向量迭代法
Vector iteration

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大型特征值问题的求解方法

定义： ⟹ 向量迭代法

$K\phi - \lambda M\phi = 0$

正交性： ⟹ 变换法

$\Phi^{\mathrm{T}} M \Phi = I$

$\Phi^{\mathrm{T}} K \Phi = \Lambda$

特征多项式： ⟹ 多项式迭代法

$p(\lambda) = |K - \lambda M| = 0$

$p(\lambda) = |K - \lambda M| = |LDL^{\mathrm{T}}| = \prod_{i=1}^{n} d_{ii}$

Sturm序列： ⟹ Sturm序列迭代法

$p(\lambda), p^{(1)}(\lambda^{(1)}), p^{(2)}(\lambda^{(2)}), \cdots, p^{(n-1)}(\lambda^{(n-1)})$

在$K - \mu M$的三角分解中，对角阵D中负元素的个数等于系统中小于μ的特征值的个数。

向量迭代法

$K\phi - \lambda M\phi = 0$ ⟹ $p(\lambda) = 0$ $\quad n > 4$ 时必须迭代求解

$K\bar{x}_{k+1} = Mx_k$ $\qquad$ K必须是正定的

$$x_{k+1} = \frac{\bar{x}_{k+1}}{(\bar{x}_{k+1}^{\mathrm{T}} M \bar{x}_{k+1})^{\frac{1}{2}}}$$

$$\rho(\bar{x}_{k+1}) = \frac{\bar{x}_{k+1}^{\mathrm{T}} K \bar{x}_{k+1}}{\bar{x}_{k+1}^{\mathrm{T}} M \bar{x}_{k+1}}$$ 瑞利商

向量迭代法 — 收敛性分析

$K\bar{x}_{k+1} = M\bar{x}_k \Leftarrow \bar{x}_k = \Phi\bar{z}_k,\ \bar{x}_{k+1} = \Phi\bar{z}_{k+1},\ x_{k+1} = \Phi z_{k+1}$

$x_{k+1} \Downarrow \phi_1$

$\Lambda\bar{z}_{k+1} = \bar{z}_k$

$\bar{z}_{k+1} = \Lambda^{-1}\bar{z}_k = \cdots = \Lambda^{-k}\bar{z}_1 \Leftarrow \bar{z}_1 = \begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix}^{\mathrm{T}}$

$$\bar{z}_{k+1} = [\ (\frac{1}{\lambda_1})^k \quad (\frac{1}{\lambda_2})^k \quad \cdots \quad (\frac{1}{\lambda_n})^k\ ]^{\mathrm{T}}$$

$$z_{k+1} = \frac{[\ (\frac{1}{\lambda_1})^k \quad (\frac{1}{\lambda_2})^k \quad \cdots \quad (\frac{1}{\lambda_n})^k\ ]^{\mathrm{T}}}{[\sum_{i=1}^{n}(\frac{1}{\lambda_i})^{2k}]^{\frac{1}{2}}} = \frac{[\ 1 \quad (\frac{\lambda_1}{\lambda_2})^k \quad \cdots \quad (\frac{\lambda_1}{\lambda_n})^k\ ]^{\mathrm{T}}}{[\sum_{i=1}^{n}(\frac{\lambda_1}{\lambda_i})^{2k}]^{\frac{1}{2}}} \Rightarrow e_1$$

特征向量收敛率

$$\lim_{k\to\infty} \frac{\|z_{k+1} - e_1\|_2}{\|z_k - e_1\|_2} = \frac{\lambda_1}{\lambda_2}$$

向量迭代法 — 收敛性分析

有重根的情况：$\lambda_1 = \lambda_2 = \cdots = \lambda_m$

$$z_{k+1} = \frac{[1 \quad (\frac{\lambda_1}{\lambda_2})^k \quad \cdots \quad (\frac{\lambda_1}{\lambda_n})^k]^{\mathrm{T}}}{[\sum_{i=1}^{n}(\frac{\lambda_1}{\lambda_i})^{2k}]^{\frac{1}{2}}} = \frac{[1 \quad 1 \quad \cdots \quad 1 \quad (\frac{\lambda_1}{\lambda_{m+1}})^k \quad \cdots \quad (\frac{\lambda_1}{\lambda_n})^k]^{\mathrm{T}}}{[m + \sum_{i=m+1}^{n}(\frac{\lambda_1}{\lambda_i})^{2k}]^{\frac{1}{2}}}$$

$$\Rightarrow \frac{1}{\sqrt{m}}[1 \quad 1 \quad \cdots \quad 1 \quad 0 \quad \cdots \quad 0]^{\mathrm{T}}$$

