

Numerical Linear Algebra

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QR factorization, Least squares

- ► Invertibility of KKT matrix
- QR factorization for constrained least squares problem
- ► Hausholder transformations and QR factorization
- Numerical eigenvalue problem
- ► Q & A

Recap of Previous Lecture

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- QR and reduced QR factorization
- Linear least squares
- Constrained least squares

Problem 14.1

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Constrained Least Squares Problem

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KKT equation

$$\begin{pmatrix} 2A^T A & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} 2A^T b \\ d \end{pmatrix}$$

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KKT equation (William Karush, Harold Kuhn and Albert Tucker)

KKT matrix

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Theorem 14.2

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KKT matrix is invertible iff

a. C has linearly independent rows

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- a. C has linearly independent rows
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- ► Necessary condition:

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- a. C has linearly independent rows
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KKT matrix is invertible \Rightarrow a. & b. of the theorem 14.2 are satisfied

- Sufficient condition:
 - a. & b. of the theorem 14.2 are satisfied \Rightarrow KKT matrix is invertible

Proof of necessary condition, part a

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- Necessary condition: KKT matrix is invertible ⇒ a. & b. of the theorem 14.2 are satisfied
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Contradiction: KKT matrix is not invertible

Proof of necessary condition, part b

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- $\tilde{\mathbf{x}} = 0, 2\mathbf{A}^T \mathbf{A} \tilde{\mathbf{x}} + \mathbf{C}^T \tilde{\mathbf{\lambda}} = 0 \Rightarrow \mathbf{C}^T \tilde{\mathbf{\lambda}} = 0$

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- $\blacktriangleright \ \ C\tilde{x} = 0 \equiv \tilde{x}^T C^T = 0 \Rightarrow \tilde{x}^T C^T \tilde{\lambda} = 0 \Rightarrow \|A\tilde{x}\|_2^2 = 0 \Rightarrow A\tilde{x} = 0 \Downarrow$
- ightharpoonup Contradiction: $\tilde{x} = 0$
- ▶ $\tilde{x} = 0, 2A^T A \tilde{x} + C^T \tilde{\lambda} = 0 \Rightarrow C^T \tilde{\lambda} = 0$ &+ condition a.(linearly independent rows of C)

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- ► $\binom{A}{C}\tilde{x} = 0$ &+ condition b.(linearly independent columns of $\binom{A}{C}$) \Downarrow
- ightharpoonup Contradiction: $\tilde{x} = 0$
- ▶ $\tilde{x} = 0, 2A^T A \tilde{x} + C^T \tilde{\lambda} = 0 \Rightarrow C^T \tilde{\lambda} = 0$ &+ condition a.(linearly independent rows of C) ↓
- ► Contradiction: $\tilde{\lambda} = 0$

Solution of KKT equation

► KKT equation:
$$\begin{pmatrix} 2A^TA & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} 2A^Tb \\ d \end{pmatrix}$$

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$$\begin{pmatrix} \hat{x} \\ \hat{\lambda} \end{pmatrix} = \begin{pmatrix} 2A^T A & C^T \\ C & 0 \end{pmatrix}^{-1} \begin{pmatrix} 2A^T b \\ d \end{pmatrix}$$

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Algorithm 14.3

► Compute $H = 2A^TA$ and $f = 2A^Tb$

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- ► Compute $H = 2A^TA$ and $f = 2A^Tb$
- ► Solve $\begin{pmatrix} H & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ d \end{pmatrix}$

Remark 14.4

Computing A^TA is not practical: expensive, may introduce errors

$Different \ Lagrangian \Rightarrow different \ KKT \ equation$

$$L(x,\lambda) = (Ax - b, Ax - b) + 2(Cx - d, \lambda)$$

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$$(A^{T}Ax - A^{T}b) + C^{T}\lambda = 0$$
$$Cx = d$$

