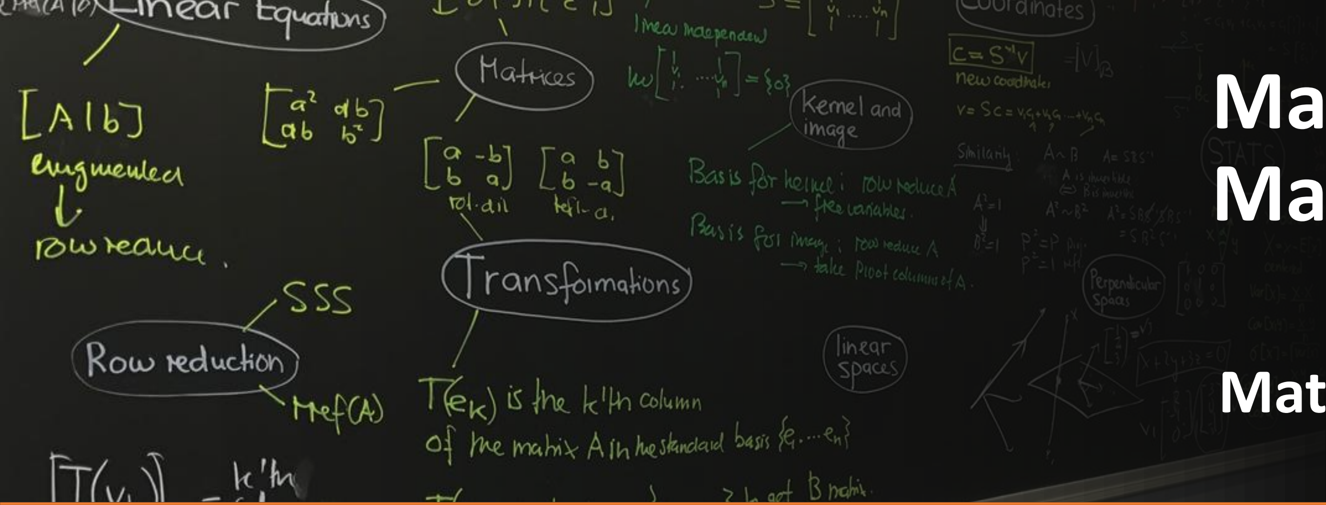

Mathematical Foundations for Machine Learning and Data Science

Matrices – Notation, Application Examples and Basic Operations

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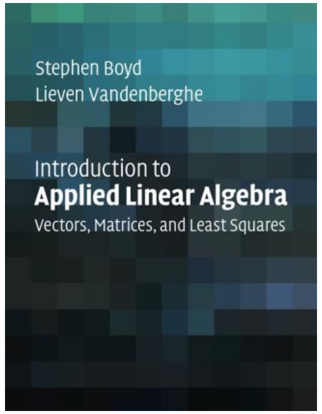
Outline

- *Matrices Notation*
- *Application Examples*
- *Operations on Matrices*
    - *Addition*
    - *Scaling*
    - *Transpose*
    - *Norm*



Chapter 6

Matrices

Definition:

A matrix is a two dimensional (2D) vector or array of numbers.

Notation:

Usually denoted by a capital letter symbol; stack the list of numbers in 2D array.

For example, consider a matrix **A** of 6 real numbers represented as stack of 3 2-vectors using square or round parentheses:

$$A = \begin{bmatrix} -1.1 & 17.3 & 2.7 \\ 30.1 & 19.1 & 8.4 \end{bmatrix} \qquad A = \begin{pmatrix} -1.1 & 17.3 & 2.7 \\ 30.1 & 19.1 & 8.4 \end{pmatrix} \qquad 2 \times 3 \text{ matrix}$$

Size of a matrix: Number of rows (m) times number of columns (n); $m \times n$

We express matrix B of size $m \times n$ as $B \in \mathbf{R}^{m \times n}$ and call it $m \times n$-matrix.

Entry of a matrix: B_{ij} - entry in the matrix at i-th row and j-th column.

For example, $A_{21} = 30.1$.

Matrices

Square Matrix: $m = n$ **Tall Matrix:** $m > n$ **Wide Matrix:** $m < n$

Zero Matrix: A matrix with all elements equal to zero.

denoted by $\mathbf{0} \in \mathbf{R}^{m \times n}$.

Identity Matrix: A square matrix with diagonal elements equal to one and off diagonal elements equal to zero.

denoted by $I \equiv I_n \in \mathbf{R}^{n \times n}$ and is defined as

$$(I)_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} = \delta_{i,j}$$

Diagonal Matrix:

Block Matrix:

$$A = \begin{bmatrix} B & C \\ D & E \end{bmatrix}$$

Triangular Matrix:

$$\begin{bmatrix} 1 & -1 & 0.7 \\ 0 & 1.2 & -1.1 \\ 0 & 0 & 3.2 \end{bmatrix} \qquad \begin{bmatrix} -0.6 & 0 \\ -0.3 & 3.5 \end{bmatrix}$$

$$U_{i,j} = \begin{cases} a_{i,j} & \text{for } i \leq j \\ 0 & \text{for } i > j. \end{cases}$$

A

Examples of Matrices - Applications

Image RGB

Each color represents a matrix.