特征向量收敛率 $\frac{\lambda_1}{\lambda_{m+1}}$

向量迭代法 — 收敛性分析

$$\rho(\bar{x}_{k+1}) = \frac{\bar{x}_{k+1}^{\mathrm{T}} K \bar{x}_{k+1}}{\bar{x}_{k+1}^{\mathrm{T}} M \bar{x}_{k+1}} \Leftarrow \begin{matrix} \bar{x}_k = \Phi\bar{z}_k,\ \bar{x}_{k+1} = \Phi\bar{z}_{k+1},\ x_{k+1} = \Phi z_{k+1} \\ K\bar{x}_{k+1} = M\bar{x}_k \end{matrix}$$

$$\rho(\bar{z}_{k+1}) = \frac{\bar{z}_{k+1}^{\mathrm{T}} \bar{z}_k}{\bar{z}_{k+1}^{\mathrm{T}} \bar{z}_{k+1}} \Leftarrow \bar{z}_{k+1} = [\ (\frac{1}{\lambda_1})^k \quad (\frac{1}{\lambda_2})^k \quad \cdots \quad (\frac{1}{\lambda_n})^k\ ]^{\mathrm{T}}$$

$$= \frac{\sum_{i=1}^{n}(\frac{1}{\lambda_i})^{2k-1}}{\sum_{i=1}^{n}(\frac{1}{\lambda_i})^{2k}} = \frac{\lambda_1 \sum_{i=1}^{n}(\frac{\lambda_1}{\lambda_i})^{2k-1}}{\sum_{i=1}^{n}(\frac{\lambda_1}{\lambda_i})^{2k}} \Rightarrow \lambda_1$$

特征值收敛率

$$\lim_{k\to\infty} \frac{\|\rho(\bar{z}_{k+1}) - \lambda_1\|_2}{\|\rho(\bar{z}_k) - \lambda_1\|_2} = \left(\frac{\lambda_1}{\lambda_2}\right)^2$$ 高于特征向量的收敛率！

向量迭代法

- 逆迭代法（K非奇异）Inverse iteration
  - 选取初始迭代向量x_1，令$k=1$
  - 迭代 $K\bar{x}_{k+1}=Mx_k$　　　$y_k = M x_k$
  - 正则化 $x_{k+1}=\dfrac{\bar{x}_{k+1}}{\left(\bar{x}_{k+1}^{T} M\bar{x}_{k+1}\right)^{1/2}}$　　　$\bar{y}_{k+1}=M\bar{x}_{k+1}$
  - 瑞利商 $\rho(\bar{x}_{k+1})=\dfrac{\bar{x}_{k+1}^{T}K\bar{x}_{k+1}}{\bar{x}_{k+1}^{T}M\bar{x}_{k+1}}$
- 收敛性
  - $x_{k+1}\to\phi_1$；$\rho\to\lambda_1$
  - 收敛率 λ_1/λ_2；$(\lambda_1/\lambda_2)^2$

迭代算法

1. 选取初始迭代向量x_1, 计算$y_1 = Mx_1$, $k=1$
2. 解方程 $K\bar{x}_{k+1}=y_k$　　　$K\bar{x}_{k+1}=Mx_k$
3. 计算 $\bar{y}_{k+1}=M\bar{x}_{k+1}$
4. 计算瑞利商 $\rho(\bar{x}_{k+1})=\dfrac{\bar{x}_{k+1}^{T}y_k}{\bar{x}_{k+1}^{T}\bar{y}_{k+1}}$　　　$\rho(\bar{x}_{k+1})=\dfrac{\bar{x}_{k+1}^{T}K\bar{x}_{k+1}}{\bar{x}_{k+1}^{T}M\bar{x}_{k+1}}$
5. 对 $\bar{x}_{k+1}$ 正则化 $y_{k+1}=\dfrac{\bar{y}_{k+1}}{(\bar{x}_{k+1}^{T}\bar{y}_{k+1})^{\frac{1}{2}}}$　　　$x_{k+1}=\dfrac{\bar{x}_{k+1}}{\left(\bar{x}_{k+1}^{T}M\bar{x}_{k+1}\right)^{1/2}}$
6. 判断 $\dfrac{|\rho(\bar{x}_{k+1})-\rho(\bar{x}_k)|}{\rho(\bar{x}_{k+1})}\le \text{tol}?$
   - 成立：$\lambda_1=\rho(\bar{x}_{k+1})$　$\phi_1=\dfrac{\bar{x}_{k+1}^{T}}{(\bar{x}_{k+1}^{T}\bar{y}_{k+1})^{1/2}}$
   - 不成立：令$k=k+1$，转向2

