做计算的感悟

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一个字：做

自学能力(生)　　　自主式学习(师)

- 学期初提要求，论文成绩在期末成绩中占 30%.
- 半学期后，组成五人左右的科研小组，最后完成 30 分钟的学术演讲. 占整个考评 25%.
- 期末的笔试：45%

值得纪念的年份

特征值与相变 1988: 30 周年

特征值计算 2015: 3 周年

- 连续: $\mathbb{R}^{\mathbb{Z}^d}$, 微分算子. $\mathbb{R}^n$
- 离散: $\mathbb{Z}_+^{\mathbb{Z}^d}$, 差分算子.

20 年后, 才回到相变研究

格子上 φ^4 欧氏量子场

$$\mathbb{R}^{\mathbb{Z}^d} \ni x : \mathbb{Z}^d \to \mathbb{R}.\ H(x) = -2J \sum_{\langle ij \rangle} x_i x_j, \quad J, \beta \geqslant 0$$

$$L = \sum_{i \in \mathbb{Z}^d} \left[\partial_{ii} - (u'(x_i) + \partial_i H)\partial_i\right], \quad u(x_i) = x_i^4 - \beta x_i^2$$

Theorem (C. 2008)

$$\inf_{\Lambda \Subset \mathbb{Z}^d} \inf_{\omega \in \mathbb{R}^{\mathbb{Z}^d}} \lambda_1^{\beta, J}(\Lambda, \omega) \approx \inf_{\Lambda \Subset \mathbb{Z}^d} \inf_{\omega \in \mathbb{R}^{\mathbb{Z}^d}} \sigma^{\beta, J}(\Lambda, \omega)$$

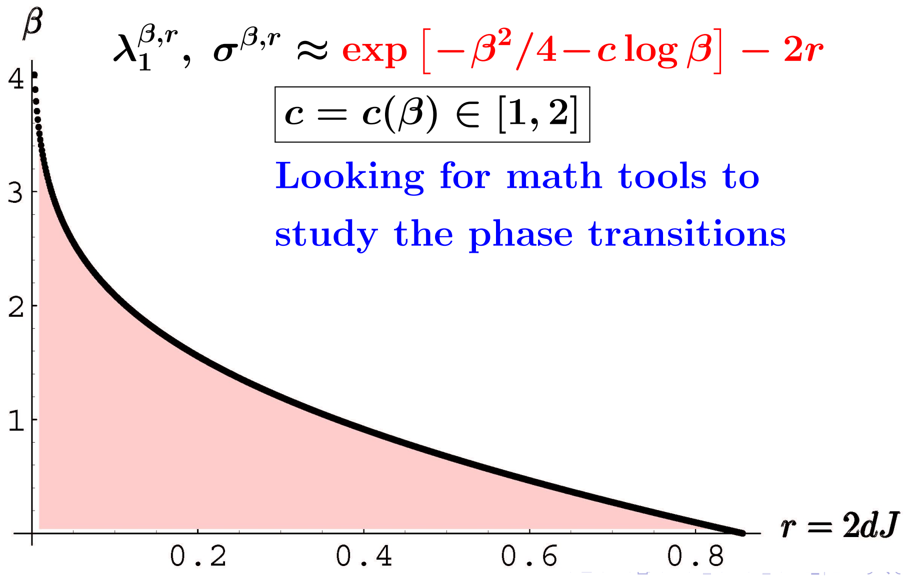
$$\approx \exp\left[-\beta^2/4 - c\log\beta\right] - 4dJ \quad \boxed{c \in [1, 2]}$$

