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

广义矩问题

$$
f_{\min} := \begin{cases} \inf\limits_{\mu \in \mathcal{M}(S)_+} & \int_S f(\mathbf{x}) \mathrm{d}\mu \\ \text{s.t.} & \int_S h_j(\mathbf{x}) \mathrm{d}\mu = \gamma_j, \quad j \in \Gamma \end{cases}
$$

$$
\Updownarrow
$$

$$
\begin{cases} \sup\limits_{\boldsymbol{\theta} \in \mathbb{R}^{|\Gamma|}} & \sum_{j \in \Gamma} \gamma_j \theta_j \\ \text{s.t.} & \sum_{j \in \Gamma} \theta_j h_j(\mathbf{x}) \geq f(\mathbf{x}), \quad \forall \mathbf{x} \in S \end{cases}
$$

广义矩问题-矩松弛

- r 阶矩松弛:

$$\lambda_r := \begin{cases} \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & \mathbf{M}_r(\mathbf{y}) \succeq 0 \\ & \mathbf{M}_{r-d_i}(g_i\mathbf{y}) \succeq 0, \quad i \in [m] \\ & L_{\mathbf{y}}(h_j) = \gamma_j, \quad j \in \Gamma \end{cases}$$

➤ $\lambda_r \nearrow f_{\min}$, $r \to \infty$ (阿基米德条件)

广义矩问题-SOS 松弛

- r 阶对偶 SOS 松弛：

$$
\begin{cases}
\sup\limits_{\boldsymbol{\theta},\sigma_i} & \sum_{j\in\Gamma}\gamma_j\theta_j \\
\text{s.t.} & \sum_{j\in\Gamma}\theta_j h_j - f = \sigma_0 + \sum_{i=1}^m \sigma_i g_i \\
 & \sigma_0,\sigma_1,\ldots,\sigma_m \in \Sigma[\mathbf{x}] \\
 & \deg(\sigma_0)\le 2r,\ \deg(\sigma_i g_i)\le 2r
\end{cases}
$$

多个测度

$$\begin{cases} \inf\limits_{\mu_i \in \mathcal{M}(S_i)_+} & \sum_{i=1}^t \int_{S_i} f_i(\mathbf{x}_i) \mathrm{d}\mu_i \\ \text{s.t.} & \sum_{i=1}^t \int_{S_i} h_{ij}(\mathbf{x}_i) \mathrm{d}\mu_i = \gamma_j, \quad j \in \Gamma \end{cases}$$

$$\Updownarrow$$

$$\begin{cases} \sup\limits_{\boldsymbol{\theta} \in \mathbb{R}^{|\Gamma|}} & \sum_{j \in \Gamma} \gamma_j \theta_j \\ \text{s.t.} & \sum_{j \in \Gamma} \theta_j h_{ij}(\mathbf{x}_i) \geq f_i(\mathbf{x}_i), \quad \forall \mathbf{x}_i \in S_i, i \in [t] \end{cases}$$

多项式动力系统

$$\begin{cases} \dot{x}_1 & = & f_1(\mathbf{x}) \\ \dot{x}_2 & = & f_2(\mathbf{x}) \\ & \vdots & \\ \dot{x}_n & = & f_n(\mathbf{x}) \end{cases} \quad \text{带控制变量} \rightsquigarrow \quad \begin{cases} \dot{x}_1 & = & f_1(\mathbf{x}, \mathbf{u}) \\ \dot{x}_2 & = & f_2(\mathbf{x}, \mathbf{u}) \\ & \vdots & \\ \dot{x}_n & = & f_n(\mathbf{x}, \mathbf{u}) \end{cases}$$

- 约束集合 $X := \{\mathbf{x} \in \mathbb{R}^n \mid p_j(\mathbf{x}) \geq 0, j = 1, \ldots, m\}$
- 最大正不变集、可达集、吸引域、全局吸引子

