lecture 18

Gram-Schmidt Orthogonalization

For simplicity, assume col's of $A = (a_1, \cdots, a_n)$ are independent. We want find orthonormal matrix $Q \in R^{m \times n}$, upper tri. $R \in R^{n \times n}$, s.t.

$$A = QR$$

This is the QR decomposition of A.

$$[a_1, \cdots, a_n] = [q_1, \cdots, q_n] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & \vdots \\ & & \ddots & \\ & & & r_{nn} \end{bmatrix}$$

For the 1st col from both sides

$$a_1 = r_{11} q_1.$$

$a_1 \neq 0$, we choose $r_{11} = \|a_1\|$, and $q_1 = a_1 / r_{11}$

Recall Q is orthonormal: $q_i^T q_j = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$

From the 2nd-col of both sides

$$a_2 = r_{12} q_1 + r_{22} q_2.$$

pre-multiply with q_1^T on both sides

$$q_1^T a_2 = r_{12} \underbrace{q_1^T q_1}_{=1} + r_{22} \underbrace{q_1^T q_2}_{=2}.$$

$$r_{12} = q_1^T a_2$$

Now $\quad r_{22} q_2 = a_2 - r_{12} q_1 \equiv \hat{q}_2$

We can choose $r_{22} = \|\hat{q}_2\|$, and $q_2 = \hat{q}_2 / r_{22}$

because $\hat{q}_2 \neq 0$

Assume we have computed $q_1, \dots, q_{k-1}$ and the first $(k-1)$-col's of R.

From the k-th of both sides of $A = QR$

$$a_k = r_{1k} q_1 + r_{2k} q_2 + \cdots + r_{k-1,k} q_{k-1} + r_{kk} q_k$$

Use the fact, $q_i^T q_j = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$.

We find $r_{1k} = q_1^T a_k$, $r_{2k} = q_2^T a_k$, $\cdots r_{k-1,k} = q_{k-1}^T a_k$

Now $r_{kk} q_k = a_k - (r_{1k} q_1 + \cdots + r_{k-1,k} q_{k-1}) \equiv \hat{q}_k$,

again $\hat{q}_k \neq 0$, we choose $r_{kk} = \hat{q}_k$, $q_k = \hat{q}_k / r_{kk}$

In R^3, $a_1 = \begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix}$, $a_2 = \begin{pmatrix} -1 \\ 0 \\ 7 \end{pmatrix}$, $a_3 = \begin{pmatrix} 2 \\ 9 \\ 11 \end{pmatrix}$

When computing by hand, it's also possible not to normalize during GS, but rather carry out normalization at the end.

$$\tilde{q}_1 = \begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix}, \quad \tilde{q}_2 = \begin{pmatrix} -1 \\ 0 \\ 7 \end{pmatrix} - \frac{-1\cdot 3 + 0 + 7\cdot 4}{25}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix} = \begin{pmatrix} -4 \\ 0 \\ 3 \end{pmatrix}$$

$$\tilde{q}_3 = \begin{pmatrix} 2 \\ 9 \\ 11 \end{pmatrix} - \frac{2\cdot 3 + 0 + 11\cdot 4}{25}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix} - \frac{2\cdot(-4) + 0 + 11\cdot 3}{25}\begin{pmatrix} -4 \\ 0 \\ 3 \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ 9 \\ 0 \end{pmatrix}$$

$$q_1 = \frac{1}{5}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix}, \quad q_2 = \frac{1}{5}\begin{pmatrix} -4 \\ 0 \\ 3 \end{pmatrix}, \quad q_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

For the case A has independent col's, the least squares $\min_x \|b - Ax\|^2$ is unique

1) Compute $b_1 = Q^T b$

2) Solve $Rx = b_1$.

Properties of GS:

1). $\mathrm{Span}\{a_1, \dots, a_k\} = \mathrm{Span}\{q_1, \dots, q_k\}$ for any $k = 1, \dots, n$. This is to say $\{q_1, \dots, q_k\}$ forms an orthonormal basis for $\mathrm{Span}\{a_1, \dots, a_k\}$ and $\{q_1, \dots, q_n\}$ forms an orthonormal basis for $C(A)$.

2). The least squares problem

$$\min_x \|[q_1 \cdots q_k]\, x - a_k\|^2$$

has sol $x = \begin{pmatrix} q_1^T a_k \\ \vdots \\ q_{k-1}^T a_k \end{pmatrix} = \begin{pmatrix} r_{1k} \\ \vdots \\ r_{k-1,k} \end{pmatrix}$

Hence $[q_1, \dots, q_{k-1}] \begin{pmatrix} r_{1k} \\ \vdots \\ r_{k-1,k} \end{pmatrix}$ is the orthogonal projection of a_k onto $\mathrm{Span}\{q_1, \dots, q_{k-1}\} = \mathrm{Span}\{a_1, \dots, a_{k-1}\}$

$\hat{q}_k = a_k - [q_1, \cdots q_{k-1}] \begin{bmatrix} r_{1k} \\ \vdots \\ r_{k-1,k} \end{bmatrix}$

is the residual.

Old problem with a new proof.

$$Q^TQ = I_n \Rightarrow QQ^T = I_n$$

Notice $Q = [q_1, \dots, q_n]$ $\quad Q^TQ = I \Rightarrow \|q_1\| = 1$.

Use Householder H_1: $\quad H_1 q_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = e_1$.

$H_1 = H_1^T$, $\; H_1^2 = I$

$$I = (H_1Q)^T(H_1Q) = \left(\begin{array}{c|c} 1 & 0 \cdots 0 \\ \hline u_1 & * \end{array}\right)\left(\begin{array}{c|c} 1 & u_1^T \\ \hline 0 \\ \vdots \\ 0 & * \end{array}\right) \Rightarrow u_1^T = 0.$$

$$H_1Q = \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & Q_1 \end{array}\right) \quad \text{and} \quad Q_1^TQ_1 = I_{n-1}$$

A sequence of Householder $\quad H_{n-1} \cdots H_1 Q = I$.

$$Q = H_1 \cdots H_{n-1}, \qquad QQ^T = H_1 \cdots H_{n-1} H_{n-1} \cdots H_1 = I$$