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$$(A^{T}Ax - A^{T}b) + C^{T}\lambda = 0$$
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${\sf Different\ Lagrangian} \Rightarrow {\sf different\ KKT\ equation}$

$$L(x,\lambda) = (Ax - b, Ax - b) + 2(Cx - d, \lambda)$$

$$(A^T A x - A^T b) + C^T \lambda = 0$$
$$Cx = d$$

$$\begin{pmatrix} A^T A & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} A^T b \\ d \end{pmatrix}$$

$$L(x,\lambda) = \frac{1}{2}(Ax - b, Ax - b) + (Cx - d, \lambda), KKT = ?$$

$Different \ Lagrangian \Rightarrow different \ KKT \ equation$

$$L(x,\lambda) = (Ax - b, Ax - b) + 2(Cx - d, \lambda)$$

$$(A^{T}Ax - A^{T}b) + C^{T}\lambda = 0$$
$$Cx = d$$

$$\begin{pmatrix} A^T A & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} A^T b \\ d \end{pmatrix}$$

$$L(x,\lambda) = \frac{1}{2}(Ax - b, Ax - b) + (Cx - d, \lambda), KKT = ?$$

$$L(x, \lambda) = \alpha(Ax - b, Ax - b) + \beta(Cx - d, \lambda), KKT = ?$$

$$(A^{T}Ax - A^{T}b) + C^{T}\lambda = 0$$
$$Cx = d$$

$$(A^{T}Ax - A^{T}b) + C^{T}\lambda = 0$$
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$$\lambda = \xi + d$$
,

$$(A^{T}Ax - A^{T}b) + C^{T}\lambda = 0$$
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$$\lambda = \xi + d$$
, $Cx = d \Rightarrow \lambda = \xi + Cx$

$$(A^{T}Ax - A^{T}b) + C^{T}\lambda = 0$$
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- $\lambda = \xi + d$, $Cx = d \Rightarrow \lambda = \xi + Cx$
- $(A^T A x A^T b) + C^T (\xi + d) = (A^T A x A^T b) + C^T (\xi + C x)$

$$(A^{T}Ax - A^{T}b) + C^{T}\lambda = 0$$
$$Cx = d$$

- $\lambda = \xi + d$, $Cx = d \Rightarrow \lambda = \xi + Cx$
- $(A^T A x A^T b) + C^T (\xi + d) = (A^T A x A^T b) + C^T (\xi + C x)$
- $(A^T A x A^T b) + C^T (\xi + C x) = (A^T A + C^T C) x A^T b + C^T \xi$

$$(A^T A x - A^T b) + C^T \lambda = 0$$
$$Cx = d$$

$$\lambda = \xi + d$$
, $Cx = d \Rightarrow \lambda = \xi + Cx$

$$(A^T A x - A^T b) + C^T (\xi + d) = (A^T A x - A^T b) + C^T (\xi + C x)$$

$$(A^T A x - A^T b) + C^T (\xi + C x) = (A^T A + C^T C) x - A^T b + C^T \xi$$

$$\begin{pmatrix} A^T A + C^T C & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ \xi \end{pmatrix} = \begin{pmatrix} A^T b \\ d \end{pmatrix}$$

QR factorization of $\begin{pmatrix} A \\ C \end{pmatrix}$, equivalent KKT equation

Assumption b.

QR factorization of $\begin{pmatrix} A \\ C \end{pmatrix}$, equivalent KKT equation

Assumption b. $\Rightarrow \begin{pmatrix} A \\ C \end{pmatrix} = QR$,

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$$\Rightarrow \begin{pmatrix} A \\ C \end{pmatrix} = QR, \Rightarrow \begin{pmatrix} A \\ C \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} R$$

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- $ightharpoonup A^T = R^T Q_1^T, C^T = R^T Q_2^T, A^T A = R^T R, C^T C = R^T R$

► Assumption b.
$$\Rightarrow$$
 $\begin{pmatrix} A \\ C \end{pmatrix} = QR, \Rightarrow \begin{pmatrix} A \\ C \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} R$

$$\begin{pmatrix} A^T A + C^T C & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ \xi \end{pmatrix} = \begin{pmatrix} A^T b \\ d \end{pmatrix}$$

