

Numerical Linear Algebra

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QR factorization, Least squares

- ▶ QR and reduced QR factorization
- ▶ Linear least squares
- ▶ Constrained least squares
- ▶ Q & A

Recap of Previous Lecture

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- ▶ Method of minimal residuals
- ▶ Steepest Descent
- ▶ Gram-Schmidt orthogonalization

QR factorization

Definition 13.1

QR Factorization of rectangular matrix:

► $A \in \mathcal{R}^{n \times m}$

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QR factorization

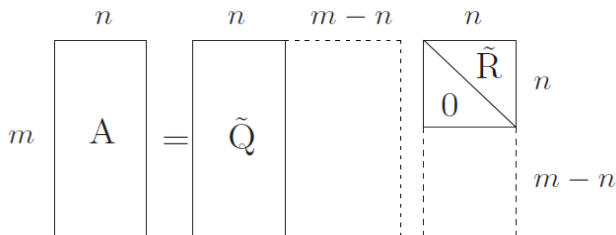


Figure: $A = QR$, $A = \tilde{Q}\tilde{R}$ - reduced QR factorization. From Quarteroni et al.

QR factorization

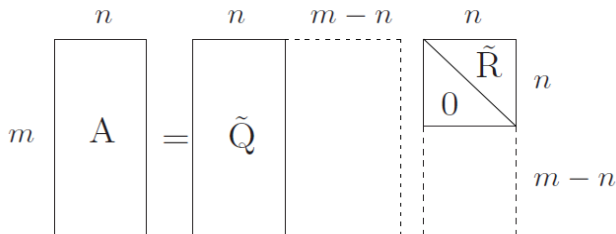


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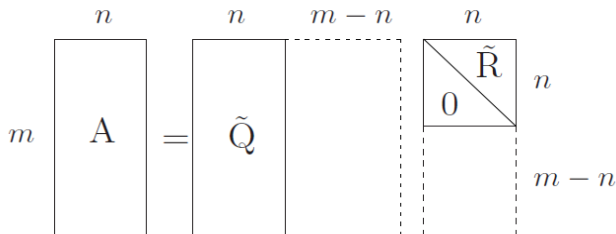


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- ▶ $A \in \mathcal{R}^{n \times m}$
- ▶ $\text{rank}(A) = m$

QR factorization

The diagram illustrates the reduced QR factorization of a matrix A . On the left, matrix A is shown as a vertical rectangle with height m and width n . This is followed by an equals sign. To the right of the equals sign, matrix \tilde{Q} is shown as a vertical rectangle with height m and width n . To its right is a dashed rectangle with width $m - n$. Further right is matrix \tilde{R} , which is a square block partitioned into two parts: an upper triangular part of size $n \times n$ containing \tilde{R} , and a lower part of size $(m - n) \times n$ containing zeros, indicated by a '0' in the bottom-left corner of the partition. The total width of the right-hand side is $n + (m - n) = m$.

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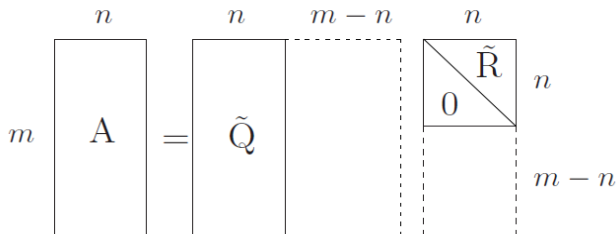


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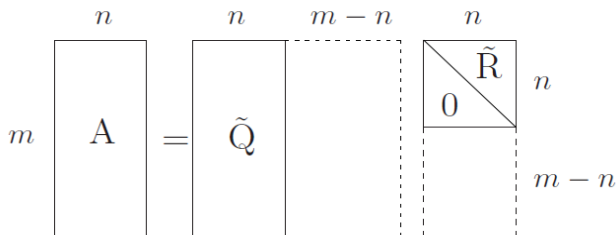
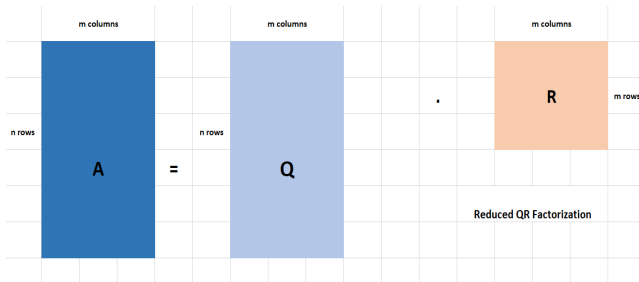
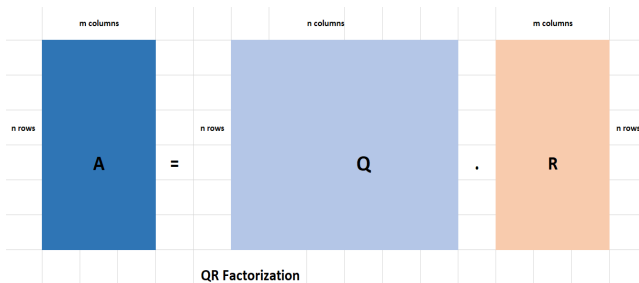


