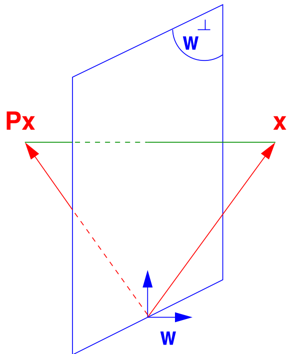
Householder QR

➤ Householder reflectors are matrices of the form

$$P = I - 2ww^T,$$

where w is a unit vector (a vector of 2-norm unity)



Geometrically, Px represents a mirror image of x with respect to the hyperplane $\text{span}\{w\}^{\perp}$.

A few simple properties:

- For real w: P is symmetric – It is also orthogonal ($P^TP = I$).
- In the complex case $P = I - 2ww^H$ is Hermitian and unitary.
- P can be written as $P = I - \beta vv^T$ with $\beta = 2/\|v\|_2^2$, where v is a multiple of w. [storage: v and β]
- Px can be evaluated $x - \beta(x^Tv) \times v$ (op count?)
- Similarly: $PA = A - vz^T$ where $z^T = \beta * v^T * A$

➤ NOTE: we work in $\mathbb{R}^m$, so all vectors are of length m, P is of size $m \times m$, etc.

➤ Next: we will solve a problem that will provide the basic ingredient of the Householder QR factorization.

Problem 1: Given a vector $x \neq 0$, find w such that

$$(I - 2ww^T)x = \alpha e_1,$$

where α is a (free) scalar.

Writing $(I - \beta vv^T)x = \alpha e_1$ yields $\boxed{\beta(v^Tx)\ v = x - \alpha e_1.}$

➤ Desired w is a multiple of $x - \alpha e_1$, i.e., we can take : $v = x - \alpha e_1$

➤ To determine α recall that $\boxed{\|(I - 2ww^T)x\|_2 = \|x\|_2}$

➤ As a result: $|\alpha| = \|x\|_2$, or $\alpha = \pm\|x\|_2$

➤ Should verify that both signs work, i.e., that in both cases we indeed get $Px = \alpha e_1$ [exercise]

.. Show that $(I - \beta vv^T)x = \alpha e_1$ when $v = x - \alpha e_1$ and $\alpha = \pm\|x\|_2$.

Solution: Equivalent to showing that

$$x - (\beta x^Tv)v = \alpha e_1 \quad \text{i.e.,} \quad x - \alpha e_1 = (\beta x^Tv)v$$

but recall that $v = x - \alpha e_1$ so we need to show that

$$\beta x^Tv = 1 \quad \text{i.e., that} \quad \frac{2}{\|x - \alpha e_1\|_2^2}(x^Tv) = 1$$

➤ Denominator $= \|x\|_2^2 + \alpha^2 - 2\alpha e_1^Tx = 2(\|x\|_2^2 - \alpha e_1^Tx)$

➤ Numerator $= 2x^Tv = 2x^T(x - \alpha e_1) = 2(\|x\|_2^2 - \alpha x^Te_1)$

Numerator/ Denominator = 1. ■

- Which sign is best? To reduce cancellation, the resulting $x - \alpha e_1$ should not be small. So, $\alpha = -\mathrm{sign}(\xi_1)\|x\|_2$, where $\xi_1 = e_1^T x$

$$v = x + \mathrm{sign}(\xi_1)\|x\|_2 e_1 \text{ and } \beta = 2/\|v\|_2^2$$

$$v = \begin{pmatrix} \hat{\xi}_1 \\ \xi_2 \\ \vdots \\ \xi_{m-1} \\ \xi_m \end{pmatrix} \quad \text{with} \quad \hat{\xi}_1 = \begin{cases} \xi_1 + \|x\|_2 & \text{if } \xi_1 > 0 \\ \xi_1 - \|x\|_2 & \text{if } \xi_1 \le 0 \end{cases}$$

- OK, but will yield a negative multiple of e_1 if $\xi_1 > 0$.