► Assumption b.
$$\Rightarrow$$
 $\begin{pmatrix} A \\ C \end{pmatrix} = QR, \Rightarrow \begin{pmatrix} A \\ C \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} R$

$$A^{T} = R^{T}Q_{1}^{T}, C^{T} = R^{T}Q_{2}^{T}, A^{T}A = R^{T}R, C^{T}C = R^{T}R$$

$$\begin{pmatrix} A^T A + C^T C & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ \xi \end{pmatrix} = \begin{pmatrix} A^T b \\ d \end{pmatrix}$$

$$\begin{pmatrix} 2R^TR & R^TQ_2^T \\ Q_2R & 0 \end{pmatrix} \begin{pmatrix} x \\ \xi \end{pmatrix} = \begin{pmatrix} R^TQ_1^Tb \\ d \end{pmatrix}$$

QR factorization of $\begin{pmatrix} A \\ C \end{pmatrix}$, equivalent KKT equation

► Assumption b.
$$\Rightarrow$$
 $\begin{pmatrix} A \\ C \end{pmatrix} = QR, \Rightarrow \begin{pmatrix} A \\ C \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} R$

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New variable: $y = Rx \Rightarrow$

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New variable:
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Proposition 14.5

Assumption a. is valid and Q_2 has linearly independent rows

Proof.

ightharpoonup Assume: Q_2 has linearly dependent rows

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- $\exists \tilde{\xi} \neq 0, Q_2^T \tilde{\xi} = 0$
- $C = Q_2 R \Rightarrow Q_2 = CR^{-1}$

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- $ightharpoonup C^T \tilde{\xi} = 0$
- C^T has linearly independent columns
- ▶ ↓
- ► Contradiction: $\xi = 0$

QR factorization of Q_2 , equivalent KKT equation

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- $\qquad \qquad \tilde{R}^T \tilde{R} \xi = \tilde{R}^T \tilde{Q}^T Q_1^T b 2d$
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QR factorization of Q_2 , equivalent KKT equation

- ▶ Q_2 has linearly independent rows $\Rightarrow Q_2^T = \tilde{Q}\tilde{R}$
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$$\tilde{R}\xi = \tilde{Q}^T Q_1^T b - 2\tilde{R}^{-T} d$$

ightharpoonup Equation for x: Rx = y

QR factorization for constrained least squares Equivalent KKT equation

Equivalent KKT equation

► KKT equation
$$\begin{pmatrix} A^TA & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} \hat{x} \\ \lambda \end{pmatrix} = \begin{pmatrix} A^Tb \\ d \end{pmatrix}$$

Equivalent KKT equation

- ► KKT equation $\begin{pmatrix} A^TA & C^T \\ C & 0 \end{pmatrix} \begin{pmatrix} \hat{x} \\ \lambda \end{pmatrix} = \begin{pmatrix} A^Tb \\ d \end{pmatrix}$
- ► Equivalent equaition

$$\tilde{R}\xi = \tilde{Q}^T Q_1^T b - 2\tilde{R}^{-T} d,$$

$$y = 0.5(Q_1^T b - Q_2^T \xi),$$

$$R\hat{x} = y$$

Algorithm 14.6

Equivalent KKT equation

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Algorithm 14.6

1. Compute QR factorization:

$$\begin{pmatrix} A \\ C \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} R$$

Equivalent KKT equation

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Algorithm 14.6

- 2. Compute QR factorization: $Q_2^T = \tilde{Q} \tilde{R}$

Equivalent KKT equation

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Algorithm 14.6

$$1. \ \, {\sf Compute} \,\, {\sf QR} \,\, {\sf factorization} \colon$$

$$\begin{pmatrix} A \\ C \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} R$$

