多項式最適化問題の半正定値計画緩和 — 疎性の活用 —

最適化:モデリングとアルゴリズム 2007年3月22-24日 統計数理研究所

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- 1. POPs (Polynomial Optimization Problems)
- 2. How do we formulate structured sparsity?
- 3. Sparse SDP relaxation of POPs
- 4. Numerical results
- 5. Concluding remarks.

1. POPs (Polynomial Optimization Problems)

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Notation and Symbols

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

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

Example: n = 3

$$\begin{array}{ll} \min & f_0(\boldsymbol{x}) \equiv x_1^3 - 2x_1x_2^2 + x_1^2x_2x_3 - 4x_3^2 \\ \text{sub.to} & f_1(\boldsymbol{x}) \equiv -x_1^2 + 5x_2x_3 + 1 \ge 0, \\ & f_2(\boldsymbol{x}) \equiv x_1^2 - 3x_1x_2x_3 + 2x_3 + 2 \ge 0, \\ & f_3(\boldsymbol{x}) \equiv -x_1^2 - x_2^2 - x_3^2 + 1 \ge 0, \\ & x_1(x_1 - 1) = 0 \text{ (0-1 integer)}, \\ & x_2 \ge 0, \ x_3 \ge 0, \ x_2x_3 = 0 \text{ (complementarity)}. \end{array}$$

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- [1] Lasserre, "Global optimization with polynomials and the problems of moments", *SIAM J. on Optim.* (2001).
- [2] Parrilo, "Semidefinite programming relaxations for semialgebraic problems", *Math. Prog.* (2003).
- [3] Henrion-Lasserre, GloptiPoly.
- [4] Prajna-Parachristodoulou-Parrilo, SOSTOOLS.
- [1,3] ⇒ a sequence of SDP relaxations primal approach.
- **9** $[2,4] \Rightarrow$ a sequence of SOS relaxations dual approach.
- (a) Lower bounds for the optimal value.
- (b) Convergence to global optimal solutions in theory.
- (c) Each relaxed problem can be solved as an SDP; its size gets larger rapidly along "the sequence" as we require a higher accuracy.
- (d) Expensive to solve large scale POPs in practice.
 - \Rightarrow Exploiting Sparsity.

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- [4] Prajna-Parachristodoulou-Parrilo, SOSTOOLS.

Exploiting sparsity to solve larger scale problem in practice

- [5] Kojima-Kim-Waki, "Sparsity in SOS Polynomials", *Math. Prog.* (2005).
- [6] Waki-Kim-Kojima-Muramatsu, "SOS and SDP Relaxations for POPs with Structured Sparsity", SIAM J. on Optim (2006).
- [7] Waki-Kim-Kojima-Muramatsu, SparsePOP (2005).

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- [3] Henrion-Lasserre, GloptiPoly.
- [4] Prajna-Parachristodoulou-Parrilo, SOSTOOLS.

Extension to polynomial SDP and SOCP

[8] Kojima, "SOS relaxations of poly. SDPs" (2003).
[9] Hol-Scherer, "SOS relaxations of poly. SDPs" (2004).
[10] Henrion-Lasserre, "Convergent relaxations of poly. mat. inequalities & static output feedback" (2006).
[11] Kojima-Muramatsu, "An Extension of SOS Relaxations to

POPs over Symmetric Cones ", to appear in *Math. Prog.*

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

How do we exploit sparsity in POP?

The answer depends on which methods we use to solve POP.

POP

↓ SDP relaxation (Lasserre 2001)

SDP *\Leftarrow Primal-Dual IPM (Interior-Point Method)*

We will assume a structured sparsity (correlative sparsity):
(a) The size of SDP gets smaller.
(b) SDP satisfies "a similar structured sparsity" under which Primal-Dual IPM works efficiently.

