Maximization of a Convex Quadratic Form on a Polytope Factorization

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Considered problem

Considered problem

- Maximization of a convex quadratic form
  on a convex polyhedral set

$$f^* = \max x^T A x \quad \text{s.t.} \qquad x \in \mathcal{M},$$

- where we consider
  - $A \in \mathbb{R}^{n \times n}$ symmetric positive semidefinite and
  - $\mathcal{M}$ convex polyhedral - system of linear inequalities

- We know that
  - For bounded $\mathcal{M}$ global optimum attained in vertex of $\mathcal{M}$
  - i.e. computationally intractable (NP-hard)

- It is NP-hard even
  - For $\mathcal{M}$ being a hypercube
  - It is in P for some special sub-classes

How to solve the problem

There are some standard approaches

- *cutting plane methods* (Konno 1980)
- *reformulation-linearization/convexification and applying branch & bound methods* (Sherali and Adams 1980)
- *polynomial time approximation methods* (Vavasis 1993)
- etc.

We consider

- Computation of cheap upper bound on f^*
  - Important due to possible relation of nonlinear model
  - Crucial for effectiveness of a branch and bound

Basic idea in transformation

- Matrix A can be factorized as $A = G^T G$
- Then $x^T A x = x^T G^T G x = \|Gx\|_2^2$
- redefine problem as

$$\max \|Gx\|_2^2 \quad \text{s.t.} \qquad x \in \mathcal{M},$$

Approximate transformed problem

Handle original problem

- For transformed problem

$$\max \|Gx\|_2^2 \quad \text{s.t.} \quad x \in \mathcal{M},$$

- replace Euclidean norm by another and use equivalences of vector norms

Example: *maximum norm*

- Using maximum norm gives

$$f^* = \max_{x \in \mathcal{M}} \|Gx\|_2^2 \leq n \cdot \max_{x \in \mathcal{M}} \|Gx\|_\infty^2 \equiv g^*(G),$$

  where $\|x\|_\infty = \max_i\{|x_i|\}$ is the maximum norm

  - Remind equivalences of norms, here $\|x\|_2 \leq \sqrt(n)\|x\|_\infty$
  - Altogether we have

$$g^*(G) = n \cdot \max_{x \in \mathcal{M}} \|Gx\|_\infty^2$$

Approximate transformed problem

Handle approximate problem

- For transformed problem

$$g^*(G) = n \cdot \max_{x \in \mathcal{M}} \|Gx\|_\infty^2$$

- How to solve?

How to compute upper bound $g^*(G)$?

- Compute using linear programming

$$g^*(G) = n \cdot \max_{x \in \mathcal{M}} \|Gx\|_\infty^2 = n \cdot \max_i \max_{x \in \mathcal{M}} (G_{i,*}x)^2$$

  - Solve $\max_{x \in \mathcal{M}} \pm(G_{i,*}x)$ for each $i = 1, \ldots, n$ ($2n$ LP)
  - Quality of $g^*(G)$ depends on $A = G^T G$ (find good)

General goal

- *Find the factorization $A = G^T G$ such that the upper bound $g^*(G)$ is as tight as possible.*

Example approach: factorizing A

Two natural choices for $A = G^T G$

- *Cholesky decomposition* $A = G^T G$ where G is upper triangular with non-negative diagonal
- *Square root* $A = G^2$ where G is symmetric positive definite

Another factorization

- Let $\mathcal{H}$ be set of orthogonal matrices
- For $H \in \mathcal{H}$ let $R := HG$
- Then

$$R^T R = (HG)^T HG = G^T G = A$$

- *Task*: Find suitable H to make $g^*(HG)$ tight upper bound

Overestimation of bounds $\max_{x \in \mathcal{M}} \|Gx\|_2^2 \leq n \cdot \max_{x \in \mathcal{M}} \|Gx\|_\infty^2$

- Utilization of maximum norm leads to overestimation
- Vanishing for vectors entries of which are same in absolute value, i.e.

