Tight Frames and Degree 4 Sum-of-Squares over the Hypercube

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Motivation

Several interesting problems (MaxCut, Grothendieck problem, $\mathbb{Z}/2\mathbb{Z}$ synchronization, statistical physics models) can be written as optimization of quadratic forms over the hypercube, or optimization of linear functions over the *cut polytope*:

$$\mathsf{M}(\boldsymbol{W}) = \max_{\boldsymbol{x}\in\{\pm1\}^N} \boldsymbol{x}^\top \boldsymbol{W}\boldsymbol{x} = \max_{\boldsymbol{X}\in\mathscr{C}^N} \langle \boldsymbol{W}, \boldsymbol{X}\rangle,$$

$$\begin{aligned}\mathscr{C}^N &= \mathsf{conv}(\{\boldsymbol{x}\boldsymbol{x}^\top : \boldsymbol{x}\in\{\pm1\}^N\}) \\ &= \text{degree 2 moments of distributions over } \{\pm1\}^N.\end{aligned}$$

Classical relaxations of $\mathsf{M}(\boldsymbol{W})$ (Goemans-Williamson, Nesterov) optimize over the *elliptope*:

$$\mathscr{E}^N = \mathscr{E}_2^N := \{\boldsymbol{X}\in\mathbb{R}^{N\times N}_{\mathsf{sym}} : \boldsymbol{X}\succeq 0, \mathsf{diag}(\boldsymbol{X}) = \boldsymbol{1}\} \supseteq \mathscr{C}^N.$$

Sum-of-squares relaxations of *degree d* compute bounds on $\mathsf{M}(\boldsymbol{W})$ by optimizing over sets $\mathscr{E}_d^N$ of (partial) *pseudomoment matrices*, giving tighter relaxations as d increases:

$$\mathscr{E}_2^N \supseteq \mathscr{E}_4^N \supseteq \cdots \supseteq \mathscr{E}_{2N}^N = \mathscr{C}^N.$$

$\mathscr{E}_2^N$ is well-studied, but little is known about the geometry and optimization performance of $\mathscr{E}_d^N$ for fixed $d > 2$.

We introduce new techniques for describing $\mathscr{E}_4^N$, which give interesting structural results that appear to be difficult to obtain by existing means.

Factorizing Pseudomoments

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

$$\begin{aligned}\mathscr{E}_2^N &= \left\{\boldsymbol{X}\in\mathbb{R}^{N\times N} : \boldsymbol{X}\succeq\boldsymbol{0}, \mathsf{diag}(\boldsymbol{X}) = \boldsymbol{1}\right\} \\ &= \left\{\boldsymbol{X}\in\mathbb{R}^{N\times N} : X_{ij} = \langle \boldsymbol{v}_i, \boldsymbol{v}_j\rangle \text{ where } \boldsymbol{v}_i\in\mathbb{S}^{r-1}\right\}.\end{aligned}$$

We do the same for degree 4, where the answer is more subtle.

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:

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

Theorem 1: Gram Matrix Description of $\mathscr{E}_4^N$ Membership

$\boldsymbol{X} = (\langle \boldsymbol{v}_i, \boldsymbol{v}_j\rangle)_{i,j=1}^N \in \mathscr{E}_4^N$ with $\boldsymbol{v}_i\in\mathbb{S}^{r-1}$ a spanning set if and only if there is $\boldsymbol{M}\in\mathcal{B}(N,r)$ with $\boldsymbol{v}^\top\boldsymbol{M}\boldsymbol{v} = N^2$, where $\boldsymbol{v}$ is the concatenation of the $\boldsymbol{v}_i$. If $\boldsymbol{M}_{[jk]}$ are the blocks of $\boldsymbol{M}$, the degree 4 pseudomoments may be recovered as

$$\tilde{\mathbb{E}}[x_i x_j x_k x_\ell] = \boldsymbol{v}_i^\top \boldsymbol{M}_{[jk]}\boldsymbol{v}_\ell.$$