- Characterized in terms of a sparse Cholesky factorization
- Characterized in terms of a sparse chordal graph structure
- Useful to solve large-scale sparse POPs in practice

Example:
$$f_0(\boldsymbol{x}) = \sum_{k=1}^n (-x_k^2)$$

 $f_j(\boldsymbol{x}) = 1 - x_j^2 - 2x_{j+1}^2 - x_n^2 \ (j = 1, \dots, n-1).$

 $Hf_0(\boldsymbol{x})$: the $n \times n$ Hes. mat. of $f_0(\boldsymbol{x})$,

 $\boldsymbol{Jf}_*(\boldsymbol{x}): \text{ the } m imes n \text{ Jacob. mat. of } \boldsymbol{f}_*(\boldsymbol{x}) = (f_1(\boldsymbol{x}), \dots, f_m(\boldsymbol{x}))^T,$

 \boldsymbol{R} : the csp matrix, the $n \times n$ sparsity pattern matrix of

 $I + H f_0(x) + J f_*(x)^T J f_*(x)$ (no cancellation in '+').

 $[\mathbf{Jf}_*(\mathbf{x})^T \mathbf{Jf}_*(\mathbf{x})]_{ij} \neq 0$ iff x_i and x_j are in a common constraint.

Example with n = 6:

the csp matrix $\boldsymbol{R}=$

$$\begin{pmatrix}
* & * & 0 & 0 & 0 & * \\
* & * & * & 0 & 0 & * \\
0 & * & * & * & 0 & * \\
0 & 0 & * & * & * & * \\
0 & 0 & 0 & * & * & * \\
* & * & * & * & * & *
\end{pmatrix}$$

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POP : c-sparse (correlatively sparse) \Leftrightarrow The $n \times n$ csp matrix $\mathbf{R} = (R_{ij})$ allows a symbolic sparse Cholesky factorization (under a row & col. ordering like a symmetric min. deg. ordering).

POP min.
$$f_0(x)$$
 s.t. $f_j(x) \ge 0$ or $= 0 \ (j = 1, ..., m)$.

Example:
$$f_0(\boldsymbol{x}) = \sum_{k=1}^n (-x_k^2)$$
 — — c-sparse
 $f_j(\boldsymbol{x}) = 1 - x_j^2 - 2x_{j+1}^2 - x_n^2 \ (j = 1, \dots, n-1).$

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* & * & * & 0 & 0 & * \\
0 & * & * & * & 0 & * \\
0 & 0 & * & * & * & * \\
0 & 0 & 0 & * & * & * \\
* & * & * & * & * & *
\end{pmatrix}$$

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Sparse (SDP) relaxation = Lasserre (2001) + c-sparsity

 \downarrow

A sequence of c-sparse SDP relaxation problems depending on the relaxation order r = 1, 2, ...;

- (a) Under a moderate assumption, opt. sol. of SDP \rightarrow opt sol. of POP as $r \rightarrow \infty$.
- (b) $r = \lceil$ "the max. deg. of poly. in POP"/2 \rceil +0 ~ 3 is usually large enough to attain opt sol. of POP in practice.
- (c) Such an r is unknown in theory except \exists special cases.
- (d) Additional method for all opt. sol. of POP, but expensive.
- (e) The size of SDP increases rapidly as $r \to \infty$.

 $\boldsymbol{R}: \hspace{0.1 cm} \mbox{the csp matrix, the } n \times n \hspace{0.1 cm} \mbox{sparsiity pattern matrix of}$

 $I + H f_0(x) + J f_*(x)^T J f_*(x)$ (no cancellation in '+').

POP : c-sparse (correlatively sparse) \Leftrightarrow The $n \times n$ csp matrix $\mathbf{R} = (R_{ij})$ allows a symbolic sparse Cholesky factorization.

 $E = \{\{i, j\} \in N \times N : \mathbf{R}_{ij} = \star, i \neq j\} \ (1)$

POP : c-sparse (correlatively sparse) \Leftrightarrow The csp graph G(N, E) has a sparse chordal extension $G(N, \overline{E})$; $E \subseteq \overline{E}$.



- The added edge $\{3, 6\}$ is corresponding to a fill-in.
- The maximal cliques = $\{1, 2\}, \{1, 3, 4\}, \{3, 4, 6\}, \{3, 5, 6\}.$

 \boldsymbol{R} : the csp matrix, the $n \times n$ sparsiity pattern matrix of

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POP : c-sparse (correlatively sparse) \Leftrightarrow The $n \times n$ csp matrix $\mathbf{R} = (R_{ij})$ allows a symbolic sparse Cholesky factorization.

Two steps to derive a sparse SDP relaxation of POP (a) Using the max. cliques J_q ($q \in L$) of $G(N, \overline{E})$, convert POP into an equivalent poly.SDP with the csp graph $G(N, \overline{E})$. (b) Linearize poly.SDP \Rightarrow SDP with a similar sparsity to poly.SDP.

