Semidefinite Programming with Applications in Geometry and Machine Learning

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A linear program (LP) is written

 $\begin{array}{ll} \mbox{minimize} & c^T x\\ \mbox{subject to} & Ax = b\\ & x \geq 0 \end{array}$

where $x \ge 0$ means that the coefficients of the vector x are nonnegative.

- Starts with Dantzig's simplex algorithm in the late 40s.
- First proofs of polynomial complexity by Nemirovskii and Yudin [1979] and Khachiyan [1979] using the ellipsoid method.
- First efficient algorithm with polynomial complexity derived by Karmarkar [1984], using interior point methods.

A semidefinite program (SDP) is written

minimize
$$\operatorname{Tr}(CX)$$

subject to $\operatorname{Tr}(A_iX) = b_i, \quad i = 1, \dots, m$
 $X \succeq 0$

where $X \succeq 0$ means that the matrix variable $X \in \mathbf{S}_n$ is **positive semidefinite**.

- Nesterov and Nemirovskii [1994] showed that the interior point algorithms used for linear programs could be extended to semidefinite programs.
- Key result: self-concordance analysis of Newton's method (affine invariant smoothness bounds on the Hessian).

Modeling

- Linear programming started as a toy problem in the 40s, many applications followed.
- Semidefinite programming has much stronger expressive power, many new applications being investigated today (cf. this talk).
- Similar conic duality theory.
- Algorithms
 - Robust solvers for solving large-scale linear programs are available today (e.g. MOSEK, CPLEX, GLPK).
 - Not (yet) true for semidefinite programs. Very active work now on first-order methods, motivated by applications in statistical learning (matrix completion, NETFLIX, structured MLE, . . .).

Outline

Introduction

Semidefinite programming

- Conic duality
- $\circ\,$ A few words on algorithms

Recent applications

- Combinatorial relaxations
- Ellipsoidal approximations
- $\circ~$ Distortion, embedding
- Mixing rates for Markov chains & maximum variance unfolding
- Moment problems & positive polynomials
- Gordon-Slepian and the maximum of Gaussian processes
- Dicitionary metrics
 - Sparse recovery conditions
 - Tractable performance bounds

Semidefinite Programming

Semidefinite programming: conic duality

Direct extension of LP duality results. Start from a semidefinite program

minimize
$$\operatorname{Tr}(CX)$$

subject to $\operatorname{Tr}(A_iX) = b_i, \quad i = 1, \dots, m$
 $X \succeq 0$

which is a convex minimization problem in $X \in \mathbf{S}_n$. The cone of positive semidefinite matrices is **self-dual**, i.e.

$$Z \succeq 0 \quad \iff \quad \mathbf{Tr}(ZX) \ge 0, \text{ for all } X \succeq 0,$$

so we can form the Lagrangian

$$L(X, y, Z) = \operatorname{Tr}(CX) + \sum_{i=1}^{m} y_i \left(b_i - \operatorname{Tr}(A_i X) \right) - \operatorname{Tr}(ZX)$$

with Lagrange multipliers $y \in \mathbb{R}^m$ and $Z \in \mathbf{S}_n$ with $Z \succeq 0$.

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Semidefinite programming: conic duality

Rearranging terms, we get

$$L(X, y, Z) = \mathbf{Tr} \left(X \left(C - \sum_{i=1}^{m} y_i A_i - Z \right) \right) + b^T y$$

hence, after minimizing this affine function in $X \in \mathbf{S}_n$, the **dual** can be written

maximize
$$b^T y$$

subject to $Z = C - \sum_{i=1}^m y_i A_i$
 $Z \succeq 0,$

which is another semidefinite program in the variables y, Z. Of course, the last two constraints can be simplified to

$$C - \sum_{i=1}^{m} y_i A_i \succeq 0.$$

Primal dual pair

 $\begin{array}{ll} \mbox{minimize} & \mathbf{Tr}(CX) & \mbox{maximize} & b^Ty \\ \mbox{subject to} & \mathbf{Tr}(A_iX) = b_i & \mbox{subject to} & C - \sum_{i=1}^m y_i A_i \succeq 0. \\ & X \succeq 0, \end{array}$

- Simple constraint qualification conditions guarantee **strong duality**.
- We can write a conic version of the KKT optimality conditions

$$\begin{cases} C - \sum_{i=1}^{m} y_i A_i = Z, \\ \mathbf{Tr}(A_i X) = b_i, \quad i = 1, \dots, m, \\ \mathbf{Tr}(XZ) = 0, \\ X, Z \succeq 0. \end{cases}$$

Semidefinite programming: conic duality

So what?

