\int_\gamma \langle (zI - A)^{-1} vv^* (zI - A)^{-1} w, w\rangle f(z)dz \\ &= \frac{1}{2\pi i}\int_\gamma \langle (zI - A)^{-1} v, w\rangle\langle (zI - A)^{-1} w, v\rangle f(z)dz.\end{aligned}$$

Note that we can write $\langle (zI - A)^{-1}v, w\rangle = \det(zI - A)^{-1}q(z)$ where q is some polynomial of degree less than n. Moreover, if A has n distinct roots and v is not orthogonal to any eigenvector of A, varying w gives all such polynomials q, so we can rewrite our object as

$$\frac{1}{2\pi i}\int_\gamma \det(zI - A)^{-2} q(z)\overline{q(\overline{z})} f(z)dz.$$

Taking $A \to 0$ reveals that

$$\frac{1}{2\pi i}\int_\gamma \frac{q(z)\overline{q(\overline{z})}}{z^{2n}} f(z)dz.$$

But actually this is all we wanted. Indeed, since by the Cauchy's integral formula we have

$$\frac{f^{(k)}(0)}{k!} = \frac{1}{2\pi i}\int_\gamma \frac{f(z)dz}{z^{k+1}}$$

for any $k \geq 0$, so we can write

$$\begin{aligned}
\sum_{1 \leq i,j \leq n} a_{i+j-1} c_i \overline{c_j} &= \sum_{1 \leq i,j \leq n} a_{i,j} \frac{1}{2\pi i}\int_\gamma \frac{f(z)dz}{z^{i+j}} \\
&= \frac{1}{2\pi i}\int_\gamma \left(\sum_{i=1}^{n} \frac{c_i}{z^i}\right)\left(\sum_{i=1}^{n} \frac{\overline{c_i}}{z^i}\right) f(z)dz \\
&= \frac{1}{2\pi i}\int_\gamma \frac{q(z)\overline{q(\overline{z})}}{z^{2n}} f(z)dz,
\end{aligned}$$

where we write $q(z) = \sum_{i=1}^{n} z^{n-i} c_i$. □

Proof "sketch" of the "only if" of 3.15. t.f.i.f. 3.16. □

Note that the proof gives also alternate interpretation for the matrix M. Positivity of M means simply that for $q \in \mathbb{C}_{n-1}[x]$ the function $f(x)q(x)\overline{q(\overline{x})} = f(x)|q(x)|^2$ has non-negative $(2n-1)$'th derivative.

Given polynomial q, we henceforth denote by q^* the polynomial with

$$q^*(z) = \overline{q(\overline{z})}.$$

Write further that $N(q) = qq^*$.

The main problem of the argument is the regularity. While we assume f to be entire mainly for convenience, we need some kind of regularity to make sense of the definition: it is a priori not even clear that functions in $P_\infty(a, b)$ should be continuous. Origin of these regularity properties is the topic of the next chapter.

3.5 Notes and references

Matrix monotone functions were first introduced by Loewner in [11]. Basic properties of the n-monotone functions are examined in numerous sources; see for instance [9]. Maximum of real maps is discussed in detail in [1]. Loewner characterized the n-monotone functions on (a, b) as functions for which the matrix

$$\begin{bmatrix} f'(\lambda_1) & \frac{f(\lambda_1)-f(\lambda_2)}{\lambda_1-\lambda_2} & \cdots & \frac{f(\lambda_1)-f(\lambda_n)}{\lambda_1-\lambda_n} \\ \frac{f(\lambda_2)-f(\lambda_1)}{\lambda_2-\lambda_1} & f'(\lambda_2) & \cdots & \frac{f(\lambda_2)-f(\lambda_n)}{\lambda_2-\lambda_n} \\ \vdots & \vdots & & \vdots \\ \frac{f(\lambda_n)-f(\lambda_1)}{\lambda_n-\lambda_1} & \frac{f(\lambda_b)-f(\lambda_2)}{\lambda_n-\lambda_2} & \cdots & f'(\lambda_n) \end{bmatrix},$$

called Loewner matrix, is positive for any $a < \lambda_1, \ldots, \lambda_n < b$. 3.16 and 3.15 were first observed by Dobsch (a student of Loewner) in [6]. Heuristics in this chapter appear essentially in (Where?).

Chapter 4

k-tone functions

4.1 Motivation

To understand the regularity properties of the matrix monotone functions we look at a closely related class of k-tone functions. k-tone functions are more or less functions with non-negative k'th derivative[1]. What should that mean?

We already know the perfect answer for the case $k = 1$: 1-tone functions should be the increasing functions.

Theorem 4.1. *Let $f : (a, b) \to \mathbb{R}$ be differentiable. Then f is increasing, if and only if $f'(x) \geq 0$ for every $x \in (a, b)$.*

Proof. If f is increasing, then all its divided differences, i.e. the quotients of the form

$$\frac{f(x) - f(y)}{x - y}$$

for $x \neq y$ are non-negative. As derivatives are limits of such quotients, also they are non-negative at any point. Conversely, by the mean value theorem for every $x \neq y$ we may find ξ such that

$$\frac{f(x) - f(y)}{x - y} = f'(\xi).$$

Now if the derivatives are non-negative, so are the divided differences, so the function is increasing. $\square$

[1]The terminology is not very established, and such functions are also occasionally called k-monotone or k-convex.

While this proof by the mean value theorem works in more general setting, if $f \in C^1$, one has more instructive proof.[2]

Alternate proof for the theorem 4.1 (in the case $f \in C^1(a,b)$). Note that if $f \in C^1(a,b)$, we may write

$$\frac{f(y)-f(x)}{y-x} = \frac{1}{y-x}\int_x^y f'(t)dt = \int_0^1 f'(tx+(1-t)y)dt.$$

Note that on the right-hand side we have average of the derivative over the interval. This means that the claim can be translated to: continuous function is non-negative, if and only if its averages over all intervals are non-negative. But this is clear. $\square$

This is a really powerful point of view. While one would like to say the increasing functions are the functions with non-negative derivative, that's a bit of a lie. Instead, one can say that they are the functions whose derivative is non-negative on average, and all the problems are gone. This should roughly mean that the derivative defines a positive distribution and it is hence a measure. Thus all increasing functions should be integrals of a positive measure (at least almost everywhere). Although this kind of thinking could be carried out, the details aren't important for us. The main point is that one should think that increasing functions, i.e. the 1-tone functions are functions whose first derivative is a (positive) measure. The divided differences are an averaged (i.e. weak) way of talking about the positivity of the derivative (measure).

This is essentially the distributional way of thinking, and we could keep going and end up with the whole business of weak derivatives and stuff. But we don't have to: the plain averages suffice. We write

$$[x,y]_f := \frac{f(x)-f(y)}{x-y},$$

and say that $[\cdot,\cdot]_f$ is the (first) divided difference of f. The domain of $[\cdot,\cdot]_f$ should naturally be $(a,b)^2$ minus the diagonal. And of course, if $f \in C^1$, we should extend $[\cdot,\cdot]_f$ to the diagonal, as the derivative. Divided differences then becomes a continuous function on the whole set $(a,b)^2$.

Aside from capturing the first derivative, divided difference have two rather convenient properties.

- For given x and y, $f \mapsto [x,y]_f$ defines a linear map, which is continuous with the topology of pointwise convergence (i.e. the product topology).

[2]The following argument would also work with slightly weaker assumptions, but that's not important to us.

- Divided differences are local in the sense that if f and g agree on $\{x, y\}$, divided differences agree.

These are the ways that divided difference is a compromise between the real derivative and the weak derivative. The first point says that one doesn't have worry too much, only about pointwise convergence, while the second says that things are still rather concrete.

What about the case $k = 2$? Again, we already know the perfect answer: 2-tone functions should be the convex functions.

Theorem 4.2. *Let $f : (a, b) \to \mathbb{R}$ be twice differentiable. Then f is convex, if and only if $f^{(2)}(x) \geq 0$ for every $x \in (a, b)$.*

Proof. While the result is true as stated, let us only prove the case $f \in C^2(a, b)$ (we'll come back to the more general case). Recall that f is convex, if and only if for any $x, y \in (a, b)$ and $t \in [0, 1]$ we have

$$tf(x) + (1 - t)f(y) \geq f(tx + (1 - t)y).$$

The alternate proof of theorem 4.1 suggests that we may write

$$tf(x) + (1 - t)f(y) - f(tx + (1 - t)y) = \int_x^y w(t)f^{(2)}(t)dt$$

for some weight w. Note that if we manage to find such weight, which is non-negative (and positive enough), we would be done.

How to find the weight w? The idea is rather simple: we want to "sieve out" the values of w by choosing f such that $f^{(2)} = \delta_a$ for $a \in \mathbb{R}$ (in some sense). Now, this should mean that $f(t) = (t - a)_+ + ct + d$ for some $c, d \in \mathbb{R}$, where we write $t_+ = \max(t, 0)$. Plugging this is on the left hand side we get

$$t(x - a)_+ + (1 - t)(y - a)_+ - (tx + (1 - t)y - a)_+ = w(a).$$

Now, while the steps taken might have contained some leaps of faith, it can be easily verified with partial integration that the given w really works. $\square$

The giveaway is that while the divided differences are a convenient averaged way to talk about first derivative, the quantity $tf(x)+(1-t)f(y)-f(tx+(1-t)y)$ is a convenient averaged way to talk about the second derivative. It captures the fact that the second derivative should be a positive measure – without talking about derivatives. We won't call the quantity the second divided difference, however, as, as it turns out, we can rewrite it in much more convenient form.

If we denote $z = tx + (1-t)y$, we can solve that $t = \frac{z-y}{x-y}$ and express

$$\begin{aligned} & tf(x) + (1-t)f(y) - f(tx + (1-t)y) \\ = & \frac{z-y}{x-y}f(x) + \frac{x-z}{x-y}f(y) - f(z) \\ = & -(z-y)(z-x)\left(\frac{f(x)}{(x-y)(x-z)} + \frac{f(y)}{(y-z)(y-x)} + \frac{f(z)}{(z-x)(z-y)}\right) \end{aligned}$$

If $t \notin \{0, 1\}$, $-(z-y)(z-x)$ is positive, so if f is convex,

$$\frac{f(x)}{(x-y)(x-z)} + \frac{f(y)}{(y-z)(y-x)} + \frac{f(z)}{(z-x)(z-y)} \geq 0$$

for any x, y and z such that z is between x and y. This new expression is symmetric in its variables, so actually there's no need to assume anything on the order of x, y and z, just that they're distinct. We can also easily carry this argument to the other direction: if the expression is non-negative for any distinct x, y and z, then f is convex. This motivates us to define

$$[x, y, z]_f := \frac{f(x)}{(x-y)(x-z)} + \frac{f(y)}{(y-z)(y-x)} + \frac{f(z)}{(z-x)(z-y)}$$

as the second divided difference of f.

One would hope that by setting

$$[x_0, x_1, \ldots, x_n]_f := \sum_{i=0}^{n} \frac{f(x_i)}{\prod_{j \neq i}(x_i - x_j)},$$

one obtains something that naturally generalizes divided differences for higher orders. This is indeed the case.

4.2 Divided differences

Define $D_n = \{x \in \mathbb{R}^n | x_i = x_j \text{ for some } 1 \leq i < j \leq n\}$.

Definition 4.3. Let $n \geq 0$. For any $f : (a, b) \to \mathbb{R}$ we define the corresponding n'th divided difference $[\cdots]_f : (a, b)^{n+1} \setminus D_{n+1}$ by setting

$$[x_0, x_1, \ldots, x_n]_f = \sum_{i=0}^{n} \frac{f(x_i)}{\prod_{j \neq i}(x_i - x_j)}.$$

We will soon prove that divided differences (of order n) are simply weighted averages of the n'th derivative.

4.2.1 Basic properties

Divided differences have the following important properties.

Proposition 4.4. *Divided differences are symmetric in the variable, i.e. for any* $f : (a,b) \to \mathbb{R}$ *and pairwise distinct* $a < x_0, x_1, \ldots, x_n < b$ *permutation* $\sigma : \{0,1,2,\ldots,n\} \to \{0,1,2,\ldots,n\}$ *we have*

$$[x_0, x_1, x_2, \ldots, x_n]_f = [x_{\sigma(0)}, x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(n)}]_f.$$

If f *is continuous, so are the divided differences. Finally, for fixed (pairwise distinct)* $a < x_0, x_1, \ldots, x_n < b$ *the map* $[x_0, x_1, \ldots, x_n]_\cdot : \mathbb{R}^{(a,b)} \to \mathbb{R}$ *is linear and continuous (with respect to the topology of pointwise convergence).*

Proof. Easy to check. □

The name "divided differences" stems from the fact that the higher order divided differences are itself (usual) divided differences of lower order ones.

Proposition 4.5. *For any* $f : (a,b) \to \mathbb{R}$ *and pairwise distinct* $x_0, x_1, \ldots, x_n \in (a,b)$ *we have*

$$[x_0, x_1, \ldots, x_n]_f = \frac{[x_0, x_1, \ldots, x_{n-1}]_f - [x_1, x_2, \ldots, x_n]_f}{x_0 - x_n} = [x_0, x_n]_{[\cdot, x_1, \ldots, x_{n-1}]_f} \tag{4.6}$$

More generally, for any pairwise distinct $x_1, x_2, \ldots, x_n, y_0, y_1, y_2, \ldots, y_m \in (a,b)$ *we have*

$$[y_0, y_1, y_2, \ldots, y_m]_{[\cdot, x_1, x_2, \ldots, x_n]_f} = [y_0, y_1, y_2, \ldots, y_m, x_1, x_2, \ldots, x_n]_f. \tag{4.7}$$

Proof. 4.6 is easy to check directly. For 4.7 note that both

$$[y_1, y_2, \ldots, y_m]_{[\cdot, x_1, x_2, \ldots, x_n]_f} \text{ and } [y_1, y_2, \ldots, y_m, x_1, x_2, \ldots, x_n]_f$$

satisfy 4.6 (as a function of the y's) and they agree when $m = 1$. □

We call 4.7 the *nesting property* of divided differences. Although the analogy isn't perfect, one could think that this identity says that m'th derivative of the n'th derivative is the $(m+n)$'th derivative.

The following observation tells us that the divided differences work as n'th derivative insomuch that it kills polynomials of degree less than n, and works with degree n as expected, up to a constant at least.

Proposition 4.8. *We have* $[x_0, x_1, \ldots, x_n]_{(x \mapsto x^n)} = 1$ *and* $[x_0, x_1, \ldots, x_n]_p = 0$ *for any polynomial* p *of degree at most* $n-1$. *In other words,* $[x_0, x_1, \ldots, x_n]_f$ *is the leading coefficient of the interpolation polynomial on pairs* $(x_0, f(x_0)), (x_1, f(x_1), \ldots, (x_n, f(x_n))$.

Proof. As the interpolation polynomial of a polynomial of degree at most n on a dataset of $(n+1)$ pairs is the polynomial itself, the second claim readily implies the first. Recall that the Lagrange form of the interpolation polynomial of a dataset $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$ is given by

$$\sum_{i=0}^{n} y_i \frac{\prod_{j\neq i}(x - x_j)}{\prod_{j\neq i}(x_i - x_j)},$$

and the leading coefficient of this polynomial is exactly the divided difference. □

4.2.2 Peano representation

Coming back to the original motivation, divided differences enjoy an integral representation also for larger n.

