**Sums of Squares Relaxation** of Polynomial Optimization Problems

Asian Mathematical Conference Singapore, July 20 - 23, 2005

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• An introduction to the recent development of SOS relaxation for computing global optimal solutions of POPs.

• Exploiting sparsity in SOS relaxation to solve large scale POPs.

- 1. POPs (Polynomial Optimization Problems)
- 2. Nonnegative polynomials and SOS (Sum of Squares) polynomials
- 3. SOS relaxation of unconstrained POPs
- 4. Conversion of SOS relaxation into an SDP (Semidefinite Program)
- 5. Exploiting structured sparsity
- 6. SOS relaxation of constrained POPs very briefly
- 7. Numerical results
- 8. Concluding remarks

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 $\mathbb{R}^n: ext{ the }n ext{-dim Euclidean space}.$  $x=(x_1,\ldots,x_n)\in\mathbb{R}^n: ext{ a vector variable}.$  $f_j(x): ext{ a multivariate polynomial in }x\in\mathbb{R}^n\;(j=0,1,\ldots,m).$ 

POP: min  $f_0(x)$  sub.to  $f_j(x) \ge 0$   $(j = 1, \ldots, m)$ .

Example: n = 3

$$egin{aligned} \min & f_0(x) \equiv x_1^3 - 2x_1x_2^2 + x_1^2x_2x_3 - 4x_3^2 \ \mathrm{sub.to} & f_1(x) \equiv -x_1^2 + 5x_2x_3 + 1 \geq 0, \ f_2(x) \equiv x_1^2 - 3x_1x_2x_3 + 2x_3 + 2 \geq 0, \ f_3(x) \equiv -x_1^2 - x_2^2 - x_3^2 + 1 \geq 0, \ x_1(x_1-1) = 0 \ (0\text{-1 integer}), \ x_2 \geq 0, \ x_3 \geq 0, \ x_2x_3 = 0 \ ( ext{complementarity}). \end{aligned}$$

• Various problems can be described as POPs.

• A unified theoretical model for global optimization in nonlinear and combinatorial optimization problems.

## POP: min $f_0(x)$ sub.to $f_j(x) \ge 0$ $(j = 1, \ldots, m)$ .

- [1] J.B.Lasserre, "Global optimization with polynomials and the problems of moments", *SIAM J. on Optim.* (2001).
- [2] P.A.Parrilo, "Semidefinite programming relaxations for semialgebraic problems". *Math. Prog.* (2003).
- $[1] \implies$  SDP relaxation primal approach.
- [2]  $\implies$  SOS relaxation dual approach.
- [1] and [2] are dual to each other.
- (a) Lower bounds for the optimal value.
- (b) Convergence to global optimal solutions in theory.
- (c) Large-scale SDPs require enormous computation.
- (d) "Exploit structured sparsity" to solve large scale POPs.

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f(x): a nonnegative polynomial  $\Leftrightarrow f(x) \ge 0 \ (\forall x \in \mathbb{R}^n).$  $\mathcal{N}$ : the set of nonnegative polynomials in  $x \in \mathbb{R}^n$ .

f(x) : an SOS (Sum of Squares) polynomial $\$   $\$   $\$   $\exists$  polynomials  $g_1(x),\ldots,g_k(x);\ f(x)=\sum_{i=1}^kg_i(x)^2.$ 

 $SOS_*$ : the set of SOS. Obviously,  $SOS_* \subset \mathcal{N}$ .  $SOS_{2r} = \{f \in SOS_* : \deg f \leq 2r\}$ : SOSs with degree ar most 2r.

$$n=2. \,\, f(x_1,x_2)=(x_1^2-2x_2+1)^2+(3x_1x_2+x_2-4)^2\in \mathrm{SOS}_4.$$

- In theory,  $SOS_*$  (SOS)  $\subset \mathcal{N}$ .  $SOS_* \neq \mathcal{N}$  in general.
- In practice,  $f(x) \in \mathcal{N} \setminus SOS_*$  is rare.
- So we replace  $\mathcal{N}$  by  $SOS_* \Longrightarrow SOS$  Relaxations.