- Weak duality produces simple bounds on e.g. combinatorial problems.
- Consider the MAXCUT relaxation

$$\begin{array}{lll} \max & x^T C x & \max & \operatorname{Tr}(XC) \\ \text{s.t.} & x_i^2 = 1 & \text{is bounded by} & \text{s.t.} & \operatorname{diag}(X) = \mathbf{1} \\ & X \succeq 0, \end{array}$$

in the variables $x \in \mathbb{R}^n$ and $X \in \mathbf{S}_n$ (more later on these relaxations).

The dual of the SDP on the right is written

$$\min_{y} n\lambda_{\max}(C - \operatorname{diag}(y)) + \mathbf{1}^{T} y$$

in the variable $y \in \mathbb{R}^n$.

By weak duality, plugging any value y in this problem will produce an upper bound on the optimal value of the combinatorial problem above. Algorithms for semidefinite programming

- Following [Nesterov and Nemirovskii, 1994], most of the attention was focused on interior point methods.
- Newton's method, with efficient linear algebra solving for the search direction.
- Fast, and robust on small problems ($n \sim 500$).
- Computing the Hessian is too hard on larger problems.

Solvers

- Open source solvers: SDPT3, SEDUMI, SDPA, CSDP, . . .
- Very powerful modeling systems: CVX

Semidefinite programming: CVX

Solving the maxcut relaxation

max. $\operatorname{Tr}(XC)$ s.t. $\operatorname{diag}(X) = 1$ $X \succeq 0$,

is written as follows in $\ensuremath{\mathsf{CVX}}\xspace/\ensuremath{\mathsf{MATLAB}}\xspace$

cvx_begin

- . variable X(n,n) symmetric
- . maximize trace(C*X)
- . subject to
- diag(X) == 1
- X==semidefinite(n)

 cvx_end

Solving large-scale problems is a bit more problematic. . .

- No universal algorithm known yet. No CVX like modeling system.
- Performance and algorithmic choices heavily depends on problem structure.
- Very basic codes only require computing one leading eigenvalue per iteration, with complexity $O(n^2 \log n)$ using e.g. Lanczos.
- Each iteration requires about 300 matrix vector products, but making progress may require many iterations. Typically $O(1/\epsilon^2)$ or $O(1/\epsilon)$ in some cases.
- In general, most optimization algorithms are purely sequential, so only the linear algebra subproblems benefit from the multiplication of CPU cores.

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- \circ Distortion, embedding
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- Many classical problems can be cast as or approximated by semidefinite programs.
- Recognizing this is not always obvious.
- At reasonable scales, numerical solutions often significantly improve on classical closed-form bounds.
- A few examples follow. . .

Combinatorial relaxations

[Goemans and Williamson, 1995, Nesterov, 1998]

Semidefinite programs with constant trace often arise in **convex relaxations** of combinatorial problems. Use MAXCUT as an example here.

The problem is written

max.
$$x^T C x$$

s.t. $x \in \{-1,1\}^n$

in the binary variables $x \in \{-1, 1\}^n$, with parameter $C \in \mathbf{S}_n$ (usually $C \succeq 0$). This problem is known to be **NP-Hard**. Using

$$x \in \{-1, 1\}^n \quad \Longleftrightarrow \quad x_i^2 = 1, \quad i = 1, \dots, n$$

we get

$$\begin{array}{ll} \max & x^T C x \\ \text{s.t.} & x_i^2 = 1, \quad i = 1, \dots, n \end{array}$$

which is a nonconvex quadratic program in the variable $x \in \mathbb{R}^n$.

