Lanczos迭代法
Lanczos Iteration Method

Tuesday, March 9, 2010

Lanczos变换

在瑞利-利兹法中，如何选取一组线性独立的里兹向量？ 利用Gram-Schmidt正交化方法

- 选取初始向量$\hat{\boldsymbol{x}}_1$： $\boldsymbol{x}_1 = \dfrac{\hat{\boldsymbol{x}}_1}{\beta_1}$ $\quad \beta_1 = \left(\hat{\boldsymbol{x}}_1^{\mathrm{T}} \boldsymbol{M} \hat{\boldsymbol{x}}_1\right)^{1/2}$
- 生成 $\boldsymbol{x}_i (i = 2, 3, \cdots, q)$

$$\boldsymbol{K}\tilde{\boldsymbol{x}}_i = \boldsymbol{M}\boldsymbol{x}_{i-1}$$

$$\hat{\boldsymbol{x}}_i = \tilde{\boldsymbol{x}}_i - \sum_{j=1}^{i-1} a_{ij}\boldsymbol{x}_j \qquad a_{ij} = \boldsymbol{x}_j^{\mathrm{T}}\boldsymbol{M}\tilde{\boldsymbol{x}}_i = \tilde{\boldsymbol{x}}_i^{\mathrm{T}}\boldsymbol{M}\boldsymbol{x}_j$$

$$\boldsymbol{x}_i = \frac{\hat{\boldsymbol{x}}_i}{\beta_i} \qquad \beta_i = \left(\hat{\boldsymbol{x}}_i^{\mathrm{T}}\boldsymbol{M}\hat{\boldsymbol{x}}_i\right)^{1/2}$$

Lanczos变换

$$a_{ij} = \boldsymbol{x}_j^{\mathrm{T}}\boldsymbol{M}\tilde{\boldsymbol{x}}_i = \tilde{\boldsymbol{x}}_i^{\mathrm{T}}\boldsymbol{M}\boldsymbol{x}_j \Leftarrow \boldsymbol{K}\tilde{\boldsymbol{x}}_i = \boldsymbol{M}\boldsymbol{x}_{i-1} \qquad \tilde{\boldsymbol{x}}_i^{\mathrm{T}}\boldsymbol{K} = \boldsymbol{x}_{i-1}^{\mathrm{T}}\boldsymbol{M}$$

$$= \tilde{\boldsymbol{x}}_i^{\mathrm{T}}\boldsymbol{K}\tilde{\boldsymbol{x}}_{j+1} \qquad \hat{\boldsymbol{x}}_i = \tilde{\boldsymbol{x}}_i - \sum_{j=1}^{i-1} a_{ij}\boldsymbol{x}_j$$

$$= \boldsymbol{x}_{i-1}^{\mathrm{T}}\boldsymbol{M}\tilde{\boldsymbol{x}}_{j+1} \Leftarrow \tilde{\boldsymbol{x}}_{j+1} = \hat{\boldsymbol{x}}_{j+1} + \sum_{k=1}^{j} a_{j+1,k}\boldsymbol{x}_k$$

$$= \boldsymbol{x}_{i-1}^{\mathrm{T}}\boldsymbol{M}\hat{\boldsymbol{x}}_{j+1} + \sum_{k=1}^{j} a_{j+1,k}\boldsymbol{x}_{i-1}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{x}_k \Leftarrow \boldsymbol{x}_i = \frac{\hat{\boldsymbol{x}}_i}{\beta_i}$$

$$= \beta_{j+1}\boldsymbol{x}_{i-1}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{x}_{j+1} + \sum_{k=1}^{j} a_{j+1,k}\boldsymbol{x}_{i-1}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{x}_k \Leftarrow \begin{array}{l} \boldsymbol{x}_j^{\mathrm{T}}\boldsymbol{M}\boldsymbol{x}_k = \delta_{jk} \\ j, k = 1, 2, \cdots, i-1 \end{array}$$

$$\Downarrow$$

$$a_{ij} = 0\ (j = i-3, i-4, \cdots, 1)$$

$$a_{i,i-2} = \beta_{i-1}$$

$$\hat{\boldsymbol{x}}_i = \tilde{\boldsymbol{x}}_i - a_{i-1}\boldsymbol{x}_{i-1} - \beta_{i-1}\boldsymbol{x}_{i-2}$$

$$a_{i-1} = a_{i,i-1} = \tilde{\boldsymbol{x}}_i^{\mathrm{T}}\boldsymbol{M}\boldsymbol{x}_{i-1}$$