Quantities

An mxn-matrix **A** can represent the amounts or quantities of n different resources or products held (or produced, or required) by an entity such as a company at m different locations or for m different customers.

For example, mxn-matrix represents the quantity of n products stocked in m number of warehouses.

Examples of Matrices - Applications

Time series grouped over time

- 12x20-matrix can represent the average monthly temperature, rainfall, pressure etc of 20 cities of Pakistan.
- 30x7-matrix can represent the number of expected COVID-19 in Pakistan cases over the next 30 days for 7 states/territories.
- Other examples include exchange rate, audio, and, in fact, any quantity that varies over time.

Operations on Matrices

Additivity and Scaling

$A \in R^{m \times n}, \quad B \in R^{m \times n}$

$A + B = C \in R^{m \times n}$

$C_{ij} = A_{ij} + B_{ij} \qquad i = 1, \dots, m, \quad j = 1, \dots, n$

$$\underbrace{\begin{bmatrix} 0 & 4 \\ 7 & 0 \\ 3 & 1 \end{bmatrix}}_{A} + \underbrace{\begin{bmatrix} 1 & 2 \\ 2 & 3 \\ 0 & 4 \end{bmatrix}}_{B} = \underbrace{\begin{bmatrix} 1 & 6 \\ 9 & 3 \\ 3 & 5 \end{bmatrix}}_{C}$$

* $A \in R^{m \times n}, \quad \alpha \in R$

$\alpha A = B$

$B_{ij} = \alpha A_{ij}$

$$(-2) \begin{bmatrix} 1 & 6 \\ 9 & 3 \\ 6 & 0 \end{bmatrix} = \begin{bmatrix} -2 & -12 \\ -18 & -6 \\ -12 & 0 \end{bmatrix}$$

Operations on Matrices

Transpose and Concept of Symmetric Matrices

* $A \in R^{m \times n}$
* $A^T \in R^{n \times m}$

$$(A^T)_{ij} = A_{ji}$$

$$\underset{A}{\begin{bmatrix} 0 & 4 \\ 7 & 0 \\ 3 & 1 \end{bmatrix}^T} = \underset{A^T}{\begin{bmatrix} 0 & 7 & 3 \\ 4 & 0 & 1 \end{bmatrix}}$$

Symmetric Matrix

$A \in R^{n \times n}$ is symmetric if $A = A^T$

Skew-Symmetric

$$A = -A^T$$

Operations on Matrices

Transpose and Concept of Symmetric Matrices

- Any square matrix can be expressed as a sum of symmetric matrix and a skew symmeytric matrix.

$B \in R^{n \times n}$

$B = A + C$

$A = A^T$

$C = -C^T$

* $A = \frac{1}{2}(B + B^T)$

* $C = \frac{1}{2}(B - B^T)$

$\frac{1}{2}(2B) = B = A + C$

Operations on Matrices

Matrix Norm

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

$$\|A\|_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2}$$

FROBENIUS Norm of a matrix

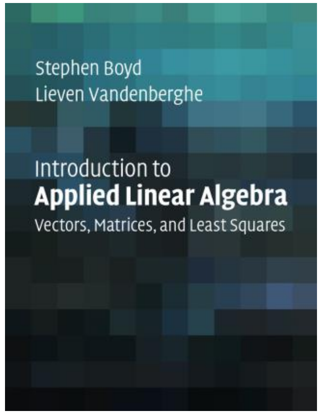
Operations on Matrices

Trace of a Matrix

- $A \in R^{n \times n}$
- $tr(A) = \sum_{i=1}^{n} a_{ii}$

Outline

- *Matrix-vector product*
- *Interpretations*
- *Application Examples*
- *Matrix-matrix product*



Chapters 6 and 10

Matrix-Vector Multiplication

$A \in \mathbf{R}^{m\times n} \qquad x \in \mathbf{R}^{n\times 1} \ (\mathbf{R}^n)$

number of columns of A equals the size of x

$y = Ax \qquad y \in \mathbf{R}^{m\times 1} \ (\mathbf{R}^m)$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$$y_i = \sum_{k=1}^{n} A_{ik}x_k = A_{i1}x_1 + \cdots + A_{in}x_n, \quad i = 1, \ldots, m$$

$= \langle$ i-th row of A, x $\rangle$

Example

$$\begin{bmatrix} 0 & 2 & -1 \\ -2 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ -1 \end{bmatrix}$$

$$= \begin{bmatrix} (0)(2) + (2)(1) + (-1)(-1) \\ (-2)(2) + (1)(1) + (1)(-1) \end{bmatrix}$$

$$= \begin{bmatrix} 3 \\ -4 \end{bmatrix}$$

Matrix-Vector Multiplication

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \Bigg\} \quad y = Ax$$

$$y_i = \sum_{k=1}^{n} A_{ik} x_k = A_{i1} x_1 + \cdots + A_{in} x_n, \quad i = 1, \dots, m$$

Interpretation In terms of Rows of Matrix

$$\underset{y}{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}} = \underset{A}{\begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_m \end{bmatrix}} \underset{x}{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}$$

$$r_i \in R^n$$

$$y_i = r_i^T x$$

$$= \langle r_i, x \rangle$$

Matrix-Vector Multiplication

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \Bigg\} \quad y = Ax$$

$$y_i = \sum_{k=1}^{n} A_{ik} x_k = A_{i1} x_1 + \cdots + A_{in} x_n, \quad i = 1, \dots, m$$

Interpretation In terms of Columns of Matrix

$$y \quad = \quad A \quad x$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = [a_1,\ a_2,\ \dots,\ a_n] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$a_i \in R^m$

$$y = x_1 a_1 + x_2 a_2 + \cdots + x_n a_n$$

$$\boxed{y = Ax}$$

- This shows that $y = Ax$ is a linear combination of the columns of A; the coefficients in the linear combination are the elements of x.