相变: φ^4 模型

$$\lambda_1^{\beta,r},\ \sigma^{\beta,r} \approx \exp\left[-\beta^2/4 - c\log\beta\right] - 2r$$

$$\boxed{c = c(\beta) \in [1,2]}$$

Looking for math tools to study the phase transitions



1. 特征值估计. 例. 生灭 Q 矩阵

三对角矩阵: $E = \{k \in \mathbb{Z}_+ : 0 \leqslant k < N+1\}$

$$Q = \begin{pmatrix} -c_0 & b_0 & & & 0 \\ a_1 & -c_1 & b_1 & & \\ & a_2 & -c_2 & b_2 & \\ & & \ddots & \ddots & \ddots \\ 0 & & & a_N & -c_N \end{pmatrix},$$

此处 $a_k,\ b_k > 0,\ c_k = a_k + b_k,\ c_N \geqslant a_N$

从简单开始

$$Q=\begin{bmatrix} -b_0 & b_0 \\ a_1 & -a_1 \end{bmatrix}, \quad \boxed{b_0=\theta,\ a_1=1-\theta}$$

$$Q=\begin{bmatrix} -b_0 & b_0 & & 0 \\ a_1 & -a_1-b_1 & b_1 & \\ & a_2 & -a_2-b_2 & b_2 \\ 0 & & a_3 & -a_3 \end{bmatrix}$$

概率、计算、几何、谱理论、调和分析

例. 生灭 Q 矩阵

最重要的一类随机过程–生灭过程有极广泛应用，理论研究起点，根据地. 最长文章 [137页, 2010]. 含 (c_k): 2014. 综述报告 C.(2016). "Unified speed estimation of various stabilities", Chin. Appl. Prob. Statis. 2016, 32(1): 1-22

$$(4\delta)^{-1} \leqslant \delta_n^{-1} \uparrow \leqslant \lambda_0(-Q) \leqslant \downarrow \delta_n'^{-1} \leqslant \delta^{-1}, \forall n$$

$$\boxed{1 \leqslant \delta_1'^{-1} / \delta_1^{-1} \leqslant 2}$$

2. 特征值计算. Perron-Frobenius 定理

非负不可约方阵最大特征对子算法:

幂法(Power iteration) 初值 v_0

$$v_k = \frac{A v_{k-1}}{\|A v_{k-1}\|}$$

初值 (v_0, z_0)

带推移逆迭代(Rayleigh quotient iteration)

$$v_k = \frac{(A - z_{k-1})^{-1} v_{k-1}}{\|(A - z_{k-1})^{-1} v_{k-1}\|}, \quad z_k = \frac{v_k^* A v_k}{v_k^* v_k}$$

例. $Q=$

$$
\begin{pmatrix}
-1 & 1^2 & & & & & & & \\
1^2 & -5 & 2^2 & & & & & 0 & \\
 & 2^2 & -13 & 3^2 & & & & & \\
 & & 3^2 & -25 & 4^2 & & & & \\
 & & & 4^2 & -41 & 5^2 & & & \\
 & & & & 5^2 & -61 & 6^2 & & \\
 & 0 & & & & 6^2 & -85 & 7^2 \\
 & & & & & & 7^2 & -113
\end{pmatrix}
$$

