Tight Frames, Quantum Information, and Degree 4 Sum-of-Squares

NYU

Dmitriy (Tim) Kunisky, joint with Afonso Bandeira

Motivation

Several interesting problems (MaxCut, little Grothendieck problem, ground states of Ising and Sherrington-Kirkpatrick models) can be written as optimization of quadratic forms over the hypercube, or optimization of linear functions over the *cut polytope*:

$$\mathsf{M}^{\mathsf{HC}}(\boldsymbol{W}) = \max_{\boldsymbol{x} \in \{\pm 1\}^N} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x} = \max_{\boldsymbol{E} \in \mathsf{CUT}^N} \langle \boldsymbol{E}, \boldsymbol{W} \rangle,$$

$$\begin{aligned} \mathsf{CUT}^N &= \mathrm{conv}(\{\boldsymbol{x}\boldsymbol{x}^\top : \boldsymbol{x} \in \{\pm 1\}^N\}) \\ &= \text{degree 2 moments of distributions over } \{\pm 1\}^N. \end{aligned}$$

Sum-of-squares (SOS) SDP relaxations of *degree* $2d$ give efficiently computable upper bounds on $\mathsf{M}^{\mathsf{HC}}(\boldsymbol{W})$ by optimizing over *pseudomoment matrices* $\mathsf{PM}^N_{2d\to 2} \supseteq \mathsf{CUT}^N$ or the associated *pseudoexpectations* $\mathsf{PE}^N_{2d} \supseteq \{\mathbb{E}_\mu : \mu \in \mathcal{M}^1(\{\pm 1\}^N)\}$:

$$\mathsf{SOS}^{\mathsf{HC}}_{2d}(\boldsymbol{W}) = \max_{\boldsymbol{E} \in \mathsf{PM}^N_{2d\to 2}} \langle \boldsymbol{E}, \boldsymbol{W} \rangle = \max_{\tilde{\mathbb{E}} \in \mathsf{PE}^N_{2d}} \tilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}].$$

To measure the computational difficulty of $M^{\mathsf{HC}}(\boldsymbol{W})$, we look at the quality of SOS relaxations as the degree grows.

Factorizing Pseudomoments

It can be useful to describe a pseudomoment matrix as a **Gram matrix** (for rounding, rank-constrained numerics, and theoretical arguments). For degree 2, this is simple:

$$\begin{aligned} \mathsf{PM}^N_{2\to 2} &= \left\{ \boldsymbol{E} \in \mathbb{R}^{N\times N} : \boldsymbol{E} \succeq \boldsymbol{0}, \mathrm{diag}(\boldsymbol{E}) = \boldsymbol{1} \right\} \\ &= \left\{ \boldsymbol{E} \in \mathbb{R}^{N\times N} : E_{ij} = \langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle \text{ where } \boldsymbol{v}_i \in \mathbb{S}^{r-1} \right\}. \end{aligned}$$

We give a more subtle answer for degree 4.

Definition. $\mathcal{B}(N,r)$ is the set of **positive semidefinite** $\mathbb{R}^{rN\times rN}$ block matrices where **every diagonal block is $\boldsymbol{I}_r$** and **every off-diagonal block is symmetric**:

$$\mathcal{B}(N,r) = \left\{ \begin{bmatrix} \boldsymbol{I}_r & \boldsymbol{S}_{\{1,2\}} & \boldsymbol{S}_{\{1,3\}} & \boldsymbol{S}_{\{1,4\}} & \boldsymbol{S}_{\{1,5\}} \\ \boldsymbol{S}_{\{1,2\}} & \boldsymbol{I}_r & \boldsymbol{S}_{\{2,3\}} & \boldsymbol{S}_{\{2,4\}} & \boldsymbol{S}_{\{2,5\}} \\ \boldsymbol{S}_{\{1,3\}} & \boldsymbol{S}_{\{2,3\}} & \boldsymbol{I}_r & \boldsymbol{S}_{\{3,4\}} & \boldsymbol{S}_{\{3,5\}} \\ \boldsymbol{S}_{\{1,4\}} & \boldsymbol{S}_{\{2,4\}} & \boldsymbol{S}_{\{3,4\}} & \boldsymbol{I}_r & \boldsymbol{S}_{\{4,5\}} \\ \boldsymbol{S}_{\{1,5\}} & \boldsymbol{S}_{\{2,5\}} & \boldsymbol{S}_{\{3,5\}} & \boldsymbol{S}_{\{4,5\}} & \boldsymbol{I}_r \end{bmatrix} \succeq \boldsymbol{0} \right\}.$$

Theorem: Gram Matrix Description of $\mathsf{SOS}^{\mathsf{HC}}_4$ Feasibility

$\boldsymbol{E} = (\langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle)^N_{i,j=1} \in \mathsf{PM}^N_{4\to 2}$ with $\boldsymbol{v}_i \in \mathbb{S}^{r-1}$ if and only if there exists $\boldsymbol{X} \in \mathcal{B}(N,r)$ with $\boldsymbol{v}^\top \boldsymbol{X} \boldsymbol{v} = N^2$, where $\boldsymbol{v}$ is the concatenation of the $\boldsymbol{v}_i$.

