Sum-of-squares

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§0. Notation

Given $n \times n$ matrices A, B, denote $\langle A, B \rangle = \mathrm{Tr}(AB) = \sum_{i,j} A_{ij} B_{ij}$.

§1. Fundamentals

1.1. Introduction

The sum-of-squares technique, at its most basic form, is a way of determining whether for some polynomial p over $\mathbb{R}^n$, $p(x) \geq 0$ for x in some base set. For now, suppose that our "base set" is $\{0,1\}^n$. Elegantly, it manages to convert *disproofs* of such inequalities to *algorithms* to determine a point where $p(x) < 0$.
More concretely, we shall show non-negativity by expressing p as a *sum of squares* of *low degree* polynomials (while low degree is not technically required, it makes the converted algorithm efficient).

Definition 1.1 (Sum-of-squares proof)**.** Given a polynomial f in variables $x_1, \ldots, x_n$, a *degree d sum-of-squares proof* or *degree d sum-of-squares certificate* (abbreviated SoS proof or SoS certificate) of $f \geq 0$ is a set $\{g_1, \ldots, g_m\}$ of polynomials of degree at most $d/2$ such that

$$f(x) = \sum_{i=1}^{m} g_i^2(x) \tag{1.1}$$

for all x. If f has a degree d sum-of-squares certificate, we write that

$$\vdash_d f(x) \geq 0.$$

Let $\mathcal{A}$ be a set of constraints of the form $A_i(x) = 0$ or $B_j(x) \geq 0$ for $i \in [k], j \in [\ell]$. Then, an *degree d SoS proof given $\mathcal{A}$* of $f \geq 0$ is a set $\{g_1, \ldots, g_m\}$ of polynomials of degree at most $d/2$ such that (1.1) holds for all x satisfying the constraints in $\mathcal{A}$. If such a set exists, we write

$$\mathcal{A} \vdash_d f \geq 0.$$

We always assume that d in this context is even.
Note that simple set restrictions can be captured by the set of constraints. In particular, we can check restrict ourselves to the boolean hypercube $\{-1,1\}^n$ by having $\mathcal{A}$ contain $x_i^2 = 1$ for all i. Note that the set of functions with degree d SoS proofs of non-negativity forms a closed convex cone.

Proposition 1.2. Any non-negative $f : \{-1,1\}^n \to \mathbb{R}$ has a degree $2n$ sum-of-squares proof.

Proof. Recall that any function $h : \{-1,1\}^n \to \mathbb{R}$ can be expressed as a polynomial of degree at most n as

$$h(x) = \sum_{S \subseteq [n]} \hat{f}(S) x_S,$$

where $x_S = \prod_{i \in S} x_i$ with the convention $x_\varnothing = 1$. Knowledgeable readers may recognize this as the *Fourier expansion* of h – we omit the details of why such an expansion exists, but refer the reader to the excellent text by O'Donnell [O'D14] for more details. In particular, $\sqrt{f}$ is a polynomial of degree at most n, so squaring both sides we get that f has a degree $2n$ SoS proof. ∎

The above is *not* true in general; not every non-negative polynomial $f : \mathbb{R}^n \to \mathbb{R}$ can be written as a sum of squares.

Definition 1.3. Given a vector $y \in \mathbb{R}^n$, the vector $y^{\otimes k} \in \mathbb{R}^{n^d}$ has entries indexed by elements of $[n]^d$, with the αth entry being $\prod_{j \in d} y_{\alpha_j}$. Also denote $v_k(x)$ to be the size $\binom{n+k}{k}$ vector with entries equal to all the monomials of x of degree at most k.

Note that for $x \coloneqq (x_1, \ldots, x_n) \in \mathbb{R}^n$, any monomial of degree at most $d/2$ appears in the vector $(1, x)^{\otimes d/2}$, where $(1, x) = (1, x_2, \ldots, x_n) \in \mathbb{R}^{n+1}$. Also recall that a matrix A is said to be positive semidefinite, denoted $A \succeq 0$, if $x^\top Ax \geq 0$ for all vectors x, which is equivalent to asserting that all eigenvalues of the matrix are non-negative.

Proposition 1.4. Let f be a polynomial. f has a degree d sum-of-squares proof iff there exists $A \succeq 0$ such that

$$f(x) = \langle v_{d/2}(x), Av_{d/2}(x) \rangle. \tag{1.2}$$

Proof. For the forward direction, suppose that $f = \sum_{i=1}^m g_i^2$, with $g_i(x) = v_i^\top v_{d/2}(x)$ by writing it out in the monomial basis. Then,

$$\begin{aligned} f(x) &= \sum_{i=1}^m v_{d/2}(x)^\top v_i v_i^\top v_{d/2}(x) \\ &= \left\langle v_{d/2}(x), \underbrace{\sum_{i=1}^m v_i v_i^\top}_{A} v_{d/2}(x) \right\rangle. \end{aligned}$$

The backward direction is straightforward by decomposing A as $\sum \lambda_i v_i v_i^\top$, where each $\lambda_i \geq 0$, and observing that each $v_i^\top v_{d/2}(x)$ is a polynomial of degree at most $d/2$. ■

As a corollary, this implies that if an f has a degree d SoS proof, it has one with at most $\binom{n+d}{d}$ squares. Also note that eq. (1.2) is *linear* in the elements of A.
If we bump up a function by enough, we can ensure non-negativity. It turns out that we can do the same to ensure SoS-ness.

Lemma 1.5. Let $f : \{-1, 1\}^n \to \mathbb{R}$ be any function of degree at most d. For sufficiently large L, $L + f$ has a degree d SoS certificate.

