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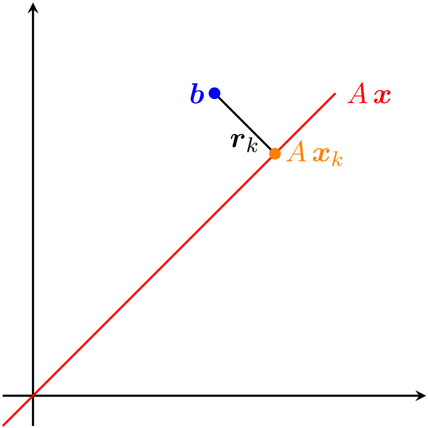
DE INFORMÁTICA

INF 285 - Computación Científica
Ingeniería Civil Informática

13: GMRes - Generalized Minimal Residual Method



Supongamos $A \in \mathbb{R}^{n\times n}$ y $\boldsymbol{b} \in \mathbb{R}^n$.

Sea $\boldsymbol{r}_k = \boldsymbol{b} - A\,\boldsymbol{x}_k$.

¿Cómo convertimos un sistema de ecuaciones lineales cuadrado en uno sobre-determinado?

Ejemplo 1

Consideremos $A\,\boldsymbol{x} = \boldsymbol{b}$ *con* $A \in \mathbb{R}^{n\times n}$, $\boldsymbol{x} \in \mathbb{R}^n$ *y* $\boldsymbol{b} \in \mathbb{R}^n$.
¿Qué sucede si restringimos el espacio de búsqueda de $\mathbb{R}^n$ *a* $\mathbb{R}$*?*

$$\boldsymbol{x}_k \approx c_1\,\boldsymbol{q}_1 \Rightarrow A\,\underbrace{c_1\,\boldsymbol{q}_1}_{\boldsymbol{x}_k} \approx \boldsymbol{b} \Rightarrow (A\,\boldsymbol{q}_1)\;c_1 \approx \boldsymbol{b}$$

GMRes

Restringimos el dominio de $\boldsymbol{x}_k$ al sub-espacio de Krylov $\mathcal{K}_k$, es decir $\boldsymbol{x}_k \in \mathcal{K}_k$.

¿Qué es $\mathcal{K}_k$?

$$\mathcal{K}_k = \operatorname{span}\left(\boldsymbol{b}, A\,\boldsymbol{b}, A^2\,\boldsymbol{b}, \dots, A^{k-1}\,\boldsymbol{b}\right)$$

¿Cómo restringimos $\boldsymbol{x}_k \in \mathcal{K}_k$?

$$\boldsymbol{x}_k = \widetilde{c}_1\,\boldsymbol{b} + \widetilde{c}_2\,A\,\boldsymbol{b} + \cdots + \widetilde{c}_k\,A^{k-1}\,\boldsymbol{b}$$

¿Qué sucede si por ejemplo $k=2$? ¿$k=3$?

GMRes

Caso general:

$$\begin{bmatrix} \boldsymbol{b} & A\,\boldsymbol{b} & \cdots & A^{k-1}\,\boldsymbol{b} \end{bmatrix} \begin{bmatrix} \widetilde{c}_1 \\ \widetilde{c}_2 \\ \vdots \\ \widetilde{c}_k \end{bmatrix} = \boldsymbol{x}_k$$

donde queremos minimizar el error cuadrático:

$$\|\boldsymbol{b} - A\,\boldsymbol{x}_k\|_2^2 = \left\| \boldsymbol{b} - A\,\begin{bmatrix} \boldsymbol{b} & A\,\boldsymbol{b} & \cdots & A^{k-1}\,\boldsymbol{b} \end{bmatrix} \begin{bmatrix} \widetilde{c}_1 \\ \widetilde{c}_2 \\ \vdots \\ \widetilde{c}_k \end{bmatrix} \right\|_2^2$$