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Matrix-Vector Multiplication

Application Examples

- For example, 200x70-matrix represents the quantity of 70 products stocked in 200 warehouses.

$$\begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{70} \end{bmatrix}$$

$x_i \rightarrow$ value of i-th product

$m = 200$

$n = 70$

We want to determine value of all products in each warehouse

$$y = Ax \in R^{200}$$

Matrix-Vector Multiplication

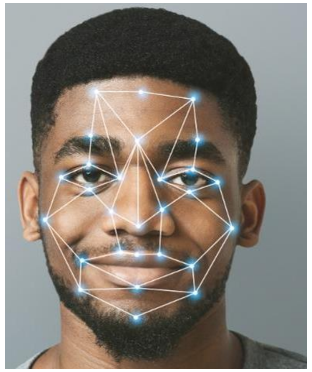
Application Examples

Feature matrix and weight vector

70 features

$$A = \begin{matrix} \text{Photo1} \\ \text{Photo2} \\ \vdots \\ 1000 \end{matrix} \begin{bmatrix} & & \\ & A_{21} & \\ & & \end{bmatrix}$$

$A \in R^{1000 \times 70}$



$$w = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_{70} \end{bmatrix}$$

$$\boxed{y = Aw} \in R^{1000}$$

Matrix-Vector Multiplication

Application Examples

Expansion in a basis

R^n, $a_1, a_2, \ldots, a_n \in R^n$

$b \in R^n$ $\quad b = \beta_1 a_1 + \beta_2 a_2 + \ldots + \beta_n a_n$

$$b = A \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix} \Rightarrow \boxed{b = A\beta}$$

Linear dependence of columns

$Ax = 0$ for some $x \neq 0$ (Linear dependence b/w columns)

$Ax = 0 \Rightarrow x = 0$ (Linear independence)

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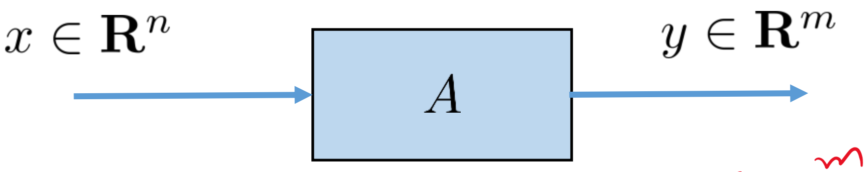
Matrix-Vector Multiplication

Linear Transformation Interpretation:

Input-Output System Interpretation

$$y = Ax$$

$f: R^n \to R^m$



$\boxed{y = Ax}$

$u \in R^n$ $\quad v \in R^m$

$A(\alpha x) = \alpha Ax$

$= \alpha y$

$x + u$ $\quad y + v$

* Scaling

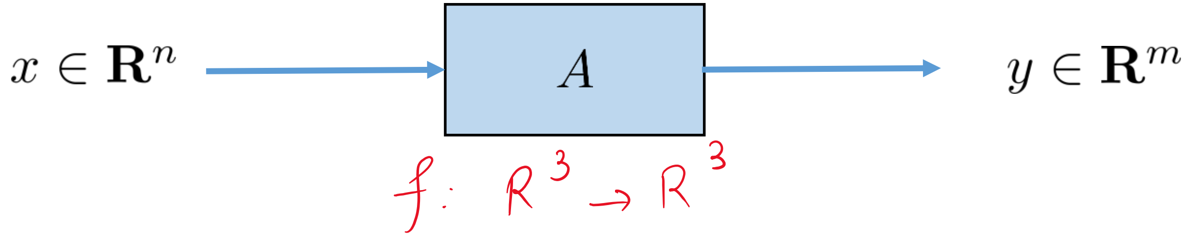
$f: R^n \to R^m$

$\boxed{f(\alpha x + \beta u) = \alpha f(x) + \beta f(u)}$

* Additivity

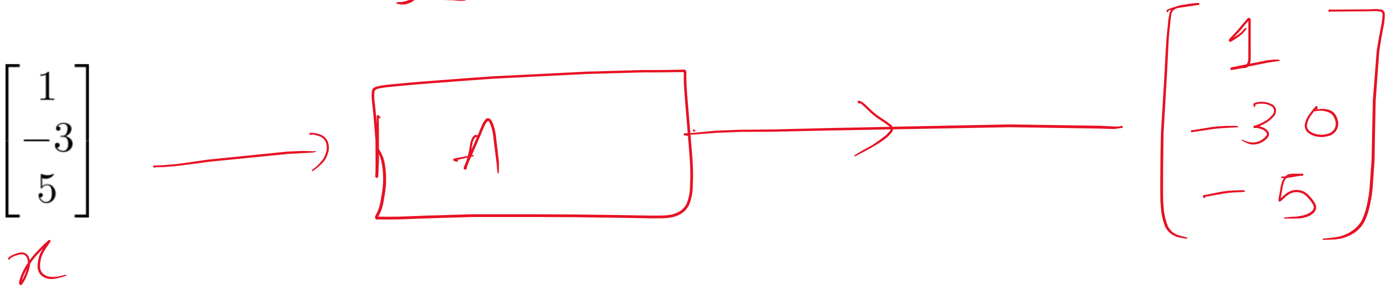
Matrix-Vector Multiplication

Input-Output System Interpretation



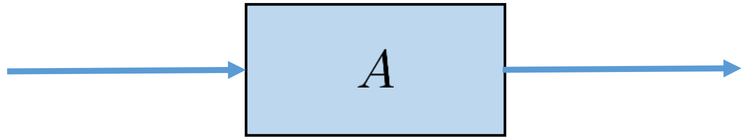
Examples

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ 10x_2 \\ -x_3 \end{bmatrix} = y$$



Matrix-Vector Multiplication

Input-Output System Interpretation



$f: R^3 \rightarrow R^2$

Examples

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 + x_2 \\ x_3 \end{bmatrix} \in R^2$$

$$\begin{bmatrix} 1 \\ -3 \\ 5 \end{bmatrix} = x$$

$$y = \begin{bmatrix} -2 \\ 5 \end{bmatrix} \in R^2$$

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Matrix-Vector Multiplication

Input-Output System Interpretation

$$x \in \mathbf{R}^n \longrightarrow \boxed{A} \longrightarrow y \in \mathbf{R}^m$$

$f: R^4 \to R^4$

Reverser

Examples

$$A = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} x_4 \\ x_3 \\ x_2 \\ x_1 \end{bmatrix}$$

Generalization: Permuation matrix

- Permutaion matrix entries $P_{i,j} \in \{0, 1\}$
- one non-zero entry equal to one per row
- one non-zero entry equal to one per column

Matrix-Matrix Multiplication

$A \in \mathbf{R}^{m\times n}$ $\quad B \in \mathbf{R}^{n\times p}$ $\quad C = AB$

no. of columns in A = no. of rows in B = n

$C \in \mathbf{R}^{m\times p}$ $\quad (m \times n) \quad (n \times p)$

$$\begin{bmatrix} C_{11} & C_{12} & \dots & C_{1p} \\ C_{21} & C_{22} & \dots & C_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ C_{m1} & C_{m2} & \dots & C_{mp} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} & \dots & B_{1p} \\ B_{21} & B_{22} & \dots & B_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \dots & B_{np} \end{bmatrix}$$

$[b_1, b_2, \dots, b_p]$

$$C = AB \iff C_{ij} = \sum_{k=1}^{p} A_{ik}B_{kj} = A_{i1}B_{1j} + \cdots + A_{ip}B_{pj}, \qquad i = 1,\dots,m, \quad j = 1,\dots,n.$$

$C_{ij} = \langle$ i-th row of A, j-th column of B $\rangle$

Matrix-Matrix Multiplication

Properties:

not *commutative:* $AB \neq BA$ in general

associative: $(AB)C = A(BC)$ so we write ABC

associative with scalar-matrix multiplication: $(\gamma A)B = \gamma(AB) = \gamma AB$

$$(AB)^T = B^T A^T$$

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} W & Y \\ X & Z \end{bmatrix} = \begin{bmatrix} AW + BX & AY + BZ \\ CW + DX & CY + DZ \end{bmatrix}$$

- Dimensions must be compatible.

Matrix-Matrix Multiplication

$$\begin{bmatrix} -1.5 & 3 & 2 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} -1 & -1 \\ 0 & -2 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 3.5 & -4.5 \\ -1 & 1 \end{bmatrix}$$

$A \in R^{2 \times 3}$ $B \in R^{3 \times 2}$ C

Outer product of Vectors:

$a \in R^n$, $b \in R^n$

$$ab^T = \begin{bmatrix} a_1b_1 & a_1b_2 & \cdots & a_1b_n \\ a_2b_1 & a_2b_2 & \cdots & a_2b_n \\ \vdots & \vdots & & \vdots \\ a_mb_1 & a_mb_2 & \cdots & a_mb_n \end{bmatrix}$$

Gram Matrix:

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

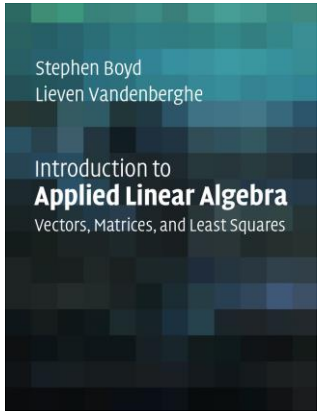
$$G = A^T A = \begin{bmatrix} a_1^T a_1 & a_1^T a_2 & \cdots & a_1^T a_n \\ a_2^T a_1 & a_2^T a_2 & \cdots & a_2^T a_n \\ \vdots & \vdots & \ddots & \vdots \\ a_n^T a_1 & a_n^T a_2 & \cdots & a_n^T a_n \end{bmatrix}$$

$(n \times m)\ (m \times n$

$$G_{ij} = a_i^T a_j$$

Outline

- *Systems of Linear Equations*
  - *Formulation*
- *Inverses*
  - *Left-inverse*
  - *Right-inverse*
  - *Inverse*
  - *Pseudo-inverse*
  - *Connection with the linear equations*