Proof. Note that for any S, $1 + x_S \geq 0$ has a degree $\lceil |S|/2 \rceil$ SoS proof. Indeed, setting $S = T_1 \sqcup T_2$ for T_1, T_2 of (almost) equal size, $1 + x_S = \frac{1}{2}(x_{T_1} + x_{T_2})^2$. Similarly, $1 - x_S$ has a degree $|S|$ SoS proof as well. Therefore,

$$\sum_{|S| \leq d} |\hat{f}(S)| + \sum_{|S| \leq d} \hat{f}(S) x_S = \sum_{|S| \leq d} |\hat{f}(S)|(1 + \operatorname{sign}(\hat{f}(S)) x_S)$$

has a degree d SoS certificate, so the statement is true with $L = \sum_{|S| \leq d} \hat{f}(S)$. ■

1.2. Semidefinite Programming

The reader is likely familiar with *linear programming*, where we are interested in

$$\min_{x \in \mathcal{P}} c^\top x, \text{ where } \mathcal{P} = \{x \geq 0 : Ax = b\}.$$

Although a linear program may in general have inequalities in the constraints, we may merge these into the $x \geq 0$ condition by introducing slack variables (if we have $\sum_i a_i x_i \geq 0$, we may add a non-negative variable y and make it $\sum_i a_i x_i - y = 0$). In *semidefinite programming*, the setting is mostly the same, albeit with the minor change that we represent the variables by a matrix instead of a vector, and we additionally have that this matrix is positive semidefinite. More concretely, denoting

$$\langle C, X \rangle = \sum_{i,j} C_{ij} X_{ij},$$

we are interested in

$$\min_{X \in \mathcal{S}} \langle C, X \rangle, \text{ where } \mathcal{S} = \{X \succeq 0 : \langle A_i, X \rangle = b_i \text{ for } i \in [m]\}.$$

We interchangeably use $\mathcal{S}$ to denote the set of constraints and the corresponding body. Proposition 1.4 suggests a link between SoS proofs and SDPs. A natural question is: can we solve SDPs efficiently?
Note that the set of all PSD matrices X forms a convex cone. In combination with the linear constraints, the intersection of this cone and the affine subspace form a so-called "spectrahedron", which we would like to minimize our quantity over. Note that any linear program is a semidefinite program, by enforcing that all off-diagonal elements of the matrix are zero. To answer our earlier question, it turns out that we cannot solve SDPs exactly.[1] However, if we enforce certain structural restrictions, we can solve them approximately (up to a small additive error).

Definition 1.6 (Separation Oracle)**.** For a convex body $K \subseteq \mathbb{R}^n$, a (*strong*) *separation oracle* for K does the following given as input any $x \in K$.

1. if $x \in K$, it returns yes.
2. if $x \notin K$, it returns no, and in addition a vector a and real b such that $\langle a, y \rangle \geq b$ for all $y \in K$ and $\langle a, x \rangle < b$ – this is a so-called "separating hyperplane" that separates x and K.

More generally, we can efficiently minimize an inner product over a convex (bounded) body up to an additive error of ϵ, given an efficient weak separation oracle.

Theorem 1.7. Let $f : \{-1, 1\}^n \to \mathbb{R}$ have a degree d sum-of-squares proof of non-negativity. Then, for $\epsilon > 0$, there exists an algorithm that finds a sum-of-squares proof of $f + \epsilon$ in $\mathrm{poly}(n^d, \log(1/\epsilon))$.

The high-level idea of the algorithm is as follows.
We first solve the "feasibility problem" of finding a point in a body K, given that $B(c, r) \subseteq K \subseteq B(0, R)$. We begin by setting $\mathcal{E}^{(0)} = B(0, R)$. Given the ellipsoid $\mathcal{E}^{(i)}$, if its center returns yes, we return the point itself. Otherwise, we use the separating hyperplane to get a halfspace H in which K is contained, and set $\mathcal{E}^{(i+1)}$ to be the smallest ellipsoid containing $\mathcal{E}^{(i)} \cap H$. This algorithm runs in $\mathrm{poly}(n, \mathrm{size}(K)) \log(R/r)$ – the proof amounts to showing that the volume of the ellipsoid decreases by a factor of at least $\exp(1/2(n+1))$ at each stage, and we have a lower bound on the volume of K by $\mathrm{vol}(B(0, r))$.
We can slightly modify this algorithm to one that approximately solves the optimization version of maximizing $c^\top x$ as well. Once we get a point α in the body, we begin looking at $K \cap \{x : c^\top x > c^\top \alpha\}$ and repeat the feasibility algorithm. This is repeatedly done until we can guarantee that we are within ϵ of the optimum. The only non-trivial part of this algorithm is showing that we can use the oracle to construct an oracle for the new body $K \cap \{x : c^\top x > c^\top \alpha\}$.
To complete the connection to SDPs, we require that the SDP constraints $\mathcal{S}$ admits an efficient weak separation oracle; we omit the details of this. Next, we require that the body $\mathcal{S}$ contains a ball and is contained in a ball. The former is not true in general because the constraints typically make our body lower-dimensional (a subspace). To get around this, we introduce an additive error in each the contraints, so the new constraints are $|\langle A, X \rangle - b_i| \leq \epsilon$ for each i. In this case, there is a ball of radius $O((\epsilon/\|A\|_F)^n)$ contained in the body, where $\|A\|_F^2 = \sum_{i,j,k} (A_i)_{jk}^2$.
In our context of finding X such that $f(x) = v_{d/2}(x)^\top X v_{d/2}(x)$, we know that $\|A\|_F^2 \leq \mathrm{Tr}(A)^2 \leq \hat{f}(\varnothing)^2$, so the body is bounded as well.

Like how LPs have duals, so do SDPs. If we have the primal

$$\min_{X \in \mathcal{S}} \langle C, X \rangle, \text{ where } \mathcal{S} = \left\{X \succeq 0 : \langle A_i, X \rangle = b_i \text{ for } i \in [m]\right\},$$

[1] It is not even known if this is in NP! It is known that it is in PSPACE however.

its dual is

$$\max_{y \in \mathcal{S}^D} b^\top y, \text{ where } \mathcal{S}^D = \left\{ S \succeq 0 : C - \sum_{i=1}^m y_i A_i = S \right\}.$$

The PSDness condition in the dual just says that $C \succeq \sum_{i=1}^m y_i A_i$.

Proposition 1.8 (Weak Duality)**.** Let X and y be solutions to the primal and dual SDPs respectively. Then, $\langle C, X \rangle \geq b^\top y$.