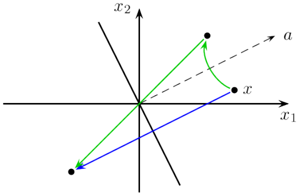
$$\|y\|_2^2 = n\|y\|_\infty^2 \quad \text{for each } y \in \{\pm 1\}^n$$

Householder matrix

Candidates for H

- Let $u \in \mathbb{R}^n \setminus \{0\}$, *Householder matrix* is

$$H(u) = I_n - \frac{2}{u^T u} uu^T$$



  - restriction is WLOG - each ortogonal matrix can be factorized into a product of $\leq n$ Householder matices

Theorem

For each $x, y \in \mathbb{R}^n$, $x \neq y$, $\|x\|_2 = \|y\|_2$ *holds* $y = H(x-y)x$.

Consider the following pair x, y with $\|x\|_2 = \|y\|_2$

$y := |G|e \qquad \Rightarrow \|y\|_2$

$x := \frac{1}{\sqrt{n}}\|y\|_2 e = \alpha e \Rightarrow \|x\|_2 = \sqrt{n\alpha^2} = \sqrt{n\left(\frac{1}{\sqrt{n}}\|y\|_2\right)^2} = \|y\|_2$

- We know that $H(u)y = \alpha \cdot e$ for

$$u := \alpha \cdot e - y$$

Bulding heuristic

Iterative search

- *Why*: No guarantee that HG has constant row absolute sums
- *How*: Keep Householder condition
- *Until (ideally)*: Search for constant row absolute sums
  Until (really): Better after some time

Algorithm 1: Factorization $A = R^T R$

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input : Let $A = G^T G$ be initial factorization
output: Factorization $A = R^T R$

```
1 Put R := G;
2 Put y := |R|e;
3 Put α := (1/√n)‖y‖₂;
4 Put H := H(α · e − y);
5 if ‖HR‖∞ < ‖R‖∞ then
6 |   put R := HR;
7 |   goto 2;
8 end
```

1 Put $R := G$;
2 Put $y := |R|e$;
3 Put $\alpha := \frac{1}{\sqrt{n}}\|y\|_2$;
4 Put $H := H(\alpha \cdot e - y)$;
5 **if** $\|HR\|_\infty < \|R\|_\infty$ **then**
6   put $R := HR$;
7   goto 2;
8 **end**

Alternative approaches

Exact method by enumeration

- Enumerate all vertices of $\mathcal{M}$ and find maximum
- Only for small dimensions

Trivial upper bound

- Let $\underline{x}, \overline{x} \in \mathbb{R}^n$ be lower and upper bounds on $\mathcal{M}$
- Compute upper bound using interval arithmetic
  - Let $\boldsymbol{x} = [\underline{x}, \overline{x}]$ be interval vector
  - We need to evaluate $\boldsymbol{f} = [\underline{f}, \overline{f}] = \boldsymbol{x}^T A \boldsymbol{x}$
  - Then $f^* \leq \overline{f}$
- Tightness of the bound
  - Use interval hull of $\mathcal{M}$
    ($\boldsymbol{x}$ is the smallest interval vector enclosing $\mathcal{M}$)
  - Compute this using $2n$ LP problems - min or max in a particular coordinate

Third approach

McCormick envelopes (relaxations for bilinear forms)

- Relaxing $x^T A x$ with McCormick envelopes (McCormick 1976)
  - *Idea*: general bilinear xy let $a := x - \underline{x}$ and $b := \overline{x} - x$

$$a \cdot b \geq 0 \quad \Rightarrow (x - \underline{x}) \cdot (\overline{x} - x) = x\overline{y} - xy - \underline{x}\overline{y} + \underline{x}y \geq 0$$

$$\text{Let } w = xy \quad \Rightarrow w \leq x\overline{y} + \underline{x}y - \underline{x}\overline{y}$$

- For quadratic form $x^T A x$
  - Let $\underline{\mathrm{x}}, \overline{\mathrm{x}} \in \mathbb{R}^n$ be lower and upper bounds on $\mathcal{M}$
  - Split A into parts $A^+, A^- \geq 0$ such that $A = A^+ - A^-$
  - *Case 1*: Set $x := x$ and $y := A^+ x$

$$\begin{aligned} x^T A^+ x &\leq \overline{\mathrm{x}}^T A^+ x + x^T A^+ \underline{\mathrm{x}} - \overline{\mathrm{x}}^T A^+ \underline{\mathrm{x}} \\ &= (\overline{\mathrm{x}} + \underline{\mathrm{x}})^T A^+ x - \overline{\mathrm{x}}^T A^+ \underline{\mathrm{x}} \\ &= 2 x_c^T A^+ x - \overline{\mathrm{x}}^T A^+ \underline{\mathrm{x}} \end{aligned}$$