Chapters 8 and 11

Systems of Linear Equations

Formulation:

$$\begin{array}{rcl} A_{11}x_1 + A_{12}x_2 + \cdots + A_{1n}x_n & = & b_1 \\ A_{21}x_1 + A_{22}x_2 + \cdots + A_{2n}x_n & = & b_2 \\ & \vdots & \\ A_{m1}x_1 + A_{m2}x_2 + \cdots + A_{mn}x_n & = & b_m \end{array}$$

$$\begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

$A \in \mathbf{R}^{m \times n}$ $\quad x \in \mathbf{R}^n$ $\quad b \in \mathbf{R}^m$

$$Ax = b$$

- one solution
- multiple solutions
- no solution

$x_1, x_2, \ldots, x_n$ - variables or unknowns

$b_1, b_2, \ldots, b_m$ - knowns, measurements, equation righ-hand side

A_{ij} - coefficient of the i-th equation associated with the j-th variable

Systems of Linear Equations

$$Ax = b$$

- $m < n$ under-determined
- $m = n$ square
- $m > n$ over-determined

Example 01

$$x_1 + x_2 = 1, \quad x_1 = -1,$$

$$x_1 - x_2 = 0$$

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 1 & -1 \end{bmatrix}, \qquad b = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

- no solution

Example 02

$$x_1 + x_2 = 1, \quad x_2 + x_3 = 2$$

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}, \qquad b = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

- multiple solutions

$$x = \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} \qquad x = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$$

Inverses

Left-Inverse:

X is a left inverse of A if

$$XA = I$$

A is left-invertible if it has at least one left inverse

Example:

$$A = \begin{bmatrix} -3 & -4 \\ 4 & 6 \\ 1 & 1 \end{bmatrix}$$

Left inverses

$$\frac{1}{9}\begin{bmatrix} -11 & -10 & 16 \\ 7 & 8 & -11 \end{bmatrix} \qquad \begin{bmatrix} 0 & -1/2 & 3 \\ 0 & 1/2 & -2 \end{bmatrix}$$

Inverses

Left-Inverse:

Left-invertibility and column independence:

If A has a left inverse X then the columns of A are linearly independent.

Assume $Ax = 0$

$$X(Ax) = 0 \qquad\qquad (XA)x = Ix = x = 0$$

Connect with independence-dimension inequality:

When A is wide; $A \in \mathbf{R}^{m \times n}$ $\quad m < n$

- Columns are linearly dependent

  A is not left invertible.

$A \in \mathbf{R}^{m \times n}$ can be left invertible

$m = n$ or $m > n$

Square or Tall

Inverses

Left Inverse: Connection with the Systems of Linear Equations

$$Ax = b$$

- $m = n$ square
- $m > n$ over-determined

- If A has a left inverse X, then we multiply with X the above system

$$X(Ax) = Xb \qquad\qquad x = Xb$$

- If solution exists for the system $Ax = b$.

  $x = Xb$ is **the** only solution of $Ax = b$.

- If there is no solution for the system $Ax = b$.

  $x = Xb$ does not **not** satisfy $Ax = b$.

If A has the left inverse X,
- there is **at most** one solution
- if exists, solution is $x = Xb$

In summary, a left inverse can be used to determine whether or not a solution of an over-determined set of linear equations exists, and when it does, find the unique solution.

Inverses

Right-Inverse:

X is a right inverse of A if

$$AX = I$$

A is right-invertible if it has at least one right inverse

Example:

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

Right inverses

$$\frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} 1 & -1 \\ 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Connection with the left Inverse:

If X is a right inverse of A, then X^T is the left inverse of A^T.

$$I = I^T = (AX)^T = X^T A^T \quad \Rightarrow \quad X^T A^T = I$$

Inverses

Right-Inverse:

Right-invertibility and row independence:

If A has a left inverse X then the columns of A are linearly independent.

↓

If A has a right inverse X then the rows of A are linearly independent.

Connect with independence-dimension inequality:

When A is tall; $A \in \mathbf{R}^{m \times n}$ $\quad m > n$

- rows are linearly dependent

A is not right invertible.

$A \in \mathbf{R}^{m \times n}$ can be right invertible

$m = n$ or $m < n$

Square or Wide

Inverses

Right Inverse: Connection with the Systems of Linear Equations

$$Ax = b$$

- $m = n$ square

- $m < n$ under-determined

- If A has a right inverse X, then we substitute $x = Xb$ in the above system

$$A(Xb) = Ib = b \qquad \Rightarrow \qquad x = Xb \text{ solution of } Ax = b$$

- If solution exists for the system $Ax = b$.

  $x = Xb$ is **the** solution out of manu solutions of $Ax = b$.

If A has the right inverse X,
- there is **at least** one solution
- one solution is $x = Xb$

- $m < n$ under-determined

- In summary, a right inverse can be used to find a solution of a square or underdetermined set of linear equations, for any vector b.

Inverses

Inverse:

If a matrix has both left and right inverses;

- they are unique and equal.

$$XA = I, \quad AY = I \qquad \Longrightarrow \qquad X = X(AY) = (XA)Y = Y$$

$X = Y$ is referred to as the inverse of the matrix A, denoted by A^{-1}.