Proof. We have

$$\begin{aligned} \langle C, X \rangle &= \left\langle \sum_{i=1}^m y_i A_i + S, X \right\rangle \\ &= \sum_{i=1}^m y_i \langle A_i, X \rangle + \langle S, X \rangle \\ &= b^\top y + \langle S, X \rangle \geq b^\top y. \end{aligned}$$

The final inequality requires showing that if $S, X \succeq 0$, then $\langle S, X \rangle \geq 0$ – this is a simple corollary of the Schur Product Theorem we shall see later, using $\mathbf{1}^\top (S \circ X) \mathbf{1} \geq 0$. ■

In linear programming, we have strong duality which asserts that the two optima are in fact *equal*. However, in SDPs, some mild conditions are required for this to be true.

Theorem 1.9 (Strong duality)**.** Let $\mathcal{S}$ be the set of constraints of a primal SDP and $\mathcal{S}^D$ the set of constraints in its dual, such that the two have optima α^*, β^*. Then, $\langle C, \alpha^* \rangle = \langle b, \beta^* \rangle$ if

1. the spectrahedron $\mathcal{S}$ is non-empty and there exists β such that $\sum_{i \in [m]} \beta_i A_i - C \succ 0$, or
2. the spectrahedron $\mathcal{S}^D$ is non-empty and there exists $\alpha \succ 0$ such that $\langle A, \alpha \rangle = b_i$ for all $i \in [m]$.

As a corollary, one may show that $\langle C, \alpha^* \rangle = \langle b, \beta^* \rangle$ if the set of optimal solutions of either of the two SDPs is non-empty and bounded.

We omit the (rather involved) proof of the above.

1.3. Pseudoexpectations

Let us again restrict ourselves to $\{-1, 1\}^n$ for a while. We have established one link between SoS proofs and SDPs, and now we shall establish another link between them and the following.

Definition 1.10 (Pseudodistribution)**.** A *degree d pseudodistribution* is a function $\mu : \{-1, 1\}^n \to \mathbb{R}$ such that the expectation operator $\widetilde{\mathbb{E}}_\mu$ defined by $\widetilde{\mathbb{E}}_\mu f = \sum_{x \in \{-1,1\}^n} f(x)\mu(x)$ satisfies

(a) $\widetilde{\mathbb{E}}_\mu 1 = 1$, and

(b) for all f of degree at most $d/2$, $\widetilde{\mathbb{E}}_\mu f^2 \geq 0$.

In this case, $\widetilde{\mathbb{E}}_\mu$ is called a *pseudoexpectation*.

Analogous to Proposition 1.2, we get that any degree $\geq 2n$ pseudodistribution is an actual distribution, in the sense that $\mu \geq 0$. Analogous to Proposition 1.4, we get the following.

Proposition 1.11. $\widetilde{\mathbb{E}}$ is a degree d pseudoexpectation iff

(a) $\widetilde{\mathbb{E}}1 = 1$, and

(b) $\widetilde{\mathbb{E}} v_{d/2}(x) v_{d/2}(x)^\top \succeq 0$.

Proof. Note that for any vector $(\hat{f})$ of Fourier coefficients of a degree $\leq d/2$ function $f : \{-1,1\}^n \to \mathbb{R}$ (so $f(x) = \hat{f}^\top v_{d/2}(x)$),

$$\begin{aligned}\widetilde{\mathbb{E}} f^2 &= \widetilde{\mathbb{E}} \left(\sum_{|S| \leq d} \hat{f}(S) x_S \right)^2 \\ &= \widetilde{\mathbb{E}} \hat{f}^\top v_{d/2}(x) v_{d/2}(x)^\top \hat{f} \\ &= \hat{f}^\top \left(\widetilde{\mathbb{E}} v_{d/2}(x) v_{d/2}(x)^\top \right) \hat{f}.\end{aligned}$$

To conclude, note that $\widetilde{\mathbb{E}} v_{d/2}(x) v_{d/2}(x) \succeq 0$ iff $\hat{f}^\top \left(\widetilde{\mathbb{E}} v_{d/2}(x) v_{d/2}(x)^\top \right) \hat{f} \geq 0$ for all vectors $\hat{f}$. ■

Given any function that is not non-negative everywhere, there exists some distribution μ such that $\mathbb{E}_\mu f < 0$. Ideally, we would like a similar result in order to distinguish between functions that have SoS certificates of degree d and those that don't.

Theorem 1.12. f has a degree d sum-of-squares proof iff for all degree d pseudoexpectations $\widetilde{\mathbb{E}}$, $\widetilde{\mathbb{E}} f \geq 0$.

Equivalently, f does not have a degree d sum-of-squares proof iff there exists a degree d pseudoexpectation $\widetilde{\mathbb{E}}$ such that $\widetilde{\mathbb{E}} f < 0$.

Proof. The forward direction is straightforward by Definition 1.10(b). For the backward direction, suppose instead that f does not have a degree d SoS proof. Then, there exists a separating hyperplane between f and this set, that is, some degree d pseudoexpectation $\widetilde{\mathbb{E}}$ such that $\widetilde{\mathbb{E}} f < 0$. If we manage to show that $\widetilde{\mathbb{E}} 1 > 0$, we are done since we can then rescale μ to make it exactly equal to 1. By Lemma 1.5, we have $L > 0$ such that $\widetilde{\mathbb{E}}(f + L) \geq 0$. Since $\widetilde{\mathbb{E}} f < 0$, this means that $\widetilde{\mathbb{E}} L = L \cdot \widetilde{\mathbb{E}} 1 > 0$, completing the proof. ■

Using our earlier discussion, given a function f without a degree d SoS certificate of positivity, we may find in $\mathrm{poly}(n^d, 1/\epsilon, \mathrm{size}(f))$ time a pseudoexpectation $\widetilde{\mathbb{E}}$ such that $\widetilde{\mathbb{E}} f < \epsilon$.

§2. Quadratic optimization on the hypercube

2.1. Max-cut

In this subsection, let us describe how the content of the previous three subsections interact through an example, and give an approximation algorithm for the max-cut problem.

Question. Given a graph $G = (V, E)$, find $S \subseteq V$ such that the size of the cut $E(S, S^c) = \left| \{\{i, j\} \in E : i \in S, j \in S^c\} \right|$ is maximized.

