Linear algebra & Numerical Analysis

Orthogonalization

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Outline

- Orthogonal matrices
- Gram-Schmidt process
- Givens rotations
- Householder transformation

Euclidean inner product

- Euclidean inner product (dot product) is a mapping
 u ∈ Rⁿ, v ∈ Rⁿ → (u, v) ∈ R
- It is defined for two vectors u, v by

$$(u, v) = u_1 v_1 + ... + u_n v_n = u^T v$$

• It satisfies for each \mathbf{u} , \mathbf{v} , \mathbf{w} a $\alpha \in \mathbb{R}$ the following properties

$$(\mathbf{u} + \mathbf{v}, \mathbf{w}) = (\mathbf{u}, \mathbf{w}) + (\mathbf{v}, \mathbf{w})$$
$$(\alpha \mathbf{u}, \mathbf{v}) = \alpha(\mathbf{u}, \mathbf{v})$$
$$(\mathbf{u}, \mathbf{v}) = (\mathbf{v}, \mathbf{u})$$
$$(\mathbf{u}, \mathbf{u}) > 0 \quad \text{pro} \quad \mathbf{u} \neq \mathbf{o}$$

Orthogonal matrices

Square matrix **Q** satisfying

$$Q^TQ = I$$

is called orthogonal matrix. This matrix has orthogonal columns and it holds

$$Q^{-1} = Q^{\mathsf{T}}.$$

The columns form an orthogonal set of vectors, i.e.

$$(\mathbf{q}_i, \mathbf{q}_j) = \mathbf{q}_i^T \mathbf{q}_j = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

QR factorization

For an arbitrary matrix $A \in \mathbb{R}^{m,n}$ there exist an orthogonal matrix $Q \in \mathbb{R}^{m,m}$ and an upper triangular matrix $R \in \mathbb{R}^{m,n}$, such that

A = QR.

QR factorization

m = n:

$$\left(\begin{array}{c|c|c} \mathbf{a}_1 & \mathbf{a}_2 & \dots & \mathbf{a}_n \end{array}\right) = \left(\begin{array}{c|c|c} \mathbf{q}_1 & \mathbf{q}_2 & \dots & \mathbf{q}_n \end{array}\right) \left(\begin{array}{c|c|c} r_{11} & r_{12} & \dots & r_{1n} \\ & r_{22} & & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{array}\right)$$

 The columns of A can be written as a linear combination of the columns of Q

$$\mathbf{a}_1 = r_{11}\mathbf{q}_1,$$

$$\mathbf{a}_2 = r_{12}\mathbf{q}_1 + r_{22}\mathbf{q}_2,$$

$$\vdots$$

$$\mathbf{a}_n = r_{1n}\mathbf{q}_1 + r_{2n}\mathbf{q}_2 + \dots + r_{nn}\mathbf{q}_n$$

Example:

For matrix

$$\mathbf{A} = \left(egin{array}{ccc} \mathbf{1} & \mathbf{1} & \mathbf{0} \ \mathbf{0} & \mathbf{1} & \mathbf{1} \ \mathbf{1} & \mathbf{0} & \mathbf{1} \end{array}
ight)$$

Find the columns $\mathbf{q}_1, \dots, \mathbf{q}_n$ and the elements of matrix **R**.

$$a_{1} = N_{11} \cdot q_{1}$$

$$a_{2} = N_{12} \cdot q_{1} + N_{22} \cdot q_{2}$$

$$a_{3} = N_{13} \cdot q_{1} + N_{23} \cdot q_{2} + N_{33} \cdot q_{3}$$

$$A_{1} = N_{13} \cdot q_{1}$$

$$A_{11} = N_{13} \cdot q_{1}$$

$$A_{12} = N_{13} \cdot q_{1}$$

$$A_{13} = N_{13} \cdot q_{1}$$

$$A_{14} = N_{13} \cdot q_{1}$$

$$A_{15} = N_{15} \cdot q_{15}$$

$$A_{17} = N_{17} \cdot q_{15}$$

$$A_{18} = N_{17} \cdot q_{15}$$

$$A_{19} = N_{19} \cdot q_{15}$$

$$A_{11} = N_{11} \cdot q_{15}$$

$$A_{11} = N_{11} \cdot q_{15}$$

$$A_{12} = N_{13} \cdot q_{15}$$

$$A_{13} = N_{14} \cdot q_{15}$$

$$A_{14} = N_{15} \cdot q_{15}$$

$$A_{15} = N_{15} \cdot q_{15}$$

$$A_{17} = N_{17} \cdot q_{15}$$

$$A_{18} = N_{17} \cdot q_{15}$$

$$A_{19} = N_{19} \cdot$$

$$0 = (q_{1}, q_{2}) = (q_{1}, q_{2} - k_{12}, q_{1}) = (q_{1}, q_{2}) - k_{12}(q_{1}, q_{2}) = 0$$