 \forall int. $s \ge 0$, $u_s(x_i : i \in J_q)$: the col. vect. of monomials with deg. at most s in var. x_i $(i \in J_q)$; e.g., if $J_q = \{1, 4\}$,

$$s = 0 \Rightarrow \boldsymbol{u}_0(x_i : i \in J_q) = 1, s = 1 \Rightarrow \boldsymbol{u}_1(x_i : i \in J_q) = (1, x_1, x_4)^T, s = 3 \Rightarrow \boldsymbol{u}_3(x_i : i \in J_q) = (1, x_1, x_4, x_1^2, x_1x_4, x_4^2, x_1^3, x_1^2x_4, x_1x_4^2, x_4^3)^T.$$

 $oldsymbol{R}$: the csp matrix, the $n \times n$ sparsiity pattern matrix of

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$$s = 1 \Rightarrow \boldsymbol{u}_1(x_i : i \in J_q) = (1, x_1, x_4)^T, \qquad 1 \quad x_1 \quad x_4 \\ s = 1 \Rightarrow \boldsymbol{u}_1(x_i : i \in J_q) \boldsymbol{u}_1(x_i : i \in J_q)^T = \begin{pmatrix} 1 & x_1 & x_4 \\ x_1 & x_1^2 & x_1 x_4 \\ x_4 & x_1 x_4 & x_4^2 \end{pmatrix}$$

Example of Sparse SDP Relaxation

POP: min
$$\sum_{i=1}^{4} (-x_i^3)$$
 s.t. $-a_i \times x_i^2 - x_4^2 + 1 \ge 0$ $(i = 1, 2, 3)$.

csp matrix
$$\mathbf{R} = \begin{pmatrix} \star & 0 & 0 & \star \\ 0 & \star & 0 & \star \\ 0 & 0 & \star & \star \\ \star & \star & \star & \star \end{pmatrix}$$

No fill-in in the Cholesky factorization \Rightarrow c-sparse.

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 s.t. $-a_i \times x_i^2 - x_4^2 + 1 \ge 0$ $(i = 1, 2, 3)$.

 \uparrow with the relaxation order $r = 2 \ge r_0 = \lceil 3/2 \rceil = 2$

poly.SDP:
min
$$\sum_{i=1}^{4} (-x_i^3)$$

s.t. $(-a_i \times x_i^2 - x_4^2 + 1)(1, x_i, x_4)^T (1, x_i, x_4) \succeq O$ $i = 1, 2, 3,$
 $(1, x_j, x_4, x_j^2, x_j x_4, x_4^2)^T (1, x_j, x_4, x_j^2, x_j x_4, x_4^2) \succeq O$ $j = 1, 2, 3.$

csp matrix
$$\mathbf{R} = \begin{pmatrix} \star & 0 & 0 & \star \\ 0 & \star & 0 & \star \\ 0 & 0 & \star & \star \\ \star & \star & \star & \star \end{pmatrix}$$

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Example of Sparse SDP Relaxation

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 $(1, x_j, x_4, x_j^2, x_j x_4, x_4^2)^T (1, x_j, x_4, x_j^2, x_j x_4, x_4^2) \succeq O$ $j = 1, 2, 3.$

Represent poly.SDP as

$$\begin{array}{l} \min \ \sum_{\boldsymbol{\alpha} \in \mathcal{A}_0} g_0(\boldsymbol{\alpha}) \boldsymbol{x}^{\boldsymbol{\alpha}} \text{ s.t. } \sum_{\boldsymbol{\alpha} \in \mathcal{A}_j} \boldsymbol{G}_j(\boldsymbol{\alpha}) \boldsymbol{x}^{\boldsymbol{\alpha}} \succeq \boldsymbol{O} \ j = 1, \dots, 6, \\ \text{where } \mathcal{A}_j \subset \mathbb{Z}_+^4 \text{ and } \boldsymbol{x}^{\alpha} = x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3} x_4^{\alpha_4} \text{; } \boldsymbol{x}^{(1,2,1,0)} = x_1 x_2^2 x_3. \end{array}$$

 \Downarrow Linearize by replacing each x^{α} by an indep. var. y_{α} ; x^0 by 1

SDP min
$$\sum_{\boldsymbol{\alpha} \in \mathcal{A}_0} g_0(\boldsymbol{\alpha}) y_{\boldsymbol{\alpha}}$$
 s.t. $\sum_{\boldsymbol{\alpha} \in \mathcal{A}_j} G_j(\boldsymbol{\alpha}) y_{\boldsymbol{\alpha}} \succeq \boldsymbol{O} \ j = 1, \dots, 6,$
which forms an SDP relaxation of POP.