Unlike min-cut, which may be solved in polynomial time using flow, the above is NP-complete.
One basic approximation algorithm was proposed by Erdős, which merely returns a random cut. With constant probability, the returned cut is a $1/2$-approximation of the max-cut. We shall in this algorithm study an algorithm due to Goemans and Williamson [GW00].
Assume wlog that $V = [n]$, and identify any $S \subseteq V$ with the vector in $\{-1, 1\}^n$ with a 1 at precisely those vertices in S. Note that the function defined by

$$f_G(x) = \frac{1}{4} \sum_{ij \in E} (x_i - x_j)^2 = \frac{1}{2} \sum_{ij \in E} (1 - x_i x_j).$$

on input S returns precisely the size of the cut corresponding to S. Equivalently, considering the *graph Laplacian* $L_G \coloneqq D_G - A_G$, where D_G is the diagonal matrix of degrees and A_G is the adjacency matrix, we have

$$f_G(x) = \frac{1}{4} x^\top L_G x. \tag{2.1}$$

We are interested in $\max_{x \in \{-1,1\}^n} f_G(x) =: \mathsf{opt}(G)$.

Theorem 2.1. Set $\alpha_{\mathrm{GW}} \coloneqq \min_{\rho \in [-1,1]} \frac{2 \arccos(\rho)}{\pi(1-\rho)} \approx 0.8786$. Then,

$$\frac{\mathsf{opt}(G)}{\alpha_{\mathrm{GW}}} - f_G(x) \geq 0$$

has a degree 2 sum-of-squares certificate.

Let $\widetilde{\mathbb{E}}_{\mathsf{opt}}$ be a pseudoexpectation that maximizes $\widetilde{\mathbb{E}}_{\mathsf{opt}} f_G$ as $\mathsf{opt}_{\mathrm{SOS}_2}(G)$. Clearly, $\mathsf{opt}_{\mathrm{SOS}_2}(G) \geq \mathsf{opt}(G)$. Furthermore, by the previous theorem,

$$\mathsf{opt}(G) \leq \mathsf{opt}_{\mathrm{SOS}_2}(G) \leq \frac{1}{\alpha_{\mathrm{GW}}} \mathsf{opt}(G).$$

By the discussion at the end of the previous subsection, we can find in $\mathrm{poly}(n, 1/\epsilon)$ a degree 2 pseudodistribution μ such that

$$\widetilde{\mathbb{E}}_{\mu} f_G \geq \mathsf{opt}_{\mathrm{SOS}_2}(G) - \epsilon.$$

So,

$$\frac{1}{\alpha_{\mathrm{GW}}} \mathsf{opt}(G) \geq \widetilde{\mathbb{E}}_{\mu} f_G \geq \mathsf{opt}(G) - \epsilon.$$

Lemma 2.2. Let μ be a degree 2 pseudodistribution on $\{-1, 1\}^n$. Then, there exists a ("real") distribution μ' on $\{-1, 1\}^n$ such that

$$\mathbb{E}_{\mu'} f_G \geq \alpha_{\mathrm{GW}} \cdot \widetilde{\mathbb{E}}_{\mu} f_G.$$

Further, it is possible to efficiently sample from μ' given μ. Plugging this back into our previous sequence of equations,

$$\mathbb{E}_{\mu'} f_G \geq \alpha_{\mathrm{GW}} (\mathsf{opt}(G) - \epsilon) \geq (\alpha_{\mathrm{GW}} - \epsilon) \mathsf{opt}(G),$$

and efficient sampling implies that we can in $\mathrm{poly}(n, 1/\epsilon)$ time sample a random cut S such that with good probability, the size of the cut of S is a $(\alpha_{\mathrm{GW}} - \epsilon)$-approximation of the max-cut.
Let us now get to the proofs of the above results.

Proof that Lemma 2.2 implies Theorem 2.1. It suffices to show that for all pseudodistributions $\widetilde{\mathbb{E}}_\mu$,

$$\widetilde{\mathbb{E}}_\mu \left[\frac{\mathsf{opt}(G)}{\alpha_{\mathrm{GW}}} - f_G \right] \geq 0.$$

Equivalently, we would like to show that

$$\widetilde{\mathbb{E}}_\mu f_G \leq \frac{\mathsf{opt}(G)}{\alpha_{\mathrm{GW}}}.$$

Letting μ' be a distribution as in Lemma 2.2,

$$\widetilde{\mathbb{E}}_\mu f_G \leq \frac{1}{\alpha_{\mathrm{GW}}} \mathbb{E}_{\mu'} f_G \leq \frac{1}{\alpha_{\mathrm{GW}}} \mathsf{opt}(G). \qquad \blacksquare$$

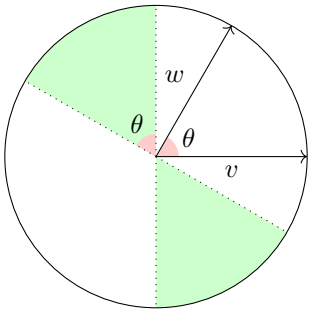
Proof of Lemma 2.2. We may assume wlog that $\widetilde{\mathbb{E}}_\mu x = 0$, by changing $\mu(x)$ to $\frac{\mu(x)+\mu(-x)}{2}$ – note that this procedure does not change $\widetilde{\mathbb{E}}_\mu f_G$ because $f_G(x) = f_G(-x)$. Using Proposition 1.11(b) and recalling that any principal submatrix of a PSD matrix is PSD, $\widetilde{\mathbb{E}}_\mu x x^\top \succeq 0$. So, let ν be a normal distribution on $\mathbb{R}^n$ with mean 0 and covariance matrix $\widetilde{\mathbb{E}}_\mu x x^\top$. Finally, define μ' by the process that samples a vector g according to ν and returns $\hat{x} = \mathrm{sign}(g)$, the vector in $\{-1, 1\}^n$ whose ith coordinate is just the sign ± 1 of g_i – this is well-defined with probability 1. Note that an $(x_i - x_j)^2$ term in f_G contributes to the cut iff $\mathrm{sign}(g_i) \neq \mathrm{sign}(g_j)$. That is,

$$\mathbb{E}_{\mu'} f_G = \sum_{ij \in E} \Pr[\mathrm{sign}(g_i) \neq \mathrm{sign}(g_j)].$$