- and similarly

$$x^T A^- x \geq \underline{\mathrm{x}}^T A^- x + x^T A^- \underline{\mathrm{x}} - \underline{\mathrm{x}}^T A^- \underline{\mathrm{x}} = 2\underline{\mathrm{x}}^T A^- x - \underline{\mathrm{x}}^T A^- \underline{\mathrm{x}}$$

$$x^T A^- x \geq \overline{\mathrm{x}}^T A^- x + x^T A^- \overline{\mathrm{x}} - \overline{\mathrm{x}}^T A^- \overline{\mathrm{x}} = 2\overline{\mathrm{x}}^T A^- x - \overline{\mathrm{x}}^T A^- \overline{\mathrm{x}}$$

McCormick formulation

Model design

- We have
$$x^T A^+ x \le 2x_c^T A^+ x - \overline{x}^T A^+ \underline{x}$$
$$x^T A^- x \ge 2\underline{x}^T A^- x - \underline{x}^T A^- \underline{x}$$
$$x^T A^- x \ge 2\overline{x}^T A^- x - \overline{x}^T A^- \overline{x}$$

- Revoking split of $A = A^+ - A^-$ gives us
  - Form $x^T A x = x^T (A^+ - A^-) x = x^T A^+ x - x^T A^- x$
  - Producing thus 2 conditions

$$\begin{aligned} \max z \text{ s.t. } \; & z \le 2x_c^T A^+ x - \overline{x}^T A^+ \underline{x} - 2\underline{x}^T A^- x - \underline{x}^T A^- \underline{x} \\ & z \le 2x_c^T A^+ x - \overline{x}^T A^+ \underline{x} - 2\overline{x}^T A^- x - \overline{x}^T A^- \overline{x} \\ & x \in \mathcal{M} \end{aligned}$$

- Standard form

$$\begin{aligned} \max z \text{ s.t. } \; & 2(\underline{x}^T A^- + x_c^T A^+) x + z \le -\overline{x}^T A^+ \underline{x} + \underline{x}^T A^- \underline{x} \\ & 2(\overline{x}^T A^- + x_c^T A^+) x + z \le -\overline{x}^T A^+ \underline{x} + \overline{x}^T A^- \overline{x} \\ & x \in \mathcal{M} \end{aligned}$$

Numerical experiments

General settings

- *Input parameter*: dimension n
- *Generated objects*: Random matrices $A \in \mathbb{R}^{n \times n}$ as

$$A := G^T G \quad \text{s.t.}$$

$G \in \mathbb{R}^{n \times n}$ generated randomly uniformly from $[-1, 1]$

Feasible set

- Set $\mathcal{M}$ defined by n^2 inequalities
- Generating inequalities $a^T x \leq b$ s.t.

  a_is are chosen randomly uniformly from $[-1, 1]$

  b is chosen randomly uniformly from $[0, e^T |a|]$

Dimension size

- Larger dimensions $n \geq 70$
  - Make 80% randomly selected entries of constraint matrix zero
  - Evaluate relative to the trivial methods: b^m / b^{triv}
- Small dimensions
  - Evaluated relative to the exact method: b^m / f^*

Summary of methods

Methods to provide upper bounds

exact : exact optimum via enumerating vertices of $\mathcal{M}$

triv : interval hull of $\mathcal{M}$

McCm : McCormick relaxation + interval hull of $\mathcal{M}$

sqrtm : using G as the quare root of A.

sqrtm-it : square root + iterative modification

chol : using G from Cholesky decomposition of A

chol-it : Cholesky decomposition + iterative modification

chol-rnd : Cholesky decomposition + iterative improvement of G - try 10 random Householder matrices