Lanczos变换 tridiagonalization

$$\boldsymbol{K}\tilde{\boldsymbol{x}}_i = \boldsymbol{M}\boldsymbol{x}_{i-1} \qquad \hat{\boldsymbol{x}}_i = \tilde{\boldsymbol{x}}_i - a_{i-1}\boldsymbol{x}_{i-1} - \beta_{i-1}\boldsymbol{x}_{i-2} \qquad \boldsymbol{x}_i = \frac{\hat{\boldsymbol{x}}_i}{\beta_i}$$

$$\boldsymbol{K}^{-1}\boldsymbol{M}\boldsymbol{x}_{i-1} = \beta_{i-1}\boldsymbol{x}_{i-2} + a_{i-1}\boldsymbol{x}_{i-1} + \beta_i\boldsymbol{x}_i \quad (i = 2, 3, \cdots, q+1) \quad \boldsymbol{x}_0 = 0$$

$$\boldsymbol{K}^{-1}\boldsymbol{M}\boldsymbol{X} = \boldsymbol{X}\boldsymbol{T} + \beta_{q+1}\boldsymbol{x}_{q+1}\boldsymbol{e}_q^{\mathrm{T}} \Rightarrow \boldsymbol{T} = \boldsymbol{X}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{K}^{-1}\boldsymbol{M}\boldsymbol{X}$$

$$\boldsymbol{X} = [\ \boldsymbol{x}_1 \quad \boldsymbol{x}_2 \quad \cdots \quad \boldsymbol{x}_q\ ] \qquad \boldsymbol{e}_q^{\mathrm{T}} = [\ 0 \quad \cdots \quad 0 \quad 1\ ]$$

$$\boldsymbol{T} = \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{q-1} & \alpha_{q-1} & \beta_q \\ & & & \beta_q & \alpha_q \end{bmatrix}$$

— 三对角阵

Lanczos变换

$$\boldsymbol{K}\boldsymbol{\phi} = \lambda\boldsymbol{M}\boldsymbol{\phi}$$

$$\Downarrow \boldsymbol{\phi} = \boldsymbol{X}\boldsymbol{z}$$

$$\boldsymbol{K}\boldsymbol{X}\boldsymbol{z} = \lambda\boldsymbol{M}\boldsymbol{X}\boldsymbol{z}$$

$$\Downarrow \boldsymbol{T} = \boldsymbol{X}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{K}^{-1}\boldsymbol{M}\boldsymbol{X}$$

$$\boldsymbol{T}\boldsymbol{z} = \frac{1}{\lambda}\boldsymbol{z}$$

$$\Downarrow$$

$$(\bar{\lambda}_i, \bar{\boldsymbol{z}}_i)$$

$$\Downarrow$$

$$(\bar{\lambda}_i, \boldsymbol{X}\bar{\boldsymbol{z}}_i)$$

Lanczos变换 解的精度

$$\boldsymbol{K}\boldsymbol{\phi} = \lambda\boldsymbol{M}\boldsymbol{\phi} \qquad \boldsymbol{K}\boldsymbol{\phi} - \lambda\boldsymbol{\phi} = \boldsymbol{0}$$

$$\Downarrow \boldsymbol{M} = \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} \qquad \min_i \left|\lambda_i - \bar{\lambda}\right| \le \left\|r\right\|_2$$

$$\boldsymbol{S}^{\mathrm{T}}\boldsymbol{K}^{-1}\boldsymbol{S}\boldsymbol{\psi} = \frac{1}{\lambda}\boldsymbol{\psi} \Rightarrow (\bar{\lambda}_i, \bar{\boldsymbol{\psi}}_i)$$

$$\boldsymbol{\psi} = \boldsymbol{S}^{\mathrm{T}}\boldsymbol{\phi} = \boldsymbol{S}^{\mathrm{T}}\boldsymbol{X}\boldsymbol{z}$$

$$\min_k \left|\frac{1}{\lambda_k} - \frac{1}{\bar{\lambda}_i}\right| \le \left\|\boldsymbol{S}^{\mathrm{T}}\boldsymbol{K}^{-1}\boldsymbol{S}\bar{\boldsymbol{\psi}}_i - \frac{1}{\bar{\lambda}_i}\bar{\boldsymbol{\psi}}_i\right\|_2$$