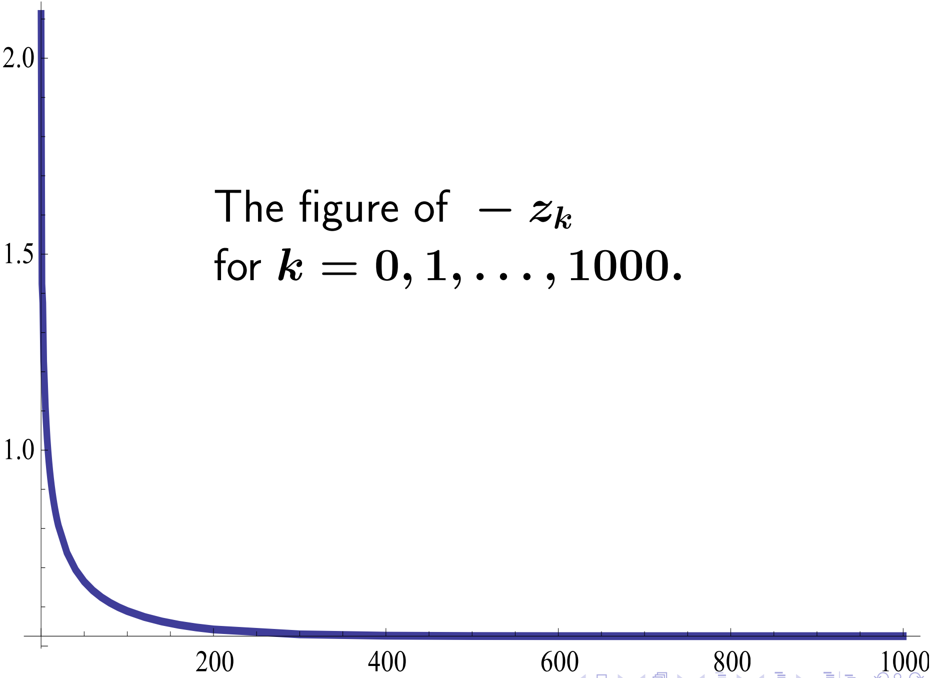
$\rho(Q) \approx -0.525268$, $\boxed{\rho(\text{Infinite } Q) = -1/4}$

k	$-z_k$	k	$-z_k$
0	2.11289	11	0.927544
1	1.42407	12	0.908975
2	1.37537	13	0.892223
3	1.22712	14	0.877012
4	1.1711	15	0.86311
5	1.10933	16	0.850338
6	1.06711	17	0.838548
7	1.02949	18	0.827619
8	0.998685	19	0.817449
9	0.971749	20	0.807953
10	0.948331	30	0.738257

Computing
180 times,
10^3 iterations
64 pages

$(k, -z_k)$

The figure of $-z_k$ for $k = 0, 1, \ldots, 1000$.



Large N. $\lambda_0 = 1/4$ if $N = \infty$. $\leqslant 30$ Sec

Use $\tilde{v}_0$ and δ_1. Let $z_0 = 7/(8\delta_1) + v_0^*(-Q)v_0/8$.

$N+1$	z_0	z_1	$z_2 = \lambda_0$
10^4	0.31437	0.302586	0.302561

Examples for $N > 8$ computed by Yue-Shuang Li

Large N. $\lambda_0 = 1/4$ if $N = \infty$. $\leqslant 30$ Sec

Use $\tilde{v}_0$ and δ_1. Let $z_0 = 7/(8\delta_1) + v_0^*(-Q)v_0/8$.

$N+1$	z_0	z_1	$z_2 = \lambda_0$	upper/lower
8	0.523309	0.525268	**0.525268**	$1+10^{-11}$
100	0.387333	0.376393	**0.376383**	$1+10^{-8}$
500	0.349147	0.338342	**0.338329**	$1+10^{-7}$
1000	0.338027	0.327254	**0.32724**	$1+10^{-7}$
5000	0.319895	0.30855	**0.308529**	$1+10^{-7}$
7500	0.316529	0.304942	**0.304918**	$1+10^{-7}$
10^4	0.31437	0.302586	**0.302561**	$1+10^{-7}$

Examples for $N > 8$ computed by Yue-Shuang Li

2. 通用算法 (Global Algorithm), ’17

三对角占优矩阵 $\Rightarrow$ 一般矩阵

Alphago

Ask computer to find efficient initials?

$v_0 =$ 一致分布: $(1, \cdots, 1)^* / \sqrt{N+1}$.

