Positivity wants to break free

Levico. July 26th, 2021

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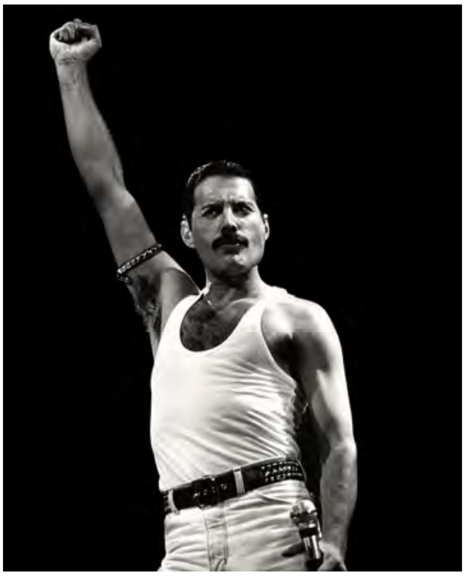

Fig. 1: What happens to positivity in the free (=non-commutative) case?

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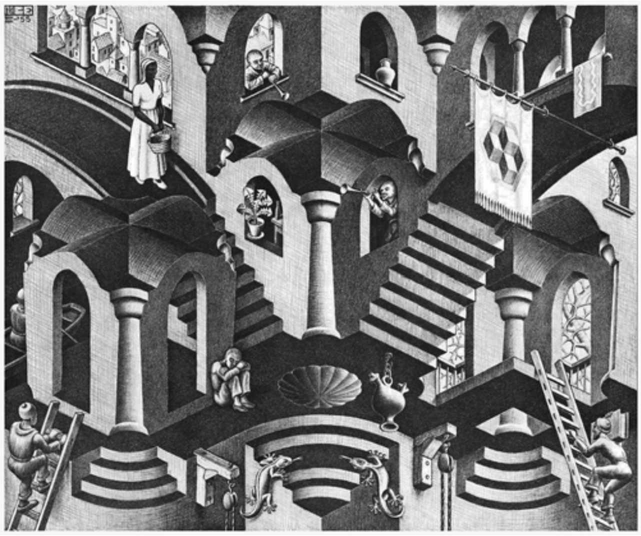


Fig. 2: The notion of positivity gives rise to convexity, which itself gives rise to many surprising effects when interacting with the multiplicity of systems, as in this lithograph by M. C. Escher.

1 Positivity

1.1 Some positive thinking

Natural numbers are used for counting and in thus "natural"—negative numbers came later.

Frequencies are described by positive numbers and hence so are probabilities. And probabilities pervade many areas of maths, physics, etc.

Positive things form cones, instead of vector spaces (because adding ends up in the cone, but subtracting not). Cones are harder to characterise than vector spaces, because they can have round walls, so may not admit a finite description.

Cones interact in a non-trivial way with the multiplicity of systems (Fig. 2). Vector spaces interact in a more "boring" way instead. This already happens for the classical (i.e. commutative) case, giving rise to nonnegative factorisations, etc (wait for a couple of minutes).

Quantum theory is like a free version of classical probability theory. So the question is, first, how to define positivity in the free setting, and second, how this 'free' positivity interacts with the multiplicity of systems (Fig. 1)—this is what this mini-lecture and open problem are about. We will see that the free setting inherits many of the weird effects from the classical setting, in particular the separations, but the biggest open question is which *new things* can happen in the quantum/free setting.

1.2 A first encounter

The **rank** of a matrix M is the number of linearly independent columns or rows. That is, it is the minimal r such that

$$M = AB \qquad \text{where } A \text{ has } r \text{ columns.} \tag{1}$$

If M is complex, A and B need to be complex. If M is real, A and B can be chosen real.

There are two main notions of positivity for matrices:

- M is *nonnegative*: it is entrywise nonnegative. This notion of positivity (or nonnegativity) is in essence the same as that of a nonnegative vector.
- M is *positive semidefinite*: it is diagonalisable and has nonnegative eigenvalues. M could thus be real and symmetric, or Hermitian—in either case with nonnegative eigenvalues. For the quantum case the latter is the important one. This notion of positivity is inherent to a matrix—the matrix itself can have complex entries, but its eigenvalues must be nonnegative. It is unnatural to map this notion of positivity to that of a vector, and much suffering is associated to doing so...