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# $\mathcal{P}: egin{array}{cc} \min_{x \, \in \, \mathbb{R}^n} \, f(x), ext{ where } f ext{ is a polynomial with deg } f = 2r \end{array}$

Here x is an index describing inequality constraints.



 $\mathcal{P} \colon egin{array}{c} \min_{x \, \in \, \mathbb{R}^n} \, f(x), ext{ where } f ext{ is a polynomial with deg } f = 2r \end{array}$ 

Here x is an index describing inequality constraints.

 $\Sigma \subset \mathrm{SOS}_{2r} \subset \mathrm{SOS}_* \subset \mathcal{N} \Downarrow$  a subproblem of  $\mathcal{P}' =$  a relaxation of  $\mathcal{P}$ 

 $\mathcal{P}$ ": max  $\zeta$  sub.to  $f(x) - \zeta \in \Sigma$ 

 $SOS_*$  ( $SOS_{2r} =$ ) the set of SOS polynomials (with degree  $\leq 2r$ ).

 $\mathcal{P} \colon \min_{x \, \in \, \mathbb{R}^n} \, f(x), ext{ where } f ext{ is a polynomial with deg } f = 2r$ 

1

Here x is an index describing inequality constraints.

 $\Sigma \subset \mathrm{SOS}_{2r} \subset \mathrm{SOS}_* \subset \mathcal{N} \Downarrow$  a subproblem of  $\mathcal{P}' =$  a relaxation of  $\mathcal{P}$ 

$$\mathcal{P}$$
": max  $\zeta$  sub.to  $f(x) - \zeta \in \Sigma$ 

 $SOS_*$  ( $SOS_{2r} =$ ) the set of SOS polynomials (with degree  $\leq 2r$ ).

• the min.val of  $\mathcal{P}$  = the max.val of  $\mathcal{P}' \geq$  the max.val of  $\mathcal{P}$ ".

- $\mathcal{P}$ " can be solved as an SDP (Semidefinite Program) next.
- In practice, we can exploit structured sparsity of the Hessian matrix of f to reduce the size of  $\Sigma$  later.

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Conversion of SOS relaxation into an SDP-1

What is an SDP (Semidefinite Program)?

• An extension of LP (Linear Program) in  $\mathbb{R}^n$  to the space  $\mathcal{S}^n$  of symmetric matrices;

variable a vector  $x \in \mathbb{R}^n \implies X \in \mathcal{S}^n$ .

inequality  $\mathbb{R}^n \ni x \ge 0 \Longrightarrow S^n \ni X \succeq O$  (positive semidefinite).

- Can be solved by the interior-point method.
- Lots of applications.

Conversion of SOS relaxation into an SDP -2

$$egin{aligned} m{a}_p \in \mathbb{R}^n \ (p=0,1,2,\ldots,m), \, b_p \in \mathbb{R} \ (p=1,2,\ldots,m): ext{ data.} \ x \in \mathbb{R}^n: ext{ variable.} \end{aligned}$$

$$a_p \cdot x = \sum_{j=1}^n [a_p]_j x_j$$
 (the inner product).

LP (Linear Program):

$$\begin{array}{l} \max \ a_0 \cdot x \\ \text{s.t.} \ \ a_p \cdot x = b_p \ (p = 1, \ldots, m), \ x \geq 0. \end{array}$$

#### **SDP** (Semidefinite Program):

$$\begin{array}{l} \max \ \boldsymbol{A}_0 \bullet X \\ \text{s.t.} \ \ \boldsymbol{A}_p \bullet X = b_p \ (p = 1, \dots, m), \ X \succeq \boldsymbol{O}. \end{array} \end{array}$$

 $egin{aligned} oldsymbol{A}_p \in \mathcal{S}^n \ (p=0,1,2,\ldots,m), \, b_p \in \mathbb{R} \ (p=1,2,\ldots,m): \ ext{data} \ X \in \mathcal{S}^n: \ ext{variable.} \ oldsymbol{A}_p ullet X = \sum_{i=1}^n \sum_{j=1}^n [oldsymbol{A}_p]_{ij} X_{ij} \ ( ext{the inner product}). \end{aligned}$ 

 $S^n$ : the set of  $n \times n$  real symmetric matrices.  $X \succeq O$ :  $X \in S^n$  is positive semidefinite.