How to choose $z_0(z_n)$ in unified way?

$$z_0 \neq \frac{v_0^* A v_0}{v_0^* v_0} \quad [RQ!], \qquad z_n = ?$$

2. 通用算法 (Global Algorithm), '17

带推移逆迭代

$$z_k = \max_{0\leqslant k\leqslant N} \frac{Av_k}{v_k}(k), \qquad k \geqslant 0.$$

设 w_k 是方程

$$(z_{k-1}I - A)w_k = v_{k-1}$$

的解，再命

$$v_k = \frac{w_k}{\|w_k\|}, \qquad k \geqslant 0.$$

3. 特征值的(次)最大实部. 2017

假定矩阵 A 有特征对子 (λ_j, g_j)，两两不同. 给定 v，表 $v = \sum_{j=0}^m c_j g_j$. 则

$$A^n v = \sum_{j=0}^m c_j \lambda_j^n g_j,$$

$$e^A v = \sum_{j=0}^\infty \frac{1}{n!} A^n v = \sum_{j=0}^m c_j g_j e^{\lambda_j}.$$

3. 特征值的(次)最大实部. 2017

$$e^{tA}v = \sum_{j=0}^{\infty} \frac{1}{n!}(tA)^n v = \sum_{j=0}^{m} c_j g_j e^{\lambda_j t}.$$

$$\frac{e^{tA}}{e^{\mathrm{Re}(\lambda_0)t}} = c_0 g_0 e^{i\mathrm{Im}(\lambda_0)t} + \sum_{j=1}^{m} c_j g_j \times$$

$$\times\ e^{(\mathrm{Re}(\lambda_j) - \mathrm{Re}(\lambda_0))t} e^{i\mathrm{Im}(\lambda_j)t}$$

$$\text{if}\ \ \mathrm{Re}(\lambda_j) < \mathrm{Re}(\lambda_0), \quad j \neq 0.$$

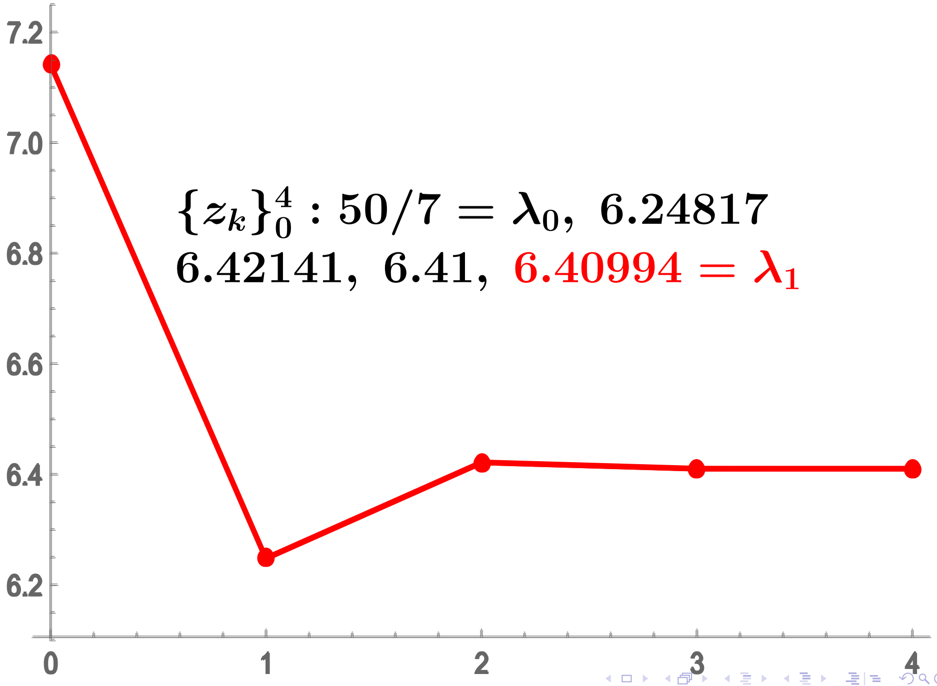
例. $Q =$

$$
\begin{bmatrix}
-1 & 1 & & & & & & \\
1/2 & -5/2 & 2 & & & \text{\Huge 0} & & \\
1/3 & & -10/3 & 3 & & & & \\
1/4 & & & -17/4 & 4 & & & \\
1/5 & & & & -26/5 & 5 & & \\
1/6 & & & & & -37/6 & 6 & \\
1/7 & & \text{\Huge 0} & & & & {\color{red}-50/7} & 7 \\
1/8 & & & & & & & -1/8
\end{bmatrix}
$$

