Matrix monotone and convex functions

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Contents

Chapter 1

Introduction

1.1 Foreword

This master's thesis is about matrix monotone and convex functions. Matrix monotonicity and convexity are generalizations of standard monotonicity and convexity of real functions: now we are just having functions mapping matrices to matrices. Formally, f is *matrix monotone* if for any two matrices A and B such that

$$A \leq B \tag{1.1}$$

we should also have

$$f(A) \leq f(B). \tag{1.2}$$

This kind of function might be more properly called *matrix increasing* but we will mostly stick to the 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 choice of words.
- Somehow I can't satisfactorily fill the following table:

monotonic	monotonicity
increasing	?

How very inconvenient.

Matrix convexity, as you might have guessed by now, is defined as follows. A function f is *matrix convex* if for any two matrices A and B and $0 \leq t \leq 1$ we have

$$f(tA + (1-t)B) \leq tf(A) + (1-t)f(B). \tag{1.3}$$

Of course, it's not really obvious how one should make any sense of these "definitions". One quickly realizes that there two things to understand.

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

Both of these questions can be (of course) answered in many ways, but for both of them, there's in a way very natural answer. In both cases we can get something more general: instead of comparing matrices we can compare linear maps, and we can apply function to linear mapping.

Just to give a short glimpse of how these things might be defined, we should first fix our ground field (for matrices): let's say it's $\mathbb{R}$, at least for now.

For matrix ordering we should first understand which matrices are *positive*, which here, a bit confusingly maybe, means "at least zero". We say that matrix is positive if all it's eigenvalues are non-negative. Having done this, we immediately restrict ourselves to (symmetric) diagonalizable matrices with real eigenvalues, but we will later see that we can't do much "better". Also, since sum of positive matrices should be positive, we should further restrict ourselves to even stricter class of matrices, called Hermitian matrices, which correspond self-adjoint linear maps. Now everything works nicely but we still preserve non-trivial non-commutative structure.

Matrix functions, i.e. "how to apply function to matrix" is bit simpler to explain. Instead of doing something arbitrary the idea is to take real function (a function $f : \mathbb{R} \to \mathbb{R}$, say) and intepret it as function $f : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$, *matrix function.* Polynomials extend rather naturally, and similarly analytic functions, or at least entire. Now, a perverse definition for matrix function for continuous functions would be some kind of a limit when function is uniformly approximated by polynomials (using Weierstrass approximation theorem). This works for Hermitian matrices, but one can do better: apply the function to the eigenvalues of the mapping to get another linear map.

As it turns out, much of the study of matrix monotone and convex functions is all about understanding these definitions of positive maps and matrix functions.

Lastly, one might wonder why should one be interested in the whole business of monotone and convex functions? It's all about point of view. Let's consider a very simple inequality:

For any real numbers $0 < x \leq y$ we have

$$y^{-1} \leq x^{-1}.$$

Of course, this is quite close to the axioms of the real numbers, but there's a rather fruitful interpretation. The function $(x \mapsto \frac{1}{x})$ is decreasing.

Now there's this matrix version of the previous inequality:

For any two matrices $0 < A \leq B$ we have

$$B^{-1} \leq A^{-1}.$$

This is already not trivial, and with previous interpretation in mind, could this be interpreted as the functions $(x \mapsto \frac{1}{x})$ could be *matrix decreasing*? And is this just a special case of something bigger? Yes, and that's exactly what this thesis is about.

1.2 Plan of attack

This master's thesis is a comprehensive review of the rich theory of matrix monotone and convex functions.

Master's thesis is to be structured roughly as follows.

1. Introduction
    - Introduction to the problem, motivation
    - Brief definition of the matrix monotonicity and convexity
    - Past and present (Is this the right place)
        - Loewner's original work, Loewner-Heinz -inequality
        - Students: Dobsch' and Krauss'
        - Subsequent simplifications and further results: Bendat-Sherman, Wigner-Neumann, Koranyi, etc.
        - Donoghue's work
        - Later proofs: Krein-Milman, general spectral theorem, interpolation spaces, short proofs etc.
        - Development of the convex case
        - Recent simplifications, integral representations
        - Operator inequalities
        - Multivariate case, other variants
        - Further open problems?
    - Scope of the thesis
2. Positive matrices

- Motivation via restriction, basics
- Spectral theorem
- Congruence
- Characterizations
- Applications
- Spectrum

3. Divided differences
    - Definition (what kind of?)
    - Mean value theorem
    - Smoothness
    - k-tone functions on $\mathbb{R}$
    - Cauchy's integral formula
    - Regularizations

4. Matrix functions
    - Several definitions: spectral and cauchy
    - Smoothness of matrix functions

5. Pick functions
    - Basic definitions and properties
    - Pick matrices/ determinants
    - Compactness
    - Pick-Nevanlinna interpolation theorem
    - Pick-Nevanlinna representations theorem

6. Monotonic and convex matrix functions
    - Basics
        - Basic definitions and properties (cone structure, pointwise limits, compositions etc.)
        - Classes P_n, K_n and their properties
        - $-1/x$

    - One directions of Loewner's theorem
    - Examples and non-examples
  - Pick matrices/determinants vs matrix monotone and convex functions
    - Proofs for (sufficiently) smooth functions
  - Smoothness properties
    - Ideas, simple cases
    - General case by induction and regularizations
  - Global characterizations
    - Putting everything together: we get original characterization of Loewner and determinant characterization

7. Local characterizations
   - Dobsch (Hankel) matrix: basic properties, easy direction (original and new proof)
   - Integral representations
     - Introducing the general weight functions for monotonicity and convexity (and beyond?)
     - Non-negativity of the weights
     - Proof of integral representations
   - Proof of local characterizations

8. Structure of the classes P_n and K_n, interpolating properties (?)
   - Strict inclusions, strict smoothness conditions
   - Strictly increasing functions
   - Extreme values
   - Interpolating properties

9. Loewner's theorem
   - Preliminary discussion, relation to operator monotone functions
   - Loewner's original proof
   - Pick-Nevanlinna proof
   - Bendat-Sherman proof

- Krein-Milman proof
- Koranyi proof
- Discussion of the proofs
- Convex case

10. Alternative characterizations (?)
    - Some discussion, maybe proofs
11. Bounded variations (?)
    - Dobsch' definition, basic properties
    - Decomposition, Dobsch' theorems

1.3 Some random ideas

1. TODO: fix Boor in the references
2. It's easy to see that [Something]. Actually, it's so so easy that we have no excuse for not doing it.
3. When is matrix of the form $f(a_i + a_j)$ positive: f is completely monotone (?).
4. Polynomial regression...
5. TODO: Maximum of two matrices (at least as big), (a + b)/2 + abs(a - b)/2
6. If $\langle Ax, y\rangle = 0$ implies $\langle x, Ay\rangle = 0$, then A is constant times hermitian.
7. Angularity preserving functions
8. If subspace of linear maps are diagonalizable with real eigenvalues, is there a inner product such that subspace consists of only Hermitian maps

Chapter 2

Positive matrices

This chapter is titled "positive matrices", although "positive maps" might be more appropriate title. We are mostly going to deal with finite-dimensional objects, but many of the ideas could be generalized infinite-dimensional settings, where matrices lose their edge. Also, one should always ask whether it really clarifies the situation to introduce concrete matrices: matrices are good at hiding the truly important properties of linear mappings. The words "matrix" and "linear map" are used somewhat synonymously, although one should always remember that the former are just special representations for the latter.

Ideas how to rewrite this section:

- Map is positive, if all of its restrictions are. One dimensional maps are positive if and only the scalar is positive.
- Map is real, if all of its restrictions are. One dimensional maps are real if and only the scalar is real.
- Adjoint commutes with restriction. Adjoint of one dimensional map is its conjugate.
- How should one restrict linear mappings? (Use inclusions and finally project)
- Central notion is adjoint
- $*$-conjugation is natural notion with adjoint
- Increasing sequence of subspaces and restriction with positive determinant $\Rightarrow$ the whole map is positive. Equivalently, map is positive if it has positive determinant and has a subspace where it is positive.

2.1 Motivation

How should one order matrices? What should we require from ordering anyway?

We would definitely like to have natural total order on the space of matrices, but it turns out there are no natural choices for that. Partial order is the next best thing. Recall that a partial order on a set X is a binary relation $\leq$ on such that

1. $x \leq x$ for any $x \in X$.
2. For any $x, y \in X$ for which $x \leq y$ and $y \leq x$, necessarily $x = y$.
3. If for some $x, y, z \in X$ we have both $x \leq y$ and $y \leq z$, also $x \leq z$.

The third point is the main point, the first two are just there preventing us from doing something crazy. But we can do better: this partial order on matrices should also respect addition.

4. For any $x, y, z \in X$ such that $x \leq y$, we should also have $x + z \leq y + z$.

There's another way to think about this last point. Instead of specifying order among all the pairs, we just say which matrices are positive: matrix is positive if and only it's at least 0.

If we know all the positive matrices, we know all the "orderings". To figure out whether $x \leq y$, we just check whether $0 = x - x \leq y - x$, i.e. whether $y - x$ is positive. Also, positive matrices are just differences of the form $y - x$ where $x \leq y$. Now, conditions on the partial order are reflected to the set of positive matrices.

1'. 0 (zero matrix) is positive.

2'. If both x and $-x$ are positive, then $x = 0$.

3'. If both x and y are positive, so is their sum $x + y$.

Here $3'$ is kind of combination of 3 and 4.

The terminology here is rather unfortunate. Natural ordering of the reals satisfies all of the above with obvious interpretation of positive numbers, which however differs from the standard definition: 0 is itself positive in our above definition. This is undoubtedly confusing, but what can you do? For real numbers we have total order, so every number is either zero, strictly positive or strictly negative, so when we say non-negative, it literally means "not negative": we get all the positive numbers and zero. But with partial orders we might get more. So the main reasons why we are using this terminology are

1. It's short.

Also, now that we have decided to preserve the word "positive" for "at least zero" one might be tempted to preserve "strictly positive" for "at least zero, but not zero". We won't do that, we save that phrase for something more important.

To figure out a correct notion for positive maps, let's start simple. If we are in a 1-dimensional vector space V over $\mathbb{R}$ there's rather canonical choice for positivity. Any linear map is of the form $v \mapsto av$ for some $a \in \mathbb{R}$ and we should obviously say that a map is positive if $a \geq 0$ (note our non-standard terminology concerning positivity). More generally, if a map if scalar multiple of identity, map should be positive if and only if the corresponding scalar is non-negative.

Natural extension of this idea could be try the following: map is positive if all of its eigenvalues are non-negative. Of course, this doesn't quite work: not every map has real eigenvalues. But even if we restrict to maps with real eigenvalues, this property is not preserved in addition. Consider for example the pair

$$\begin{bmatrix} 0 & 4 \\ 1 & 0 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & -1 \\ -4 & 0 \end{bmatrix}$$

The two matrices have both distinct eigenvalues -2 and 2 and are hence diagonlizable, but their sum has characteristic polynomial x^2+9, which most definitely has no real zeros. In general one should not except summation and eigenvalues go very well together.

2.2 Real maps

2.2.1 Restricting linear maps

There's however quite clever way to go around this. Instead of requiring non-negativity of eigenvalues, we require that map "restricts" to positive map. The idea is: we already know which maps should be positive in one-dimensional spaces, or more generally, which scalar multiples of identity should be positive. Now we should require that when we restrict our look to one-dimensional subspaces, we should get a positive map.

Of course, one should first understand what restricting linear maps means. Usually if we have a linear map $A : V \to V$, we could take subspace $W \subset V$ and consider the usual restriction map $A\big|_W : W \to V$ given by $A\big|_W(w) = Aw$ for any $w \in W \subset V$. In other words $A\big|_W = A \circ J_W$, where J_W denotes the natural inclusion from W to V. But this map is going to wrong space. Instead we would like to define something satisfying

- Restriction is a linear map $(\cdot)_{V,W} = (\cdot)_W : \mathcal{L}(V) \to \mathcal{L}(W)$.
- If $A \in \mathcal{L}(V)$ and $A(W) \subset W$, restriction should coincide with the original map, in the sense that $A = J_W \circ A_W$.

- If $W' \subset W \subset V$, we should have $(\cdot)_{W'} = ((\cdot)_W)_{W'}$.

These properties don't uniquely define a linear map but they say that A_W should be of the form $P_{V,W} \circ A \circ J_W$ where $P_{V,W}$ is a projection, i.e. a map for which $P_{V,W} \circ J_W = I_W$. Moreover, these projections should satisfy $P_{V,W'} = P_{W,W'} \circ P_{V,W}$.