Example:

$$A = \begin{bmatrix} -1 & 1 & -3 \\ 1 & -1 & 1 \\ 2 & 2 & 2 \end{bmatrix} \qquad A^{-1} = \frac{1}{4}\begin{bmatrix} 2 & 4 & 1 \\ 0 & -2 & 1 \\ -2 & -2 & 0 \end{bmatrix}$$

Inverses

Inverse: Connection with the Systems of Linear Equations

$$Ax = b$$

- If A is invertible, $Ax = b$ has the unique solution given by

$$x = (A^{-1})\, b$$

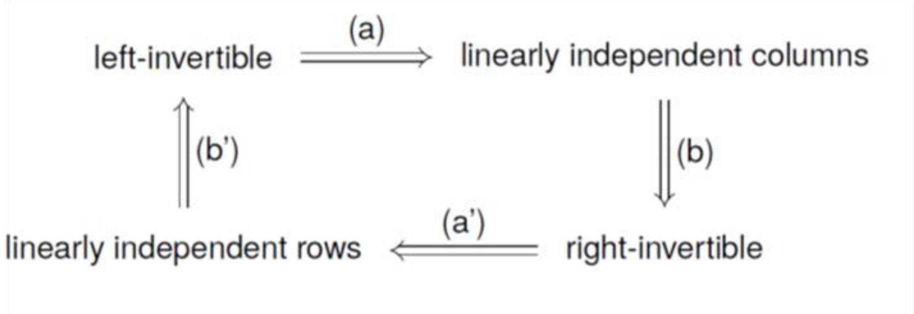
Inverses

Inverse: Properties of Nonsingular or Invertible Matrix

Square matrix A is nonsingular if it is invertible.

Following statements are equivalent for a square matrix A.

1. A is left-invertible
2. the columns of A are linearly independent
3. A is right-invertible
4. the rows of A are linearly independent



Inverses

Inverse: Examples

- The identity matrix I is invertible, with inverse $I^{-1} = I$, since $II = I$.
- A diagonal matrix A is invertible if and only if its diagonal entries are nonzero. The inverse of an $n \times n$ diagonal matrix A with nonzero diagonal entries is

$$A^{-1} = \begin{bmatrix} 1/A_{11} & 0 & \cdots & 0 \\ 0 & 1/A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/A_{nn} \end{bmatrix},$$

since

$$AA^{-1} = \begin{bmatrix} A_{11}/A_{11} & 0 & \cdots & 0 \\ 0 & A_{22}/A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{nn}/A_{nn} \end{bmatrix} = I.$$

In compact notation, we have

$$\mathrm{diag}(A_{11}, \ldots, A_{nn})^{-1} = \mathrm{diag}(A_{11}^{-1}, \ldots, A_{nn}^{-1}).$$

Vandermonde Matrix

$$A = \begin{bmatrix} 1 & t_1 & t_1^2 & \cdots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \cdots & t_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_n & t_n^2 & \cdots & t_n^{n-1} \end{bmatrix}$$

Inverses

Inverse: Examples

the *Gram matrix* associated with a matrix

$$A = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}$$

is the matrix of column inner products

$$A^T A = \begin{bmatrix} a_1^T a_1 & a_1^T a_2 & \cdots & a_1^T a_n \\ a_2^T a_1 & a_2^T a_2 & \cdots & a_2^T a_n \\ \vdots & \vdots & & \vdots \\ a_n^T a_1 & a_n^T a_2 & \cdots & a_n^T a_n \end{bmatrix}$$

the Gram matrix is nonsingular if only if A has linearly independent columns

$$\begin{aligned} A^T A x = 0 \quad &\Longrightarrow \quad x^T A^T A x = (Ax)^T (Ax) = \|Ax\|^2 = 0 \\ &\Longrightarrow \quad Ax = 0 \\ &\Longrightarrow \quad x = 0 \end{aligned}$$

Example

- $A \in \mathbf{R}^{m \times n}$ with orthonormal columns

$$A^T A = I$$

Inverses

Inverse: Examples

Orthonormal Matrix

- $A \in \mathbf{R}^{n \times n}$ with orthonormal columns

$$A^T A = I$$

$$A^{-1} = A^T$$

- A^T is also orthonormal.

Orthogonal Matrix

- $A \in \mathbf{R}^{n \times n}$ with orthonormal columns

$$A^T A = I$$

$$A^{-1} = A^T$$

- A^T is also orthogonal.

Matrix with orthonormal columns

- $A \in \mathbf{R}^{m \times n}$ with orthonormal columns

$$A^T A = I$$

Inner product $(Ax)^T(Ay) = x^T A^T Ay = x^T y$

Norm $\|Ax\| = \left((Ax)^T(Ax)\right)^{1/2} = (x^T x)^{1/2} = \|x\|$

Distance $\|Ax - Ay\| = \|x - y\|$

Angle $\angle(Ax, Ay) = \angle(x, y)$

Linear transformation using 'matrix with orthonormal columns' preserves norm, distance, angle and inner product.