Results - small dimensions

Efficiency of the methods

- the best ones highlighted in boldface

n	runs	triv	McCm	sqrtm	sqrtm-it	chol	chol-it	chol-rnd
3	100	65.55	51.17	65.22	67.52	78.33	75.12	**48.96**
5	100	24.01	19.31	25.20	23.16	33.54	27.43	**18.98**
7	100	26.47	21.90	20.63	21.36	28.15	23.26	**16.59**
9	20	19.57	16.48	14.90	14.83	19.81	13.65	**11.27**
10	20	22.26	18.75	13.25	13.54	19.75	14.08	**11.92**

Computational times of the methods

- in 10^{-3}sec.

n	runs	exact	triv	McCm	sqrtm	sqrtm-it	chol	chol-it	chol-rnd
3	100	0.8256	38.83	44.87	36.95	36.94	36.78	36.85	369.6
5	100	101.5	64.10	69.79	61.10	61.60	61.19	61.39	616.1
7	100	7160	91.87	97.62	89.01	88.86	88.48	88.01	887.7
9	20	141900	119.1	123.8	114.8	115.2	115.0	114.6	1145
10	20	240000	132.3	137.7	126.4	126.9	125.2	125.9	1257

Results - higher dimensions (eff+times-bottom sparse)

n	runs	triv	McCm	sqrtm	sqrtm-it	chol	chol-it	chol-rand
20	100	1	0.8737	0.4614	0.4625	0.6682	0.5013	**0.4260**
30	100	1	0.8879	0.3730	0.3731	0.5587	0.4046	**0.3582**
40	100	1	0.9019	**0.3170**	**0.3170**	0.4707	0.3471	0.3216
50	100	1	0.9102	0.2725	**0.2719**	0.4273	0.3113	0.2940
60	100	1	0.9196	**0.2396**	0.2401	0.3806	0.2781	0.2692
70	20	1	0.9101	**0.2709**	**0.2709**	0.4344	0.3133	0.3062
80	20	1	0.9127	**0.2445**	**0.2445**	0.3905	0.2923	0.2900
90	20	1	0.9201	**0.2237**	**0.2237**	0.3604	0.2845	0.2779
100	20	1	0.9229	**0.1993**	**0.1993**	0.3496	0.2706	0.2677

n	runs	triv	McCm	sqrtm	sqrtm-it	chol	chol-it	chol-rand
20	100	0.4686	0.4799	0.4587	0.4575	0.4601	0.4573	4.583
30	100	2.115	2.150	2.075	2.073	2.087	2.087	20.80
40	100	7.889	7.983	7.735	7.725	7.812	7.780	77.74
50	100	25.16	25.44	24.71	24.72	24.93	24.85	248.4
60	100	64.89	63.97	63.97	64.19	64.92	64.43	641.1
70	20	12.36	12.57	12.99	12.94	12.89	13.25	131.2
80	20	24.09	24.23	24.61	24.64	25.34	25.19	251.5
90	20	43.97	44.10	45.71	45.45	46.25	46.62	465.9
100	20	78.92	79.77	84.74	84.22	85.08	86.19	855.7

Conclusions

Proposed

- Simple and cheap *method to compute an upper bound* for **convex quadratic form on a convex polyhedron**
- method based on factorization of quadratic form and application of Chebyshev vector norm

Numerical experiments

- Method gives tighter bounds
- Basically the same running time
  - compared to trivial or McCormick
- Effect of dimensions
  - *Small dimensions*: efficiency is low
  - *Medium and larger*: efficiency is significantly higher

Open problems and challanges

- *Task*: Compare with approximation methods
  - s.a. semidefinite programming
- *Open*: Find suitable approximation
  - Random Householder ⇒ achieve even better results

Rethink the problem

What is the best solution

- For original problem

$$f^* = \max x^T A x \quad \text{s.t.} \quad x \in \mathcal{M},$$

- Define **best upper bound by factorization**

$$g^* = \min_{R \in \mathbb{R}^{n \times m}; A = R^T R} \max_{x \in \mathcal{M}} \|Rx\|_\infty^2$$

- How about any ortogonal $H \in \mathcal{H}$
  - Overestimation of g^* is the same as **max-min inequality**

