

## 疎半正定値計画緩和法による偏微分方程式の数値解法

Martin Mevissen (ETH → 東京工業大学),

小島政和 (東京工業大学),

Jiawang Nie (University of California at San Diego),

高山信毅 (神戸大学) [発表者]

## 代数方程式、不等式系と疎半正定値計画緩和法 (sparse semi-definite programming relaxation)

連立代数方程式系を解くための一般的方法

1. Newton 法 : 大域的に解けない. 全部の根の求解はむつかしい.
2. Gröbner 基底法 : 厳密算法. 大きい問題を解くのが大変. 現状では 6~10 変数程度.
3. 多面体 homotopy 法: Gröbner 基底法よりも大きいサイズの問題を解ける. 確率 1 算法. 複素数解を全部求めてしまう (並列化も容易).

しかし偏微分方程式系の差分化から生じるような方程式系に適用するには全部の解を求めてしまうので不向きである.

## 差分化より生じる代数方程式系

$u(x)$  を未知関数,  $a$  をパラメータとする次の非線形常微分方程式の境界値問題

$$xu'' + u' + axu(1 - u) = 0, \quad u(1/2) = u(1) = 0.$$

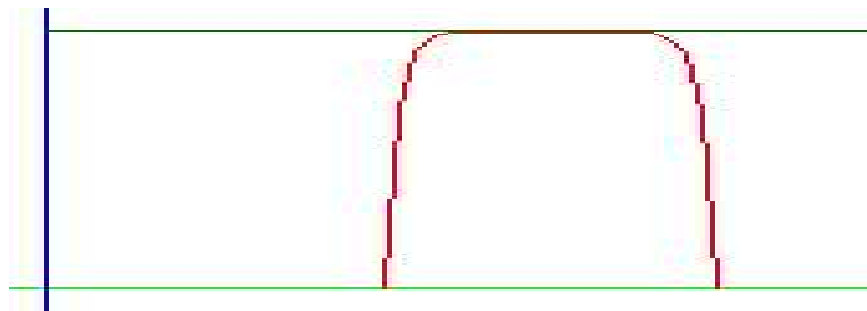
を差分法で解くことを考えよう. さて区間  $[1/2, 1]$  を4つの区間に等しく分割してこの方程式を差分法で書き下す.

$$\begin{aligned} (1/2 + ih) \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} \\ + \frac{u_{i+1} - u_i}{h} + a(1/2 + ih)u_i(1 - u_i) = 0, \\ i = 1, 2, 3, \\ u_0 = 0, u_4 = 0, h = \frac{1}{2 \cdot 4} \end{aligned} \tag{1}$$

なる3つの方程式を得る (非線型連立代数方程式系).

複素数解の個数: 8.

$a = 2000$ . 非負実数解. 2 つ.  $u_i \geq 0$ .



実数解のみをとらえ、また適当な不等式制約を加えることにより、解空間を狭めることが可能となる方法がないか？

### 疎半正定値計画緩和法

- J.Lasserre, Global Optimization with Polynomials and the Problem of Moments, SIAM J. Optim, (2001). [収束条件]
- H.Waki, S.Kim, M.Kojima, M.Muramatsu, Sums of Squares and Semidefinite Programming Relaxations for Polynomial Optimization Problems with Structured Sparsity, SIAM J. Optim, (2006)
- J.Lasserre, Semidefinite Relaxation in Polynomial Optimization with Sparsity, to appear [収束条件]
- ソフトウェア: matlab 上の SeDuMi, SparsePOP

$$\begin{aligned}
 \text{(LP)} \quad & \min \quad \mathbf{a}_0 \cdot \mathbf{x} \\
 & \text{sub.to} \quad \mathbf{a}_p \cdot \mathbf{x} = b_p \quad (p = 1, \dots, m), \quad \mathbb{R}^n \ni \mathbf{x} \geq \mathbf{0}.
 \end{aligned}$$