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- ▶ \exists reduced QR factorization $A = \tilde{Q}\tilde{R}$

QR and reduced QR



QR factorization

Example 13.4

```
A= [[ 1  2  3]
     [ 4  5  6]
     [ 7  8  9]
     [10 11 12]]
Q= [[-0.07761505 -0.83305216  0.53358462]
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Figure: Reduced QR factorization

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Figure: Reduced QR factorization

► A - tall matrix

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Figure: Reduced QR factorization

- ▶ A - tall matrix
- ▶ Q - tall matrix, orthogonal

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Figure: Reduced QR factorization

- ▶ A - tall matrix
- ▶ Q - tall matrix, orthogonal
- ▶ R - square matrix, upper triangular

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$$A = QR$$

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- ▶ $q_i = \frac{\tilde{q}_i}{\|\tilde{q}_i\|}$
- ▶ $a_i = \sum_{j=1}^{i-1} (q_j, a_i) q_j + \|\tilde{q}_i\| q_i$

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- ▶ $q_i = \frac{\tilde{q}_i}{\|\tilde{q}_i\|}$
- ▶ $a_i = \sum_{j=1}^{i-1} (q_j, a_i) q_j + \|\tilde{q}_i\| q_i$
- ▶ $r_{ij} = \begin{cases} i < j : r_{ij} = (a_j, q_i) \\ i = j : r_{ii} = \|\tilde{q}_i\| \\ i > j : r_{ij} = 0 \end{cases}$

Reduced QR factorization, 3

$$\blacktriangleright a_i = \sum_{j=1}^{i-1} (q_j, a_i) q_j + \|\tilde{q}_i\| q_i$$

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Reduced QR factorization, 3

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$$a_1 = r_{11} q_1 = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{11} \\ 0 \\ \dots \\ 0 \end{pmatrix}$$

Reduced QR factorization, 3

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$$a_2 = r_{12} q_1 + r_{22} q_2 = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{12} \\ r_{22} \\ \dots \\ 0 \end{pmatrix}$$

Reduced QR factorization, 3

$$\blacktriangleright a_i = \sum_{j=1}^{i-1} (q_j, a_i) q_j + \|\tilde{q}_i\| q_i$$

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$$a_k = r_{1k} q_1 + r_{2k} q_2 + \dots + r_{kk} q_k = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{1k} \\ r_{2k} \\ \dots \\ r_{kk} \end{pmatrix}$$

Reduced QR factorization, 4



$$a_1 = r_{11}q_1 = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{11} \\ 0 \\ \dots \\ 0 \end{pmatrix}$$



$$a_2 = r_{12}q_1 + r_{22}q_2 = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{12} \\ r_{22} \\ \dots \\ 0 \end{pmatrix}$$



$$a_k = r_{1k}q_1 + r_{2k}q_2 + \dots + r_{kk}q_k = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{1k} \\ r_{2k} \\ \dots \\ r_{kk} \end{pmatrix}$$

Reduced QR factorization, 4



$$a_1 = r_{11}q_1 = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{11} \\ 0 \\ \dots \\ 0 \end{pmatrix}$$



$$a_2 = r_{12}q_1 + r_{22}q_2 = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{12} \\ r_{22} \\ \dots \\ 0 \end{pmatrix}$$



$$a_k = r_{1k}q_1 + r_{2k}q_2 + \dots + r_{kk}q_k = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{1k} \\ r_{2k} \\ \dots \\ r_{kk} \end{pmatrix}$$



$$\begin{pmatrix} a_1 & a_2 & \dots & a_k \end{pmatrix} = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1k} \\ 0 & r_{22} & \dots & r_{2k} \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & r_{kk} \end{pmatrix}$$

Reduced QR factorization, 5



$$\begin{pmatrix} a_1 & a_2 & \dots & a_k \end{pmatrix} = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1k} \\ 0 & r_{22} & \dots & r_{2k} \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & r_{kk} \end{pmatrix}$$



$$A = QR$$

- ▶ Q: Is reduced QR factorization always possible?

Reduced QR factorization, 5



$$\begin{pmatrix} a_1 & a_2 & \dots & a_k \end{pmatrix} = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1k} \\ 0 & r_{22} & \dots & r_{2k} \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & r_{kk} \end{pmatrix}$$



$$A = QR$$

► Q: Is reduced QR factorization always possible?

► A:

Theorem 13.5

For $A \in \mathcal{R}^{n \times m}$ of full rank always exist $Q \in \mathcal{R}^{n \times m}$ with orthonormal columns and upper triangular $R \in \mathcal{R}^{m \times m}$ such that $A = QR$

Reduced QR factorization