## Conversion of SOS relaxation into an SDP -3

Representation of

$$\mathrm{SOS}_{2r} \equiv \left\{ \sum_{j=1}^k g_j(x)^2 : \exists k \geq 1, \; g_j(x) : \; \mathrm{degree \; at \; most } \; \; r 
ight\} \subset \mathrm{SOS}_*.$$

$$\forall r$$
-degree poly.  $g(x) \exists a \in \mathbb{R}^{d(r)}; g(x) = a^T u_r(x)$ , where  
 $u_r(x) = (1, x_1, x_2, \dots, x_n, x_1^2, x_1 x_2, x_1 x_3, \dots, x_n^2, \dots, x_1^r, \dots, x_n^r)^T$ ,

 $\downarrow$ 

$$d(r)=inom{(1,01,02)}{r}$$
 (a column vector of a basis of  $r$ -degree polynomial), $d(r)=inom{(n+r)}{r}$ : the dimension of  $u_r(x)$ .

$$egin{aligned} \mathrm{SOS}_{2r} &= \left\{ \sum_{j=1}^k \left( a_j^T u_r(x) 
ight)^2 \ : \ k \geq 1, \ a_j \in \mathbb{R}^{d(r)} 
ight\} \ &= \left\{ u_r(x)^T \left( \sum_{j=1}^k a_j a_j^T 
ight) u_r(x) \ : \ k \geq 1, \ a_j \in \mathbb{R}^{d(r)} 
ight\} \ &= \left\{ u_r(x)^T V u_r(x) \ : \ V \ ext{ is a positive semidefinite matrix} 
ight\}. \end{aligned}$$

### Conversion of SOS relaxation into an SDP — 4

Example. n = 2, SOS of at most deg.2 polynomials in  $x = (x_1, x_2)$ .

$$\mathbf{SOS}_4 \equiv \left\{ egin{array}{l} \sum\limits_{i=1}^k g_i(x)^2 : k \ge 1, \; g_i(x) \; ext{ is at most deg.2 polynomial} 
ight\} \ = \left\{ egin{pmatrix} 1 & & & \ x_1 & & \ x_2 & & \ x_1^2 & & \ x_1x_2 & & \ x_2^2 &$$

Conversion of SOS relaxation into an SDP - 5Example :  $f(x) = -x_1 + 2x_2 + 3x_1^2 - 5x_1^2x_2^2 + 7x_2^4$  $\max \zeta$  sub.to  $f(x) - \zeta \in SOS_4$  (SOS of at most deg. 2 polynomials) **Sum of Squares**  $\max \zeta$  $\text{s.t.} \quad f(x) - \zeta = \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_1 x_2 \\ x_2^2 \\ x_2^2 \end{pmatrix}^T \begin{pmatrix} V_{11} & V_{12} & V_{13} & V_{14} & V_{15} & V_{16} \\ V_{12} & V_{22} & V_{23} & V_{24} & V_{25} & V_{26} \\ V_{13} & V_{23} & V_{33} & V_{34} & V_{35} & V_{36} \\ V_{14} & V_{24} & V_{34} & V_{44} & V_{45} & V_{46} \\ V_{15} & V_{25} & V_{35} & V_{45} & V_{55} & V_{56} \\ V_{16} & V_{26} & V_{36} & V_{46} & V_{56} & V_{66} \end{pmatrix} \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_1 x_2 \\ x_2^2 \end{pmatrix}$  $(\forall (x_1, x_2)^T \in \mathbb{R}^n), \quad 6 \times 6 \ V \succ O$ 

