The Gram-Schmidt orth. via Orthogonal Projectors

Note Title 4/23/2012

To understand the behavior of the classical GS algorithm and to discuss the better version, let's view the classical GS alg. using ortho. projectors.

$A \in \mathbb{R}^{m\times n}$, $m \ge n$, full rank

i.e., $\operatorname{rank}(A) = n$.

$$q_1 = \frac{a_1}{r_{11}}, \quad q_2 = \frac{a_2 - r_{12} q_1}{r_{22}}, \quad \cdots, \quad q_n = \frac{a_n - \sum_{i=1}^{n-1} r_{in} q_i}{r_{nn}}$$

$$\updownarrow \qquad\qquad \updownarrow \qquad\qquad \updownarrow$$

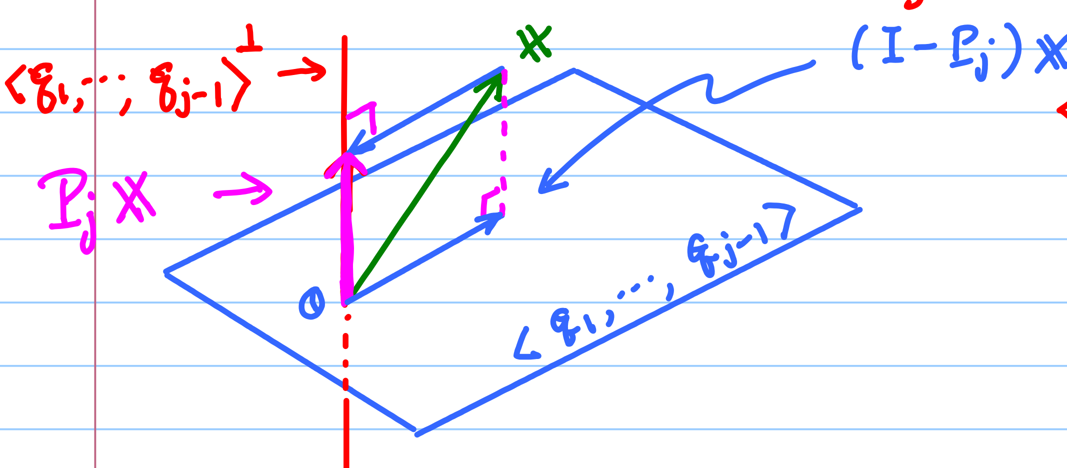
$$q_1 = \frac{P_1 a_1}{\|P_1 a_1\|}, \quad q_2 = \frac{P_2 a_2}{\|P_2 a_2\|}, \quad \cdots, \quad q_n = \frac{P_n a_n}{\|P_n a_n\|}$$

where P_j = Ortho. proj. onto

$$\underbrace{\langle q_1, \cdots, q_{j-1} \rangle^{\perp}}_{\text{orthogonal complement to } \langle q_1, \cdots, q_{j-1}\rangle}$$

$j = 1, 2, \cdots, n$

orthogonal complement to $\langle q_1, \cdots, q_{j-1} \rangle$



$$\mathbb{R}^m = \langle q_1, \cdots, q_{j-1} \rangle \oplus \langle q_1, \cdots, q_{j-1} \rangle^{\perp}$$

$$= \underbrace{\operatorname{null}(P_j)}_{\dim = j-1} \oplus \underbrace{\operatorname{range}(P_j)}_{\dim = m-(j-1)}$$

Note: $q_j \perp \langle q_1, \cdots, q_{j-1} \rangle$,

$q_j \in \langle a_1, \cdots, a_j \rangle$,

and $\|q_j\| = 1$, by construction.

Now let $\hat{Q}_{j-1} := [\, q_1 \ \cdots \ q_{j-1} \,] \in \mathbb{R}^{m \times (j-1)}$

Then clearly, $P_j = I - \hat{Q}_{j-1} \hat{Q}_{j-1}^T$, $j > 1$

$P_1 = I$.

☆ Modified Gram-Schmidt Algorithm

Recall the CGS algorithm:

$$
\begin{array}{l}
\text{for } j = 1 : n \\
\left\{
\begin{array}{l}
v_j = a_j \\
\text{for } i = 1 : j-1 \\
\quad \left\{
\begin{array}{l}
r_{ij} = q_i^T a_j \\
v_j = v_j - r_{ij} q_i
\end{array}
\right. \\
r_{jj} = \|v_j\| \\
q_j = v_j / r_{jj}
\end{array}
\right.
\end{array}
$$

This part computes $P_j a_j$ and store it as v_j

Since $\operatorname{rank}(P_j) = m - (j-1)$, rank of $P_j \downarrow$ as $j \uparrow$, which is not good. Also, numerical error accumulates in the inner "for" loop.

