多项式优化入门

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课程内容

1. 半定规划
2. 平方和理论
3. 测度和矩
4. 矩-平方和松弛分层
5. 项稀疏（TS）
6. 变量稀疏（CS）
7. 扩展与应用
8. 软件与实验

求解矩-平方和松弛

	矩松弛	SOS 松弛
n_{sdp}	$\binom{n+r}{r}$	$\binom{n+r}{r}$
m_{sdp}	$\frac{1}{2}\binom{n+r}{r}\left(\binom{n+r}{r}+1\right)-\binom{n+2r}{2r}$	$\binom{n+2r}{2r}$

$$n = 20$$

r	n_{sdp}	矩松弛	SOS 松弛
1	21	0	231
2	231	16,170	10,626
3	1771	1,338,876	230,230

SOS 松弛问题的结构

$$
\begin{cases}
\sup\limits_{X_1, X_2, x} & c^\intercal x \\
\text{s.t.} & \langle A_i, X_1 \rangle + \langle B_i, X_2 \rangle + d_i^\intercal x = b_i, \quad i = 1, \ldots, m \\
 & X_1, X_2 \succeq 0
\end{cases}
$$

- 正交性：$\langle A_i, A_j \rangle = 0, \quad \forall i \neq j$
- 稀疏性：A_i, B_i 是稀疏矩阵
- 低秩性：$\operatorname{rank}(X_1^*)) \ll n$

➤ 高效 ADMM 算法

矩松弛问题的结构

$$\begin{cases} \inf\limits_{X \in \mathbb{R}^{n\times n}} & \langle C, X\rangle \\ \text{s.t.} & \langle A_i, X\rangle = b_i, \quad i = 1, \dots, m \\ & X \succeq 0 \end{cases}$$

- 低秩性：$\text{rank}(X^*) \ll n$
- 单位对角元：$\text{diag}(X) = \mathbf{1}$
- 单位迹：$\text{tr}(X) = 1$

基于流形优化求解低秩结构化 SDP

- **低秩性**： $\mathrm{rank}(X^*) \ll n \rightsquigarrow X = YY^\intercal,\ Y \in \mathbb{R}^{n \times p}$ **Burer-Monteiro**
  - ➤ $\mathcal{N} := \{Y \in \mathbb{R}^{n \times p}\}$
- **单位对角元**： $\mathrm{diag}(x) = \mathbf{1}$
  - ➤ $\mathcal{N} := \{Y \in \mathbb{R}^{n \times p} \mid \|Y(k,:)\| = 1, k = 1, \ldots, n\}$
- **单位迹**： $\mathrm{tr}(x) = 1$
  - ➤ $\mathcal{N} := \{Y \in \mathbb{R}^{n \times p} \mid \|Y\|_F = 1\}$

➤ J. Wang and L. Hu, Solving low-rank semidefinite programs via manifold optimization. arXiv preprint arXiv:2303.01722, 2023.

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复 SDP 的实 SDP 等价转化

$$
\begin{cases}
\sup\limits_{H\in\mathbb{C}^{n\times n}} & \langle C, H\rangle \\
\text{s.t.} & \mathscr{A}(H) = b \\
& H \succeq 0
\end{cases}
$$

$$
\Longleftrightarrow
\begin{cases}
\sup\limits_{Y\in\mathbb{R}^{2n\times 2n}} & \langle C_R, H_R\rangle + \langle C_I, H_I\rangle \\
\text{s.t.} & \mathscr{A}_R(H_R) + \mathscr{A}_I(H_I) = b_R \\
& \mathscr{A}_R(H_I) - \mathscr{A}_I(H_R) = b_I \\
& Y = \begin{bmatrix} H_R & -H_I \\ H_I & H_R \end{bmatrix} \succeq 0
\end{cases}
$$

复 SDP 的实 SDP 等价转化

$$
\Longleftrightarrow \begin{cases}
\sup\limits_{X \in \mathbb{R}^{2n \times 2n}} & \langle C_R, X_1 + X_2 \rangle + \langle C_I, X_3 - X_3^\intercal \rangle \\
\text{s.t.} & \mathscr{A}_R(X_1 + X_2) + \mathscr{A}_I(X_3 - X_3^\intercal) = b_R \\
& \mathscr{A}_R(X_3 - X_3^\intercal) - \mathscr{A}_I(X_1 + X_2) = b_I \\
& X = \begin{bmatrix} X_1 & X_3^\intercal \\ X_3 & X_2 \end{bmatrix} \succeq 0
\end{cases}
$$