Theorem 4.9. *If $f \in C^n(a, b)$, then for any pairwise distinct $a < x_0, x_1, x_2, \ldots, x_n < b$ we have*

$$[x_0, x_1, \ldots, x_n]_f = \int_{\mathbb{R}} f^{(n)}(t) w(t) dt, \tag{4.10}$$

where

$$w(t) := w_{x_0,x_1,\ldots,x_n}(t) = \frac{1}{(n-1)!} \sum_{i=0}^{n} \frac{((x_i - t)_+)^{n-1}}{\prod_{j\neq i}(x_i - x_j)}. \tag{4.11}$$

In addition, w is non-negative, supported on $[\min(x_i), \max(x_i)]$ and integrates to $(n!)^{-1}$.

Proof. Note that the weight is simply the n'th divided difference of the map $g_{t,n} : x \mapsto ((x-t)_+)^{n-1}/(n-1)!$. This is not very surprising: one should think that $g_{t,n}$ is the function whose n'th derivative is δ_t. If we plug in $f = g_{t,n}$, (as in the proof of 4.2), we, at least morally, get the claim. While the previous argument could be pushed through, we take safer route. To prove that the formula even makes sense, we should prove the claim on the support. It is clear that w is zero whenever $t \geq \max(x_i)$. If on the other hand $t \leq \min(x_i)$, $w(t)$ agrees with the n'th divided difference of the map $x \mapsto (x - t)^{n-1}/(n-1)!$, which is zero by the proposition 4.8.

We may hence repeatedly partially integrate the right-hand side:

$$\begin{aligned}\int_{\mathbb{R}} f^{(n)}(t)w(t)dt &= \int_{\mathbb{R}} f^{(n-1)}(t)(-1)w'(t)dt \\ &= \int_{\mathbb{R}} f^{(n-2)}(t)w^{(2)}(t)dt \\ &= \dots \\ &= \int_{\mathbb{R}} f^{(1)}(t)(-1)^n w^{(n-1)}(t)dt,\end{aligned}$$

where

$$(-1)^n w^{(n-1)}(t) = \sum_{i=0}^{n} \frac{\chi_{(t,\infty)}(x_i)}{\prod_{j\neq i}(x_i - x_j)}.$$

Note that $w^{(j)}$ is continuous, piecewise C^1, and compactly supported for every $0 \leq j < n-1$, so the partial integration is legitimate. The final step is a easy calculation.

Applying the identity to $x \mapsto x^n$ shows the claim on the integral of w.

Only non-negativity remains: we prove it by induction on n. The case $n = 1$ is clear. The idea is rather simple: we should prove that the functions $g_{t,n}$ have non-negative divided differences, which should roughly mean it has non-negative n'th derivative (being δ_t). By the nesting property we have

$$[x_0, x_1, \dots, x_n]_{g_{t,n}} = [x_0, x_1, \dots, x_{n-1}]_{[\cdot, x_n]_{g_{t,n}}}.$$

Now if we could replace $[\cdot, x_n]_{g_{t,n}}$ with the derivative of $g_{t,n}$, which is conveniently $g_{t,n-1}$, we would be done by the induction hypothesis. Note that while these functions aren't the same in general, they agree (up to constant) if $x_n = t$. But if $x_n \neq t$, we can play the same game as before: $[\cdot, x_n]_{g_{t,n}}$ is weighted average of the derivative $g'_{t,n} = g_{t,n-1}$. Indeed, as

$$[\cdot, x_n]_{g_{t,n}} = \int_0^1 g_{t,n-1}(s \cdot +(1-s)x_n)ds,$$

we have

$$[x_0, x_1, \dots, x_{n-1}]_{[\cdot, x_n]_{g_{t,n}}} = \int_0^1 [x_0, x_1, \dots, x_{n-1}]_{g_{t,n-1}(s\cdot+(1-s)x_n)}ds,$$

Now since all the divided differences of $g_{t,n-1}$ are non-negative, the same is clearly true for $g_{t,n-1}(s \cdot +(1-s)x_n)$, so we are done. □

The weight 4.11 is called **Peano kernel** (of order n). The points $x_0, x_1, \ldots, x_n$ are called the **nodes** of w.

As a very important corollary we get the following.

Theorem 4.12 (Mean value theorem for divided differences)**.** *Let $f \in C^n(a,b)$. Then for any pairwise distinct $x_0, x_1, \ldots, x_n \in (a,b)$ we have*

$$\min_{0\le i\le n}(x_i) < \xi < \max_{0\le i\le n}(x_i)$$

such that

$$[x_0, x_1, \ldots, x_n] = \frac{f^{(n)}(\xi)}{n!}. \tag{4.13}$$

Proof. t.f.i.f. 4.9 and mean value theorem for integrals. □

Alternate proof. By linearity and proposition 4.8 it suffices to verify the claim in the case where $f(x_i) = 0$ for $0 \le i \le n$.

Lemma 4.14. *If f is n times differentiable, and has $n+1$ roots, then $f^{(n)}$ has a root (in the interior of the convex hull of the roots).*

Proof. If f has $n+1$ roots, by the mean value theorem its derivative has n roots (in the interior of the convex hull of the roots of f) and is $(n-1)$ times differentiable. Since the derivative satisfies the same assumptions for $n-1$, the claim follows by induction. □

□

Note that the alternate proofs works even if f is merely n times differentiable.

The mean value theorem could be also used to prove the non-negativity of the weight w: if w were somewhere negative, one could construct a function with non-negative derivative and negative divided difference, which would contradict 4.13.

As in the case $n = 1$, if for $n > 1$ we can continuously extend divided differences to the set D_{n+1}, we should do that; we identify the resulting function with the original one. We will later prove that, as expected, this can be done, if and only $f \in C^n(a,b)$. In this case by 4.13 the extesion satisfies

$$[x_0, x_0, \ldots, x_0]_f = \frac{f^{(n)}(x_0)}{n!},$$

which together with 4.6 is enough to expand the divided differences with values of the function and its derivative.

4.2.3 Cauchy's integral formula

Complex analysis offers a nice view on divided differences: if f is analytic, we may interpret divided differences as contour integrals.

Lemma 4.15 (Cauchy's integral formula for divided differences)**.** *If γ is a simple closed counter-clockwise curve enclosing the numbers $x_0, x_1, \dots, x_n$, we have*

$$[x_0, x_1, \dots, x_n]_f = \frac{1}{2\pi i} \int_\gamma \frac{f(z)}{(z - x_0)(z - x_1) \cdots (z - x_n)} dz.$$

Proof. This is a direct consequence of the Residue theorem. □

If all the points coincide, we get the familiar formula for the n'th derivative. If f is a polynomial of degree at most $n-1$, the integrand decays as $|z|^{-2}$ (at infinity) and the divided differences vanish, as expected. Also, for $z \mapsto z^n$ one can use the formula to calculate the n'th divided difference with a residue at infinity. This formula is slightly more concisely expressed by writing for a sequence $X = (x_i)_{i=0}^n$ $p_X(x) = \prod_{i=0}^n (x - x_i)$. Now we have

$$[x_0, x_1, \dots, x_n]_f = \frac{1}{2\pi i} \int_\gamma \frac{f(z)}{p_X(z)} dz.$$

Cauchy's integral formula is a convenient way to think about severel identities.

Example 4.16. We may express an interpolation polynomial of an analytic function f and sequence $X = (x_i)_{i=0}^n$ by

$$P_{X,f}(x) := \frac{1}{2\pi i} \int_\gamma \frac{p_X(x) - p_X(z)}{x - z} \frac{f(z)}{p_X(z)} dz = [x_0, x_1, \dots, x_n]_{f[x,\cdot]p_X}.$$

Indeed: $P_{X,f}(x_i)$ evaluates to $f(x_i)$ by Cauchy's integral formula. More generally, if some of the points coincide, we get the Hermite interpolation polynomial, as can be shown with slightly more careful considerations. △

While the previous argument works stricly speaking only for analytic function (and even then one would have to be careful with domains and γ), the identity holds more generally. The expression for $P_{X,f}$ can be expanded as some kind polynomial, coefficients of which are linear combinations of evaluations $f(x_i)$: such expressions make perfect sense irrespective of the regularity of f. Same is true for the evaluations of this polynomial at points x_i, numbers $P_{X,f}(x_i)$. We know that $P_{X,f}(x_i) = f(x_i)$ holds for all analytic (or at least entire) functions. On the other hand the map $f \mapsto P_{X,f}(x_i) - f(x_i)$ is simply a finite linear combination of point evaluations, so it vanishes for any function if we manage to prove that

Lemma 4.17. *For any pairwise distinct $x_0, x_1, \dots, x_n \in \mathbb{C}$ and $y_0, y_1, \dots, y_n \in \mathbb{C}$ there exists an entire function f with $f(x_i) = y_i$.*

Proof. Simply take f to be the interpolating polynomial. □

One can also interpret such identities to be strictly formal: Cauchy's integral formula can be thought as a bijection between rational functions with simple poles and the span of δ-measures. Such signed measures look often simpler as rational functions.

4.2.4 Identities

Many of the familiar identities for the derivatives have analogs with divided differences. We won't need these formulas, but it's nevertheless nice to know that there are such. Also, they are not really more complicated than the derivative counterparts. On the contrary; the author honestly thinks that they are in fact easier to remember. One of the downsides of the divided difference identities is however that they are usually not symmetric with respect to the sequence $x_0, x_1, \dots, x_n$ anymore. That's life.

Proposition 4.18. *Let n, k, f, g, $f_1, f_2, \dots, f_k$ and $x_0, x_1, \dots, x_n$ be such that the folliowing identities make sense.*

(i) (Newton expansion)

$$\begin{aligned} f(x) = {} & [x_0]_f + [x_0, x_1]_f (x - x_0) + [x_0, x_1, x_2]_f (x - x_0)(x - x_1) + \dots \\ & + [x_0, x_1, \dots, x_n]_f (x - x_0)(x - x_1) \cdots (x - x_{n-1}) \\ & + [x, x_0, x_1, \dots, x_n]_f (x - x_0)(x - x_1) \cdots (x - x_n), \end{aligned} \tag{4.19}$$

in particular, if the points coincide we get the familiar Taylor expansion

$$f(x) = \sum_{k=0}^{n-1} \frac{f^{(k)}(x_0)}{k!} + [x, x_0, x_0, \dots, x_0]_f (x - x_0)^n, \tag{4.20}$$

(ii) (Product rule)

$$[x_0, x_1]_{fg} = [x_0]_f [x_0, x_1]_g + [x_0, x_1]_f [x_1]_g.$$

(iii) (Leibniz rule)

$$\begin{aligned} [x_0, x_1, \dots, x_n]_{fg} = {} & [x_0]_f [x_0, \dots, x_n]_g + [x_0, x_1]_f [x_1, \dots, x_n]_g + \dots \\ & + [x_0, x_1, \dots, x_{n-1}]_f [x_{n-1}, x_n]_g + [x_0, x_1, \dots, x_n]_f [x_n]_g. \end{aligned} \tag{4.21}$$

More generally

$$[x_0, x_1, \ldots, x_n]_{f_1 f_2 \cdots f_k} = \sum_{0=i_0<i_1<i_2<\ldots<i_{k-1}<i_k=n} \prod_{j=1}^{k} [x_{i_{j-1}}, \ldots, x_{i_j}]_{f_j}$$

(iv) (Chain rule)

$$[x_0, x_1]_{f\circ g} = [g(x_0), g(x_1)]_f [x_0, x_1]_g$$

(v) (Faà di Bruno formula)

$$[x_0, x_1, \ldots, x_n]_{f\circ g}$$
$$= \sum_{k=1}^{n} \sum_{0=i_0<i_1<i_2<\ldots<i_{k-1}<i_k=n} [g(x_{i_0}), g(x_{i_1}) \ldots, g(x_{i_k})]_f \prod_{j=1}^{k} [x_{i_{j-1}}, \ldots, x_{i_j}]_g$$

Proof sketches. (i) Easy induction using 4.6. Notice that also this formula makes it clear that the divided difference agrees with the degree n coefficient of the interpolating polynomial.

(ii) Easy to check.

(iii) Induction using the product rule (i.e. the case $n = 1$) and the nesting rule 4.7. Alternatively one could write Newton expansions of both f and g with sequences $(x_0, x_1, \ldots, x_n)$ and $(x_n, x_{n-1}, \ldots, x_0)$ and notice that the given sum gives exactly the leading term of the interpolating polynomial of fg. The more general case follows from the case of two functions by induction.

(iv) Easy to check.

(v) A bit tedious induction using the Leibniz rule and 4.6.

□

One might ask under what kind of conditions 4.19 leads to Newton series, i.e. we have

$$f(z) = \sum_{i=0}^{\infty} [z_0, z_1, \ldots, z_i]_f (z - z_0)(z - x_0) \cdots (z - z_{i-1}), \tag{4.22}$$

for some sequence $x_0, x_1, \ldots$ and analytic f. While Newton series can be globally rather subtle, locally they work almost like Taylor series.

Proposition 4.23. *Let $f : \mathbb{D}(z_\infty, \rho) \to \mathbb{C}$ be analytic and $z_0, z_1, \ldots \in \mathbb{D}(z_\infty, r)$ sequence converging to z_∞. Then 4.22 holds for any $z \in \mathbb{D}(z_\infty, r)$.*

Proof. We need to verify that the error term $[z, z_0, z_1, \ldots, z_n]_f(z - z_0)(z - z_1)\cdots(z - z_n)$ in Newton expansion tends to zero as $n \to \infty$. But for any $\rho' < \rho$ such that $z, z_0, z_1, \ldots \in \mathbb{D}(z_\infty, \rho')$ we have

$$\begin{aligned}&[z, z_0, z_1, \ldots, z_n]_f(z - z_0)(z - z_1)\cdots(z - z_n)\\ =&\frac{1}{2\pi i}\int_{\partial\mathbb{D}(z_\infty,\rho')}\frac{(z - z_0)(z - z_1)\cdots(z - z_n)}{(w - z)(w - z_0)(w - z_1)\cdots(w - z_n)}f(w)dw.\end{aligned}$$

As $z_n \to z_\infty$, the absolute values of the quotients $(z - z_n)/(w - z_n)$ tend to $|z - z_\infty|/|\rho'| < 1$ uniformly on $\partial\mathbb{D}(z_\infty, \rho')$ and hence the integrand tends uniformly to 0. □

In similar vein one could prove that if f is entire, its Newton series converge whenever $(z_i)_{i\geq 0}$ is bounded. Note that 4.22 easily implies the identity theorem for analytic functions.

4.2.5 k-tone functions

Definition 4.24. Function $f : (a, b) \to \mathbb{R}$ is called k-tone if for any $x_0, x_1, \ldots, x_n \in (a, b)$ of distinct points we have

$$[x_0, x_1, \ldots, x_n]_f \geq 0,$$

i.e. the n'th divided difference is non-negative.

We denote the space of k-tone functions by on interval (a, b) by $P^{(k)}(a, b)$.

Theorem 4.25. *Let k be an non-negative integer. Then $P^{(k)}(a, b) \subset \mathbb{R}^{(a,b)}$ is a closed convex cone.*

Proof. t.f.i.f 2.6. □

Mean value theorem tells us that C^k k-tone functions are exactly the functions with non-negative k'th derivative.

