QR-factorizations:

Two vectors $x, y \in \mathbb{R}^n$ are orthogonal if $x^T y = \sum_{i=1}^{n} x_i y_i = 0$

A matrix $Q \in \mathbb{R}^{n \times n}$, is orthogonal if $Q^T Q = I_n$

So Q is invertible with $Q^{-1} = Q^T$.

Examples:

1) The identity matrix: $Q = I$

2) Permutations: $Q = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$

3) Rotations : $Q = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$

4) Reflections: $v \in \mathbb{R}^n$

$$Q = I - 2 \frac{v \cdot v^T}{v^T v}$$

Properties:

- $(m = n)$ If Q_1, Q_2 are orthogonal, so is $Q = Q_1 \cdot Q_2$.

  Proof: $Q^T Q = (Q_1 Q_2)^T (Q_1 Q_2) = Q_2^T \underbrace{Q_1^T Q_1}_{I_n} Q_2 = Q_2^T Q_2 = I_n$

- $\| Q \cdot x \|_2 = \| x \|$.

  Proof: $\| Q x \|_2^2 = x^T Q^T Q x = x^T x = \| x \|_2^2$.

  NB! This holds even if $Q \in \mathbb{R}^{n \times m}$, $Q^T Q = I_m$.

  Corollary: $(m = n)$ $|\lambda(Q)| = 1$.

Some applications:

- If $A = A^T$ then $Q^T A Q = \mathrm{diag}\{\lambda_1, \cdots, \lambda_m\}$
- QR-factorization: $A = Q \cdot R$, R upper triangular.
- Singular value decomposition: $A = U \Sigma V$, U, V orthogonal, Σ diagonal.

QR - factorizations

Applications

- Least square problems:

  Given the overdetermined system

  $$Ax = b \quad , \quad A \in \mathbb{R}^{n \times m} \quad , \quad n > m.$$

  Find x s.t. $\|b - Ax\|_2$ is as small as possible.
  This is the solution of the normal equation

  $$A^T A x = A^T b$$

  With $A = \tilde{Q} \cdot \tilde{R} \Rightarrow \tilde{R}^T \tilde{R} x = \tilde{R}^T \tilde{Q} b \Rightarrow \boxed{\tilde{R} x = \tilde{Q}^T b}$

- QR - iterations for finding eigenvalues:

  Given $A \in \mathbb{R}^{n \times n}$

  for $k = 0, 1, 2$
      Find Q, R s.t. $A^{(k)} = QR$
      $A^{(k+1)} = R \cdot Q$
  end

  If $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$ then

  $$A^{(k)} \xrightarrow[k \to \infty]{} \begin{bmatrix} \lambda_1 & \times & \times \cdots & \times \\ & \lambda_2 & & \vdots \\ & & \ddots & \times \\ 0 & & & \lambda_n \end{bmatrix},$$

Algorithm: How to compute Q and R.

Gram - Schmidt:

Let $A = [a_1, \cdots, a_m]$, a_i is column i of A

Assume A has full rank, a_i are linear. independent.

- Let $q_1 = a_1 / \|a_1\|_2$

- Find $v_2 = a_2 - r_{12} q_1$ so that $v_2 \perp q_1$

  that $v_2^T q_1 = a_2^T q_1 - r_{12} \underbrace{q_1^T q_1}_{=1} = 0 \Rightarrow r_{12} = a_2^T q_1$

and let $q_2 = \frac{v_2}{\|v_2\|_2}$.

Assume we have found $q_1, \cdots q_{j-1}$, based on $a_1, a_2, \cdots a_{j-1}$. Then, find v_j

$$v_j = a_j - \sum_{i=1}^{j-1} r_{ij}\, q_i \qquad \text{s.t. } v_j \perp q_\ell ,\ \ell = 1,2,\cdots j-1$$

$$\Rightarrow \quad v_j^T q_\ell = a_j^T q_\ell - \sum_{i=1}^{j-1} r_{ij} \underbrace{q_i^T q_\ell}_{= \delta_{i\ell}} = a_j^T q_\ell - r_{\ell j} = 0$$

$$\Rightarrow r_{\ell j} = a_j^T q_\ell$$

Which together give us

Gram-Schmidt algorithm

Given $A \in \mathbb{R}^{n \times m}$ $n \geq m$ with full rank.