GMRes

$$\left\| \boldsymbol{b} - \underbrace{\underbrace{A}_{n\times n} \underbrace{\begin{bmatrix} \boldsymbol{b} & A\,\boldsymbol{b} & \cdots & A^{k-1}\,\boldsymbol{b} \end{bmatrix}}_{K_{n\times k}}}_{n\times k} \begin{bmatrix} \widetilde{c}_1 \\ \widetilde{c}_2 \\ \vdots \\ \widetilde{c}_k \end{bmatrix} \right\|_2^2$$

Hemos convertido un sistema de ecuaciones lineales cuadrado a un problema de mínimos cuadrados 😃

La matriz $K_{n\times k}$ es mal condicionada porque sus columnas son "casi" linealmente independientes 😟

GMRes

Ortonormalización de Gram-Schmidt modificada al rescate!

$$\downarrow$$

Iteración de Arnoldi

$$\operatorname{span}\left(\boldsymbol{b}, A\,\boldsymbol{b}, A^2\,\boldsymbol{b}, \ldots, A^{k-1}\,\boldsymbol{b}\right)$$

$$\Downarrow$$

$$\operatorname{span}\left(\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3, \ldots, \boldsymbol{q}_k\right)$$

$$\Downarrow$$

$$\operatorname{span}\left(\boldsymbol{q}_1, A\,\boldsymbol{q}_1, A\,\boldsymbol{q}_2, \ldots, A\,\boldsymbol{q}_{k-1}\right)$$

¿Cómo se obtiene?

$$\downarrow$$

Descomposición parcial de Hessenberg

Descomposición parcial de Hessenberg

$$\underbrace{A}_{n\times n}\underbrace{Q_k}_{n\times k} = \underbrace{Q_{k+1}}_{n\times(k+1)}\underbrace{\widetilde{H}_k}_{(k+1)\times k}$$

$$A\begin{bmatrix}\boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_k\end{bmatrix} = \begin{bmatrix}\boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_{k+1}\end{bmatrix}\begin{bmatrix}h_{11} & h_{12} & \cdots & h_{1,k}\\ h_{21} & h_{22} & \cdots & h_{2,k}\\ 0 & h_{32} & \ddots & \vdots\\ \vdots & \ddots & \ddots & h_{k,k}\\ 0 & \cdots & 0 & h_{k+1,k}\end{bmatrix}$$

Descomposición parcial de Hessenberg

$$A\,Q_k = Q_{k+1}\,\widetilde{H}_k$$

$$A\begin{bmatrix}\boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_k\end{bmatrix} = \begin{bmatrix}\boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_{k+1}\end{bmatrix}\begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1,k} \\ h_{21} & h_{22} & \cdots & h_{2,k} \\ 0 & h_{32} & \ddots & \vdots \\ \vdots & \ddots & \ddots & h_{k,k} \\ 0 & \cdots & 0 & h_{k+1,k} \end{bmatrix}$$

$$\begin{aligned} A\,\boldsymbol{q}_1 &= h_{11}\,\boldsymbol{q}_1 + h_{21}\,\boldsymbol{q}_2 \\ A\,\boldsymbol{q}_2 &= h_{21}\,\boldsymbol{q}_1 + h_{22}\,\boldsymbol{q}_2 + h_{32}\,\boldsymbol{q}_3 \\ &\vdots \end{aligned}$$

$$\boldsymbol{q}_1 = \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|} \qquad \boldsymbol{q}_i^*\,\boldsymbol{q}_j = 0\ , i \neq j \qquad \|\boldsymbol{q}_i\| = 1$$

$$\left\| \boldsymbol{b} - A \underbrace{\begin{bmatrix} \boldsymbol{b} & A\,\boldsymbol{b} & \cdots & A^{k-1}\,\boldsymbol{b} \end{bmatrix}}_{K} \underbrace{\begin{bmatrix} \widetilde{c}_1 \\ \vdots \\ \widetilde{c}_k \end{bmatrix}}_{\widetilde{\boldsymbol{c}}} \right\|_2^2 = \|\boldsymbol{b} - A\,K\,\widetilde{\boldsymbol{c}}\|_2^2$$