The cones $P^{(k)}(a, b)$ aren't quite salient. Instead we have

$$[\cdot, \cdot, \ldots, \cdot]_f = 0 \Leftrightarrow f \text{ is a polynomial of degree less than } k.$$

This suggests that a better object of study should be $\mathbb{R}^{(a,b)}$ quotiented by polynomials of degree less than k. We won't follow that trail, however.

4.3 Locality

One of the properties of the divided differences, which might not be clear from the definition, is that they can also be used to model local phenomena. One of the important properties of the k-tone functions is that if a function is k-tone on two overlapping intervals, then the function is k-tone on their union. While this definitely holds for C^k functions, it's not really clear how to change the argument for the general case.

If one thinks that k-tone functions have k'th derivative as a positive measure, the locality property should be thought of a special case of a general property of distributions.

Proposition 4.26. *Let $a < c < b < d$ and μ distribution on (a, d), restriction of which to (a, b) and (c, d) is a positive measure. Then μ is a positive measure.*

Proof. We should prove that $\mu(f)$ is non-negative for every non-negative test function f on (a, d). But every such function can be written as sum of two non-negative test functions, f_1 and f_2, f_1 supported on (a, b) and f_2 on (c, d), so $\mu(f) = \mu(f_1) + \mu(f_2) \geq 0$ by the assumption. □

They key idea in the proof was to split the test functions to two parts, one supported on (a, b) and one on (c, d). One can do the same with Peano kernels, except larger the order k, the more parts we need.

Lemma 4.27. *Let $a < c < b < d$ be reals and w a Peano kernel supported on (a, d). Then w can written as a (finite) weighted average of Peano kernels, all of which are supported either on (a, b) or on (c, d).*

Proof. Let n be the order of the Peano kernel and let $a < x_0 < x_1 < \ldots < x_n < d$ be the nodes or w.

The case $n = 1$ is rather clear: we simply split characteristic function of an interval to characteristic function of two intervals. In terms of the kernels, if $a < x_0 < c < b < x_1 < d$, we can pick $c < y_0 < b$ and write

$$w_{x_0,x_1} = \frac{y_0 - x_0}{x_1 - x_0} w_{x_0,y_0} + \frac{x_1 - y_0}{x_1 - x_0} w_{y_0,x_1} :$$

this is a sought decomposition.

The case $n = 2$ is not much harder. Peano kernels of order 2 are essentially triangles sitting on x-axis, corners of which have distinct x-coordinates. So we have one such triangle and we should split it to smaller triangles in such a way that

- No triangle has two equal x-coordinates.
- All triangles have all their corners' x-coordinates either on (a, b) and (c, d).

We call such triangles good. While the above picture should be rather convincing already, one can write an general algorithm generating such decomposition.
Input: A triangle (Peano kernel of order 2) supported on (a, d).
Output: A decomposition of the input as a positive linear combination of triangles all supported completely either on (a, b) or (c, d).

Step 1. If the triangle is good already, we are done.

Step 2. Pick $y_0 \in (c, b)$, which does not coincide with any of the x_0, x_1, x_2.

Step 3. Divide the triangle into two triagles with x-coordinates (x_0, x_1, y_0) and (x_1, x_2, y_0).

Step 4. Run this algorithm recursively for these two triangles.

Why does this algorithm terminate? Note that if any of the x_i's are in (c, b), the triangle is either good or $x_1 \in (c, b)$ (or maybe both). In the former case we are done, and in the latter the two parts of the split are both good. If none of x_i's are in (c, b), both of the parts of the split has a coordinate in (c, b), so also this case leads to a good split. In other words we can keep splitting triangles in such a way that they either become good or they have more nodes on (c, b).

It's easy to verify that splitting the triangle corresponds to the identity

$$w_{x_0,x_1,x_2} = \frac{y_0 - x_0}{x_2 - x_0} w_{x_0,x_1,y_0} + \frac{x_2 - y_0}{x_2 - x_0} w_{x_1,x_2,y_0}.$$

When $n > 2$, the geometric picture is largely lost (at least by the author), but the algebra generalizes perfectly: we can still split Peano kernels using the following identity:

$$w_{x_0,x_1,\ldots,x_n} = \frac{y_0 - x_0}{x_n - x_0} w_{x_0,x_1,\ldots,x_{n-1},y_0} + \frac{x_n - y_0}{x_n - x_0} w_{x_1,\ldots,x_n,y_0}. \tag{4.28}$$

Where does this come from? Recall that the Peano kernels are just the divided differences of the functions $g_{t,n} = ((\cdot - t)_+)^{n-1}/(n-1)!$. The first identity immediately generalizes to

$$[x_0, x_1]_f = \frac{y_0 - x_0}{x_1 - x_0}[x_0, y_0]_f + \frac{x_1 - y_0}{x_1 - x_0}[y_0, x_1]_f,$$

where f is now any function. By the nesting property the identity 4.28 is nothing more than the previous identity applied to $f = [\cdot, x_1, \ldots, x_{n-1}]_{g_{t,n}}$. Note that we need $x_0 < y_0 < x_n$, so that the weighted average is really a convex combination.

Now we are ready to generalize the algorithm to bigger n:
Input: A Peano kernel of order n supported on (a, d).
Output: A Decomposition of the input as a positive linear combination of Peano kernels of order n, all supported completely either on (a, b) or (c, d).

Step 1. If the kernel is good already, we are done.

Step 2. Pick $y_0 \in (c, b)$, which does not coincide with any of the $x_0, x_1, \ldots, x_n$.

Step 3. Divide the kernel to two kernels with nodes $(x_0, x_1, \ldots, y_0)$ and $(x_1, \ldots, x_n, y_0)$ as in the 4.28.

Step 4. Run this algorithm recursively for these two kernels.

This algorithm terminates basically because of the same reason: if the kernel isn't good already, the two splits have more nodes on (c, b), and this quantity cannot increase forever. $\square$

While this property is of independent interest, the real use of it is its generalization to divided differences.

Lemma 4.29. *Let $a < c < b < d$ be reals and $x_0, x_1, \ldots, x_n \in (a, d)$. Then we may find $N, M \in \mathbb{N}$, sequences $(y_{0,i}, \ldots, y_{n,i})$ and $(z_{0,j}, \ldots, z_{n,j})$ and numbers p_i and q_j for $1 \leq i \leq N$ and $1 \leq j \leq M$, such that*

- $\sum_{i=1}^{N} p_i + \sum_{j=1}^{M} q_j = 1$ *and $p_i, q_j \geq 0$ for every $1 \leq i \leq N$ and $1 \leq j \leq M$.*
- $y_{0,i}, y_{1,i}, \ldots, y_{n,i}$ *are pairwise distinct elements of (a, b) for every $1 \leq i \leq N$.*
- $z_{0,j}, z_{1,j}, \ldots, z_{n,j}$ *are pairwise distinct elements of (c, d) for every $1 \leq j \leq M$.*
- *For every $f : (a, d) \to \mathbb{R}$ we have*

$$[x_0, x_1, \ldots, x_n]_f = \sum_{i=1}^{N} p_i [y_{0,i}, y_{1,i}, \ldots, y_{n,i}]_f + \sum_{j=1}^{M} q_j [z_{0,j}, z_{1,j}, \ldots, z_{n,j}]_f.$$

Proof. Proof is almost identical to that of the lemma 4.27: we more or less just replace the identity 4.28 by

$$[x_0, x_1, \ldots, x_n]_f = \frac{y_0 - x_0}{x_n - x_0} [x_0, x_1, \ldots, x_{n-1}, y_0]_f + \frac{x_n - y_0}{x_n - x_0} [x_1, \ldots, x_n, y_0]_f, \tag{4.30}$$

which is valid because of essentially the same reasoning, and replace the word "kernel" with word "tuple". $\square$

The proof of 4.27 gives that we may take N and M (in 4.29) with $N + M \leq 2^n$. With slightly more careful argument one can achieve $M + N \leq n + 1$.

We are now ready to prove the locality property of the k-tone functions.

Proposition 4.31. *$P^{(k)}$ is a local property i.e. $P^{(k)}(a,b) \cap P^{(k)}(c,d) \subset P^{(k)}(a,d)$ for any $-\infty \leq a \leq c < b \leq d \leq \infty$. To be more precise, if $f : (a,d) \to \mathbb{R}$ such that $f\big|_{(a,b)} \in P^{(k)}(a,b)$ and $f\big|_{(c,d)} \in P^{(k)}(c,d)$, then $f \in P^{(k)}(a,d)$.*

Proof. t.f.i.f. lemma 4.29. □

Note that we could have also used the splitting property 4.30 to slightly simplify the proof of theorem 4.9. In the induction step we managed to prove that we have

$$[x_0, x_1, \ldots, x_{n-1}, t]_{g_{t,n}} = \frac{1}{n-1}[x_0, x_1, \ldots, x_{n-1}]_{g_{t,n-1}} = \frac{1}{n-1} w_{x_0,\ldots,x_{n-1}}(t) \geq 0$$

for any $x_0, x_1, \ldots, x_{n-1}$. But this readily implies that the divided differences are non-negative on all tuples as we have

$$\begin{aligned}
w_{x_0,x_1,\ldots,x_{n-1},x_n} &= [x_0, x_1, \ldots, x_{n-1}, x_n]_{g_{t,n}} \\
&= \frac{t - x_0}{x_n - x_0}[x_0, x_1, \ldots, x_{n-1}, t]_{g_{t,n}} + \frac{x_n - t}{x_n - x_0}[x_1, \ldots, x_n, t]_{g_{t,n}} \\
&= \frac{1}{n-1}\frac{t - x_0}{x_n - x_0}[x_0, x_1, \ldots, x_{n-1}]_{g_{t,n-1}} + \frac{1}{n-1}\frac{x_n - t}{x_n - x_0}[x_1, \ldots, x_n]_{g_{t,n-1}} \\
&= \frac{1}{n-1}\frac{t - x_0}{x_n - x_0} w_{x_0,x_1,\ldots,x_{n-1}} + \frac{1}{n-1}\frac{x_n - t}{x_n - x_0} w_{x_1,\ldots,x_n} \\
&\geq 0.
\end{aligned}$$

Of course, this approach only works if $\min(x_i) \leq t \leq \max(x_i)$, but if this is not the case, the divided differences are zero anyway. The previous identity can be also used to recursively compute Peano kernels.

Remark 4.32. The above arguments are a bit awkward and one might be tempted to think that one should instead consider positive linear combinations of Peano kernels, called (positive) splines, to get better analogue for the "locality of distributions" -proof. For $k \leq 3$ positive splines can be also characterized as suitable non-negative piecewise polynomial functions, but for $k > 3$ there's a problem: positive splines are merely subclass thereof. △

4.4 Regularity

The real power of the divided differences comes in when they are used to carry regularity information.

Theorem 4.33. *Let $k \geq 2$. Then $f \in P^{(k)}(a,b)$, if and only if $f \in C^{k-2}(a,b)$ and $f^{(k-2)}$ is convex.*

"Proof". Let $f \in P^{(k)}(a,b)$. Since $f^{(k)}$ is a positive measure, $f^{(k-1)}$ is increasing and $f^{(k-2)}$ is convex. As convex functions are continuous, we are done with $\Rightarrow$. Conversely, if $f \in C^{k-2}(a,b)$ and $f^{(k-2)}$ is convex, then $f^{(k-2)}$ has second derivative as a positive measure. But this measure is also the k'th derivative of f, so $f \in P^{(k)}(a,b)$. $\square$

Even though the previous argument isn't exactly sound (at least given our current machinery), the result is true. In this section we will translate the proof to the language of the divided differences.

The first step is to connect the divided differences of a function to the divided differences (of one lower order) of the derivative.

Lemma 4.34. *Let $f \in C^1(a,b)$. Then for any (pairwise distinct) $x_0, x_1, \ldots, x_n \in (a,b)$ we have*

$$[x_0, x_1, \ldots, x_{n-1}]_{f'} = \sum_{i=0}^{n-1} [x_0, x_1, \ldots, x_{i-1}, x_i, x_i, x_{i+1}, \ldots, x_{n-1}]_f \tag{4.35}$$

and

$$\begin{aligned} [x_0, x_1, \ldots, x_n]_f &= \int_0^1 [x_0, x_1, \ldots, x_{n-1}]_{f'(s\cdot+(1-s)x_n)} ds \\ &= \int_0^1 [s x_0 + (1-s)x_n, \ldots, s x_{n-1} + (1-s)x_n]_{f'} s^{n-1} ds. \end{aligned} \tag{4.36}$$

Proof. Note that divided differences of f have repeated entries in the first identity. As mentioned, these values of the divided difference are defined as a continuous extension. We will take the existence of this extension given for now.

We have

$$\begin{aligned} [x_0, x_1, \ldots, x_{n-1}]_{f'} &= \lim_{h \to 0} [x_0, x_1, \ldots, x_{n-1}]_{\frac{f(\cdot+h)-f(\cdot)}{h}} \\ &= \lim_{h \to 0} \frac{[x_0, x_1, \ldots, x_{n-1}]_{f(\cdot+h)} - [x_0, x_1, \ldots, x_{n-1}]_f}{h} \\ &= \lim_{h \to 0} \frac{[x_0 + h, x_1 + h, \ldots, x_{n-1} + h]_f - [x_0, x_1, \ldots, x_{n-1}]_f}{h}. \end{aligned}$$

Now the approach is basically the same as with differentiation of multivariate functions: we write the difference as sum of n differences: the difference can be expressed as sum of differences where only one of the entries are changed at a time.

$$
\begin{aligned}
&\lim_{h\to 0}\frac{[x_0+h,x_1+h,\ldots,x_{n-1}+h]_f-[x_0,x_1,\ldots,x_{n-1}]_f}{h}\\
=&\lim_{h\to 0}\left(\frac{[x_0+h,x_1+h,\ldots,x_{n-1}+h]_f-[x_0+h,x_1+h,\ldots,x_{n-2}+h,x_{n-1}]_f}{h}\right.\\
+&\frac{[x_0+h,x_1+h,\ldots,x_{n-2}+h,x_{n-1}]_f-[x_0+h,x_1+h,\ldots,x_{n-2},x_{n-1}]_f}{h}\\
+&\ldots\\
+&\left.\frac{[x_0+h,x_1,\ldots,x_{n-1}]_f-[x_0,x_1,\ldots,x_{n-1}]_f}{h}\right)\\
&=\lim_{h\to 0}\left(\sum_{i=0}^{n}[x_0+h,\ldots,x_{i-1}+h,x_i+h,x_i,x_{i+1},\ldots,x_{n-1}]_f\right).
\end{aligned}
$$

Now assuming the claim on the continuity, the limit is exactly what we wanted.

First equality of second claim was already essentially proved in the proof of theorem 4.9; the second is a simple computation. □

Note that the proof essentially gives also the following identity.