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

Constraints from Complementarity and Sum-of-Squares Eagerness

Theorem 1 gives a new SDP describing membership in $\mathscr{E}_4^N$, different from the pseudomoment one. We examine this program through convex duality:

$$\left\{\begin{array}{ll}\max & \langle \boldsymbol{v}\boldsymbol{v}^\top, \boldsymbol{M}\rangle \\ \text{s.t.} & \boldsymbol{M}\succeq 0, \boldsymbol{M}_{[ii]} = \boldsymbol{I}_r, \boldsymbol{M}_{[ij]} = \boldsymbol{M}_{[ij]}^\top\end{array}\right\} = \left\{\begin{array}{ll}\min & \mathrm{Tr}(\boldsymbol{D}) \\ \text{s.t.} & \boldsymbol{D}\succeq \boldsymbol{v}\boldsymbol{v}^\top, \boldsymbol{D}_{[ij]} = -\boldsymbol{D}_{[ij]}^\top\end{array}\right\}.$$

While the primal problem is as hard as the pseudomoment extension problem, it is easy to match the optimal value in the dual problem using the **partial transpose**:

$$(\boldsymbol{v}\boldsymbol{v}^\top)_{[ij]} = \boldsymbol{v}_i\boldsymbol{v}_j^\top \rightsquigarrow \mathsf{PT}(\boldsymbol{v}\boldsymbol{v}^\top)_{[ij]} = \boldsymbol{v}_j\boldsymbol{v}_i^\top.$$

The partial transpose is studied in **quantum information**; its spectrum for a rank-one matrix is known exactly. We build a dual optimizer $\boldsymbol{D}^* := \boldsymbol{v}\boldsymbol{v}^\top - \mathsf{PT}(\boldsymbol{v}\boldsymbol{v}^\top) + \boldsymbol{I}_N\otimes\left(\sum_{i=1}^N \boldsymbol{v}_i\boldsymbol{v}_i^\top\right)$, with $\mathrm{Tr}(\boldsymbol{D}^*) = N^2$. By complementarity, $\boldsymbol{M}^*(\boldsymbol{D}^* - \boldsymbol{v}\boldsymbol{v}^\top) = \boldsymbol{0}$, constraining $\boldsymbol{M}^*$.

Theorem 2: Gram Matrix Certificate Constraints

If $\boldsymbol{v}_i\in\mathbb{S}^{r-1}$, $\boldsymbol{v}$ is the concatenation of the $\boldsymbol{v}_i$, $\boldsymbol{V}$ has $\boldsymbol{v}_i$ as columns, and $\boldsymbol{M}^*\in\mathcal{B}(N,r)$ with $\boldsymbol{v}^\top\boldsymbol{M}^*\boldsymbol{v}$, then all positive eigenvectors of $\boldsymbol{M}^*$ lie in the subspace

$$V_S = \left\{\mathsf{vec}(\boldsymbol{S}\boldsymbol{V}) : \boldsymbol{S}\in\mathbb{R}^{r\times r}_{\mathsf{sym}}\right\}\subset\mathbb{R}^{rN}.$$

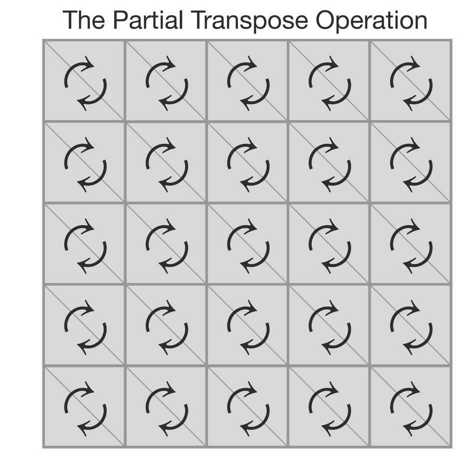
The blocks of $\boldsymbol{M}^*$ control the pseudomoments, so we find pseudomoment identities.