$\|\boldsymbol{X}\| \le N$ when $\boldsymbol{X} \in \mathcal{B}(N,r)$, so $\boldsymbol{v}$ is a top eigenvector of $\boldsymbol{X}$.

Separability and Partial Transposition

Some simple constructions of a witness $\boldsymbol{X}$ are guaranteed to produce "trivial" pseudomoment matrices, those arising from true probability distributions.

Proposition: Low-Rank and Separable Feasibility Witnesses are Trivial

If $\boldsymbol{E} = (\langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle)^N_{i,j=1}$ with $\boldsymbol{v}_i \in \mathbb{S}^{r-1}$, $\boldsymbol{X} \in \mathcal{B}(N,r)$ with $\boldsymbol{v}^\top \boldsymbol{X} \boldsymbol{v} = N^2$, and $\mathrm{rank}(\boldsymbol{X}) = r$ or $\frac{1}{rN}\boldsymbol{X}$ is the density matrix of a separable bipartite quantum state, then $\boldsymbol{E} \in \mathsf{CUT}^N$.

Therefore, all interesting applications of the Theorem must have $\frac{1}{rN}\boldsymbol{X}$ be the density matrix of an entangled state.

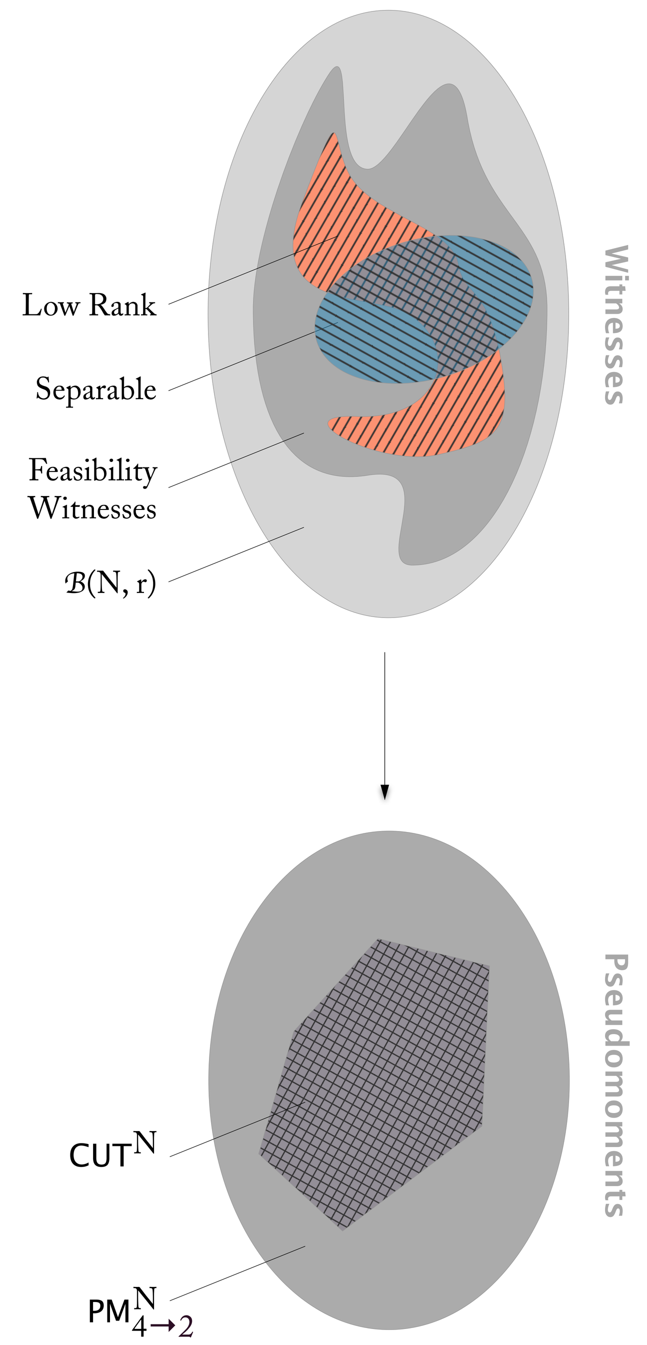
Any $\boldsymbol{X} \in \mathcal{B}(N,r)$ equals its own *partial transpose* $\mathsf{PT}(\boldsymbol{X})$, the matrix with all blocks transposed. In particular, $\mathsf{PT}(\boldsymbol{X}) \succeq 0$, making $\frac{1}{rN}\boldsymbol{X}$ a *positive partial transpose (PPT)* state. The structure of PPT entangled states is an active subject in quantum information theory.