Combinatorial relaxations

We now do a simple change of variables, setting $X = xx^T$, with

$$X = xx^T \quad \Longleftrightarrow \quad X \in \mathbf{S}_n, \ X \succeq 0, \ \operatorname{\mathbf{Rank}}(X) = 1$$

and we also get

$$\mathbf{Tr}(CX) = x^T C x$$

$$\mathbf{diag}(X) = \mathbf{1} \quad \Longleftrightarrow \quad x_i^2 = 1, \quad i = 1, \dots, n$$

so the original combinatorial problem is equivalent to

max.
$$\operatorname{Tr}(CX)$$

s.t. $\operatorname{diag}(X) = 1$
 $X \succeq 0, \operatorname{Rank}(X) = 1$

which is now a nonconvex problem in $X \in \mathbf{S}_n$.

If we simply drop the rank constraint, we get the following relaxation

 $\begin{array}{ll} \max & x^T C x & \max & \operatorname{Tr}(CX) \\ \text{s.t.} & x \in \{-1,1\}^n & \text{ is bounded by } & \text{s.t. } & \operatorname{diag}(X) = 1 \\ & X \succeq 0, \end{array}$

which is a semidefinite program in $X \in \mathbf{S}_n$.

- Rank constraints in semidefinite programs are usually hard. All semi-algebraic optimization problems can be formulated as rank constrained SDPs.
- Randomization techniques produce bounds on the approximation ratio. When $C \succeq 0$ for example, we have

$$\frac{2}{\pi}SDP \leq OPT \leq SDP$$

for the MAXCUT relaxation (more details in [Ben-Tal and Nemirovski, 2001]).

Applications in graph, matrix approximations (CUT-Norm, $\|\cdot\|_{2\to 1}$) [Frieze and Kannan, 1999, Alon and Naor, 2004, Nemirovski, 2005]

We cannot hope to always get low rank solutions, unless we are willing to admit some **distortion**. . . The following result from [Ben-Tal, Nemirovski, and Roos, 2003] gives some guarantees.

Theorem

Approximate S-lemma. Let $A_1, \ldots, A_N \in \mathbf{S}_n$, $\alpha_1, \ldots, \alpha_N \in \mathbb{R}$ and a matrix $X \in \mathbf{S}_n$ such that

$$A_i, X \succeq 0, \quad \mathbf{Tr}(A_i X) = \alpha_i, \quad i = 1, \dots, N$$

Let $\epsilon > 0$, there exists a matrix X_0 such that

$$\alpha_i(1-\epsilon) \le \operatorname{Tr}(A_iX_0) \le \alpha_i(1+\epsilon) \quad \text{and} \quad \operatorname{Rank}(X_0) \le 8 \frac{\log 4N}{\epsilon^2}$$

Proof. Randomization, concentration results on Gaussian quadratic forms. See [Barvinok, 2002, Ben-Tal, El Ghaoui, and Nemirovski, 2009] for more details.

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A particular case: Given N vectors $v_i \in \mathbb{R}^d$, construct their Gram matrix $X \in \mathbf{S}_N$, with

$$X \succeq 0, \quad X_{ii} - 2X_{ij} + X_{jj} = ||v_i - v_j||_2^2, \quad i, j = 1, \dots, N.$$

The matrices $D_{ij} \in \mathbf{S}_n$ such that

$$\mathbf{Tr}(D_{ij}X) = X_{ii} - 2X_{ij} + X_{jj}, \quad i, j = 1, \dots, N$$

satisfy $D_{ij} \succeq 0$. Let $\epsilon > 0$, there exists a matrix X_0 with

$$m = \operatorname{Rank}(X_0) \le 16 \frac{\log 2N}{\epsilon^2},$$

from which we can extract vectors $u_i \in \mathbb{R}^m$ such that

$$\|v_i - v_j\|_2^2 \ (1 - \epsilon) \le \|u_i - u_j\|_2^2 \le \|v_i - v_j\|_2^2 \ (1 + \epsilon).$$

In this setting, the Johnson-Lindenstrauss lemma is a particular case of the approximate S lemma...