Corollary: Strong Subspace Identities

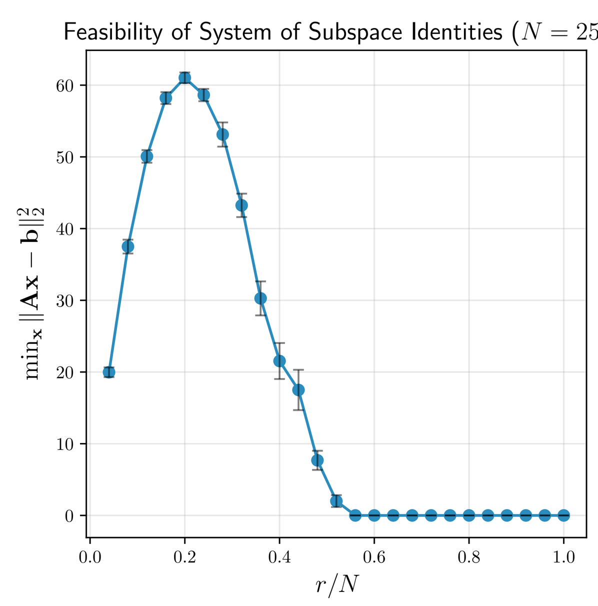
If $\tilde{\mathbb{E}}$ is a degree 4 pseudoexpectation over $\{\pm1\}^N$, and $\boldsymbol{P}$ is the projector to the range of $\tilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top]$, then for all $i\in[N]$ and $p\in\mathbb{R}[x_1,\dots,x_N]_{\le 3}$,

$$\tilde{\mathbb{E}}[x_i p(\boldsymbol{x})] = \tilde{\mathbb{E}}[(\boldsymbol{P}\boldsymbol{x})_i p(\boldsymbol{x})].$$

These identities admit simple sum-of-squares proofs at degree 6, but seem difficult to prove without our methods at degree 4—this is the phenomenon of *eagerness*.



A schematic illustration of the partial transpose operation of transposing each block of a block matrix, which plays an important role in our dual certificate construction.



We observe a phase transition in the feasibility of the subspace identities (together with the symmetry constraints, but no other constraints) when $\boldsymbol{P}$ is taken to be a projection to a random subspace of dimension r. When r is too small, no degree 4 pseudoexpectation can have $\mathsf{img}(\tilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top]) = \mathsf{img}(\boldsymbol{P})$.

Equiangular Tight Frame Gram Matrices are (Usually) in $\mathscr{E}_4^N$

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 $i\neq j$, $|\langle \boldsymbol{v}_i, \boldsymbol{v}_j\rangle| = \mu$.

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

Theorem 3: Membership in $\mathscr{E}_4^N$ of Equiangular Tight Frame Gram Matrices

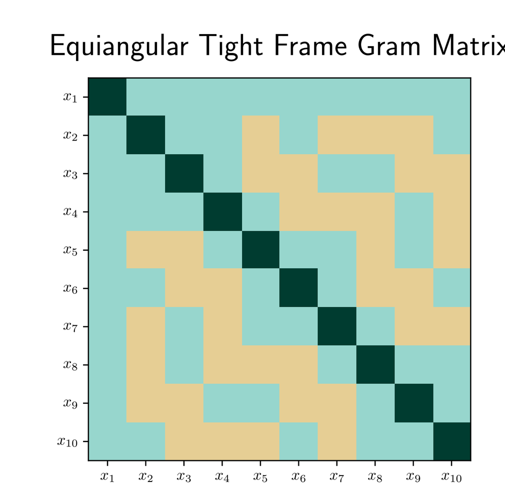
If $\boldsymbol{v}_1,\dots,\boldsymbol{v}_N\in\mathbb{S}^{r-1}$ form an ETF, and $\boldsymbol{X} = (\langle \boldsymbol{v}_i, \boldsymbol{v}_j\rangle)_{i,j=1}^N$ is the Gram matrix, then $\boldsymbol{X}\in\mathscr{E}_4^N$ if and only if $N < \frac{r(r+1)}{2}$.