$$= \lambda_{12} = (q_{1}, q_{2}) = \frac{1}{12!}(1+0+0) = \frac{1}{12!}$$

$$\mathcal{T}_{2} = \mathcal{Z}_{2} - \mathcal{N}_{12} \cdot \mathcal{Y}_{1} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} - \frac{1}{12!} \cdot \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix} \\
\mathcal{N}_{22} = ||\mathcal{T}_{2}||^{2} + ||\mathcal{T}_{2}||^{2} + ||\mathcal{T}_{1}||^{2} + ||\mathcal{T}_{1}||^{2} = ||\mathcal{T}_{1}||^{2} + ||\mathcal{T}_{1}||^{2} = ||\mathcal{T}_{2}||^{2} + ||\mathcal{T}_{1}||^{2} = ||\mathcal{T}_{2}||^{2} = ||\mathcal{T}_{2}||^{2} + ||\mathcal{T}_{2}||^{2} = ||\mathcal{T}_{2}||^{2} + ||\mathcal{T}_{2}||^{2} = ||\mathcal{T}_{2$$

$$Q_{3} = \frac{r_{3}}{|r_{3}|} = \frac{13}{2} \cdot \frac{2}{3} \cdot \frac{1}{1} = \frac{1}{3} \cdot \frac{1}{1}$$

$$Q = \begin{bmatrix} \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \end{bmatrix}$$

$$R = \begin{bmatrix} \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \end{bmatrix}$$

$$R = \begin{bmatrix} \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \end{bmatrix}$$

Problem: Find the columns q_1, \dots, q_n and the elements of matrix **R**

Process:

•
$$\mathbf{v}_1 = \mathbf{a}_1, \quad \mathbf{q}_1 = \frac{\mathbf{v}_1}{\|\mathbf{v}_1\|}, \quad r_{11} = \|\mathbf{v}_1\|$$
 $\|\mathbf{a}\|^2 = (\mathbf{a}, \mathbf{a})$

• Let us consider that we already know $\mathbf{q}_1, \dots, \mathbf{q}_{j-1}$

$$\mathbf{a}_{j} = r_{1j}\mathbf{q}_{1} + \dots + r_{ij}\mathbf{q}_{i} + \dots + r_{j-1,j}\mathbf{q}_{j-1} + \underbrace{r_{jj}\mathbf{q}_{j}}_{\mathbf{v}_{j}}$$

$$\mathbf{v}_{j} = \mathbf{a}_{j} - r_{1j}\mathbf{q}_{1} - \dots - r_{ij}\mathbf{q}_{i} - \dots - r_{j-1,j}\mathbf{q}_{j-1}$$

• Requirement: V_j is orthogonal to q_1, \dots, q_{j-1}

for k = 1, ..., j - 1



• Since $(\mathbf{q}_k, \mathbf{q}_i) = 0$ for $k \neq i$ $(\mathbf{q}_i, \mathbf{a}_j - r_{ij}\mathbf{q}_i) = (\mathbf{q}_i, \mathbf{a}_j) - r_{ij}\underbrace{(\mathbf{q}_i, \mathbf{q}_i)} = 0 \implies r_{ij} = (\mathbf{q}_i, \mathbf{a}_j)$

$$\mathbf{q}_{j} = \frac{\mathbf{v}_{j}}{\|\mathbf{v}_{j}\|} = \frac{\mathbf{v}_{j}}{r_{jj}} \Rightarrow r_{jj} = \|\mathbf{v}_{j}\|$$

$$- || v_j ||^2 = r_{jj}^2 q_j^T q_j = r_{jj}^2$$

Algorithm

```
function [Q,R] = my_gram_schmidt(A)
n = size(A,1); Q = zeros(n); R = zeros(n);
for j=1:n
                                                            modify A(:,j) to v
      v=A(:,j);
                                                            for more accuracy
       for i=1:j-1
              R(i,j)=Q(:,i)'*A(:,j);
                                                       r_{ij} = (\mathbf{q}_i, \mathbf{a}_j)
              v=v-R(i,j)*Q(:,i);
                                                       \mathbf{v}_i = \mathbf{a}_i - r_{1i}\mathbf{q}_1 - \ldots - r_{ii}\mathbf{q}_i - \ldots - r_{j-1,i}\mathbf{q}_{j-1}
       end
                                                        r_{ii} = || v_i ||
      R(j,j) = norm(v);
                                                        \mathbf{q}_j = \frac{\mathbf{v}_j}{r_{ij}}
      Q(:,j)=v/R(j,j);
end
```