Theorem

We have

$$f^* = n \cdot {\color{blue}\max_{x \in \mathcal{M}}} {\color{red}\min_{H \in \mathcal{H}}} \|HGx\|_\infty^2 \leq n \cdot {\color{red}\min_{H \in \mathcal{H}}} {\color{blue}\max_{x \in \mathcal{M}}} \|HGx\|_\infty^2 = g^* \qquad (1)$$

Max-min overestimation

Theorem

$$f^* = n \cdot \max_{x \in \mathcal{M}} \min_{H \in \mathcal{H}} \|HGx\|_\infty^2 \leq n \cdot \min_{H \in \mathcal{H}} \max_{x \in \mathcal{M}} \|HGx\|_\infty^2 = g^*$$

Proof

Start with first equation $\|Gx\|_2^2 = f^* = n \cdot \max_{x \in \mathcal{M}} \min_{H \in \mathcal{H}} \|HGx\|_\infty^2$

First direction $\leq$:

- Let $H \in \mathcal{H}$ and $x \in \mathcal{M}$ we have
- Remind: $\|Gx\|_2^2 = xG^TGx$ and $(HG)^T HG = G^T G$ and $\|y\|_2 = \frac{1}{\sqrt{n}} \|y\|_\infty$

$$\|Gx\|_2^2 = \|HGx\|_2^2 \leq n \cdot \|HGx\|_\infty^2$$

- Take minimum over H

$$\|Gx\|_2^2 \leq n \cdot \min_{H \in \mathcal{H}} \|HGx\|_\infty^2$$

Oposite direction $\geq$:

- Let $x \in \mathcal{M}$ and denote $y := Gx$
- Utilize Householder transformation $Hy = \alpha \cdot e$ with $\alpha = \frac{1}{\sqrt{n}} \|y\|_2$

$$n \cdot \|Hy\|_\infty^2 = n \cdot \|\alpha \cdot e\|_\infty^2 = n \cdot \alpha^2 = \|y\|_2^2$$

- Therefore $\|Gx\|_2^2 = n \cdot \max_{x \in \mathcal{M}} \min_{H \in \mathcal{H}} \|HGx\|_\infty^2$ for each $x \in \mathcal{M}$

Max-min overestimation dtto

Theorem

$$f^* = n \cdot \max_{x \in \mathcal{M}} \min_{H \in \mathcal{H}} \|HGx\|_\infty^2 \leq n \cdot \min_{H \in \mathcal{H}} \max_{x \in \mathcal{M}} \|HGx\|_\infty^2 = g^*$$

Proof

Right-hand side, i.e. (substitute g^*)

$$\min_{H \in \mathcal{H}} \max_{x \in \mathcal{M}} \|HGx\|_\infty^2 = \min_{A = R^T R} \max_{x \in \mathcal{M}} \|Rx\|_\infty^2.$$

Let $H \in \mathcal{H}$ be arbitrary

- Put $R := HG$, again we know

$$R^T R = (HG)^T HG = G^T H^T HG = G^T G = A$$

- Conversely, let $A = G^T G = R^T R$ be two factorizations of A then

$$I_n = (G^T)^{-1} R^T R G^{-1} = (RG^{-1})^T RG^{-1}$$

  so $H := RG^{-1}$ is an orthogonal matrix

- It remains to show $f^* \leq g^*$
  - This is given by max-min inequality

$\square$

Strictness of the bound

We can show example of strictness

- Let's believe (example not very nice) How far we can go?

Proposition

We have $g^* \leq n \cdot f^*$

Proof

Thanks to general $\|x\|_\infty \leq \|x\|_2$ we have

$$g^* = n \cdot \min_{H \in \mathcal{H}} \max_{x \in \mathcal{M}} \|HGx\|_\infty^2 \leq n \cdot \min_{H \in \mathcal{H}} \max_{x \in \mathcal{M}} \|HGx\|_2^2$$
$$= n \cdot \min_{H \in \mathcal{H}} \max_{x \in \mathcal{M}} x^T A x = n \cdot f^*. \qquad \square$$

Proposition

Let $H^* \in \mathcal{H}$ and $x^* \in \mathcal{M}$ be optimal solutions for g^*. If $|H^* G x^*|$ has all entries the same, then $f^* \leq g^*$ holds as equation.

