Sparsity in Polynomial Optimization

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•Some joint works with S.Kim, K.Kobayashi, M.Muramatsu & H.Waki

•Applications to nonlinear PDEs (partial differential equations) --- Ongoing joint work with M.Mevissen, J.Nie & N.Takayama

- 1. How do we formulate structured sparsity?
 - 1-1. Unconstrained cases.
 - 1-2. Constrained and linear objective function cases.
 - (Recent Joint work with S.Kim & K.Kobayashi)
- 2. Sparse SDP relaxation of constrained POPs.
- 3. Applications to PDEs (partial differential equations).

4. Concluding remarks.

POP --- Polynomial Optimization Problem

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POP --- Polynomial Optimization Problem

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

 $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$: a vector variable.

 $f_j(x)$: a multivariate polynomial in $x \in \mathbb{R}^n$ (j = 0, 1, ..., m).

How do we exploit sparsity in POP? ↓

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

POP

 \Downarrow 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.

1. How do we formulate structured sparsity?

- 1-1. Unconstrained cases.
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POP --- Polynomial Optimization Problem
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Unconstrained POP: minimize $f_0(x)$, $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$.

Define $n \times n$ csp (correlative sparsity pattern) matrix R

$$R_{ij} = \begin{cases} \star \text{ (nonzero symbol) if } i = j \text{ or if } \partial^2 f(x) / \partial x_i \partial x_j \not\equiv 0, \\ 0 & \text{otherwise.} \end{cases}$$

(The sparsity pattern of the Hessian matrix of $f_0(x)$ except the diagonal)

Unconstrained POP : c-sparse (correlatively sparse) \Leftrightarrow R allows a sparse (symbolic) Cholesky factorization (under an ordering like the min. degree ordering).

Example.
$$f(x) = x_1^4 + 2x_1^2x_2 + x_2^4 - x_2x_3 + x_3^4 - 3x_3x_4^2 + x_4^4 - x_4x_5 + x_5^6$$
$$\begin{pmatrix} \star & \star & 0 & 0 \\ \star & \star & \star & 0 \\ 0 & \star & \star & \star \\ 0 & 0 & \star & \star \\ 0 & 0 & 0 & \star & \star \end{pmatrix} = LL^T, \text{ where } L = \begin{pmatrix} \star & 0 & 0 & 0 \\ \star & \star & 0 & 0 \\ 0 & \star & \star & 0 \\ 0 & 0 & \star & \star \\ 0 & 0 & 0 & \star & \star \end{pmatrix}.$$

No fill-in in the Cholesky factorization.

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Unconstrained POP : c-sparse (correlatively sparse) \Leftrightarrow
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(under an ordering like the min. degree ordering).

Numerical results on a sparse SDP relaxation applied to three nonconvex test problems with opt.values = 0 from globalib

	B. tridiagon	al	C. Wood		G. Rosenbrock	
\boldsymbol{n}	approx.opt.val	\mathbf{cpu}	apprx.opt.val	\mathbf{cpu}	apprx.opt.val	\mathbf{cpu}
600	1.0e-7	9.3	1.4e-5	0.9	3.9e-7	3.4
800	2.2e-7	12.6	1.8e-5	1.3	2.1e-7	5.1
1000	2.6e-7	16.0	3.8e-5	1.6	4.5e-7	5.9

Broyden tridiagonal function

$$f(x) = \sum_{i=1}^{n} \left((3 - 2x_i)x_i - x_{i-1} - 2x_{i+1} + 1 \right)^2, \text{ where } x_0 = x_{n+1} = 0.$$

1. How do we formulate structured sparsity? 1-1. Unconstrained cases.

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We consider cases where objective functions are linear.
LP, SOCP and SDP + Primal-Dual Interior-Point Method.

$$M = \{1, \dots, m\}, \ N = \{1, \dots, n\}, \ I_p \subset N \ (p \in M)$$

$$(y_i : i \in I_p)$$
 : a subvector of $y = (y_1, \dots, y_n) \in \mathbb{R}^n$
consisting of elements y_i $(i \in I_p)$,

 C_p : a nonempty subset of the set of all $(y_i : i \in I_p)$.