$$\begin{aligned}
 \text{(SDP)} \quad & \min \quad \mathbf{A}_0 \bullet \mathbf{X} \\
 & \text{sub.to} \quad \mathbf{A}_p \bullet \mathbf{X} = b_p \quad (p = 1, \dots, m), \quad \mathbb{S}^n \ni \mathbf{X} \succeq \mathbf{O}.
 \end{aligned}$$

$$\uparrow \left\{ \begin{array}{l} m = 2, n = 2, b_1 = 7, b_2 = 9, X_{12} = X_{21}, \\ \mathbf{X} = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix}, \mathbf{A}_0 = \begin{pmatrix} -1 & -1 \\ -1 & -5 \end{pmatrix}, \\ \mathbf{A}_1 = \begin{pmatrix} 2 & 1.5 \\ 1.5 & 1 \end{pmatrix}, \mathbf{A}_2 = \begin{pmatrix} 2 & 0.5 \\ 0.5 & 3 \end{pmatrix}. \end{array} \right.$$

$$\begin{aligned}
 \min \quad & -X_{11} - 2X_{12} - 5X_{22} \\
 \text{sub.to} \quad & 2X_{11} + 3X_{12} + X_{22} = 7, \quad 2X_{11} + X_{12} + 3X_{22} = 9, \\
 & \begin{pmatrix} X_{11} & X_{12} \\ X_{12} & X_{22} \end{pmatrix} \succeq \mathbf{O}.
 \end{aligned}$$

例 3 の SDP 緩和 :  $f(\mathbf{x}) = -11x + 2x^2 - 3x^3 + 4x^4 \rightarrow$  最小化

Polynomial SDP  $\Updownarrow$  自明な不等式の追加

$$\begin{array}{ll} \min & f(\mathbf{x}) = -11x + 2x^2 - 3x^3 + 4x^4 \\ \text{sub.to} & \begin{pmatrix} 1 \\ x \\ x^2 \end{pmatrix} \begin{pmatrix} 1 \\ x \\ x^2 \end{pmatrix}^T \equiv \begin{pmatrix} 1 & x & x^2 \\ x & x^2 & x^3 \\ x^2 & x^3 & x^4 \end{pmatrix} \succeq \mathbf{O}. \end{array}$$

線形化  $\Updownarrow$  各  $x^\alpha$  を  $y_\alpha$  で置き換える

$$\begin{array}{ll} \min & -11y_1 + 2y_2 - 3y_3 + 4y_4 \\ \text{sub.to} & \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} y_1 + \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} y_2 \\ & + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} y_3 + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} y_4 \succeq \mathbf{O}. \end{array}$$

$$\text{例: } \min f_0(\mathbf{x}) = \sum_{i=1}^4 (-x_i^3)$$

$$\text{s.t. } f_j(x_j, x_4) = -j \times x_j^2 - x_4^2 + 1 \geq 0 \quad (j = 1, 2, 3).$$

$$\omega = 2 \geq \lceil \{\max\{\text{deg } f_j(\mathbf{x})/2 \ (j = 0, 1, \dots, 3)\}\rceil, \quad r_j = 1$$

**sparse SDP 緩和  $\omega$  — Primal approach : 以下の展開・線形化 :**

$$\min f_0(\mathbf{x})$$

$$\text{s.t. } \begin{pmatrix} 1 \\ x_j \\ x_4 \end{pmatrix} \begin{pmatrix} 1 \\ x_j \\ x_4 \end{pmatrix}^T f_j(x_j, x_4) \succeq \mathbf{O} \quad (j = 1, 2, 3),$$

$$\begin{pmatrix} 1 \\ x_i \\ x_4 \\ x_i^2 \\ x_i x_4 \\ x_4^2 \end{pmatrix} \begin{pmatrix} 1 \\ x_i \\ x_4 \\ x_i^2 \\ x_i x_4 \\ x_4^2 \end{pmatrix}^T \succeq \mathbf{O} \quad (i = 1, 2, 3).$$