Inverses

Pseudo Inverse: Matrix with linearly independent columns

- suppose $A \in \mathbf{R}^{m \times n}$ has linearly independent columns
- this implies that A is tall or square ($m \geq n$)

the *pseudo-inverse* of A is defined as

$$A^{\dagger} = (A^T A)^{-1} A^T$$

(Left Pseudo-Inverse)

Equivalent Statements

- A is left-invertible
- the columns of A are linearly independent
- $A^T A$ is nonsingular

- A is left-invertible

$$A^{\dagger} A = (A^T A)^{-1} (A^T A) = I$$

Inverses

Pseudo Inverse: Matrix with linearly independent rows

- suppose $A \in \mathbf{R}^{m \times n}$ has linearly independent rows
- this implies that A is wide or square ($m \leq n$)

the *pseudo-inverse* of A is defined as

$$A^{\dagger} = A^T (AA^T)^{-1}$$

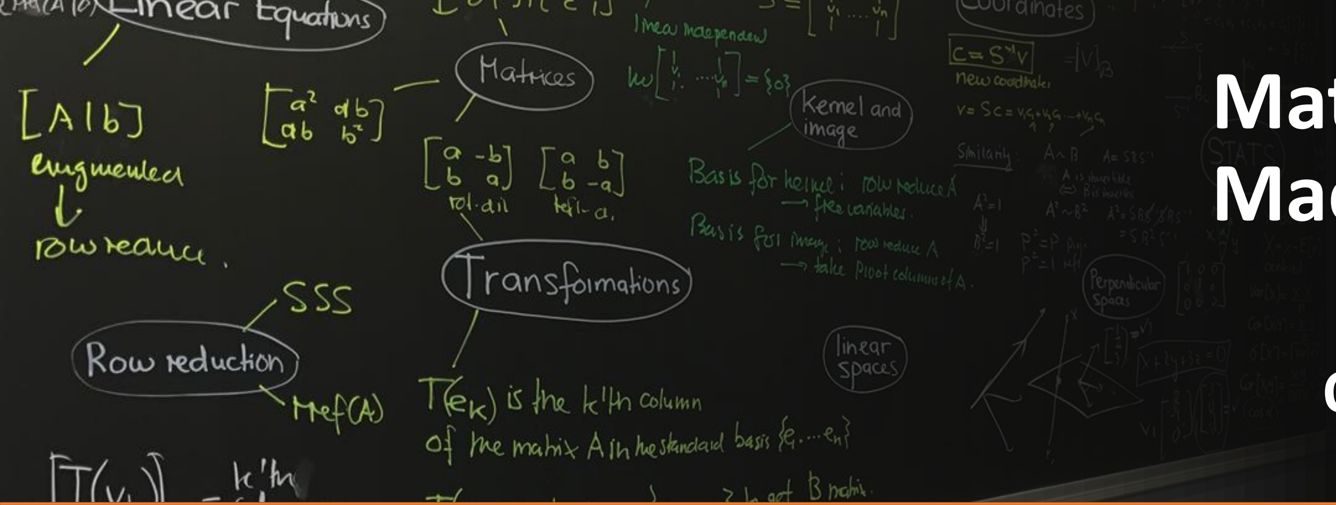
(Right Pseudo-Inverse)

Equivalent Statements

- A is right-invertible
- the rows of A are linearly independent
- AA^T is nonsingular

- A is right-invertible

$$AA^{\dagger} = (AA^T)(AA^T)^{-1} = I$$



Mathematical Foundations for Machine Learning and Data Science

QR Factorization and Solution of Linear Equations

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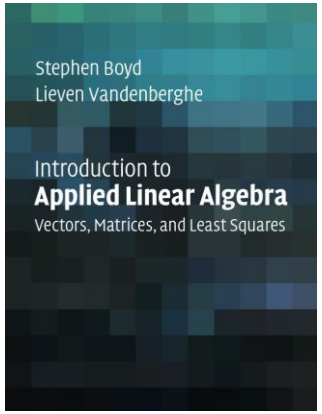
Outline

- *Systems of Linear Equations*
    - *Formulation*
- *Inverses*
    - *Left-inverse*
    - *Right-inverse*
    - *Inverse*
    - *Pseudo-inverse*
    - *Connection with the linear equations*



Chapters 10.4 and 11.3

Triangular Matrix

- Square matrix $A \in \mathbf{R}^n$ is lower triangular if

$$A_{ij} = 0, \quad j > i$$

$$A = \begin{bmatrix} A_{11} & 0 & \cdots & 0 & 0 \\ A_{21} & A_{22} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & 0 & 0 \\ A_{n-1,1} & A_{n-1,2} & \cdots & A_{n-1,n-1} & 0 \\ A_{n1} & A_{n2} & \cdots & A_{n,n-1} & A_{nn} \end{bmatrix}$$

- Square matrix $A \in \mathbf{R}^n$ is upper triangular if $A_{ij} = 0$ for $j < i$

- Triangular matrix A with nonzero diagonal elements is nonsingular.

$$Ax = 0 \quad \Longrightarrow \quad x = 0$$

Triangular Matrix

Linear Equations with Lower Triangular Matrix

$Ax = b$ $\qquad$ $A \in \mathbf{R}^n$ is lower triangular

$$\begin{bmatrix} A_{11} & 0 & \cdots & 0 & 0 \\ A_{21} & A_{22} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & 0 & 0 \\ A_{n-1,1} & A_{n-1,2} & \cdots & A_{n-1,n-1} & 0 \\ A_{n1} & A_{n2} & \cdots & A_{n,n-1} & A_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