Proposition 4.37. *Let $x_0,x_1,\ldots,x_n$ and $y_0,y_1,\ldots,y_n$ be pairwise distinct points on (a,b). Then for any $f:(a,b)\to\mathbb{R}$ we have*

(4.38)

$$[y_0,y_1,\ldots,y_{n-1}]_f-[x_0,x_1,\ldots,x_{n-1}]_f=\sum_{i=0}^{n-1}[x_0,\ldots,x_{i-1},x_i,y_i,y_{i+1},\ldots,y_{n-1}]_f(y_i-x_i).$$

Next step is to connect the regularity of divided differences to regularity of divided differences of the derivative. Denote

$$D_{n,m}=\{x\in\mathbb{R}^n|x_{i_1}=x_{i_2}=\ldots=x_{i_m}\text{ for some }1\le i_1<i_2<\ldots<i_m\le n\}.$$

Note that $D_{n+1,2}$ is exactly the set where the divided differences aren't defined. Still, if f is smooth enough, we should be able to continuously extend the divided differences to this set, or at least to some subset set of it. This thinking leads to the following notion of the regularity of a function.

Definition 4.39. Let $f:(a,b)\to\mathbb{R}$ and $k\ge 0$. We call f *weakly C^k* (on (a,b)), or write $f\in C^k_w(a,b)$, if its order k divided differences can be continuously extended to $(a,b)^{k+1}$.

Our aim is to prove that function is weakly C^k, if and only if it's C^k. Note that this trivially holds for $k = 0$.

Lemma 4.40. *Let $n \geq k$. Then $f \in C^k_w(a, b)$, if and only if the order n divided differences of f extend continuously to $(a, b)^{n+1} \setminus D_{n+1,k+2}$.*

Proof. Let us denote

$S(n, k, f) =$ "order n divided differences of f extend continuously to $(a, b)^{n+1} \setminus D_{n+1,k+2}$".

As $S(k, k, f)$ is just saying that $f \in C^k_w(a, b)$, it is enough to prove that for any $n > k$ we have $S(n-1, k, f) \Leftrightarrow S(n, k, f)$.

$\Rightarrow$: Assume $S(n-1, k, f)$ and take any $x = (x_0, x_1, \ldots, x_n) \in (a, b)^{n+1} \setminus D_{n+1,k+2}$. Since $n + 1 \geq k + 2$, we may assume that $x_0 \neq x_n$. But now by the assumption the map

$$(y_0, y_1, \ldots, y_n) \mapsto \frac{[y_0, y_1, \ldots, y_{n-1}]_f - [y_1, y_2, \ldots, y_n]_f}{y_0 - y_n}$$

extends continuously to some neighbourhood of x (in $(a, b)^{n+1} \setminus D_{n+1,k+2}$), and since this map agrees with the n'th order divided differences on $(a, b)^{n+1} \setminus D_{n+1,2}$ by 4.6, it gives the continuous extension to x.

$\Leftarrow$: Assume then $S(n, k, f)$. Take any $x = (x_0, x_1, \ldots, x_{n-1}) \in (a, b)^n \setminus D_{n,k+2}$ and additional point $(z_0, z_1, \ldots, z_{n-1})$ with pairwise distinct components and $x_i \neq z_j$ for $0 \leq i, j \leq n-1$. Now the map

$$(y_0, \ldots, y_{n-1}) \to [z_0, z_1, \ldots, z_{n-1}]_f + \sum_{i=0}^{n-1} [z_0, \ldots, z_{i-1} z_i, y_i, y_{i+1}, \ldots, y_{n-1}]_f (y_i - z_i)$$

is continuous on some neighbourhood of x in $(a, b)^n \setminus D_{n,k+2}$, and since it agrees with the order n divided differences on $(a, b)^n \setminus D_{n,2}$ (by proposition 4.37), it gives the extension at x. $\square$

Lemma 4.41. *Let $f : (a, b) \to \mathbb{R}$, $k \geq 1$. Then $f \in C^k_w(a, b)$, if and only if $f \in C^1(a, b)$ and $f' \in C^{k-1}_w(a, b)$.*

Proof. "$\Rightarrow$": Let's start by proving that f is continuouly differentiable. Lemma 4.40 easily implies that it is sufficient prove this for the case $k = 1$. But in this case we know that the limits $\lim_{x \to x_0} [x, x_0]_f = [x_0, x_0]_f$ exist and f is hence differentiable with $f'(x) = [x, x]_f$. Also, $x \mapsto [x, x]_f = f'(x)$ is continuous.

Now the identity 4.35 easily implies the claim.

"$\Leftarrow$": By 4.36 it suffices to prove that the map

$$(x_0, x_1, \ldots, x_k) \to \int_0^1 [sx_0 + (1-s)x_k, \ldots, sx_{k-1} + (1-s)y_k]_{f'} s^{k-1} ds.$$

is continuous. Since $f' \in C_w^{k-1}(a,b)$, the order $(k-1)$ divided differences are uniformly continuous on any compact subset of $(a,b)^k$. The integrand is consequently continuous with sup-norm and hence the whole map continuous. $\square$

Corollary 4.42. *$f \in C_w^k(a,b)$ if and only if $f \in C^k(a,b)$.*

Proof. Simply apply Lemma 4.41 inductively. $\square$

This continuity results implies (among many other things) that mean value theorem also holds for general tuples.

Corollary 4.43 (General mean value theorem for divided differences)**.** *Let $f \in C^n(a,b)$ and $a < x_0, x_1, \ldots, x_n < b$. Then there exists ξ with*

$$\min_{0 \le i \le n} (x_i) \le \xi \le \max_{0 \le i \le n} (x_i)$$

such that

$$[x_0, x_1, \ldots, x_n] = \frac{f^{(n)}(\xi)}{n!}. \tag{4.44}$$

Proof. t.f.i.f 4.13 and 4.42. $\square$

Just like one can carry regularity information, one can carry boundedness information.

Lemma 4.45. *Let $f : (a,b) \to \mathbb{R}$ and $k \ge 2$. Then the k'th order divided differences of f are bounded, if and only if $f \in C^1$ and the order $(k-1)$ divided differences of f' are bounded. Moreover, the bounds satisfy*

$$\sup_{a<x_0<x_1<\ldots<x_{k-1}<b} |[x_0, x_1, \ldots, x_{k-1}]_{f'}| = k \sup_{a<x_0<x_1<\ldots<x_k<b} |[x_0, x_1, \ldots, x_k]_f|$$

Proof. The bounds follow rather immediately from the identities 4.35 and 4.36, so it only remains to verify that $f \in C^1$ given the conditions. Since the k'th divided difference corresponds to k'th derivative, if it is bounded, $(k-1)$'th derivative should be continuous. Thus we should prove that this is indeed the case by proving that $(k-1)$'th divided differences of f extend continuously to the whole of $(a,b)^k$.

Note that lemma 4.37 immediately implies that $(k-1)$'th divided difference of f is Lipschitz. But Lipschitz functions on dense set can be always extended to the whole space (as Lipschitz functions), so we are done by lemma 4.41. $\square$

Theorem 4.46. *Let $f : (a, b) \to \mathbb{R}$. Then $f \in C^{k-1}(a, b)$ and $f^{(k-1)}$ is Lipschitz, if and only if k:th divided difference of f is bounded. Moreover,*

$$\sup_{a<x_0<x_1<\ldots<x_k<b} |[x_0, x_1, \ldots, x_k]_f| = \frac{\mathrm{Lip}(f^{(k-1)})}{k!}$$

Proof. Again, simply apply lemma 4.45 inductively. $\square$

Finally, one can carry positivity.

Lemma 4.47. *Let $f : (a, b) \to \mathbb{R}$ and $k \geq 3$. Then f is k-tone, if and only if $f' \in C^1(a, b)$ and f' is $(k-1)$-tone.*

Proof. Again, only the claim on the regularity is non-trivial as the k-tone claim follows straightforwardly from 4.35 and 4.36. As with the bounded case the idea is that if f is k-tone $f^{(k)}$ is positive and hence $f^{(k-1)}$ is increasing, and consequently locally bounded. We should hence prove that the $(n-1)$'th divided differences are bounded, as then 4.45 would imply the claim. But this follow easily from 4.37. $\square$

Proof of the theorem 4.33. Yet again, simply apply lemma 4.47 inductively. $\square$

4.5 Analyticity

Theorem 4.48. *Let $f : (a, b) \to \mathbb{R}$. Then f is real analytic, if and only if for every closed subinteval $[c, d]$ of (a, b) there exists constant c such that for any $n \geq 1$*

$$\sup_{a<x_0<x_1<\ldots<x_n<b} |[x_0, x_1, \ldots, x_n]_f| \leq C_{c,d}^{n+1}.$$

Proof. "$\Leftarrow$": We need to prove that the for any $x_0 \in (a, b)$ Taylor series at x_0 converges in some neighbourhood of x_0. As observed before, the n:th error term in Taylor series is given by

$$[x, x_0, x_0, \ldots, x_0]_f (x - x_0)^n$$

with n x_0's. Now choose $a < c < x_0 < d < b$ and take any x with $x \in [c, d]$ and $|x - x_0| C_{c,d} < 1$. But then the error term tends to zero and we are done.

"$\Rightarrow$": Note that if $x_0 \in (a, b)$ and f extends to analytic function on $\mathbb{D}(x_0, r)$, we definititely have $\left|\frac{f^{(n)}(x_0)}{n!}\right| \leq C_{x_0}^{n+1}$ for some C_{x_0}. For $|x - x_0| < r$ we have

$$\frac{f^{(k)}(x)}{k!} = \sum_{n=k}^{\infty} \binom{n}{k} \frac{f^{(n)}(x_0)}{n!} (x - x_0)^{n-k},$$

which may be estimated by

$$\left|\frac{f^{(k)}(x)}{k!}\right| \leq C_{x_0}^{k+1}\sum_{n=k}^{\infty}\binom{n}{k}C_{x_0}^{n-k}(x-x_0)^{n-k} = \frac{C_{x_0}^{k+1}}{(1-|x-x_0|C_{x_0})^k},$$

whenever $|x-x_0|C_{x_0} < 1$. By the mean value theorem for divided differences it follows that we get required bound for some neighbourhood of x_0 and consequently, by compactness for any closed subinteval of (a, b). □

The previous result is some kind of relative of 4.46. Also theorem 4.33 has rather interesting relative.

Theorem 4.49 (Bernstein's theorem)**.** *If $f : (a, b) \to \mathbb{R}$ is k-tone for every $k \geq 0$, then f is real-analytic on (a, b).*

Proof. We prove that the conditions of the theorem 4.48 are satisfied. Pick any $a < x_0 < x < b$. Now for any $n \geq 0$ we have

$$f(x) = \sum_{k=0}^{n-1}\frac{f^{(k)}(x_0)}{k!}(x-x_0)^k + \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n + [x, x_0, x_0, \ldots, x_0]_f(x-x_0)^{n+1}.$$

Note that all the terms on the right-hand side are non-negative, and hence

$$0 \leq \frac{f^{(n)}(x_0)}{n!} \leq f(x)(x-x_0)^{-n}.$$

Now given any interval $[c, d] \subset (a, b)$ we can make such estimate uniform over $x_0 \in [c, d]$ simply by picking $x \in (d, b)$. □

4.6 Notes and references

Results of this chapter, with plentiful of illustrations, can be found in [5] (?).

Chapter 5

Matrix monotone functions – part 2

5.1 Characterization

5.1.1 Main theorem

Let's come back to theorem 3.15: with the k-tone language it rewrites to

Theorem 5.1. *$f \in P_n(a, b)$, if and only if $fN(q)$ is $(2n-1)$-tone for any $q \in \mathbb{C}_{n-1}[x]$.*

Main goal of this chapter is to prove this theorem. Note that in contrast to theorem 3.15 theorem 5.1 makes sense without any regularity assumptions. The new version also gives a resolution to the regularity issues related to its predecessor. Recall that $(2n-1)$-tone functions are C^{2n-3} and their $(2n-3)$'th derivative is convex. As convex functions are twice differentiable almost everywhere (see for instance TODO), $fN(q)$ is $(2n-1)$ times differentiable almost everywhere. We won't need these regularity properties, however.

There are also many different ways to talk about the polynomial part.

Lemma 5.2. *Let $h : \mathbb{C} \to \mathbb{C}$. Then the following are equivalent:*

(i) h is a non-negative polynomial on real line with $\deg(h) \leq 2n$.

(ii) There exists $q \in \mathbb{C}_n[x]$ such that $h = N(q)$.

(iii) There exists $q_1, q_2 \in \mathbb{R}_n[x]$ such that $h = q_1^2 + q_2^2$.

Proof. $(i) \Rightarrow (ii)$: If h is non-negative on real axis, it's roots all appear in pairs (of which there are at most n): either with strict complex conjugate pairs, of pairs of double real roots. We may take q to be $\sqrt{a_n} \prod (z - z_i)$ where z_i range over representatives of all the pairs and a_n is the leading coefficient of h.

$(ii) \Rightarrow (iii)$: If q has single conjugate pair $(z_0, \overline{z_0})$ of roots we have

$$(z - z_0)(z - \overline{z_0}) = z^2 - 2\Re(z_0) + |z_0|^2 = (z - \Re(z_0))^2 + \Im(z_0)^2,$$

so we may take $q_1 = \cdot - \Re(z_0)$ and $q_2 = \Im(z_0)$. But if $N(q) = q_1^2 + q_2^2$ and $N(r) = r_1^2 + r_2^2$, then

$$N(qr) = N(q)N(r) = (q_1 r_1 + q_2 r_2)^2 + (q_1 r_2 - q_2 r_1)^2,$$

so polynomial of higher order can be dealt with inductively.

$(iii) \Rightarrow (i)$: This is clear. □

To prove 5.1 we are going to verify that for any $f : (a, b) \to \mathbb{R}$, we have

$$f \in P_n(a, b)$$
$$\Leftrightarrow$$
$$[x_0, x_1, x_2, \ldots, x_{2n-1}]_{fN(q)} \geq 0 \text{ for any } q \in \mathbb{C}_{n-1}[x] \text{ and } a < x_0 < \ldots < x_{2n-1} < b.$$

Note that the proof of 3.15 can be interpreted as saying

$$Df_A(H) \geq 0 \text{ for any } A \in \mathcal{H}_{(a,b)} \text{ and } H \geq 0 \text{ with } \operatorname{rank}(H) = 1$$
$$\Leftrightarrow$$
$$[\lambda_1, \lambda_1, \ldots, \lambda_n, \lambda_n]_{fN(q)} \geq 0 \text{ for any } q \in \mathbb{C}_{n-1}[x] \text{ and } a < \lambda_1 < \ldots < \lambda_n < b.$$

The idea of the proof was to note that the quadratic form of the derivative rewrites to such divided difference, where λ's are the eigenvalues of A.

To avoid regularity issues we simply do the same thing without limits.

Definition 5.3. Let us call a triplet $(A, B, v) \in \mathcal{H}(V)^2 \times V$ a **projection pair** if $B - A = vv^*$. Let us further say that a projection pair (A, B, v) is **strict**, if v is not orthogonal to any eigenvector of A.

Lemma 5.4. *If $a < \lambda_0 < \lambda_1 < \ldots < \lambda_{2n-1} < b$ and $q \in \mathbb{C}_{n-1}[x]$, we may find a strict projection pair (A, B, v) such that*

$$\langle (f(B) - f(A))w, w \rangle = [\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_{2n-1}]_{fN(q)}$$

for any $f : (a, b) \to \mathbb{R}$.