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The problem of reconstructing an N-point Euclidean metric, given partial information on pairwise distances between points v_i, i = 1, ..., N can also be cast as an SDP, known as and Euclidean Distance Matrix Completion problem.

find
$$D$$

subject to $\mathbf{1}v^T + v\mathbf{1}^T - D \succeq 0$
 $D_{ij} = ||v_i - v_j||_2^2, \quad (i, j) \in S$
 $v \ge 0$

in the variables $D \in \mathbf{S}_n$ and $v \in \mathbb{R}^n$, on a subset $S \subset [1, N]^2$.

- We can add further constraints to this problem given additional structural info on the configuration.
- Applications in sensor networks, molecular conformation reconstruction etc...



[Dattorro, 2005] 3D map of the USA reconstructed from pairwise distances on 5000 points. Distances reconstructed from Latitude/Longitude data.

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Theorem

Embedding. [Bourgain, 1985] Every *n*-point metric space (X,d) can be embedded in an $O(\log n)$ -dimensional Euclidean space with an $O(\log n)$ distortion.

Let $(X = \{x_1, \ldots, x_n\}, d)$ be a finite metric space, we can find the **minimum** distortion embedding by solving

minimize z
subject to
$$X_{ii} + X_{jj} - 2X_{ij} \ge d(x_i, x_j)^2$$

 $X_{ii} + X_{jj} - 2X_{ij} \le z d(x_i, x_j)^2$, $i, j = 1, ..., n$
 $X \ge 0$

in the variables $X \in \mathbf{S}_n$ and $z \in \mathbb{R}$.

The result above shows $\sqrt{z^*}$ is $O(\log n)$ in the worst case.

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Minimum volume ellipsoid \mathcal{E} s.t. $C \subseteq \mathcal{E}$ (Löwner-John ellipsoid).

- parametrize \mathcal{E} as $\mathcal{E} = \{v \mid ||Av + b||_2 \le 1\}$ with $A \succ 0$.
- $\operatorname{vol} \mathcal{E}$ is proportional to $\det A^{-1}$; to compute minimum volume ellipsoid,

minimize (over A, b)
$$\log \det A^{-1}$$

subject to $\sup_{v \in C} ||Av + b||_2 \le 1$

convex, but the constraint can be hard (for general sets C).

Finite set $C = \{x_1, \ldots, x_m\}$, or polytope with polynomial number of **vertices**:

minimize (over A, b)
$$\log \det A^{-1}$$

subject to $\|Ax_i + b\|_2 \le 1, \quad i = 1, \dots, m$

also gives Löwner-John ellipsoid for polyhedron $Co\{x_1, \ldots, x_m\}$.

Similar result for the maximum volume inscribed ellipsoid when C is a polyhedron given by its facets $\{x \mid a_i^T x \leq b_i, i = 1, ..., m\}$.

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D-Optimal Experiment Design.

Given experiment vectors $v_i \in \mathbb{R}^n$, we minimize the MLE estimation error in

$$y_j = v_j^T x + w_j$$

for Gaussian noise w. Assuming we run λ_i times experiment v_i , the covariance matrix of the estimation error $x - \hat{x}$ is given by $\sum_{i=1}^{p} \lambda_i v_i v_i^T$ and we solve

minimize
$$\log \det \left(\sum_{i=1}^{p} \lambda_i v_i v_i^T\right)^{-1}$$

subject to $\mathbf{1}^T \lambda = 1, \ \lambda \ge 0$

in the variable $\lambda \in \mathbb{R}^p$. The **dual** of this last problem is written

minimize $\log \det(W)^{-1}$ subject to $v_i^T W v_i \leq 1$

which is a minimum volume ellipsoid problem in the variable $W \in \mathbf{S}_n$.

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 $C \subseteq \mathbb{R}^n$ convex, bounded, with nonempty interior

- Löwner-John ellipsoid, shrunk by a factor n, lies inside C
- maximum volume inscribed ellipsoid, expanded by a factor n, covers C

example (for two polyhedra in \mathbb{R}^2)



factor n can be improved to \sqrt{n} if C is symmetric. See [Boyd and Vandenberghe, 2004] for further examples.

