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Gram-Schmidt orthogonalization

At the j-th step, $q_j$ , $||q_j|| = 1$, is orthogonal to { $q_1, q_2, \ldots, q_{j-1}$ }.

Consider $$\mathrm{v}_j = \mathrm{a}_j + \sum_{i=1}^{j-1} \beta_i q_i$$

Since $$0 = q_k^T \mathrm{v}_j = q_k^T \mathrm{a}_j + \sum_{i=1}^{j-1} \beta_i (q_k^T q_i) \qquad k = 1, \ldots, j-1$$

$$= q_k^T \mathrm{a}_j + \beta_k q_k^T q_k$$

$$\beta_k = -q_k^T \mathrm{a}_j \qquad\qquad (q_k^T q_k = 1)$$

$$\Rightarrow \qquad \mathrm{v}_j = \mathrm{a}_j - \sum_{i=1}^{j-1} (q_i^T a_j) q_i$$

Normalize it -> $q_j = v_j / ||v_j||$

Hence
$$q_1 = \tfrac{1}{r_{11}} a_1$$
$$q_2 = \tfrac{1}{r_{22}} (a_2 - r_{12} q_1)$$
$$\vdots$$
$$q_n = \tfrac{1}{r_{nn}} (a_n - \sum_{i=1}^{n-1} r_{in} q_i)$$

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

## Gram-Schmidt algorithm

for $j = 1, 2, . . . , n$

  $v_j = a_j$

  for $i = 1, 2, . . . , j-1$

    $r_{ij} = q_i^T a_j$

    $v_j = v_j - r_{ij} q_i$

  end

  $r_{jj} = ||v_j||$

  $q_j = v_j / r_{jj}$

end

## Modified Gram-Schmidt

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

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

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

:

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

At i=k, $r_{kj} = q_k^T a_j$

$= q_k^T (a_j - \text{sum } r_{ij} q_i)$ ($q_k$ orth to $\{q_1, ..., q_{k-1}\}$)

$= q_k^T v_j^{(k-1)}$

Thus, change "$r_{ij} = q_i^T a_j$" -> "$r_{ij} = q_i^T v_j$".

Complexity of Gram-Schmidt

Consider the i-loop:

$r_{ij} = q_i^T a_j$ or $q_i^T v_j$ $\rightarrow$ m mults, m-1 adds

$v_j = v_j - r_{ij} q_i$ -> m mults, m subs

$\therefore$ flops ~ 4m

$$\text{Total flops} = \sum_{j=1}^{n} \sum_{i=1}^{j-1} 4m$$

$$= \sum_{j=1}^{n} (j-1)4m \sim 4m \sum_{j=1}^{n} j$$

$$= 4m \frac{n(n+1)}{2}$$

$$\sim 2mn^2$$

Note

When m = n, then flops(QR) = $2n^3 + O(n^2)$

$\approx$ 3 x flops(LU)

Example: Find the QR factorization of A = $\begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}$

$$v_1 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}. \qquad \text{Then} \quad r_{11} = \|v_1\| = \sqrt{1^2 + 2^2 + 3^2} = 3$$

$$\therefore \quad q_1 = \tfrac{1}{3} v_1 = \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix}$$

$$a_2 = \begin{bmatrix} -4 \\ 3 \\ 2 \end{bmatrix} \qquad r_{12} = q_1^T a_2 = \left(\tfrac{1}{3}\right)\left(-4\right) + \left(\tfrac{2}{3}\right)(3) + \left(\tfrac{2}{3}\right)(2) = 2$$

$$v_2 = \begin{bmatrix} -4 \\ 3 \\ 2 \end{bmatrix} - 2 \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix} = \tfrac{1}{3} \begin{bmatrix} -14 \\ 5 \\ 2 \end{bmatrix}$$

$$r_{22} = \|v_2\| = \tfrac{1}{3}\sqrt{(14)^2 + 5^2 + 2^2} = 5$$

$$\therefore \quad q_2 = \tfrac{1}{5} v_2 = \tfrac{1}{15} \begin{bmatrix} -14 \\ 5 \\ 2 \end{bmatrix}$$

$$\text{Hence} \qquad \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix} = \begin{bmatrix} \frac{1}{3} & \frac{-14}{3} \\ \frac{2}{3} & \frac{1}{3} \\ \frac{2}{3} & \frac{2}{15} \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 0 & 5 \end{bmatrix}$$