Conversely, if (A, B, v) is a strict projection pair and $w \in V$, then there exists $a < \lambda_0 < \lambda_1 < \ldots < \lambda_{2n-1} < b$ and polynomial $q \in \mathbb{C}_{n-1}[x]$, such that for any $f : (a, b) \to \mathbb{R}$ we have

$$\langle (f(B) - f(A))w, w \rangle = [\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_{2n-1}]_{fN(q)}.$$

Before trying to understand the lemma we use it to prove theorem 5.1.

Proof. "$\Rightarrow$": t.f.i.f lemma 5.4.

"$\Leftarrow$": Take any $aI < A \leq B < bI$. Write $B - A = \sum_{i=1}^{n} c_i P_{v_i}$ for some $c_i \geq 0$. To prove that $f(B) - f(A) \geq 0$ we simply need to prove that $f(A + \sum_{i=1}^{k} c_i P_{v_i}) - f(A + \sum_{i=1}^{k-1} c_i P_{v_i}) \geq 0$ for any $1 \leq k \leq n$. We may hence assume that (A, B, v) projection pair.

We may also assume that (A, B, v) is strict. Indeed, if this is not the case, we can decompose $V = (v_1) \oplus V'$, where v_1 is an eigenvector of A orthogonal to v, and factorize $A = A_{(v_1)} \oplus A_{V'}$ and $B = A_{(v_1)} \oplus B_{V'}$. But now $f(B) - f(A) \geq 0$, if and only if $f(B_{V'}) - f(A_{V'}) \geq 0$, which would follow if we could prove that $f \in P_{n-1}(a, b)$. So we should just add the sentence "We induct on n." as the first sentence of this proof.

The strict case follows immediately from the lemma 5.4. □

Corollary 5.5. *P_n is a local property: if $a < c < b < d$ and $f : (a, d) \to \mathbb{R}$ such that $f\big|_{(a,b)} \in P_n(a, b)$ and $f\big|_{(c,d)} \in P_n(c, d)$, then $f \in P_n(a, d)$.*

Proof. t.f.i.f Theorem 5.1 and Proposition 4.31. □

5.1.2 Main lemma

It remains to understand what is going on with lemma 5.4. The surprising part about it is the following fact about eigenvalues of real maps.

Lemma 5.6. *Let (A, B, v) be a projection pair. Then*

$$\lambda_1(B) \geq \lambda_1(A) \geq \lambda_2(B) \geq \lambda_2(A) \geq \ldots \geq \lambda_n(B) \geq \lambda_n(A).$$

(A, B, v) is strict if and only if all the inequalities are strict.

Conversely, given any two interlacing sequences $b_1 \geq a_1 \geq b_2 \geq a_2 \geq \ldots \geq b_n \geq a_n$ there exists a projection pair (A, B, v) with $\lambda_i(A) = a_i$ and $\lambda_i(B) = b_i$.

This lemma is based on the following explicit relationship between characteristic polynomials of a projection pair.

Lemma 5.7. *Let (A, B, v) be a projection pair. Then*

$$\det(B - zI) = \det(A - zI) \left(1 + \langle (A - zI)^{-1} v, v \rangle\right)$$

and

$$\det(zI - B)(zI - B)^{-1} v = \det(zI - A)(zI - A)^{-1} v$$

Proof. Both of these identities should be understood as equalities between rational functions (to avoid problems at the spectra of A and B).

By the basic properties of the determinant we have

$$\begin{aligned}\det(B - zI) &= \det(A - zI)\\ &\quad + \|v\|^2 \det((A - zI)_{(v)^\perp})\\ &= \det(A - zI) + \|v\|^2 \det(A - zI)\langle (A - zI)^{-1} v, v\rangle / \|v\|^2\\ &= \det(A - zI)\left(1 + \langle (A - zI)^{-1} v, v\rangle\right),\end{aligned}$$

where the second equality follows from the Cramer rule.

Multiplying both sides of the second claim from left by $zI - A$ simplifies to an equivalent claim

$$\det(zI - B)v = \det(zI - A)(1 + \langle (A - zI)^{-1} v, v\rangle)v,$$

which is just the first identity (multiplied by v). □

Proof of lemma 5.6. Note that if v is orthogonal to one of the eigenvectors of A, P_v doesn't affect this eigenspace. Hence, as one easily checks, we may forget this eigenvector and restrict our attention to a smaller space. Similarly for the converse: if $a_i = b_j$ for some $1 \leq i, j \leq n$ we can forget a_i and b_j, and solve the remaining problem on smaller space. Consequently, we may assume that the pair (A, B, v) and the inequalities in the converse are strict.

Let $(e_i)_{i=1}^n$ be the eigenbasis of A and consider the rational function

$$z \mapsto 1 + \langle (A - zI)^{-1} v, v\rangle = 1 + \sum_{i=1}^{n} \frac{|\langle v, e_i\rangle|^2}{\lambda_i(A) - z}.$$

It has n poles of negative residue so it has a root between any two poles. Also it tends to 1 at infinity so it has a root on $(\lambda_1(A), \infty)$. It has hence n distinct roots. All these roots are eigenvalues of B by Lemma 5.7 so they are exactly the eigenvalues. This implies the first claim.

For the converse, first take A with the given eigenvalues. By Lemma 5.7 we now just want to choose v in such a way that

$$\frac{p_B(z)}{p_A(z)} = 1 + \langle (A - zI)^{-1} v, v\rangle = 1 + \sum_{i=1}^{n} \frac{|\langle v, e_i\rangle|^2}{a_i - z},$$

But this is clearly achieveable if can show that the residues of $p_B(z)/p_A(z)$ are negative, which follows easily from the interlacing property. Hence the converse. □

Let us then complete the proof of theorem 5.1 by proving the lemma 5.4.

Proof of lemma 5.4. Assume first that f is entire and fix a strict projection pair (A, B, v) and $w \in V$. Similarly to the "proof" of 3.16 we have

$$\begin{aligned}
&\langle (f(B) - f(A))w, w\rangle \\
&= \frac{1}{2\pi i}\int_\gamma \langle (zI - B)^{-1}v, w\rangle\langle (zI - A)^{-1}w, v\rangle f(z)dz \\
&= \frac{1}{2\pi i}\int_\gamma \frac{\det(zI - A)}{\det(zI - B)}\langle (zI - A)^{-1}v, w\rangle\langle (zI - A)^{-1}w, v\rangle f(z)dz \\
&= \frac{1}{2\pi i}\int_\gamma \frac{N(q)}{\det(zI - A)\det(zI - B)} f(z)dz \\
&= [\lambda_1(A), \ldots, \lambda_n(A), \lambda_1(B), \ldots, \lambda_n(B)]_{fN(q)}.
\end{aligned}$$

where Lemma 5.7 was used in the second equality and we write $q(z) = \det(zI - A)\langle (zI - A)^{-1}v, w\rangle$. By 4.17 or by suitable formal interpretation one sees that this identity holds without any regularity assumptions.

Now when (A, B, v) ranges over all strict projection pairs, the permutations of tuples

$$(\lambda_1(A), \ldots, \lambda_n(A), \lambda_1(B), \ldots, \lambda_n(B)) \tag{5.8}$$

range over all tuples of $2n$ distinct numbers on (a, b). Hence to prove the lemma, we should verify that for fixed strict projection pair (A, B, v), as w ranges over V, q ranges over $\mathbb{C}_{n-1}[x]$. Note that the components of $\det(zI - A)(zI - A)^{-1}v$ with respect to an eigenbasis of A, $(e_j)_{j=1}^n$, are $p_j(z) = \langle v, e_j\rangle \prod_{i\neq j}(z - \lambda_i(A))$. But since $p_j(\lambda_i(A)) \neq 0$, if and only if $i = j$, the components are linearly independent over $\mathbb{C}$ and hence span $\mathbb{C}_{n-1}[x]$. $\square$

To recap, the map

$$\begin{aligned}
&V \to \mathbb{C}_{n-1}[x] \\
&w \mapsto \det(zI - A)\langle (zI - A)^{-1}v, w\rangle = \sum_{j=1}^n p_j(z)\langle e_j, w\rangle
\end{aligned}$$

is antilinear bijection, the correspondence between w and q.

5.1.3 Dual pairing

Proof of theorem 5.1 is actually missing one more detail we need in the induction step.

Lemma 5.9. *If $fN(q)$ is $(2n+1)$-tone for $q \in \mathbb{C}_n[x]$, then $fN(\tilde{q})$ is $(2n-1)$-tone for every $\tilde{q} \in \mathbb{C}_{n-1}[x]$.*

To understand this result, recall that for analytic f and $a < x_0 < x_1 < \ldots < x_{2n-1} < b$ we have

$$[x_0, x_1, \ldots, x_{2n-1}]_{fN(q)} = \frac{1}{2\pi i}\int_\gamma \frac{N(q)}{(z-z_0)(z-z_1)\cdots(z-z_{2n-1})} f(z)dz,$$

for suitable γ. One way to interpret this identity is to consider it as a linear map: for given analytic f we have the map

$$r \mapsto \frac{1}{2\pi i}\int_\gamma r(z)f(z)dz,$$

where r is a rational functions with its poles in the domain of f. Note that all this makes formally sense for arbitrary f given that the poles of r are simple. This motivates us to define a dual pairing $\langle \cdot, \cdot \rangle_L$ (over $\mathbb{R}$) between $\mathbb{R}^{(a,b)}$ and rational functions with simple poles on (a,b), for which

$$\langle f, r \rangle_L = \frac{1}{2\pi i}\int_\gamma r(z)f(z)dz,$$

for analytic f. We could of course replace (a,b) by any subset of $\mathbb{C}$.

Now theorem 5.1 is just saying that $f \in P_n(a,b)$, if and only if $\langle f, r\rangle_L \geq 0$ whenever r is of the form

$$r(z) = \frac{N(q)}{(z-z_0)(z-z_1)\cdots(z-z_{2n-1})}$$

where $a < z_0 < \ldots < z_{2n-1} < b$ and $q \in \mathbb{C}_{n-1}[x]$. Let us denote this family of rational functions by $R_{+,n}(a,b)$. Now, in order to prove the lemma we should prove that we have

$$\mathrm{cone}(R_{+,n}(a,b)) \subset \mathrm{cone}(R_{+,n+1}(a,b))$$

Proof lemma 5.9. Take any $r \in R_{+,n}(a,b)$. If there was no condition on the order of the poles, we could simply note that

$$r = r\frac{N(z-c)}{(z-c)(z-c)} \in R_{+,n+1}(a,b).$$

Even though that doesn't quite work, we can modify the idea a little: we have

$$r = \frac{1}{2}r\frac{N((z-c))}{(z-c)(z-\frac{c+d}{2})} + \frac{1}{2}r\frac{N((z-d))}{(z-d)(z-\frac{c+d}{2})} \in \mathrm{cone}(R_{+,n+1}(a,b))$$

as soon as we choose $c, d \in (a,b)$ so that the poles remain simple. □

5.2 Loewner's theorems

Let's move our focus to the classes $P_\infty(a,b)$. Using the earlies ideas we can rewrite theorem 3.15 in the following form.

Theorem 5.10. *$f \in P_\infty(a,b)$, if and only if f is analytic and for every $n \geq 1$ and $q \in \mathbb{C}_{n-1}[x]$ the function $fN(q)$ is $(2n-1)$-tone.*

Without the analyticity condition this would immediately follow from 5.1, and the statement would also make perfect sense without it. It is nevertheless true that the functions in class $P_\infty(a,b)$ are analytic. One could use Bernstein type arguments and tricks (see proof of the theorem 4.49) to convince oneself that this indeed the case, but there's actually a lot more going on.

First of all, the dual pairing thinking leads to much more satisfactory conclusion in the case $n = \infty$.

Lemma 5.11. *We have*

$$\begin{aligned} R_+(a,b) &:= \bigcup_{n=1}^{\infty} R_{+,n}(a,b) = \operatorname{cone}\left(\bigcup_{n=1}^{\infty} R_{+,n}(a,b)\right) \\ &= \{\textit{rational functions with only simple, real poles; non-negative} \\ &\quad \textit{on } \mathbb{R}\setminus(c,d) \textit{ for some } a < c < d < b\textit{; and decay } r(z) = O(|z|^{-2}) \textit{ at } \infty\}. \end{aligned}$$

Proof. It is sufficient to prove that if r is a rational function as in the lemma statement, then $r \in R_{+,n}(a,b)$ for some $n \geq 1$. So pick such r.

Note that r changes its sign even number of times, and only on interval (a,b), say at points $a < x_0 < x_1 < \ldots < x_{2n-1} < b$. Write $p := \prod_{i=0}^{2n-1}(\cdot - x_i)$. Now pr is a polynomial of degree less than $2n$ non-negative on $\mathbb{R}$, so it is of the form $N(q)$ for some $q \in \mathbb{C}_{n-1}[x]$. Hence we have

$$r = \frac{N(q)}{p} \in R_{+,n}(a,b).$$

$\square$

Now, it might not be too big of a surprise that the class $R(a,b) := \operatorname{span} R_+(a,b)$ is dense in $C_c(\mathbb{R}\setminus(a,b))$, compactly supported continuous functions on $\mathbb{R}\setminus(a,b)$ with sup-norm. This should imply, by the Riesz representation theorem, that for any $f \in P_\infty(a,b)$ there exists a Radon measure μ_f on $\mathbb{R}\setminus(a,b)$ with $\mu_f((\lambda^2+1)^{-1}) < \infty$ such that for any $r \in R_+(a,b)$

$$\langle f, r\rangle_L = \int_{\mathbb{R}\setminus(a,b)} r(\lambda)\, d\mu_f(\lambda).$$

This is almost true. As the functions $R_+(a,b)$ are not compactly supported, there's a problem at infinity. Nevertheless, the previous holds with slight modification.

Theorem 5.12 (Loewner's theorem, version 1)**.** *Let $f \in P_\infty(a,b)$. Then there exists a unique Radon measure μ_f on $\mathbb{R} \setminus (a,b)$ with $\mu_f((\lambda^2+1)^{-1}) < \infty$ and $\alpha \geq 0$ such that for any $r \in R_+(a,b)$ we have*

$$\langle f, r\rangle_L = \alpha\left(\lim_{\lambda\to\infty} r(\lambda)\lambda^2\right) + \int_{\mathbb{R}\setminus(a,b)} r(\lambda)d\mu_f(\lambda).$$

In particular for any $x, y \in (a,b)$ we have

$$[x,y]_f = \alpha + \int_{\mathbb{R}\setminus(a,b)} \frac{d\mu_f(\lambda)}{(\lambda-x)(\lambda-y)}.$$

Note that the limit $(\lim_{\lambda\to\infty} r(\lambda)\lambda^2)$ exists and is non-negative for any $r \in R_+(a,b)$. It is clear that the converse of this theorem also holds. Note also that examples 3.6 fit in the this framework: they correspond to positive linear combinations of δ-measures. Theorem 5.12 can be interpreted as saying that all functions in the class $P_\infty(a,b)$ are more or less of the form 3.6; only summation is replaced with integration with respect to (somewhat) arbitrary measure.

Although it would not be terribly tricky to fill in the details to the previous argument, we will not prove 5.12. Instead we look into one of its corollaries:

Corollary 5.13. *Every $f \in P_\infty(a,b)$ has an analytic extension $\tilde{f}$ on $\mathbb{H}_+ \cup \mathbb{H}_-$. This extension maps (open) upper half-plane $\mathbb{H}_+$ to closed upper half-plane $\overline{\mathbb{H}_+}$.*

In fact, also this corollary has a converse.