加强实矩松弛

$$\rho'_r := \begin{cases} \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & y_{\mathbf{0}} = 1 \\ & \mathbf{M}^{\mathbb{R}}_{r-d_i}(g_i\mathbf{y}) \succeq 0, \quad i \in [m] \\ & \begin{bmatrix} \mathbf{M}^{\mathbb{R}}_r(\mathbf{y}) & \mathbf{M}^{\mathbb{R}}_r(x_i\mathbf{y}) \\ \mathbf{M}^{\mathbb{R}}_r(x_i\mathbf{y}) & \mathbf{M}^{\mathbb{R}}_r(x_i^2\mathbf{y}) \end{bmatrix} \succeq 0, \quad i \in [n] \end{cases}$$

- $\rho_r \leq \rho'_r \leq \rho_{r+1}$

加强实矩松弛

$$\rho_r' := \begin{cases} \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & y_{\mathbf{0}} = 1 \\ & \mathbf{M}^{\mathbb{R}}_{r-d_i}(g_i\mathbf{y}) \succeq 0, \quad i \in [m] \\ & \begin{bmatrix} \mathbf{M}^{\mathbb{R}}_r(\mathbf{y}) & \mathbf{M}^{\mathbb{R}}_r(x_i\mathbf{y}) \\ \mathbf{M}^{\mathbb{R}}_r(x_i\mathbf{y}) & \mathbf{M}^{\mathbb{R}}_r(x_i^2\mathbf{y}) \end{bmatrix} \succeq 0, \quad i \in [n] \end{cases}$$

- $\rho_r \le \rho_r' \le \rho_{r+1}$

加强复矩松弛

$$\tau'_{r,s} := \begin{cases} \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & \mathbf{M}_r^{\mathbb{C}}(\mathbf{y}) \succeq 0, \quad y_{\mathbf{0},\mathbf{0}} = 1 \\ & \mathbf{M}_{r-d_i}^{\mathbb{C}}(g_i\mathbf{y}) \succeq 0, \quad i \in [m] \\ & \begin{bmatrix} \mathbf{M}_s^{\mathbb{C}}(\mathbf{y}) & \mathbf{M}_s^{\mathbb{C}}(x_i\mathbf{y}) \\ \mathbf{M}_s^{\mathbb{C}}(\overline{x}_i\mathbf{y}) & \mathbf{M}_s^{\mathbb{C}}(|x_i|^2\mathbf{y}) \end{bmatrix} \succeq 0, \quad i \in [n] \end{cases}$$

- $\tau_r \leq \tau'_{r,s} \leq \tau'_{r,s+1}$, $\tau'_{r,s} \leq \tau'_{r+1,s}$

加强复矩松弛

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- $\tau_r \leq \tau'_{r,s} \leq \tau'_{r,s+1}$, $\tau'_{r,s} \leq \tau'_{r+1,s}$

求解大规模多项式优化


POP结构（对称性、稀疏性、商环）
结构化Moment-SOS分层
Moment-SOS性质（低秩、单位对角、常数迹、部分正交）
结构化SDP问题
大规模多项式优化全局求解

Julia 语言

- **官方网站：** **https://julialang.org**
- **中文网站：** **https://cn.julialang.org**
  - 高性能
  - 动态执行
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TSSOS、NCTSSOS、ManiSDP

- TSSOS：基于 JuMP，支持交换/复多项式优化、多项式矩阵优化、SOS 规划等

https://github.com/wangjie212/TSSOS

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相关 Julia 包

- DynamicPolynomials：定义多项式
- MultivariatePolynomials：多项式运算
- JuMP：优化建模平台
- Graphs：图操作
- CliqueTrees：计算弦扩张
- SemialgebraicSets：计算 Gröbner 基
- SymbolicWedderburn：计算群的不可约表示

TSSOS 用法

```
using TSSOS
using DynamicPolynomials
@polyvar x[1:2]
f = 1 + x[1]^4*x[2]^2 + x[1]^2*x[2]^4 - 3x[1]^2*x[2]^2 # define the objective
g = 1 - sum(x.^2) # define the inequality constraint
pop = [f, g] # define the POP
d = 3 # set a relaxation order
opt,sol,data = tssos_first(pop, x, d, numeq=0) # k = 1
opt,sol,data = tssos_higher!(data) # k > 1
opt,sol,data = cs_tssos_first(pop, x, d, numeq=0) # k = 1
opt,sol,data = cs_tssos_higher!(data) # k > 1
```