## 非線型波動方程式, $y$ について周期的

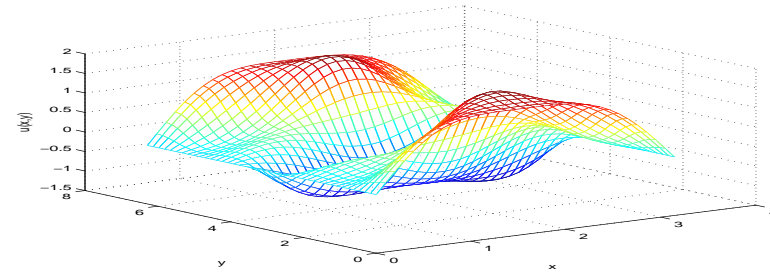
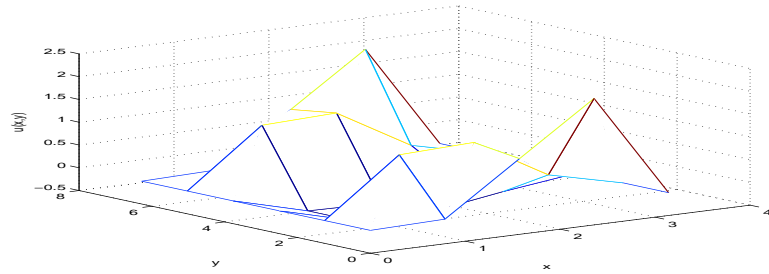
$$\begin{aligned}
 & -u_{xx} + u_{yy} + u(1-u) + 0.2 \sin(2x) = 0 \\
 & \quad \forall (x, y) \in [0, \pi] \times [0, 2\pi], \\
 & u(0, y) = u(\pi, y) = 0 \quad \forall y \in [0, 2\pi], \\
 & u(x, 0) = u(x, 2\pi) \quad \forall x \in [0, \pi], \\
 & -3 \leq u(x, y) \leq 3 \quad \forall (x, y) \in [0, \pi] \times [0, 2\pi].
 \end{aligned} \tag{1}$$

目的関数

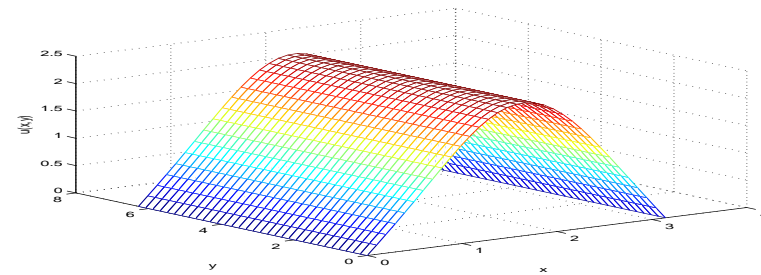
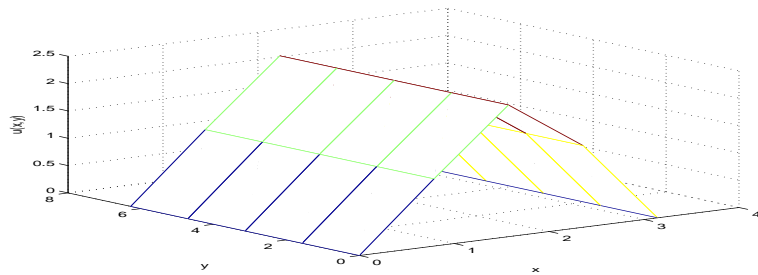
$$F_1(u) = \sum_{i,j} \sigma_{i,j} u_{i,j}, \quad F_2(u) = \sum_{i,j} u_{i,j},$$

係数  $\sigma_{i,j}$  ( $i = 1, \dots, N_x, j = 1, \dots, N_y$ ) は  $[-0.5, 0.5]$  の範囲の乱数.