for $j = 1, 2, \cdots, m$

$$v_j = a_j - \sum_{i=1}^{j-1} r_{ij}\, q_i , \qquad r_{ij} = a_j^T q_i$$

$$q_j = v_j / \|v_j\|_2 , \qquad r_{jj} = \|v_j\|_2$$

end

As long as $a_1, a_2, \cdots, a_m$ are linear independent, $v_j \neq 0$ and the algorithm will continue.
If $v_j = 0$, then $a_j \in \text{span}\{a_1, \cdots, a_{j-1}\}$

Notice that

$$v_j = r_{jj} \cdot q_j = a_j - \sum_{i=1}^{j-1} r_{ij}\, q_i$$

$$\Rightarrow a_j = \sum_{i=1}^{j} r_{ij}\, q_i$$

so, with $\tilde{Q} = [q_1, \cdots, q_m]$ and $R = \begin{bmatrix} r_{11} & \cdots & r_{1m} \\ & \ddots & \vdots \\ 0 & & r_{mm} \end{bmatrix} \in \mathbb{R}^{m \times m}$

we have $\tilde{A} = \tilde{Q} \cdot \tilde{R}$. upper triangular.

This is called the reduced QR-factorization.

Each $A \in \mathbb{R}^{n \times m}$ of full column rank has a unique, reduced QR-factorization

$$A = \tilde{Q}\tilde{R} \quad \text{with} \quad r_{ii} > 0$$

We can extend $\tilde{Q}$: $Q = [\hat{Q}, q_{m+1}, \cdots q_n] \in \mathbb{R}^{n \times n}$

Where $q_{m+1}, \cdots q_m$ are arbitrary chosen orthogonal vectors, and

$$R = \begin{bmatrix} \tilde{R} \\ 0 \end{bmatrix} \in \mathbb{R}^{n \times m}$$

If A do not have full column rank, then some $v_j = 0 \Rightarrow r_{jj} = 0$. Then pick some q_j orthogonal to the previous ones.
In fact

Every $A \in \mathbb{R}^{n \times m}$, $n \geq m$ has a QR-factorization

$$A = Q \cdot R$$

where Q is orthogonal and $R \in \mathbb{R}^{n \times m}$ is upper triangular.

But: Gram-Schmidt orthogalization is numerical unstable.

Householder triangulation.

This is an alternative way to construct the QR-factorization. The main tool is the

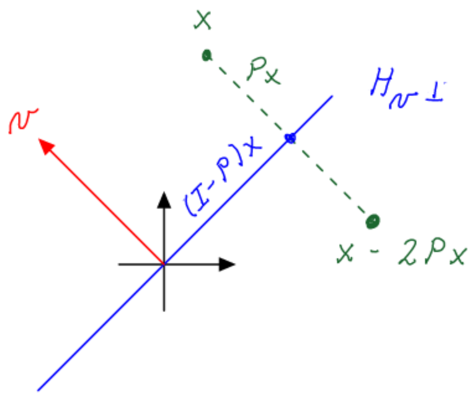
Householder reflection:

Given some $v \in \mathbb{R}^n$. Then

$$P = \frac{vv^T}{\|v\|^2}$$

is an orthogonal projection onto $H = \text{span}\{v\}$.
So

$$Q = I - 2P = I - 2\frac{vv^T}{\|v\|_2^2}$$



is an orthogonal reflection over the hyperplane $\{z \in \mathbb{R}^n,\ z^T v = 0\} := H_{v\perp}$.
Moreover $Q = Q^T = Q^{-1}$.

In the following, assume $\|v\|_2 = 1$, so our Householder reflection is

$$Q = I - 2vv^T.$$

Also, notice that

$$Q \cdot x = x - 2v\underbrace{v^T \cdot x}_{\mathbb{R}} = x - 2v^T x \cdot v.$$

So we never store Q, only v.

Application

Given $x \in \mathbb{R}^n$. Find Q (or v) s.t.