 $\updownarrow$  Compare the coef. of 1,  $x_1$ ,  $x_2$ ,  $x_1^2$ ,  $x_1x_2$ ,  $x_2^2$  on both side of =

#### **SDP** (Semidefinite Program)

$$egin{aligned} \max \ \zeta \ ext{s.t.} & -\zeta = V_{11}, \ -1 = 2V_{12}, \ 2 = 2V_{13}, \ 3 = 2V_{14} + V_{22}, \ -5 = 2V_{46} + V_{55}, \ 7 = V_{66}, \ ext{all others} \ \ 0 = \cdots, \ V \succeq O \end{aligned}$$

In general, each equality constraint is a linear equation in  $\zeta$  and V.

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- $\mathcal{P}{:} \ \overline{\min_{x \ \in \ \mathbb{R}^n} \ f(x), \ ext{where} \ f \ ext{is a polynomial with} \ ext{deg} \ f = 2r}$
- H: the sparsity pattern of the Hessian matrix of f(x) $H_{ij} = \begin{cases} \star \text{ if } i = j \text{ or } \partial^2 f(x) / \partial x_i \partial x_j \not\equiv 0, \\ 0 \text{ otherwise.} \end{cases}$

f(x): correlatively sparse  $\Leftrightarrow \exists$  a sparse Cholesky fact. of H.

(a) A sparse Chol. fact. is characterized as a sparse (chordal) graph G(N, E);  $N = \{1, \ldots, n\}$  and

$$E = \{(i,j): H_{ij} = \star\} + ext{"fill-in"}.$$

(b) Let  $C_1, C_2, \ldots, C_q \subset N$  be the maximal cliques of G(N, E).

 $\begin{array}{l} \text{Dense SOS relaxation} \\ \max \ \zeta \\ \text{s.t.} \ \ f(x) - \zeta \in (\text{SOS of polynomials in } x_i \ (i \in N)) \end{array}$ 

• Sparse relaxation is weaker but less expensive in practice.

Example: Generalized Rosenbrock function.

$$f(x) = \sum_{i=2}^n \left( 100(x_i - x_{i-1}^2)^2 + (1-x_i)^2 
ight).$$

• The size of Dense grows very rapidly, so we can't apply Dense to the case  $n \ge 20$  in practice.

- The Hessian matrix is sparse (tridiagonal).
- No fill-in in the Cholesky factorization.

•  $C_i = \{i - 1, i\} \ (i = 2, ..., n - 1)$ : the max. cliques.

• The size of Sparse grows linearly in n, and Sparse can process the case n = 800 in less than 10 sec.

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POP: min  $f_0(x)$  sub.to  $f_j(x) \ge 0$   $(j = 1, \dots, m)$ .

• Rough sketch of SOS relaxation of POP

"Generalized Lagrangian Dual" + "SOS relaxation of unconstrained POPs" ↓ SOS relaxation of POP

• Exploiting sparsity in SOS relaxation of POP

$$\begin{array}{l} \text{POP: } \min f_0(x) \quad \text{sub.to} \quad f_j(x) \geq 0 \ (j = 1, \dots, m). \\ \hline \textbf{Generalized Lagrangian function} \\ \boldsymbol{L}(x, \lambda_1, \dots, \lambda_m) = f_0(x) - \sum_{j=1}^m \lambda_j(x) f_j(x) \\ \quad \text{for } \forall x \in \mathbb{R}^n, \ \forall \lambda_j \in \textbf{SOS}_* \\ \textbf{If } \mathbb{R} \ni \lambda_j \geq 0 \ \textbf{then } \textbf{L} \ \textbf{is the standard Lagrangian function.} \\ \hline \textbf{Generalized Lagrangian Dual} \\ \lambda_1 \in \textbf{SOS}_*, \dots, \lambda_m \in \textbf{SOS}_* \ x \in \mathbb{R}^n \\ \boldsymbol{L}(x, \lambda_1, \dots, \lambda_m) \\ \boldsymbol{\chi}_1 \in \textbf{SOS}_*, \dots, \lambda_m \in \textbf{SOS}_* \\ \textbf{s.t.} \quad \boldsymbol{L}(x, \lambda_1, \dots, \lambda_m) - \zeta \geq 0 \ (\forall x \in \mathbb{R}^n), \\ \lambda_1 \in \textbf{SOS}_*, \dots, \lambda_m \in \textbf{SOS}_* \\ \boldsymbol{\psi} \ \textbf{SOS relaxation} \\ \hline \textbf{max } \zeta \\ \textbf{s.t.} \quad \boldsymbol{L}(x, \lambda_1, \dots, \lambda_m) - \zeta \in \Sigma_0 \\ \lambda_1 \in \Sigma_1, \dots, \lambda_m \in \Sigma_m. \\ \textbf{Here } \Sigma_j \ \textbf{denotes a set of SOS polynomials with a finite degree.} \end{array}$$