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Numerical result on unconstrained optimization

Unconstrained POP: min. $f(\boldsymbol{x}), \ \boldsymbol{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$.

Broyden tridiagonal function with min.val.= 0 $f(\mathbf{x}) = \sum_{i=1}^{n} ((3 - 2x_i)x_i - x_{i-1} - 2x_{i+1} + 1)^2, \ x_0 = x_{n+1} = 0.$

Generalized Rosenbrock function with min.val.= 0 $f(\boldsymbol{x}) = \sum_{i=2}^{n} \left(100(x_i - x_{i-1}^2)^2 + (1 - x_i)^2 \right), \ x_1 \ge 0..$

		B. tridiagon	al	G. Rosenbro	ck
n	r	approx.opt.val cpu		approx.opt.val	cpu
600	2	1.0e-7	9.3	3.9e-7	3.4
800	2	2.2e-7	12.6	2.1e-7	5.1
1000	2	2.6e-7	16.0	4.5e-7	5.9

An optimal control problem from Coleman et al. 1995

min
$$\frac{1}{M} \sum_{i=1}^{M-1} (y_i^2 + x_i^2)$$

s.t. $y_{i+1} = y_i + \frac{1}{M} (y_i^2 - x_i), \quad (i = 1, \dots, M-1), \quad y_1 = 1.$

Numerical results on sparse relaxation

M	r	# of variables	ϵ obj	ϵ feas	cpu
600	2	1198	3.4e-08	2.2e-10	3.4
800	2	1598	5.9e-08	1.6e-10	3.8
1000	2	1998	6.3e-08	2.7e-10	5.0

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

alkyl.gms : a benchmark problem from globalib

$$\min \quad -6.3x_5x_8 + 5.04x_2 + 0.35x_3 + x_4 + 3.36x_6$$

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

		Sparse		Dense (Lasserre)		
r	ϵ obj	ϵ feas	cpu	ϵ obj	ϵ feas	cpu
2	1.0e-02	7.1e-01	1.8	7.2e-3	4.3e-2	14.4
3	5.6e-10	2.0e-08	23.0	out of	memory	

 $\epsilon_{obj} = approx.opt.val. - lower bound for opt.val.$ $<math>\epsilon_{feas} = the maximum error in the equality constraints$

Some other benchmark problems from globalib

		Sparse			Dense (Lasserre)	
problem	n	€obj	ϵ feas	cpu	€obj	cpu
ex3_1_1	8	6.3e-9	4.7e-4	5.5	0.7e-8	597.8
st_bpaf1b	10	3.8e-8	2.8e-8	1.0	4.6e-9	1.7
st_e07	10	0.0	8.1e-5	0.4	0.0	3.0
ex2_1_3	13	5.1e-09	3.5e-9	0.5	1.6e-9	7.7
ex9_1_1	13	0.0	4.5e-6	1.5	0.0	7.7
ex9_2_3	16	0.0	5.7e-6	2.3	0.0	49.7
ex2_1_8	24	1.0e-5	0.0	304.6	3.4e-6	1946.6
ex5_2_2	9	1.0e-2	3.2e+1	1.8	1.6e-5	2.6

- ex5_2_2 Dense is better.
- Sparse attains approx. opt. solutions with the same quality as Dense except ex5_2_2.
- Sparse is much faster than Dense in large dim. cases.