Partial transposition also constrains $\boldsymbol{X}$ when $\boldsymbol{E}$ is the Gram matrix of a *unit norm tight frame (UNTF)*, i.e. when $\boldsymbol{E}$ is a scaled projection matrix.

Proposition: Partial Transpose Constraint for Feasibility Witness

If $\boldsymbol{E} = (\langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle)^N_{i,j=1}$ with $\boldsymbol{v}_i \in \mathbb{S}^{r-1}$ forming a UNTF and $\boldsymbol{X} \in \mathcal{B}(N,r)$ with $\boldsymbol{v}^\top \boldsymbol{X} \boldsymbol{v} = N^2$, then $\boldsymbol{X} = \boldsymbol{v}\boldsymbol{v}^\top + \tilde{\boldsymbol{X}}$ where $\tilde{\boldsymbol{X}} \succeq \boldsymbol{0}$ and its positive eigenvectors belong to the positive eigenspace of $\mathsf{PT}(\boldsymbol{v}\boldsymbol{v}^\top)$.

This positive eigenspace may be computed through the *Schmidt decomposition* and is related to the SVD of the matrix with columns $\boldsymbol{v}_i$.



Equiangular Tight Frames are (Usually) $\mathsf{SOS}^{\mathsf{HC}}_4$ Feasible

Definition. Vectors $\boldsymbol{v}_1, \dots, \boldsymbol{v}_N \in \mathbb{R}^r$ form an *equiangular tight frame (ETF)* if

1. (Unit Norm) $\|\boldsymbol{v}_i\|_2 = 1$.
2. (Tight Frame) $\sum_{i=1}^N \boldsymbol{v}_i \boldsymbol{v}_i^\top = \frac{N}{r}\boldsymbol{I}_r$.
3. (Equiangular) For any $i \ne j$, $|\langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle| = \mu$.

ETFs are rare and rigidly structured, with connections to strongly regular graphs, tight spherical designs, Steiner systems, and other exceptional combinatorial objects.

Theorem: $\mathsf{SOS}^{\mathsf{HC}}_4$ Feasibility of Equiangular Tight Frames

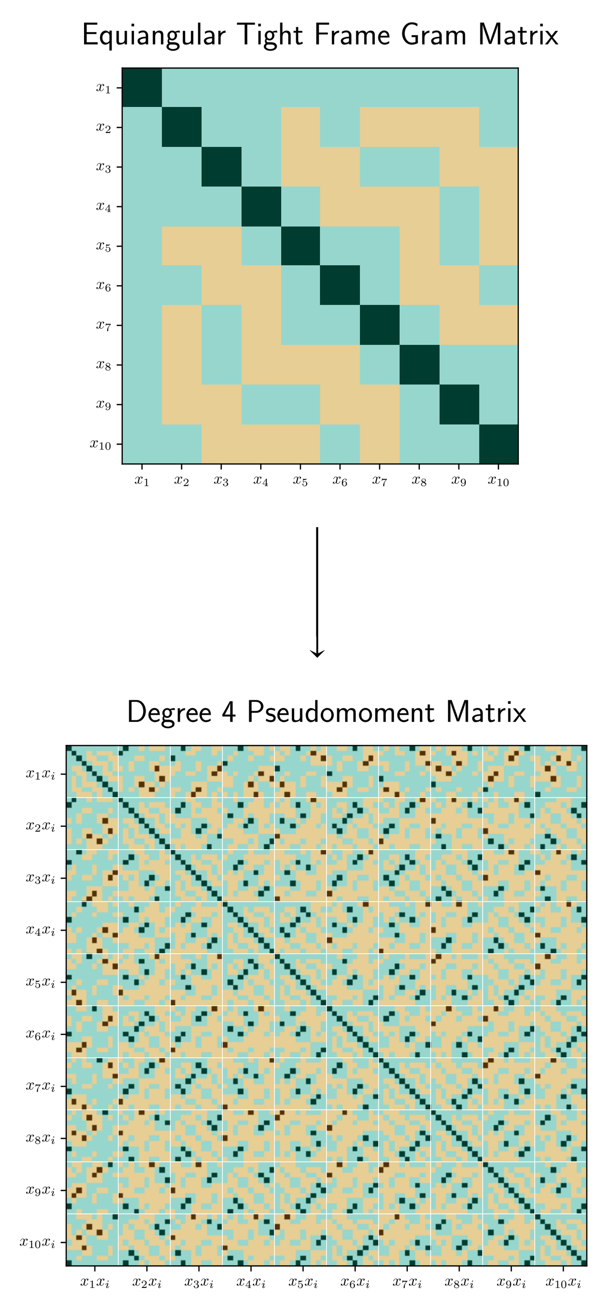
If $\boldsymbol{v}_1, \dots, \boldsymbol{v}_N \in \mathbb{S}^{r-1}$ form an ETF, and $\boldsymbol{E} = (\langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle)^N_{i,j=1}$ is the Gram matrix, then $\boldsymbol{E} \in \mathsf{PM}^N_{4\to 2}$ if and only if $N < \frac{r(r+1)}{2}$.