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- 最大正不变集、可达集、吸引域、全局吸引子

最大正不变集（maximum positively invariant set）

- **最大正不变集**：$M := \{\mathbf{x}_0 \in X \mid \varphi_t(\mathbf{x}_0) \subseteq X, \forall t \geq 0\}$

$$
\begin{cases}
\inf\limits_{a_j,b_j,c_j,v,w} & \int_X w(\mathbf{x})\,\mathrm{d}\mathbf{x} \\
\text{s.t.} & v \in \mathbb{R}[\mathbf{x}]_{2d+1-d_f},\ w \in \mathbb{R}[\mathbf{x}]_{2d} \\
& \beta v - \nabla v \cdot \mathbf{f} = a_0 + \sum_{j=1}^m a_j p_j \\
& w = b_0 + \sum_{j=1}^m b_j p_j \\
& w - v - 1 = c_0 + \sum_{j=1}^m c_j p_j \\
& a_j, b_j, c_j \in \Sigma[\mathbf{x}]_{2d-d_j},\ j = 0, 1, \ldots, m
\end{cases}
$$

- $S_d := w^{-1}([1, +\infty]) = \{\mathbf{x} \in X : w(\mathbf{x}) \geq 1\} \supseteq S_{d+1} \supseteq \cdots \supseteq M$

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优化有理函数之和

- $S := \{\mathbf{x} \in \mathbb{R}^n \mid g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0\}$
- $q_1(\mathbf{x}) > 0, \ldots, q_N(\mathbf{x}) > 0, \ \forall \mathbf{x} \in S$

$$\begin{cases} \inf\limits_{\mathbf{x} \in \mathbb{R}^n} & \sum_{i=1}^{N} \frac{p_i(\mathbf{x})}{q_i(\mathbf{x})} \\ \text{s.t.} & \mathbf{x} \in S \end{cases}$$

测度转化

$$
\begin{cases}
\inf\limits_{\mu_i \in \mathcal{M}(S)_+} & \sum\limits_{i=1}^{N} \int_S p_i \, \mathrm{d}\mu_i \\
\text{s.t.} & \int_S q_1 \, \mathrm{d}\mu_1 = 1, \\
& \int_S \mathbf{x}^{\boldsymbol{\alpha}} q_i \, \mathrm{d}\mu_i = \int_S \mathbf{x}^{\boldsymbol{\alpha}} q_1 \, \mathrm{d}\mu_1, \quad \forall \boldsymbol{\alpha} \in \mathbb{N}^n, i \in [N] \setminus \{1\}
\end{cases}
$$

非负多项式转化

$$
\begin{cases}
\sup\limits_{\lambda, h_i} \lambda \\
\text{s.t. } p_1(\mathbf{x}) + \left(\sum\limits_{i=2}^{N} h_i(\mathbf{x}) - \lambda \right) q_1(\mathbf{x}) \geq 0, \quad \forall \mathbf{x} \in S \\
\qquad p_i(\mathbf{x}) - h_i(\mathbf{x}) q_i(\mathbf{x}) \geq 0, \quad \forall \mathbf{x} \in S, i \in [N] \setminus \{1\} \\
\qquad h_i \in \mathbb{R}[\mathbf{x}], \quad i \in [N] \setminus \{1\}
\end{cases}
$$

联合谱半径

- 联合谱半径（JSR）：给定 $\mathcal{A} = \{A_1, \ldots, A_m\} \subseteq \mathbb{R}^{n \times n}$

$$\rho(\mathcal{A}) := \lim_{k \to \infty} \max_{\sigma \in \{1,\ldots,m\}^k} ||A_{\sigma_1} A_{\sigma_2} \cdots A_{\sigma_k}||^{\frac{1}{k}}$$