Mixing rates for Markov chains & maximum variance unfolding

[Sun, Boyd, Xiao, and Diaconis, 2006]

- Let G = (V, E) be an **undirected graph** with n vertices and m edges.
- We define a **Markov chain** on this graph, and let $w_{ij} \ge 0$ be the transition rate for edge $(i, j) \in V$.
- Let $\pi(t)$ be the state distribution at time t, its evolution is governed by the heat equation

$$d\pi(t) = -L\pi(t)dt$$

with

$$L_{ij} = \begin{cases} -w_{ij} & \text{if } i \neq j, \ (i,j) \in V \\ 0 & \text{if } (i,j) \notin V \\ \sum_{(i,k) \in V} w_{ik} & \text{if } i = j \end{cases}$$

the graph Laplacian matrix, which means

$$\pi(t) = e^{-Lt}\pi(0).$$

• The matrix $L \in \mathbf{S}_n$ satisfies $L \succeq 0$ and its smallest eigenvalue is zero (associated with the uniform distribution).

With

$$\pi(t) = e^{-Lt}\pi(0)$$

the **mixing rate** is controlled by the second smallest eigenvalue $\lambda_2(L)$.

Since the smallest eigenvalue of L is zero, with eigenvector 1, we have

$$\lambda_2(L) \ge t \iff L(w) \succeq t(\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^T),$$

Maximizing the mixing rate of the Markov chain means solving

$$\begin{array}{ll} \text{maximize} & t\\ \text{subject to} & L(w) \succeq t(\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^T) \\ & \sum_{(i,j) \in V} d_{ij}^2 w_{ij} \leq 1 \\ & w \geq 0 \end{array}$$

in the variable $w \in \mathbb{R}^m$, with (normalization) parameters $d_{ij}^2 \ge 0$.

- Since L(w) is an affine function of the variable $w \in \mathbb{R}^m$, this is a semidefinite program in $w \in \mathbb{R}^m$.
- Numerical solution usually performs better than Metropolis-Hastings.

- We can also form the **dual** of the maximum MC mixing rate problem.
- The dual means solving

maximize
$$\mathbf{Tr}(X(\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^T))$$

subject to $X_{ii} - 2X_{ij} + X_{jj} \leq d_{ij}^2$, $(i, j) \in V$
 $X \succeq 0$,

in the variable $X \in \mathbf{S}_n$.

• Here too, we can interpret X as the gram matrix of a set of n vectors $v_i \in \mathbb{R}^d$. The program above maximizes the variance of the vectors v_i

$$\mathbf{Tr}(X(\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^T)) = \sum_i \|v_i\|_2^2 - \|\sum_i v_i\|_2^2$$

while the constraints bound pairwise distances

$$X_{ii} - 2X_{ij} + X_{jj} \le d_{ij}^2 \iff ||v_i - v_j||_2^2 \le d_{ij}^2$$

This is a maximum variance unfolding problem [Weinberger and Saul, 2006, Sun et al., 2006].





From [Sun et al., 2006]: we are given pairwise 3D distances for k-nearest neighbors in the point set on the right. We plot the maximum variance point set satisfying these pairwise distance bounds on the right.

Moment problems & positive polynomials

Moment problems & positive polynomials

[Nesterov, 2000]. Hilbert's 17^{th} problem has a positive answer for univariate polynomials: a polynomial is nonnegative iff it is a **sum of squares**

$$p(x) = x^{2d} + \alpha_{2d-1}x^{2d-1} + \ldots + \alpha_0 \ge 0$$
, for all $x \iff p(x) = \sum_{i=1}^{N} q_i(x)^2$

We can formulate this as a linear matrix inequality, let v(x) be the moment vector

$$v(x) = (1, x, \dots, x^d)^T$$

we have

$$\sum_{i} \lambda_{i} u_{i} u_{i}^{T} = M \succeq 0 \quad \Longleftrightarrow \quad p(x) = v(x)^{T} M v(x) = \sum_{i} \lambda_{i} (u_{i}^{T} v(x))^{2}$$

where (λ_i, u_i) are the eigenpairs of M.

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The dual to the cone of Sum-of-Squares polynomials is the cone of moment matrices

$$\mathbf{E}_{\mu}[x^{i}] = q_{i}, \ i = 0, \dots, d \quad \Longleftrightarrow \quad \begin{pmatrix} q_{0} & q_{1} & \cdots & q_{d} \\ q_{1} & q_{2} & & q_{d+1} \\ \vdots & & \ddots & \vdots \\ q_{d} & q_{d+1} & \cdots & q_{2d} \end{pmatrix} \succeq 0$$

- [Putinar, 1993, Lasserre, 2001, Parrilo, 2000] These results can be extended to multivariate polynomial optimization problems over compact semi-algebraic sets.
- This forms exponentially large, ill-conditioned semidefinite programs however.