Theorem 5.14 (Loewner's theorem, version 2)**.** *Let $f : (a,b) \to \mathbb{R}$. Then $f \in P_\infty(a,b)$, if and only there exists a analytic function $\tilde{f}$ on $(\mathbb{H}_+ \cup \mathbb{H}_-) \cup (a,b)$ such that $\tilde{f}\Big|_{(a,b)} = f$ and $\tilde{f}$ maps the upper half-plane to its closure.*

This is the version of the Loewner's theorem we are going to focus on.

5.3 Notes and references

This chapter is largely original (?), although heavily inspired by multiple sources. Key ideas are an extension to [8]. 5.1 is new formulation of 3.16. Lemma 5.6 (or some variant of it) is present in many discussions of the matrix monotonicity, see for instance [7]. While

5.4 is new (?) it can be seen as a variant of lemma 1 in [14]. Theorem 5.14 appears in the original paper of Loewner [11]. 5.12 was first discussed in [2]. Sparr in [14] gives proof of 5.12 somewhat similar in nature to our argument sketch (...). Bernstein type arguments for the analyticity are discussed in [2].

Chapter 6

Pick-Nevanlinna functions

Pick-Nevanlinna function is an analytic function defined in upper half-plane with a non-negative imaginary part. Such functions are sometimes also called Herglotz or $\mathbb{R}$ functions; we will call them just *Pick functions*. The class of Pick functions is denoted by $\mathcal{P}$.

6.1 Examples and basic properties

Most obvious examples of Pick functions might be functions of the form $\alpha z + \beta$ where $\alpha, \beta \in \mathbb{R}$ and $\alpha \geq 0$. Of course one could also take $\beta \in \overline{\mathbb{H}}_+$. As non-constant analytic functions are open mappings, real constants are the only Pick functions failing to map $\mathbb{H}_+ \to \mathbb{H}_+$.

Pick functions can be thought of a set of "positive analytic functions".

Theorem 6.1. *$\mathcal{P} \subset \{$analytic maps on $\mathbb{H}_+\}$ is a closed convex cone.*

Proof. Again, t.f.i.f 2.6. □

Also a composition of Pick functions is a Pick function.

The map $z \mapsto -\frac{1}{z}$ is evidently a Pick function. Hence are also all functions of the form

$$\alpha z + \beta + \sum_{i=1}^{N} \frac{m_i}{\lambda_i - z},$$

where N is non-negative integer, $\alpha, m_1, m_2, \ldots, m_N \geq 0$, $\beta \in \mathbb{H}_+$ and $\lambda_1, \ldots, \lambda_N \in \mathbb{H}_-$.

There are (luckily) more interesting examples. All the functions of the form x^p (with natural branch) where $0 < p < 1$ are Pick functions; similarly for log. Another classic example is tan. Indeed, by the addition formula

$$\begin{aligned}\tan(x+iy) &= \frac{\tan(x)+\tan(iy)}{1-\tan(x)\tan(iy)} = \frac{\tan(x)+i\tanh(y)}{1-i\tan(x)\tanh(y)} \\ &= \frac{\tan(x)(1+\tanh^2(y))}{1+\tan^2(x)\tanh^2(y)} + i\frac{(1+\tan^2(x))\tanh(y)}{1+\tan^2(x)\tanh^2(y)},\end{aligned}$$

and y and $\tanh(y)$ have the same sign.

$\mathcal{P}$ is almost salient: if φ is analytic and $\Im(\varphi) = 0$, then φ is a real constant (by Cauchy-Riemann equations, for instance). And again, this suggests that one should think about Pick functions up to a real constant.

So far we have made no mention on the topology, as it's usually taken to be the topology of locally uniform convergence. This definitely works (as it makes the evaluation functionals continuous), but we can do much better. It namely turns out that we can consider the set of Pick functions as a proper cone of $\mathbb{C}^{\mathbb{H}_+}$, set of all functions, with the topology of pointwise convergence.

Proposition 6.2. *If $(\varphi_i)_{i=1}^{\infty}$ is a sequence of Pick functions converging pointwise, the limit function is also a Pick function.*

This result is far from clear: pointwise limits of analytic functions need not analytic in general. We will not prove the result yet, but it strongly suggests that there is something more going on; Pick functions are very rigid. Note also that if Pick functions are thought of a subset of all functions, the definition of the cone doesn't really fit the general framework of theorem 2.6. This suggests that question one should ask is:

Question 6.3. What is the "correct" predual for $\mathcal{P}$?

6.2 Rigidity

6.2.1 Boundary

To understand the rigidity phenomena we take a brief look at a close relative to Pick functions, *Schur functions.* Schur funtions are analytic maps from open unit disc to closed unit disc. Classic fact about these functions is the Schwarz lemma.

Theorem 6.4 (Schwarz lemma). *Let $\psi : \mathbb{D} \to \mathbb{D}$ be analytic such that $\psi(0) = 0$. Then $|\psi(z)| \leq |z|$ for any $z \in \mathbb{D}$.*

The textbook proof is based on two observations about analytic functions.

- If φ is analytic at a with $\varphi(a) = 0$, then $\varphi/(\cdot - a)$ is also analytic.
- If φ is analytic on closed unit disc and $|\varphi| \leq 1$ on the boundary of the disc, then $|\varphi| \leq 1$ inside the disc.

The first observation might not be very surprising, and it holds for smooth functions also. The second, on the other hand, is a true manifestation of the nature of the analytic maps: we can bound analytic functions simply by bounding them on the boundary of the domain. More generally: one knows everything about an analytic function on a domain simply by knowing it on a boundary, by Cauchy's integral formula.

This suggests that we should be able to recognize also Pick functions looking only at their boundary values. Actually even more is true: it suffices to look at the imaginary parts.

Proposition 6.5. *Let $\varphi : U \to \mathbb{C}$ be analytic, such that $\overline{\mathbb{H}_+} \subset U$, and φ is continuous at ∞. Then if the imaginary part of φ is non-negative on the real axis, φ is Pick function.*

Proof. t.f.i.f the minimum principle applied to the harmonic function $\Im(\varphi)$. $\square$

6.2.2 Integral representations

Recall that imaginary part of an analytic function determines also its real part, up to a constant, so we can also recover the function itself. This can be also done explicitly.

Theorem 6.6. *Let $\varphi : U \to \mathbb{C}$ be analytic, such that $\overline{\mathbb{H}_+} \subset U$, and $\varphi(z) = O(|z|^{-\varepsilon})$ for some $\varepsilon > 0$ at infinity. Then for any $z \in \mathbb{H}_+$ we have*

$$\varphi(z) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{\Im(\varphi)(\lambda)}{\lambda - z} d\lambda$$

Proof. Note that the integral defines an analytic function, imaginary part of which equals

$$\frac{\Im(z)}{\pi} \int_{\mathbb{R}} \frac{\Im(\varphi)(\lambda)}{(\lambda - z)(\lambda - \overline{z})} d\lambda.$$

This expression however equals $\Im(\varphi(z))$ by Poisson integral formula. By letting $z \to \infty$ one sees that also the real constants match.

Alternatively one could observe that for a closed counter clockwise oriented curves γ on the upper half-plane, enclosing z, we have

$$\varphi(z) = \frac{1}{2\pi i} \int_{\gamma} \frac{\varphi(\lambda)}{\lambda - z} d\lambda.$$

Now given the bound, we may deform the contour to real axis. By comparing this identity and our goal, we are left to prove that

$$\frac{1}{2\pi i}\int_\gamma \frac{\overline{\varphi(\lambda)}}{\lambda - z} d\lambda = \frac{1}{2\pi i}\overline{\int_\gamma \frac{\varphi(\lambda)}{\lambda - \overline{z}} d\lambda} = 0.$$

But this is clear as $\varphi/(\cdot - \overline{z})$ is analytic in the upper half-plane. $\square$

There's of course nothing really special about the decay assumption $\varphi(z) = O(|z|^{-\varepsilon})$; it's there just to make everything converge.

One can guarantee the convergence also by other means. Note that as the integrand behaves like $(\lambda - z)^{-1}$, if we subtract from it something (not depending on z) behaving the same way at the infinity, we ought to improve convergence, but only change the value of the function by a constant. As an example, consider the integral

$$\frac{1}{\pi}\int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{[|\lambda| > 1]}{\lambda}\right) \Im(\varphi)(\lambda) d\lambda. \tag{6.7}$$

It converges to an analytic function as long as, say, $\Im(\varphi)$ is bounded. As before, its imaginary part coincides with φ's so the functions are equal up to a real constant. Now, however, there's no reason for the real constants to match and indeed they need not.

Note that the previous idea could be used to construct Pick functions. Everything still makes sense if we replace $\Im(\varphi)$ by some other positive function, as long as the integral converges. Heck, we could replace it by any positive measure for which $\mu((\lambda^2+1)^{-1}) < \infty$.

(Almost) all the examples given before are actually just special cases of this construction. The rational functions $\frac{1}{\lambda - z}$, where $\lambda \in \mathbb{R}$ are obtained by setting $\mu = \delta_\lambda$. The power functions are obtained as

$$\begin{aligned} z^p &= 1 + \frac{1}{\pi}\int_{-\infty}^{0} \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - 1}\right) \Im(\lambda^p) d\lambda \\ &= 1 + \frac{1}{\pi}\int_{-\infty}^{0} \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - 1}\right) |\lambda|^p \sin(\pi p) d\lambda, \end{aligned}$$

Logarithm is even simpler:

$$\log(z) = \int_{-\infty}^{0} \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - 1}\right) d\lambda.$$

Tangent function could be obtained by putting δ-measures to its poles, the points of the form $\frac{\pi}{2} + n\pi$, where $n \in \mathbb{Z}$.

The only exception is the function $z \mapsto \alpha z$ – it can't be expressed as such integral. But even this failure is really more about poor point of view, as we will see in a minute. With these observations in mind it ought to be not too surprising that we have the following.

Theorem 6.8. *$\varphi \in \mathcal{P}$, if and only*

$$\varphi(z) = \alpha z + \beta + \int_{-\infty}^{\infty} \left(\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right) d\mu(\lambda) \tag{6.9}$$

for some $\alpha \geq 0$ and $\beta \in \mathbb{R}$ and a Radon measure μ with $\int_{-\infty}^{\infty} (\lambda^2 + 1)^{-1} d\mu(\lambda) < \infty$.

Choosing $\lambda \mapsto \frac{\lambda}{\lambda^2+1}$ is common choice in the literature and is convenient as

- It's real, so the integrand is Pick function for any $\lambda \in \mathbb{R}$.
- We may recover the constant β as $\Re(\varphi(i))$.

To better explain the appearance of the linear term, we can write the integral in a sligtly different form. Denoting $d\nu(\lambda) = \frac{d\mu(\lambda)}{\lambda^2+1}$, the formula reads

$$\varphi(z) = \alpha z + \beta + \int_{-\infty}^{\infty} \frac{\lambda z + 1}{\lambda - z} d\nu(\lambda).$$

Here ν is just a finite Borel measure. Now it kind of makes sense to extend the domain of this measure to infinity: the linear term merely corresponds to δ-measure at infinity point. Of course, should one formalize this line of thought, the question on the type of extended real line had to be asked and one should address the topology. The answer is that one should glue the real line into a circle. One shouldn't worry about such issues, though, as these thoughts are here merely for intuition. The giveaway is that α should be really thought as a part of the measure μ, even though this might not make perfect sense.

We will not prove theorem 6.8, but it shall work as a motivation. Instead, we prove somewhat weaker claim.

Lemma 6.10. *Under the topology of pointwise convergence one has*

$$\mathcal{P} \subset \overline{\text{cone}}\{(\lambda - z)^{-1} | \lambda \in \mathbb{R}\}.$$

Proof. Denote the closure of the cone by $\mathcal{P}_e$. As $\lim_{\lambda \to \pm\infty} |\lambda|(\lambda - z)^{-1} = \pm 1$, $\mathbb{R} \in \mathcal{P}_e$ Now by 6.7 all the bounded Pick functions extending analytically over $\mathbb{R}$ are also in $\mathcal{P}_e$. We finish the proof by showing that such functions are dense in the set of all Pick functions: we denote this class by $\mathcal{P}_b$.

It is straightforward to check that

$$g_\varepsilon(z) = \frac{z + i\varepsilon}{1 - i\varepsilon z} \in \mathcal{P}_b$$

for any $\varepsilon > 0$. But now for any $\varphi \in \mathcal{P}$ and $\varepsilon > 0$ also $\varphi \circ g_\varepsilon \in \mathcal{P}_b$. Finally $\varphi = \lim_{\varepsilon \to 0} \varphi \circ g_\varepsilon \in \mathcal{P}_b$, as we wanted. $\square$

6.3 Dual thinking

6.3.1 Pick functionals

Theorem 6.8 sheds light to Question 6.3: linear functionals on $\mathcal{P}$ should be thought of some kind of rational functions.

Definition 6.11. Let $X \subset \mathbb{H}_+$. We will denote by $R(X)$ the $\mathbb{C}$-vector space of rational functions r such that

- All poles of r are simple and lie in $X \cup X^* = X \cup \{z \in \mathbb{C} | \, \overline{z} \in X\}$.
- $r(\lambda) = O(|\lambda|^{-2})$ at infinity.

We will also write $R_+(X)$ for the functions in $R(X)$, which are non-negative on $\mathbb{R}$.

It is useful to note that

$$\begin{aligned} \operatorname{span}_{\mathbb{R}}(R_+(X)) &= \{r \in R(X) | r(\mathbb{R}) \subset \mathbb{R}\} =: R_\pm(X) \\ &\text{and} \\ \operatorname{span}_{\mathbb{C}}(R_+(X)) &= R(X). \end{aligned} \tag{6.12}$$

Similarly to the previous chapter we have the dual pairing $\langle f, r \rangle_L$ between $\mathbb{C}^X$ and $R(X)$. Indeed, we may set

$$\langle f, (z-a)^{-1} \rangle_L = \begin{cases} f(a) & \text{if } a \in X \\ \overline{f(\overline{a})} & \text{if } a \in X^* \end{cases}$$

and extend linearly.

Theorem 6.13. *$R_+(\mathbb{H}_+)$ is the dual cone of $\mathcal{P}$ in the sense of $\langle \cdot, \cdot \rangle_L$. In other words: all continuous linear functionals $p^* \in \mathbb{C}^{\mathbb{H}_+}$ such that $p^*(\varphi) \geq 0$ for any $\varphi \in \mathcal{P}$ are of the form $p^*(\varphi) = \langle \varphi, r \rangle_L$ for some $r \in R_+(\mathbb{H}_+)$.*

Proof. $\mathcal{P}^* \subset R_+(\mathbb{H}_+)$: It is well known that continuous dual of a product is direct sum of duals (see for instance TODO). In other words, the elements of $\mathcal{P}$ are finitely supported (i.e. finite linear combinations of evaluation functionals)[1]. We may hence interpret $p^* \in \mathcal{P}^*$ as an rational function, r, with poles on $\mathbb{H}_+ \cup \mathbb{H}_-$ and $r(\infty) = 0$, acting as $\varphi \to$

[1]This fact is not important to us and we could have restricted our attention to finitely supported functionals anyway.