If we are working in a inner-product space, there's rather natural choice for the map $P_{V,W}$: orthogonal projections. Orthogonal projections are projections with $\ker(P) = \mathrm{im}(P)^{\perp}$. Such maps are easily seen to satisfy all the requirements. Finally, we will call our new concept *compression* instead of restriction, to distinguish between the two.

Definition 2.1. Let $(V, \langle \cdot, \cdot \rangle)$ be an inner product space and $W \subset V$ a subset. We define the map A_W, *compression* of A to W to be the linear map given by $P_W \circ A \circ J_W$.

Theorem 2.2. *Let $(V, \langle \cdot, \cdot \rangle)$ be an inner product space and $W \subset V$ subspace of V. Then the compression to W is unique linear contraction from $\mathcal{L}(V)$ to $\mathcal{L}(W)$, such that for any $A \in L(V, W)$ we have $(J_W \circ A)_W = A \circ J_W$. Moreover, if $W' \subset W$, we have $(\cdot)_{W'} = ((\cdot)_W)_{W'}$.*

Proof. TODO $\square$

For one-dimensional compressions we have convenient representation. As one easily checks, one dimensional projection onto subspace spanned by vector v is given by

$$P_{(v)} = \frac{\langle \cdot, v \rangle}{\langle v, v \rangle} v,$$

as long as $v \neq 0$, and thus

$$A_{(v)} = \frac{\langle A \cdot, v \rangle}{\langle v, v \rangle} v.$$

If $w \in (v) \setminus \{0\}$, we could rewrite the previous in the form

$$A_{(v)}(w) = \frac{\langle Av, v \rangle}{\langle v, v \rangle} w = \frac{\langle Aw, w \rangle}{\langle w, w \rangle} w.$$

This gives rise to so called Rayleigh quotient $R(A, \cdot) : V \setminus \{0\} \to \mathbb{C}$, given by

$$R(A, v) = \frac{\langle Av, v \rangle}{\langle v, v \rangle}.$$

Compression in the direction of v is given by scaling by the corresponding Rayleigh quotient.

We will call $\langle Av, v \rangle$ the quadratic form of A, and denote it by $Q_A(v)$.

There's one more important property of compression we need. When map is compressed to a subspace, we naturally lose some information about the map. Knowing about all of the compressions, however, we can get our map back.

Lemma 2.3 (Injectivity of compression)**.** *If $A, B \in \mathcal{L}(V)$, $A = B$ if and only if $A_W = B_W$ for any one-dimensional subspace $W \subset V$.*

Proof. By linearity, it is sufficient to prove that if $Q_A(v) = 0$ for any $v \in V$, then $A = 0$. TODO polarization identity. □

2.2.2 Positive maps

Now that we have defined the compression we are ready define positive maps.

Definition 2.4. Let $(V, \langle\cdot,\cdot\rangle)$ be an inner product space. We say that a map $A \in \mathcal{L}(V)$ is positive, and write $A \geq 0$, if for any one-dimensional subspace $W \subset V$ the map A_W is positive, i.e. is induced by a non-negative real.

We denote the space of positive maps by $\mathcal{H}_+(V)$. Positive maps have the following useful properties.

Proposition 2.5. *Let $(V, \langle\cdot,\cdot\rangle)$ be an inner product space over $\mathbb{C}$. Then*

(i) $A \in \mathcal{L}(V)$ is positive if and only if A_W is positive for every subspace $W \subset V$.

(ii) If $A, B \in \mathcal{L}(V)$ are positive and $\alpha, \beta \geq 0$, also $\alpha A + \beta B$ is positive.

(iii) If $(A_i)_{i=1}^{\infty}$ are positive and $\lim_{i\to\infty} A_i = A$, also A is positive.

(iv) $A \in \mathcal{L}(V)$, A is positive if and only for any $v \in V$, or for any $v \in V$ with $|v| = 1$ we have $\langle Av, v\rangle \geq 0$, or still equivalently, for any $v \in V \setminus \{0\}$ the Rayleigh quotient $R(A, v)$ is non-negative.

(v) If both A and $-A$ are positive, then $A = 0$.

(vi) If A is positive, all of its eigenvalues are non-negative.

Proof. (i) Other direction is immediate. Also if for any subspace $W \subset V$ take any one-dimensional $W' \subset W$. Now $(A_W)_{W'} = A_{W'}$, is positive by assumption, and so is A_W.

(ii) The claim evidently holds for one-dimensional spaces. Now for any one-dimesional $W \subset V$ we have $(\alpha A + \beta B)_W = \alpha A_W + \beta B_W \geq 0$, by the one-dimensional case, so $\alpha A + \beta B \geq 0$.

(iii) Again, the claim evidently holds for one-dimensional spaces. Now for any one-dimesional $W \subset V$ we have $(\lim_{i\to\infty} A_i)_W = \lim_{i\to\infty}(A_i)_W \geq 0$, by the one-dimensional case, so $A \geq 0$.

(iv) These claims are immediate from our representation for one-dimensional compressions.

(v) If $A, -A \geq 0$, all the one-dimensional compressions of A are both non-negative and non-positive, so zero. But by the injectivity of compression, it follows that $A = 0$.

(vi) Note that if v is any eigenvector of v, $A_{(v)}w = \frac{\langle Av,v\rangle}{\langle v,v\rangle}w = \lambda w$, so by assumption $\lambda \geq 0$.

$\square$

The map $v \mapsto \langle Av, v\rangle$ is called the quadratic form of A, and is denoted by Q_A.

We can also lift other important notions.

Definition 2.6. Let $(V, \langle\cdot,\cdot\rangle)$ be an inner product space. We say that a map $A \in \mathcal{L}(V)$ is real, if for any one dimensional subspace $W \subset V$ the map A_W is real, i.e. is induced by real number.

Definition 2.7. Let $(V, \langle\cdot,\cdot\rangle)$ be an inner product space. We say that a map $A \in \mathcal{L}(V)$ is imaginary, if for any one dimensional subspace $W \subset V$ the map A_W is imaginary, i.e. is induced by imaginary number.

The previous two families of maps are usually called Hermitian and Skew-Hermitian and as with positive maps, many of their properties are lifted form usual complex numbers. Hermitian maps will have a special role in our discussion. 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.

2.2.3 Adjoint

We can also lift the notion of complex conjugate. If V is one-dimensional, $\overline{A}$, conjugate of A should be a linear map which is induced by the complex conjugate of the scalar inducing A.

Theorem 2.8. *Let $(V, \langle\cdot,\cdot\rangle)$ be an inner product space. Then for any $A \in \mathcal{L}(V)$ there exists unique map $A^* \in \mathcal{L}(V)$, which we will call adjoint of A, for which for any one-dimensional subspace W we have $(A^*)_W = \overline{A_W}$.*

Proof. The uniqueness of adjoint is immediate from the injectivity of compression. 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.

Note that the Rayleigh quotient for such map is given by

$$R(A,x) = \frac{\langle x,v\rangle\langle w,x\rangle}{\langle x,x\rangle}.$$

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

$$R(A^*,x) = \frac{\langle x,w\rangle\langle v,x\rangle}{\langle x,x\rangle} = \frac{\overline{\langle w,x\rangle\langle x,w\rangle}}{\langle x,x\rangle} = \overline{R(A,x)}.$$

□

Real maps are their own adjoints, and that is why they are often called *self-adjoint*.

There is also a meaningful way to extend the notion of adjoint for general (non-endomorphism) linear maps. In general setting, we don't have a notion of compression of linear map: there's no canonical way to restrict the codomain. We can however interpret a map in a bigger space. Indeed, any map $A \in \mathcal{L}(V,W)$ can be canonically interpreted as a map $\tilde{A} \in \mathcal{L}(V \oplus W)$: define $\tilde{A}(v,w) = (0, Av)$. We call this map the *symmetrization* of A. Now it makes sense to consider $(\tilde{A})^*$, the symmetrization has a unique adjoint. This adjoint does not in general live in $\mathcal{L}(V,W)$ anymore: but it turns out that it does live in $\mathcal{L}(W,V)$!

Theorem 2.9. *For any $A \in \mathcal{L}(V,W)$ there exists a unique map $A^* \in \mathcal{L}(W,V)$ which we call the adjoint of A, such that $(\tilde{A})^* = (\tilde{A^*})$. Moreover, if $V = W$, the new notion of adjoint coincides with the old one.*

Proof. Of course, strictly speaking $\tilde{A^*}$ would be map in $\mathcal{L}(W \oplus V)$, not in $\mathcal{L}(V \oplus W)$, but the two spaces are canonically isomorphic.

The uniqueness follows from the already known uniqueness for the old notion. The map $(\cdot)^* : \mathcal{L}(V,W) \to \mathcal{L}(W,V)$ should again evidently be conjugate linear. Also, the same construction for basis elements of the form $A = (x \mapsto \langle x,v\rangle_V w)$ (where $v \in V$ and $w \in W$) works again. Indeed, for any $(x,y) \in V \oplus W$ the corresponding Rayleigh quotient is given by

$$R(\tilde{A},(x,y)) = \frac{\langle (0,Ax),(x,y)\rangle_{V\oplus W}}{\langle (x,y),(x,y)\rangle_{V\oplus W}} = \frac{\langle Ax,y\rangle_W}{\langle x,x\rangle_V + \langle y,y\rangle_W} = \frac{\langle x,v\rangle_V\langle w,y\rangle_W}{\langle x,x\rangle_V + \langle y,y\rangle_W},$$

and it's clear that we may set $A^* = (x \mapsto \langle x,w\rangle_W v)$. Our construction also makes it clear that this notion coincides with the old one. □

The previous proof also gives a convenient corollary, which is the most common definition for adjoint.

Corollary 2.10. *For any $A \in \mathcal{L}(V, W)$, the adjoint $A^* \in \mathcal{L}(W, V)$ is unique linear map such that for any $v \in V$ and $w \in W$ we have*

$$\langle Av, w \rangle_W = \langle v, A^* w \rangle_V.$$

In particular, map $A \in \mathcal{L}(V)$ is real for any $v, w \in V$ we have

$$\langle Av, w \rangle = \langle v, Aw \rangle.$$

and imaginary if for any $v, w \in V$

$$\langle Av, w \rangle = -\langle v, Aw \rangle.$$

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

Theorem 2.11. *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)* $(AB)^* = B^* A^*$.
- *vi)* $\ker(A) = \operatorname{im}(A)^\perp$

2.2.4 Examples

It's high time to have some examples.

Most obvious, although not very interesting, representatives of real/imaginary/positive maps are real/imaginary/positive scalar multiples of the identity. Projections are stereotypical examples of positive and hence real maps. Projections, proper definition. Indeed, one-dimensional projections are given by $A = (x \mapsto \langle x, v \rangle v)$ for some $v \in V$ with $|v| = 1$. For such maps $\langle Ax, x \rangle = \langle x, v \rangle \langle v, x \rangle = |\langle x, v \rangle|^2 \geq 0$. Higher dimensional projections are simply sums of one-dimensional ones, so they are also positive and real. More generally one could take any positive linear combination of projections to get much more positive maps, and real linear combination of projections to get real maps.

As we earlier noticed, however, not every map with real eigenvalues is real, and not every map non-negative eigenvalues is positive. It turns out that the basis elements of the form $A = (x \mapsto \langle x, v\rangle w)$ are real if and only if v and w are real multiples of each other, or to be precise, if there exists $\alpha, \beta \in \mathbb{R}$, not both 0, such that $\alpha v + \beta w = 0$. Indeed, by the corollary, the map is real if for any $x, y \in V$ we have

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

Now if v and w are not parallel, we can find x such that $\langle x, v\rangle = 0 \neq \langle x, w\rangle$, which contradicts the previous. The case of parallel v and w is easy to check.

While hunting for examples, it's worthwhile to note that in some sense $\mathcal{H}(V)$ is not essentially bigger than $\mathcal{H}_+(V)$: if $A \in \mathcal{H}(V)$ we can always find a positive real number λ such that $A + \lambda I \in \mathcal{H}_+(V)$. To this end, note that the quadratic form of $A + \lambda I$ at $v \in V$ is $\langle (A + \lambda I)v, v\rangle = \langle Av, v\rangle + \lambda\langle v, v\rangle$. But if $\lambda \geq \|A\|$, the operator norm of A, the previous quantity is non-negative for any $v \in V$.

TODO: 2×2 case.

2.3 Spectral theorem

One might wonder if there are other examples of positive maps than positive linear combination of projections. Rather surprisingly, there are none.

Theorem 2.12. *$A \in \mathcal{L}(V)$ is positive if and only for some $m \geq 0$, $\lambda_i > 0$ and $v_i \in V$ for $1 \leq i \leq m$ we have*

$$A = \sum_{1 \leq i \leq m} \lambda_i P_{v_i}.$$

Proof. 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 by any orthonormal basis of the corresponding subspace and λ_i's 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 2.13. *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 $A = J_W \circ A_W \circ P_W = A$. Now A_W is also positive, and $\dim(W) < n$. By induction assumption we have numbers λ_i and vectors $v_i \in V$ for the map A_W, but such representation for A_W immediately gives representation for A also.