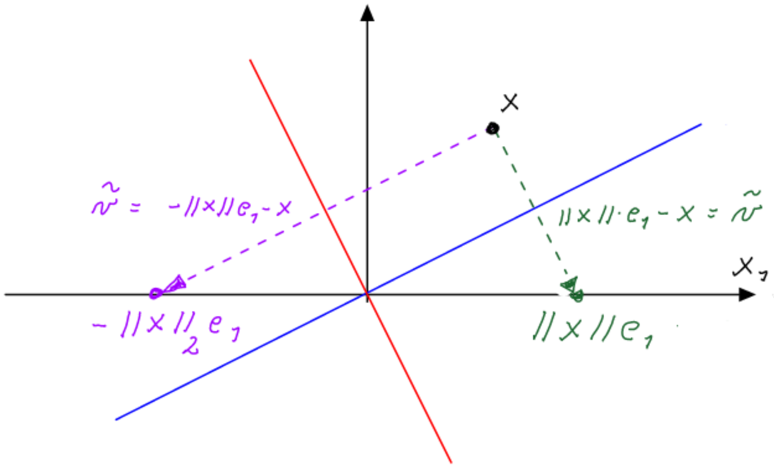
$$Q \cdot x = \pm \begin{bmatrix} \|x\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \pm \|x\|_2 \cdot e_1, \qquad e_1 = [1, 0, \cdots, 0]^T$$

$$\Rightarrow \quad \left(I - 2\frac{vv^T}{v^Tv}\right)x = \pm \|x\|_2 \cdot e_1$$

$$\Rightarrow \quad v = \frac{v^Tv}{v^Tx}\left(x \mp \|x\|_2 \cdot e_1\right)$$

NB! We only want the direction of v.

Choose v such that $\|v\|_2 = 1$. Moreover, if we are free to choose the sign, choose the sign of x_1, to avoid subtraction of almost equal numbers.



This figure is supposed to illustrate the situation.

In conclusion: Choose

$$\tilde{v} = x + \text{sign}(x_1) \cdot \|x\| \cdot e_1 \quad , \quad v = \frac{\tilde{v}}{\|\tilde{v}\|_2} .$$

Given $A \in \mathbb{R}^{n \times m}$, with full column rank.
We want to find $Q_1, Q_2, \cdots$ so that

$$Q_1 \cdot A = \begin{bmatrix} x & x & \cdots & x \\ 0 & x & & x \\ 0 & x & & x \\ \vdots & & & \vdots \\ \vdots & x & & x \end{bmatrix} , \quad Q_2 Q_1 A = \begin{bmatrix} x & x & x & \cdots & x \\ 0 & x & x & \cdots & x \\ 0 & 0 & x & & x \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & x & \cdots & x \end{bmatrix}$$

Until

$$Q_m Q_{m-1} \cdots Q_1 A = R \qquad \text{(upper triangular)}$$

Then $A = Q_1 Q_2 \cdots Q_m \cdot R = Q R$.

Householder QR-factorization

$R = A$

for $k = 1:m$

$\quad x = R_{k:n,k}$

$\quad v_k = \text{sign}(x_1) \cdot \|x\|_2 \cdot e_1 + x$

$\quad v_k = v_k / \|v_k\|_2$

$\quad R_{k:n,k:m} = R_{k:n,k:m} - 2 v_k (v_k^T R_{k:n,k:m})$

end.

Notice that $v_k \in \mathbb{R}^{n-k+1}$, and Q_k, as used above is

$$Q_k = \begin{pmatrix} I_{k-1} & 0 \\ 0 & I_{n-k+1} - 2 v_k v_k^T \end{pmatrix}$$

The algorithm produce R but not Q.
Usually, we do not need Q itself, only the operation it perform.

For example:

$$Ax = b \qquad A = QR \quad \text{nonsingular}$$

$$\Rightarrow \quad QRx = b \Rightarrow Rx = Q^T b = Q_1 Q_2 \cdots Q_n b$$

The computation of $y = Q^T b$ is then

$y = b$

for $k = 1:n$

$\quad y_{k:n} = y_{k:n} - 2v_k (v_k^T y_{k:n})$

end