Define the $n \times n$ csp (correlative sparsity pattern) matrix R by

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Opt.Problem: c-sparse (correlatively sparse) \Leftrightarrow *R* allows a sparse (symbolic) Cholesky factorization.

Example

$$\begin{split} C_p &= \{ \begin{array}{l} (y_p, y_{p+1}, y_n) \in \mathbb{R}^n : \ 1 - y_p^2 - y_{p+1}^2 - y_n^2 \geq 0, \\ & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} b_p & c_p \\ c_p & d_p \end{pmatrix} y_p + \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} y_p y_{p+1} + \begin{pmatrix} -2 & 1 \\ 1 & -1 \end{pmatrix} y_{p+1} \succeq O, \\ & \begin{pmatrix} 0.3(y_p^3 + y_n) + 1 \end{pmatrix} - \|(y_p + \beta_p, y_n)\| \geq 0 \, \} \qquad (p = 1, \dots, n-1). \end{split}$$
 Here $a_i, b_p, d_p \in (-1, 0), \ c_p, \beta_p \in (0, 1)$ denote random numbers.

$$M = \{1, \ldots, m\}, \ N = \{1, \ldots, n\}, \ I_p \subset N \ (p \in M)$$

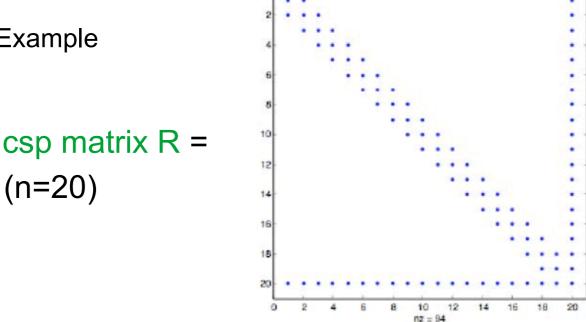
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Example

SDP size # of cpu $\epsilon_{\rm obj} \epsilon_{\rm feas}$ size of A, SeDuMi nonzeros in A sec. \boldsymbol{n} 25.7 4.0e-12 235.612600 0.0 $11,974 \times 113,022$ 800 34.8 3.2e-12 $0.0 | 15,974 \times 150,822$ 314,412 1000 | 44.5 | 1.6e-120.0 $19,974 \times 188,622$ 393,212

Numerical results on the sparse SDP relaxation

$$M = \{1, \ldots, m\}, \ N = \{1, \ldots, n\}, \ I_p \subset N \ (p \in M)$$

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Opt.Problem: c-sparse (correlatively sparse) \Leftrightarrow *R* allows a sparse (symbolic) Cholesky factorization.

- (a) $\forall C_p$ is described by poly. (matrix or second-order cone) inequalites. \Rightarrow A sparse SDP relaxation whose csp matrix R' is of "a similar sparsity pattern" to R; the size of $R' \geq$ the size of R.
- (b) $\forall C_p$ is described by linear matrix inequalities (SDP) \Rightarrow The coef. matrix B of the Schur complement eq. Bdy = r, which is the most time consuming in Primal-dual IPMs, for a search direction dy has the same pattern as the csp matrix R' of SDP.

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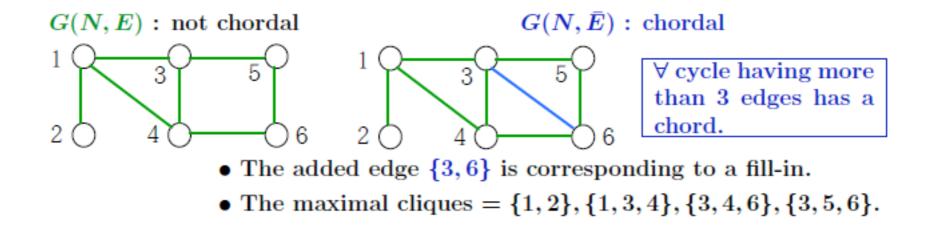
Sections 1-1 + 1-2 ==> Section 2