Alternative:

- Define $\sigma = \sum_{i=2}^m \xi_i^2$.
- Always set $\hat{\xi}_1 = \xi_1 - \|x\|_2$. Update OK when $\xi_1 \le 0$
- When $\xi_1 > 0$ compute $\hat{x}_1$ as

$$\hat{\xi}_1 = \xi_1 - \|x\|_2 = \frac{\xi_1^2 - \|x\|_2^2}{\xi_1 + \|x\|_2} = \frac{-\sigma}{\xi_1 + \|x\|_2}$$

So: $$\hat{\xi}_1 = \begin{cases} \frac{-\sigma}{\xi_1 + \|x\|_2} & \text{if } \xi_1 > 0 \\ \xi_1 - \|x\|_2 & \text{if } \xi_1 \le 0 \end{cases}$$

- It is customary to compute a vector v such that $v_1 = 1$. So v is scaled by its first component.
- If $\sigma == 0$, wll get $v = [1; x(2:m)]$ and $\beta = 0$.

- Matlab function:

```
function [v,bet] = house (x)
%% computes the householder vector for x
m = length(x);
v = [1 ; x(2:m)];
sigma = v(2:m)' * v(2:m);
if (sigma == 0)
   bet = 0;
else
   xnrm = sqrt(x(1)^2 + sigma) ;
   if (x(1) <= 0)
      v(1) = x(1) - xnrm;
   else
      v(1) = -sigma / (x(1) + xnrm) ;
   end
   bet = 2 / (1+sigma/v(1)^2);
   v = v/v(1) ;
end
```


Problem 2: Generalization.

Given an $m \times n$ matrix X, find $w_1, w_2, \ldots, w_n$ such that

$$(I - 2w_n w_n^T) \cdots (I - 2w_2 w_2^T)(I - 2w_1 w_1^T)X = R$$

where $r_{ij} = 0$ for $i > j$

- First step is easy : select w_1 so that the first column of X becomes αe_1
- Second step: select w_2 so that x_2 has zeros below 2nd component.
- etc.. After $k-1$ steps: $X_k \equiv P_{k-1} \ldots P_1 X$ has the following shape:

$$X_k = \begin{pmatrix} x_{11} & x_{12} & x_{13} & \cdots & \cdots & \cdots & x_{1n} \\ & x_{22} & x_{23} & \cdots & \cdots & \cdots & x_{2n} \\ & & x_{33} & \cdots & \cdots & \cdots & x_{3n} \\ & & & \ddots & \cdots & \cdots & \vdots \\ & & & & x_{kk} & \cdots & \vdots \\ & & & & x_{k+1,k} & \cdots & x_{k+1,n} \\ & & & & \vdots & \vdots & \vdots \\ & & & & x_{m,k} & \cdots & x_{m,n} \end{pmatrix}.$$

- To do: transform this matrix into one which is upper triangular up to the k-th column...
- ... while leaving the previous columns untouched.

- To leave the first $k-1$ columns unchanged w must have zeros in positions 1 through $k-1$.

$$P_k = I - 2w_k w_k^T, \quad w_k = \frac{v}{\|v\|_2},$$

where the vector v can be expressed as a Householder vector for a shorter vector using the matlab function house,

$$v = \begin{pmatrix} 0 \\ house(X(k:m,k)) \end{pmatrix}$$

- The result is that work is done on the $(k:m, k:n)$ submatrix.

ALGORITHM : 1. *Householder QR*

1. *For* $k = 1 : n$ *do*
2. $\quad [v, \beta] = house(X(k:m,k))$
3. $\quad X(k:m, k:n) = (I - \beta vv^T) X(k:m, k:n)$
4 $\quad$ *If* $(k < m)$
5 $\quad\quad X(k+1:m, k) = v(2:m-k+1)$
6 $\quad$ *end*
7 *end*

- In the end:

$$X_n = P_n P_{n-1} \dots P_1 X = \text{upper triangular}$$

Yields the factorization: $\quad X = QR$

where: $\quad Q = P_1 P_2 \dots P_n$ and $R = X_n$

Example:
Apply to system of vectors: $X = [x_1, x_2, x_3] = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & -1 \\ 1 & 0 & 4 \end{pmatrix}$