If M has some notion of positivity, can we decompose M so that it preserves this notion of positivity? If M is nonnegative, the **nonnegative factorisation** is defined as

$$M = AB \qquad \text{where } A \text{ and } B \text{ are nonnegative} \tag{2}$$

and the **nonnegative rank** is the minimal number of columns of A. We denote it by nn-rank, although often is it is called rank_+.This was defined in the early 1990's in the context of communication complexity.

The following is a noncommutative version of the nonnegative factorisation. The **positive semidefinite (psd) factorisation** is defined as

$$M_{i,j} = \text{tr}(A_i B_j) \quad \text{where all } A_i \text{ and } B_j \text{ are positive semidefinite} \tag{3}$$

Note that there need to be as many A_i's as the number of rows of M, and as many B_j's as the number of columns of M, so that cannot define a rank. The **psd rank** is defined as the minimal size of all A_i's and B_j's, i.e. the minimal r such that there exist $A_i \in \text{PSD}_r$ and $B_j \in \text{PSD}_r$ such that $M_{i,j} = \text{tr}(A_i B_j)$ for all i, j (where PSD_r is the set of psd matrices of size r). Usually these psd matrices are defined in the reals (i.e. they are real symmetric matrices with nonnegative eigenvalues); for the quantum stuff we care about the Hermitian case. This was defined in [FMP⁺12] and surveyed some time ago in [FGP⁺15].

In the psd factorisation we could choose the matrices A_i and B_j diagonal, and we would recover a nonnegative factorisation. So it sort of holds that

$$\text{rank} \leq \text{psd-rank} \leq \text{nn-rank} \tag{4}$$

(There are some missing factors: the actual inequalities are $\frac{1}{2}\sqrt{1+8\text{rank}(M)} - \frac{1}{2} \leq \text{psd-rank}_{\mathbb{R}}(M) \leq \text{nn-rank}(M)$). In plain words this says that it is harder to decompose with nonnegative numbers than with real numbers (rank $\leq$ nn-rank), that noncommutativity helps (psd-rank $\leq$ nn-rank), and that it doesn't get smaller than the rank.

1.3 Separations

Now, why is all this interesting? Because *the nonnegative rank and the psd rank are much more expensive than the rank*. That is, negative numbers allow for massive shortcuts in a finite set of sums (even if the result of these sums needs to be positive).

Formally, there is a **separation** between each of these ranks. That is, there is a sequence of matrices M_n (whose size increases with n) such that rank(M_n) is bounded but nn-rank(M_n) diverges. This means that rank cannot be upper bounded by a function of nn-rank exclusively. We write

$$\text{rank} \ll \text{nn-rank} \tag{5}$$

The size of M_n needs to grow with n because both ranks can always be upper bounded by a function of the size of M_n. This is long known. The same is true for the rank and psd rank

$$\text{rank} \ll \text{psd-rank} \tag{6}$$

and for the psd rank and nonnegative rank:

$$\text{psd-rank} \ll \text{nn-rank} \tag{7}$$

(This was first shown in [GPT13].) So there are separations everywhere!

> Message: Imposing local positivity makes a big difference, i.e. it requires *many* more terms.

1.4 With symmetry

If M is symmetric (i.e. $M = M^t$ if real, and $M = M^\dagger$ if complex), it is natural to consider the three decompositions above in the symmetric case:

- The **symmetric factorisation** of M is defined as

$$M = AA^t \qquad \text{where } A \text{ is complex} \tag{8}$$

  and the minimal number of columns of A is the **symmetric rank**.

- The **cp factorisation** (standing for completely positive) is defined as

$$M = AA^t \qquad A \text{ nonnegative} \tag{9}$$

  and the minimal number of columns of A is the **cp rank**.

- The **cpsd factorisation** (standing for completely positive semidefinite) is defined as

$$M_{i,j} = \mathrm{tr}(A_i A_j) \qquad A_i \text{ psd} \tag{10}$$

  and the minimal size of all A_i's is the **cpsd rank** (see Fig. 3).

So 'completely' here means 'symmetric'.

$$\begin{array}{ccc}
\text{minimal factorisation} & \xrightarrow{\text{symmetric}} & \text{symmetric factorisation} \\
\text{nonnegative}\downarrow & & \downarrow\text{nonnegative} \\
\text{nonnegative factorisation} & \xrightarrow{\text{symmetric}} & \text{cp factorisation} \\
\text{non-commutative}\downarrow & & \downarrow\text{non-commutative} \\
\text{psd factorisation} & \xrightarrow{\text{symmetric}} & \text{cpsdt factorisation}
\end{array}$$

Fig. 3: Factorisations of nonnegative matrices.