strategy	$\omega$	$N_N$	$N_x$	$N_y$	$\epsilon_{feas}$	$t_C$	$m_e$
initial SPOP, obj. $F_1$	2	5	5	6	-3e-9	151	7
grid-refining 3b		5	33	40	-1e-6	427	415
initial SPOP, obj. $F_2$	2	5	5	5	-5e-10	19	3
grid-refining 3b		5	33	33	-4e-9	86	411



Solution for nonlinear wave equation (1), objective  $F_1$



Solution for nonlinear wave equation (1), objective  $F_2$

三村の方程式の定常解 M. Mimura, Asymptotic Behaviors of a Parabolic System Related to a Planktonic Prey and Predator Model, SIAM Journal on Applied Mathematics, 37 (1979), no. 3, pp. 499-512.

$$\begin{aligned}
 \frac{1}{20} u''(x) + \frac{1}{9} (35 + 16u(x) - u(x)^2) u(x) - u(x)v(x) &= 0, \\
 4 v''(x) - \left(1 + \frac{2}{5}v(x)\right) v(x) + u(x)v(x) &= 0, \\
 \dot{u}(0) = \dot{u}(5) = \dot{v}(0) = \dot{v}(5) &= 0, \\
 0 \leq u(x) \leq 14, \\
 0 \leq v(x) \leq 14, \\
 \forall x \in [0, 5].
 \end{aligned} \tag{1}$$

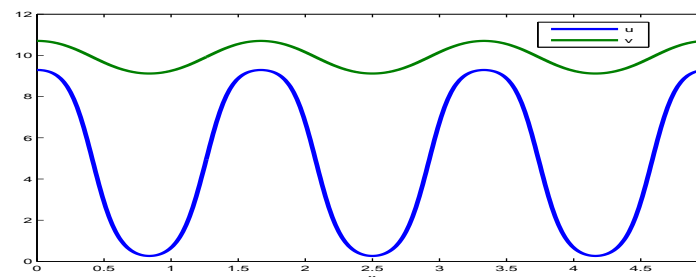
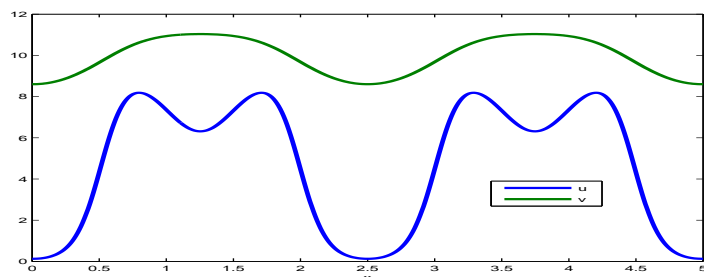
$$\begin{aligned}
 F_1(u, v) &= u_{\lceil \frac{N}{2} \rceil}, \quad F_2(u, v) = \sum_{i=1}^N u_i, \quad F_3(u, v) = u_2, \\
 F_4(u, v) &= u_{N-1}, \quad F_5(u, v) = u_2 + u_{N-1}.
 \end{aligned} \tag{2}$$

$u_2$	$u_3$	$u_4$	$v_2$	$v_3$	$v_4$	obj	ubd <sub>2</sub>	ubd <sub>4</sub>	$\epsilon_{\text{feas}}$
4.623	6.787	0.939	9.748	10.799	5.659	$F_3$	5	1.5	-2e-6
4.607	6.930	0.259	9.737	10.831	5.166	$F_3$	5	0.5	-3e-6
0.259	6.930	4.607	5.166	10.831	9.737	$F_2$	0.5	6	-5e-7
5.683	2.971	5.683	10.388	8.248	10.388	$F_3$	6	6	-1e-6
6.274	0.177	6.274	10.638	6.404	10.638	$F_3$	7	7	-7e-5
0.970	7.812	0.970	5.735	10.94	5.735	$F_3$	2	2	-2e-7
0.297	7.932	0.966	5.230	10.94	5.729	$F_4$	0.5	2	-1e-7
0.962	7.932	0.297	5.729	10.94	5.230	$F_3$	2	0.5	-2e-7
0.304	8.045	0.304	5.234	10.94	5.234	$F_1$	14	14	-5e-9
0.939	6.787	4.623	5.659	10.80	9.748	$F_4$	2	14	-1e-3
5.000	5.000	5.000	10.000	10.000	10.000	$F_2$	14	14	-2e-7