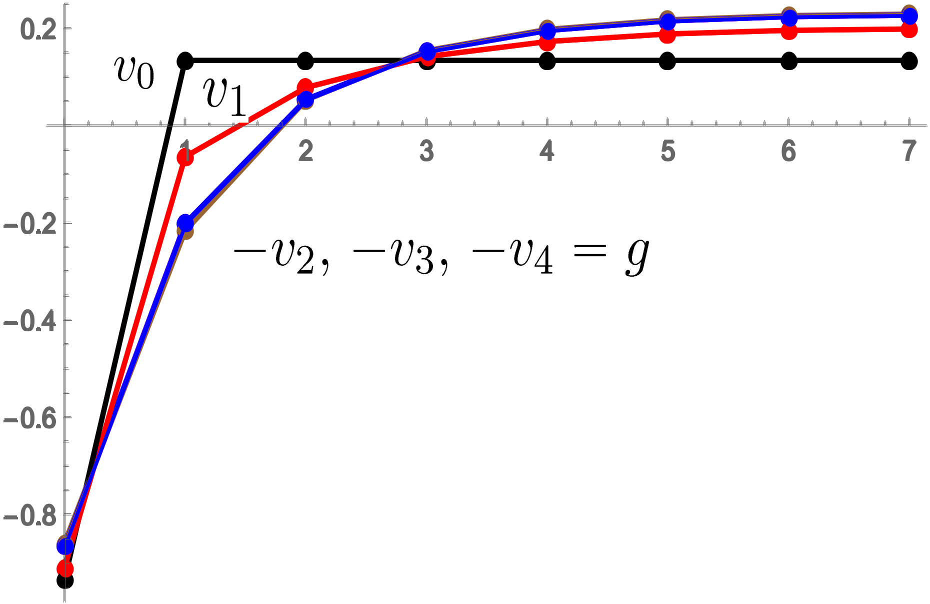
$A = Q + 50\,I/7$. Eigenvalues of A:

$$\lambda_0 = 50/7,\ \lambda_1 = 6.40994,$$
$$4.26332 \pm 0.835966\,i,$$
$$2.24838 \pm 0.593141\,i,$$
$$0.824966,\ 0.0238239.$$

$$w_0 = (-7, 1, 1, 1, 1, 1, 1, 1)^*.$$
$$v_0 = w_0/\sqrt{w_0^* w_0}. \quad z_0 = \lambda_0 = 50/7.$$



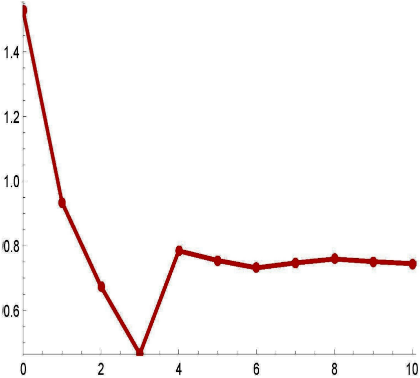
$$\{z_k\}_0^4 : 50/7 = \lambda_0,\ 6.24817$$
$$6.42141,\ 6.41,\ 6.40994 = \lambda_1$$


0.2
−0.2
−0.4
−0.6
−0.8
1
2
3
4
5
6
7
v_0
v_1
$-v_2, -v_3, -v_4 = g$

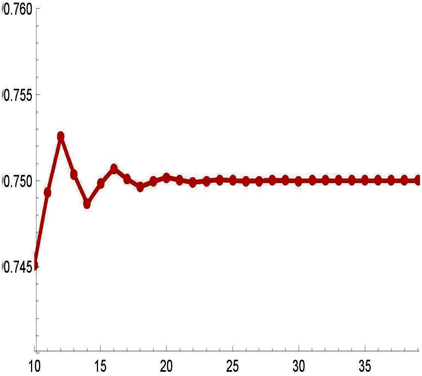
复共轭情形

$$Q = \begin{bmatrix} -1/2 & 1/2 & 0 \\ 0 & -1 & 1 \\ 1 & 0 & -1 \end{bmatrix}. \quad A = Q + 2I$$