Sparse SDP relaxation = Modification of Lasserre's relaxation

 $\begin{array}{l} \text{POP: max. } f_0(x) \text{ s.t. } (x_i: i \in I_p) \in C_p \ (p \in M) \\ M = \{1, \ldots, m\}, \ N = \{1, \ldots, n\}, \ I_p \subset N \ (p \in M) \\ C_p \subset \text{ the set of all } (x_i: i \in I_p), \text{ described as poly. inequalites.} \\ R_{ij} = \begin{cases} \star \ (\text{nonzero symbol}) \ \text{if } i = j, \ \partial^2 f_0(x) / \partial x_i \partial x_j \not\equiv 0, \\ 0 & \text{or } i, \ j \in I_p \ \text{for } \exists p \in M, \\ 0 & \text{otherwise.} \end{cases} \\ \begin{array}{c} \text{POP: c-sparse (correlatively sparse) } \Leftrightarrow \\ \text{The } n \times n \ \text{csp matrix } R = (R_{ij}) \ \text{allows a sparse Cholesky factorization.} \end{cases} \end{array}$

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

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



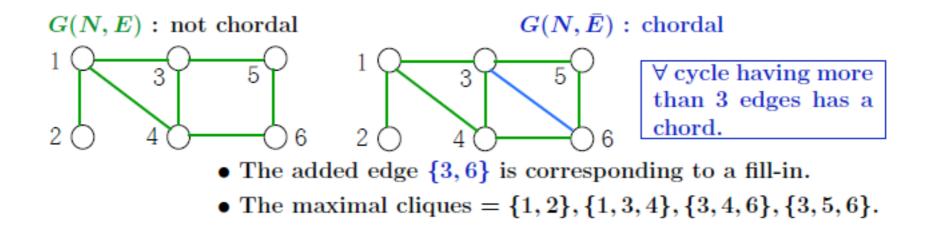
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POP : c-sparse (correlatively sparse) \Leftrightarrow The csp graph G(N, E) has a sparse chordal extension $G(N, \overline{E}); E \subseteq \overline{E}$.

Two steps to derive a sparse SDP relaxation of POP

- (a) Using the max. cliques J_q $(q \in L)$ of $G(N, \overline{E})$, we 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.



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Notation: For every nonnegative integer s, let $u_s(x_i : i \in J_q)$ denote the column vector of monomials with degree at most s in variables x_i $(i \in J_q)$. Example: Let $J_q = \{1, 4\}$. Then

$$s = 0 \Rightarrow u_0(x_i : i \in J_q) = 1,$$

$$s = 1 \Rightarrow u_1(x_i : i \in J_q) = (1, x_1, x_4)^T,$$

$$s = 3 \Rightarrow u_3(x_i : i \in J_q) = (1, x_1, x_4, x_1^2, x_1x_4, x_4^2, x_1^3, x_1^2x_4, x_1x_4^2, x_4^3)^T,$$

$$s = 1 \Rightarrow u_1(x_i : i \in J_q)u_1(x_i : i \in J_q)^T = \begin{pmatrix} 1 & x_1 & x_4 \\ x_1 & x_1^2 & x_1x_4 \\ x_4 & x_1x_4 & x_4^2 \end{pmatrix}$$

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(a-1) Let
$$r_0 = \lceil \deg(\text{POP})/2 \rceil \equiv \lceil \text{"the max.deg. of the poly. in POP"}/2 \rceil$$
.

(a-2) Choose $r \ge r_0$; a sequence of poly.SDPs depending on $r \ge r_0$.

r: the relaxation order of the sparse SDP relaxation of POP; $r = \lceil \deg(\text{poly.SDP})/2 \rceil$

(a-3) Replace each $f(x_i : i \in I_p) \ge 0$ involved in C_p by an equivalent $f(x_i : i \in I_p)u_s(x_i : i \in J_q)u_s(x_i : i \in J_q)^T \succeq O$,

where $s = r - \lceil$ "the degree of $f(x_i : i \in I_p)"/2 \rceil$ and $I_p \subseteq J_q$.

