Sec 3.3 Gram-Schmidt Orthogonalization

Topics: 1. Gram-Schmidt (G-S) projection

2. Modified Gram-Schmidt (MGS)

3. MGS as triangular orthogonalization

Goal: $\{\vec{a}_1, \cdots, \vec{a}_n\}$, linearly independent $\longrightarrow$ $\{\vec{q}_1, \cdots, \vec{q}_n\}$, orthonormal.

1. Gram-Schmidt projections:

Recall: classical Gram-Schmidt (CGS):

$$\vec{v}_j = \vec{a}_j - \vec{q}_1(\vec{q}_1^{\,*}\vec{a}_j) - \vec{q}_2(\vec{q}_2^{\,*}\vec{a}_j) - \cdots - \vec{q}_{j-1}(\vec{q}_{j-1}^{\,*}\vec{a}_j)$$

$$\vec{q}_j = \vec{v}_j / \|\vec{v}_j\|$$

- Orthogonal projection: $P_j = I - \vec{q}_1\vec{q}_1^{\,*} - \vec{q}_2\vec{q}_2^{\,*} - \cdots - \vec{q}_{j-1}\vec{q}_{j-1}^{\,*}$, $j = 2, \cdots, n$

$\Rightarrow$ CGS: $\vec{v}_j = P_j\vec{a}_j$ $\quad (P_1 = I)$

$\vec{q}_j = \vec{v}_j / \|v_j\|$

- Let $\hat{Q}_j = [\vec{q}_1, \vec{q}_2, \cdots, \vec{q}_{j-1}]$. Then $P_j = I - \hat{Q}_j\hat{Q}_j^*$,

rank$(P_j) = m - (j-1)$, range$(P_j) \perp$ range$(\hat{Q})$ $\leftarrow \langle \vec{q}_1, \cdots, \vec{q}_{j-1} \rangle$

2. Modified Gram-Schmidt (MGS) orthogonalization:

To compute $\vec{q}_j$ (assuming $\{\vec{q}_1, \cdots, \vec{q}_{j-1}\}$ orthonormal):

$$\vec{v}_j^{(1)} = \vec{a}_j,$$

$$\vec{v}_j^{(2)} = P_{\perp\vec{q}_1}\vec{v}_j^{(1)} = \vec{v}_j^{(1)} - \vec{q}_1(\vec{q}_1^{\,*}\vec{v}_j^{(1)})$$

$$\vec{v}_j^{(3)} = P_{\perp\vec{q}_2}\vec{v}_j^{(2)} = \vec{v}_j^{(2)} - \vec{q}_2(\vec{q}_2^{\,*}\vec{v}_j^{(2)})$$

$$\vdots$$

$$\vec{v}_j = \vec{v}_j^{(j)} = P_{\perp\vec{q}_{j-1}}\vec{v}_j^{(j-1)} = \vec{v}_j^{(j-1)} - \vec{q}_{j-1}(\vec{q}_{j-1}^{\,*}\vec{v}_j^{(j-1)})$$

- Let $P_{\perp\vec{q}} = I - \vec{q}\vec{q}^{\,*}$ for $\vec{q} \in \mathbb{C}^m$. Then $\vec{v}_j = \underbrace{P_{\perp\vec{q}_{j-1}} \cdots P_{\perp\vec{q}_2}P_{\perp\vec{q}_1}}_{P_j} a_j$

Remark: Mathematically $P_j = I - \hat{Q}_j\hat{Q}_j^* = P_{\perp\vec{q}_{j-1}} \cdots P_{\perp\vec{q}_1}$

But numerically, modified G-S is more stable and has smaller errors.