TSSOS 用法

- For large-scale POPs, it is more efficient to define the supports and coefficients directly:

$$x_1^4 x_2^2 \longrightarrow [1;1;1;1;2;2]$$

```
using TSSOS
supp = Vector{Vector{UInt16}}[[[], [1; 1; 1; 1; 2; 2], [1; 1; 2; 2; 2; 2], [1; 1; 2; 2]], [[], [1; 1], [2 ;2]]] # define the support array of the POP
coe = Vector{Float64}[[1; 1; 1; -3], [1; -1; -1]] # define the coefficient array of the POP
opt,sol,data = cs_tssos_first(supp, coe, 2, 3, numeq=0) # k = 1
opt,sol,data = cs_tssos_higher!(data) # k > 1
```

NCTSSOS 用法

```
using NCTSSOS
using DynamicPolynomials
@ncpolyvar x[1:2]
f = 2 - x[1]^2 + x[1]*x[2]^2*x[1] - x[2]^2
g1 = 4 - x[1]^2 - x[2]^2
g2 = x[1]*x[2] + x[2]*x[1] - 2
pop = [f, g1, g2]
opt,data = nctssos_first(pop, x, 2, numeq=1, TS="MD", obj="eigen", QUIET=true)
opt,data = nctssos_higher!(data, TS="MD", QUIET=true)
```

应用一：低秩矩阵补全

给定 $\{M_{ij}\}_{(i,j)\in\Omega}$：

$$\begin{cases} \inf\limits_{Z\in\mathbb{R}^{s\times s}} & \|Z\|_* \\ \text{s.t.} & Z_{ij} = M_{ij}, \quad \forall (i,j)\in\Omega \end{cases}$$

$$\Longleftrightarrow \begin{cases} \inf\limits_{X\in\mathbb{R}^{2s\times 2s}} & \mathrm{Tr}(X) \\ \text{s.t.} & \left\langle \begin{bmatrix} 0_{s\times s} & E_{ij}^\mathsf{T} \\ E_{ij} & 0_{s\times s} \end{bmatrix}, X \right\rangle = 2M_{ij}, \quad \forall (i,j)\in\Omega \\ & X = \begin{bmatrix} U & Z^\mathsf{T} \\ Z & V \end{bmatrix} \succeq 0 \end{cases}$$

应用一：低秩矩阵补全

n	m	MOSEK 10.0		SDPLR 1.03		SDPNAL+		ManiSDP	
		$\eta_{\max}$	time	$\eta_{\max}$	time	$\eta_{\max}$	time	$\eta_{\max}$	time
4000	1,318,563	-	-	1.0e-06	88.7	4.8e-08	532	3.2e-10	**48.3**
5000	1,711,980	-	-	1.2e-06	157	1.4e-09	1143	1.5e-10	**86.3**
6000	2,107,303	-	-	2.2e-07	272	2.1e-09	1883	4.7e-09	**139**
8000	2,900,179	-	-	2.1e-06	498	1.5e-08	3417	5.2e-11	**210**
10000	3,695,929	-	-	1.1e-06	800	1.4e-09	8370	1.9e-10	**369**
12000	4,493,420	-	-	7.8e-07	1310	$*$	$*$	8.3e-11	**568**

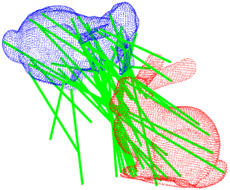
应用二：BQP 问题 $\min_{\mathbf{x}\in\{-1,1\}^d} \mathbf{x}Q\mathbf{x}^\intercal$

表: 二阶矩 SDP 松弛[1]

d	n	m	MOSEK 10.0		SDPNAL+		STRIDE		ManiSDP	
			$\eta_{\max}$	time	$\eta_{\max}$	time	$\eta_{\max}$	time	$\eta_{\max}$	time
10	66	1871	4.4e-11	0.96	3.9e-09	0.86	4.9e-13	0.87	3.2e-15	**0.45**
20	231	20,791	2.7e-11	99.7	9.4e-09	10.3	4.8e-09	5.32	1.2e-14	**1.56**
30	496	91,761	-	-	1.9e-08	173	6.1e-13	54.6	2.4e-14	**6.42**
40	861	269,781	-	-	1.6e-08	1056	5.0e-13	265	4.1e-14	**17.3**
50	1,326	629,851	-	-	$*$	$*$	8.3e-09	992	6.4e-14	**48.4**
60	1,891	1,266,971	-	-	$*$	$*$	1.3e-09	3020	7.9e-14	**101**