For distinct i, j, set $\rho_{ij} = \mathbb{E}_\mu[x_i x_j] = \mathbb{E}[g_i g_j]$. Let $h \sim \mathcal{N}(0, \mathrm{Id}_2)$. Then, to analyze the above probability (for a fixed i, j), we can assume that $g_i = \langle h, v \rangle$ and $g_j = \langle h, w \rangle$ for some v, w such that $\langle v, w \rangle = \rho_{ij}$. So, $\mathrm{sign}(g_i) \neq \mathrm{sign}(g_j)$ iff $\langle h, v \rangle$ and $\langle h, w \rangle$ have opposite signs. Because the "direction" $h/\|h\|$ of h is uniformly distributed on $\mathbb{S}^1$, we get that

$$\Pr[\mathrm{sign}(g_i) \neq \mathrm{sign}(g_j)] = \frac{\arccos(\rho_{ij})}{\pi},$$

as seen in the following diagram, where h must lie in the green region for the signs to be different.



The angle between v, w is $\theta = \arccos(\rho_{ij})$.

Using the facts that $\mathbb{E}[g_i^2] = 1$ and $\mathbb{E}[g_i g_j] = \rho_{ij}$, we have that $\mathbb{E}[(g_i - g_j)^2] = 2(1 - \rho_{ij})$ and so

$$\begin{aligned}
\mathbb{E}_{\mu'} f_G &= \sum_{ij \in E} \Pr[\mathrm{sign}(g_i) \neq \mathrm{sign}(g_j)] \\
&= \sum_{ij \in E} \frac{\arccos(\rho_{ij})}{2\pi(1 - \rho_{ij})} \mathbb{E}[(g_i - g_j)^2] \\
&\geq \frac{\alpha_{\mathrm{GW}}}{4} \cdot \mathbb{E} \left[\sum_{ij \in E} (g_i - g_j)^2 \right] = \alpha_{\mathrm{GW}} \widetilde{\mathbb{E}}_\mu f_G.
\end{aligned}$$

$\blacksquare$

Now, we have managed to get roughly an α_{GW}-approximation using degree 2 SoS. Is it possible to do any better using degree 2 SoS? What about with a higher (but constant) degree? It might even be interesting to see if we can get a better approximation with non-constant degree, say $O(\log n)$.
To answer the first question, it turns out that what we have done is indeed the best possible. A strong result regarding the constant degree case is due to Khot-Kindler-Mossel-O'Donnell [KKMO07], where it is proved that Khot's *Unique Games Conjecture* (UGC) [Kho02] implies that an $(\alpha_{\text{GW}} + \epsilon)$-approximation is NP-hard for any $\epsilon > 0$. While it is unknown at the time of writing this whether the unique games conjecture is true, we have strong reason to believe that it is due to a recent result [DKK+18] which proves the "2-to-2 Games Conjecture", a close variant of the unique games conjecture. We shall later look at the UGC in more detail.

Let us get back to the Goemans-Williamson algorithm. Instead of looking at the best approximation ratio, can we parametrize the output result in terms of the optimal value?

Proposition 2.3. Let G be a graph with $\mathsf{opt}(G) = (1-\delta)|E|$. For the output distribution μ' of the Goemans-Williamson algorithm, $\mathbb{E}_{\mu'} f_G = (1 - O(\sqrt{\delta}))|E|$.

Proof. *** INCOMPLETE *** ■

Is this rounding we have done, called "Gaussian rounding", the best possible? It turns out that it is not, and we can in general do better using the "RPR^2" scheme of roundings. We shall soon study this in more detail.

Let us now return to our earlier statement that it is impossible to do better using degree 2 SoS. That is, for graphs in general, if we can get a degree 2 SoS certificate of non-negativity for

$$\frac{\mathsf{opt}(G)}{c} - f_G(x),$$

how large can c be? We shall show that $c = \alpha_{\text{GW}}$ is optimal, by looking at the cycle C_n for odd n. This serves as a "gap" example. It is easily seen that the max-cut in this graph is $n - 1 = \left(1 - \frac{1}{n}\right)|E|$. We shall show that there exists a degree 2 pseudodistribution μ such that

$$\widetilde{\mathbb{E}}_{\mu} f_{C_n} \geq \left(1 - O\left(\frac{1}{n^2}\right)\right)|E|.$$

Due to Proposition 2.3, this shows that the Goemans-Williamson algorithm is tight, at least up to constant factors. We can think of the cycle as something of a discretization of the 2-dimensional sphere. If we instead look at the discretization of a high-dimensional sphere, it can be shown that this is tight even up to constant factors. We refer the reader to [FS02] for details. The sketch of the proof for the cycle is as follows.
Recall eq. (2.1), so we are interested in $\max_{x \in \{-1,1\}^n} x^\top L_G x$. This is at most $\max_{x:\|x\|_2 = \sqrt{n}} x^\top L_G x = n\|L_G\|_2$, which can be computed in polynomial time. Now, how do we construct a pseudodistribution $\widetilde{\mathbb{E}}$ for the cycle as mentioned earlier? Note that a given $\widetilde{\mathbb{E}}$ is a well-defined degree 2 pseudodistribution iff $\widetilde{\mathbb{E}}(1, x)(1, x)^\top$ is a PSD matrix with 1s on the diagonal. Now,

$$\begin{aligned}
\widetilde{\mathbb{E}} f_G(x) &= \widetilde{\mathbb{E}} x^\top L_G x \\
&= \widetilde{\mathbb{E}} \langle L_G, xx^\top \rangle \\
&= \left\langle L_G, \widetilde{\mathbb{E}} xx^\top \right\rangle.
\end{aligned}$$

Observe that the top eigenvalue of L_G is indeed $1 - O(1/n^2)$, and this eigenspace is 2-dimensional. It turns out that for an appropriate choice of v_1, v_2 in this eigenspace, we can ensure that $v_1 v_1^\top + v_2 v_2^\top$ does have only 1s on the diagonal (this is essentially a consequence of the fact that $\sin^2\theta + \cos^2\theta = 1$).

