Advanced Numerical Methods

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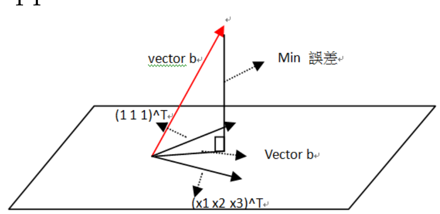
- Review: Interpolation v.s Approximation
  - Interpolation

$$
\begin{aligned}
ex : ax^2 + bx + c &= y \\
\begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} &= \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}
\end{aligned}
$$

  - Approximation



$$
\begin{aligned}
ax_1 + b &\approx y_1 \\
ax_2 + b &\approx y_2 \\
ax_3 + b &\approx y_3
\end{aligned}
$$

$$
\left.\begin{aligned} A = QR \\ \vec{b'} = QQ^T\vec{b} \end{aligned}\right] \qquad \Rightarrow A\vec{x} = \vec{b'}
$$

$$
\begin{aligned}
QR\vec{x} &= QQ^T\vec{b} \\
Q^TQR\vec{x} &= Q^TQQ^T\vec{b} \\
\vec{x} &= R^{-1}(Q^T\vec{b})
\end{aligned}
$$

- Given a linear equation:

$$A\vec{x} = \vec{b}$$

Def:

$$A^{-1} = f(A)$$

$$\begin{aligned} \Rightarrow \vec{x} &= A^{-1}\vec{b} \\ &= f(A)\vec{b} \\ &\approx p(A)\vec{b} \end{aligned}$$

$$\begin{aligned} P(A)\vec{b} &= (\alpha_{m-1}A^{m-1} + \alpha_{m-2}A^{m-2} + \cdots + \alpha_1 A + \alpha_0 I) \\ &\in K_m\left(A, \frac{\vec{(b)}}{||\vec{(b)}||}\right) \end{aligned}$$

and because

$$K_m\left(A, \frac{\vec{(b)}}{||\vec{(b)}||}\right) = span\{\vec{b}, A\vec{b}, \cdots, A^{m-1}\vec{b}\}$$

So the goal becomes finding:

$$\vec{y} = \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{m-1} \end{bmatrix} \Rightarrow \quad Q_m\vec{y} \approx A^{-1}\vec{b}$$

$$\Rightarrow \quad Solving\ \vec{y}\ then\ we\ can\ obtain\ \vec{x} = A^{-1}\vec{b}$$

- FOM(Full orthogonol method):

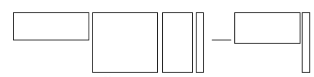
$$\begin{aligned} X_m &= Q_m\vec{y_n}, \\ residual\ \vec{r} &= A\vec{X_m} - \vec{b} \\ &\Rightarrow Minimun\ Error\ when\ \vec{r} \perp\ Q_m \\ &\Rightarrow Galerkin\ condition \end{aligned}$$

Let $\vec{r} \perp \ Q_m, Q_m = [q_1, q_2, \cdots, q_m]$

$$\begin{cases} \vec{q_1^T} \vec{r} = 0 \\ \vec{q_2^T} \vec{r} = 0 \\ \qquad \vdots \\ \vec{q_m^T} \vec{r} = 0 \end{cases}$$

$$\Rightarrow 0 \qquad = Q_m^T \vec{r}$$

$$\begin{aligned} &= \quad Q_m^T (A Q_m \vec{y_m} - \vec{b}) \\ &= \quad Q_m^T A Q_m^T \vec{y_m} - Q_m^t \vec{b} \end{aligned}$$



$$\Rightarrow y_m = \underbrace{(Q_m^t A Q_m^T)^{-1}}_{Rayleigh\ quotient} Q_m^T \vec{b}$$

By Arnoldirelation,we know

$$\begin{aligned} A Q_m &= Q_m H_m + \beta \vec{q_{m+1}} \vec{e_m^t} \\ Q_m^T A Q_m &= \underbrace{Q_m^T Q_m H_m}_{I} + \beta \underbrace{Q_m^T \vec{q_{m+1}}}_{0} \vec{e_m^T} \\ &= H_m \end{aligned}$$

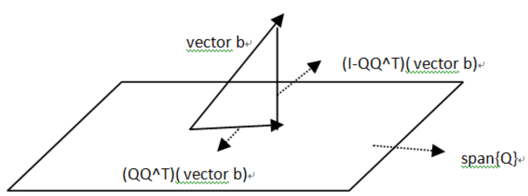
Algorithm 1 Full orthogonol method Algorithm