Answer:

$$x_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \; \|x_1\|_2 = 2, \; v_1 = \begin{pmatrix} 1+2 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \; w_1 = \frac{1}{2\sqrt{3}} \begin{pmatrix} 1+2 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$P_1 = I - 2w_1w_1^T = \frac{1}{6}\begin{pmatrix} -3 & -3 & -3 & -3 \\ -3 & 5 & -1 & -1 \\ -3 & -1 & 5 & -1 \\ -3 & -1 & -1 & 5 \end{pmatrix},$$

$$P_1X = \begin{pmatrix} -2 & -1 & -2 \\ 0 & 1/3 & -1 \\ 0 & -2/3 & -2 \\ 0 & -2/3 & 3 \end{pmatrix}$$

Next stage:

$$\tilde{x}_2 = \begin{pmatrix} 0 \\ 1/3 \\ -2/3 \\ -2/3 \end{pmatrix}, \ \|\tilde{x}_2\|_2 = 1, \ v_2 = \begin{pmatrix} 0 \\ 1/3 + 1 \\ -2/3 \\ -2/3 \end{pmatrix},$$

$$P_2 = I - \frac{2}{v_2^Tv_2}v_2v_2^T = \frac{1}{3}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 2 & 2 \\ 0 & 2 & 2 & -1 \\ 0 & 2 & -1 & 2 \end{pmatrix},$$

$$P_2P_1X = \begin{pmatrix} -2 & -1 & -2 \\ 0 & -1 & 1 \\ 0 & 0 & -3 \\ 0 & 0 & 2 \end{pmatrix}$$

Last stage:

$$\tilde{x}_3 = \begin{pmatrix} 0 \\ 0 \\ -2 \\ 3 \end{pmatrix}, \ \|\tilde{x}_3\|_2 = \sqrt{13}, \ v_1 = \begin{pmatrix} 0 \\ 0 \\ -2 - \sqrt{13} \\ 3 \end{pmatrix},$$

$$P_2 = I - \frac{2}{v_3^Tv_3}v_3v_3^T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -.83205 & .55470 \\ 0 & 0 & .55470 & .83205 \end{pmatrix},$$

$$P_3P_2P_1X = \begin{pmatrix} -2 & -1 & -2 \\ 0 & -1 & 1 \\ 0 & 0 & \sqrt{13} \\ 0 & 0 & 0 \end{pmatrix} = R,$$

$$P_3P_2P_1 = \begin{pmatrix} -.50000 & -.50000 & -.50000 & -.50000 \\ -.50000 & -.50000 & .50000 & .50000 \\ .13868 & -.13868 & -.69338 & .69338 \\ -.69338 & .69338 & -.13868 & .13868 \end{pmatrix}$$

- So we end up with the factorization $\boxed{X = \underbrace{P_1P_2P_3}_{Q}R}$

End Example

MAJOR difference with Gram-Schmidt: Q is $m \times m$ and R is $m \times n$ (same as X). The matrix R has zeros below the n-th row. Note also : this factorization always exists.

- Cost of Householder QR? Compare with Gram-Schmidt

Question: How to obtain $X = Q_1R_1$ where Q_1 = same size as X and R_1 is $n \times n$ (as in MGS)?

Answer: simply use the partitioning

$$X = (Q_1 \; Q_2) \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \quad \to \quad X = Q_1 R_1$$

➤ Referred to as the "thin" QR factorization (or "economy-size QR" factorization in matlab)

➤ How to solve a least-squares problem $Ax = b$ using the Householder factorization?

➤ Answer: no need to compute Q_1. Just apply Q^T to b.

➤ This entails applying the successive Householder reflections to b

The rank-deficient case

➤ Result of Householder QR: Q_1 and R_1 such that $Q_1 R_1 = X$. In the rank-deficient case, can have $\mathrm{span}\{Q_1\} \neq \mathrm{span}\{X\}$ because R_1 may be singular.