Eigenvalues of A:
$\lambda_0 = 2, \ \lambda_{1\pm} = 0.75 \pm 0.661438\, i.$



$n = 0, \ldots 10$



$n = 10, \ldots 39$

$\{v_n\}$ 不收敛，循环(不相关向量):

$(.707107, -4.23422\cdot 10^{-7}, -.707107)^*$

$(.408248, -.816497, .498248)^*$

将 A 换成 $A + i\,I$. 分离共轭对

n	$m=0$	$m=4$
0	$5/3$	$5/3$
1	$.973214+.598214\,i$	$.973214+.598214\,i$
2	$.712632+.434641\,i$	$.849115+.481596\,i$
3	$.755776+.334411\,i$	$.767798+.422326\,i$
4	$.750037+.338573\,i$	$.735231+.376756\,i$
5	$.75+.338562\,i$	$.750863+.337752\,i$
6		$.750001+.338562\,i$
7		$.75+.338562\,i$

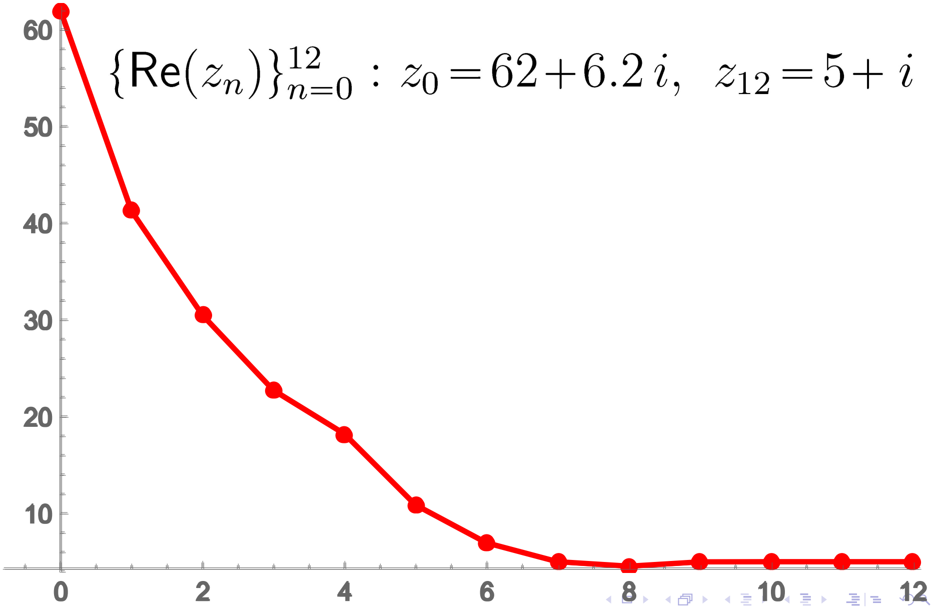
更多测试 $B =$ $\boxed{\lambda = 5 + i}$

$$
\begin{bmatrix}
4+3i & & & & & & \\
 & 4-3i & & & & & \\
 & & 3+2i & & & & \\
 & & & 3-2i & & & \\
 & & & & 2+i & & \\
 & & & & & 2-i & \\
 & & & & & & \color{red}{\lambda}
\end{bmatrix}
$$