- p 是正的 $2d$ 次齐次多项式使得 $p(A_i\mathbf{x}) \leq \gamma^{2d} p(\mathbf{x}), i \in [m] \Rightarrow \rho(\mathcal{A}) \leq \gamma$

$$\rho_{2d}(\mathcal{A}) := \begin{cases} \inf_{p \in \mathbb{R}[\mathbf{x}]_{2d}, \gamma} & \gamma \\ \text{s.t.} & p(\mathbf{x}) - ||\mathbf{x}||_2^{2d} \in \Sigma[\mathbf{x}]_{2d} \\ & \gamma^{2d} p(\mathbf{x}) - p(A_i\mathbf{x}) \in \Sigma[\mathbf{x}]_{2d}, \quad i \in [m] \end{cases}$$

- $m^{-\frac{1}{2d}} \rho_{2d}(\mathcal{A}) \leq \rho(\mathcal{A}) \leq \rho_{2d}(\mathcal{A})$

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SOS 矩阵和矩阵测度

- **SOS 矩阵**：$F(\mathbf{x}) = R(\mathbf{x})^\intercal R(\mathbf{x})$
- $\langle \cdot, \cdot \rangle_p \colon \mathbb{R}^{pq \times pq} \times \mathbb{R}^{q \times q} \to \mathbb{R}^{p \times p}$

$$\langle C, D \rangle_p := \begin{pmatrix} \langle C_{11}, D \rangle & \cdots & \langle C_{1p}, D \rangle \\ \vdots & \ddots & \vdots \\ \langle C_{p1}, D \rangle & \cdots & \langle C_{pp}, D \rangle \end{pmatrix}$$

- **矩阵测度** $\Phi \colon B(\mathcal{X}) \to \mathbb{R}^{p \times p}$

$$\Phi(\mathbf{A}) := [\phi_{ij}(\mathbf{A})] \in \mathbb{R}^{p \times p}, \quad \forall \mathbf{A} \in B(\mathcal{X})$$

多项式矩阵优化

$$\inf_{\mathbf{x}\in\mathbb{R}^n} \lambda_{\min}(F(\mathbf{x})) \quad \text{s.t.} \quad G_1(\mathbf{x}) \succeq 0, \ldots, G_m(\mathbf{x}) \succeq 0$$

$$\begin{cases} \inf\limits_{\mathbf{S}} & L_{\mathbf{S}}(F) \\ \text{s.t.} & \mathbf{M}_r(\mathbf{S}) \succeq 0 \\ & \mathbf{M}_{r-d_i}(G_i\mathbf{S}) \succeq 0, i \in [m] \\ & L_{\mathbf{S}}(I_p) = 1 \end{cases} \Longleftrightarrow \begin{cases} \sup & \lambda \\ \text{s.t.} & F - \lambda I_p = S_0 + \sum_{i=1}^m \langle S_i, G_i \rangle_p \\ & S_0 \in \Sigma^p[\mathbf{x}]_{2r}, S_i \in \Sigma^{pq_k}[\mathbf{x}]_{2(r-d_i)}, i \in [m] \end{cases}$$

多项式矩阵优化

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复多项式优化

- $f, g_1, \ldots, g_m$ 是实值复多项式

$$f_{\min} := \begin{cases} \inf\limits_{\mathbf{z} \in \mathbb{C}^n} & f(\mathbf{z}, \overline{\mathbf{z}}) \\ \text{s.t.} & g_i(\mathbf{z}, \overline{\mathbf{z}}) \geq 0, \quad i = 1, \ldots, m \end{cases}$$

- 复矩方阵 $\mathbf{M}_r^{\mathbb{C}}(\mathbf{y})$: $[\mathbf{M}_r^{\mathbb{C}}(\mathbf{y})]_{\beta\gamma} = y_{\beta,\gamma}, \forall \boldsymbol{\beta}, \boldsymbol{\gamma} \in \mathbb{N}_r^n$
- 复局部化矩阵 $\mathbf{M}_r^{\mathbb{C}}(g\mathbf{y})$:

$[\mathbf{M}_r^{\mathbb{C}}(g\mathbf{y})]_{\beta\gamma} = \sum_{(\beta',\gamma')} g_{\beta',\gamma'} y_{\beta+\beta',\gamma+\gamma'}, \forall \boldsymbol{\beta}, \boldsymbol{\gamma} \in \mathbb{N}_r^n$