The modified GS (MGS) algorithm "uses the fresh material immediately rather than waiting to avoid staleness."

what I mean above is:

to use

$$\begin{cases} P_j = P_{\perp q_{j-1}} P_{\perp q_{j-2}} \cdots P_{\perp q_1} \ ; \ j>1 \\ P_1 = I \end{cases}$$

Note that each $P_{\perp q_i}$ has rank $m-1$

$P_{\perp q_i}$ = the complementary projection to P_{q_i}

$= I - q_i q_i^T$

Mathematically,

$$v_j = P_j a_j = (I - \hat{Q}_{j-1} \hat{Q}_{j-1}^T) a_j$$

and

$$v_j = P_j a_j = P_{\perp q_{j-1}} \cdots P_{\perp q_1} a_j$$
$$= (I - q_{j-1} q_{j-1}^T) \cdots (I - q_1 q_1^T) a_j$$

are equivalent. But the sequence of arithmetic operations are different. The MGS computes and updates:

$$\begin{cases} v_j^{(1)} = a_j \rightarrow q_1 \\ v_j^{(2)} = P_{\perp q_1} v_j^{(1)} = v_j^{(1)} - q_1 q_1^T v_j^{(1)} \rightarrow q_2 \\ v_j^{(3)} = P_{\perp q_2} v_j^{(2)} = v_j^{(2)} - q_2 q_2^T v_j^{(2)} \rightarrow q_3 \\ \vdots \end{cases}$$

$\vdots$

$$v_j^{(j)} = P_{\perp q_{j-1}} v_j^{(j-1)} = v_j^{(j-1)} - q_{j-1} q_{j-1}^T v_j^{(j-1)}$$

$$\rightarrow = v_j \rightarrow q_j$$

This process is applied for $j = 1, \cdots, n$

Algorithm (Modified Gram-Schmidt)

for $i = 1 : n$

  $v_i = a_i$

for $i = 1 : n$

$$\left\{\begin{array}{l} r_{ii} = \| v_i \| \\ q_i = v_i / r_{ii} \\ \text{for } j = i+1 : n \\ \quad \left\{\begin{array}{l} r_{ij} = q_i^T v_j \\ v_j = v_j - r_{ij} q_i \end{array}\right. \end{array}\right.$$

Note the order of r_{ij} computation

i:					
1	r_{11}	r_{12}	r_{13}	$\cdots$	r_{1n}
2		r_{22}	r_{23}	$\cdots$	r_{2n}
3			r_{33}	$\cdots$	r_{3n}
$\vdots$					$\vdots$
n					r_{nn}

Let's consider the previous example.

$$A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix}.$$

ε : small s.t. ε^2 can be ignored.

Now apply the MGS algorithm!

$$v_j^{(1)} = a_j , \quad j = 1, 2, 3$$

$$r_{11} = \| v_1^{(1)} \| = \sqrt{1+\varepsilon^2} \approx 1.$$

$$q_1 = v_1^{(1)} / r_{11} = [1 \ \varepsilon \ 0 \ 0]^T$$

Now immediately compute r_{12}, r_{13}:

$$\begin{cases} r_{12} = q_1^T v_2^{(1)} = [1 \ \varepsilon \ 0 \ 0] \begin{bmatrix} 1 \\ 0 \\ \varepsilon \\ 0 \end{bmatrix} = 1. \\ v_2^{(2)} = v_2^{(1)} - r_{12} q_1 \\ \quad = \begin{bmatrix} 1 \\ 0 \\ \varepsilon \\ 0 \end{bmatrix} - 1 \cdot \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -\varepsilon \\ \varepsilon \\ 0 \end{bmatrix} \\ r_{13} = q_1^T v_3^{(1)} = [1 \ \varepsilon \ 0 \ 0] \begin{bmatrix} 1 \\ 0 \\ 0 \\ \varepsilon \end{bmatrix} = 1 \\ v_3^{(2)} = v_3^{(1)} - r_{13} q_1 \\ \quad = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \varepsilon \end{bmatrix} - 1 \cdot \begin{bmatrix} 1 \\ \varepsilon \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -\varepsilon \\ 0 \\ \varepsilon \end{bmatrix} \end{cases}$$

$$r_{22} = \| v_2^{(2)} \| = \sqrt{2}\, \varepsilon$$

$$q_2 = v_2^{(2)} / r_{22} = [0 \ -1/\sqrt{2} \ 1/\sqrt{2} \ 0]^T$$

Now immediately compute r_{23} :

$$\begin{cases} r_{23} = q_2^T v_3^{(2)} = [0 \ -1/\sqrt{2} \ 1/\sqrt{2} \ 0] \begin{bmatrix} 0 \\ -\varepsilon \\ 0 \\ \varepsilon \end{bmatrix} = \frac{\varepsilon}{\sqrt{2}} \end{cases}$$

$$v_3^{(3)} = v_3^{(2)} - r_{23}\, q_2 = \begin{bmatrix} 0 \\ -\varepsilon \\ 0 \\ \varepsilon \end{bmatrix} - \frac{\varepsilon}{\sqrt{2}} \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -\varepsilon/2 \\ -\varepsilon/2 \\ \varepsilon \end{bmatrix}$$

$$r_{33} = \| v_3^{(3)} \| = \varepsilon \cdot \sqrt{(-\tfrac{1}{2})^2 + (\tfrac{1}{2})^2 + 1^2} = \sqrt{\tfrac{3}{2}}\,\varepsilon$$

$$q_3 = v_3^{(3)} / r_{33} = \begin{bmatrix} 0 \\ -1/\sqrt{6} \\ -1/\sqrt{6} \\ \sqrt{2/3} \end{bmatrix}$$