[1] -: 内存不足，$*$: $>$10000s

应用三：鲁棒旋转搜寻问题



$$\min_{q \in \mathcal{R}^3} \sum_{i=1}^{N} \min \left\{ \frac{\|\tilde{z}_i - q \circ \tilde{w}_i \circ q^{-1}\|^2}{\beta_i^2}, 1 \right\}$$

$$\Updownarrow$$

$$\min_{\substack{q \in \mathcal{R}^3, \\ \theta_i \in \{1,-1\}, i=1,\ldots,N}} \sum_{i=1}^{N} \frac{1+\theta_i}{2} \frac{\|\tilde{z}_i - q \circ \tilde{w}_i \circ q^{-1}\|^2}{\beta_i^2} + \frac{1-\theta_i}{2}$$

应用三：鲁棒旋转搜寻问题

表: 二阶矩 SDP 松弛

N	n	m	`MOSEK 10.0`		`SDPNAL+`		`STRIDE`		`ManiSDP`	
			$\eta_{\max}$	time	$\eta_{\max}$	time	$\eta_{\max}$	time	$\eta_{\max}$	time
50	204	8,151	4.7e-10	16.4	1.1e-02	106	2.8e-09	18.3	6.6e-09	**3.27**
100	404	31,301	2.0e-11	622	7.1e-02	642	3.1e-09	73.0	1.0e-09	**25.1**
150	604	69,451	-	-	8.0e-02	1691	4.3e-11	249	1.5e-09	**43.2**
200	804	122,601	-	-	8.3e-02	2799	1.4e-09	254	6.3e-10	**71.7**
300	1204	273901	-	-	5.2e-02	3528	4.1e-10	1176	1.1e-09	**188**
500	2004	756,501	-	-	$*$	$*$	7.1e-09	5627	5.2e-10	**601**

应用四：最近结构秩退化矩阵

给定矩阵 $L_0, \ldots, L_{2s-1} \in \mathbb{R}^{s\times s}$ 和 $\theta \in \mathbb{R}^{2s-1}$：

$$\min_{u\in\mathbb{R}^{2s-1}} \left\{ \|u-\theta\|^2 \middle| L_0 + \sum_{i=1}^{2s-1} u_i L_i \text{ is rank deficient} \right\}$$

$$\Updownarrow$$

$$\min_{z\in\mathcal{S}^{s-1}, u\in\mathbb{R}^{2s-1}} \left\{ \|u-\theta\|^2 \middle| z^\intercal \left(L_0 + \sum_{i=1}^{2s-1} u_i L_i \right) = 0 \right\}$$

应用四：最近结构秩退化矩阵

表: 二阶矩 SDP 松弛

s	n	m	MOSEK 10.0		SDPNAL+		STRIDE		ManiSDP	
			$\eta_{\max}$	time	$\eta_{\max}$	time	$\eta_{\max}$	time	$\eta_{\max}$	time
10	200	10,551	3.0e-11	22.9	7.2e-08	64.1	3.5e-12	8.97	1.0e-09	**1.26**
20	800	164,201	-	-	3.8e-03	894	3.0e-10	174	9.7e-09	**58.3**
30	1800	823,951	-	-	$*$	$*$	4.2e-10	1042	4.9e-09	**108**
40	3200	2,592,801	-	-	$*$	$*$	$*$	$*$	4.4e-09	**1984**

应用五：多相码设计

- **多相码集**：一组单位模复数 $z_1, \ldots, z_n \in \mathbb{C}$
- **非周期自相关函数**： $A(j) = \sum_{i=1}^{n-j} z_i \bar{z}_{i+j}, j = 1, \ldots, n-2$

$$\inf_{\mathbf{z} \in \mathbb{C}^n} \left\{ \max_{1 \le j \le n-2} |A(j)| \text{ s.t. } |z_i|^2 = 1, i = 1, \ldots, n \right\}$$

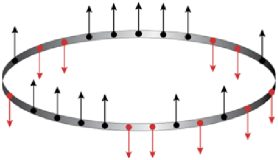
$$\rightsquigarrow \begin{cases} \inf\limits_{(\mathbf{z},u) \in \mathbb{C}^{n+1}} & |u|^2 \\ \text{s.t.} & |A(j)|^2 \le |u|^2, \quad j = 1, \ldots, n-2, \\ & |z_i|^2 = 1, \quad i = 1, \ldots, n. \end{cases}$$

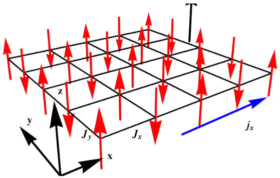
应用五：多相码设计

表: $r = 4$

n	opt	time	n	opt	time
4	0.5000*	0.01	10	0.5805	2.30
5	0.7703*	0.02	11	0.4943	6.37
6	1.0000*	0.05	12	0.4928	19.3
7	0.5219*	0.14	13	0.4189	105
8	0.6483*	0.37	14	0.3309	324
9	0.1119*	1.03	15	0.3098	1096