SparsePOP solutions for (1) with discretization  $N = 5$  grid points.  $\omega = 3$ . ubd=upper bound. 182個の複素数解 (by PHoM).

strategy	$N_N$	N	solution	$\epsilon_{\text{feas}}$	$\epsilon_{\text{scaled}}$	$m_e$
init SPOP with $F_2$	10	7		-1e-8	-5e-9	-2.2
mGrid 3b	10	13		-1e+6	-2e+0	2.7
mGrid 3b	10	25		-6e-5	-2e-6	-0.9
mGrid 3b	10	193		-9e-2	-2e-4	0.3
mGrid 3b	10	385	2teeth	-1e-1	-5e-5	0.2
init SPOP with $F_5$	10	26		-3e+0	-1e-1	2.09
mGrid 3b	10	51		-8e-1	-5e-2	-0.18
mGrid 3b	10	101		-6e-12	-2e-15	-0.07
mGrid 3b	10	401	2,3peak	-1e-10	-6e-16	-0.07

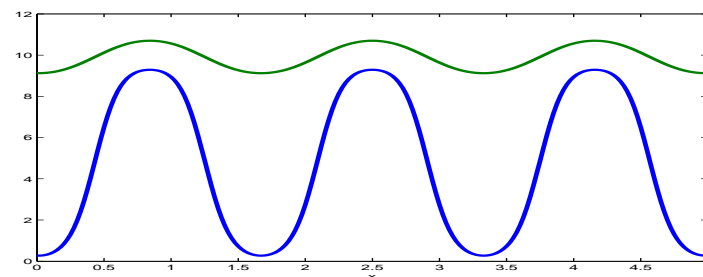
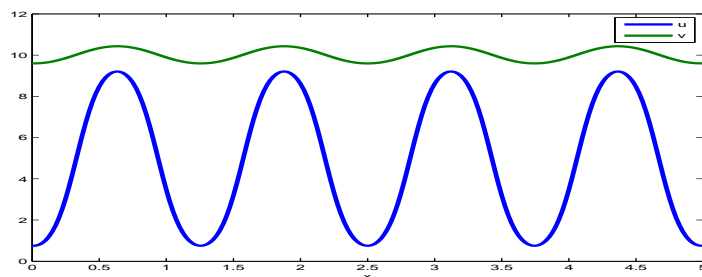
Results of grid-refining strategy 3b for solutions 2teeth and 2,3peak.  $N_N$  は Newton step.



不安定解 (2teeth) (左), 安定解 (2,3peak) (右)

strategy	obj	$N_N$	N	solution	$\epsilon_{\text{feas}}$	$\epsilon_{\text{scaled}}$	$m_e$	$t_C$
init SPOP	$F_5$	10	26		-3e+1	-2e-1	2.09	203
mGrid 3a/b	$F_M$	10	51		-8e-1	-4e-2	-0.05	224
mGrid 3a/b	$F_M$	10	101		-3e-2	-4e-4	-0.02	383
mGrid 3a/b	$F_M$	10	201	4peak	-1e-8	-3e-11	-0.02	1082
init SPOP	$F_1$	10	26		-1e-1	-1e-3	-0.12	270
mGrid 3a/b	$F_M$	10	51		-1e-1	-4e-3	-0.08	348
mGrid 3a/b	$F_M$	10	101		-9e-12	-3e-16	-0.08	511
mGrid 3a/b	$F_M$	10	201	3peak	-5e-9	-2e-11	-0.07	1192