We just have to get rid of the extra assumption on the existence of such v. But for this, note that if $\lambda = \inf_{|v|=1}\langle Av, v\rangle$, 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. Now cook up a representation for B and add orthonormal basis of V with λ_i's equal to λ: this is required representation for A. □

TODO: image of the proof process in $\mathbb{R}^3$.

Proof of lemma 2.13. Take any $w \in V$. Now by assumption for any $c \in \mathbb{C}$ we have

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

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 $w \in V$. □

As discussed, there should be obvious generalization for real maps: they real linear combinations for projections. We can however still improve the statement: we can take v_i's to be orthogonal, and hence $m \leq n$. We have thus arrived at Spectral theorem.

Theorem 2.14 (Spectral theorem)**.** *Let $A \in \mathcal{H}(V)$. Then there exists real numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$ and orthonormal vectors $v_1, v_2, \ldots, v_n$ such that*

$$A = \sum_{i=1}^{n} \lambda_i P_{v_i}. \tag{2.15}$$

Proof. Let's first check case of positive A. There's not very many things to change from the proof of theorem 2.12. Indeed, we again argue by induction. The case $n = 0$ is again clear. In the induction step we found that induction assumption applies to $A - \lambda I$ compressed to suitable $(n-1)$-subspace. There we can cook up required representation, and bring back the representation for $A - \lambda I$ itself. That is we have

$$A - \lambda I = \sum_{i=1}^{n-1} \lambda_i P_{v_i}$$

for orthonormal v_i's and non-negative λ_i's. But then if v_n is a missing orthonormal vector, we find that

$$A = \sum_{i=1}^{n} (\lambda_i + \lambda) P_{v_i},$$

where $\lambda_n = 0$. But this is what we wanted.

For non-positive A, simply add suitable multiple of identity to get $B := A + \lambda I \geq 0$ and apply what we have proved to B. If we have representation for B, we can easily cook up one for A: just subtract λ for λ_i's in the representation of B. □

In the representation 2.15 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.* Such representation is of course not unique: if $A = I$, we could again choose v_i's to be any orthonormal basis of V.

There is way to make the Spectral representation unique, however. For this we have to change v_i to corresponding eigenspaces.

Theorem 2.16 (Spectral theorem)**.** *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 orthogonal subspaces of V, $E_{\lambda_1}, E_{\lambda_2}, \ldots E_{\lambda_m}$ with $E_{\lambda_1} + E_{\lambda_2} + \ldots + E_{\lambda_m} = V$, such that*

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

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. □

Although the latter version is definitely of theoretical importance, we will mostly stick the former: it only contains one-dimensional projections.

Spectral representation makes many of the properties of real maps obvious. For instance any power of 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 for higher powers. In other words: eigenspaces are preserved under compositional powers, and eigenvalues are ones to get powered up. From the original definition this is not all that clear. One could even extend to polynomials. If $p(x) = c_n x^n + c_{n-1}x^{n-1} + \dots c_1 x + c_0$, with $c_i \in \mathbb{R}$, we should write

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

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.

Also, given $A \in \mathcal{H}(V)$, we may write any $x \in V$ in the form $v = \sum_{1 \le i \le n} x_i v_i$, where $(v_i)_{i=1}^n$ is a eigenbasis for A and $x_i = \langle x, v_i \rangle$. Now $Ax = \sum_{1 \le i \le n} \lambda_i x_i v_i$, so for instance

- $Q_A(x) = \langle Ax, x \rangle = \sum_{1 \le i \le n} \lambda_i x_i^2$. Thus Q_A is just a positive linear combination of eigenvalues, and $R(A, \cdot)$ convex combination.
- $\|Ax\|^2 = \langle Ax, Ax \rangle = \sum_{1 \le i \le n} \lambda_i^2 x_i^2 \le (\max_{1 \le i \le n} \lambda_i^2) \sum_{1 \le i \le n} x_i^2 = (\max_{1 \le i \le n} \lambda_i^2) \|x\|^2$. It follows that $\|A\| = \max_{1 \le i \le n} |\lambda_i|$.

Similarly, if $A \ge 0$, A has a unique positive square root, which we denote by $A^{\frac{1}{2}}$: map such that $A^{\frac{1}{2}} A^{\frac{1}{2}} = A$. Given the spectral reprsentation $A = \sum_{1 \le i \le n} \lambda_i P_{v_i}$, we can simply set $A^{\frac{1}{2}} = \sum_{1 \le i \le n} \lambda_i^{\frac{1}{2}} P_{v_i}$. As for the uniqueness, note that if B is a positive square root for A and $B = \sum_{1 \le i \le n} \lambda'_i P_{v'_i}$, then $B^2 = \sum_{1 \le i \le n} \lambda'^2_i P_{v'_i}$. It follows that eigenvalues of B are simply square roots of eigenvalues of A and the corresponding eigenspaces are equal. Of course, the whole uniqueness argument floats more naturally with unique spectral representation.

2.3.1 Commuting real maps

Warning! Composition of positive maps need not be positive!

If $A, B \in \mathcal{H}_+(V)$, then, as we noticed, $(AB)^* = B^* A^* = BA$, so for AB to be even real, A and B would at least need to commute. Natural question follows: when do two positive maps commute? Since $(c_1 I + A)$ and $(c_2 I + B)$ commute if and only if A and B do, this is same as asking when do two real maps commute.

It turns out that real maps commute only if they "trivially" commute, in the following sense. If there exists vectors $v_1, v_2, \dots, v_n$ and numbers $\lambda_1, \lambda_2, \dots, \lambda_n$ and $\lambda'_1, \lambda'_2, \dots, \lambda'_n$ such that

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

then A and B are said to be *simultaneously diagonalizable*. Simultaneosly diagonalizable maps trivially commute, and it turns out that if two real maps commute, they are indeed simultenously diagonalizable.

To prove this statement, we start with a lemma, simplest non-trivial case of the statement.

Lemma 2.17. *Let $W_1, W_2 \subset V$ be two subspaces. Then P_{W_1} and P_{W_2} commute if and only if there exists orthogonal subspaces U_1, U_2 and U_0 such that*

$$W_1 = U_1 + U_0 \quad and \quad W_2 = U_2 + U_0.$$

We then have $P_{W_1} = P_{U_1} + P_{U_0}$ and $P_{W_2} = P_{U_2} + P_{U_0}$, and $U_0 = W_1 \cap W_2$.

Proof. Write $U_0 := W_1 \cap W_2$ and $W_i = U_0 + U_i$ for some $U_i \perp U_0$ for $i \in \{1,2\}$. Now $P_{W_i} = P_{U_i} + P_{U_0}$ for $i \in \{1,2\}$ so it suffices to check that $U_1 \perp U_2$. Equivalently, it suffices to prove that if $W_1 \cap W_2 = \{0\}$, and P_{W_1} and P_{W_2} commute, then $W_1 \perp W_2$ or equivalently $P_{W_1}P_{W_2} = 0 = P_{W_2}P_{W_1}$. But for any $v \in V$ we have $W_1 \ni P_{W_1}P_{W_2}v = P_{W_2}P_{W_1}v \in W_2$, so indeed $P_{W_1}P_{W_2} = 0 = P_{W_2}P_{W_1}$. $\square$

Definition 2.18. We say that two $W_1, W_2 \subset V$ subspaces commute if the respective projections commute.

Theorem 2.19. *Let $\mathcal{A} = (A_j)_{j \in J}$ by an arbitrary family of commuting real maps. Then there exists non-trivial orthogonal subspaces of V, $E_1, E_2, \ldots E_m$ with $E_1 + E_2 + \ldots + E_m = V$ and numbers $\lambda_{i,j}$ for $j \in J$ and $1 \leq i \leq n$ such that*

$$A_j = \sum_{1 \leq i \leq m} \lambda_{i,j} P_{E_i}$$

for any $j \in J$.

Proof. The main idea is the following: like in the spectral theorem, we would like to somehow find the subspaces $E_1, E_2, \ldots E_m$. Also, at least for finite families, we could probably use induction, so we should get far just by proving the theorem for a family of only two maps. For two projections we have already proved the statement as lemma 2.17.

Now here's the trick: if two maps commute, so do all their polynomials. Hence if we have two commuting A and B, we know that all the respective eigenspaces commute. Now if we could prove the statement at least for finite families of projections, we could conclude the case of two general maps. Indeed we could write any eigenprojection of A or B as a linear combination of sum finite family of orthogonal (orthogonal) projections, but those projections would then also span A and B.

More generally, if we could prove the statement for arbitrary families of projections, the same argument would yield it for any family of more general linear maps, so we can safely assume that all the maps A_j are projections.

Let's first deal with the finite case by induction. As mentioned, we already dealt with the case $|J| = 2$, but we can draw better conclusions. If we have two commuting projections P_{W_1} and P_{W_2} in $\mathcal{A}$. Now by the lemma we may write $P_{W_1} = P_{U_1} + P_{U_0}$ and $P_{W_2} = P_{U_2} + P_{U_0}$. The nice things is that any map in $\mathcal{A}$ also commutes with $P_{W_1} + P_{W_2} = P_{U_1} + P_{U_2} + 2P_{U_0}$, so also with it's eigenprojections, P_{U_0} and $P_{U_1+U_2}$. It follows that any map in $\mathcal{A}$ commutes with U_0, U_1 and U_2.

We have split the subspaces W_1 and W_2 in pieces, and we could actually forget W_1 and W_2 altogether and replace them by U_0, U_1 and U_2: note that all the same assumption hold for this new family, and U_0, U_1 and U_2 span W_1 and W_2.

Problem here is of course: it's not clear that the new family, say $\mathcal{A}'$ is any simpler than $\mathcal{A}$! It could well have more elements than $\mathcal{A}$ so we can't just do straightforward induction. What could happen also is that some of the subspaces U_0, U_1, U_2 coincide with the subspaces already present in the family, so the size of the family doesn't increase, and it could even decrease. This will indeed happen. One way to see this is to look at the sum of dimensions of all the projections of the family: if we change the family this sum cannot increase. Moreover, if we pick two subspaces W_1 and W_2 which are not orthogonal, this sum will decrease!

The conclusion is: pick pairs projections with non-orthogonal subspaces and do the replacing procedure as explained before; this process will eventually stop since the sum of dimesions can't drop below zero. But the only reason this process could stop is that all subspaces are pairwise orthogonal in which case we are done. The proof of finite case is complete.

There are many ways to bootstrap the previous argument for arbitrary families. For any finite subfamily we can form the set of generating projections. If add one more map, the set projections get refined: some of the subspaces get split to pieces. Now sizes of all these generating families are bounded by n so we may pick one with most number of elements. Now if A is any projection in $\mathcal{A}$, by maximality, adding it to the family does not refine the generating set. But this means that the generating set generates any element of $\mathcal{A}$ and we are done.

We also see that there exists unique minimal family of generating projections TODO.

Alternative approach to the theorem could be to look at the commutative $\mathbb{R}$-algebra of real maps generated by $\mathcal{A}$: generating projections will be in some sense minimal projections in this algebra. □

The previous theorem sends a very important message.

Philosophy 2.20. Commutativity kills the exciting phenomena.

One would naturally hope that product of positive maps is still positive, but as soon as we try to make such restriction, everything degenerates to $\mathbb{R}^m$, or to diagonal maps. Dealing with diagonal maps is then again just dealing with many real numbers at the same time: of course this makes sense and all, but doesn't lead to very interesting concept.

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

TODO: independence of random variables.

2.4 Congruence

2.4.1 $*$-conjugation

There is one very important way to produce positive maps from others, called congruence. 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 $Q_{BAB}(v) = \langle BABv, v\rangle = \langle A(Bv), (Bv)\rangle \geq 0$ for any $v \in V$. We didn't really need the assumption on the positivity of B, but realness was not that important either. Namely for arbitrary linear B we could consider the product B^*AB instead: this is positive whenever A is. If $C = B^*AB$ for some $B \in \mathcal{L}(V)$, we say that C is $*$-conjugate of A.

We also see that $Q_{B^*AB} = Q_A \circ B$: conjugation is a change of basis in the quadratic form. This is the main motivation for the definition of the $*$-conjugation. We have already seen that the quadratic form of a map is a good way to characterize many of its good properties, so to some extent to understand maps, we just to need to understand structure of their quadratic forms. By change of basis of the quadratic form we have a good control of what happens. We might however lose some information: if $B = 0$, for instance, the quadratic form after $*$-conjugation by B doesn't tell much about A. But if B is invertible, or equivalently if C and B are $*$-conjugates of each other, we shouldn't lose any information. If this is the case, we say that A and C are congruent. It is easily verified that congruence is a equivalence relation.