Descomposición de Hessenberg: $A\,Q_k = Q_{k+1}\,\widetilde{H}_k$

$$\operatorname{span}\left(\boldsymbol{b}, A\,\boldsymbol{b}, A^2\,\boldsymbol{b}, \dots, A^{k-1}\,\boldsymbol{b}\right)$$
$$\Downarrow$$
$$\operatorname{span}\left(\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3, \dots, \boldsymbol{q}_k\right)$$
$$\Downarrow$$
$$\operatorname{span}\left(\boldsymbol{q}_1, A\,\boldsymbol{q}_1, A\,\boldsymbol{q}_2, \dots, A\,\boldsymbol{q}_{k-1}\right)$$

$$\|\boldsymbol{b} - A\,K\,\widetilde{\boldsymbol{c}}\|_2^2 = \|\boldsymbol{b} - A\,Q_k\,\boldsymbol{c}\|_2^2 = \|\boldsymbol{b} - Q_{k+1}\,\widetilde{H}_k\,\boldsymbol{c}\|_2^2$$

Recordemos que $\boldsymbol{q}_1 = \dfrac{\boldsymbol{b}}{\|\boldsymbol{b}\|_2}$,

por lo tanto, se obtiene que $\boldsymbol{b} = \|\boldsymbol{b}\|_2\,Q_{k+1}\,\boldsymbol{e}_1$

$$\begin{aligned}\|Q_{k+1}\,\widetilde{H}_k\,\boldsymbol{c} - \boldsymbol{b}\|_2^2 &= \|Q_{k+1}\,\widetilde{H}_k\,\boldsymbol{c} - \|\boldsymbol{b}\|_2\,Q_{k+1}\,\boldsymbol{e}_1\|_2^2 \\ &= \|Q_{k+1}\left(\widetilde{H}_k\,\boldsymbol{c} - \|\boldsymbol{b}\|_2\,\boldsymbol{e}_1\right)\|_2^2 \\ &= \|\widetilde{H}_k\,\boldsymbol{c} - \|\boldsymbol{b}\|_2\,\boldsymbol{e}_1\|_2^2\end{aligned}$$

$$\underbrace{\|\boldsymbol{b} - A\,K\,\widetilde{\boldsymbol{c}}\|_2^2}_{\text{Mínimos cuadrados de } m\times k} \quad = \quad \underbrace{\|\widetilde{H}_k\,\boldsymbol{c} - \|\boldsymbol{b}\|_2\,\boldsymbol{e}_1\|_2^2}_{\text{Mínimos cuadrados de } (k+1)\times k}$$

$$\begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1,k} \\ h_{21} & h_{22} & \cdots & h_{2,k} \\ 0 & h_{32} & \ddots & \vdots \\ \vdots & \ddots & \ddots & h_{k,k} \\ 0 & \cdots & 0 & h_{k+1,k} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ \vdots \\ c_k \end{bmatrix} = \begin{bmatrix} \|\boldsymbol{b}\|_2 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix}$$

$\mathbf{x}_0 =$ "initial guess"
$\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$
$\mathbf{q}_1 = \dfrac{\mathbf{r}_0}{\|\mathbf{r}_0\|_2}$
for k **in** **range**(1,m+1):
    $\mathbf{y} = A\mathbf{q}_k$
    for j **in** **range**(1,k+1):
        $h_{jk} = \mathbf{q}_j^T \cdot \mathbf{y}$
        $\mathbf{y} = \mathbf{y} - h_{jk}\mathbf{q}_j$
    $h_{k+1,k} = \|\mathbf{y}\|_2$
    if $h_{k+1,k} > 0$:
        $\mathbf{q}_{k+1} = \dfrac{\mathbf{y}}{h_{k+1,k}}$
    $\overline{\mathbf{c}}_k = \underset{\mathbf{c}_k \in \mathbb{R}^k}{\operatorname{argmin}} \left\| \|\mathbf{r}_0\| \, \mathbf{e}_1 - \widetilde{H}_k \mathbf{c}_k \right\|_2$
    $\mathbf{x}_k = Q_k \overline{\mathbf{c}}_k + \mathbf{x}_0$