These factorisations have been kind of studied.

1.5 Positivity breaks free

Now, *what happens if M is a positive semidefinite matrix*, instead of a nonnegative one? The nonnegative and the psd factorisation of M are not defined, since M can have negative and complex entries. We need to consider free[1] versions of the decompositions above.

So let M be positive semidefinite (let's say complex), and bipartite i.e.

$$M \geqslant 0 \qquad \text{and } M \in \mathcal{M}_d \otimes \mathcal{M}_d, \tag{11}$$

[1] Free from the commutation relation, obviously.

where $\geqslant 0$ means positive semidefinite, and $\mathscr{M}_d$ is the space of $d \times d$ complex matrices. The following are free / quantum version of the previous factorisations (Fig. 4):

- The **operator Schmidt decomposition** of M is

$$M = \sum_{\alpha=1}^{r} A_\alpha \otimes B_\alpha \tag{12}$$

  and the minimal such r is the **osr** (standing for operator Schmidt rank).

- The **separable decomposition** of M is

$$M = \sum_{\alpha=1}^{r} \sigma_\alpha \otimes \tau_\alpha \quad \text{where } \sigma_\alpha, \tau_\alpha \geqslant 0 \tag{13}$$

  where the minimal such r is the **separable rank**. This only exists if M is in the convex cone of $\mathrm{PSD}_d \times \mathrm{PSD}_d$ i.e. separable.

- The **local purification** of M is

$$M = LL^\dagger, \qquad L = \sum_{\alpha=1}^{r} A_\alpha \otimes B_\alpha \tag{14}$$

  where L need not be a square matrix (for the physicists: this the same as a purification $M = \mathrm{tr}_{\mathrm{aux}}|\psi\rangle\langle\psi|$.) The minimal such r is the **purification rank**.

- There is also the **quantum square root** of M where L is the psd square root of M, and the **q-sqrt-rank** is the osr of M.

Now with symmetry. Let M be symmetric, i.e. given $M = \sum_{\alpha=1}^{r} A_\alpha \otimes B_\alpha$, $T(M) = \sum_{\alpha=1}^{r} B_\alpha \otimes A_\alpha = M$.

- The **t.i. operator Schmidt decomposition** (where t.i. stands for translationally invariant) is defined as

$$M = \sum_{\alpha=1}^{r} A_\alpha \otimes A_\alpha \tag{15}$$

  and the minimal such r is the **ti-osr**.

- The **t.i. separable decomposition** is

$$M = \sum_{\alpha=1}^{r} \sigma_\alpha \otimes \sigma_\alpha \qquad \text{where } \sigma_\alpha \geqslant 0 \tag{16}$$

  and the minimal such r is the **ti-separable rank**.

$$
\begin{array}{ccc}
\text{operator Schmidt decomp.} & \xrightarrow{\text{symmetric}} & \text{t.i. operator Schmidt decomp.} \\
{\scriptstyle\text{nonnegative}}\big\downarrow & & \big\downarrow{\scriptstyle\text{nonnegative}} \\
\text{separable decomp.} & \xrightarrow{\text{symmetric}} & \text{t.i. separable decomp.} \\
{\scriptstyle\text{non-commutative}}\big\downarrow & & \big\downarrow{\scriptstyle\text{non-commutative}} \\
\text{local purification} & \xrightarrow{\text{symmetric}} & \text{t.i. local purification}
\end{array}
$$

Fig. 4: Factorisations of psd matrices.

- And the **t.i. local purification** is

$$M = AA^\dagger \qquad \text{where } A = \sum_{\alpha=1}^{r} B_\alpha \otimes B_\alpha \tag{17}$$

and the minimal such r is the **t.i. purification rank**.

If M is diagonal in the computational basis, we recover the "classical" case above (Table 1), i.e. the generalisation is sensible. Namely, if $M = \text{diag}(N)$ where N is a nonnegative matrix and $\text{diag}(N)$ rearranges the entries of N into a diagonal, the factorisations of the psd matrix M coincide with the factorisations of the nonnegative matrix N.[2]

Decomposition of $M = \text{diag}(N)$	Decomposition of N
operator Schmidt decomposition	minimal factorisation
separable decomposition	nonnegative factorisation
local purification	complex psd factorisation
t.i. operator Schmidt decomposition	symmetric factorisation
t.i. separable decomposition	cp factorisation
t.i. local purification	complex cpsdt factorisation

Tab. 1: If a psd matrix M is diagonal in the computational basis, $M = \text{diag}(N)$ where N is the nonnegative matrix containing the diagonal of M, then the decompositions of M on the left hand side are the same as the decompositions of N on the right hand side [DN20].