The construction of $*$-conjugation makes also sense for general linear map A, i.e. we could just as well $*$-conjugate non-positive, or even non-real maps. The result then need not be positive or real, and in general, $*$-conjugation loses its usefulness.

The previous construction can be also performed between two spaces V and W: given any map $B \in \mathcal{L}(V, W)$ and $A \in \mathcal{H}_+(W)/\mathcal{H}(W)/\mathcal{L}(W)$, we note that $B^*AB \in \mathcal{H}_+(V)/\mathcal{H}(W)/\mathcal{L}(W)$. For self-adjoint maps we can say a lot more: while congruence doesn't in general preserve eigenvalues, it preserves their signs.

Theorem 2.21 (Sylvester's Law of Inertia)**.** *$A, B \in \mathcal{H}(V)$ are congruent, if and only if A and B have equally many positive, negative and zero eigenvalues, counted with multiplicity.*

Proof. Let's start with the "if" part. Let's denote the eigenvalues of A and B by $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ and $\lambda'_1 \leq \lambda'_2 \leq \ldots \leq \lambda'_n$, respectively, and the corresponding eigenvectors with $v_1, v_2, \ldots, v_n$ and $v'_1, v'_2, \ldots, v'_n$. By assumption λ_i and λ'_i have the same sign (or are both zero) for any $1 \leq i \leq n$, so we may find non-zero real numbers $t_1, t_2, \ldots, t_n$ such that $\lambda_i = \lambda'_i t_i^2$. Now consider a linear map C with $Cv_i = t_i v'_i$. C is clearly a surjection and hence a bijection. Also if $v = \sum_{i=1}^n x_i v_i$ $(Q_B \circ C)(v) = Q_B(\sum_{i=1}^n x_i t_i v'_i) = \sum_{i=1}^n |x_i|^2 t_i^2 \lambda'_i = \sum_{i=1}^n |x_i|^2 \lambda_i = Q_A(v)$ so $Q_{C^*BC} = Q_B \circ C = Q_A$. It follows that $C^*BC = A$ and hence A and B are congruent.

The "only if" - part is a bit trickier. The idea is to find a good description for the number of positive non-negative eigenvalues. We noticed before that we can write quadratic forms in the form $Q_A(v) = \sum_{i=1}^n \lambda_i |x_i|^2$ if $v = \sum_{i=1}^n x_i v_i$, and v_i are the eigenvectos of A with $\lambda'_i s$ as the corresponding eigenvectors. In particular if say first k eigenvalues are negative, Q_A will be negative on $\operatorname{span}\{v_i | 1 \leq i \leq k\}$, a k-dimensional subspace, minus zero. Similarly, now $n-k$ of the eigenvalues are non-negative, so the quadratic form is non-negative on a subspace of dimension of at least $n-k$. But the dimensions can't be any bigger: if Q_A were for instance negative on some $k+1$ dimesional subspace, this subspace would necessarily intersect a subspace where Q_A is non-negative, which is non-sense.

Congruence preserves the previous notion: if Q_B is negative on a subspace of dimension k, so is $Q_B \circ C$ for any invertible C; namely in the inverse image. Same reasoning holds for the the subspace on which Q_B is non-negative, so again, $Q_B \circ C$ has to have similar structure. We are done. □

If n_0, n_- and n_+ denote the number of zero, negative and positive eigenvalues of A, *inertia* of A is the triplet $\{n_0, n_-, n_+\} := \{n_0(A), n_-(A), n_+(A)\}$. The previous theorem can be hence restated, that inertia is invariant under congruence.

The proof also gives a useful characterization for the number of non-negative eigenvalues.

Corollary 2.22. *If $A \in \mathcal{H}(V)$, number of non-negative eigenvalues of A equals largest non-negative integer k such that for some subspace $W \subset V$ of dimension k the quadratic form Q_A is non-negative on W, or equivalently, $A_W \geq 0$.*

Sylvester's Law of inertia gives another proof of the fact that strictly positive maps are exactly the maps congruent to the identity, and positive maps are the maps congruent to some projection. More precisely, the positive maps are partitioned to $n+1$ congruence classes depending on their rank, k:th congruence class containing the projections to k-dimensional subspaces. 0:th class contains only the zero map, the only rank 0 positive map, and the n:th class is the class of strictly positive maps.

If one $*$-conjugates with non-invertible, the inertia may change, but in quite obvious way only: some eigenvalues may move to 0. In particular, we have the following even a bit more general version of the law.

Theorem 2.23 (General Sylvester's Law of Inertia)**.** *For $A, B \in \mathcal{N}(V)$ and A is $*$-conjugate of B, if and only if $n_\pm(A) \leq n_\pm(B)$.*

Proof. TODO $\square$

This extension draws a picture about the relation of previously mentioned congcruence classes. We can move to the congruence classes of lower indeces by $*$-conjugation, but cannot move up the ladder: the complexity of quadratic forms cannot increase. One could also think that $*$-congruence for linear maps corresponds to multiplication by non-negative real for real numbers.

2.4.2 Block decomposition

Congruence is a convenient to tool to investigate positivity. The idea is that with conguence we can perform sort of a Gaussian elimination. If $n = 2$ for instance, we can write any real map in the matrix form

$$M = \begin{bmatrix} a & b \\ \overline{b} & c \end{bmatrix}$$

for some $a, c \in \mathbb{R}$ and $b \in \mathbb{C}$. Now if $a \neq 0$, we could eliminate with

$$D = \begin{bmatrix} 1 & -\frac{b}{a} \\ 0 & 1 \end{bmatrix}$$

to get

$$MD = \begin{bmatrix} a & b \\ \overline{b} & c \end{bmatrix} \begin{bmatrix} 1 & -\frac{b}{a} \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} a & 0 \\ \overline{b} & \frac{ac-|b|^2}{a}. \end{bmatrix}$$

If we however eliminate from the other side by D^*, we get

$$D^*MD = \begin{bmatrix} a & 0 \\ 0 & \frac{ac-|b|^2}{a}. \end{bmatrix} =: M'$$

Now D is evidently invertible, it's determinant being 1, so M and M' are congruent. Sylvester's law of inertia tell's us hence that that if $a > 0$ and $\det(M) \geq 0$, then $M \geq 0$.

We can generalize this thinking. For general n if we have decomposition $V = W_1 \oplus W_2$, then we can decompose any mapping M as

$$M = \begin{bmatrix} A & B \\ B^* & C \end{bmatrix},$$

where A, B and C are the *blocks* of M given by $A = P_{W_1} \circ M \circ J_{W_1} = M_{W_1}$, $B = P_{W_1} \circ M \circ J_{W_2}$ and $C = P_{W_2} \circ M \circ J_{W_2} = M_{W_2}$. Now we can generalize the previous elimination: if A happens to be invertible and we let

$$D = \begin{bmatrix} I & -A^{-1}B \\ 0 & I \end{bmatrix}$$

then

$$D^* = \begin{bmatrix} I & 0 \\ -B^*A^{-1} & I \end{bmatrix}$$

and

$$D^*MD = \begin{bmatrix} I & 0 \\ -B^*A^{-1} & I \end{bmatrix} \begin{bmatrix} A & B \\ B^* & C \end{bmatrix} \begin{bmatrix} I & -A^{-1}B \\ 0 & I \end{bmatrix} = \begin{bmatrix} A & 0 \\ 0 & C - B^*A^{-1}B \end{bmatrix}. \tag{2.24}$$

The map $(C - B^*A^{-1}B) : W_2 \to W_2$ is called the *Schur complement* of block A of M, or maybe one should say Schur complement of M with respect to W_1. We denote the Schur complement by M/A.

Now again if A is invertible, $M \geq 0$ if and only if $A > 0$ and $M/A \geq 0$.

This observations leads to convenient characterization for strictly positivity, called Sylvester's criterion. If W_2 is 1-dimensional, M/A is just a real number and M is stricly positive if and only if $A > 0$ and this real number is positive. On the other hand, by computing determinants we see that

$$\det(M) = \det\left(\begin{bmatrix} A & 0 \\ 0 & M/A \end{bmatrix}\right) = \det(A)\det(M/A),$$

as $\det(D) = 1$. Hence M is positive if and only if $\det(M)$ is positive and $A > 0$. Applying the same idea inductively we arrive at

Theorem 2.25 (Sylvester's criterion)**.** *$A \in \mathcal{H}(V)$ is stricly positive if and only for some (and then for any) sequence of subspaces $W_1 \subset W_2 \subset \ldots \subset W_{n-1} \subset W_n = V$ with $\dim(W_m) = m$ we have $\det(A_{W_m}) > 0$ for any $1 \leq m \leq n$.*

One can solve M from 2.24 to arrive at so-called *LDL-decomposition* of M:

$$M = \begin{bmatrix} A & B \\ B^* & C \end{bmatrix} = \begin{bmatrix} I & 0 \\ B^*A^{-1} & I \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & C - B^*A^{-1}B \end{bmatrix} \begin{bmatrix} I & A^{-1}B \\ 0 & I \end{bmatrix}. \tag{2.26}$$

2.5 Loewner Order

Definition 2.27. If $A, B \in \mathcal{H}(V)$, we write that $A \leq B$ (A is smaller than B) if $B - A \geq 0$, $B - A$ is positive. If $B - A$ is strictly positive, we write $A < B$.

We could of course have made such definition immediately after defining positive maps, but now we have proper tools to investigate such order. Proposition 2.5 tells us that such order is indeed partial order on the $\mathbb{R}$-vector space of real maps. More explicitly, we have the following properties:

Proposition 2.28. *(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) If $\lambda I \leq A$, all the eigenvalues of A are at least λ.

Example 2.29. 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 $P_{W_2} = P_{W_1} + P_{W_3} \geq P_{W_1}$. Conversely if $P_{W_1} \leq P_{W_2}$, for any $v \in W_1$ we have $Q_{P_{W_1}}(v) = \|v\|^2 \leq \langle P_{W_2} v, v \rangle = Q_{P_{W_2}}(v)$, where the inequality can hold if and only if $v \in W_2$.

Key thing here is to note what is missing from the standard real ordering: multiplication by positive map doesn't preserve usual ordering. This is the reason many standard arguments don't work for general real maps.

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

Congruence is way to at least partially fix this deficit: it's almost like multiplying by positive number. We have

Proposition 2.30. *If $A \leq B$, then for any C we have $C^* A C \leq C^* B C$.*

Using the previous we can mimic the previous proof to make it work.

Theorem 2.31. *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. If A and B commute, this would work though. We can almost multiply by A^{-1}: $*$-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 sort of want to multiply B^{-1}; so $*$-conjugate by $B^{-\frac{1}{2}}$, but B is in the middle, so this doesn't quite work. But now we can follow the original strategy: since $I \leq X := A^{-\frac{1}{2}}BA^{-\frac{1}{2}}$ we have $X^{-1} \leq I$, that is

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

This is already almost what we wanted: simply $*$-conjugate by $A^{-\frac{1}{2}}$. $\square$

There's one wee bit non-trivial part in the proof: if $I \leq X$ then $X^{-1} \leq I$. But if $I \leq X$, all the eigenvalues of X are at least 1, so all the eigenvalues of its inverse are at most 1, so $X \leq 1$.

Remark 2.32. Alternatively, we could conjugate both sides by $X^{-\frac{1}{2}}$ to arrive at the conclusion. Note that 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. It turns out that this mean, denoted by $G(A, B)$ satifies

$$G(A, B) = G(B, A) \quad \text{and} \quad G(A, B)^{-1} = G(A^{-1}, B^{-1}),$$

and if A and B commute we have $G(A, B) = (AB)^{\frac{1}{2}}$. The defining property of it we used it was that $G(A, B)$ is unique real map with

$$B = G(A, B)A^{-1}G(A, B).$$

The point is: somewhat curiously we can almost do the original proof: just replace multiplication by congruence by squareroot, and replace squareroot of product by geometric mean.

To further highlight the importance of Congruence, we can use it to change map inequalities to usual real inequalities. For instance, one can generalize so called (two variable) arithmetic-harmonic mean inequality, which states that for any two positive real numbers a and b we have

$$\frac{a+b}{2} \geq \frac{2}{\frac{1}{a} + \frac{1}{b}}.$$

This classic inequality, which can be seen as a restatement of the convexity of the map $x \mapsto \frac{1}{x}$, can be verified for instance by multiplying out the denominator and rewriting it as $\frac{(a-b)^2}{ab} \geq 0$.