2.2. The positive semidefinite case

In the previous subsection, we looked at $\max_{x\in\{-1,1\}^n} x^\top L_G x$, where L_G is the (positive semidefinite) Laplacian of a graph. This is an example of quadratic optimization, where we are more generally interested in

$$\mathsf{opt}(B) \coloneqq \max_{x\in\{-1,1\}^n} x^\top B x$$

for some $n \times n$ matrix B.
In the case where $B \succeq 0$, it turns out that we can do something similar to what we had done in the max-cut algorithm.

Theorem 2.4 (Nesterov)**.** Let B be a positive semidefinite $n \times n$ matrix. Then,

$$\frac{\mathsf{opt}(B)}{c} - x^\top B x$$

has a degree 2 sum-of-squares certificate for $c = 2/\pi \approx 0.63$.

By the discussion in the previous section, this means as a corollary that we have a $\mathrm{poly}(n, 1/\epsilon)$-time $(2/\pi - \epsilon)$-approximation algorithm for any $\epsilon > 0$.

Definition 2.5. Let $M \in \mathbb{R}^{n\times n}$. Given $f : \mathbb{R} \to \mathbb{R}$, define $f[M] \in \mathbb{R}^{n\times n}$ by $f[M]_{ij} = f(M_{ij})$ for all i, j.

Proposition 2.6. Suppose M is a positive semidefinite matrix and f a function whose Taylor series has all positive Taylor coefficients and is uniformly convergent on $[-1, 1]$. Then, $f[M]$ is positive semidefinite.

The above is a corollary of the following simple observation.

Proposition 2.7 (Schur Product Theorem)**.** Let M, M' be positive semidefinite matrices. Denote by $M \circ M'$ the *Hadamard product* of M, M' defined by $(M \circ M')_{ij} = M_{ij}M'_{ij}$. Then, $M \circ M'$ is positive semidefinite.

Proof. Let $M = \sum_i \lambda_i v_i v_i^\top$ and $M' = \sum_j \lambda'_j v'_j v'^\top_j$. Using linearity of the Hadamard product,

$$M \circ M' = \sum_{i,j} \lambda_i\lambda'_j (v_i v_i^\top) \circ (v_j v_j'^\top) = \sum_{i,j} \lambda_i\lambda'_j (v_i \circ v'_j)(v_i \circ v'_j)^\top \succeq 0. \qquad \blacksquare$$

Proof of Proposition 2.6. Denote $[M]^2 = M \circ M$, and $[M]^i = [M]^{i-1} \circ M$ more generally. By the Schur Product Theorem, $[M]^i \succeq 0$ for all i. Therefore, $\sum c_i[M]^i \succeq 0$, that is, $(\sum c_i x^i)[M] \succeq 0$. $\blacksquare$

Proof of Nesterov. As in the previous subsection, let μ be a zero mean degree 2 pseudodistribution on $\{-1, 1\}^n$, g a normal random variable with zero mean and covariance matrix $\widetilde{\mathbb{E}}_\mu xx^\top$, and $\hat{x} \coloneqq \mathrm{sign}(g)$ distributed as μ'. A straightforward byproduct of the final part of the proof of Lemma 2.2 is that

$$\mathbb{E}_{\mu'}[\hat{x}_i\hat{x}_j] = \frac{2}{\pi}\arcsin \mathbb{E}[g_i g_j].$$

Therefore,

$$\begin{aligned}
\mathbb{E}_{\mu'}\hat{x}^\top B\hat{x} &= \sum_{i,j} B_{ij}\mathbb{E}[\hat{x}_i\hat{x}_j] \\
&= \sum_{i,j} B_{ij}\frac{2}{\pi}\arcsin[g_i g_j] \\
&= \frac{2}{\pi}\left\langle B, \arcsin\left[\mathbb{E}gg^\top\right]\right\rangle.
\end{aligned}$$

Recall that if $B, C \succeq 0$, then $\langle B, C \rangle \geq 0$. In particular,

$$\left\langle B, \arcsin\left[\mathbb{E} gg^\top\right] - \mathbb{E} gg^\top \right\rangle \geq 0,$$

so

$$\mathbb{E}_{\mu'} \hat{x}^\top B \hat{x} \geq \frac{2}{\pi} \langle B, \mathbb{E} gg^\top \rangle = \frac{2}{\pi} \widetilde{\mathbb{E}}_\mu x^\top B x.$$

The remainder of the proof is identical to that in the previous subsection. ■

2.3. The most general case

Let us next look at the case where B is any arbitrary matrix. First of all, we may assume that B is symmetric by looking at its symmetrization $(B + B^\top)/2$ instead. We may also assume that all diagonal entries of B are 0, since if we set $B = D + N$ where D is diagonal and N has all diagonal entries zero,

$$\max_{y \in \{-1,1\}^n} y^\top B y = \operatorname{Tr}(B) + \max_{y \in \{-1,1\}^n} y^\top N y.$$

We assume so for the remainder of this subsection.
We shall give an $O(\log n)$-approximation algorithm. First of all, is $\mathsf{opt}(B)$ even non-negative?

Proposition 2.8. Let $y \in [-1, 1]^n$. Then, there exists $\hat{y} \in \{-1, 1\}^n$ such that $\hat{y}^\top B y \geq y^\top B y$.

In particular, setting $y = 0$ implies that the desired value is non-negative.

Proof. Consider the random variable $\hat{y}$ on $\{-1, 1\}^n$ which has $\hat{y}_i = 1$ with probability $(1+y_i)/2$ and 0 with probability $(1 - y_i)/2$, independently for different coordinates i. Note that $\mathbb{E}\hat{y}_i \hat{y}_j = y_i y_j$ for distinct i, j. Consequently,

$$\mathbb{E}_\mu \hat{y}^\top B \hat{y} = y^\top B y,$$

so the desideratum follows. ■

The above result is also true in the more general case where $\operatorname{Tr}(B) \geq 0$, but we do not require it.

We can in fact get a stronger lower bound than just the 0 in the above proposition.