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## Numerical results

Software

- MATLAB for constructing sparse and dense SDP relaxation problems
- SeDuMi to solve SDPs.

Hardware

• 2.4GHz Xeon cpu with 6.0GB memory.

**G.Rosenbrock function:** 

$$f(x) = \sum_{i=2}^n ig( 100(x_i - x_{i-1}^2)^2 + (1-x_i)^2 ig)$$

- Two minimizers on  $\mathbb{R}^n$ :  $x_1 = \pm 1, \, x_i = 1 \, (i \geq 2).$
- Add  $x_1 \ge 0 \Rightarrow$  a single minimizer.

		cpu in sec.			
n	$\epsilon_{\rm obj}$	Sparse	Dense		
10	2.5e-08	0.2	10.6		
15	6.5e-08	<b>0.2</b>	756.6		
200	5.2e-07	2.2			
400	2.5e-06	3.7			
800	5.5e-06	6.8			

 $\epsilon_{\rm obj} = \frac{|{\rm the\ lower\ bound\ for\ opt.\ value-the\ approx.\ opt.\ value}|}{\max\{1, |{\rm the\ lower\ bound\ for\ opt.\ value}|\}}.$ 

An optimal control problem from Coleman et al. 1995

$$egin{aligned} \min \ rac{1}{M} \sum_{i=1}^{M-1} \left(y_i^2 + x_i^2
ight) \ ext{s.t.} \ \ y_{i+1} = y_i + rac{1}{M} (y_i^2 - x_i), \quad (i = 1, \dots, M-1), \quad y_1 = 1. \end{aligned}$$

Numerical results on sparse relaxation

M	# of variables	$\epsilon_{\rm obj}$	$\epsilon_{\mathrm{feas}}$	cpu
600	1198	<b>3.4e-08</b>	2.2e-10	3.4
700	1398	2.5e-08	8.1e-10	<b>3.3</b>
800	$\boldsymbol{1598}$	<b>5.9e-08</b>	1.6e-10	<b>3.8</b>
900	$\boldsymbol{1798}$	1.4e-07	6.8e-10	4.5
1000	1998	6.3e-08	2.7e-10	5.0

$$\begin{split} \epsilon_{\rm obj} &= \frac{|{\rm the\ lower\ bound\ for\ opt.\ value\ -\ the\ approx.\ opt.\ value|}}{\max\{1, |{\rm the\ lower\ bound\ for\ opt.\ value|}\}},\\ \epsilon_{\rm feas} &= {\rm the\ maximum\ error\ in\ the\ equality\ constraints,}\\ {\rm cpu:\ cpu\ time\ in\ sec.\ to\ solve\ an\ SDP\ relaxation\ problem.} \end{split}$$

alkyl.gms : a benchmark problem from globallib

$$egin{aligned} \min & -6.3x_5x_8+5.04x_2+0.35x_3+x_4+3.36x_6\ \mathrm{sub.to} & -0.820x_2+x_5-0.820x_6=0,\ & 0.98x_4-x_7(0.01x_5x_{10}+x_4)=0,\ & -x_2x_9+10x_3+x_6=0,\ & x_5x_{12}-x_2(1.12+0.132x_9-0.0067x_9^2)=0,\ & x_8x_{13}-0.01x_9(1.098-0.038x_9)-0.325x_7=0.574,\ & x_{10}x_{14}+22.2x_{11}=35.82,\ & x_1x_{11}-3x_8=-1.33,\ & \mathrm{lbd}_i\leq x_i\leq \mathrm{ubd}_i\ (i=1,2,\ldots,14). \end{aligned}$$