Gordon-Slepian and the maximum of Gaussian processes

Gordon-Slepian & the max. of Gaussian processes

[Massart, 2007]

• Let $x \sim \mathcal{N}(0, X)$ and $y \sim \mathcal{N}(0, Y)$ be two Gaussian processes such that

$$\begin{cases} X_{ij} \leq Y_{ij} \\ X_{ii} = Y_{ii}, \quad i, j = 1, \dots, n, \end{cases}$$

then

$$\mathbf{E}\left[\prod_{i=1}^{N} f(x_i)\right] \le \mathbf{E}\left[\prod_{i=1}^{N} f(y_i)\right]$$

for every nonnegative and nonincreasing differentiable f such that f and f' are bounded on \mathbb{R} . This is **first order stochastic dominance**.

This implies in particular that

$$\mathbf{E}\left[\sup_{i=1,\dots,N} y_i\right] \le \mathbf{E}\left[\sup_{i=1,\dots,N} x_i\right]$$

Lemma

Simple bound on Gaussian processes. Let $y \sim \mathcal{N}(0, Y)$ be a Gaussian vector with covariance $Y \in \mathbf{S}_n$. Suppose $X \succeq 0$ satisfies

$$Y_{ii} - 2Y_{ij} + Y_{jj} \le X_{ii} - 2X_{ij} + X_{jj}, \quad i, j = 1, \dots, n$$

which are convex inequalities in $X \in \mathbf{S}_n$, then

$$\mathbf{E}\left[\sup_{i=1,\dots,n} y_i\right] \le 2\left(\mathbf{Rank}(X) \max_{i=1,\dots,n} X_{ii}\right)^{1/2}$$

Proof. Use Gordon-Slepian together with Cauchy inequality. Write x = Vg with $V \in \mathbb{R}^{n \times k}$ such that $X = VV^T$ and k = Rank(X), so $\sup_{i=1,...,n} x_i = \sup_{i=1,...,n} \sum_{j=1}^k V_{ij}g_j \leq \left(\sup_{i=1,...,n} \|V_i\|_2\right) \|g\|_2$ where g i.i.d. Gaussian, with $\mathbf{E}[\|g\|_2] \leq \sqrt{k}$ and $\|V_i\|_2 = X_{ii}$.

Proposition

SDP bounds on Gaussian processes. Let $y \sim \mathcal{N}(0, Y)$ be a Gaussian vector with covariance $Y \in \mathbf{S}_n$. From a matrix $X \in \mathbf{S}_n$ satisfying

$$Y_{ii} - 2Y_{ij} + Y_{jj} \le (X_{ii} - 2X_{ij} + X_{jj}), \quad i, j = 1, \dots, n$$

which are convex inequalities in $X \in \mathbf{S}_n$, we can construct a low rank matrix X^r such that

$$\mathbf{E}\left[\sup_{i=1,\dots,n} y_i\right] \le c_2 \sqrt{\log n} \left(\max_{i=1,\dots,n} \sqrt{X_{ii}}\right)$$

where $c_1, c_2 > 0$ are absolute constants.

Proof. Combine previous lemma with approximate S-lemma. Explicit randomized procedure to find X^r .

The previous result shows that the SDP bound always does as well as the classical bound

$$\mathbf{E}\left[\sup_{i=1,\dots,n} y_i\right] \le 2\sqrt{\log n} \left(\max_{i=1,\dots,n} \sqrt{Y_{ii}}\right),$$

up to a multiplicative constant.

We can exploit symmetries in the matrix Y to block diagonalize the SDP and reduce its complexity. [Gatermann and Parrilo, 2002, Vallentin, 2009]

- Semidefinite programming formulation to some problems in geometry, probability, statistics.
- Improvements over classical closed-form bounds on reasonably large problems.

Next: applications to compressed sensing. . .

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