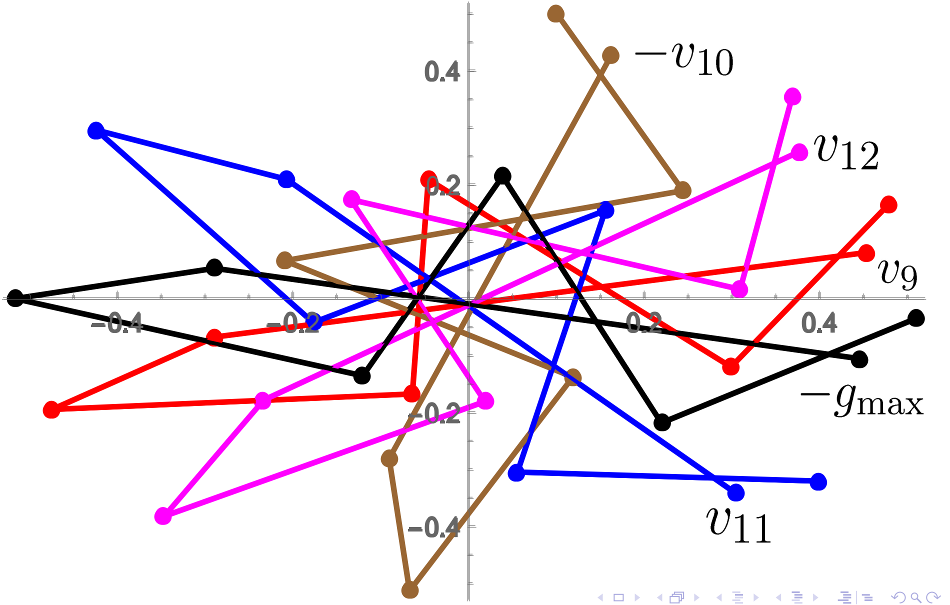
更多测试. $A := P^{-1}BP$

$$P=\begin{bmatrix} 3 & 5 & 3+i & 2 & 3 & 1 & 3+i \\ 5 & 4 & 2+i & 4 & 5 & 1 & i \\ 3-i & 2-i & 5 & 1+i & 2 & 1 & 3+i \\ 2 & 4 & 1-i & 2 & i & 1 & 2 \\ 3 & 5 & 2 & -i & 1 & 1 & 2 \\ 1 & 2 & 3 & 4 & 5 & 2 & 3 \\ 7 & 6 & 5 & 4 & 3 & 2 & 1 \end{bmatrix}$$

$\{z_n\}$ 实部的收敛性



The vectors $\{v_n\}_{n=9}^{12}$



$\{v_n\}$ 收敛？不计常数因子，是的！

$$v_{12} = (-\alpha)\, g_{\max},$$

$$\alpha = (.672245 + .740328\, i), \quad |\alpha| = 1.$$

$$\frac{cv}{\|cv\|} = \mathrm{sgn}(c)\frac{v}{\|v\|} \quad \text{if } c \text{ is real;}$$

$$\frac{cv}{\|cv\|} = e^{i\theta}\frac{v}{\|v\|} \quad \text{if } c = re^{i\theta}\ (r > 0).$$

4. 何时复方阵有实谱?

(实)对称 (symmetry) $\Rightarrow$ 实谱,
复对称阵谱不必实的, 如

$$A = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \qquad \lambda = \pm i$$

(实)对称→Hermite: $a_{ij} = \bar{a}_{ji} \Rightarrow$ 实谱. 如

$$A = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \qquad \lambda = \pm 1$$

复可配称矩阵. 意义: 代数, 量子力学

(实)可配称 (symmetrizable),

$\exists(\mu_k > 0)$: $\mu_i a_{ij} = \mu_j a_{ji}, \quad i, j \in E$

复可配称 (Hermitizable) [a_{ii} 为实]

$\exists(\mu_k > 0)$: $\mu_i a_{ij} = \mu_j \bar{a}_{ji}, \quad i, j \in E$

矩阵 $A = (a_{ij})$ 复可配称的必要条件:

- 零同性: 对于任意的 i, j,
  $a_{ij} = 0 \Leftrightarrow a_{ji} = 0$. 不可约. a_{ii} 为实
- 正比值: 如 $a_{ji} \neq 0$, 则$a_{ij}/\bar{a}_{ji} > 0$.