(a-4) Add (redundant) $u_r(x_i : i \in J_q)u_r(x_i : i \in J_q)^T \succeq O \ (q \in L)$ to POP.

An equiv.poly.SDP with the csp graph G(N, E) of the form max. $f_0(x)$ s.t. $P_j(x) \succeq O$ $(j = 1, ..., \ell)$. Here $P_j(x)$: a poly. with sym. mat. coefficients.

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An equiv.poly.SDP with the csp graph $G(N, \overline{E})$ of the form max. $f_0(x)$ s.t. $P_j(x) \succeq O$ $(j = 1, ..., \ell)$. Here $P_j(x)$: a poly. with sym. mat. coefficients.

Represent poly.SDP as

max. $\sum_{\alpha \in \mathcal{A}_0} g_0(\alpha) x^{\alpha}$ s.t. $\sum_{\alpha \in \mathcal{A}_j} G_j(\alpha) x^{\alpha} \succeq O \ (j = 1, \dots, \ell).$

 \downarrow (b) Linearize by replacing each x^{α} by an indep. var. y_{α}

SDP: max. $\sum_{\alpha \in \mathcal{A}_0} g_0(\alpha) y_\alpha$ s.t. $\sum_{\alpha \in \mathcal{A}_j} G_j(\alpha) y_\alpha \succeq O \ (j = 1, \dots, \ell)$, which forms a sparse SDP relaxation of POP.

- poly.SDP dep.on $r \ge r_0 = \lceil \deg(\text{POP})/2 \rceil \Rightarrow$ a seq.of SDPs dep.on $r \ge r_0$.
- Under an assump., opt.val.SDP \rightarrow opt.val.POP as $r \rightarrow \infty$ (Lasserre '05).

Example

 $\begin{array}{l} \text{POP: min. } \sum_{i=1}^{3}(-x_{i}^{3}) \text{ s.t. } -i \times x_{i}^{2} - x_{4}^{2} + 1 \geq 0 \ (i = 1, 2, 3). \\ \textcircled{} (a) \text{ with the relaxation order } r = 2 \geq r_{0} = \lceil 3/2 \rceil = 2 \\ \hline \text{poly.SDP} \\ \text{min. } \sum_{i=1}^{3}(-x_{i}^{3}) \\ \text{s.t. } (-i \times x_{i}^{2} - x_{4}^{2} + 1)(1, x_{i}, x_{4})^{T}(1, x_{i}, x_{4}) \succeq O \ (i = 1, 2, 3), \\ (1, x_{i}, x_{4}, x_{i}^{2}, x_{i}x_{4}, x_{4}^{2})^{T}(1, x_{i}, x_{4}, x_{i}^{2}, x_{i}x_{4}, x_{4}^{2}) \succeq O \ (i = 1, 2, 3). \end{array}$

Represent poly.SDP as

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

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

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

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- Various numerical methods have been developed for (nonlinear) PDEs.
- Is SDP relaxation of POPs useful in solving PDEs?
- We are not sure how far we can go; so far only small size PDEs with at most two independent variables and two unknown functions.
- Challenge to PDEs using SDP relaxation of POPs.

Basic idea of solving a PDE by using SDP relaxation of POPs.

PDE with some boundary conditions such as Dirichlet, Neumann and periodic conditions

Assump. **PDE** is described as "a mult. poly. equation." in unknown functions and their derivatives for each fixed independent variables.

Example 1 (A nonlinear elliptic equation with an inhomogeneous term): $u_{xx}(x,y) + u_{yy}(x,y) + 22u(x,y)(1 - u(x,y)^2) + 5\sin(\pi x)\sin(2\pi y) = 0,$ $u(0,y) = u(1,y) = u(x,0) = u(x,1) = 0, \ \forall (x,y) \in [0,1] \times [0,1].$

Example 2 - A nonlinear wave equation with a periodic condition.