1. $\vec{q_1} = \frac{\vec{b}_1}{\|\vec{b}_1\|}$, $Q_1 = [\vec{q_1}]$, $H_1 = \vec{q_1}^T A \vec{q_1}$
2. For $i = 0, 1, 2, \ldots, until\ converge$
3. $\quad \vec{y_i} = H_i^{-1}(Q_i \vec{b})$
4. $\quad if \|r_m\| = \|AQ_i \vec{(y)}_i - \vec{b}\|\ is\ small\ enough$
5. $\quad return\ \vec{x}_i = Q_i \vec{y_i}$
6. $\quad expand\ Q_{i+1} = [Q_i \vec{q}_{i+1}]$, $H_{i+1} = \begin{bmatrix} H_i \vec{h} \\ - \end{bmatrix}$ $by\ Arnoldi\ relation$

$End\ for$

Note:For reducing the time complexity:

$$\begin{aligned}
\vec{r_i} &= AQ_i\vec{y_i} - \vec{b} \\
&= (Q_iH_i + \beta_i\vec{q}_{i+1}\vec{e^T}_i)\vec{y_i} - \vec{b}
\end{aligned}$$



$$\begin{aligned}
&= Q_iH_i\vec{y_i} + \beta_i\vec{q}_{i+1}\vec{e^T}_i\vec{y_i} - \vec{b} \\
&= Q_iH_i(H_i^{-1}Q_i^T\vec{b}) + (\beta_iy_i)\vec{q}_{i+1} - \vec{b} \\
&= \underbrace{(Q_iQ_i^T - I)}_{Note\ below}\vec{b} + (\beta_iy_i)\vec{q}_{i+1} \\
&= (\beta_iy_i)\vec{q}_{i+1} \\
For \quad & \underbrace{Q_i \underbrace{Q_i^T\vec{b}}_{\|\vec{b}\|\vec{e}_1} - I\vec{b}}_{\|\vec{b}\|\vec{q}_1 - \vec{b} = 0}
\end{aligned}$$

More attention:from the above result,we can find

$$\arg\min_{\vec{y_i}} \|\vec{r_i}\| = \arg\min_{\vec{y_i}} \|AQ_i\vec{y_i} - \vec{b}\| = \|\beta_i\vec{y_i}\|$$

$$\Rightarrow \textit{ But } \vec{y_i} \textit{ appear in argument and result} \Rightarrow \textit{ Can't be solve}!$$

We need GMERS method.

- GMERS method
  Refer to the original matrix structure:

$$\begin{aligned} r_i &= AQ_i\vec{y_i} - \vec{b} \\ &= (Q_iH_i + \beta_i\vec{q_{i+1}}\vec{e_i}^T)\vec{y_i} - Q_i\vec{e_i}\|\vec{b}\| \\ &= Q_{i+1}\begin{bmatrix} H_i \\ \beta_i\vec{e_1}^T \end{bmatrix}\vec{y_i} - Q_{i+1}\vec{e_1}\|\vec{b}\| \\ &= Q_{i+1}[\hat{H}\vec{y_i} - \|\vec{b}\|\vec{e_1}] \end{aligned}$$

The problem becomes:

$$\Rightarrow \arg\min_{\vec{y_i}} \|\hat{H}\vec{y_i} - \|\vec{b}\|\vec{e_1}\| \Rightarrow \textit{ least square error problem}$$

Algorithm 2 GMERS(alteration from Full orthogonol method)Algorithm

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1. $\vec{q_1} = \frac{\vec{b_1}}{\|\vec{b_1}\|}$, $Q_1 = [\vec{q_1}]$, $H_1 = \vec{q_1}^T A\vec{q_1}$
2. For $i = 0, 1, 2, \ldots,$ *until converge*
3. $\arg\min_{\vec{y_i}} \|\hat{H}\vec{y_i} - \|\vec{b}\|\vec{e_1}\|$
4. $\quad if \|r_i\| = \|AQ_i\vec{(y)}_i - \vec{b}\|$ *is small enough*
5. $\quad return\ \vec{x_i} = Q_i\vec{y_i} - \vec{b}$
6. $\quad expand\ Q_{i+1} = [Q_i\vec{q}_{i+1}]$, $H_{i+1} = \begin{bmatrix} H_i\vec{h} \\ - \end{bmatrix}$ *by Arnoldi relation*

End for