Moreover, since the quantum version is a generalisation of the classical case, the separations are inherited:

$$\text{osr} \ll \text{puri-rank} \ll \text{sep-rank} \tag{18}$$

Some other results are inherited too (in a non-trivial way), like what happens for rank two / operator Schmidt rank two (Table 2).

[2]Up to an extra transpose in the cpsd factorisation (giving rise to the cpsdt factorisation).

Nonnegative matrix M	rank(M)	
	1	Trivial (all ranks the same)
	2	nn-rank = psd-rank = 2
	3	nn-rank and psd-rank can be unbounded

Psd matrix ρ	osr(ρ)	
	1	Product state (all ranks the same)
	2	Separable, and sep-rank = puri-rank = 2
	3	puri-rank and sep-rank can be unbounded

Tab. 2: The case of rank 1 is trivial, of rank 2 is easy and fully characterised, and of rank 3 is as hard as the general case. This is true both for a nonnegative matrix M [FGP+15] and for a bipartite psd matrix ρ (where rank needs to be substituted by osr) [DDN19].

1.6 Positivity breaks free and multipartite

What if M is positive semidefinite and multipartite? That is,

$$M \in \mathcal{M}_d \otimes \ldots \otimes \mathcal{M}_d \qquad \text{where } M \geqslant 0 \tag{19}$$

We should first ask the simpler question where we forget about the positivity: *If M is an element of a tensor product space, in how many ways can it be decomposed?* Namely if

$$M \in V_1 \otimes \ldots \otimes V_n \qquad \text{where } V_i \text{ are vector spaces,} \tag{20}$$

then M can clearly be expressed as a sum of individual tensor elements, but how are the summation indices arranged? In the **tensor rank** decomposition there is a single, common summation index:

$$M = \sum_{\alpha=1}^{r} a_\alpha \otimes b_\alpha \otimes \ldots \otimes z_\alpha \tag{21}$$

(where the minimal such r is the tensor rank), but in the operator Schmidt decomposition the summation indices are shared between neighbors drawing in a 1D line:

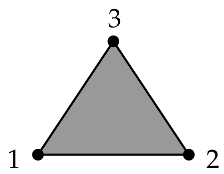
$$M = \sum_{\alpha_1,\ldots,\alpha_n=1}^{r} a_{\alpha_1} \otimes b_{\alpha_1,\alpha_2} \otimes \ldots \otimes z_{\alpha_{n-1}} \tag{22}$$

(where the minimal such r is the operator Schmidt rank). In between there are many other cases: there could be a shared index among the first 3 factors and a linear structure for the rest, etc, etc.

We model all of these cases with a weighted simplicial complex Ω,[3] where

[3] This is like a hypergraph where the facets can have multiplicity. In fact it is a "well-behaved"

the vertices are associated to the individual vector spaces and the facets to the summation indices. For example, for the tensor rank decomposition, the simplicial complex is the full simplex (here for 3 vertices),

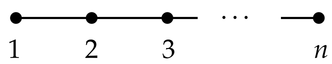


meaning that in

$$M = \sum_{\alpha=1}^{r} v_\alpha^{[1]} \otimes v_\alpha^{[2]} \otimes v_\alpha^{[3]} \tag{23}$$

the index α lives in the facet shared by vertices $1, 2, 3$.

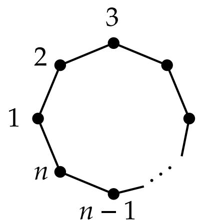
In the operator Schmidt decomposition, the simplicial complex is the line graph



meaning that in

$$M = \sum_{\alpha_1,\ldots,\alpha_{n-1}=1}^{r} v_{\alpha_1}^{[1]} \otimes v_{\alpha_1,\alpha_2}^{[2]} \otimes v_{\alpha_2,\alpha_3}^{[3]} \otimes \ldots \otimes v_{\alpha_{n-1}}^{[n]} \tag{24}$$

the indices α_i live in the edges (which are the facets in this case). If we had periodic boundary conditions in 1D, we would model this with a circle graph



For every simplicial complex Ω, the minimal number of terms defines the $\text{rank}_\Omega(M)$.