- 2. Compute QR factorization: $Q_2^T = \tilde{Q}\tilde{R}$
- 3. Solve $\tilde{R}^T \eta = d$

Equivalent KKT equation

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Algorithm 14.6

1. Compute QR factorization:

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- 2. Compute QR factorization: $Q_2^T = \tilde{Q}\tilde{R}$
- 3. Solve $\tilde{R}^T \eta = d$
- 4. Compute $\tilde{\eta} = \tilde{Q}^T Q_1^T b 2\eta$
- 5. Solve $\tilde{R}\xi = \tilde{\eta}$
- 6. Compute $y = 0.5(Q_1^T b Q_2^T \xi)$
- 7. Find solution of constrained least squares problem: solve $R\hat{x} = y$

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Hausholder transformation, full QR factorization

Definition 14.7

$$H = I - \frac{2vv^T}{v^Tv}$$

Hausholder transformation, full QR factorization

Definition 14.7

$$H = I - \frac{2vv^T}{v^Tv}$$

H - Hausholder matrix

Hausholder transformation, full QR factorization

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$$H = I - \frac{2vv^T}{v^Tv}$$

H - Hausholder matrix

v - Hausholder vector

Definition 14.7

$$H = I - \frac{2vv^T}{v^Tv}$$

H - Hausholder matrix

v - Hausholder vector

Alston Hausholder (1904-1993)

American mathematician, celebrated numerical analyst, former director of Mathematics and Computer Science Division of Oak Ridge National Laboratory.

Hausholder transformation

Hausholder transformation

ightharpoonup v - unit vector, $\|v\|_2=1$, normal to hyperplane

Hausholder transformation

- ightharpoonup v unit vector, $||v||_2 = 1$, normal to hyperplane

Hausholder transformation

- ightharpoonup v unit vector, $||v||_2 = 1$, normal to hyperplane
- $v^T x = ||v|| ||x|| \cos(\hat{vx})$
- \triangleright \hat{vx} angle between vectors v and x

Hausholder transformation

- \triangleright v unit vector, $||v||_2 = 1$, normal to hyperplane
- $V V^T x = ||v|| ||x|| \cos(\hat{vx})$
- $ightharpoonup \hat{vx}$ angle between vectors v and x
- ► Geometric interpetation

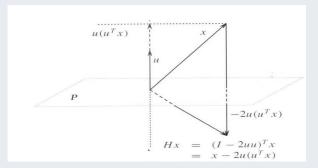


Figure: Source: Biswa Nath Datta

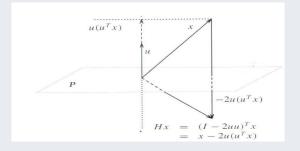


Figure: Source: Biswa Nath Datta

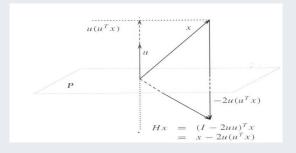


Figure: Source: Biswa Nath Datta

$$\|Hx\|_2 = \|x\|_2$$

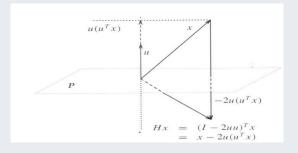


Figure: Source: Biswa Nath Datta

►
$$||Hx||_2 = ||x||_2$$
 ↓

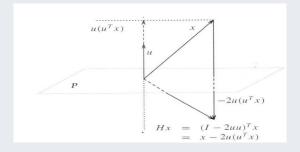


Figure: Source: Biswa Nath Datta

- ► $||Hx||_2 = ||x||_2$ ↓
- ► *H* is an orthogonal matrix:

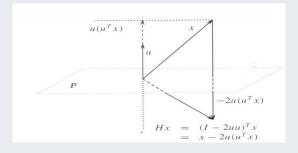


Figure: Source: Biswa Nath Datta

- ► $||Hx||_2 = ||x||_2$ ↓
- \blacktriangleright H is an orthogonal matrix: $||Hx||_2^2 = ||x||_2^2, (Hx, Hx) = (H^T Hx, x)$