Examples 3 & 4

- 2 unknown cases with Dirichlet and Neumann conditions, respectively (modifications of the Ginzburg-Landau equation for superconductivity).

We will show some numerical results on these examples later.

Basic idea of solving a PDE by using SDP relaxation of POPs.

PDE with some boundary conditions such as Dirichlet, Neumann and periodic conditions

↓ discretize on finite grid points; approximate partial derivatives by finite differences

A system of polynomial equations

↓ add an objective function and/or polynomial inequality constraints

A POP (Polynomial Optimization Problem)

 \Downarrow apply SDP relaxation with \exists relaxation order r

A discretized solution of PDE

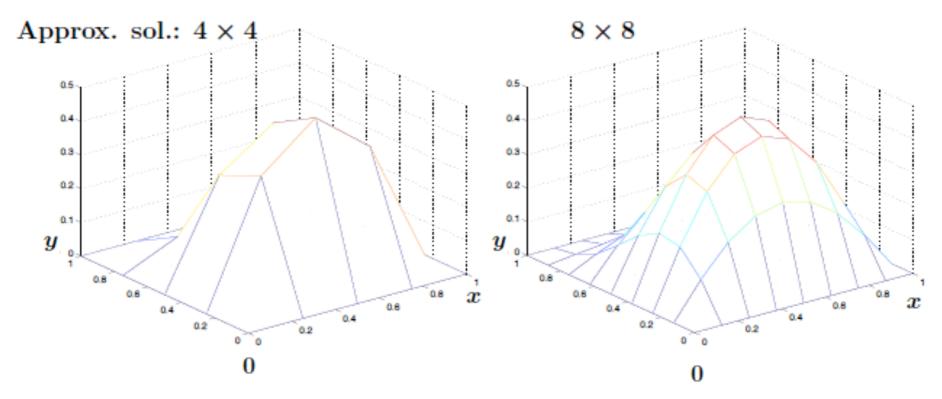
Advantage

- (a) We can add an objective function and/or polynomial inequality constraints to pick up a specific solution which we want to compute.
- (b) The system of polynomial equations induced from PDE satisfies the correlative sparsity.

But (c) Expensive, depending on a relaxation order r unknown in advance.

Example 1 (A nonlinear elliptic equation with an inhomogeneous term): $\begin{aligned} u_{xx}(x,y) + u_{yy}(x,y) + 22u(x,y)(1-u(x,y)^2) + 5\sin(\pi x)\sin(2\pi y) &= 0, \\ u(0,y) &= u(1,y) = u(x,0) = u(x,1) = 0, \ \forall (x,y) \in [0,1] \times [0,1]. \end{aligned}$

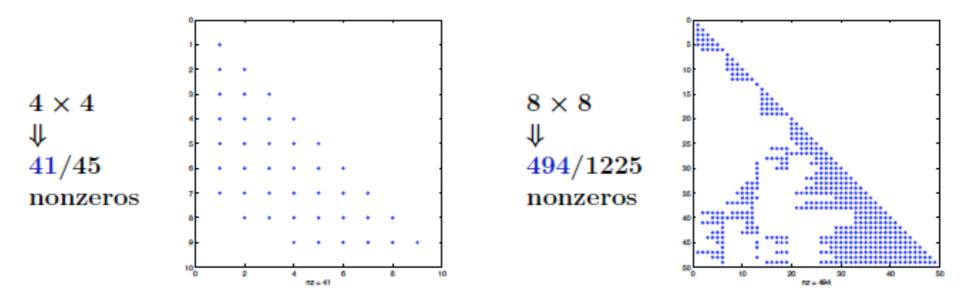
grid	# of	\mathbf{cpu}	relax.		SDP size	# of
size	var.	sec.	order \boldsymbol{r}	$\epsilon_{\rm feas}$	size of A, SeDuMi	nonzeros in A
4×4	9	0.92	2	8.4e-11	183 imes 1,506	2013
8×4	21	1.7	2	4.7e-10	544 imes 4,807	6,380
8×8	49	33.1	2	1.5e-10	$3,\!642 imes 31,\!907$	$42,\!425$