```
A= [[ 1  2  3]
     [ 4  5  6]
     [ 7  8  9]
     [10 11 12]]
Q= [[-0.07761505 -0.83305216  0.53358462]
     [-0.31046021 -0.45123659 -0.8036038 ]
     [-0.54330537 -0.06942101  0.00645373]
     [-0.77615053  0.31239456  0.26356544]]
R= [[-1.28840987e+01 -1.45916299e+01 -1.62991610e+01]
     [ 0.00000000e+00 -1.04131520e+00 -2.08263040e+00]
     [ 0.00000000e+00  0.00000000e+00 -3.39618744e-15]]
A-QR= [[-1.33226763e-15 -7.10542736e-15 -5.32907052e-15]
        [-8.88178420e-16 -1.77635684e-15 -8.88178420e-16]
        [ 0.00000000e+00 -3.55271368e-15 -3.55271368e-15]
        [-1.77635684e-15 -5.32907052e-15 -3.55271368e-15]]
Pseudo inverse = [[-0.48333333 -0.24444444 -0.00555556  0.23333333]
                   [-0.03333333 -0.01111111  0.01111111  0.03333333]
                   [ 0.41666667  0.22222222  0.02777778 -0.16666667]]
```

Figure: Pseudo inverse, $A^\dagger = R^{-1}Q^T$

Linear Least Squares

Problem 13.6

Linear Least Squares Problem

Linear Least Squares

Problem 13.6

Linear Least Squares Problem

► $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$

Linear Least Squares

Problem 13.6

Linear Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$
- ▶ $Ax = b$ - over determined system

Linear Least Squares

Problem 13.6

Linear Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$
- ▶ $Ax = b$ - over determined system
- ▶ $f(x) = \|Ax - b\|_2$

Linear Least Squares

Problem 13.6

Linear Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$
- ▶ $Ax = b$ - over determined system
- ▶ $f(x) = \|Ax - b\|_2$
- ▶ $x_* = \arg \min f(x)$

Linear Least Squares

Problem 13.6

Linear Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$
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- ▶ $f(x) = \|Ax - b\|_2$
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Definition 13.7

- ▶ If the least squares problem has more than one solution

Linear Least Squares

Problem 13.6

Linear Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$
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- ▶ $f(x) = \|Ax - b\|_2$
- ▶ $x_* = \arg \min f(x)$

Definition 13.7

- ▶ If the least squares problem has more than one solution
- ▶ **minimal-length solution** **minimal-norm solution** = solution with least Euclidean norm

Linear Least Squares

Solution of Linear Least Squares Problem

► $x_* = \arg \min f(x) \Rightarrow \nabla f(x) = 0$

Linear Least Squares

Solution of Linear Least Squares Problem

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Linear Least Squares

Solution of Linear Least Squares Problem

► $x_* = \arg \min f(x) \Rightarrow \nabla f(x) = 0$



► $A^T A x = A^T b$

Linear Least Squares

Solution of Linear Least Squares Problem

► $x_* = \arg \min f(x) \Rightarrow \nabla f(x) = 0$



► $A^T A x = A^T b$ - Normal equation

Linear Least Squares

Solution of Linear Least Squares Problem

► $x_* = \arg \min f(x) \Rightarrow \nabla f(x) = 0$



► $A^T A x = A^T b$ - Normal equation

► $\exists (A^T A)^{-1},$

Linear Least Squares

Solution of Linear Least Squares Problem

► $x_* = \arg \min f(x) \Rightarrow \nabla f(x) = 0$