例3-1

用向量迭代法求广义特征值问题 $K\phi=\lambda M\phi$ 的第一阶特征对(λ_1,ϕ_1)，其中：

$$K=\begin{bmatrix}2&-1&0&0\\-1&2&-1&0\\0&-1&2&-1\\0&0&-1&1\end{bmatrix},\quad M=\begin{bmatrix}0&&&\\&2&&\\&&0&\\&&&1\end{bmatrix}$$

并取误差范数tol = 10^{-6}。

$$\lambda_1=\frac{1}{2}-\frac{\sqrt{2}}{4}=0.146446609,\quad \phi_1=\begin{bmatrix}1/4\\1/2\\(1+\sqrt{2})/4\\\sqrt{2}/2\end{bmatrix}\qquad \lambda_2=\frac{1}{2}+\frac{\sqrt{2}}{4},\quad \phi_2=\begin{bmatrix}-\frac{1}{4}\\-\frac{1}{2}\\\frac{-1+\sqrt{2}}{4}\\\frac{\sqrt{2}}{2}\end{bmatrix}$$

例3-1

取初始向量为 $x_1=\begin{bmatrix}1&1&1&1\end{bmatrix}^T$

对$k=1$，有

$$y_1=\begin{bmatrix}0\\2\\0\\1\end{bmatrix};\quad \bar{x}_2=\begin{bmatrix}3\\6\\7\\8\end{bmatrix};\quad \bar{y}_2=\begin{bmatrix}0\\12\\0\\8\end{bmatrix}$$

$$\rho(\bar{x}_2)=0.1470588,\quad y_2=\begin{bmatrix}0\\1.02899\\0\\0.68599\end{bmatrix}$$

例3-1

k	$\bar{x}_{k+1}$	$\bar{y}_{k+1}$	$\rho(\bar{x}_{k+1})$	$\dfrac{\lvert\lambda_1^{(k+1)}-\lambda_1^{(k)}\rvert}{\lambda_1^{(k+1)}}$	y_k
1	$\begin{bmatrix}3\\6\\7\\8\end{bmatrix}$	$\begin{bmatrix}0\\12\\0\\8\end{bmatrix}$	0.1470588	–	$\begin{bmatrix}0\\1.02899\\0\\0.68599\end{bmatrix}$
2	$\begin{bmatrix}1.71499\\3.42997\\4.11597\\4.10896\end{bmatrix}$	$\begin{bmatrix}0\\6.85994\\0\\4.80196\end{bmatrix}$	0.1464646	0.004057	$\begin{bmatrix}0\\1.00504\\0\\0.70353\end{bmatrix}$

例3-1

3	$\begin{bmatrix}1.70856\\3.41713\\4.12066\\4.82418\end{bmatrix}$	$\begin{bmatrix}0\\6.83426\\0\\4.82418\end{bmatrix}$	0.1464471	0.0001195	$\begin{bmatrix}0\\1.00087\\0\\0.70649\end{bmatrix}$
4	$\begin{bmatrix}1.70736\\3.41472\\4.12121\\4.82771\end{bmatrix}$	$\begin{bmatrix}0\\6.82944\\0\\4.82771\end{bmatrix}$	0.1464466	0.000003519	$\begin{bmatrix}0\\1.00015\\0\\0.70700\end{bmatrix}$
5	$\begin{bmatrix}1.70715\\3.41430\\4.12130\\4.82830\end{bmatrix}$	$\begin{bmatrix}0\\6.82860\\0\\4.82830\end{bmatrix}$	0.1464466	0.000000104	$\begin{bmatrix}0\\1.00003\\0\\0.70709\end{bmatrix}$

例3-1

$$\lambda_1 \approx 0.146447; \quad \phi_1 \approx \begin{bmatrix} 0.25001 \\ 0.50001 \\ 0.60355 \\ 0.70709 \end{bmatrix}$$