To prove the matrix version, namely

$$\frac{A+B}{2} \geq (A^{-1}+B^{-1})^{-1}$$

for any $A, B > 0$, we can $*$-conjugate both sides by $A^{-\frac{1}{2}}$ to arrive at

$$\frac{I + A^{-\frac{1}{2}}BA^{-\frac{1}{2}}}{2} \geq 2(I + A^{\frac{1}{2}}B^{-1}A^{\frac{1}{2}})^{-1}.$$

If one writes $X = A^{-\frac{1}{2}}BA^{-\frac{1}{2}}$, this rewrites to

$$\frac{I+X}{2} \geq 2(I + X^{-1})^{-1}.$$

But now since I and X commute, the claim is evident form the scalar inequality.

2.6 Absolute Value

As adjoint behaves as conjugate, it would be natural to guess that

$$|A| := (A^*A)^{\frac{1}{2}},$$

absolute value of a map, would have many similar properties as the standard absolute value. Note that in general we have $|A| \neq |A^*|$, and maps need not even go between the same spaces.

The following list of properties of the absolute value make it clear that this is indeed good definition.

- $|A| \geq 0$ for any $A \in \mathcal{L}(V)$ and $|A| = A$, if and only if $A \geq 0$.
- For any $A \in \mathcal{H}(V)$ we have $-|A| \leq A \leq |A|$, or equivalently $|Q_A(v)| \leq Q_{|A|}(v)$ for any $v \in V$
- For any $v \in V$ we have $\|Av\| = \||A|v\|$.

One might be tempted to think that the previous absolute value leads to an triangle inequality, i.e.

$$|A+B| \leq |A| + |B|,$$

for any $A, B \in \mathcal{L}(V)$, or at least $A, B \in \mathcal{H}^n$. Such inequality doesn't hold, but it's not that far from being true. Like in the real case, one would like to add

$$-|A| \leq A \leq |A| \ \text{ and } \ -|B| \leq B \leq |B|,$$

to get

$$-(|A| + |B|) \leq A + B \leq |A| + |B|.$$

The problem is that we can't make any further conclusions: just because $-Y \leq X \leq Y$, it is not necessarily the case that $|X| \leq Y$. Thinking in quadratic forms we get the inequality

$$|Q_{A+B}(v)| \leq Q_{|A|+|B|}(v), \tag{2.33}$$

for any $v \in V$, but this does not imply that $Q_{|A+B|}(v) \leq Q_{|A|+|B|}(v)$. Indeed $|Q_{A+B}(v)| \leq Q_{|A+B|}(v)$, as we noticed, so the inequality is going to the wrong direction. If however v is an eigenvector of $A + B$, we have $|Q_{A+B}(v)| = Q_{|A+B|}(v)$, and it follows that

$$Q_{|A+B|}(v) \leq Q_{|A|+|B|}(v)$$

holds for eigenvectors v of $|A + B|$. Summing over the eigenvector we see that

$$\mathrm{tr}|A + B| \leq \mathrm{tr}|A| + \mathrm{tr}|B|,$$

so instead of the full inequality, we get inequality for traces. There is a nice generalization for the previous we'll get back to.

2.7 Notes and references

2.8 Ideas

- Normal maps
- Square root of a matrix
- Ellipses map to ellipses
- Sylvester's criterion
- adjoints of vectors
- projections with inclusions
- order of projections
- Loewner order
- Schur complements

- Moore-Penrose pseudoinverse
- (canonical, löwdin) orthogonalization, polar decomposition and orthogonal Procrustes problem
- projection matrices
- Hilbert-Schmidt norm ($\to$ matrix functions?) and inner product
- Hilbert spaces
- Real vs. complex
- Positive definite kernels
- Weakly positive matrices
- Hlawka inequality for determinant
- Trace-characterization of positive maps.
- Splitting positive maps to pseudo square roots
- Product of maps
- AM-GM-HM
- Exponential formula for geometric mean?
- Maximum of matrices with powerlimit

Ideas how to rewrite this section:

- Spectral theorem for positive maps
- Map is positive, if all of its restrictions are. One dimensional maps are positive if and only the scalar is positive.
- Map is real, if all of its restrictions are. One dimensional maps are real if and only the scalar is real.
- Adjoint commutes with restriction. Adjoint of one dimensional map is its conjugate.
- How should one restrict linear mappings? (Use inclusions and finally project)
- Central notion is adjoint

- $*$-conjugation is natural notion with adjoint
- More generally, adjoint of a map $A \in L(V, W)$ is a unique map $A^* \in \mathcal{L}(V, W)$ such that $A \oplus A^*$ is real.
- Increasing sequence of subspaces and restriction with positive determinant $\Rightarrow$ the whole map is positive. Equivalently, map is positive if it has positive determinant and has a subspace where it is positive: $A \geq 0$ if and only if for any $B \geq 0$ we have $\operatorname{tr}(AB) \geq 0$.

Chapter 3

Divided differences

3.1 Motivation

Divided differences are derivatives without limits.

Consider a function $f : \mathbb{R} \to \mathbb{R}$. Its (first) divided difference is defined as

$$
\begin{aligned}
[\cdot, \cdot]_f : \mathbb{R}^2 \setminus \{x \neq y\} \to \mathbb{R} \\
[x, y]_f = \frac{f(x) - f(y)}{x - y}.
\end{aligned}
$$

If f is sufficiently smooth, we should also define $[x, x]_f = f'(x)$: if $f \in C^1(\mathbb{R})$, this gives continuous extension to $[\cdot, \cdot]_f$. Much of the power of divided differences comes however from the fact that they conveniently carry same information even if we do not do such extension.

Consider the case of increasing f. This information is exactly carried by the inequality $[x, y]_f \geq 0$. Again, if f is differentiable, this is equivalent to $f'(x) = [x, x]_f \geq 0$. There are many ways to see this fact, one of the more standard being the mean value theorem: If $x \neq y$, for some ξ between x and y we have

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

Now if the derivative is everywhere non-negative, so are divided differences. Also divided differences are sort of approximations for derivative.

We can push these ideas to higher orders. Second order divided differences should be something that captures second order behaviour of a function. In particular, if $f \in C^2(\mathbb{R})$ has non-negative second derivative everywhere, i.e. it is convex, its second divided difference should be non-negative, and vice versa. Standard definition of convexity is almost what we are looking for: f is convex if for any $x, y \in \mathbb{R}$ and $0 \leq t \leq 1$ we have $tf(x) + (1-t)f(y) \geq f(tx + (1-t)y)$. So if we define the mapping $[\cdot,\cdot,\cdot]_f : \mathbb{R}^2 \times [0,1]$ by $tf(x) + (1-t)f(y) - f(tx + (1-t)y)$, we have $[x, y, t]_f \geq 0$ for any $(x, y, t) \in \mathbb{R}^2 \times [0,1]$ if and only if $f^2(x) \geq 0$ for any $x \in \mathbb{R}$.

There is however much better version for the function. If we write $z = tx + (1-t)y$, we can solve that $t = \frac{z-y}{x-y}$ and express

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

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 is new expression is symmetric in its variables, so actually there's no need to assume anything on the fo x, y and z, just that they're distinct. We can also easily carry this argument to the other direction. If this expression is non-negative any distinct x, y and z, f is convex. This motivates us to crap the previous definition and set instead

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

One would naturally except 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.

3.2 Basic properties

For $n \geq 1$ define $D_n = \{x \in \mathbb{R}^n | x_i = x_j \text{ for some } 1 \leq i \leq n\}$.

Definition 3.1. Let $n \geq 0$. For any real function $f : (a, b) \to \mathbb{R}$ we define the corresponding n'th divided difference $[\cdots]_f : (a, b)^{n+1} \setminus D_{n+1}$ by setting

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

As with the first order divided differences, if we can continuously extend divided differences to the set D_{n+1}, we should do that, and we identify the resulting function with the original one.

Albeit a rather direct generalization for the cases $n = 1$ and $n = 2$, We defined divided differences only for real valued functions, but codomain could just as well any real or complex vector space. it's not very clear why such definition should correspond to anything useful. We have however the following important properties.

Proposition 3.2. *Divided differences are symmetric in the variable and linear in the function, i.e. for any $\alpha, \beta \in \mathbb{R}$, $f, g : (a, b) \to \mathbb{R}$ and $0 < x_0, x_1, \ldots, x_n < b$ we have*

$$[x_0, x_1, \ldots, x_n]_{\alpha f + \beta g} = \alpha [x_0, x_1, \ldots, x_n]_f + \beta [x_0, x_1, \ldots, x_n]_g.$$

In addition, divided differences can be calculated recursively as

$$[x_0, x_1, \ldots, x_n]_f = \frac{[x_0, x_1, \ldots, x_{n-1}]_f - [x_1, \ldots, x_n]_f}{x_0 - x_n}.$$

Proof. Easy to check. □

Also, we have following classic characterization.

Proposition 3.3. *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 of degree at most n−1. In other words, $[x_0, x_1, \ldots, x_n]_f$ is the leading coefficient of the Lagrange interpolation polynomial on pairs $(x_0, f(x_0)), (x_1, f(x_1), \ldots, (x_n, f(x_n))$.*

Proof. Claims are easily derived from each other since if f is itself a polynomial of degree at most n, its lagrange interpolation polynomial is f itself. Recall that the Lagrange 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 in our case the leading coefficient of this polynomial leads exactly to our definition for the divided differences. □

These observation already partially justify the terminology: as higher order derivatives are defined recursively using (first order) derivatives, higher order divided differences can be calculated recursively using (the usual) divided differences.

The most important property of the divided differences is the following.

Theorem 3.4 (Mean value theorem for divided differences)**.** *Let $n \geq 1$ and $f \in C^n(a,b)$. Then for any $x_0, x_1, \ldots, x_n$ we have $\min_{0 \leq i \leq n}(x_i) \leq \xi \leq \max_{0 \leq i \leq n}(x_i)$ such that*

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

Proof. We prove the statement assuming additionally that the divided differences define a continuous function on the whole set $(a,b)^{n+1}$: this will proven later. Note that if one manages to prove the statement for distinct points, one may take sequence of tuples of distinct points, $((x_i^{(j)})_{i=0}^{n})_{j=1}^{\infty}$ converging to $(x_i)_{i=0}^{\infty}$. Now the left-hand side will converge to the respective divided difference (assuming the continuity), and by moving to a convergent subsequence, so will the ξ_n's on the right-hand side. By the continuity of $f^{(n)}$ we are done.

For the case of distinct x_i's note that we have already proven the statement for polynomials of order at most n. By linearity it hence suffices to prove the statement for $C^n(a,b)$ functions vanishing on the set $\{x_i | 0 \leq i \leq n\}$. This we know already for $n = 1$; this is the mean value theorem. Let us prove the statement by induction on n. To simplify notation we may assume that $x_0 < x_1 < \ldots < x_n$. Note that by the mean value theorem, given that $f(x_i) = 0$ for any $0 \leq i \leq n$, we also have $f'(y_i) = 0$ for some $x_i < y_i < y_{i+1}$, for $0 \leq i \leq n-1$. By the induction hypothesis the $(n-1)$:th derivative of f', $f^{(n)}$ has a zero ξ with $x_0 \leq \xi \leq x_n$. But this is exactly what we wanted.

TODO: figure of recursive procedure. □

We'll get back to smoothness in a minute. This is already a very precise sense in which divided differences work like derivatives, up to a constant. In some sense though $\frac{f^{(n)}}{n!}$, the Taylor coefficients are even more natural objects than the pure derivatives. They are the coefficients in the Taylor expansion, and they satisfy very natural Leibniz rule

$$\frac{(fg)^{(n)}(x)}{n!} = \sum_{k=0}^{n} \left(\frac{f^{(k)}(x)}{k!}\right) \left(\frac{g^{(n-k)}(x)}{(n-k)!}\right),$$

which is of course just a formula for polynomial convolution.

Divided differences enjoy similar Leibniz formula, which is related to a generalization of Taylor expansion, called Newton expansion. In Newton expansion we first fix a sequence of points $x_0, x_1, \ldots x_n \in (a,b)$, say pairwise distinct for starters. For $f : (a,b) \to \mathbb{R}$ and

$x \in (a, b)$ we may start a process of rewriting

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

By taking first $1, 2, \ldots$ terms of the sum, one obtains Newton form of interpolating polynomial for the first $1, 2, \ldots,$ points of the sequence $x_0, x_1, \ldots$. If the points x_i coincide, the previous coincides with the usual Taylor expansion and, as usual, the joy is that we can approximate $[x, x_0, x_1, \ldots, x_n]_f$ by a n'th derivative of f.