Proof

All entries the same $\Rightarrow n\|H^* G x^*\|_\infty^2 = \|H^* G x^*\|_2^2$

$$g^* = n\|H^* G x^*\|_\infty^2 = \|H^* G x^*\|_2^2 = \|Gx^*\|_2^2 \leq f^*. \qquad \square$$

Simple not tight case: interval box

Reformulation

- *Feasible set*: int. vector $\boldsymbol{x} = [\underline{x}, \overline{x}] = \{x \in \mathbb{R}^n;\ \underline{x} \leq x \leq \overline{x}\}$
- *Reformulation*: $f^* = \max\ x^T A x$ subject to $x \in \boldsymbol{x}$
- *Assumptions*:

$$x_\Delta = \frac{1}{2}(\overline{x} - \underline{x}) = e \qquad \text{(scaling)}$$

$$x_c = \frac{1}{2}(\underline{x} + \overline{x}) = 0 \qquad \text{(slightly less obvious)}$$

  - Introduce z and consider

$$q(y,z) := (y^T, z)\begin{pmatrix} A & Ax_c \\ x_c^T A & x_c^T A x_c \end{pmatrix}\begin{pmatrix} y \\ z \end{pmatrix} = (y + zx_c)^T A (y + zx_c)$$

    on the interval domain $y \in [-x_\Delta, x_\Delta]$, $z \in [-1, 1]$.
  - Maximum attained for $z \in \{\pm 1\}$
  - Since $q(y,z) = q(-y,-z)$, we can consider only $z = 1$
  - Substitute $x := y + x_c$ and obtain the original one.

Upper bound

- Base on the original formulation it is

$$g^* := n \cdot \min_{R \in \mathbb{R}^{n \times n} : A = R^T R}\ \max_{x \in \boldsymbol{x}}\ \|Rx\|_\infty^2$$

Interval case is not tight

Reformulation continues

- We have $x_c = 0$ and $x_\Delta = e$, then

$$\max_{x \in \boldsymbol{x}} \|Rx\|_\infty^2 = \max_{x : \|x\|_\infty = 1} \|Rx\|_\infty^2 = \||R|e\|_\infty^2 = \|R\|_\infty^2,$$

- *Reformulation*

$$g^* := n \cdot \min_{R \in \mathbb{R}^{n \times n} : A = R^T R} \max_{x \in \boldsymbol{x}} \|Rx\|_\infty^2 \quad \to \quad g^* = n \cdot \min_{R \in \mathbb{R}^{n \times n} : A = R^T R} \|R\|_\infty^2$$

- Now, consider trivial upper bound $f^* = \max x^T A x \le e^T |A| e$

Proposition (Interval box not tight)

We have $f^* \le e^T |A| e \le g^*$.

Proof

For any factorization $A = R^T R$, we have

$$e^T |A| e = e^T |R^T R| e \le e^T |R^T| |R| e = \||R|e\|_2^2$$

Again applying equality of norms

$$e^T |A| e = \||R|e\|_2^2 \le n \|R\|_\infty^2$$

The factorization, for which g^* is attained then yields $e^T |A| e \le g^*$. $\square$

Note: There are cases for which the bound is tight!

Some final notes

General preconditioning

- Matrices *suitable for upper bounds*

$$\begin{aligned}\mathcal{B} &:= \{B \in \mathbb{R}^{n\times n};\ \|x\|_2 \leq \sqrt{n}\|Bx\|_\infty\ \forall x \in \mathbb{R}^n\}\\ &= \{B \in \mathbb{R}^{n\times n};\ 1 \leq \sqrt{n}\|Bx\|_\infty\ \forall x \in \mathbb{R}^n : \|x\|_2 = 1\}.\end{aligned}$$

Proposition

We have $f^* \leq n \cdot \max_{x\in\mathcal{M}} \|BGx\|_\infty^2$ for each $B \in \mathcal{B}$.

Some other notes

- We can see $\mathcal{H} \subseteq \mathcal{B}$
- We can show some properties
  - lower bounds on smallest singular number, etc.
- Unfortunately, the general case remain complicated

Proposition

Checking $B \in \mathcal{B}$ is a co-NP-hard problem.

Thank you