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A sparse Cholesky factorization of the CSP matrix under a symmetric minimum degree ordering:



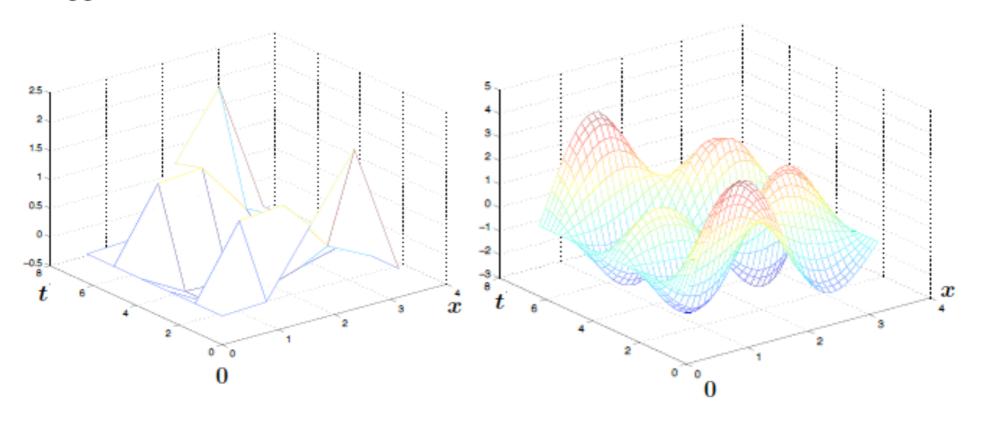
Example 2 (A nonlinear wave equation on $[0,\pi] \times [0,2\pi]$): $-u_{xx}(x,t) + u_{tt}(x,t) + u(x,t)(1 - u(x,t)) + 0.2\sin(x) = 0,$ $u(0,t) = u(\pi,t) = 0, \ \forall t \in [0,2\pi], \ u(x,0) = u(x,2\pi), \ \forall x \in [0,\pi].$

	grid	# of	cpu	relax.		SDP size	# of
	\mathbf{size}	var.	sec.	order \boldsymbol{r}	$\epsilon_{\rm feas}$	size of A, SeDuMi	nonzeros in A
4	4×5	15	159.5	2	9.4e-10	$2,616 \times 36,029$	43,689



Approx. sol.: $4 \times 5 \implies$

 32×40



Example 2 (A nonlinear wave equation on $[0, \pi] \times [0, 2\pi]$): $-u_{xx}(x, t) + u_{tt}(x, t) + u(x, t)(1 - u(x, t)) + 0.2 \sin(x) = 0,$ $u(0, t) = u(\pi, t) = 0, \ \forall t \in [0, 2\pi], \ u(x, 0) = u(x, 2\pi), \ \forall x \in [0, \pi].$

grid	# of	cpu	relax.		SDP size	# of
size	var.	sec.	order r	$\epsilon_{\rm feas}$	size of A, SeDuMi	nonzeros in A
4×5					$2,616 \times 36,029$	43,689

 32×40

"Multigrid technique"

- 1. A rough approx. sol. u^0 for 8×5 case by interpolation to the solution of 4×5 case.
- 2-a. Sparse SDP relax. to 8×5 case with obj.funct. $||u - u^0||^2 \downarrow$, $u_k^0 - \epsilon \le u_k \le u^0 + \epsilon, \forall k$ $(\epsilon = 0.5)$, and r = 1, or
- 2-b. Newton meth. to 8×5 case with the init. pt. u^0 .

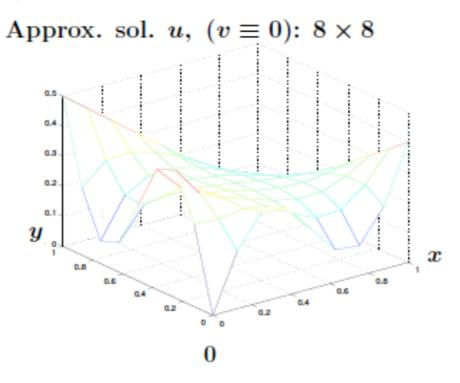
(2-a is more expensive, but robust(?))