TODO: Smoothness: Tohoku

3.3 Cauchy's integral formula

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

Lemma 3.5 (Cauchy's integral formula for divided differences)**.** *If γ is a closed counter-clockwise curve enclosing the numbers $x_0, x_1, \ldots, x_n$, we have*

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

Proof. Easy induction, by taking Cauchy's integral formula as a base case. Alternatively, the claim is a direct consequence of the Residue theorem. □

If all the points coincide, we get the familiar formula for the n'th derivative. Also, if f is polynomial of degree at most $n - 1$, the integrand decays as $|z|^{-2}$ and hence the divided differences vanish. Also, for $z \mapsto z^n$ one can use the formula to calculate the n'th divided difference with a residue at infinity. Formula is slightly more concisely expressed by writing for a sequence $X = (x_i)_{i=0}^n$ $p_X(x) = \prod_{i=0}^n (x - x_i)$. Also if one shortens $[X]_f = [x_0, x_1, \ldots, x_n]_f$, we have

$$[X]_f = \frac{1}{2\pi i} \int_\gamma \frac{f(z)}{p_X(z)} dz.$$

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

Example 3.6. For instance we may express the Lagrange interpolation polynomial of a analytic function f and sequence $X = (x_i)_{i=0}^n$ by

$$P_X(x) = \frac{1}{2\pi i}\int_\gamma \frac{p_X(x) - p_X(z)}{x - z}\frac{f(z)}{p_X(z)}dz = [X]_{f[x,\cdot]p_X}.$$

TODO: use the previous for some tricks. Lagrange interpolation polynomial, Leibniz formula for divided differences.

3.4 k-tone functions

Definition 3.7. $f : (a, b) \to \mathbb{R}$ is called k-tone if for any $X = (x_i)_{i=0}^n$ of distinct points we have

$$[X]_f \geq 0,$$

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

As we noticed, 1-tone and 2-tone functions are exactly the monotone increasing and convex functions. The terminology is not very established, and such functions are also occasionally called k-monotone or k-convex.

Mean value theorem for divided differences tells us that C^k k-tone functions are exactly the functions with non-negative k'th derivative. In some sense the further smoothness assumption is not that much of a game changer. It turns out k-tone functions are always k times differentiable in a weak sense (?), and the weak derivative is non-negative. One can also usually use regularization techniques discussed in ? to reduce a problem about general k-tone functions to smooth k-tone functions. In general:

Philosophy 3.8. One should not worry about smoothness issues.

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

Proposition 3.9. *For any positive integer k and open interval (a, b) $P^{(k)}(a, b)$ is a closed (under pointwise convergence) convex cone.*

Proof. Convex cone property is immediate form the linearity of divided differences. Also, if $f_i \to f$ pointwise, the respective divided differences converge, so also the closedness is clear. □

Proposition 3.10. *$P^{(k)}$ 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. For $f \in C^k$ the statement is immediate form the mean value theorem. For more general functions: regularizations TODO. □

3.5 Basis k-tone functions

We noticed that k-tone functions correspond more or less to functions with non-negative k'th derivative. In other words, k-tone functions should be k-fold integrals of positive functions, at least in sufficiently smooth setting. For instance $f : (a,b) \to \mathbb{R}$ is increasing and smooth if and only if it's of the form

$$f(x) = \int_{x_0}^{x} \rho(t)dt \tag{3.11}$$

for some positive $\rho \in C^\infty(a,b)$ and $x_0 \in (a,b)$, up to a constant at least. For non-smooth case, we could require ρ only to be a positive L^1-function: this gives us absolutely continuous increasing functions. If we further drop ρ but replace the Lebesgue measure by an arbitrary Radon measure μ, we get every right-continuous increasing function. Measuretheoretically these are already all the increasing functions, although we miss some functions like $\chi_{(0,\infty)}$.

If $\mu = \delta_0$, for instance, $f = \chi_{[0,\infty)}$. One could think that δ_0 gives a jump for f at 0. More generally, if μ is positive linear combination if m (distinct) Dirac deltas, f is a function with m jumps. Now every Radon measure is a weak limit of positive linear combination Dirac deltas, so every increasing function is limit of finite sums of jump functions, at least in some weak sense.

This is fact is actually contained in 3.11: we may rewrite

$$f(x) = \int_a^b \chi_{[t,\infty)}(x)d\mu(t),$$

f is essentially sum of functions of the form $\chi_{[t,\infty)}$, again up to a constant. We will call those the basis functions for

The point is: whenever something holds for any step function, it should hold for any increasing function. In this context by "something" I mean linear inequalities: if ν is a signed Radon measure such that for any step function $\chi_{[t,\infty)}$ we have

$$\int \chi_{[x,\infty)}(t)d\nu(t),$$

then also

$$\int f(t) d\nu(t)$$

for any increasing function. Actually we should also require that $\int d\nu(t) = 0$. I'm being deliberately vague about the domains, they don't really matter too much.

Things get much more interesting when we move to k-tone functions of higher order. For k-tone functions, i.e. convex functions we can make similar statements.

We can write any (smooth enough) convex function in the form

$$f(x) = \int_{x_0}^{x} \int_{x_0}^{x_1} \rho(t) dt dx_1,$$

at least up to a constant and linear term. By simple partial integration this can be rewritten as

$$f(x) = \int_{x_0}^{x} (x - t)\rho(t) dt,$$

or even, better, as

$$f(x) = \int_{a}^{b} (x - t)_+ \rho(t) dt,$$

where $(x-t)_+$ denotes $\max(0, x-t)$. What this means is that the functions $(\cdot - t)_+$ work as a basis functions for convex functions, up to a affine term. By affine transformation we could equivalently take the functions of the form $|\cdot - t|$ as a basis functions.

Now if a linear equality holds for functions of the form $|x-t|$, it holds for any convex function. So since for any $x_1, x_2, \ldots, x_m \in \mathbb{R}$ we have

$$\sum_{1 \le i \le m} |x_i - t| \ge m \left|\frac{\sum_{1 \le i \le m} x_i}{m} - t\right|,$$

also for any convex function

$$\sum_{1 \le i \le m} f(x_i) \ge m f\left(\frac{\sum_{1 \le i \le m} x_i}{m}\right),$$

Jensen's inequaltity.

3.6 Majorization

Of course there should be a larger family of inequalities which hold for functions of the form $|x-t|$: it turns out that there is a rather simple characterization for such inequalities, by *majorization.*

Definition 3.12. Let $x = (x_i)_{i=1}^n$ and $y = (y_i)_{i=1}^n$ be two sequences of reals. We say that y majorizes x, and write $x \prec y$, if TODO

Theorem 3.13 (Polya-Hardy-Littlewood-Karamata-Inequality)**.** *Let (a, b) be an open interval, n positive integer, and $x = (x_i)_{i=1}^n \in (a, b)^n$ and $y = (y_i)_{i=1}^n \in (a, b)^n$. Then the following are equivalent.*

1. *$x \prec y$*
2. *For any real number t we have*
$$\sum_{1 \le i \le n} |x_i - t| \le \sum_{1 \le i \le n} |y_i - t|.$$
3. *For any convex $f : (a, b) \to \mathbb{R}$ we have*
$$\sum_{1 \le i \le n} f(x_i) \le \sum_{1 \le i \le n} f(y_i).$$

Proof. TODO $\square$

3.7 Spectral majorization

In addition to being convenient notion to discuss k-tone functions, majorization explains many phenomena related to spectra of real maps. Basic fact is the following.

Proposition 3.14. *If $A \le B$, the spec$(A) \prec_1$ spec(B).*

Proof. By Theorem (?) it suffices to check that for any $t \in \mathbb{R}$ we have $\#([t, \infty) \cap \text{spec}(A)) \le \#([t, \infty) \cap \text{spec}(B))$. Translating by tI this amounts to proving that if $A \le B$, B has at least as many non-negative eigenvalues as A. But this follows from Lemma 2.22. $\square$

TODO: Higher orders, majorization

3.8 TODO

- Mean value theorem, coefficient of the interpolating polynomial
- Basic properties, product rule.

- k-tone functions, smoothness, and representation
- Majorization, Jensen and Karamata inequalities, generalizations, and corollaries concerning spectrum and trace functions. Schur-Horn conjectures and Honey-Combs
- Tohoku contains nice proof of Lidskii inequality
- How to understand the inequalities arising from k-tone functions: is there nice way to parametrize the tuples coming from the k-majorization.
- For $k = 3$ and 3 numbers, it's all about the biggers number: one with the largest largest number dominates.
- The previous probably generalizes: for k-tone functions and k numbers on both sides, with all polynomials of degree less than k vanishing on both tuples, one with largest largest value dominates, or equivalently, it's all about the constant term. This is clearly necessary, by is it also sufficient? Should be: express the whole thing as an integral, differentiate with respect to the constant term, and finally interpret as a divided difference.
- What if we add more terms: is there simple characterization? Why have similar integral representation, and can probably differentiate.
- Peano Kernels: Smoothness properties, Bernstein (?) polynomials as examples.
- Opitz formula
- Regularization techniques
- Notion of midpoint-convexity should generalize by regularization techniques.
- Should Legendre transform generalize to higher orders? For smooth enough functions probably with derivatives being inverses of each other, but what is the correct definition? And is it of any use? Maybe differentiating $k-2$ times and then having similar characterization. Is there higher order duality?
- Is there elementary transformations for k-tone Karamata?

Chapter 4

Matrix functions

TODO:

- Basic definition
- Equivalent definitions
- Continuity properties
- Examples
- Calculating with matrix functions
- Smoothness properties, derivative formulas, Hadamard product
- Cauchy's integral formula
- Jordan block formula

Chapter 5

Pick-Nevanlinna functions

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

Pick functions have many interesting properties related to positive matrices and that is why they are central objects to the theory of matrix monotone functions.

5.1 Basic properties and examples

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 $\beta \in \overline{\mathbb{H}}_+$. Actually real constants are the only Pick functions failing to map $\mathbb{H}_+ \to \mathbb{H}_+$: non-constant analytic functions are open mappings.

Sum of two Pick functions is a Pick function and one can multiply a Pick function by non-negative constant to get a new Pick function. Same is true for composition.

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 $\lambda_1, \ldots, \lambda_N \in \mathbb{H}_+$. So far we have constructed our function by adding simple poles to the closure of lower half-plane. We could further add poles of higher order at lower half plane, and change residues and so on, but then we have to be a bit more careful.

There are (luckily) more interesting examples: all the functions of the form x^p where $0 < p < 1$ are Pick functions. To be precise, one should choose branch for the previous so that they are real at positive real axis. Also log yields Pick function when branch is chosen properly i.e. naturally again. 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.

We observe the following useful fact.

Proposition 5.1. *If $(\varphi_i)_{i=1}^{\infty}$ is a sequence of Pick functions converging locally uniformly, the limit function is also a Pick function.*

Proof. Locally uniform limits of analytic functions are analytic. Also the limit function has evidently non-negative imaginary part. □

This is one of the main reasons we include real constants to Pick functions, although they are exceptional in many ways. Note that for any $z \in \mathbb{H}_+$ we have $\log(z) = \lim_{p\to 0^+}(z^p - 1)/p$: log can be understood as a limit of Pick functions. There's actually a considerable strengthening of the previous result.

Proposition 5.2. *If $(\varphi_i)_{i=1}^{\infty}$ is a sequence of Pick functions converging pointwise, the limit function is also a Pick function.*

We will not prove this quite surprising result yet.

5.2 Schur functions

As we have noticed, Pick functions need not be injections or surjections. Some are both: simple examples are functions of the form $\alpha z + \beta$ and $\frac{\alpha}{\lambda - z} + \beta$ for $\alpha > 0$ and $\beta, \lambda \in \mathbb{R}$. And that's all.

Before trying to understand why is that, we have to change the point of view. All the previous functions are rational functions, but even more is true: they are all Möbius transformations. Möbius transformations are analytic bijections of extended complex plane i.e. Riemann sphere, to itself. Our examples all exactly those Möbius transformation which map the extended real axis to itself, and don't change the orientation, so the upper half-plane is mapped to itself and not to the lower half-plane. When viewed as a part of the Riemann sphere, upper half-plane is just a hemisphere. Of course it shouldn't matter too much which hemisphere we are looking at, so we could also consider mappings from unit disc to itself (or closed unit disc, to be precise). These mappings are called *Schur* *functions* and class of Schur functions is denoted by $\mathcal{S}$. It's then natural to conjecture that bijective Schur functions are exactly the Möbius transformations which map unit circle to unit circle, and don't change the orientation so that the inside is mapped to the inside.

These claims are easily derivable from each other as follows. Consider the pair of Möbius transformations

$$\begin{aligned} \xi : \mathbb{D} \to \mathbb{H}_+ \qquad \xi(z) &= i\frac{1-z}{1+z} \\ \eta : \mathbb{H}_+ \to \mathbb{D} \qquad \eta(z) &= \frac{i-z}{i+z}. \end{aligned}$$

They are inverses of each other and map the (open) unit disc to upper half-plane and back, respectively. Now take any bijective Schur function $\psi : \mathbb{D} \to \mathbb{D}$. Then $\varphi = \xi \circ \psi \circ \eta$ is bijective Pick function. Similarly one could invert $\psi = \eta \circ \varphi \circ \xi$. This means that bijections can be paired: if all bijective Pick functions are Möbius transformations, so are all bijective Schur functions, since non-Möbiusness on one side would give rise to non-Möbiusness on the other side.