Algorithm (Modified Gram-Schmidt)

for $i = 1$ to n
  $v_j = a_j$

for $i=1$ to n
  $r_{ii} = \|v_i\|$
  $q_i = v_i / r_{ii}$
  for $j = i+1$ to n
    $r_{ij} = q_i^* v_j$
    $v_j = v_j - r_{ij} q_i$

operation Count:

flops: floating point operations, such as $+, -, *, /$, or $\sqrt{\ }$

$r_{ii} = \|\vec{v}_i\| = \left(\sum_{j=1}^{m} (\vec{v}_i(j))^2\right)^{1/2}$: m multiplications, $(m-1)$ additions, 1 square root

$\vec{q}_j = \vec{v}_j / r_{jj}$: m divisions

$\vec{r}_{ij} = \vec{q}_i^* \vec{v}_j = \sum_{k=1}^{m} \vec{q}_j(k) \cdot \vec{v}_j(k)$: m multiplications, $(m-1)$ additions

$\vec{v}_j = \vec{v}_j - r_{ij} \vec{q}_i$: m multiplications, m subtractions

$$\text{Total flop count} = \sum_{i=1}^{n} (m + (m-1) + 1 + m) + \sum_{i=1}^{n} \sum_{j=i+1}^{n} [m + (m-1) + m + m]$$
$$= \sum_{i=1}^{n} 3m + \sum_{i=1}^{n} \sum_{j=i+1}^{n} (4m-1) = 3mn + (4m-1) \sum_{i=1}^{n} (n-i)$$
$$= 3mn + (4m-1) \sum_{j=1}^{n-1} j = 3mn + (4m-1) \frac{n(n-1)}{2} \sim 2mn^2$$

eg. Compare classical and modified G-S for the vectors

$\vec{a}_1 = (1, \varepsilon, 0, 0)^T$, $\vec{a}_2 = (1, 0, \varepsilon, 0)^T$, $\vec{a}_3 = (1, 0, 0, \varepsilon)^T$,

assuming $1 + \varepsilon^2 \approx 1$.

① Classical G-S: $\vec{v}_1 = \vec{a}_1$, $r_{11} = \|\vec{a}_1\| = \sqrt{1+\varepsilon^2} \approx 1$, $\vec{q}_1 = \vec{v}_1 / r_{11} = (1, \varepsilon, 0, 0)^T$

$r_{12} = \vec{q}_1^T \vec{a}_2 = (1, \varepsilon, 0, 0) \cdot (1, 0, \varepsilon, 0)^T = 1$, $\vec{v}_2 = \vec{a}_2 - r_{12} \vec{q}_1 = (0, -\varepsilon, \varepsilon, 0)^T$.

$r_{22} = \sqrt{2}\, \varepsilon$, $\vec{q}_2 = \vec{v}_2 / r_{22} = \frac{1}{\sqrt{2}} (0, -1, 1, 0)^T$

$r_{13} = \vec{q}_1^T \cdot \vec{a}_3 = (1, \varepsilon, 0, 0) \cdot (1, 0, 0, \varepsilon)^T = 1$, $r_{23} = \vec{q}_2^T \vec{a}_3 = \frac{1}{\sqrt{2}} (0, -1, 1, 0) \cdot (1, 0, 0, \varepsilon)^T = 0$

$$\vec{v}_3 = \vec{a}_3 - \underbrace{r_{13}}_{1}\vec{q}_1 - \underbrace{r_{23}}_{0}\vec{q}_2 = (0, -\varepsilon, 0, \varepsilon)^T, \qquad r_{33} = \|\vec{v}_3\| = \sqrt{2}\,\varepsilon$$

$$\vec{q}_3 = \vec{v}_3 / r_{33} = \frac{1}{\sqrt{2}}(0, -1, 0, 1)^T$$

② Modified G-S: $\vec{v}_1 = \vec{a}_1$, $r_{11} = \|\vec{a}_1\| = \sqrt{1+\varepsilon^2} \approx 1$, $\vec{q}_1 = \vec{v}_1 / r_{11} = (1, \varepsilon, 0, 0)^T$

$\vec{v}_2 = \vec{a}_2 = (1, 0, \varepsilon, 0)^T$, $r_{12} = \vec{q}_1^{\,T}\vec{v}_2 = (1, \varepsilon, 0, 0)\cdot(1, 0, \varepsilon, 0)^T = 1$