		Sparse			Dense (Lasserre)		
problem	$\boldsymbol{n}$	$\epsilon_{\rm obj}$	$\epsilon_{\mathrm{feas}}$	cpu	$\epsilon_{\rm obj}$	$\epsilon_{\mathrm{feas}}$	cpu
alkyl	14	5.6e-10	2.0e-08	23.0	out of	memory	

$$\begin{split} \epsilon_{\rm obj} &= \frac{|{\rm the\ lower\ bound\ for\ opt.\ value\ -\ the\ approx.\ opt.\ value|}}{\max\{1, |{\rm the\ lower\ bound\ for\ opt.\ value}|\}},\\ \epsilon_{\rm feas} &= {\rm the\ maximum\ error\ in\ the\ equality\ constraints,}\\ {\rm cpu:\ cpu\ time\ in\ sec.\ to\ solve\ an\ SDP\ relaxation\ problem.} \end{split}$$

Some	other	benchmark	problems	from	globallib
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		Sparse			Dense (Lasserre)		
problem	n	$\epsilon_{\rm obj}$	$\epsilon_{\mathrm{feas}}$	$\mathbf{cpu}$	$\epsilon_{ m obj}$	$\epsilon_{\mathrm{feas}}$	$\mathbf{cpu}$
$ex3_1_1$	8	6.3e-09	4.7e-04	5.5	0.7e-08	2.5e-03	597.8
$st_bpaf1b$	10	3.8e-08	2.8e-08	1.0	4.6e-09	7.2e-10	1.7
$st_e07$	10	0.0e+00	8.1e-05	0.4	0.0e+00	8.8e-06	<b>3.0</b>
st_jcbpaf2	10	1.1e-07	0.0e+00	2.1	1.1e-07	0.0e+00	<b>2.0</b>
$ex2_1_3$	13	5.1e-09	3.5e-09	0.5	1.6e-09	1.5e-09	7.7
$ex9_1_1$	13	0.0	4.5e-06	1.5	0.0	9.2e-07	7.7
$ex9_2_3$	16	0.0e+00	5.7e-06	2.3	0.0e+00	7.5e-06	49.7
$ex2_1_8$	<b>24</b>	1.0e-05	0.0e+00	304.6	3.4e-06	0.0e+00	1946.6
$ex5_2_c1$	9	<b>1.0e-2</b>	3.2e+01	1.8	<b>1.6e-05</b>	<b>2.1e-01</b>	2.6
$ex5_2_c2$	9	1.0e-02	7.2e + 01	<b>2.1</b>	<b>1.3e-04</b>	2.7e-01	<b>3.5</b>

- $ex5_2_c1$  and  $ex5_2_c2$  Dense is better.
- Sparse attains approx. opt. solutions with the same quality as Dense except  $ex5_2_c1$  and  $ex5_2_c2_c2$ .
- Sparse is much faster than Dense in large dim. cases.

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- Lasserre's (dense) relaxation
  - theoretical convergence but expensive in practice.
- The proposed sparse relaxation
  - = Lasserre's (dense) relaxation + sparsity
  - no theoretical convergence but very powerful in practice.
- There remain many issues to be studied further.
  - Exploiting sparsity.
  - -Large-scale SDPs.
  - Numerical difficulty in solving SDP relaxations of POPs.

This presentation material is available at

http://www.is.titech.ac.jp/~kojima/talk.html

Thank you!

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