Still before proving anything we should think about this relation a bit further. We noticed that every bijective Pick function has a corresponding Schur function pair. This correspondence is however by no means unique, it was merely our choice to choose such ξ and η. Still, there is need to restrict ourselves to bijections anymore. If one takes **any** Schur function $\psi : \mathbb{D} \to \mathbb{D}$ we can form the corresponding Pick function by taking $\varphi = \xi \circ \psi \circ \eta$. This gives rise to bijection $\mathcal{S} \to \mathcal{P}$, and the inverse should be rather obvious by now. Of course, it's not a big surprise that there would be such bijection, that is to say that the sets are equal in size, but our bijection preserves composition of functions. All this is to say that in some sense these classes are almost the same.

One should be a bit more careful here though: we have included also real constant functions to our class $\mathcal{P}$ and we should also add unimodular constants to $\mathcal{S}$. For these the bijection doesn't quite work; we can mostly do a natural extension, but then one would be forced to map the constant function -1 to the constant ∞. This means that we should add the constant infinity function to our Pick functions. We will not do this, as it would change the whole business to Riemann sphere, since it will bring other technical problems, but we will try to indicate when you should think about this extension.

If one only thinks about composition one can of course do lot more. Take any simply connected domain in $U \subset \mathbb{C}$. By Riemann mapping theorem there's a analytic bijection $\xi_U : \mathbb{D} \to U$. For the domain U we could define similar class of functions, and via ξ_U and it's inverse we could connect the classes. Again, one should be a bit careful with the boundary.

In many ways Pick and Schur functions are most natural of these classes: they are closed under addition and multiplication, respectively. Also, they both contain the identity of the respective operations, so these properties are barely true.

5.2.1 Automorphisms of the unit disc

As mentioned, the functions ξ and η are not unique. All such mappings are however of a very simple form. If $\rho : \mathbb{D} \to \mathbb{D}$ is analytic bijection, the function $\xi \circ \rho$ is an analytic bijection from unit disc to upper half-plane. Conversely, if ξ_1 is an analytic bijection from unit disc to upper half-plane, $\eta \circ \xi_1$ is an analytic bijection. Hence to understand the diversity of the analytic mappings from $\mathbb{D}$ to $\mathbb{H}_+$, we need to understand the analytic self-maps of the unit disc.

All analytic bijections from the unit disc to itself, called the automorhphisms of the unit disc, are given by

$$\rho_{a,\omega}(z) = \omega \frac{a - z}{1 - \overline{a}z},$$

where $a \in \mathbb{D}$ and $\omega \in \mathbb{S}$. We will write $\rho_a = \rho_{a,1}$. As $|1 - \overline{a}z|^2 - |a - z|^2 = (1 + |a||z|^2 - \overline{a}z - \overline{z}a) - (|a|^2 + |z|^2 - \overline{a}z - \overline{z}a) = (1 - |z|^2)(1 - |a|^2)$, one readily sees that such mappings are indeed analytic bijections. Schwarz lemma explains why these are the all.

5.3 Schwarz lemma

At first sight one might not guess that Pick function have strong regularity properties. In some sense they however work like Schur functions, and they feel much more restrictive. If one considers a Schur function ψ mapping zero to itself very classic lemma of Schwarz states that $|\psi(z)| \leq z$ for any $z \in \mathbb{D}$. For completeness let's review a standard proof.

Theorem 5.3 (Schwarz lemma)**.** *Let $\psi : \mathbb{D} \to \mathbb{D}$ be analytic such that $\psi(0) = 0$. Then $|\psi(z)| \leq |z|$ for any $z \in \mathbb{D}$ and hence also $|\psi'(0)| \leq 1$. If $|\psi(z)| = |z|$ for some $z \in \mathbb{D} \setminus \{0\}$ or $|\psi'(0)| = 1$, $\psi(z) = \omega z$ for some $\omega \in \mathbb{S}$.*

Proof. By the assumption ψ can be represented as a locally uniformly convergent power series in unit disc, of the form $\sum_{n=1}^{\infty} a_n z^n$. Now $\psi(z)/z := \sum_{n=0}^{\infty} a_{n+1} z^n$ defines also an analytic function in unit disc. For any $0 < r < 1$, by the maximum modulus principle, we have

$$\sup_{z \in \mathbb{D}(0,r)} \left| \frac{\psi(z)}{z} \right| \leq \sup_{z \in \mathbb{S}(0,r)} \left| \frac{\psi(z)}{z} \right| \leq \frac{1}{r},$$

so by letting $r \to 1$ we get $\sup_{z \in \mathbb{D}} \left| \frac{\psi(z)}{z} \right| \leq 1$ and hence for any $z \in \mathbb{D}$

$$|\psi(z)| \leq \left| \frac{\psi(z)}{z} \right| |z| \leq |z|$$

TODO $\square$

One might argue that this proof hides all the mysteriousness in the maximum modulus principle, which is quite surprising itself too. Maximum modulus principle can be seen as a consequence of the Cauchy's integral formula.

There is somewhat better form of the Schwarz lemma, called the invariant form or Schwarz-Pick theorem.

Theorem 5.4 (Schwarz-Pick theorem)**.** *Let $\psi : \mathbb{D} \to \mathbb{D}$ be analytic. Then for any $z_1, z_2 \in \mathbb{D}$ we have*

$$\left| \frac{\psi(z_1) - \psi(z_2)}{1 - \overline{\psi(z_1)}\psi(z_2)} \right| \leq \left| \frac{z_1 - z_2}{1 - \overline{z_1} z_2} \right|,$$

and

$$\frac{|\psi'(z_1)|}{1 - |\psi(z_1)|^2} \leq \frac{1}{1 - |z_1|^2}.$$

If the equality holds in one of the inequalities, ψ is an automorphism of the unit disc.

Note that one obtains the usual Schwarz lemma if $z_1 = 0 = \psi(z_1)$. One may check that if ψ is indeed automorphism, the inequalities hold as equalities.

Proof. Consider the map $\psi_1 = \rho_{\psi(z_1)} \circ \psi \circ \rho_{z_1}$. The claim follows by using the previous form of the Schwarz lemma for the ψ_1 and point z_2. $\square$

There are many ways to think about these results. One immediate interpretation is that Schur functions are in some precise sense very rigid. Knowing a Schur function in a point immediately restricts the values the functions might attain at some other points. We could make this more precise. If we consider the points z_1, z_2 and the value $\psi(z_1)$ how exactly is the value $\psi(z_2)$ restricted? If $z_1 = 0 = \psi(z_1)$, we are in the original Schwarz lemma and $\psi(z_2)$ is simply restricted in a closed disc of radius $|z_2|$ around 0. More generally, the restriction is bit more subtle, but the values are still restricted in a closed disc. Indeed, the set of admissible $\psi(z_2)$ is inverse of image of disc $\mathbb{D}(0, r)$, where

$$r = \left| \frac{z_1 - z_2}{1 - \overline{z_1} z_2} \right|,$$

under the map $\rho_{\psi(z_1)}$, thus a disc.

Other interpretation is that we may factor Schur functions. If ψ is a Schur function with $\psi(z) = 0$, then also $\frac{\psi(z)}{z}$ is a Schur function; this is the main step in the proof of Schwarz lemma. More generally, for any Schur function ψ, the function

$$\psi_{z_0}(z) = \frac{1 - \overline{z_0} z}{z_0 - z} \frac{\psi(z_0) - \psi(z)}{1 - \overline{\psi(z_0)}\psi(z)}$$

is also a Schur function for any $z_0 \in \mathbb{D}$. In particular, if $\psi(z_0) = 0$ for some $z_0 \in \mathbb{D}$, we can write

$$\psi(z) = \frac{z - z_0}{1 - \overline{z_0} z} \psi_{z_0}(z).$$

There is a correponding variant of the Schwarz-Pick theorem for the upper half-plane, for the Pick functions.

Theorem 5.5 (Schwarz-Pick theorem for the upper half-plane)**.** *Let $\varphi : \mathbb{H}_+ \to \mathbb{H}_+$ be analytic. Then for any $z_1, z_2 \in \mathbb{H}_+$ we have*

$$\left| \frac{\varphi(z_1) - \varphi(z_2)}{\varphi(z_1) - \overline{\varphi(z_2)}} \right| \leq \left| \frac{z_1 - z_2}{z_1 - \overline{z_2}} \right|.$$

Proof. Apply the Schwarz-Pick theorem to the map $\xi \circ \varphi \circ \eta$. □

In a way there's no natural variant of the original Schwarz lemma for the upper half-plane. Direct analogue would be to consider Pick functions with $\varphi(i) = i$, but one might wonder if this is really any simpler. The problem is that there's no canonical center to the upper half-plane, although we've been implicitely taking it as i (by choosing ξ and η). One might however argue that there's no canonical center to the unit disc either. With automorphisms ρ_a we may map any point of the unit disc to any other point. For any Schur function ψ and $a \in \mathbb{D}$ we can consider the map $\rho_a \circ \psi \circ \rho_a$. TODO

5.3.1 Poincaré metric

There's really nice interpretation for the Schwarz-Pick theorem. The unit disc $\mathbb{D}$ can be equipped with a hyperbolic metric, which for any two points $z_1, z_2 \in \mathbb{D}$ is given by

$$2 \tanh^{-1} \left| \frac{z_1 - z_2}{1 - \overline{z_1} z_2} \right|.$$

This is space is called Poincaré disc. One may check that the previous is indeed a metric, and automorhisms of the unit disc are exactly the isometries of this space. Now Schwarz-Pick theorem states that any Schur function decreases distances i.e. Schur functions are contractions on Poincaré disc.

Because of this intepretation, we abuse the notation and write

$$\rho(z_1, z_2) := \rho_{z_1}(z_2) = \frac{z_1 - z_2}{1 - \overline{z_1} z_2}.$$

Now the metric is given by

$$2 \tanh^{-1} |\rho(z_1, z_2)|.$$

Analogously one could interpret that the Pick functions are contractions in Poincaré upper half-plane, metric space in upper half-plane in which the metrix is given by

$$2\tanh^{-1}\left|\frac{z_1 - z_2}{z_1 - \overline{z_2}}\right|.$$

5.3.2 Pick Matrices

Schwarz-Pick theorem was about restricting Schur functions at one point. If we fix two points instead, things get more complicated. Let's say we have a Schur function ψ and we know that $\psi(\frac{1}{2}) = \frac{1}{3}$ and $\psi(\frac{i}{2}) = \frac{i}{3}$. Surely there are such Schur functions, since $|\rho(\frac{1}{3}, \frac{i}{3})|^2 = \frac{9}{41} < \frac{8}{17} = |\rho(\frac{1}{2}, \frac{i}{2})|^2$, but at least Schwarz-Pick theorem doesn't immediately fix such function, which it would do should we change the $\frac{1}{3}$'s to $\frac{1}{2}$. The question is: what kind of values could a Schur function attain at some other point, say at 0.

There are two immediate restrictions: values at $-\frac{1}{2}$ and $\frac{1}{2}$ restrict the value at 0 in the intersection of two discs. The value at $-\frac{1}{2}$ restricts the value in a closed disc of radius $\frac{16}{35}$ at $-\frac{9}{35}$ and, symmetrically, the value at $\frac{1}{2}$ of radius $\frac{16}{35}$ at $\frac{9}{35}$. Considering these bounds, there's nothing in principle preventing us from having $\psi(0) = 0$. This value is however not attainable. The problem is that if $\psi(0) = 0$, then also $\tilde{\psi}(z) := \frac{\psi(z)}{z}$ should be Schur function. But $\tilde{\psi}(\frac{1}{2}) = \frac{2}{3}$ and $\tilde{\psi}(\frac{i}{2}) = \frac{2i}{3}$. But $|\rho(\frac{2}{3}, \frac{2i}{3})|^2 = \frac{72}{97} > |\rho(\frac{1}{2}, \frac{i}{2})|^2$ violating the Schwarz-Pick theorem.