Remark: The Gram-Schmidt process can be stabilized by a small modification → modified Gram-Schmidt, which gives the same result as the original formula in exact arithmetic and introduces smaller errors in finite-precision arithmetic.

Givens transformation

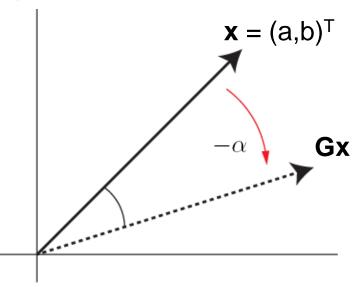
Let us consider Givens matrix (rotation matrix)

$$\mathbf{G} = \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix}$$

which rotates a vector $(a,b)^T$ in the xy-plane through an angle $-\alpha$ about the origin.

We will use a notation

$$c = \cos \alpha \text{ a } s = \sin \alpha$$



Example in Matlab: givens_rotation

Givens transformation

 We can use matrix G to zeroing elements. Let us consider that

$$\mathbf{G}^T \mathbf{x} = \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \sqrt{a^2 + b^2} \\ 0 \end{pmatrix}$$

It is easy to see that

$$c = \frac{a}{\sqrt{a^2 + b^2}}$$
 a $s = \frac{-b}{\sqrt{a^2 + b^2}}$

Givens transformation

Generalization for vectors of the order n

$$\mathbf{G}_{ij} = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & c & s & \\ & & \ddots & \\ & & -s & c & \\ & & & \ddots & \\ & & & & 1 \end{pmatrix} j \qquad \mathbf{y} = \mathbf{G}_{ij}^T \mathbf{x}$$

$$y_k = \begin{cases} cx_i - sx_j, & k = i, \\ sx_i + cx_j, & k = j, \\ x_k, & k \neq i, j. \end{cases}$$

To zeroing the element in the j-th row we have

$$c = \frac{x_i}{\sqrt{x_i^2 + x_j^2}}, \quad s = \frac{-x_j}{\sqrt{x_i^2 + x_j^2}}$$

Givens QR method

 Form of the rotation matrix to zeroing element in the i-th row is

$$\mathbf{G}(i-1,i), \text{ where } c = \frac{x_{i-1}}{\sqrt{x_{i-1}^2 + x_i^2}}, \quad s = \frac{-x_i}{\sqrt{x_{i-1}^2 + x_i^2}}$$

Using the rotation matrices we will edit matrix A:

$$\mathbf{A} = \begin{pmatrix} * & * & * \\ * & * & * \\ * & * & * \end{pmatrix} \quad \mathbf{G}(2,3)^T \quad \begin{pmatrix} * & * & * \\ * & * & * \\ 0 & * & * \end{pmatrix} \quad \mathbf{G}(1,2)^T \quad \begin{pmatrix} * & * & * \\ 0 & * & * \\ 0 & * & * \end{pmatrix} \quad \mathbf{G}(2,3)^T \quad \begin{pmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & * \end{pmatrix} = \mathbf{R}.$$

$$\left\{ egin{aligned} \mathbf{G}_p^T \dots \mathbf{G}_1^T \mathbf{A} &= \mathbf{R} &\Leftrightarrow & \mathbf{Q}^T \mathbf{A} &= \mathbf{R}
ight\} \ && \downarrow & \\ \mathbf{A} &= \mathbf{Q} \mathbf{R}, & \mathbf{Q} &= \mathbf{G}_1 \dots \mathbf{G}_p. \end{aligned}
ight.$$

Example:

$$\mathbf{A} = \begin{pmatrix} -1 & 4 & -1 \\ -2 & -1 & -11 \\ 2 & 10 & 2 \end{pmatrix}$$

Solution:

Foliation: G(i-1,i) To set A(3,1) = 0, we need to build matrix
$$G_1(2,3)$$
 $c = \frac{-2}{\sqrt{(-2)^2 + 2^2}} = \frac{-\sqrt{2}}{2}, \quad s = \frac{-2}{\sqrt{(-2)^2 + 2^2}} = \frac{-\sqrt{2}}{2}$ $s = \frac{-x_i}{\sqrt{x_{i-1}^2 + x_i^2}}$ $s = \frac{-x_i}{\sqrt{x_{i-1}^2 + x_i^2}}$

$$\mathbf{G}_{1}(2,3) = \begin{pmatrix} 1 & & & \\ & -\sqrt{2}/2 & -\sqrt{2}/2 \\ & \sqrt{2}/2 & -\sqrt{2}/2 \end{pmatrix} \qquad \mathbf{G(i-1,i)} = \begin{pmatrix} 1 & & c & s & \\ & c & s & \\ & -s & c & \\ & & 1 \end{pmatrix} \mathbf{i} \mathbf{1}$$

$$G(i-1,i)$$

$$c = \frac{x_{i-1}}{\sqrt{x_{i-1}^2 + x_i^2}}$$

$$s = \frac{-x_i}{\sqrt{x_{i-1}^2 + x_i^2}}$$

$$\mathbf{G(i-1,i)} = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & c & s & & & \\ & & & \ddots & & & \\ & & -s & c & & & \\ & & & \ddots & & \\ & & & & 1 \end{pmatrix} \mathbf{i-1}$$

$$\mathbf{A}_1 = \mathbf{G}_1(2,3)^T \mathbf{A} = \begin{pmatrix} -1 & 4 & -1 \\ 2\sqrt{2} & 11\sqrt{2}/2 & 13\sqrt{2}/2 \\ 0 & -9\sqrt{2}/2 & 9\sqrt{2}/2 \end{pmatrix}$$

• To set $A_1(2,1) = 0$, we need to build matrix $G_2(1,2)$

$$c = -1/3,$$

 $s = -2\sqrt{2}/3$ $\mathbf{G}_2(1,2) = \begin{pmatrix} -1/3 & -2\sqrt{2}/3 \\ 2\sqrt{2}/3 & -1/3 \\ 1 \end{pmatrix}$

$$\mathbf{A}_2 = \mathbf{G}_2(1,2)^T \mathbf{A}_1 = \begin{pmatrix} 3 & 6 & 9 \\ 0 & -9\sqrt{2}/2 & -3\sqrt{2}/2 \\ 0 & -9\sqrt{2}/2 & 9\sqrt{2}/2 \end{pmatrix}$$

• To set $A_2(3,2) = 0$, we need matrix $G_3(2,3)$

$$c = -\sqrt{2}/2,$$

 $s = -\sqrt{2}/2$ $\mathbf{G}_3(2,3) = \begin{pmatrix} 1 & & \\ & -\sqrt{2}/2 & \sqrt{2}/2 \\ & -\sqrt{2}/2 & -\sqrt{2}/2 \end{pmatrix}$

$$\mathbf{A}_3 = \mathbf{G}_3(2,3)^T \mathbf{A}_2 = \begin{pmatrix} 3 & 6 & 9 \\ 0 & 9 & -3 \\ 0 & 0 & -6 \end{pmatrix} = \mathbf{R}$$

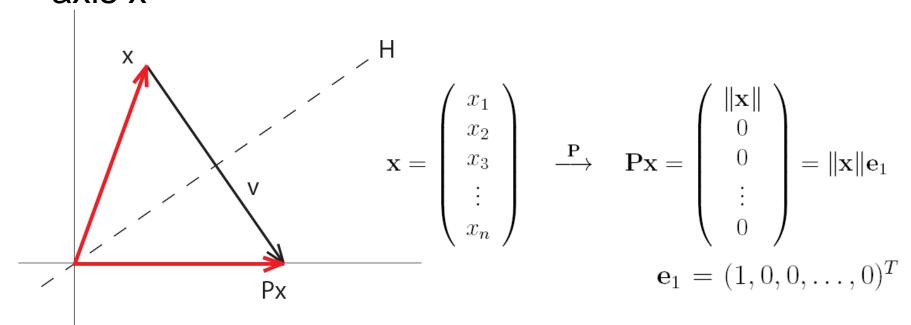
$$\mathbf{Q} = \mathbf{G}_1(2,3)\mathbf{G}_2(1,2)\mathbf{G}_3(2,3) = \begin{pmatrix} -1/3 & 2/3 & -2/3 \\ -2/3 & 1/3 & 2/3 \\ 2/3 & 2/3 & 1/3 \end{pmatrix}$$