应用六：量子多体系统的基态能量





☞ 计算基态能量：QMA-hard

应用六：量子多体系统的基态能量

- 自旋-$\frac{1}{2}$ 粒子
- Pauli 矩阵

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^y = \begin{bmatrix} 0 & -\mathbf{i} \\ \mathbf{i} & 0 \end{bmatrix}, \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- $a \in \{x, y, z\}, \quad i, N \in \mathbb{N}$

$$\sigma_i^a = \underbrace{I_2 \otimes \cdots \otimes I_2}_{i-1} \otimes \sigma^a \otimes \underbrace{I_2 \otimes \cdots \otimes I_2}_{N-i} \in M_2(\mathbb{C})^{\otimes N} = M_{2^N}(\mathbb{C})$$

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- Pauli 矩阵

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- $a \in \{x, y, z\}$, $i, N \in \mathbb{N}$

$$\sigma_i^a = \underbrace{I_2 \otimes \cdots \otimes I_2}_{i-1} \otimes \sigma^a \otimes \underbrace{I_2 \otimes \cdots \otimes I_2}_{N-i} \in M_2(\mathbb{C})^{\otimes N} = M_{2^N}(\mathbb{C})$$

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- 自旋-$\frac{1}{2}$ 粒子
- Pauli 矩阵

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^y = \begin{bmatrix} 0 & -\mathbf{i} \\ \mathbf{i} & 0 \end{bmatrix}, \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- $a \in \{x, y, z\}$, $i, N \in \mathbb{N}$

$$\sigma_i^a = \underbrace{I_2 \otimes \cdots \otimes I_2}_{i-1} \otimes \sigma^a \otimes \underbrace{I_2 \otimes \cdots \otimes I_2}_{N-i} \in M_2(\mathbb{C})^{\otimes N} = M_{2^N}(\mathbb{C})$$

应用六：量子多体系统的基态能量

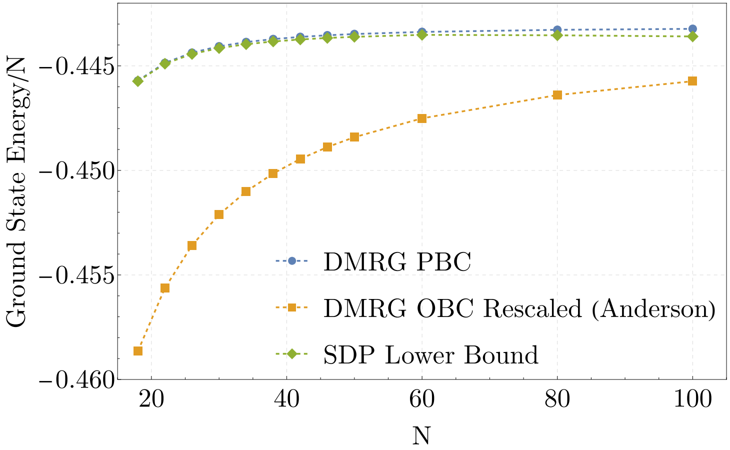
考虑一维 Heisenberg 模型：

$$
\begin{cases}
\min\limits_{\{|\psi\rangle,\sigma_i^a\}} & \frac{1}{4}\sum_{i=1}^{N}\sum_{a\in\{x,y,z\}}\langle\psi|\sigma_i^a\sigma_{i+1}^a|\psi\rangle \\
\text{s.t.} & (\sigma_i^a)^2 = 1, \quad i = 1,\ldots,N, a\in\{x,y,z\}, \\
& \sigma_i^x\sigma_i^y = \mathbf{i}\sigma_i^z, \sigma_i^y\sigma_i^z = \mathbf{i}\sigma_i^x, \sigma_i^z\sigma_i^x = \mathbf{i}\sigma_i^y, \quad i = 1,\ldots,N, \\
& \sigma_i^y\sigma_i^x = -\mathbf{i}\sigma_i^z, \sigma_i^z\sigma_i^y = -\mathbf{i}\sigma_i^x, \sigma_i^x\sigma_i^z = -\mathbf{i}\sigma_i^y, \quad i = 1,\ldots,N, \\
& \sigma_i^a\sigma_j^b = \sigma_j^b\sigma_i^a, \quad 1\le i\ne j\le N, a,b\in\{x,y,z\}.
\end{cases}
$$

应用六：量子多体系统的基态能量

1. 商环
2. 稀疏性
3. 符号对称性
4. 平移对称性
5. 置换对称性
6. 镜像对称性

应用六：量子多体系统的基态能量



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