$$= \left\|\boldsymbol{S}^{\mathrm{T}}\boldsymbol{K}^{-1}\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}}\boldsymbol{X}\bar{\boldsymbol{z}}_i - \frac{1}{\bar{\lambda}_i}\boldsymbol{S}^{\mathrm{T}}\boldsymbol{X}\bar{\boldsymbol{z}}_i\right\|_2 \Leftarrow \begin{array}{l} \boldsymbol{M} = \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} \\ \boldsymbol{T}\boldsymbol{z} = \dfrac{1}{\lambda}\boldsymbol{z} \end{array}$$

$$= \left\|\boldsymbol{S}^{\mathrm{T}}(\boldsymbol{K}^{-1}\boldsymbol{M}\boldsymbol{X} - \boldsymbol{X}\boldsymbol{T})\bar{\boldsymbol{z}}_i\right\|_2 \Leftarrow \boldsymbol{K}^{-1}\boldsymbol{M}\boldsymbol{X} = \boldsymbol{X}\boldsymbol{T} + \beta_{q+1}\boldsymbol{x}_{q+1}\boldsymbol{e}_q^{\mathrm{T}}$$

$$= \left\|\boldsymbol{S}^{\mathrm{T}}\beta_{q+1}\boldsymbol{x}_{q+1}\boldsymbol{e}_q^{\mathrm{T}}\bar{\boldsymbol{z}}_i\right\|_2 \Leftarrow \left\|\boldsymbol{S}^{\mathrm{T}}\boldsymbol{x}_{q+1}\right\|_2 = 1 \qquad \boldsymbol{e}_q^{\mathrm{T}}\bar{\boldsymbol{z}}_i = \bar{z}_{iq}$$

$$\le \left|\beta_{q+1}\bar{z}_{iq}\right|$$

例3-7

利用Lanczos变换法求解广义特征值问题$\boldsymbol{K\phi} = \lambda \boldsymbol{M\phi}$的最小二阶特征值，其中

$$\boldsymbol{K} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{bmatrix} \qquad \boldsymbol{M} = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1/2 \end{bmatrix}$$

本问题的精确解为

$$\lambda_1 = 0.09789,\ \lambda_2 = 0.824,\ \lambda_3 = 2,\ \lambda_4 = 3.18,\ \lambda_5 = 3.90$$

例3-7

取初始迭代向量$\hat{\boldsymbol{x}}_1 = [1 \quad 1 \quad 1 \quad 1 \quad 1]^{\mathrm{T}}$

$$\beta_1 = 2.121 \qquad \boldsymbol{x}_1 = 0.4714[1 \quad 1 \quad 1 \quad 1 \quad 1]^{\mathrm{T}}$$

$$i = 2 \quad \tilde{\boldsymbol{x}}_2 = \begin{bmatrix} 2.121 \\ 3.771 \\ 4.950 \\ 5.657 \\ 5.893 \end{bmatrix} \quad a_1 = 9.167 \quad \hat{\boldsymbol{x}}_2 = \begin{bmatrix} -2.20 \\ -0.55 \\ 0.6285 \\ 1.336 \\ 1.571 \end{bmatrix}$$

$$\beta_2 = 2.925 \qquad \boldsymbol{x}_2 = \begin{bmatrix} -0.7521 \\ -0.1880 \\ 0.2149 \\ 0.4566 \\ 0.5372 \end{bmatrix}$$

例3-7

$$i = 3 \quad \tilde{\boldsymbol{x}}_3 = \begin{bmatrix} 0.00 \\ 0.7521 \\ 1.692 \\ 2.417 \\ 2.686 \end{bmatrix} \quad a_2 = 2.048 \quad \hat{\boldsymbol{x}}_3 = \begin{bmatrix} 0.1612 \\ -0.2417 \\ -0.1266 \\ 0.1036 \\ 0.2072 \end{bmatrix}$$

$$\beta_3 = 0.3642 \qquad \boldsymbol{x}_3 = \begin{bmatrix} 0.4425 \\ -0.6637 \\ -0.3477 \\ 0.2845 \\ 0.5689 \end{bmatrix}$$