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

We obtain the degree 4 pseudomoments explicitly by solving the subspace identities, and find that they are intricately structured and "fine-tuned" to satisfy positive semidefiniteness:

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

Some ETF Gram matrices (of simplex and Paley ETFs) provably belong to the difference set $\mathscr{E}_4^N\setminus\mathscr{C}^N$, and appear to be the first explicit examples of members of this set.



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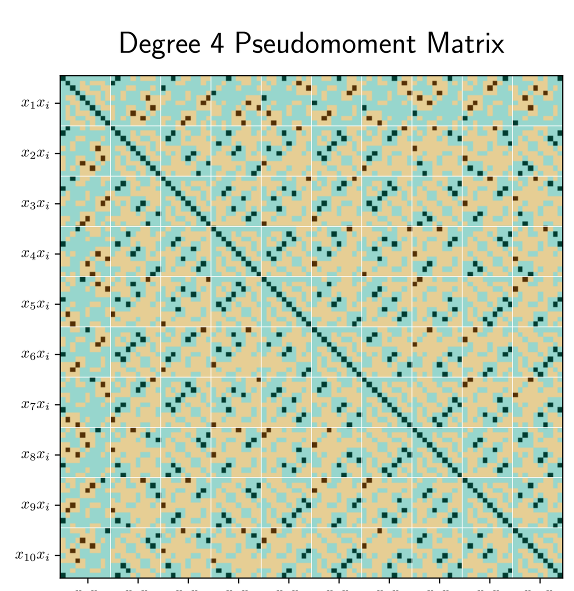

Applications

New sum-of-squares inequalities. The only known family of quadratic inequalities satisfied by degree 4 but not degree 2 pseudoexpectations appear to be the *triangle inequalities*,

$$(x_i + x_j + x_k)^2 \ge 1 \Leftrightarrow x_i x_j + x_j x_k + x_i x_k \ge -1.$$

We show that the triangle inequalities are but the first of a larger family corresponding to maximal ETFs.

Violation of hypermetric inequalities. In the opposite direction, we also show that the similar inequalities

$$\left(\textstyle\sum_{i\in\mathcal{I}} x_i\right)^2 \ge 1 \text{ for } |\mathcal{I}|\ge 5, |\mathcal{I}| \text{ odd}$$

over $\mathscr{C}^N$, called *hypermetric inequalities*, are *not* satisfied by all degree 4 pseudoexpectations.

MaxCut integrality gaps. Extending our result on ETFs to some other *two-distance tight frames* gives the value of the degree 4 sum-of-squares relaxation of MaxCut on associated strongly regular graphs (for example, Johnson and Hamming graphs). A direct computation of the MaxCut value shows that in fact these exhibit a small *integrality gap* between the true MaxCut value and the relaxation value:

$$\text{MaxCut} = (1+\epsilon_N)\frac{|E|}{2} < \left(1 + \epsilon_N + \Omega(\epsilon_N^2)\right)\frac{|E|}{2} = \text{relaxation}.$$

Questions for Future Work

Eagerness. Does the phenomenon of eagerness occur at higher degrees of sum-of-squares, or with other identities?

Factorizing SDPs. When can feasibility for a more general SDP (sum-of-squares over other constraints, or entirely different problems) be described by another SDP on the Gram vectors of the original variable? When does a complementary slackness argument like ours give new constraints?

Random problems. We were motivated originally by relaxing the *Sherrington-Kirkpatrick model*, where $W_{ij}\sim_{\text{iid}}\mathcal{N}(0,1)$. This relates to whether $\boldsymbol{X}\in\mathscr{E}_4^N$ can have "most of its mass near a random subspace." The subspace identities preclude this in some sense, but are they strong enough?

References

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