$\langle \varphi, r\rangle_L$. It is easy to see that $r \in R_+(\mathbb{H}_+)$ if we can verify that r is non-negative. But as $(\lambda - z)^{-1} \in \mathcal{P}$ for any $\lambda \in \mathbb{R}$, we have

$$p^*((\lambda - z)^{-1}) = \langle (\lambda - z)^{-1}, r\rangle_L = r(\lambda) \geq 0$$

for any $\lambda \in \mathbb{R}$, as desired.

$R_+(\mathbb{H}_+) \subset \mathcal{P}^*$: As by the previous part $\langle (\lambda - z)^{-1}, r\rangle_L$ for any $\lambda \in \mathbb{R}$ and $r \in R_+(\mathbb{H}_+)$, we are done by Lemma 6.10. □

The rational functions $R_+(X)$ (identified with the respective linear maps $f \mapsto \langle f, r\rangle_L$) are called **Pick functionals** (on $X \subset \mathbb{H}_+$).

One can also interpret the Pick functionals also with divided differences. Indeed, if $r \in R_+(X)$, it is easy to see that

$$r(z) = \frac{N(q)}{|z - z_1|^2 \cdots |z - z_n|^2}$$

for some $n \geq 1$, $q \in \mathbb{C}_{n-1}[x]$ and pairwise distinct $z_1, z_2, \ldots, z_n \in X$. But this means that the respective Pick functional is given by

$$\varphi \mapsto [z_1, \overline{z_1}, \ldots, z_n, \overline{z_n}]_{\varphi N(q)}.$$

6.3.2 Weakly Pick functions

While Theorem 6.13 implies that $R_+(\mathbb{H}_+)$ is the dual cone of $\mathcal{P}$, it turns out that it is also the predual we were looking for.[2]

Definition 6.14. We will denote

$$\mathcal{P}(X) := (R_+(X))^*$$

and call elements of $\mathcal{P}(X)$ **weakly Pick functions** (on X).

First off: why should the elements of $\mathcal{P}(X)$ be called weakly Pick functions? Note that every $p^* \in R(X)^*$ can be represented as a function $\varphi_{p^*} : X \cup X^* \to \mathbb{C}$ by setting

$$\varphi_{p^*}(z) = p^*((\lambda - z)^{-1}).$$

[2]While preduals are not unique in general, as $R_+(\mathbb{H}_+)$ is the dual cone of $\mathcal{P}$, if $R_+(\mathbb{H}_+)$ is a predual of $\mathcal{P}$, it is unique maximal predual.

Strictly speaking $(\lambda - z)^{-1} \notin R(X)$, so the above equality should be interpreted suitably and function φ_{p^*} will be only defined up to a constant. Apart from that the correspondence is bijective and the resulting map

$$R(X)^* \to \mathbb{C}^{X \cup X^*}/\mathbb{C}$$

is isomorphism, as one easily checks. If one restricts the domain to $R_+(X)^*$, additional reflectional symmetry is obtained

Lemma 6.15. *There exists a unique injection*

$$\mathcal{P}(X) \to \mathbb{C}^X/\mathbb{R}$$
$$p^* \mapsto \varphi_{p^*}$$

satisfying

$$\varphi_{p^*}(z) - \overline{\varphi_{p^*}(w)} = p^*\left(\frac{1}{(\lambda - z)} - \frac{1}{(\lambda - \overline{w})}\right) \tag{6.16}$$

for any $z, w \in X$ and $p^* \in (R_+(X))^*$.

Proof. Fix $z_0 \in X$. Condition 6.16 implies that such map φ_{p^*} should also satisfy

$$\begin{gathered}\Im(\varphi_{p^*}(z)) = p^*\left(\frac{\Im(z)}{|\lambda - z|^2}\right)\\ \text{and}\\ \Re(\varphi_{p^*}(z)) - \Re(\varphi_{p^*}(z_0)) = p^*\left(\frac{\lambda}{|\lambda - z|^2} - \frac{\lambda}{|\lambda - z_0|^2}\right)\end{gathered} \tag{6.17}$$

for any $z \in X$. By 6.12 these equalities determine a unique function in $\mathbb{C}^X/\mathbb{R}$, and it's straighforward to check that such function also satisfies 6.16.

For injectivity, note that if $p^* \in R(X)^*$ such that φ_{p^*} is real constant, then p^* kills functions of the form $(\lambda - z)^{-1} - (\lambda - \overline{w})^{-1}$. Since such functions span $R(X)$, $p^* = 0$. □

Now the statement "$R_+(\mathbb{H}_+)$ is the predual of $\mathcal{P}$" makes sense.

Theorem 6.18. *The natural map $\mathcal{P}/\mathbb{R} \to \mathcal{P}(\mathbb{H}_+)$ is bijection.*

Why is this useful? The message is that Pick functions are completely determined by Pick functionals. If function on $\mathbb{C}$ looks like a Pick function, in the sense that it gives non-negative values on every Pick functional, then it is a Pick function. As set of such functions is certainly closed, so is $\mathcal{P}$. In particular:

Proof of theorem 6.2. t.f.i.f 6.18. □

Theorem 6.18 is kind of a result that would definitely benefit from quotient point of view: Pick functions should be defined up to a constant in the first place. One shouldn't worry too much, however: whether one thinks that weakly Pick functions (elements of $R_+(X)$) are really functions (elements of $\mathbb{C}^X$) or functions up to a constant (elements of $\mathbb{C}^X/\mathbb{R}$) doesn't make much difference.

Proof of Theorem 6.18. Well-definedness: this follows immediately from 6.13.

Injectivity: Take any $\varphi \in \mathbb{C}^X/\mathbb{R}$ such that $\langle \varphi, r \rangle_L = 0$ for any $r \in R_+(X)$. As $R(X) = \overline{\operatorname{span}_{\mathbb{C}}(R_+(X))}$, for any $z, w \in \mathbb{H}_+$ we have $0 = \langle \varphi, (\lambda - z)^{-1} - (\lambda - \overline{w})^{-1} \rangle_L = \varphi(z) - \overline{\varphi(w)}$, which immediately implies that φ is constant.

Surjectivity: This is the tricky part. We should prove that for any $p^* \in \mathcal{P}(\mathbb{H}_+)$ the map φ_{p^*} is a Pick function. Note that (6.17) implies that φ_{p^*} maps upper half-plane to its closure. So "only" analyticity remains to be checked.

Let us first prove something slightly easier: φ_{p^*} is continuous. This amounts to showing that for any $w \in \mathbb{H}_+$

$$\lim_{z \to w} p^* \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - w} \right) = \lim_{z \to w} \left(\varphi_{p^*}(z) - \varphi_{p^*}(w) \right) = 0.$$

The function $r_{z,w}(\lambda) = (\lambda - z)^{-1} - (\lambda - w)^{-1}$ tends to zero (in some sense) as $z \to w$, so something like this should be true: $R(\mathbb{H}_+)$ should have topology for which this convergence happens and the map $r \to p^* r$ is continuous.

And indeed, there is one:

$$\|r\|_R = \sup_{x \in \mathbb{R}} |r(x)|(x^2 + 1).$$

Lemma 6.19. *For every $p^* \in \mathcal{P}(\mathbb{H}_+)$ there exists constant $C(p^*)$ such that*

$$|p^*(r)| \leq C(p^*) \|r\|_R$$

for any $r \in R(\mathbb{H}_+)$

Proof. Write $r = r_1 + i r_2$ where $r_1, r_2 \in R_\pm(\mathbb{H}_+)$. Since clearly

$$\max(\|r_1\|_R, \|r_2\|_R) \leq \|r\| \leq \|r_1\|_R + \|r_2\|_R$$

it suffices cook up such bound for $R_\pm(\mathbb{H}_+)$. But such functions satisfy

$$-\frac{\|r\|_R}{\lambda^2 + 1} \leq r(\lambda) \leq \frac{\|r\|_R}{\lambda^2 + 1}$$

so $|p^*(r)| \leq \Im(\varphi_{p^*}(i)) \|r\|_R$. □

Now in order to prove the continuity is suffices to check that $\lim_{w\to z}\|r_{z,w}\|_R = 0$. But this follows from

$$\begin{aligned}\|r_{z,w}\|_R =&|z-w|\sup_{\lambda\in\mathbb{R}}\left|\frac{\lambda^2+1}{(\lambda-z)(\lambda-w)}\right|\\ =&|z-w|\sup_{\lambda\in\mathbb{R}}\left|\left(1+\frac{z-i}{\lambda-z}\right)\left(1+\frac{w+i}{\lambda-w}\right)\right|\\ \leq&|z-w|\left(1+\frac{|z-i|}{\Im(z)}\right)\left(1+\frac{|w+i|}{\Im(w)}\right).\end{aligned}$$

Proving analyticity is not much harder. Note that if we manage to show that the order 2 divided differences of φ_{p^*} are locally bounded, Theorem 4.46 implies the claim. Strictly speaking we only proved 4.46 on real line, but the proof would be almost identical in the complex case. Observe that for any $z_0, z_1, z_2 \in \mathbb{H}_+$ we have

$$[z_0, z_1, z_2]_{\varphi_{p^*}} = p^*\left(\frac{1}{(\lambda-z_0)(\lambda-z_1)(\lambda-z_2)}\right).$$

Hence, by 6.19 we can bound the divided difference just by estimating $\|(\lambda-z_0)^{-1}(\lambda-z_1)^{-1}(\lambda-z_2)^{-1}\|_R$. But this is straighforward: one has, for instance,

$$\left\|\frac{1}{(\lambda-z_0)(\lambda-z_1)(\lambda-z_2)}\right\|_R \leq \frac{1}{\Im(z_0)}\left(1+\frac{|z-i|}{\Im(z)}\right)\left(1+\frac{|w+i|}{\Im(w)}\right).$$

□

It can be easily checked that the estimates in the proof can be generalized and pushed to local setting. We for instance have:

Lemma 6.20. *Let $X \subset \mathbb{H}_+$ and $p^* \in \mathcal{P}(X)$. Then there exists a constant $C(p^*)$ such that*

$$|p^*(r)| \leq C(p^*)\|r\|_R$$

for any $r \in R_+(X)$.

Proposition 6.21. *Let $X \subset \mathbb{H}_+$ and $p^* \in \mathcal{P}(X)$. Then for every compact $K \subset \mathbb{H}_+$ there exists a constant $C(K, p^*)$ such that*

$$\left|[z_0, z_1, \ldots, z_k]_{\varphi_{p^*}}\right| \leq \frac{C(K, p^*)}{\Im(z_0)\Im(z_1)\cdots\Im(z_k)}$$

for any $k \geq 1$ and $z_0, z_1, \ldots, z_k \in X \cap K$. In particular φ_{p^*} is continuous and analytic at every interior point of X.

6.4 Pick-Nevanlinna interpolation theorem

There's an interesting generalization to Theorem 6.18.

Theorem 6.22 (Pick-Nevanlinna interpolation theorem)**.** *Let $X \subset \mathbb{H}_+$. Then the restriction map $\mathcal{P}(\mathbb{H}_+) = \mathcal{P}/\mathbb{R} \to \mathcal{P}(X)$ is surjection. In other words: for any $\varphi \in \mathcal{P}(X)$ there exists a Pick function $\tilde{\varphi}$ such that $\tilde{\varphi}\big|_X = \varphi$.*

Proof. So we have an element in $p^* \in (R(X))^*$ such that $p^*(r) \geq 0$ for any $r \in R_+(X)$ and should prove that there exists $\tilde{p^*} \in R(\mathbb{H}_+)^*$ such that $\tilde{p^*}\big|_{R(X)} = p^*$ and $\tilde{p^*}(r) \geq 0$ for any $r \in R_+(\mathbb{H}_+)$: we should extend a linear functional preverving its positivity.

Such extension is not unique in general. Nevertheless, if it so happens that $R(X)$ is dense in $R(\mathbb{H}_+)$ with respect to $\|\cdot\|_L$, then, as p^* is Lipschitz by 6.20, $\tilde{p^*}$ is unique. In this case $R_+(X)$ is dense in $R_+(\mathbb{H}_+)$ so the extension is really a Pick function. This already covers large variety of sets X.

Lemma 6.23. *If $X \subset \mathbb{H}_+$ has an accumulation point in $\mathbb{H}_+$, then $R(X)$ is dense in $R(\mathbb{H}_+)$.*

Proof. Take a sequence of distinct points $z_0, z_1, \ldots$ in X converging to $z_\infty \in \mathbb{H}_+$. We may assume w.l.o.g. that $z_\infty = i$. By Newton expansion, for any $w \in \mathbb{H}_+$

$$\frac{1}{\lambda - w} - \sum_{i=0}^{n} \frac{(w - z_0)\cdots(w - z_{i-1})}{(\lambda - z_0)\cdots(\lambda - z_{i-1})(\lambda - z_i)} = \frac{(w - z_0)\cdots(w - z_n)}{(\lambda - w)(\lambda - z_0)\cdots(\lambda - z_n)}.$$

If $|w - i| < 1$, norm of the error term tends to zero. It follows that $R(X)$ is dense in $R(X \cup \mathbb{D}(i, 1))$. But as $2i$ is an accumulation point of $X \cup \mathbb{D}(i, 1)$, we may repeat the previous argument: $R(X)$ is dense in $R(X \cup \mathbb{D}(2i, 2))$. Bootstrapping along the sequence $(2^n i)_{n=1}^{\infty}$ yields the claim. □

For the general case one has to work slighty harder. Observe first that one only needs to prove the following lemma.

Lemma 6.24. *For any $X \in \mathbb{H}_+$ and $w \in \mathbb{H}_+ \setminus X$ the restriction map $\mathcal{P}(X \cup \{w\}) \to \mathcal{P}(X)$ is surjective.*

Given this lemma one can, for instance, use transfinite induction (or Zorn's lemma if one so prefers) to extend any element of $\mathcal{P}(X)$ to $\mathcal{P}(\mathbb{H}_+)$. Or one may inductively extend X by a countable set with an accumulation point, after which there exists a unique extension by the already proven dense case.

Proof of Lemma 6.24. Fix $z_0 \in X$. Note that any $r \in R_+(X \cup \{w\})$ is of the form

$$\Re\left(a\left(\frac{1}{\lambda - w} - \frac{1}{\lambda - z_0}\right)\right) + s,$$

where $a \in \mathbb{C}$ and $s \in R(X)$. Writing $r_w(\lambda) = (\lambda - w)^{-1} - (\lambda - z_0)^{-1}$, the extension should satisfy

$$\Re\left(ap^*(r_w)\right) + p^*(s) \geq 0 \tag{6.25}$$

for some family of $\mathcal{F}$ pairs $(a, s) \in \mathbb{C} \times R(X)$. Note that if we find a value $p^*(r_w)$ which satisfies all such inequalities, it determines an extension for p^* to $\mathcal{P}(X \cup \{w\})$.

Each of the inequalities of the form 6.25 (where $a \neq 0$) force $p^*(r_w)$ in some closed half-space of $\mathbb{C}$. It is easy to check that for any $a \in \mathbb{C}$ there exist $(a, s) \in \mathcal{F}$: $p^*(r_w)$ is constrained by half-spaces of all directions. This implies that set of suitable $p^*(r_w)$'s can be expressed as intersection of compact sets, certain finite intersections of half-spaces in $\mathcal{F}$. We hence just have to verify that all such finite intersections are non-empty.