讨论

- 正迭代 Forward iteration

$$M\bar{x}_{k+1} = Kx_k \qquad \text{M必须是正定的}$$

$$x_{k+1} = \frac{\bar{x}_{k+1}}{(\bar{x}_{k+1}^{\mathrm{T}} M \bar{x}_{k+1})^{\frac{1}{2}}}$$

$$K\phi = \lambda M\phi \iff M\phi = \lambda^{-1} K\phi$$

正迭代 ⇔ 逆迭代

$$k \to \infty: \quad x_{k+1} \to \phi_n, \ \rho(\bar{x}_{k+1}) \to \lambda_n$$

收敛率：$\dfrac{\lambda_{n-1}}{\lambda_n}, \left(\dfrac{\lambda_{n-1}}{\lambda_n}\right)^2$

讨论

- 正交化 Gram-Schmidt orthogonalization

如迭代向量与已求得的特征向量$\phi_1, \phi_2, \cdots, \phi_m$ 正交，则迭代不可能收敛于这些向量中的任何一个。

$$\tilde{x}_1 = x_1 - \sum_{i=1}^{m} \alpha_i \phi_i \Rightarrow \alpha_i = \phi_i^{\mathrm{T}} M x_1$$

正交条件：$\phi_j^{\mathrm{T}} M \tilde{x}_1 = 0 \quad j = 1, 2, \cdots, m$

如以$\tilde{x}_1$作为初始迭代向量：$z_1 = [\overbrace{0 \ \cdots \ 0}^{m} \quad 1 \ \cdots \ 1]^{\mathrm{T}}$

$$k \to \infty: \quad x_{k+1} \to \phi_{m+1}, \ \rho(\bar{x}_{k+1}) \to \lambda_{m+1}$$

收敛率：$\dfrac{\lambda_{m+1}}{\lambda_{m+2}}, \left(\dfrac{\lambda_{m+1}}{\lambda_{m+2}}\right)^2$

讨论

- 移轴法 Shifting $\quad (K - \alpha M)\phi = \hat{\lambda} M \phi \qquad \hat{\lambda}_i = \lambda_i - \alpha$
  - 如何提高收敛率？
  - 如何求解除λ_1和λ_n以外的特征值？

$$\bar{z}_{k+1} = [\ (1/\hat{\lambda}_1)^k \quad (1/\hat{\lambda}_2)^k \quad \cdots \quad (1/\hat{\lambda}_n)^k\ ]^{\mathrm{T}}$$

$$z_{k+1} = \frac{[\quad (\hat{\lambda}_j/\hat{\lambda}_1)^k \quad \cdots \quad (\hat{\lambda}_j/\hat{\lambda}_{j-1})^k \quad 1 \quad (\hat{\lambda}_j/\hat{\lambda}_{j+1})^k \quad \cdots \quad (\hat{\lambda}_j/\hat{\lambda}_n)^k\ ]^{\mathrm{T}}}{[\sum_{i=1}^{n} (\hat{\lambda}_j/\hat{\lambda}_i)^{2k}]^{\frac{1}{2}}}$$

$$\rho(\bar{z}_{k+1}) = \frac{\bar{z}_{k+1}^{\mathrm{T}} \bar{z}_k}{\bar{z}_{k+1}^{\mathrm{T}} \bar{z}_{k+1}} = \frac{\hat{\lambda}_j \sum_{i=1}^{n} (\hat{\lambda}_j/\hat{\lambda}_i)^{2k-1}}{\sum_{i=1}^{n} (\hat{\lambda}_j/\hat{\lambda}_i)^{2k}}$$

$$k \to \infty: \quad x_{k+1} \to \phi_j, \ \rho(\bar{x}_{k+1}) \to \lambda_j - \alpha$$

收敛率：$\max\left(\left|\hat{\lambda}_j/\hat{\lambda}_{j-1}\right|, \left|\hat{\lambda}_j/\hat{\lambda}_{j+1}\right|\right) \quad \max\left(\left(\hat{\lambda}_j/\hat{\lambda}_{j-1}\right)^2, \left(\hat{\lambda}_j/\hat{\lambda}_{j+1}\right)^2\right)$

例3-2

用带移轴的向量迭代法（移轴量取为1）求广义特征值问题 $K\phi = \lambda M\phi$ 的第一阶特征对(λ_1, ϕ_1)

其中：

$$K = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}, \quad M = \begin{bmatrix} 0 & & & \\ & 2 & & \\ & & 0 & \\ & & & 1 \end{bmatrix}$$