例3-7

$$\boldsymbol{T} = \begin{bmatrix} 9.167 & 2.925 \\ 2.925 & 2.048 \end{bmatrix}$$

$$\boldsymbol{T}\boldsymbol{z} = \frac{1}{\lambda}\boldsymbol{z} \Rightarrow \bar{\lambda}_1 = 0.0979, \quad \bar{\boldsymbol{z}}_1 = \begin{bmatrix} -0.9414 \\ -0.3372 \end{bmatrix}$$

$$\bar{\lambda}_2 = 1.0, \quad \bar{\boldsymbol{z}}_2 = \begin{bmatrix} 0.3372 \\ -0.9414 \end{bmatrix}$$ 误差大！

$$\left| \frac{1}{\lambda_1} - \frac{1}{\bar{\lambda}_1} \right| = 0.0016 \le \left| \beta_3 \bar{z}_{12} \right| = 0.1228$$

$$\left| \frac{1}{\lambda_2} - \frac{1}{\bar{\lambda}_2} \right| = 0.213 \le \left| \beta_3 \bar{z}_{22} \right| = 0.3429$$

Lanczos变换法

- 存在的问题
  - 结果的精度取决于所生成的Lanczos向量的质量；
  - Lanczos向量之间可能会丧失正交性；
- 解决办法
  - 引入迭代法
  - 已收敛的特征向量$\boldsymbol{\phi}_i$不再参与迭代：使迭代向量与$\boldsymbol{\phi}_i$正交
  - 使用移轴法加快收敛
  - 引入重正交化（Reorthogonalization）
    - 对Lanczos向量进行重正交化

Lanczos迭代法　　将Lanczos法与迭代法结合

- 选取与所有已收敛的特征向量正交的初始迭代向量$\hat{\boldsymbol{x}}_1$，并正则化

$$\boldsymbol{x}_1 = \frac{\hat{\boldsymbol{x}}_1}{\beta_1} \qquad \beta_1 = \left(\hat{\boldsymbol{x}}_1^{\mathrm{T}} \boldsymbol{M} \hat{\boldsymbol{x}}_1\right)^{1/2}$$

- 选取一移轴量μ（对第一轮Lanczos循环取$\mu = 0$），生成Lanczos基向量$\boldsymbol{x}_i (i = 2, 3, \cdots, q)$

$$(\boldsymbol{K} - \mu \boldsymbol{M})\tilde{\boldsymbol{x}}_i = \boldsymbol{M}\boldsymbol{x}_{i-1} \qquad a_{i-1} = \tilde{\boldsymbol{x}}_i^{\mathrm{T}} \boldsymbol{M} \boldsymbol{x}_{i-1}$$

$$\hat{\boldsymbol{x}}_i' = \tilde{\boldsymbol{x}}_i - a_{i-1}\boldsymbol{x}_{i-1} - \beta_{i-1}\boldsymbol{x}_{i-2}$$

$$\boxed{\hat{\boldsymbol{x}}_i = \hat{\boldsymbol{x}}_i' - \sum_{k=1}^{i-1} \left(\hat{\boldsymbol{x}}_i'^{\mathrm{T}} \boldsymbol{M} \boldsymbol{x}_k\right) \boldsymbol{x}_k - \sum_{j=1}^{n_c} \left(\hat{\boldsymbol{x}}_i'^{\mathrm{T}} \boldsymbol{M} \boldsymbol{\phi}_j\right) \boldsymbol{\phi}_j}$$

$$\beta_i = \left(\hat{\boldsymbol{x}}_i^{\mathrm{T}} \boldsymbol{M} \hat{\boldsymbol{x}}_i\right)^{1/2} \qquad \boldsymbol{x}_i = \frac{\hat{\boldsymbol{x}}_i}{\beta_i}$$

Lanczos迭代法

- 求解 $\boldsymbol{T}z=\frac{1}{\lambda}z$，得到在本次循环中收敛的$r$个特征值$\lambda_{n_c+1},\lambda_{n_c+2},\cdots,\lambda_{n_c+r}$及相应的特征向量，并令 $n_c=n_c+r$
- 如果$n_c<p$，转向1进行新一轮的Lanczos循环

讨论

- 部分正交或选择性重正交
- 检测Lanczos向量正交性的方法
- 生成初始迭代向量的方法
- 更有效的移轴法
- 块Lanczos方法
- Sturm序列
- BLZPACK、ARPACK

LANCZOS90