$N \le \frac{r(r+1)}{2}$ always holds; only four cases with equality are known.

In the course of the proof, we obtain the degree 4 pseudomoments explicitly, which are themselves intricately structured and "fine-tuned" to satisfy positive semidefiniteness. They are given by the highly symmetric formula:

$$\tilde{\mathbb{E}}[x_i x_j x_k x_\ell] = \frac{\frac{r(r-1)}{2}}{\frac{r(r+1)}{2} - N}(E_{ij}E_{k\ell} + E_{ik}E_{j\ell} + E_{i\ell}E_{jk}) - \frac{r^2\left(1 - \frac{1}{N}\right)}{\frac{r(r+1)}{2} - N} \sum_{m=1}^N E_{im}E_{jm}E_{km}E_{\ell m}.$$

Some ETF Gram matrices (of simplex and Paley ETFs) provably belong to the difference set $\mathsf{PM}^N_{4\to 2} \setminus \mathsf{CUT}^N$, and appear to be the first explicit examples of members of this set.



Applications

- **SOS inequalities.** The only known family of inequalities satisfied by degree 4 but not degree 2 pseudoexpectations are the *triangle inequalities*, $(x_i + x_j + x_k)^2 \ge 1$, equivalently $x_i x_j + x_j x_k + x_i x_k \ge -1$. We show that **the triangle inequalities are the first of a larger family** corresponding to maximal ETFs. We also show that the similar facts $(\sum_{i\in\mathcal{I}} x_i)^2 \ge 1$ for $|\mathcal{I}| \ge 5$ and odd called **hypermetric inequalities are *not* satisfied by degree 4 pseudoexpectations**.
- **ETF sparsity and spark.** If $\boldsymbol{v}_1, \dots, \boldsymbol{v}_N \in \mathbb{S}^{r-1}$ form an ETF and $\boldsymbol{V} \in \mathbb{R}^{r\times N}$ has the $\boldsymbol{v}_i$ as its columns, we give new upper bounds for $\|\mathrm{row}(\boldsymbol{V})\|_{2\to 4}$ and $\|\ker(\boldsymbol{V})\|_{2\to 4}$. These give **lower bounds on the sparsity and spark** of $\boldsymbol{V}$, which are related to efficient encoding and the restricted isometry property for ETFs.
- **MaxCut integrality gaps.** A correspondence between ETFs and strongly regular graphs gives graphs where the $\mathsf{SOS}^{\mathsf{HC}}_2$ and $\mathsf{SOS}^{\mathsf{HC}}_4$ relaxations of MaxCut are equal. This does not give an integrality gap, but numerics on a generalization to non-equiangular tight frames indicate that **several families of strongly regular graphs have MaxCut integrality gaps**.

Future Work

We are interested in particular in the $\mathsf{SOS}^{\mathsf{HC}}_4$ relaxation of the **Sherrington-Kirkpatrick model**, where $\boldsymbol{W} \sim \mathsf{GOE}(N)$. It is known that $\mathsf{SOS}^{\mathsf{HC}}_2(\boldsymbol{W}) \sim 2N^{3/2}$, and we investigate whether $\mathsf{SOS}^{\mathsf{HC}}_4$ achieves a constant factor improvement. Using the results shown here and others, this may be related to the following random optimization problem:

$$\max_{\substack{\boldsymbol{X} \in \mathbb{R}^{rN\times rN} \\ \boldsymbol{X} \succeq 0,\ \text{diagonal blocks} = \boldsymbol{I}_r}} \langle \boldsymbol{X}, \mathsf{PT}(\boldsymbol{g}\boldsymbol{g}^\top) \rangle \text{ with } \boldsymbol{g} \sim \mathcal{N}(0, \boldsymbol{I}_{rN}).$$

This is an instance of the *orthogonal cut* SDP relaxation, which admits several Grothendieck-type inequalities and efficient rank-constrained numerical methods.

References

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