## Householder triangularization

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

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

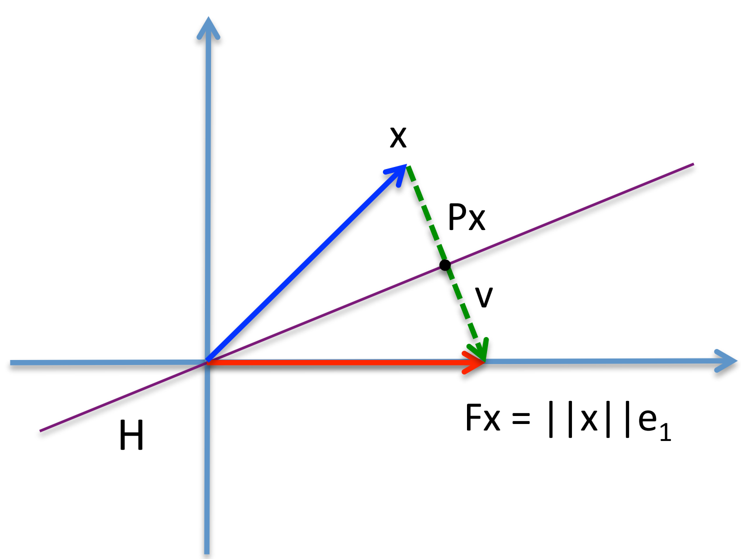
$$
\underset{A}{\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}}
\xrightarrow{Q_1}
\underset{Q_1A}{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}}
\xrightarrow{Q_2}
\underset{Q_2Q_1A}{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{bmatrix}}
\xrightarrow{Q_3}
\underset{Q_3Q_2Q_1A}{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{bmatrix}}
$$

## Householder reflections

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



Suppose $x = \begin{bmatrix} \times \\ \times \\ \vdots \\ \times \end{bmatrix}$ Then $Fx = \begin{bmatrix} \|x\| \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|x\| e_1$

- F "reflects" x across hyperplane H orthogonal to v = $||x||e_1$ - x.

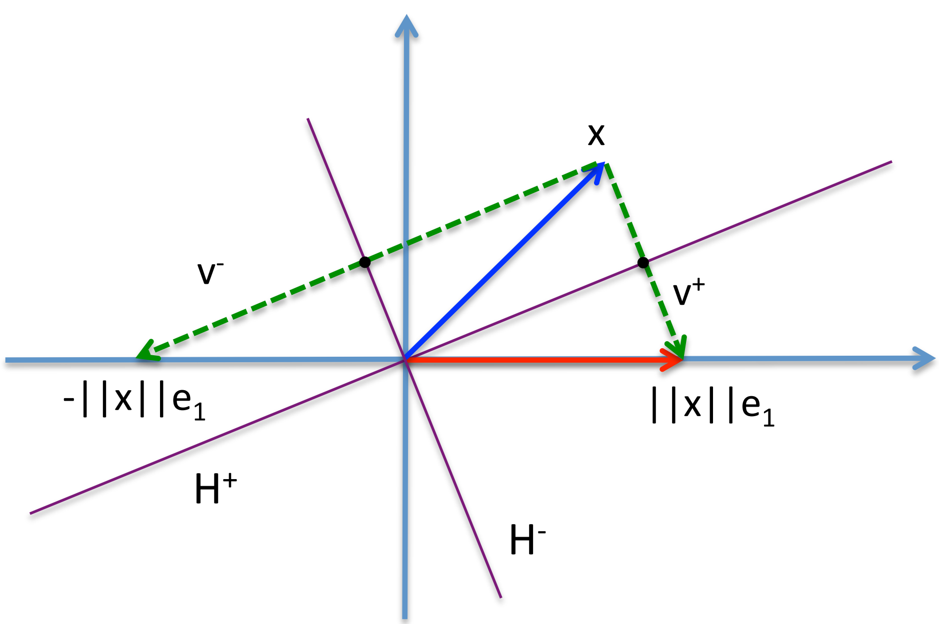
- The orthogonal projector of x onto H:

$$Px = x - [(\tfrac{v}{\|v\|})^T x]\tfrac{v}{\|v\|} = x - v\,\tfrac{v^T x}{v^T v}$$

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

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

- Another possibility:




- For stability reason, the one which is farther away is chosen.

E.g. v = -sign($x_1$) $||x||e_1$ - x

i.e. v = sign($x_1$) $||x||e_1$ + x

Another derivation

Let $F = I - 2\,(vv^T/v^Tv)$. Find $v$ s.t. $Fx \in \operatorname{span}\{e_1\}$.

$$Fx = x - 2\,(v^Tx/v^Tv)\,v$$

$$\in \operatorname{span}\{e_1\} \quad \Leftrightarrow \quad v \in \operatorname{span}\{x, e_1\}$$

Let $v = x + \alpha\, e_1$

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

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

$$= x^Tx + 2\,\alpha\, x_1 + \alpha^2$$

$$\therefore \quad Fx = x - 2\,\tfrac{v^Tx}{v^Tv}(x + \alpha e_1)$$

$$= (1 - 2\,\tfrac{v^Tx}{v^Tv})x - 2\alpha\,\tfrac{v^Tx}{v^Tv}\,e_1$$

$$= (1 - 2\,\tfrac{x^Tx+\alpha x_1}{x^Tx+2\alpha x_1+\alpha^2})x - 2\alpha\,\tfrac{v^Tx}{v^Tv}\,e_1$$

$$= \underbrace{\tfrac{x^Tx+2\alpha x_1+\alpha^2-2x^Tx-2\alpha x_1}{x^Tx+2\alpha x_1+\alpha^2}}_{=0}\,x - 2\alpha\,\tfrac{v^Tx}{v^Tv}\,e_1$$

if $\alpha^2 - x^Tx = 0$

$\alpha = \pm||x||$

Hence $$v = x \pm \|x\| e_1$$

and $$Fx = \mp \|x\| e_1$$