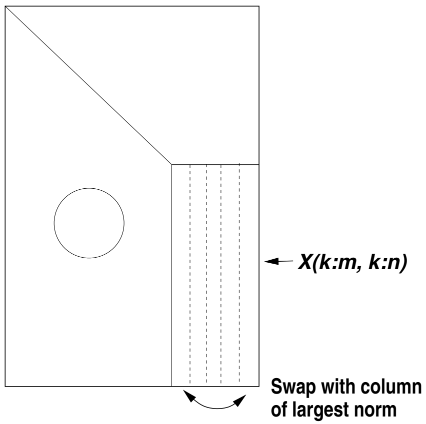
➤ Remedy: Householder QR with column pivoting. Result will be:

$$A\Pi = Q \begin{pmatrix} R_{11} & R_{12} \\ 0 & 0 \end{pmatrix}$$

➤ R_{11} is nonsingular. So rank(X) = size of R_{11} = rank(Q_1) and Q_1 and X span the same subspace.

➤ Π permutes columns of X.

Algorithm: At step k, active matrix is $X(k:m, k:n)$. Swap k-th column with column of largest 2-norm in $X(k:m, k:n)$. If all the columns have zero norm, stop.



Practical Question: How to implement this ???

✍ Suppose you know the norms of each column of X at the start. What happens to each of the norms of $X(2:m, j)$ for $j = 2, \cdots, n$? Generalize this to step k and obtain a procedure to inexpensively compute the desired norms at each step.

Properties of the QR factorization

Consider the 'thin' factorization $A = QR$, (size(Q) = [m,n] = size (A)). Assume $r_{ii} > 0$, $i = 1, \ldots, n$

1. When A is of full column rank this factorization exists and is unique

2. It satisfies:

$$\text{span}\{a_1, \cdots, a_k\} = \text{span}\{q_1, \cdots, q_k\}, \quad k = 1, \ldots, n$$

3. R is identical with the Cholesky factor G^T of $A^T A$.

➤ When A in rank-deficient and Householder with pivoting is used, then

$$Ran\{Q_1\} = Ran\{A\}$$

Cost of Householder QR

Look at the algorithm: each step works in rectangle $X(k : m, k : n)$. Step k : twice $2(m - k + 1)(n - k + 1)$

$$\begin{aligned} T(n) &= \sum_{k=1}^{n} 4(m - k + 1)(n - k + 1) \\ &= 4 \sum_{k=1}^{n} [(m - n) + (n - k + 1)](n - k + 1) \\ &= 4[(m - n) * \frac{n(n + 1)}{2} + \frac{n(n + 1)(2n + 1)}{6}] \\ &\approx (m - n) * 2n^2 + 4n^3/3 \\ &= 2mn^2 - \frac{2}{3} n^3 \end{aligned}$$

Givens Rotations

➤ Matrices of the form

$$G(i, k, \theta) = \begin{array}{cc} \begin{pmatrix} 1 & \ldots & 0 & & \ldots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & c & \cdots & s & \cdots & 0 \\ \vdots & \cdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \cdots & -s & \cdots & c & \cdots & 0 \\ \vdots & \cdots & \vdots & \cdots & \vdots & \cdots & \vdots \\ 0 & \ldots & 0 & & \ldots & & 1 \end{pmatrix} & \begin{array}{c} \\ \\ i \\ \\ k \\ \\ \\ \end{array} \end{array}$$

with $c = \cos\theta$ and $s = \sin\theta$

➤ represents a rotation in the span of e_i and e_k.

Main idea of Givens rotations consider $y = Gx$ then

$$\begin{aligned} y_i &= c * x_i + s * x_k \\ y_k &= -s * x_i + c * x_k \\ y_j &= x_j \quad \text{for} \quad j \neq i, k \end{aligned}$$

➤ Can make $y_k = 0$ by selecting

$$s = x_k/t; \quad c = x_i/t; \quad t = \sqrt{x_i^2 + x_k^2}$$

➤ This is used to introduce zeros in the first column of a matrix A (for example $G(m-1, m)$, $G(m-2, m-1)$ etc..$G(1, 2)$)..

➤ See text for details