Discretization of Mimura's ODE with 2 unknowns
$$u, v : [0,5] \rightarrow \mathbb{R}$$

 $u_{xx} = -(\delta_1/9)(35 + 16u - u^2)u + (\delta_1)(kuv),$
 $v_{xx} = (\delta_2)((1 + (2/5)v)v - kuv),$
 $u_x(0) = u_x(5) = v_x(0) = v_x(5) = 0,$
where $k = 1, \delta_1 = 20$ and $\delta_2 = 1/4$. Discretize:
 $x_i = i\Delta x \ (i = 0, 1, 2, ...), \ u_x(x_i) \approx (u(x_{i+1}) - u(x_{i-1}))/(2\Delta x).$
Discretized system of polynomials with $\Delta x = 1$:
 $f_1(u, v) = 76.8u_1 + u_3 + 35.6u_1^2 - 20.0u_1v_1 - 2.22u_2^3,$
 $f_2(u, v) = -1.25v_1 + v_2 + 0.25u_1v_1 - 0.1v_1^2,$
 $f_3(u, v) = u_1 + 75.8u_2 + u_3 + 35.6u_2^2 - 20.0u_2v_2 - 2.22u_2^3,$
 $f_4(u, v) = v_1 - 2.25v_2 + v_3 + 0.25u_2v_2 - 0.1v_2^2,$
 $f_5(u, v) = u_2 + 75.8u_3 + u_4 + 35.6u_3^2 - 20.0u_3v_3 - 2.22u_3^2,$
 $f_6(u, v) = v_2 - 2.25v_3 + v_4 + 0.25u_3v_3 - 0.1v_3^2,$
 $f_7(u, v) = u_3 + 76.8u_4 + 35.6u_4^2 - 20.0u_4v_4 - 2.22u_4^3,$
 $f_8(u, v) = v_3 - 1.25v_4 + 0.25u_4v_4 - 0.1v_4^2.$
Here $u_i = u(x_i), v_i = v(x_i) \ (i = 0, 1, 2, 3, 4, 5),$
 $u_0 = u_1, u_5 = u_4, v_0 = v_1 \text{ and } v_5 = v_4.$ \Rightarrow c-sparse

Discretization of Mimura's ODE with 2 unknowns $u, v : [0,5] \rightarrow \mathbb{R}$ $u_{xx} = -(\delta_1/9)(35 + 16u - u^2)u + (\delta_1)(kuv),$ $v_{xx} = (\delta_2)((1 + (2/5)v)v - kuv),$ $u_x(0) = u_x(5) = v_x(0) = v_x(5) = 0,$ where $k = 1, \delta_1 = 20$ and $\delta_2 = 1/4$. Discretize: $x_i = i\Delta x \ (i = 0, 1, 2, ...), \ u_x(x_i) \approx (u(x_{i+1}) - u(x_{i-1}))/(2\Delta x).$

Numerical results on SparsePOP

Δx	n	obj.funct.	r	A in SeDuMi	cpu
1.0	8	$\sum r_i u(x_i) \uparrow$	3	[1,084, 18,732]	11.3
0.5	18	$\sum r_i u(x_i) \uparrow$	3	[3,025, 48,285]	57.8

Here $r_i \in (0, 1)$: random numbers.



Discretization of DAE with 3 unknowns $y_1, y_2, y_3 : [0, 2] \rightarrow \mathbb{R}$ $y'_1 = y_3, \ 0 = y_2(1 - y_2), \ 0 = y_1y_2 + y_3(1 - y_2) - t, \ y_1(0) = y_1^0.$ 2 solutions : y(t) = (t, 1, 1) and $y(t) = (y_1^0 + t^2, 0, t).$

Numerical results on SparsePOP

- c-sparse

y_1^0	Δt	n	obj.funct.	r	A in SeDuMi	cpu
0	0.02	297	$\sum y_2(t_i)\uparrow$	2	[3,557, 25,413]	30.9
1	0.02	297	$\sum y_1(t_i)\uparrow$	2	[3,557, 25,413]	33.9



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- 1. POPs (Polynomial Optimization Problems)
- 2. How do we formulate structured sparsity?
- 3. Sparse SDP relaxation of POPs
- 4. Numerical results
- 5. Concluding remarks

- Lasserre's (dense) relaxation
 - Theoretical convergence but expensive in practice.
- Sparse relaxation (Waki-Kim-Kojima-Muramatsu)
 - = Lasserre's (dense) relaxation + sparsity
 - Very powerful in practice and theoretical convergence (Lasserre)
- There remain many issues to be studied further.
 - Exploiting sparsity.
 - Large-scale SDPs.
 - Numerical difficulty in solving SDP relaxations of POPs.

Thank you!