► $A^T A x = A^T b$ - Normal equation

► $\exists (A^T A)^{-1}, \Rightarrow x = (A^T A)^{-1} A^T b$

Linear Least Squares

Solution of Linear Least Squares Problem

► $x_* = \arg \min f(x) \Rightarrow \nabla f(x) = 0$



► $A^T A x = A^T b$ - Normal equation

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Definition 13.8

Pseudo inverse of a matrix

► $A \in \mathbb{R}^{n \times m}, n > m$

Linear Least Squares

Solution of Linear Least Squares Problem

► $x_* = \arg \min f(x) \Rightarrow \nabla f(x) = 0$



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► $\exists (A^T A)^{-1}$

► $A^\dagger = (A^T A)^{-1} A^T$

Linear Least Squares

Pseudo inverse and QR factorization

Linear Least Squares

Pseudo inverse and QR factorization

► $A \in \mathbb{R}^{n \times m}, n > m$

Linear Least Squares

Pseudo inverse and QR factorization

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
- ▶ $\text{rank}(A) = m, A = QR$

Linear Least Squares

Pseudo inverse and QR factorization

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Linear Least Squares

Pseudo inverse and QR factorization

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- ▶ $A^T = (QR)^T = R^T Q^T,$

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Linear Least Squares

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Linear Least Squares

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Linear Least Squares

Pseudo inverse and QR factorization

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Linear Least Squares

Pseudo inverse and QR factorization

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Least squares solution and QR factorization

Linear Least Squares

Pseudo inverse and QR factorization

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Least squares solution and QR factorization

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Linear Least Squares

Pseudo inverse and QR factorization

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
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Least squares solution and QR factorization

- ▶ $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$
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Linear Least Squares

Pseudo inverse and QR factorization

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Least squares solution and QR factorization

- ▶ $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$
- ▶ $\text{rank}(A) = m, A = QR$
- ▶ $Ax = b$

Linear Least Squares

Pseudo inverse and QR factorization

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
- ▶ $\text{rank}(A) = m, A = QR$
- ▶ $A^\dagger = (A^T A)^{-1} A^T$
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- ▶ $A^\dagger = R^{-1} Q^T$

Least squares solution and QR factorization

- ▶ $A \in \mathbb{R}^{n \times m}, n > m, x \in \mathbb{R}^m, b \in \mathbb{R}^n$
- ▶ $\text{rank}(A) = m, A = QR$
- ▶ $Ax = b$
- ▶ $c = Q^T b, Rx = c, x = R^{-1} c$

Linear Least Squares

Least squares solution and QR factorization

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