Hence

$$\hat{Q} = \begin{bmatrix} 1 & 0 & 0 \\ \varepsilon & -1/\sqrt{2} & -1/\sqrt{6} \\ 0 & 1/\sqrt{2} & -1/\sqrt{6} \\ 0 & 0 & \sqrt{2/3} \end{bmatrix} \qquad \hat{R} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & \sqrt{2}\,\varepsilon & \varepsilon/\sqrt{2} \\ 0 & 0 & \sqrt{3/2}\,\varepsilon \end{bmatrix}$$

Notice that $A = \hat{Q}\hat{R}$ holds.

Moreover,

$$\hat{Q}^T \hat{Q} = \begin{bmatrix} 1+\varepsilon^2 & -\varepsilon/\sqrt{2} & -\varepsilon/\sqrt{6} \\ -\varepsilon/\sqrt{2} & 1 & 0 \\ -\varepsilon/\sqrt{6} & 0 & 1 \end{bmatrix}$$

This is closer to $I_{3\times 3}$

$$\approx \begin{bmatrix} 1 & -\varepsilon/\sqrt{2} & -\varepsilon/\sqrt{6} \\ -\varepsilon/\sqrt{2} & 1 & \underline{\underline{0}} \\ -\varepsilon/\sqrt{6} & \underline{\underline{0}} & 1 \end{bmatrix}$$

than this

Compare this with the CGS result:

$$\hat{Q}^T \hat{Q} \approx \begin{bmatrix} 1 & -\varepsilon/\sqrt{2} & -\varepsilon/\sqrt{2} \\ -\varepsilon/\sqrt{2} & 1 & \underline{\underline{1/2}} \\ -\varepsilon/\sqrt{2} & \underline{\underline{1/2}} & 1 \end{bmatrix}$$

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- <u>Note:</u> The best algorithm for QR factorization is the so-called "Householder Triangularization", which will be discussed in the next lecture.

☆ Application to the LS problem

Recall the solution $\mathbb{x} \in \mathbb{R}^n$ of the LS problem: $\| \mathbb{b} - A\mathbb{x} \|^2 \to \min$ where $A \in \mathbb{R}^{m \times n}$, $m \geq n$, $\mathbb{b} \in \mathbb{R}^m$, satisfies the normal eqn.

$$A^T A \mathbb{x} = A^T \mathbb{b}$$

(Suppose A is full rank)

Now plug in the reduced QR fact. of $A = \hat{Q}\hat{R}$

$$\Leftrightarrow \quad \hat{R}^T \underbrace{\hat{Q}^T \hat{Q}}_{= I} \hat{R} \mathbb{x} = \hat{R}^T \hat{Q}^T \mathbb{b}$$

$$\Leftrightarrow \quad \hat{R}^T \hat{R} \mathbb{x} = \hat{R}^T \hat{Q}^T \mathbb{b}$$

Now notice that $\hat{R}^T$ is the same on both sides and it's

If A is full rank → nonsingular. So we can remove it to get

$$\hat{R} \mathbb{x} = \hat{Q}^T \mathbb{b}$$

So, the LS solution via QR proceeds:

(1) Compute reduced QR of A.
(2) Compute $y = \hat{Q}^T \mathbb{b}$.
(3) Solve $\hat{R}\mathbb{x} = \mathbb{y}$

Note that $\hat{R}$: upper triangular helps solve this system (3)

$\rightarrow$ back substitution

$$\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & & r_{n-1\,n-1} & r_{n-1\,n} \\ 0 & \cdots & 0 & r_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-1} \\ y_n \end{bmatrix}$$

Start solving $r_{nn} x_n = y_n$

$x_n = y_n / r_{nn}$

then go backward:

$r_{n-1\,n-1} x_{n-1} + r_{n-1\,n} x_n = y_{n-1}$

$\Rightarrow \quad x_{n-1} = \dfrac{1}{r_{n-1\,n-1}} \left(y_{n-1} - r_{n-1\,n} x_n \right)$

Next solve for $x_{n-2}, \cdots,$ up to x_1 //

Direct consequence of the GS procedure!

☆ Existence & Uniqueness of QR

Thm Every $A \in \mathbb{R}^{m \times n}$ $(m \geq n)$ has a full QR factorization, hence also $\hat{Q}\hat{R}$.

Thm Each $A \in \mathbb{R}^{m \times n}$ $(m \geq n)$ of full rank matrix has a unique $\hat{Q}\hat{R}$ with $r_{ii} > 0$.