Proposition 2.9.

$$\max_{y \in \{-1,1\}^n} y^\top B y \geq \frac{1}{n} \sum_{i,j} |B_{ij}|.$$

Proof. *** INCOMPLETE *** ■

The sum-of-squares proof we shall give is due to [Meg01, CW04].

Theorem 2.10. For sufficiently large n and $c = O(\log n)$,

$$\frac{\mathsf{opt}(B)}{c} - x^\top B x$$

has a degree 2 sum-of-squares certificate.

While we do not compute the exact constants exactly, the above is true for roughly $n > 60$ and $c = 4 \log n$.

Proof. As in the max-cut and PSD cases, we prove that given any pseudodistribution μ, there exists an (efficiently sampleable) distribution μ' on $\{-1,1\}^n$ such that $\mathbb{E}_{\mu'} \hat{x}^\top B \hat{x} \geq \frac{1}{O(\log n)} \widetilde{\mathbb{E}}_\mu x^\top B x$. By Proposition 2.8, it suffices to show this for a distribution on the continuous hypercube $[-1,1]^n$ instead of $\{-1,1\}^n$.
As before, choose $g \sim \mathcal{N}(0, \mathbb{E}_\mu x x^\top)$, so

$$\mathbb{E}[g^\top B g] = \widetilde{\mathbb{E}}_\mu [x^\top B x].$$

Make the mild assumption that $\mathbb{E}[g^\top B g] \geq 0$; the analysis of the general case is nearly identical. For a suitable constant C, we have that

$$\Pr[\|g\|_\infty > C \log n] \cdot \mathbb{E}[g^\top B g \mid \|g\|_\infty > C \log n] \leq \frac{1}{n^2} \mathbb{E}[g^\top B g], \text{ so}$$
$$\Pr[\|g\|_\infty \leq C \log n] \cdot \mathbb{E}[g^\top B g \mid \|g\|_\infty \leq C \log n] \geq \left(1 - \frac{1}{n^2}\right) \mathbb{E}[g^\top B g] \tag{2.2}$$

Our assumption that $\mathbb{E}[g^\top B g] \geq 0$ also implies that all the quantities above are non-negative. The final random variable $\hat{x}$ on the solid hypercube is defined by

$$\hat{x}_i = \begin{cases} \frac{g_i}{C\sqrt{\log n}}, & |g_i| \leq C\sqrt{\log n}, \\ \frac{g_i}{|g_i|}, & \text{otherwise.} \end{cases}$$

Then,

$$\begin{aligned} \mathbb{E}[\hat{x}^\top B x] &\geq \Pr[\|g\|_\infty \leq C\sqrt{\log n}] \cdot \mathbb{E}[\hat{x}^\top B \hat{x} \mid \|g\|_\infty \leq C\sqrt{\log n}] \\ &\geq \frac{1}{2C^2 \log n} \mathbb{E}[g^\top B g \mid \|g\|_\infty \leq C\sqrt{\log n}] \\ &\overset{(2.2)}{\geq} \frac{1}{O(\log n)} \mathbb{E}[g^\top B g] = \frac{1}{O(\log n)} \widetilde{\mathbb{E}}_\mu [x^\top B x], \end{aligned}$$

completing the proof. ∎

This above rounding is a specific case of the more general RPR^2 scheme of roundings that we mentioned earlier. In this, we "modify" $\widetilde{\mathbb{E}}_\mu x x^\top$ in some way (in the above method of Nesterov, we scale it down), sample a Gaussian with this modified covariance matrix, then do randomized rounding. In the setting of max-cut, we search over all RPR^2 roundings and output whichever returns the maximum cut value.

2.4. The bipartite support case

In this section, we shall look at the specific case where the *support* $\mathrm{supp}(B) \coloneqq \{\{i,j\} : B_{ij} \neq 0\}$ defines a bipartite graph (on vertex set $[n]$). We also assume that B is symmetric by symmetrizing it. The constant-factor approximation we shall describe is due to Alon and Naor [AN04].
Since $\mathrm{supp}(B)$ is bipartite, there exists some bipartition $X \cup Y$ of $[n]$ such that $B_{xx'} = B_{yy'} = 0$ for any $x, x' \in X$ and $y, y' \in Y$. Letting B' be the submatrix of B consisting of the X-rows and Y-columns (note that the submatrix consisting of the Y-rows and X-columns is then $B'^\top$) and splitting a given vector $x \in \mathbb{R}^n$ into two parts (x_X, x_Y), we have that

$$x^\top B x = 2 x_X^\top B' x_Y.$$

Therefore, our optimization problem is equivalent to the following: given an arbitrary $n \times n$ matrix B, determine

$$\max_{x,y \in \{-1,1\}^n} x^\top B y.$$

For simplicity, denote the above maximum by $\mathsf{opt}(B)$.

While the B' we looked at above in the bipartite setting need not be square, we can assume it is by appending appropriately many rows/columns filled with zeros.
Given norms $\|\cdot\|$ and $\|\cdot\|$ on $\mathbb{R}^n$, we have an associated *operator norm* on matrices defined by

$$\|A\| = \inf\{c \geq 0 : \|Ax\| \leq \|x\| \text{ for all } x \in \mathbb{R}^n\}.$$

When the first norm is the L^p and the second is the L^q, the operator norm is denoted the $\|\cdot\|_{q\to p}$ norm. That is,

$$\|A\|_{q\to p} \coloneqq \max_{\substack{x\in\mathbb{R}^n \\ x\neq 0}} \frac{\|Ax\|_p}{\|x\|_q}.$$

Now, note that for a given x,

$$\max_{y\in\{-1,1\}^n} x^\top By = \max_{y\in\{-1,1\}^n} \langle Bx, y\rangle = \|Bx\|_1,$$

since we can just choose the sign of y_i opposite to that of $(Bx)_i$. Further,

$$\begin{aligned}\|B\|_{\infty\to 1} &= \max_{\|x\|\le 1} \sum_i \left|\sum_j B_{ij}x_j\right| \\ &= \max_{|x_i|=1} \left|\sum_j B_{ij}x_j\right| \\ &= \max_{x\in\{-1,1\}^n} \|Bx\|_1 = \max_{x,y\in\{-1,1\}^n} x^\top By,\end{aligned}$$

where the second equality is because the summation is a convex function of the (x_i), so it is maximized at a vertex of the cube $[-1,1]^n$, namely at a point in $\{-1,1\}^n$. Therefore, our problem is equivalent to approximating $\|B\|_{\infty\to 1}$ for an arbitrary matrix $B\in\mathbb{R}^{n\times n}$.

