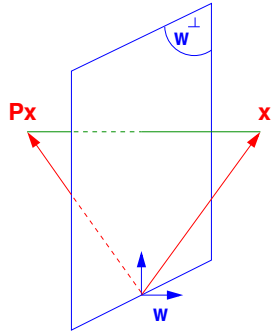


The Householder QR

► Householder reflectors are matrices in $\mathbb{R}^{m \times m}$ of the form

$$P = I - 2ww^T, \quad \text{where } w \text{ is a unit vector (a vector of 2-norm unity)}$$



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

8-1 GvL 5.1 – HouQR

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 $\beta(v^T x)v = x - \alpha e_1$.

► 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 $\|(I - 2ww^T)x\|_2 = \|x\|_2$

► 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]

8-3 GvL 5.1 – HouQR

A few simple properties:

- For real w : P is symmetric – It is also orthogonal ($P^T P = I$).
- 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 $x - \beta(x^T v) \times v$ (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. In complex case $(\cdot)^T \rightarrow (\cdot)^H$, 'symmetric' \rightarrow Hermitian, ...

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

8-2 GvL 5.1 – HouQR

Q1 .. Show that $(I - \beta vv^T)x = \alpha e_1$ when $v = x - \alpha e_1$ and $\alpha = \pm \|x\|_2$.

Q2 $Pw = ?$

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

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

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

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

8-4 GvL 5.1 – HouQR

Alternative:

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

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

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

- It is customary to compute a vector v such that $v_1 = 1$. So v is scaled by its first component.
- If $\sigma == 0$, will 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
    xnorm = sqrt(x(1)^2 + sigma) ;
    if (x(1) <= 0)
        v(1) = x(1) - xnorm;
    else
        v(1) = -sigma / (x(1) + xnorm) ;
    end
    bet = 2 / (1+sigma/v(1)^2);
    v = v/v(1) ;
end
```

Problem 2: Generalization.

Want to transform x into $y = Px$ where first k components of x and y are the same and $y_j = 0$ for $j > k + 1$. In other words:

Problem 2: Given $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, $x_1 \in \mathbb{R}^k$, $x_2 \in \mathbb{R}^{m-k}$, find: Householder transform $P = I - 2ww^T$ such that:
 $Px = \begin{pmatrix} x_1 \\ \alpha e_1 \end{pmatrix}$ where $e_1 \in \mathbb{R}^{m-k}$.

- Solution $w = \begin{pmatrix} 0 \\ \hat{w} \end{pmatrix}$, where \hat{w} is s.t. $(I - 2\hat{w}\hat{w}^T)x_2 = \alpha e_1$

- This is because:
$$P = \left[\begin{array}{c|c} I & 0 \\ \hline 0 & I - 2\hat{w}\hat{w}^T \end{array} \right]$$

Overall Procedure:

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

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

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: $X_k \equiv P_{k-1} \dots P_1 X$ 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.

ALGORITHM : 1 ■ Householder QR

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

- In the end:

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

- 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`,

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

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

Yields the factorization:

$$X = QR \quad \text{where:} \quad Q = P_1 P_2 \dots P_n \quad \text{and} \quad R = X_n$$

Example: Apply to

$$X = [x_1, x_2, x_3] = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & -1 \\ 1 & 0 & 4 \end{pmatrix}$$

Answer:

$$x_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad \|x_1\|_2 = 2, \quad v_1 = \begin{pmatrix} 1 + 2 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad v_1 = \begin{pmatrix} 3 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$P_1 = I - \frac{2}{v_1^T v_1} v_1 v_1^T = \frac{1}{6} \begin{pmatrix} -3 & -3 & -3 & -3 \\ -3 & 5 & -1 & -1 \\ -3 & -1 & 5 & -1 \\ -3 & -1 & -1 & 5 \end{pmatrix}.$$

$$P_1 X = \begin{pmatrix} -2 & -1 & -2 \\ 0 & 1/3 & -1 \\ 0 & -2/3 & -2 \\ 0 & -2/3 & 3 \end{pmatrix} \quad \text{Next stage:}$$

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

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

$$P_2 P_1 X = \begin{pmatrix} -2 & -1 & -2 \\ 0 & -1 & 1 \\ 0 & 0 & -3 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{Last stage:}$$

$$\tilde{x}_3 = \begin{pmatrix} 0 \\ 0 \\ -3 \\ 2 \end{pmatrix}, \|\tilde{x}_3\|_2 = \sqrt{13}, v_3 = \begin{pmatrix} 0 \\ 0 \\ -3 - \sqrt{13} \\ 2 \end{pmatrix},$$

$$P_3 = I - \frac{2}{v_3^T v_3} v_3 v_3^T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -.83205 & .55470 \\ 0 & 0 & .55470 & .83205 \end{pmatrix},$$

$$P_3 P_2 P_1 X = \begin{pmatrix} -2 & -1 & -2 \\ 0 & -1 & 1 \\ 0 & 0 & \sqrt{13} \\ 0 & 0 & 0 \end{pmatrix} = R,$$

$$P_3 P_2 P_1 = \begin{pmatrix} -.50000 & -.50000 & -.50000 & -.50000 \\ -.50000 & -.50000 & .50000 & .50000 \\ .13868 & -.13868 & -.69338 & .69338 \\ -.69338 & .69338 & -.13868 & .13868 \end{pmatrix}$$

► So we end up with the factorization

$$X = \underbrace{P_1 P_2 P_3}_Q R$$

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 $X = Q_1 R_1$ where $Q_1 =$ same size as X and R_1 is $n \times n$ (as in MGS)?

Answer: simply use the partitioning

$$X = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \rightarrow X = Q_1 R_1$$

- 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

8-17 GvL 5.1 – HouQR

The rank-deficient case

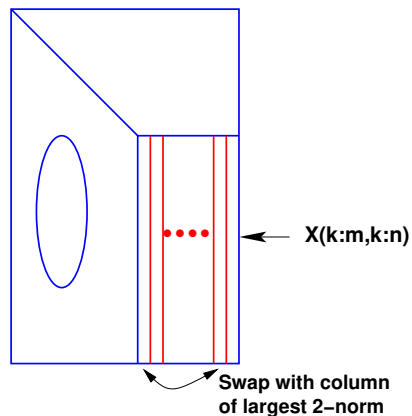
- Result of Householder QR: Q_1 and R_1 such that $Q_1 R_1 = X$. In the rank-deficient case, can have $\text{span}\{Q_1\} \neq \text{span}\{X\}$ because R_1 may be singular.
- Remedy: Householder QR with column pivoting. Result will be:

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

- R_{11} is nonsingular. So $\text{rank}(X) = \text{size of } R_{11} = \text{rank}(Q_1)$ and Q_1 and X span the same subspace.
- Π permutes columns of X .

8-18 GvL 5.1 – HouQR

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 columns have zero norm, stop.



8-19 GvL 5.1 – HouQR

Practical Question: How to implement this ???

- 4 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 $j = 2, \dots, n$? Generalize this to step k and obtain a procedure to inexpensively compute the desired norms at each step.

8-20 GvL 5.1 – HouQR

Properties of the QR factorization

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

1. When A is of full column rank this factorization exists and is unique
2. It satisfies:

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

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

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

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

Ex 5 Consider the mapping that sends any point x in \mathbb{R}^2 into a point y in \mathbb{R}^2 that is **rotated** from x by an angle θ . Find the matrix representing the mapping. [Hint: observe how the canonical basis is transformed.] Show an illustration. What is the mapping corresponding to an angle $-\theta$?

Main idea of Givens QR

Consider $y = Gx$ then:

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

► 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 appropriate locations of first column of a matrix A (for example $G(m-1, m)$, $G(m-2, m-1)$ etc.. $G(1, 2)$). Then similarly for second column, etc.

Givens Rotations and the Givens QR

► Givens rotations are matrices of the form:

$$G(i, k, \theta) = \begin{pmatrix} 1 & \dots & 0 & & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & c & \dots & s & \dots & 0 \\ \vdots & \dots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & -s & \dots & c & \dots & 0 \\ \vdots & \dots & \vdots & \dots & \vdots & \dots & \vdots \\ 0 & \dots & 0 & & \dots & & 1 \end{pmatrix} \begin{matrix} i \\ \\ k \\ \\ \end{matrix}$$

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

► $G(i, k, \theta)$ represents a rotation in the span of e_i and e_k