This, finally, follows almost immediately from the Farkas' lemma.

Lemma 6.26 (Farkas' lemma)**.** *Let $m \geq 1$, $a_1, a_2, \ldots, a_m \in \mathbb{R}^n$ and $c_1, c_2, \ldots, c_m \in \mathbb{R}$. Assume that whenever $t_1, t_2, \ldots, t_m \geq 0$ are such that*

$$t_1 a_1 + t_2 a_2 + \ldots + t_m a_m = 0,$$

then also

$$t_1 c_1 + t_2 c_2 + \ldots + t_m c_m \geq 0.$$

Then there exists $b \in \mathbb{R}^n$ such that $a_i \cdot b + c_i \geq 0$ for any $1 \leq i \leq m$.

Indeed: the inequalities in 6.25 can be interpreted in $\mathbb{R}^2$, in the sense of Farkas' lemma. Let's then check the condition. Pick any finite set of pairs $(a_1, s_1), (a_2, s_2), \ldots, (a_m, s_m) \in \mathcal{F}$. Take also $t_1, t_2, \ldots, t_m \geq 0$ with $\sum_{i=1}^m t_i a_i = 0$. Now

$$0 \leq \sum_{i=1}^m t_i \left(\Re(a_i r_w) + s_i\right) = \Re\left(\sum_{i=1}^m t_i a_i r_w\right) + \sum_{i=1}^m t_i s_i = \sum_{i=1}^m t_i s_i$$

and hence $\sum_{i=1}^m t_i p^*(s_i) \geq 0$. By Farkas' lemma we can find $p^*(r_w) \in \mathbb{C}$ such that

$$\Re(a_i p^*(r_w)) + p^*(s_i) \geq 0$$

for any $1 \leq i \leq m$. This is just what we wanted. $\square$

$\square$

For completeness, we also prove Farkas' lemma.

Proof of Lemma 6.26. Proof is by induction on n.

The case $n = 1$: We may clearly ignore all the zeros from the a_i's. If all a_i's are positive or negative, claim is trivial. Assume then that there are both positive and negative a_i's. We may scale a_i's (with c_i's) such that they are all 1 or -1: w.l.o.g. first k a_i's are ones. We should prove that one may choose b such that $b + c_i \geq 0$ for any $1 \leq i \leq k$ and $-b + c_j \geq 0$ for any $k + 1 \leq j \leq m$. This is clearly possible if $c_i + c_j \geq 0$ for any $1 \leq i \leq k < j \leq m$. But if one sets $t_i = 1$ and $t_j = 1$ and other t_l's to zero in the main condition, this is exactly the inequality one gets.

Induction step: We split into two cases.

- Case 1: There exists $t_1, t_2, \ldots, t_m \geq 0$, not all zero, such that $\sum_{i=1}^m t_i a_i = 0$.
- Case 2: The complement of case 1.

Let us also denote

$$C = \operatorname{cone}\{a_i | 1 \leq i \leq m\}.$$

Case 1: it follows that there exist nonzero $v \in \mathbb{R}^n$ such that $v, -v \in C$. Decompose $\mathbb{R}^n = \operatorname{span}(v) \oplus W$, $a_i = a_i^{(v)} + a_i^W$ and $b = b^{(v)} + b^W$. The idea is to interpret the problem of finding b as parametrized problem of finding b^W. We should find $b^{(v)}$ such that the following condition holds: whenever $t_1, t_2, \ldots, t_m$ are such that

$$\sum_{i=1}^m t_i a_i^W = 0$$

then

$$0 \leq \sum_{i=1}^m t_i (c_i + a_i^{(v)} b^{(v)}) = \sum_{i=1}^m t_i c_i + b^{(v)} \sum_{i=1}^m t_i a_i^{(v)}.$$

Then by $n - 1$ dimensional case there exists b^W such that

$$0 \leq c_i + a_i^{(v)} b^{(v)} + a_i^W \cdot b^W = a_i \cdot b + c_i.$$

This can be interpreted as one-dimensional problem where a_i's are sums $\sum_{i=1}^m t_i a_i^{(v)}$ and c_i's sums $\sum_{i=1}^m t_i c_i$ where t_i's range over all tuples of non-negative numbers with $\sum_{i=1}^m t_i a_i^W = 0$. But now there are infinitely many conditions so we can't immediately use the case $n = 1$. However, by the extra assumption $v, -v \in C$, so one can find t_i's such that $\sum_{i=1}^m t_i a_i^W = 0$ and $\sum_{i=1}^m t_i a_i^{(v)}$ is both positive and negative. This means that it suffices to check that the condition holds for all pairs of such tuples. So take $s_1, s_2 \geq 0$ and numbers $t_{i,1}, t_{i,2} \geq 0$ for $1 \leq i \leq m$ such that $\sum_{i=1}^m t_{i,1} a_i^W = \sum_{i=1}^m t_{i,2} a_i^W = 0$ and

$$s_1 \sum_{i=1}^m t_{i,1} a_i^{(v)} + s_2 \sum_{i=1}^m t_{i,2} a_i^{(v)} = 0.$$

Then $\sum_{i=1}^m (s_1 t_{i,1} + s_2 t_{i,2}) a_i = 0$ so by the main condition

$$0 \leq \sum_{i=1}^m (s_1 t_{i,1} + s_2 t_{i,2}) c_i = s_1 \sum_{i=1}^m t_{i,1} c_i + s_2 \sum_{i=1}^m t_{i,2} c_i,$$

as desired.

Case 2: We first claim that there exists $v \in \mathbb{R}^n$ such that $v, -v \notin C$. Assuming otherwise, take $1 \leq j < l \leq m$ (the case $m = 1$ is clear as $n > 1$). Now as $a_j - a_l \in C$ or $a_j - a_l \in C$, w.l.o.g. $a_j = a_l + \sum_{i=1}^m t_i a_i$ for some $t_1, \ldots, t_m \geq 0$. If $t_j \geq 1$, we have found non-trivial decomposition for 0, a contradiction. If on the other hand $t_j < 1$, we see that $a_j \in \operatorname{cone}\{a_i | i \neq j\}$, so we may forget a_j. Inducting on m finishes the claim.

Again, decompose $\mathbb{R}^n = \operatorname{span}(v) \oplus W$, $a_i = a_i^{(v)} + a_i^W$ and $b = b^{(v)} + b^W$. We prove that we may set $b^{(v)} = 0$ and also the reduced problem falls in the case 2. Indeed, if $t_1, t_2, \ldots, t_m \geq 0$ are such that $\sum_{i=1}^m t_i a_i^W = 0$ then $\sum_{i=1}^m t_i a_i^{(v)} \in C \cap \operatorname{span}(v) \subset \{0\}$. Consequently $\sum_{i=1}^m t_i a_i = 0$ and hence $t_i = 0$ for any $1 \leq i \leq m$. $\square$

Remark 6.27. Pick Nevanlinna interpolation can be extended in many ways. One such extension concerns Taylor sections.

Definition 6.28. Let $d : \mathbb{H}_+ \to \mathbb{N} \cup \{\infty\}$. Extend d to $\mathbb{C}$ with $d(z) = d(\overline{z})$ for any $z \in \mathbb{H}_+$ and $d(\lambda) = 0$ for any $\lambda \in \mathbb{R}$. We denote by $R(d)$ the set of rational functions r with the properties

- Pole of r at $z \in \mathbb{C}$ (if any) has order at most $d(z)$.
- $r(\lambda) = O(|\lambda|^{-2})$ at infinity.

Note that $R(X) = R(\chi_X)$.

Theorem 6.29. *Let $d : \mathbb{H}_+ \to \mathbb{N} \cup \{\infty\}$. Then the natural map $\mathcal{P}/\mathbb{R} \to \mathcal{P}(d) =: (R(d))^*$ is surjection.*

What does this result has to do with Taylor sections? Fix any $d : \mathbb{H}_+ \to \mathbb{N} \cup \{\infty\}$. Now Theorem 6.29 is just saying that for any $p^* \in \mathcal{P}(d)$, there exists a Pick function φ_{p^*} for which

$$\frac{\varphi_{p^*}^{(m)}(z)}{m!} = p^* \left(\frac{1}{(\lambda - z)^{m+1}} \right)$$

for any $z \in \mathbb{H}_+$ and $1 \leq m \leq d(z) - 1$.

Theorem 6.29 could be proved with pretty much same ideas as Theorem 6.22; we're not going to do that, however. $\triangle$

6.5 Notes and references

Pick functions and representation theorem 6.8 are discussed in numerous sources; see for example (?). Pick-Nevanlinna interpolation theorem 6.22 was first observed and proved independently by Pick [13] and Nevanlinna [12]. Since then, many different approaches exist, see (?) for a survey. Approach taken in this text is similar to (?).

Chapter 7

Matrix monotone functions – part 3

7.1 Loewner's theorem

Aim of this chapter is to prove Theorem 5.14. Before we start with the proof, we reinterpret Theorem 5.14 in terms of duals.

Definition 7.1. We will denote

$$\mathcal{P}(a,b) := (R_+(a,b))^*$$

and call elements of $\mathcal{P}(a,b)$ **weakly Pick functions** (on (a,b)).

Let us first come back to Theorem 5.10. With the dual language it rewrites to (modulo analyticity) to

Theorem 7.2. *The natural map $P_\infty(a,b)/\mathbb{R} \to \mathcal{P}(a,b)$ is bijection.*

Proof. We already observed in the end of the chapter 5 that every function $f \in P_\infty(a,b)$ defines an element in $\mathcal{P}(a,b)$. Using the arguments of the proof of theorem 6.15 it's easy to check that any element in $\mathcal{P}(a,b)$ is induced by an function $\mathbb{R}^{(a,b)}$ up to a constant, and such function is in $P_\infty(a,b)$ by Theorem 5.10. $\square$

Let us denote

$$\tilde{\mathcal{P}}(a,b) := \varphi \text{ extends analytically to } (\mathbb{H}_+ \cup \mathbb{H}_-) \cup (a,b) \text{ such that } \varphi[(a,b)] \subset \mathbb{R}.\}.$$

We prove Theorem 5.14 in the following form.

Theorem 7.3. *The restriction $\tilde{\mathcal{P}}(a,b) \to P_\infty(a,b)$ is bijection.*

Proof. Well-definedness: Pick any $\varphi \in \tilde{\mathcal{P}}(a,b)$. Note that for any $q \in \mathbb{C}_{n-1}[x]$ and $t \in (a,b)$ one has

$$\frac{(\varphi N(q))^{(2n-1)}(t)}{(2n-1)!} = \lim_{\substack{z_1,\ldots,z_n \in \mathbb{H}_+ \\ z_1,\ldots,z_n \to t}} [z_1, \overline{z_1}, \ldots, z_n, \overline{z_n}]_{\varphi N(q)} \geq 0.$$

By Theorem 5.1 $\varphi\big|_{(a,b)} \in P_\infty(a,b)$.

Injectivity: This follows immediately from the basic properties of analytic functions.

Surjectivity: The main idea is to interpret the claim via duals. Recall that by Theorem 7.2 any $f \in P_\infty(a,b)$ corresponds to some $p^* \in \mathcal{P}(a,b)$. The class $R(a,b) := \operatorname{span}_{\mathbb{C}}(R_+(a,b))$ can be given norm $\|r\|_{(a,b)} = \sup_{\lambda \in \mathbb{R}\setminus(a,b)} |r(\lambda)|(\lambda^2+1)$.

Lemma 7.4. *For every $p^* \in \mathcal{P}(a,b)$ there exists constant $C(p^*)$ such that*

$$|p^*(r)| \leq C(p^*)\|r\|_{(a,b)}$$

for any $r \in R(a,b)$.

Proof. Not much changes from the proof of Lemma 6.19. We can again assume that $r \in R_\pm(a,b) := \operatorname{span}_{\mathbb{R}}(R_+(a,b))$. Fix $a < c < d < b$. It's easy to see that there exists a constant $C_{c,d}$ such that

$$-\frac{C_{c,d}\|r\|_{(a,b)}}{(\lambda-c)(\lambda-d)} \leq r(\lambda) \leq \frac{C_{c,d}\|r\|_{(a,b)}}{(\lambda-c)(\lambda-d)}$$

holds for $\lambda \in \mathbb{R} \setminus (c', d')$ for some $a < c' < c < d < d' < b$. But now just by the definition of $\mathcal{P}(a,b)$ we have $|p^*(r)| \leq C_{c,d}\|r\|_{(a,b)}[c,d]_{\varphi_{p^*}}$. □

Lemma 7.5. *$\mathcal{P}(a,b)$ is dense in $\mathcal{P}((a,b)\cup\mathbb{H}_+)$ with norm $\|\cdot\|_{(a,b)}$.*

Proof. Again, not much changes from the proof of Lemma 6.23. We take sequence $x_0, x_1, \ldots$ converging to $x_\infty \in (a,b)$. Note that

$$\left\|\frac{(w-x_0)\cdots(w-x_n)}{(\lambda-w)(\lambda-x_0)\cdots(\lambda-x_n)}\right\|_{(a,b)}$$

tends to zero as $n \to \infty$ whenever $|w - x_\infty| < \min(x_\infty - a, b - x_\infty)$. But this means that $\mathcal{P}(a,b)$ is dense in $\mathcal{P}((a,b)\cup\mathbb{D}(x_\infty, \min(x_\infty - a, b - x_\infty)))$, which is dense in $\mathcal{P}((a,b)\cup\mathbb{H}_+)$ by Lemma 6.23 (and the fact that $\|\cdot\|_{(a,b)} \leq \|\cdot\|_R$). □

By Lemmas 7.4 and 7.5 we may extend $p^* \in \mathcal{P}(a,b)$ to $R((a,b)\cup\mathbb{H}_+)^*$. It is easy to see that the extension satisfies the estimate of Lemma 7.4 and $p^*(r) \geq 0$ for any $r \in R_+((a,b)\cup\mathbb{H}_+)$. The extension lies hence in $\mathcal{P}((a,b)\cup\mathbb{H}_+)$ and so defines an extension φ_{p^*} for f on $\mathbb{H}_+\cup\mathbb{H}_-\cup(a,b)$. That such function lies in $\tilde{\mathcal{P}}(a,b)$ follows immediately from the following estimate, which can be easily shown.

Lemma 7.6. *For every compact $K \subset \mathbb{H}_+\cup\mathbb{H}_-\cup(a,b)$ and $p^* \in \mathcal{P}((a,b)\cup\mathbb{H}_+)$ there exists a constant $C(K,p^*)$ such that*

$$\left|[z_0, z_1, \ldots, z_k]_{\varphi_{p^*}}\right| \leq \frac{C(K,p^*)}{\operatorname{dist}(z_0,\mathbb{R}\setminus(a,b))\operatorname{dist}(z_1,\mathbb{R}\setminus(a,b))\cdots\operatorname{dist}(z_n,\mathbb{R}\setminus(a,b))}$$

for any $k \geq 1$ and $z_0, z_1, \ldots, z_k \in K$. In particular φ_{p^*} is analytic.

□

Note that by the Schwarz reflection principle the class $\tilde{\mathcal{P}}(a,b)$ coincides with the set of Pick functions that continuously extend to (a,b) in such a way that the extension is real on (a,b).

7.2 Notes and references

Proofs of this chapter are new but heavily inspired by the respective arguments on Pick functions.

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