TODO (Introduce Pick matrices earlier)

5.4 Pick-Nevanlinna interpolation theorem

We have seen that the Schur functions are contractions in Poincaré disc and Pick function are contractions in Poincaré upper half-plane. Not every contraction in these spaces is however analytic. Take disc for instance. It turns out that $z \mapsto \Re(z)$ is **not** contraction in the Poincaré disc, but for small enough positive ε, $z \mapsto \varepsilon\Re(z)$ definitely is. One could immediately push this example to upper half-plane, by using the maps ξ and η, or do something similar from the scratch and take, say, $z \to i + \varepsilon\Re(1 + 2i - \frac{2i}{z+i})$. In the both examples the philosophy is the same: the hyperbolic metric in both cases look locally like (a scaled version of) standard metric. So if we map everything to small neighbourhood everyhing behaves nicely. In the disc, this is very simple, just scale. In the upper half-plane, we can for instance first map everything to some compact set in the upper half-plane. Then break the analyticity and scale to get contractivity.

5.4.1 Pick Matrices

There is however rather simple characterization for Schur functions requiring a bit more than contractivity. It turns out, that the condition "$\psi : \mathbb{D} \to \mathbb{D}$ is contraction" is equivalent to the matrix

$$\begin{bmatrix} \frac{1-|\psi(z_1)|^2}{1-|z_1|^2} & \frac{1-\overline{\psi(z_1)}\psi(z_2)}{1-\overline{z_1}z_2} \\ \frac{1-\overline{\psi(z_2)}\psi(z_1)}{1-\overline{z_2}z_1} & \frac{1-|\psi(z_2)|^2}{1-|z_2|^2} \end{bmatrix}$$

being positive. Such matrix is called Pick matrix. Conveniently, even the condition "ψ maps $\mathbb{D}$ to itself" is built-in in the positivity. This is not entirely obvious but it may straighforwardly, although tediously verified by checking that the Schwarz-Pick inequality is equivalent to the determinant of the Pick matrix being non-negative.

Similarly, for any sequence of say n points in the unit disc we may form the matrix

$$\begin{bmatrix} \frac{1-|\psi(z_1)|^2}{1-|z_1|^2} & \frac{1-\overline{\psi(z_1)}\psi(z_2)}{1-\overline{z_1}z_2} & \cdots & \frac{1-\overline{\psi(z_1)}\psi(z_n)}{1-\overline{z_1}z_n} \\ \frac{1-\overline{\psi(z_2)}\psi(z_1)}{1-\overline{z_2}z_1} & \frac{1-|\psi(z_2)|^2}{1-|z_2|^2} & \cdots & \frac{1-\overline{\psi(z_2)}\psi(z_n)}{1-\overline{z_2}z_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1-\overline{\psi(z_n)}\psi(z_1)}{1-\overline{z_n}z_1} & \frac{1-\overline{\psi(z_n)}\psi(z_2)}{1-\overline{z_n}z_2} & \cdots & \frac{1-|\psi(z_n)|^2}{1-|z_n|^2} \end{bmatrix}$$

TODO:

- Poincaré metric: discs are discs, Apollonius circle
- Pick matrices
- 2 proofs of the Pick-Nevanlinna interpolation theorem
- Hindmarsh's theorem
- Pick-Nevanlinna-Herglotz representation theorem
- Compactness
- Examples of representing measures behind functions and functions behind representing measures
- "Pointed" Pick-Nevanlinna interpolation: two proofs (one with Pick-Nevanlinna, one with congretely extending)
- Spectral commutant lifting theorem

Chapter 6

Monotone and Convex matrix functions

We already introduced monotone and convex matrix functions in the introduction, but now that we have properly defined and discussed underlying structures we should take a deeper look. As mentioned, monotone and convex matrix functions are sort of generalizations for the standard properties of reals, and this is why we should undestand which of the phenomena for the real functions carry to matrix functions and which do not.

We will start with the matrix monotone functions; much of the discussion carries quite directly to the convex case.

6.1 Basic properties of the matrix monotone functions

We first state the definition.

Definition 6.1. 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, if for any $A, B \in \mathcal{H}^n_{(a,b)}$, 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 $P_n(a,b)$. One immediately sees that that all the matrix monotone functions are monotone as real functions.

Proposition 6.2. *If $f \in P_n(a,b)$, f is increasing.*

Proof. Take any $a < x \leq y < b$. Now for $xI, yI \in \mathcal{H}^n_{(a,b)}$ we have $xI \leq yI$ so by definition

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

from which it follows that $f(x) \leq f(y)$. This is what we wanted. $\square$

Actually, increasing functions have simple and expected role in n-monotone matrices.

Proposition 6.3. *Let (a, b) be an open interval and $f : (a, b) \to \mathbb{R}$. Then the following are equivalent:*

(i) f is increasing.

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

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

Proof. TODO $\square$

The equivalence of the first two is almost obvious and from this point on we shall identify 1-monotone and increasing functions. But the third point is very important: it is exactly the non-commutative nature which makes the classes of higher order interesting.

Let us then have some examples.

Proposition 6.4. *For any positive integer n, open interval (a, b) and $\alpha, \beta \in \mathbb{R}$ such that $\alpha \geq 0$ we have that $(x \mapsto \alpha x + \beta) \in P_n(a, b)$.*

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. $\square$

That was easy. It's not very easy to come up with other examples, though. Most of the common monotone functions fail to be matrix monotone. Let's try some non-examples.

Proposition 6.5. *Function $(x \mapsto x^2)$ is not n-monotone for any $n \geq 2$ and any open interval $(a, b) \subset \mathbb{R}$.*

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

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

Note that $H^2 \geq 0$, but as we have seen in TODO, $AH + HA$ need not be positive! Also, if H is small enough, H^2 is negligible compared to $AH + HA$. We are ready to formulate our proof strategy: find $A \in \mathcal{H}^n_{a,b}$ and $\mathbb{H}^n_+$ such that $AH + HA \not\geq 0$. Then choose parameter $t > 0$ so small that $A + tH \in \mathcal{H}^n(a, b)$ and

$$(A + tH)^2 - A^2 = t(AH + HA + tH^2) \not\geq 0$$

and set the pair $(A, A + tH)$ as the counterexample.

TODO $\square$

In a similar manner one could show the similar statement for the functions $(x \mapsto x^k)$.

At this point several other important properties of the matrix monotone functions should be clear.

Proposition 6.6. *For any positive integer n and open interval (a, b) the set $P_n(a, b)$ is a convex cone, i.e. it is closed under taking summation and multiplication by non-negative scalars.*

Proof. This is easy: closedness under summation and scalar multiplication with non-negative scalars correspond exaclty to the same property of positive matrices. $\square$

We should be a bit careful though. 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; similar statement holds for increasing functions. Similarly, taking maximums doesn't preserve monotonicity.

Proposition 6.7. *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 $n = 1$.

Fix open interval (a, b), positive integer $n \geq 2$ and two functions $f, g \in P^n(a, b)$. Take any two $A, B \in \mathcal{H}^n_{(a,b)}$ with $A \leq B$. Now $f(A) \leq f(B) \leq \max(f, g)(B)$ 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? This is an interesting question and we will come back to it a bit later, but it turns out that however you try to define it, you can't satisfy the above inequality.

We still need proper counterexamples though. Let's try $f \equiv 0$ and $g = \mathrm{id}$. So far the only n-monotone functions we know are affine functions so that's essentially our only hope for counterexamples.

TODO $\square$

Similarly we have composition and pointwise limits.

Proposition 6.8. *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 $A, B \in \mathcal{H}^n_{(a,b)}$ with $A \leq B$. By assumption $f(A) \leq f(B)$ and $f(A), f(B) \in \mathcal{H}^n_{(c,d)}$ so again by assumption, $g(f(A)) \leq g(f(B))$, our claim. $\square$

Proposition 6.9. *If n-monotone functions $f_i : (a, b) \to \mathbb{R}$ converge pointwise to $f : (a, b) \to \mathbb{R}$ as $i \to \infty$, also f is n-monotone.*

Proof. As always, fix $A, B \in \mathcal{H}^n_{(a,b)}$ with $A \leq B$. Now by assumption

$$f(B) - f(A) = \lim_{i\to\infty} f_i(B) - \lim_{i\to\infty} f_i(A) = \lim_{i\to\infty} (f_i(B) - f_i(A)) \geq 0,$$

so also $f \in P_n(a, b)$. $\square$

We shall be using especially the previous result a lot.

One of the main properties of the classes of matrix monotone functions has still avoided our discussion, namely the relationship between classes of different orders. We already noticed that matrix monotone functions of all orders all monotonic, or $P_n(a, b) \subset P_1(a, b)$ for any $n \geq 1$. It should not be very surprising that we can make much more precise inclusions.

Proposition 6.10. *For any open interval (a, b) and positive integer n we have $P_{n+1}(a, b) \subset P_n(a, b)$.*

Proof. TODO $\square$

One might ask whether these inclusions are strict. It turns out they are, as long as our interval is not the whole $\mathbb{R}$. We will come back to this.

There are also more trivial inclusions: $P_n(a, b) \subset P_n(c, d)$ for any $(a, b) \supset (c, d)$. More interval, more matrices, more restrictions, less functions. To be precise, we only allowed functions with domain (a, b) to the class $P_n(a, b)$, so maybe one should say instead something like: if $(a, b) \supset (c, d)$ and $f \in P_n(a, b)$, then also $f\big|_{(c,d)} \in P_n(c, d)$. We will try not to worry too much about these technicalities.

6.2 Pick functions are monotonic

One of the main reasons for introducing Pick functions is that they are monotone of all orders. After understanding real valued monotone functions, it should be clear how to prove the previous statement: as Pick functions are essentially sums of functions of the form $x \mapsto \frac{1}{\lambda - x}$, we should verify that these are monotone. Also λ should not have effect on anything so we only need the following. But the increasing nature of the function of $x \mapsto -\frac{1}{x}$ is something we know already. We have hence proved

Theorem 6.11. *If $f \in P(a,b)$, then $f \in P_n(a,b)$ for any $n \geq 1$.*

This is obviously why we chose the notation P_n for classes of matrix monotone functions.

TODO:

- Examples
- Pick functions are monotone
- Heaviside function
- Trace inequalities: if f is monotone/convex then $\mathrm{tr} f$ is monotone/convex. Proof idea: we may write $\mathrm{tr} f$ as a limit of finite sum of translations of Heaviside functions (monotone case) or absolute values (convex case), so its sufficient to prove the claim for these functions. For monotone case it hence suffices to prove that if $A \leq B$, B has at least as many non-negative eigenvalues as A. But this is clear by subspace characterization of non-negative eigenvalues. For convex case, it suffices to prove that $\mathrm{tr}|A| + \mathrm{tr}|B| \geq \mathrm{tr}|A+B|$ for any $A, B \in \mathcal{H}^n(a,b)$. For this, note that if $(e_i)_{i=1}^n$ is eigenbasis of $A+B$, we have

$$\begin{aligned} \mathrm{tr}|A+B| &= \sum_{i=1}^n \langle |A+B| e_i, e_i \rangle \\ = \sum_{i=1}^n |\langle (A+B) e_i, e_i \rangle| &\leq \sum_{i=1}^n |\langle A e_i, e_i \rangle| + \sum_{i=1}^n |\langle B e_i, e_i \rangle| \\ \leq \sum_{i=1}^n \langle |A| e_i, e_i \rangle + \sum_{i=1}^n \langle |B| e_i, e_i \rangle &= \mathrm{tr}|A| + \mathrm{tr}|B| \end{aligned}$$

- What about trace inequalities for k-tone functions? Eigen-package seems to find a counterexample for 6-tone functions and $n = 2$, but it's hard to see if there's enough numerical stability. At divided differences of polynomials vanish. First non-trivial question would be: If $A_j = A + jH$ for $0 \leq j \leq 3$ and $H \geq 0$. Then is it necessarily the case that

$$\operatorname{tr}(A_3|A_3| - 3A_2|A_2| + 3A_1|A_1| - A_0|A_0|) \geq 0?$$

This would imply that 3-tone functions would lift to trace 3-tone functions. Maybe expressing this as a contour integral from $-i\infty \to i\infty$ a same tricks as in the paper. First projection case: H is projection. Or: approximate by integrals of heat kernels. It should be sufficient to proof things for k-fold integrals or heat kernel, or by scaling just for gaussian function.

- How is the previous related to the $|\cdot|$ not being operator-convex: quadratic form inequality for eigenvectors is not enough.
- The previous also implies that

  $$f(Q_A(v)) \leq Q_{f(A)}(v)$$

  for any convex f. Using this and Minkowski one sees that p-schatten norms are indeed norms.
- For f, g generalization (Look at $h(X) = g(\operatorname{tr} f(X))$) we need that f is convex. What else? h is convex if it is convex for diagonalizable matrices and f is convex and g increasing. For the diagonalizable maps it is sufficient that f is increasing and $g = f^{-1}$ and $\log \circ f \circ \exp$ is convex.
- Von Neumann trace inequality, more trace inequalities.
- On Generalizations of Minkowski's Inequality in the Form of a Triangle Inequality, Mulholland
- Positive derivative
- Smoothness properties
- Characterizations

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