复矩松弛

$$\lambda_r := \begin{cases} \inf\limits_{\mathbf{y}\in\mathbb{C}^{\mathbb{N}_r^n}\times\mathbb{C}^{\mathbb{N}_r^n}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & \mathbf{M}_r^{\mathbb{C}}(\mathbf{y}) \succeq 0 \\ & \mathbf{M}_{r-d_i}^{\mathbb{C}}(g_i\mathbf{y}) \succeq 0, \quad i\in[m] \\ & y_{\mathbf{0},\mathbf{0}} = 1 \end{cases}$$

- 存在球面约束（$\sum_{i=1}^n |z_i|^2 = R$）：$\lambda_r \nearrow f_{\min}$，$r\to\infty$

HSOS 松弛

- HSOS： $p(\mathbf{z}, \overline{\mathbf{z}}) = |p_1(\mathbf{z})|^2 + \cdots + |p_t(\mathbf{z})|^2$

$$\begin{cases} \sup\limits_{\lambda, \sigma_i} & \lambda \\ \text{s.t.} & f - \lambda = \sigma_0 + \sigma_1 g_1 + \cdots + \sigma_m g_m \\ & \sigma_0 \in \Sigma^{\mathbb{C}}[\mathbf{z}, \overline{\mathbf{z}}]_r,\ \sigma_i \in \Sigma^{\mathbb{C}}[\mathbf{z}, \overline{\mathbf{z}}]_{r-d_i},\ i \in [m] \end{cases}$$

三角多项式优化

$$\begin{cases} \inf\limits_{\mathbf{x}\in[0,2\pi)^n} & f(\sin x_1,\ldots,\sin x_n,\cos x_1,\ldots,\cos x_n) \\ \text{s.t.} & g_i(\sin x_1,\ldots,\sin x_n,\cos x_1,\ldots,\cos x_n) \geq 0, \quad i=1,\ldots,m \end{cases}$$

$$\Updownarrow$$

$$\begin{cases} \inf\limits_{\mathbf{z}\in\mathbb{C}^n} & f(\mathbf{z},\overline{\mathbf{z}}) \\ \text{s.t.} & g_i(\mathbf{z},\overline{\mathbf{z}}) \geq 0, \quad i=1,\ldots,m \\ & |z_j|^2 = 1, \quad j=1,\ldots,n \end{cases}$$

非交换多项式与 SOHS

- $f(\mathbf{x}) = 3x_1x_2 + 3x_2x_1 + x_3x_2x_1^2 + x_1^2x_2x_3$
- $x_1, \ldots, x_n \in \cup_{\ell=1}^{\infty} \mathbb{S}^{\ell}$
- involution $*$： $(x_1x_2x_3)^* = x_3x_2x_1$
- $f = \sum_w f_w w$
- SOHS： $f(\mathbf{x}) = f_1(\mathbf{x})^* f_1(\mathbf{x}) + \cdots + f_t(\mathbf{x})^* f_t(\mathbf{x}) \rightsquigarrow$ SDP
- $f \geq 0 \iff f$ 是 SOHS

非交换多项式的特征值优化

- $f^* = f, g_1^* = g_1, \ldots, g_m^* = g_m$:

$$\begin{cases} \inf\limits_{x_i \in \cup_{\ell=1}^{\infty} \mathbb{S}^{\ell}} & \lambda_{\min}(f(\mathbf{x})) \\ \text{s.t.} & g_i(\mathbf{x}) \geq 0, \quad i = 1, \ldots, m \end{cases}$$