Theorem 2.11. There exists a constant K_G such that

$$K_G\mathsf{opt}(B) - x^\top By$$

has a degree 2 sum-of-squares certificate.

Interestingly, the exact value of K_G is an open problem, and the interested reader may look up *Grothendieck's inequality* for more details. It is known that

$$1.57 \approx \frac{\pi}{2} \le K_G \le \frac{\pi}{2\ln(1+\sqrt{2})} \approx 1.78.$$

We shall give a proof due to Krivine in 1977 which yields the bound on the right.

Proof. This proof is slightly different from previous ones in terms of execution. We shall show that given a degree 2 pseudodistribution μ (on $\{-1,1\}^n$), there exists a real distribution μ' such that

$$\mathbb{E}_{\mu'}\hat{x}\hat{y}^\top = \frac{2\ln(1+\sqrt{2})}{\pi}\widetilde{\mathbb{E}}_\mu xy^\top.$$

Given this,

$$\begin{aligned}\mathbb{E}_{\mu'}\hat{x}^\top B\hat{y} &= \left\langle B, \mathbb{E}_{\mu'}\hat{x}\hat{y}^\top\right\rangle \\ &= \frac{2\ln(1+\sqrt{2})}{\pi}\left\langle B, \widetilde{\mathbb{E}}_\mu xy^\top\right\rangle = \frac{2\ln(1+\sqrt{2})}{\pi}\widetilde{\mathbb{E}}_\mu x^\top By,\end{aligned}$$

so we are done by methods similar to previous proofs. We shall first modify the "covariance matrix" of $\widetilde{\mathbb{E}}$ in some manner to get another matrix M' before creating the Gaussian used in rounding. Let $c = \ln(1+\sqrt{2})$. This matrix M' is defined by

$$M' = \begin{pmatrix} \sinh\left[c\widetilde{\mathbb{E}}_\mu xx^\top\right] & \sin\left[c\widetilde{\mathbb{E}}_\mu xy^\top\right] \\ \sin\left[c\widetilde{\mathbb{E}}_\mu yx^\top\right] & \sinh\left[c\widetilde{\mathbb{E}}_\mu yy^\top\right]\end{pmatrix}.$$

We shall explain the reasoning behind this choice in the proof. Then, we choose Gaussians $g,h\sim\mathcal{N}(0,M')$, and we finally define $\hat{x}=\operatorname{sign}(g)$ and $\hat{y}=\operatorname{sign}(h)$. To complete the proof, we need to show three things.

(a) $\mathbb{E}_{g,h}\hat{x}\hat{y}^\top = (2c/\pi)\widetilde{\mathbb{E}}_\mu xy^\top$. Recall that

$$\mathbb{E}\hat{x}\hat{y}^\top = \frac{2}{\pi}\arcsin[\mathbb{E}gh^\top].$$

We want this expression on the left to be some constant times $\widetilde{\mathbb{E}}_\mu xy^\top$. So, it makes sense to choose $\mathbb{E}gh^\top = \sin[c\widetilde{\mathbb{E}}_\mu xy^\top]$. This means that the bottom-left and bottom-right of our modified matrix should look like that of M'. While this might inspire us to choose sins on the diagonal blocks as well, doing so causes problems when it comes to PSD-ness, so we choose $\sinh$ instead. The reason for the precise choice of $\sinh$ is explained when we look at why $M' \succeq 0$.
Recalling the definition of $\mathbb{E}gh^\top$ from M',

$$\mathbb{E}[\hat{x}\hat{y}^\top] = \frac{2}{\pi}\arcsin[\mathbb{E}gh^\top] = \frac{2}{\pi}\arcsin[\sin[c\widetilde{\mathbb{E}}_\mu xy^\top]] = \frac{2\ln(1+\sqrt{2})}{\pi}\widetilde{\mathbb{E}}_\mu xy^\top.$$

(b) $M' \succeq 0$. We saw earlier in the proof of Proposition 2.6 that if M is PSD, so is $[M]^i$. It turns out, in fact, that if

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$$

is PSD, so is

$$\begin{pmatrix} [M_{11}]^i & -[M_{12}]^i \\ -[M_{21}]^i & [M_{22}]^i \end{pmatrix}.$$

Indeed,

$$\begin{pmatrix} v \\ w \end{pmatrix}^\top \begin{pmatrix} [M_{11}]^i & -[M_{12}]^i \\ -[M_{21}]^i & [M_{22}]^i \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} v \\ -w \end{pmatrix}^\top \begin{pmatrix} [M_{11}]^i & [M_{12}]^i \\ [M_{21}]^i & [M_{22}]^i \end{pmatrix} \begin{pmatrix} v \\ -w \end{pmatrix}$$

and the matrix on the right is PSD. Recalling that the Taylor series expansions of $\sin$ and $\sinh$ are given by

$$\sinh(x) = \sum_{n=0}^{\infty} \frac{1}{(2n+1)!}x^{2n+1} \text{ and}$$
$$\sin(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!}x^{2n+1},$$

it follows by a proof very similar to that of Proposition 2.6 that $M' \succeq 0$.

(c) $M'_{ii} = 1$ for each i. The value of c is forced by this requirement, and indeed $\sinh(\ln(1+\sqrt{2})) = 1$. ■

Krivine conjectured in his original paper that K_G is exactly equal to this quantity. Later however, it was shown [BMMN11] that K_G is strictly less than this.

Here, we looked at matrices with bipartite support. More generally, if the support of the matrix is some graph G, [AMMN06] give an $O(\log(\chi(G)))$-approximation algorithm. They also show it is get an $o(\log(\omega(g)))$-approximation algorithm. Recall that $\chi(G)$ and $\omega(G)$ are the chromatic number and clique number of a graph G respectively.

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