Algorithm

```
function [Q,R] = my_givens_QR(A)
n = size(A,1); Q=eye(n); R=A;
for j=1:n
    for i=n:(-1):j+1
        x=R(:,j);
        if norm([x(i-1),x(i)])>0
            c=x(i-1)/norm([x(i-1),x(i)]);
            s=-x(i)/norm([x(i-1),x(i)]);
            G=eye(n); G([i-1,i],[i-1,i])=[c,s;-s,c];
            R=G'*R;
            Q=Q*G;
        end
    end
end
```

Householder transformation

 For vector x we are able to find its reflection Px to axis x



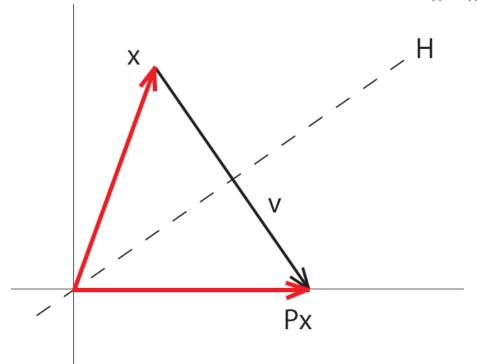
Both vectors have the same length

$$\|\mathbf{P}\mathbf{x}\| = [\mathbf{P}\mathbf{x}]_1 = \|\mathbf{x}\|$$

Householder transformation

 Px is mirror image of x with axis H. H is orthogonal to vector

$$\mathbf{v} = \mathbf{P}\mathbf{x} - \mathbf{x} = \|\mathbf{x}\|\mathbf{e}_1 - \mathbf{x}$$

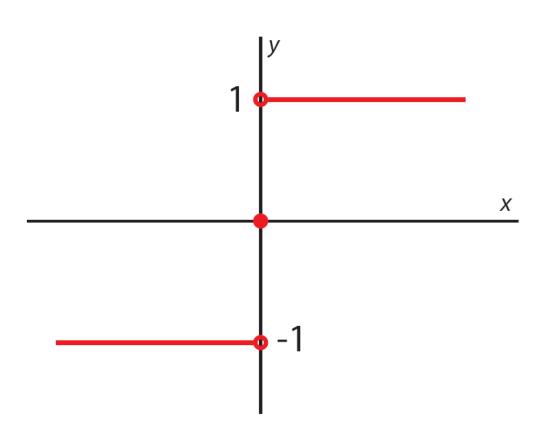


Reflection matrix:

$$\mathbf{P} = \mathbf{I} - 2 \frac{\mathbf{v} \mathbf{v}^T}{\|\mathbf{v}\|^2} = \mathbf{I} - 2 \frac{\mathbf{v} \mathbf{v}^T}{\mathbf{v}^T \mathbf{v}}$$

Function sign

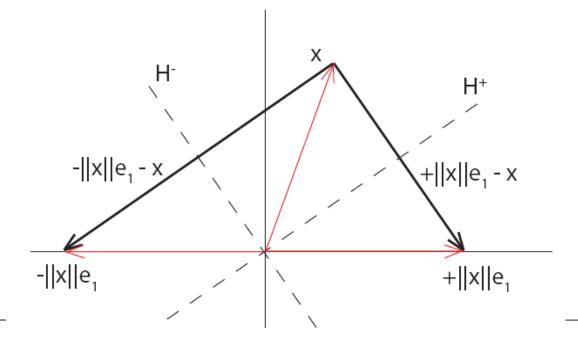
$$sign(x) = \begin{cases} -1 & \text{if } x < 0, \\ 0 & \text{if } x = 0, \\ 1 & \text{if } x > 0. \end{cases}$$



Householder transformation

- The image of **x** is not unique: $z ||\mathbf{x}|| \mathbf{e}_1$ for all |z| = 1
- For numerical stability we choose $z = -\mathrm{sign}(x_1)$

$$\mathbf{v} = -\operatorname{sign}(x_1) \|\mathbf{x}\| \mathbf{e}_1 - \mathbf{x}$$



Householder QR method

Using the reflections P we can modify matrix A

$$\mathbf{P}_n \cdots \mathbf{P}_2 \mathbf{P}_1 \mathbf{A} = \mathbf{Q}^T \mathbf{A} = \mathbf{R}$$



$$A = QR, \quad Q = P_1 \dots P_n$$

• Example:

$$\mathbf{A} = \begin{pmatrix} -1 & 4 & -1 \\ -2 & -1 & -11 \\ 2 & 10 & 2 \end{pmatrix}$$