$\rightsquigarrow$ quantum information, ground state energy

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NPA 松弛分层

- $L_{\mathbf{y}}(\sum_w f_w w) = \sum_w f_w y_w$
- 二次模：$\mathcal{Q}(\mathbf{g}) := \{\sum_\sigma \sigma^* g_\sigma \sigma \mid g_\sigma \in \{1\} \cup \mathbf{g}\}$

$$
\begin{cases}
\inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\
\text{s.t.} & \mathbf{M}_r(\mathbf{y}) \succeq 0 \\
& \mathbf{M}_{r-d_i}(g_i \mathbf{y}) \succeq 0,\ i \in [m] \\
& \mathbf{M}_r(\mathbf{y})_{uv} = \mathbf{M}_r(\mathbf{y})_{wz},\ \forall u^* v = w^* z \\
& y_1 = 1
\end{cases}
\quad \Longleftrightarrow \quad
\begin{cases}
\sup\limits_{\lambda} & \lambda \\
\text{s.t.} & f - \lambda \in \mathcal{Q}(\mathbf{g})_{2r}
\end{cases}
$$

非交换多项式的迹优化

- $\mathrm{tr}(A) := \frac{1}{k}\sum_{i=1}^{k} A_{ii}$

$$\begin{cases} \inf\limits_{x_i \in \cup_{\ell=1}^{\infty} \mathbb{S}^{\ell}} & \mathrm{tr}(f(\mathbf{x})) \\ \text{s.t.} & g_i(\mathbf{x}) \geq 0, \quad i = 1, \ldots, m \end{cases}$$

$\rightsquigarrow$ Connes' embedding conjecture

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$\rightsquigarrow$ Connes' embedding conjecture

迹优化的 SDP 松弛分层

- **交换子**: $[g, h] := gh - hg$
- $g \overset{\text{cyc}}{\sim} h$: $g - h$ 可以写成若干个交换子之和

$$
\begin{cases}
\inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\
\text{s.t.} & \mathbf{M}_r(\mathbf{y}) \succeq 0 \\
& \mathbf{M}_{r-d_i}(g_i\mathbf{y}) \succeq 0,\ i \in [m] \\
& \mathbf{M}_r(\mathbf{y})_{uv} = \mathbf{M}_r(\mathbf{y})_{wz},\ \forall u^* v \overset{\text{cyc}}{\sim} w^* z \\
& y_1 = 1
\end{cases}
\iff
\begin{cases}
\sup\limits_{\lambda} & \lambda \\
\text{s.t.} & f - \lambda \in \mathcal{Q}^{\text{cyc}}(\mathbf{g})_{2r}
\end{cases}
$$

态多项式优化

- $\mathcal{H}$：Hilbert 空间
- $\mathcal{B}(\mathcal{H})$：$\mathcal{H}$ 上的有界线性算子空间
- $\mathcal{S}(\mathcal{H})$：$\mathcal{B}(\mathcal{H})$ 上的正有界 $*$-线性泛函（$X \mapsto \mathrm{tr}(\rho X)$）
- **态多项式**：$\varsigma(x_1^2)x_2x_1 + \varsigma(x_1)\varsigma(x_2x_1x_2)$, $x_1, \ldots, x_n \in \mathcal{B}(\mathcal{H})$, $\varsigma \in \mathcal{S}(\mathcal{H})$

$$\begin{cases} \inf\limits_{(\mathcal{H},\mathbf{x},\varsigma)} & \varsigma(f(\mathbf{x};\varsigma)) \\ \text{s.t.} & g_i(\mathbf{x};\varsigma) \geq 0, \quad i = 1, \ldots, m \end{cases}$$

➤ quantum information, quantum states

态多项式优化的 SDP 松弛

$$\begin{cases} \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & \mathbf{M}_r(\mathbf{y}) \succeq 0 \\ & \mathbf{M}_{r-d_i}(g_i\mathbf{y}) \succeq 0,\ i \in [m] \\ & \mathbf{M}_r(\mathbf{y})_{uv} = \mathbf{M}_r(\mathbf{y})_{wz},\ \forall \varsigma(u^* v) = \varsigma(w^* z) \\ & y_1 = 1 \end{cases} \quad \Longleftrightarrow \quad \begin{cases} \sup\limits_{\lambda} & \lambda \\ \text{s.t.} & f - \lambda \in \mathcal{Q}^{\mathrm{st}}(\mathbf{g})_{2r} \end{cases}$$

- Igor Klep et al. “State polynomials: positivity, optimization and nonlinear bell inequalities.” Mathematical Programming 207(1)(2024): 645-691.