$\vec{v}_2 = \vec{v}_2 - r_{12}\vec{q}_1 = (0, -\varepsilon, \varepsilon, 0)^T$, $r_{22} = \|\vec{v}_2\| = \varepsilon\sqrt{2}$, $\vec{q}_2 = \vec{v}_2 / r_{22} = \frac{1}{\sqrt{2}}(0, -1, 1, 0)^T$

$\vec{v}_3 = \vec{a}_3 = (1, 0, 0, \varepsilon)^T$, $r_{13} = \vec{q}_1^{\,T}\vec{v}_3 = (1, \varepsilon, 0, 0)\cdot(1, 0, 0, \varepsilon)^T = 1$,

$\vec{v}_3 = \vec{v}_3 - r_{12}\vec{q}_1 = (0, -\varepsilon, 0, \varepsilon)^T$. $r_{23} = \vec{q}_2^{\,T}\cdot\vec{v}_3 = \frac{1}{\sqrt{2}}(0, -1, 1, 0)\cdot(0, -\varepsilon, 0, \varepsilon) = \frac{\varepsilon}{\sqrt{2}}$

$\vec{v}_3 = \vec{v}_3 - r_{23}\vec{q}_2 = (0, -\varepsilon, 0, \varepsilon)^T - \frac{\varepsilon}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}(0, -1, 1, 0)^T = (0, -\varepsilon, 0, \varepsilon)^T - (0, -\frac{\varepsilon}{2}, \frac{\varepsilon}{2}, 0)^T = (0, -\frac{\varepsilon}{2}, -\frac{\varepsilon}{2}, \varepsilon)^T$

$r_{33} = \|\vec{v}_3\| = \varepsilon\sqrt{\frac{1}{4}+\frac{1}{4}+1} = \frac{\varepsilon\sqrt{6}}{2}$, $\vec{q}_3 = \vec{v}_3 / r_{33} = \frac{1}{\sqrt{6}}(0, -1, -1, 2)$

③ Check orthogonality:

- Classical G-S: $\vec{q}_2^{\,T}\vec{q}_3 = \frac{1}{\sqrt{2}}(0, -1, 1, 0)\cdot\frac{1}{\sqrt{2}}(0, -1, 0, 1) = \frac{1}{2}$
- Modified G-S: $\vec{q}_2^{\,T}\cdot\vec{q}_3 = \frac{1}{\sqrt{2}}(0, -1, 1, 0)\cdot\frac{1}{\sqrt{6}}(0, -1, -1, 2) = 0$

3. Modified Gram-Schmidt as triangular orthogonalization:

step 1: $(i=1)$.

$$\underbrace{\begin{bmatrix} \vec{v}_1 & \vec{v}_2 & \cdots & \vec{v}_n \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} \frac{1}{r_{11}} & -\frac{r_{12}}{r_{11}} & -\frac{r_{13}}{r_{11}} & \cdots \\ & 1 & & \\ & & 1 & \\ & & & \ddots\ 1 \end{bmatrix}}_{R_1} = \begin{bmatrix} \vec{q}_1 & \vec{v}_2^{(2)} & \cdots & \vec{v}_n^{(2)} \end{bmatrix}$$

step 2 $(i=2)$:

$$R_2 = \begin{bmatrix} 1 & & & \\ & \frac{1}{r_{22}} & -\frac{r_{23}}{r_{22}} & \cdots \\ & & 1 & \\ & & & \ddots\ 1 \end{bmatrix}, \quad \cdots \quad R_i = \begin{bmatrix} 1 & & & & \\ & \ddots\ 1 & & & \\ & & \frac{1}{r_{ii}} & -\frac{r_{i,i+1}}{r_{ii}} & \cdots \\ & & & 1 & \\ & & & & \ddots\ 1 \end{bmatrix}$$

$$A\underbrace{R_1 R_2 \cdots R_n}_{\hat{R}^{-1}} = \hat{Q} = [\vec{q}_1 | \cdots \vec{q}_n] \qquad \Rightarrow \quad A = \hat{Q}\hat{R}.$$

So the G-S is a method of triangular orthogonalization.