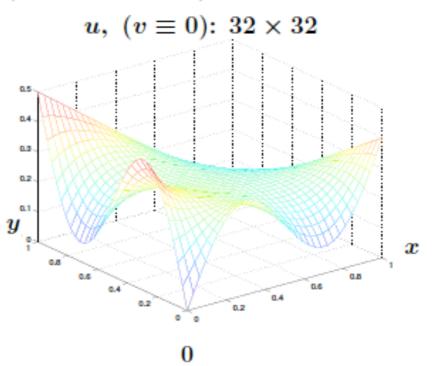
• $4 \times 5 \Rightarrow 8 \times 5 \Rightarrow 8 \times 10 \cdots 32 \times 40$

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Ε	Example 3 (2 unknown case on $[0, 1] \times [0, 1]$, Dirichlet condition):										
	$u_{xx}(x,y) + u_{yy}(x,y) + u(x,y)(1 - u(x,y)^{\rho} - v(x,y)^{\rho}) = 0,$										
	$v_{xx}(x,y) + v_{yy}(x,y) + v(x,y)(1 - u(x,y)^{\rho} - v(x,y)^{\rho}) = 0,$										
	$u(0,y) = 0.5y + 0.3\sin(2\pi y), \ u(1,y) = 0.4 - 0.4y, \ \forall y \in [0,1],$										
	u(:	x, 0) =	= 0.4x +	$-0.2\sin(2)$	$(2\pi x), u($	(x,1) = 0.5 - 0.5x,	$\forall x \in [0,1],$				
	$v(x,0)=v(x,1)=v(0,y)=v(1,y)=0,\;\forall x\in[0,1],\;\forall y\in[0,1].$										
	grid # of cpu relax. SDP size # of										
ρ	$ ho$ size var. sec. order r ϵ_{feas} size of A, SeDuMi nonzeros in A										
1	8×8	98	19.0	1	6.2e-07	$1,999 \times 21,377$	21,865				
2	8×8	98	10,959	2	9.4 e- 07	$25,\!699 \times 235,\!471$	319,306				

 $\rho=2$ case, Sparse SDP relaxation + 2.b (Newton Method)

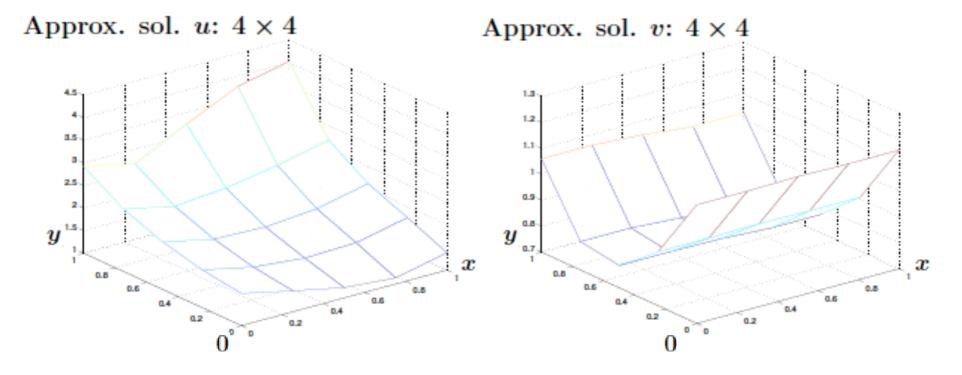




Example 4 (2 unknown case on $[0,1] \times [0,1]$, Neumann condition):

$$\begin{split} & u_{xx}(x,y) + u_{yy}(x,y) + u(x,y)(1 - u(x,y)^2 - v(x,y)^2) = 0, \\ & v_{xx}(x,y) + v_{yy}(x,y) + v(x,y)(1 - u(x,y)^2 - v(x,y)^2) = 0, \\ & u_x(0,y) = -1, \ u_x(1,y) = 1, \ \forall y \in [0,1], \\ & u_y(x,0) = 2x, \ u_y(x,1) = x + 5\sin(\pi x/2), \ \forall x \in [0,1], \\ & v_x(0,y) = 0, \ v_x(1,y) = 0, \ \forall y \in [0,1], \\ & v_y(x,0) = -1, \ v_y(x,1) = 1, \ \forall x \in [0,1]. \end{split}$$

