CS475 / CS675
Lecture 11: June 7, 2016

QR Factorization and

Gram-Schmidt Orthogonalization

Reading: [TB] Chapters 7, 8

Gram-Schmidt Orthogonalization

- QR factorization algorithm

  $A = QR$ (Q orthogonal and R upper Δ)

  Picture:

- At the j^{th} step

  q_j is orthogonal to $\{q_1, \ldots, q_{j-1}\}$

  $\left|\left|q_j\right|\right| = 1$

Gram-Schmidt Orthogonalization

- Consider $v_j = a_j + \sum_{i=1}^{j-1} \beta_i q_i$
- Since $0 = q_k^T v_j$ $\quad\quad\quad\quad k = 1, \dots, j-1$

$$= q_k^T a_j + \sum_{i-1}^{j-1} \beta_i (q_k^T q_i)$$
$$= q_k^T a_j + \beta_k q_k^T q_k$$

$$\therefore \beta_k = -q_k^T a_j \quad\quad\quad\quad (q_k^T q_k = 1)$$
$$\Longrightarrow v_j = a_j - \sum_{i=1}^{j-1} (q_i^T a_j) q_i$$

Gram-Schmidt Orthogonalization

- Normalize v_j → $q_j = \frac{v_j}{||v_j||}$
- Hence $q_1 = \frac{a_1}{r_{11}}$

$$q_2 = \frac{a_2 - r_{12} q_1}{r_{22}}$$

$$\vdots$$

$$q_n = \frac{a_n - \sum_{i=1}^{n-1} r_{in} q_i}{r_{nn}}$$

- Where $r_{ij} = q_i^T a_j, \quad r_{jj} = \left|\left| a_j - \sum_{i=1}^{j-1} r_{ij} q_i \right|\right|_2$

Gram-Schmidt Algorithm

For $j = 1,2, \dots, n$

$v_j = a_j$

for $i = 1, \dots, j-1$

$r_{ij} = q_i^T a_j$

$v_j = v_j - r_{ij} q_i$

end

$r_{jj} = \left|\left|v_j\right|\right|$

$q_j = \frac{v_j}{r_{jj}}$

end

Modified Gram-Schmidt

- Change: "$r_{ij} = q_i^T a_j$" → "$r_{ij} = q_i^T v_j$" (more stable)

- In the i-loop, v_j changes for each i

$$i = 1: v_j^{(1)} = a_j - r_{1j}q_1$$

$$i = 2: v_j^{(2)} = v_j^{(1)} - r_{2j}q_2 = a_j - r_{1j}q_1 - r_{2j}q_2$$

$$\vdots$$

$$i = k-1: v_j^{(k-1)} = a_j - \sum_{i=1}^{k-1} r_{ij}q_i$$

- At $i = k$,

$$\begin{aligned} r_{kj} &= q_k^T a_j \\ &= q_k^T\left(a_j - \sum_{i=1}^{k-1} r_{ij}q_i\right) \quad (q_k \perp \{q_1, \dots, q_{k-1}\}) \\ &= q_k^T v_j^{k-1} \end{aligned}$$

Complexity of Gram-Schmidt

- Consider the i-loop:
  $r_{ij} = q_i^T a_j$ or $q_i^T v_j$ → m mult, $m-1$ adds
  $v_j = v_j - r_{ij} q_i$ → m mult, m subs
  $\therefore flops \backsim 4m$
- Total flops $= \sum_{j=1}^{n} \sum_{i=1}^{j-1} 4m$
  $= \sum_{j=1}^{n} (j-1)4m \sim 4m \sum_{j=1}^{n} j$
  $= \frac{4mn(n+1)}{2}$
  $\sim 2mn^2$
- Note: when $m = n$, then $flops(QR) = 2n^3 + O(n^2)$
  $\approx 3 \times flops(LU)$

Example

Householder triangularization

- More stable than Gram-Schmidt
- Idea: $Q_n \dots Q_2\, Q_1\, A = R$

  $Q_k \in \Re^{m \times m}$ orthogonal matrices
- Similar to GE, each Q_k will make the entries of col j become zero
- Picture:

Householder reflectors

- Define $Q_k = \begin{bmatrix} I & 0 \\ 0 & F \end{bmatrix} \begin{matrix} \} \, k-1 \\ \} \, m-(k-1) \end{matrix}$
- F is chosen to be a Householder reflector
- Picture

Householder Reflector

- Suppose $x = \begin{bmatrix} \times \\ \times \\ \vdots \\ \times \end{bmatrix}$ then $Fx = \begin{bmatrix} ||x|| \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \big||x|\big| e_1$
- F "reflects" x across hyperplane H orthogonal to $v = \big||x|\big| e_1 - x$
- The orthogonal projector of x onto H:

$$Px = x - \left[\left(\frac{v}{\big||v|\big|} \right)^T x \right] \frac{v}{\big||v|\big|} = x - v \frac{v^T x}{v^T v}$$

- Since F is a reflector, it should go twice as far:

$$Fx = x - 2v \frac{v^T x}{v^T v}$$

Householder Reflectors

- Two possibilities:

- For stability reason, the further one is chosen
  - i.e., $v = -sign(x_1)||x||e_1 - x$

  Upon clearing the minus signs, we obtain

$$v = sign(x_1)||x||e_1 + x$$

Another Derivation

- Let $F = I - 2\frac{vv^T}{v^T v}$. Find v s.t. $Fx \in span\{e_1\}$.
- $Fx = x - 2\frac{v^T x}{v^T v} v$

  $\in span\{e_1\} \Leftrightarrow v \in span\{x, e_1\}$
- Let $v = x + \alpha e_1$

  $v^T x = x^T x + \alpha e_1^T x = x^T x + \alpha x_1$

  $v^T v = (x + \alpha e_1)^T (x + \alpha e_1)$

  $= x^T x + 2\alpha x_1 + \alpha^2$

Derivation Continued

- $\therefore Fx =$

- Hence $v = x \pm ||x||e_1$
  and $Fx = \mp ||x||e_1$

Example