复三对角矩阵

$$A=\begin{pmatrix} -c_0 & b_0 & & & 0 \\ a_1 & -c_1 & b_1 & & \\ & a_2 & -c_2 & b_2 & \\ & & \ddots & \ddots & \ddots \\ 0 & & & a_N & -c_N \end{pmatrix},$$

此处 a_k, b_k c_k 均为复数

Theorem

三对角复矩阵 $A \sim (a_k, -c_k, b_k)$ 复可配称的充要条件是下述两条件同时成立.

- (c_k) 为实的.
- 或 a_{i+1} 和 b_i 同时为零, 或 $a_{i+1}b_i > 0$

注　a_{i+1} 和 b_i 同时为零, 则此矩阵可分块处理. 故常省略此条件.

$a_{i+1}b_i > 0 \Rightarrow \dfrac{b_i}{\bar{a}_{i+1}} > 0$. 如 $\bar{a}_{i+1} \neq 0$, 反隐含也对

三对角复矩阵: $A \sim (a_k, -c_k, b_k)$

配称测度 (μ_n):

$$\mu_0 = 1, \mu_n = \mu_{n-1}\frac{b_{n-1}}{\bar{a}_n}, \quad 1 \leqslant n \leqslant N+1$$

$$Q = \begin{pmatrix} -1 & 1 & & 0 \\ 1 & -5 & 4 & \\ & 4 & -13 & 9 \\ 0 & & 9 & -25 \end{pmatrix}.$$

同时改变某些 (b_{n-1}, a_n) 的符号，谱不变

复可配称三对角矩阵的等谱变换

Theorem (Algorithm)

假定 $c_k \geqslant |a_k|+|b_k|$, 并设 $u_k = a_k b_{k-1}$ 及 $\tilde{c}_k = c_k, 0 \leqslant k < N+1$. 定义 $\tilde{b}_0 = c_0 > 0$,

$$\begin{cases} \tilde{b}_k = c_k - u_k / \tilde{b}_{k-1}, \quad \tilde{a}_k = c_k - \tilde{b}_k, \\ \qquad 1 \leqslant k < N \\ \tilde{a}_N = u_N / \tilde{b}_{N-1} \quad \text{如 } N < \infty. \end{cases}$$

则 $\tilde{a}_k, \tilde{b}_k > 0$; $c_N \geqslant |a_N|$ 如 $N < \infty$.
$A \sim (a_k, -c_k, b_k)$ 等谱于 $\tilde{A} \sim (\tilde{a}_k, -\tilde{c}_k, \tilde{b}_k)$.

$$\tilde{b}_k = \qquad \text{显式 } u_k = a_k b_{k-1} = |a_k b_{k-1}|$$

$$c_k - \cfrac{u_k}{c_{k-1} - \cfrac{u_{k-1}}{c_{k-2} - \cfrac{u_{k-2}}{\ddots\, c_2 - \cfrac{u_2}{c_1 - \cfrac{u_1}{c_0}}}}}$$

来自不易 2014–2018/2/1-2

$$\tilde{a}_k = c_k - \tilde{b}_k, \quad \tilde{a}_N = u_N / \tilde{b}_{N-1} \text{ 如 } N < \infty.$$

For Further Reading I

- C. (2016): Efficient initials for computing the maximal eigenpair, Front. Math. China 11(6): 1379–1418.

- C. (2017). Global algorithms for maximal eigenpair. Front. Math. China 12(5): 1023–1043.

- C. (2018a). Hermitizable, isospectral complex matrices or differential operators. Front. Math. China.

For Further Reading II

C. (2018b). Computing (sub-)maximal real part of eigenvalues. Preprint

http://math0.bnu.edu.cn/~chenmf

4 volumes, 22 popularizing papers, 9 videos

The end!

Thank you, everybody!

谢谢大家!

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