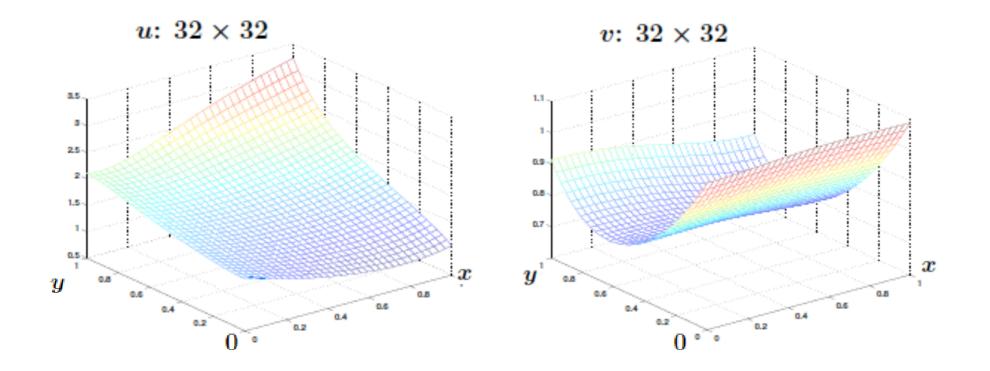
grid	# of	\mathbf{cpu}	relax.		SDP size	# of
size	var.	sec.	order \boldsymbol{r}	$\epsilon_{\rm feas}$	size of A, SeDuMi	nonzeros in A
4×4	18	6.9	2	1.7e-10	$979 imes9,\!165$	12,598



Example 4 (2 unknown case on $[0, 1] \times [0, 1]$, Neumann condition):

$$\begin{aligned} u_{xx}(x,y) + u_{yy}(x,y) + u(x,y)(1 - u(x,y)^2 - v(x,y)^2) &= 0, \\ v_{xx}(x,y) + v_{yy}(x,y) + v(x,y)(1 - u(x,y)^2 - v(x,y)^2) &= 0, \\ u_x(0,y) &= -1, \ u_x(1,y) = 1, \ \forall y \in [0,1], \\ u_y(x,0) &= 2x, \ u_y(x,1) = x + 5\sin(\pi x/2), \ \forall x \in [0,1], \\ v_x(0,y) &= 0, \ v_x(1,y) = 0, \ \forall y \in [0,1], \\ v_y(x,0) &= -1, \ v_y(x,1) = 1, \ \forall x \in [0,1]. \end{aligned}$$

(Sparse SDP relaxation + 2.b (Newton Method))



- 1. How do we formulate structured sparsity?
 - 1-1. Unconstrained cases.
 - 1-2. Constrained and linear objective function cases.
- 2. Sparse SDP relaxation of constrained POPs.
- 3. Applications to PDEs (partial differential equations).
- 4. Concluding remarks.

Some difficulties in SDP relaxation of POPs

- (a) Sparse SDP relaxation problems of a POP are sometimes difficult to solve accurately (by the primal-dual interior-point method).
- (b) The efficiency of the (sparse) SDP relaxation of a POP depends on the relaxation order r which is required to get an accurate optimal solution but is unknown in advance.

A difficulty in application of the sparse SDP relaxation to PDEs
(c) A polynomial system induced from a PDE is not c-sparse enough to process finer grid discretization.

₩

• More powerful and stable software to solve SDPs.

• Some additional techniques.

Thank you!