Now imagine that M is symmetric under some group action G (i.e. $g \cdot M = M$ where $g \in G$ and $g \cdot M$ means that g permutes the local vector spaces). Can this invariance be made explicit? For example

$$M = \sum_{\alpha=1}^{r} v_\alpha \otimes v_\alpha \otimes \ldots \otimes v_\alpha \tag{25}$$

multi-hypergraph, as there are some compatibility relations.

is clearly invariant under the full symmetry group S_n. In general this invariant decomposition is called an (Ω, G)**-decomposition**, and the minimal number of terms needed is the (Ω, G)**-rank** [DHN19]. For example the **symmetric tensor rank** is the minimal r in (25). The **ti-operator Schmidt decomposition** is

$$M = \sum_{\alpha=1}^{r} v_{\alpha_1,\alpha_2} \otimes v_{\alpha_2,\alpha_3} \otimes \ldots \otimes v_{\alpha_n,\alpha_1} \tag{26}$$

where G is the cyclic group of order n, and the minimal such r is the **ti-osr**.

(The main result of [DHN19] is in fact: If M is G-symmetric, it has an (Ω, G)-decomposition if G acts *freely* on Ω, and the multiplicity of the facets of Ω can always be increased so that G acts freely on it.)

Finally we add positivity to obtain the **sep-rank**$_{(\Omega,G)}$ and **puri-rank**$_{(\Omega,G)}$.

Fig. 5: Andreas Klingler.

In the approximate case, many separations disappear [DKN20] (Fig. 5). Approximate means that we consider an ε ball around the element, in some norm (Schatten p-norm or ℓ_p norm) and we define e.g.

$$\text{rank}^{\varepsilon}_{(\Omega,G)}(M) = \min_{N \in B_\varepsilon(M)} \text{rank}_{(\Omega,G)}(N), \tag{27}$$

where $B_\varepsilon(M)$ is the ball around M, and similarly for the other cases. Our only tool so far to study the approximate case is the approximate Caratheodory Theorem, which says that the number of elements needed to express an element of a convex set as a convex combination of terms at the boundary is independent of the ambient dimension.

1.7 Some open problems

Open problem 1 What new things can happen in the free case? Can we prove stronger separations in the free case? We don't have any tool so far.

Intuition: lots of new things should happen because matrices are very special kinds of tensors. More generally: 2 is easy and 3 is as hard as it gets (e.g. 2SAT vs. 3SAT). Even more generally: Quantum is very different than classical.

Open problem 2 What happens for the border rank? Namely what is the (Ω, G) border rank, purirank, seprank, and their approximate versions?

2 Extra: Tensor-stable positivity

All maps are linear.

A map $\mathscr{P} : \mathscr{M}_d \to \mathscr{M}_d$ is *positive* if it maps positive semidefinite matrices to positive semidefinite matrices, i.e. $X \geqslant 0 \implies \mathscr{P}(X) \geqslant 0$. It's very hard to tell whether a map is positive.

A map is *tensor-stable positive* if $\mathscr{P}^{\otimes n}$ is positive for all n [MHRW16]. If $\mathscr{P}$ is completely positive or co-completely positive (i.e. completely positive followed by transposition) then it is tensor-stable positive. These are trivial tensor-stable positive maps.

(A map is *completely positive* if $\mathrm{id}_n \otimes \mathscr{P}$ is positive for all n. These are very easy to characterise.)

Fig. 6: Mirte van der Eyden.

Are there non-trivial tensor-stable positive maps?

If this is the case, then there exist bound entangled states with a non-positive partial transpose [MHRW16].

Let the "matrix multiplication tensor" be

$$|\chi_n\rangle = \sum_{\alpha_1,\ldots,\alpha_n=1}^{D} |\alpha_1, \alpha_2\rangle \otimes |\alpha_2, \alpha_3\rangle \otimes \ldots \otimes |\alpha_n, \alpha_1\rangle$$

and denote the projector on this state by $\chi_n = |\chi_n\rangle\langle\chi_n|$.

Theorem [DVN21]: Given a map $\mathscr{P}$, it is undecidable whether $\mathscr{P}^{\otimes n}(\chi_n) \geqslant 0$ for all n.

The proof is a reduction from an undecidable matrix product operator problem in [DCC+16], which itself is a reduction from the matrix mortality problem.

Conjecture: Given a map $\mathscr{P}$, it is undecidable whether $\mathscr{P}^{\otimes n}$ is positive for all n.

Open problem: Can we prove this conjecture? In particular, are there undecidable problems with a similar structure which could be reduced to the tensor-stable positivity problem?

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