迹多项式优化

- $\mathcal{H}$：Hilbert 空间
- $\mathcal{B}(\mathcal{H})$：$\mathcal{H}$ 上的有界线性算子空间
- $\mathrm{tr}(A) := \frac{1}{k}\sum_{i=1}^{k} A_{ii}$：$u \overset{\text{cyc}}{\sim} v, u^* \overset{\text{cyc}}{\sim} v \Rightarrow \mathrm{tr}(u) = \mathrm{tr}(v)$
- **迹多项式**：$\mathrm{tr}(x_1^2)x_2x_1 + \mathrm{tr}(x_1)\mathrm{tr}(x_2x_1x_2)$, $x_1, \ldots, x_n \in \mathcal{B}(\mathcal{H})$

$$\begin{cases} \inf\limits_{\mathbf{x}\in\cup_{k\geq 1}(\mathbb{S}_k)^n} & \mathrm{tr}(f(\mathbf{x})) \\ \text{s.t.} & g_i(\mathbf{x}) \geq 0, \quad i = 1, \ldots, m \end{cases}$$

➤ quantum information, maximal entanglement states

迹多项式优化的 SDP 松弛

$$
\left\{
\begin{array}{ll}
\inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\
\text{s.t.} & \mathbf{M}_r(\mathbf{y}) \succeq 0 \\
 & \mathbf{M}_{r-d_i}(g_i\mathbf{y}) \succeq 0,\ i \in [m] \\
 & \mathbf{M}_r(\mathbf{y})_{uv} = \mathbf{M}_r(\mathbf{y})_{wz},\ \forall \mathrm{tr}(u^* v) = \mathrm{tr}(w^* z) \\
 & y_1 = 1
\end{array}
\right.
\iff
\left\{
\begin{array}{ll}
\sup\limits_{\lambda} & \lambda \\
\text{s.t.} & f - \lambda \in \mathcal{Q}^{\mathrm{tr}}(\mathbf{g})_{2r}
\end{array}
\right.
$$

- Igor Klep, Victor Magron, and Jurij Volčič. “Optimization over trace polynomials.” Annales Henri Poincaré. Vol. 23. Springer International Publishing, 2022.

矩多项式优化

- 概率测度 μ：$\mathfrak{m}(\mathbf{x}^{\boldsymbol{\alpha}}) \to \int \mathbf{x}^{\boldsymbol{\alpha}} \mathrm{d}\mu$
- 矩多项式：$f = \mathfrak{m}(x_1 x_3^2) x_1 x_2 - \mathfrak{m}(x_1^2)^3 x_2^2 + x_2 - \mathfrak{m}(x_2)\mathfrak{m}(x_1 x_2) - 2$
- 矩多项式优化

➤ Igor Klep, Victor Magron, and Jurij Volčič. "Sums of squares certificates for polynomial moment inequalities." Foundations of Computational Mathematics, pp.1-43, 2025.

矩多项式优化

- 概率测度 μ： $\mathfrak{m}(\mathbf{x}^{\boldsymbol{\alpha}}) \to \int \mathbf{x}^{\boldsymbol{\alpha}} \mathrm{d}\mu$
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- 矩多项式优化

➤ Igor Klep, Victor Magron, and Jurij Volčič. “Sums of squares certificates for polynomial moment inequalities.” Foundations of Computational Mathematics, pp.1-43, 2025.

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- ...

下次课

- 软件与实验

参考文献

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2. Jean B. Lasserre, **An Introduction to Polynomial and Semi-Algebraic Optimization**, Cambridge University Press, 2015.
3. Jie Wang and Victor Magron, **Sparse Polynomial Optimization: Theory and Practice**, World Scientific Publishing, 2023.

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