 - ▶ $\text{rank}(A) = m, A = QR$
 - ▶ $Ax = b$
 - ▶ $c = Q^T b, Rx = c, x = R^{-1}c$
-
- ▶ Rank deficient case: $\text{rank}(A) < m$

Linear Least Squares

Least squares solution and QR factorization

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
 - ▶ $\text{rank}(A) = m, A = QR$
 - ▶ $Ax = b$
 - ▶ $c = Q^T b, Rx = c, x = R^{-1}c$
-
- ▶ Rank deficient case: $\text{rank}(A) < m$
 - ▶ Solution is not unique

Linear Least Squares

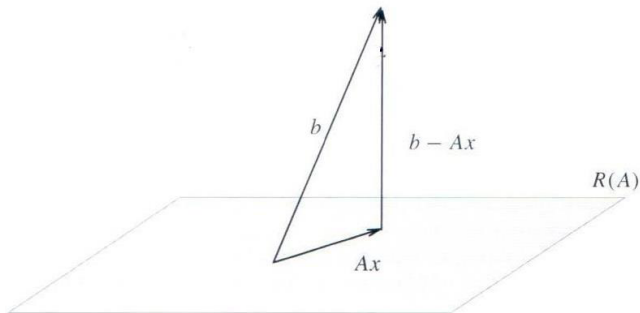


Figure: Geometric interpretation of Least Squares, Biswa Natt Datta

- $A \in \mathcal{R}^{n \times m}$, $R(A) = \{y : y = Ax, \forall x \in \mathcal{R}^m\}$

Linear Least Squares

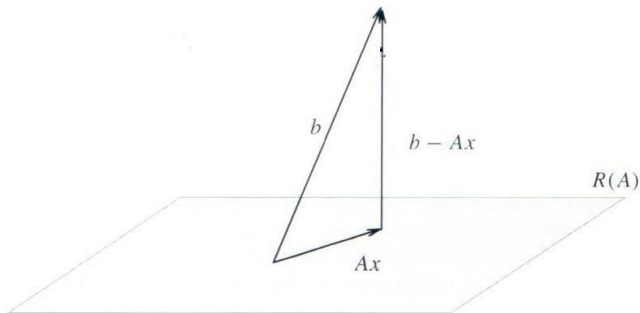


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Linear Least Squares

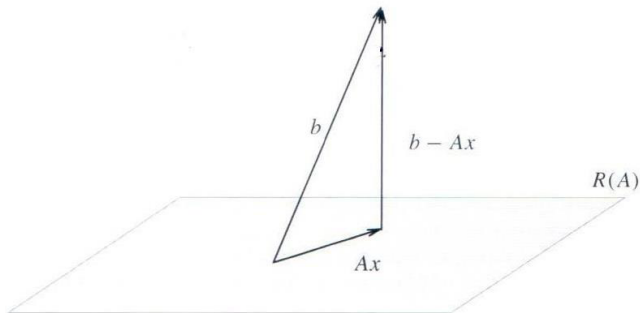


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- ▶ $x_* \in R(A)$, minimal distance to b

Linear Least Squares

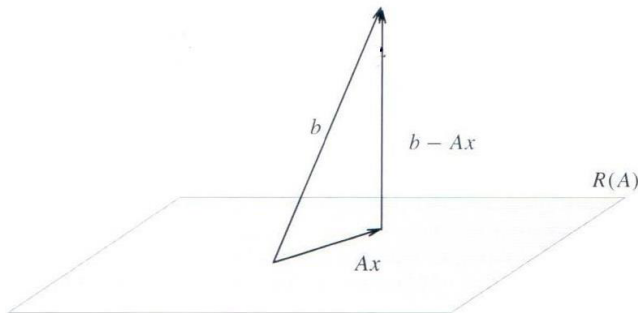


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- ▶ $x_* \in R(A)$, minimal distance to b



- ▶ $(b - Ax) \perp R(A)$

Linear Least Squares

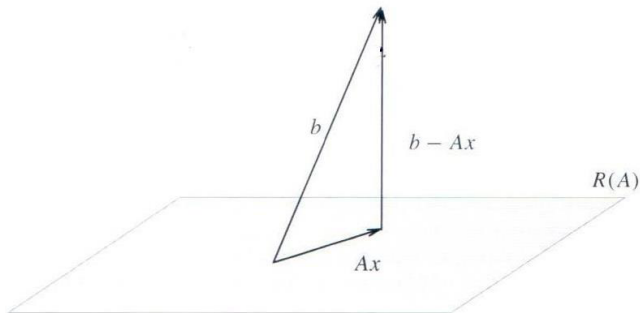


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- ▶ $x_* \in R(A)$, minimal distance to b



- ▶ $(b - Ax) \perp R(A)$
- ▶ Solution to linear least squares problem always exists

Constrained Least Squares

Problem 13.9

Constrained Least Squares Problem

Constrained Least Squares

Problem 13.9

Constrained Least Squares Problem

► $A \in \mathbb{R}^{n \times m}, n > m$

Constrained Least Squares

Problem 13.9

Constrained Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
- ▶ $C \in \mathbb{R}^{p \times m}$

Constrained Least Squares

Problem 13.9

Constrained Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
- ▶ $C \in \mathbb{R}^{p \times m}$
- ▶ $x \in \mathbb{R}^m, b \in \mathbb{R}^n, d \in \mathbb{R}^p$

Constrained Least Squares

Problem 13.9

Constrained Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
- ▶ $C \in \mathbb{R}^{p \times m}$
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- ▶ $Ax = b$ - over determined system

Constrained Least Squares

Problem 13.9

Constrained Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
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- ▶ $x \in \mathbb{R}^m, b \in \mathbb{R}^n, d \in \mathbb{R}^p$
- ▶ $Ax = b$ - over determined system
- ▶ $f(x) = \|Ax - b\|_2$

Constrained Least Squares

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Constrained Least Squares Problem

- ▶ $A \in \mathbb{R}^{n \times m}, n > m$
- ▶ $C \in \mathbb{R}^{p \times m}$
- ▶ $x \in \mathbb{R}^m, b \in \mathbb{R}^n, d \in \mathbb{R}^p$
- ▶ $Ax = b$ - over determined system
- ▶ $f(x) = \|Ax - b\|_2$
- ▶ $x_* = \arg \min_{Cx=d} f(x)$

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Problem 13.9

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Lagrange multipliers



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- ▶ *C has linearly independent rows*
- ▶ *$\begin{pmatrix} A \\ C \end{pmatrix}$ has linearly independent columns*

Q & A