Solution:

$$\mathbf{x} = (-1, -2, 2)^T, \quad \|\mathbf{x}\| = \sqrt{1 + 4 + 4} = 3, \quad \operatorname{sign}(x_1) = -1$$

$$\mathbf{v} = -\operatorname{sign}(x_1)\|\mathbf{x}\|\mathbf{e}_1 - \mathbf{x} = \|\mathbf{x}\|\mathbf{e}_1 - \mathbf{x} =$$

$$= \begin{pmatrix} 3\\0\\0 \end{pmatrix} - \begin{pmatrix} -1\\-2\\2 \end{pmatrix} = \begin{pmatrix} 4\\2\\-2 \end{pmatrix}$$

$$\mathbf{P}_1 = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} = \begin{pmatrix} -1/3 & -2/3 & 2/3 \\ -2/3 & 2/3 & 1/3 \\ 2/3 & 1/3 & 2/3 \end{pmatrix}$$

$$\mathbf{R}_1 = \mathbf{P}_1 \mathbf{A} = \begin{pmatrix} 3 & 6 & 9 \\ 0 & 0 & -6 \\ 0 & 9 & -3 \end{pmatrix}$$

$$\mathbf{x} = (0,9)^T, \quad \|\mathbf{x}\| = 9, \quad \text{sign}(x_1) = 1$$

$$\mathbf{v} = -\|\mathbf{x}\|\mathbf{e}_1 - \mathbf{x} = \begin{pmatrix} -9 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 9 \end{pmatrix} = \begin{pmatrix} -9 \\ -9 \end{pmatrix}$$

$$\mathbf{P'}_2 = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad \Rightarrow \quad \mathbf{P}_2 = \begin{pmatrix} \frac{1}{0} & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$\mathbf{R}_2 = \mathbf{P}_2 \mathbf{P}_1 \mathbf{A} = \begin{pmatrix} 3 & 6 & 9 \\ 0 & -9 & 3 \\ 0 & 0 & 6 \end{pmatrix}$$

$$\mathbf{Q} = \mathbf{P}_1 \mathbf{P}_2 = \begin{pmatrix} -1/3 & -2/3 & 2/3 \\ -2/3 & -1/3 & -2/3 \\ 2/3 & -2/3 & -1/3 \end{pmatrix}$$

Algorithm

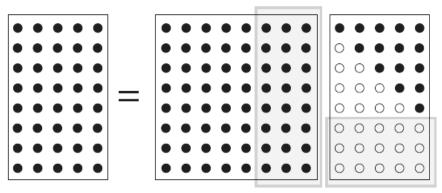
```
function [Q,R] = my householder QR(A)
n = size(A,1); Q=eye(n); R=A; I = eye(n);
for j=1:n-1
    x=R(j:n,j);
    v=-sign(x(1))*norm(x)*eye(n-j+1,1)-x;
    if norm(v) > 0,
        v=v/norm(v);
        P=I; P(j:n,j:n)=P(j:n,j:n)-2*v*v';
        R=P*R;
        Q=Q*P;
    end
end
```

QR factorization

m > n:

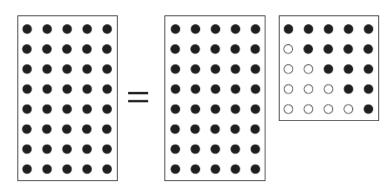
Full QR factorization

$$A = QR$$



Reduced QR factorization

$$\mathbf{A} = \tilde{\mathbf{Q}}\tilde{\mathbf{R}}$$



Matlab function: qr

- [Q,R] = qr(A), where A is m-by-n, produces an m-by-n upper triangular matrix R and an m-by-m unitary matrix Q so that A = Q*R.
- [Q,R] = qr(A,0) produces the "economy size" decomposition. If m>n, only the first n columns of Q and the first n rows of R are computed. If m<=n, this is the same as [Q,R] = qr(A)

For more details see: help qr

References

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- Lloyd Nicholas Trefethen, David Bau, Numerical linear algebra (available on Google books)
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- Gram-Schmidt in 9 Lines of MATLAB
 http://ocw.mit.edu/courses/mathematics/18-06-linear-algebra-spring-2010/related-resources/MIT18_06S10_gramschmidtmat.pdf