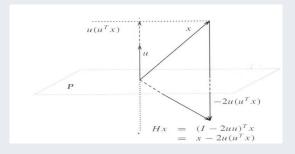


Figure: Source: Biswa Nath Datta

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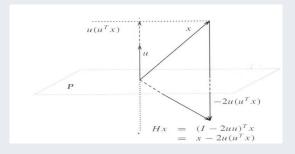


Figure: Source: Biswa Nath Datta

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- ► *H* is an orthogonal matrix: $||Hx||_2^2 = ||x||_2^2$, $(Hx, Hx) = (H^T Hx, x) \Rightarrow (H^T Hx, x) = (x, x) \Rightarrow ((H^T H I)x, x) = 0 \forall x$

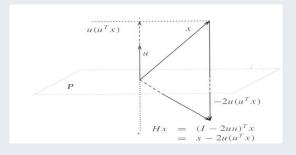


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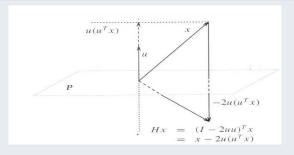


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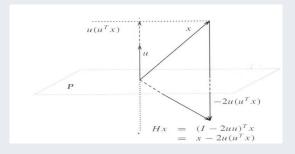


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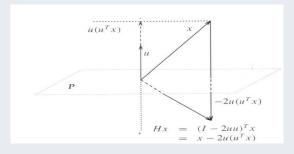


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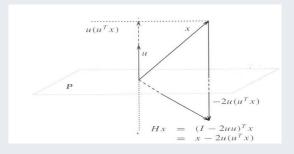


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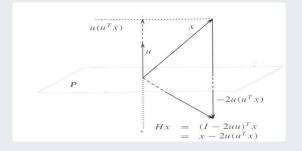


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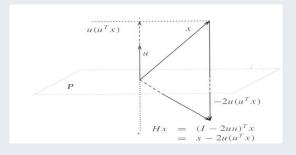


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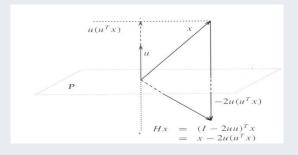


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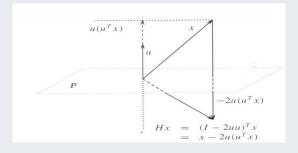


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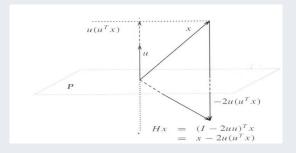


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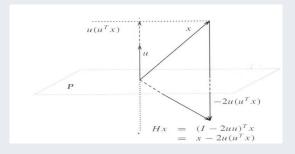


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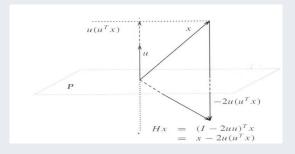


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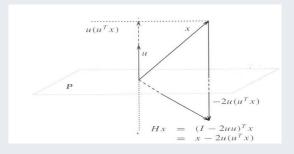


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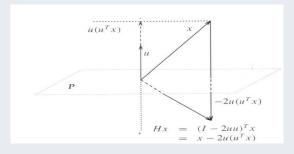


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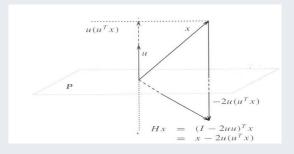


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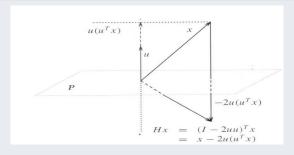


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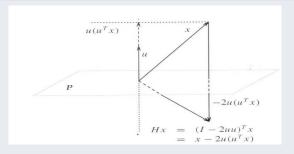


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Proof by direct verification (Exercise)

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Proof by direct verification (Exercise)

Hausholder's method of QR factorization

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- ightharpoonup A = QR

Q & A