并取误差范数tol = 10^{-6}。

例3-2

$$K - \alpha M = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

$$(K - \alpha M)\phi = \hat{\lambda} M \phi$$

$$\rho(\bar{x}_7) = -0.1464466, \quad x_7 = \begin{bmatrix} -0.250006 \\ -0.50001 \\ 0.103538 \\ 0.707089 \end{bmatrix}$$

$$\lambda_2 \approx \alpha + \rho(\bar{x}_7) = 0.85355339$$

$$\phi_2 \approx x_7$$

讨论

- 瑞利商迭代法 **Rayleigh quotient iteration**

  在带移轴的迭代法中如何选取合适的移轴量？

  将瑞利商 $\rho(\bar{\boldsymbol{x}}_k)$ 取为移轴量

1. $\boldsymbol{x}_1$： $\boldsymbol{y}_1 = \boldsymbol{M}\boldsymbol{x}_1,\ \rho(\bar{\boldsymbol{x}}_1),\ k = 1$
2. 解方程 $[\boldsymbol{K} - \rho(\bar{\boldsymbol{x}}_k)\boldsymbol{M}]\bar{\boldsymbol{x}}_{k+1} = \boldsymbol{y}_k$
3. 计算 $\bar{\boldsymbol{y}}_{k+1} = \boldsymbol{M}\bar{\boldsymbol{x}}_{k+1}$
4. 计算瑞利商 $\rho(\bar{\boldsymbol{x}}_{k+1}) = \dfrac{\bar{\boldsymbol{x}}_{k+1}^{\mathrm{T}} \cdot \boldsymbol{y}_k}{\bar{\boldsymbol{x}}_{k+1}^{\mathrm{T}} \cdot \bar{\boldsymbol{y}}_{k+1}} + \rho(\bar{\boldsymbol{x}}_k)$
5. 对 $\bar{\boldsymbol{x}}_{k+1}$ 正则化 $\boldsymbol{y}_{k+1} = \dfrac{\bar{\boldsymbol{y}}_{k+1}}{(\bar{\boldsymbol{x}}_{k+1}^{\mathrm{T}}\bar{\boldsymbol{y}}_{k+1})^{1/2}}$
6. 判断 $\dfrac{|\rho(\bar{\boldsymbol{x}}_{k+1}) - \rho(\bar{\boldsymbol{x}}_k)|}{\rho(\bar{\boldsymbol{x}}_{k+1})} \le \mathrm{tol}?$

讨论

- 成立：$\lambda_i = \rho(\bar{\boldsymbol{x}}_{k+1})$ $\quad \phi_i = \boldsymbol{x}_{k+1}^{\mathrm{T}} = \dfrac{\bar{\boldsymbol{x}}_{k+1}^{\mathrm{T}}}{(\bar{\boldsymbol{x}}_{k+1}^{\mathrm{T}}\bar{\boldsymbol{y}}_{k+1})^{1/2}}$
- 不成立： 令$k = k+1$，转向2

收敛结果(λ_i, ϕ_i)取决于$\boldsymbol{x}_1$和 $\rho(\bar{\boldsymbol{x}}_1)$ 。

$$[\boldsymbol{\Lambda} - \rho(\bar{\boldsymbol{z}}_k)\boldsymbol{I}]\bar{\boldsymbol{z}}_{k+1} = \bar{\boldsymbol{z}}_k$$

$$\rho(\bar{\boldsymbol{z}}_{k+1}) = \frac{\bar{\boldsymbol{z}}_{k+1}^{\mathrm{T}}\bar{\boldsymbol{z}}_k}{\bar{\boldsymbol{z}}_{k+1}^{\mathrm{T}}\bar{\boldsymbol{z}}_{k+1}} + \rho(\bar{\boldsymbol{z}}_k)$$

$$\bar{\boldsymbol{z}}_k^{\mathrm{T}} = [\ 1 \quad O(\varepsilon) \quad O(\varepsilon) \quad \cdots \quad O(\varepsilon)\ ]$$

$$\rho(\bar{\boldsymbol{z}}_k) = \lambda_1 + O(\varepsilon^2)$$

$$\bar{\boldsymbol{z}}_{k+1}^{\mathrm{T}} = [\ \frac{1}{O(\varepsilon^2)} \quad \frac{O(\varepsilon)}{\lambda_2 - \lambda_1} \quad \cdots \quad \frac{O(\varepsilon)}{\lambda_n - \lambda_1}\ ]$$

$$\boldsymbol{z}_{k+1}^{\mathrm{T}} = [\ 1 \quad O(\varepsilon^3) \quad \cdots \quad O(\varepsilon^3)\ ]$$ 具有三阶收敛性！