Results for grid-refining strategy 3a/3b (3/a:  $\omega_1 = 3, \omega_2 = 2$ )

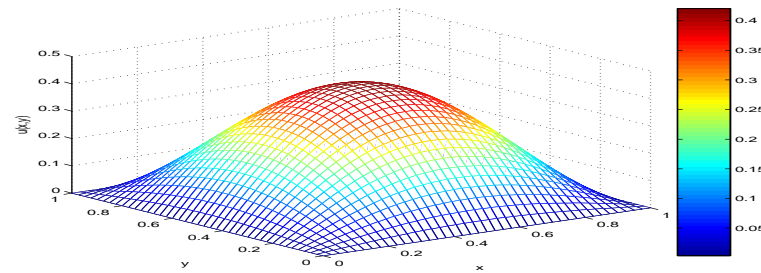
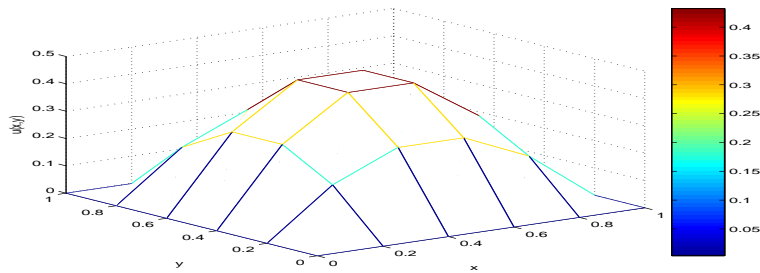


安定解 (grid-refining strategy 3a/b)

1. M.Mevisse, M.Kojima, J.W.Nie, N.Takayama, Solving Partial Differential Equations via Sparse SDP Relaxations, この講演のプレプリント <http://www.is.titech.ac.jp/~kojima>
2. <http://fe.math.kobe-u.ac.jp/Movies/cm/2007-07-kojima.html> 小島政和, 半正定値計画 — 多項式最適化への応用 (入門用サーベイビデオ)

## 非線型楕円型方程式

$$\begin{aligned}
 u_{xx}(x, y) + u_{yy}(x, y) + \lambda u(x, y) (1 - u(x, y)^2) &= 0 \quad \forall (x, y) \in [0, 1]^2, \\
 u(x, y) &= 0 \quad \forall (x, y) \in \partial[0, 1]^2, \\
 0 \leq u(x, y) &\leq 1 \quad \forall (x, y) \in [0, 1]^2,
 \end{aligned}
 \tag{1}$$



Solution for (1) if  $\lambda = 22$ ,  $(N_x, N_y) = (6, 6)$  and  $(N_x, N_y) = (41, 41)$ .  $\Delta x = 1/(N_x - 1)$



$F(u) = \sum_{i,j} u_{i,j}$  : 目的関数

微分方程式の差分化を制約条件に

$\omega = 2$ (relaxation order),  $N_x = N_y = 8$  ( $6^2$  変数): SparsePOP での近似解.

時間: 253.88s

以後 SparsePOP での近似解を種にして grid refining で  $41 \times 41$ -grid まで.

$W[u] = \int_D u_x^2 + u_y^2 - \lambda(\frac{u^2}{2} - \frac{u^4}{4}) dx dy$  : 目的関数  $F(u)$  はこれの差分化. 微分方程式の差分化を制約条件からはずす.

$\omega = 2$ (relaxation order),  $N_x = N_y = 9$  ( $7^2$  変数): SparsePOP での近似解.

時間: 67.22 s

緩和次数 (relaxation order) をあげると計算が困難になっていくので、目的関数の次数が高いのは一般に不利だがこの場合は、エネルギー積分を最小化の方が早い.