Using forward substitution:

$$\begin{aligned} x_1 &= b_1/A_{11} \\ x_2 &= (b_2 - A_{21}x_1)/A_{22} \\ x_3 &= (b_3 - A_{31}x_1 - A_{32}x_2)/A_{33} \\ &\vdots \\ x_n &= (b_n - A_{n1}x_1 - A_{n2}x_2 - \cdots - A_{n,n-1}x_{n-1})/A_{nn} \end{aligned}$$

Triangular Matrix

Linear Equations with Upper Triangular Matrix

$Ax = b$ $\qquad$ $A \in \mathbf{R}^n$ is upper triangular

Using back substitution:

$$
\begin{aligned}
x_n &= b_n / A_{nn} \\
x_{n-1} &= (b_{n-1} - A_{n-1,n} x_n) / A_{n-1,n-1} \\
x_{n-2} &= (b_{n-2} - A_{n-2,n-1} x_{n-1} - A_{n-2,n} x_n) / A_{n-2,n-2} \\
&\vdots \\
x_1 &= (b_1 - A_{12} x_2 - A_{13} x_3 - \cdots - A_{1n} x_n) / A_{11}
\end{aligned}
$$

QR Factorization

if $A \in \mathbf{R}^{m \times n}$ has linearly independent columns then it can be factored as

$$A = \begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1n} \\ 0 & R_{22} & \cdots & R_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_{nn} \end{bmatrix}$$

- vectors $q_1, \ldots, q_n$ are orthonormal m-vectors:

$$\|q_i\| = 1, \qquad q_i^T q_j = 0 \quad \text{if } i \neq j$$

- diagonal elements R_{ii} are nonzero

QR Factorization

if $A \in \mathbf{R}^{m \times n}$ has linearly independent columns then it can be factored as

$$A = QR$$

Q-factor

- Q is $m \times n$ with orthonormal columns ($Q^T Q = I$)
- if A is square ($m = n$), then Q is orthogonal ($Q^T Q = QQ^T = I$)

R-factor

- R is $n \times n$, upper triangular, with nonzero diagonal elements
- R is nonsingular (diagonal elements are nonzero)

QR Factorization

How to compute?

Gram–Schmidt algorithm

Gram–Schmidt QR algorithm computes Q and R column by column

- after k steps we have a partial QR factorization

$$\begin{bmatrix} a_1 & a_2 & \cdots & a_k \end{bmatrix} = \begin{bmatrix} q_1 & q_2 & \cdots & q_k \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1k} \\ 0 & R_{22} & \cdots & R_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_{kk} \end{bmatrix}$$

- columns $q_1, \ldots, q_k$ are orthonormal
- diagonal elements $R_{11}, R_{22}, \ldots, R_{kk}$ are positive

Orthogonalization

$$\tilde{q}_i = a_i - \sum_{j=1}^{i-1} (q_j^T a_i)\, q_j$$

Normalization

$$q_i = \frac{\tilde{q}_i}{\|\tilde{q}_i\|}$$

QR Factorization

How to compute?

Gram–Schmidt algorithm

$$A = \begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1n} \\ 0 & R_{22} & \cdots & R_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_{nn} \end{bmatrix}$$

- column k of the equation $A = QR$ reads

$$a_k = R_{1k}q_1 + R_{2k}q_2 + \cdots + R_{k-1,k}q_{k-1} + R_{kk}q_k$$

$$R_{1k} = q_1^T a_k, \qquad R_{2k} = q_2^T a_k, \qquad \ldots, \qquad R_{k-1,k} = q_{k-1}^T a_k$$

QR Factorization

Example

$$
\begin{bmatrix} a_1 & a_2 & a_3 \end{bmatrix} = \begin{bmatrix} -1 & -1 & 1 \\ 1 & 3 & 3 \\ -1 & -1 & 5 \\ 1 & 3 & 7 \end{bmatrix}
$$

$$
= \begin{bmatrix} q_1 & q_2 & q_3 \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & R_{13} \\ 0 & R_{22} & R_{23} \\ 0 & 0 & R_{33} \end{bmatrix}
$$

First column of Q and R

$$
\tilde{q}_1 = a_1 = \begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \end{bmatrix}, \qquad R_{11} = \|\tilde{q}_1\| = 2, \qquad q_1 = \frac{1}{R_{11}}\tilde{q}_1 = \begin{bmatrix} -1/2 \\ 1/2 \\ -1/2 \\ 1/2 \end{bmatrix}
$$

QR Factorization

Example

Second column of Q and R

- compute $R_{12} = q_1^T a_2 = 4$
- compute

$$\tilde{q}_2 = a_2 - R_{12} q_1 = \begin{bmatrix} -1 \\ 3 \\ -1 \\ 3 \end{bmatrix} - 4 \begin{bmatrix} -1/2 \\ 1/2 \\ -1/2 \\ 1/2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

- normalize to get

$$R_{22} = \|\tilde{q}_2\| = 2, \qquad q_2 = \frac{1}{R_{22}} \tilde{q}_2 = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}$$

QR Factorization

Example

Third column of Q and R

- compute $R_{13} = q_1^T a_3 = 2$ and $R_{23} = q_2^T a_3 = 8$
- compute

$$\tilde{q}_3 = a_3 - R_{13}q_1 - R_{23}q_2 = \begin{bmatrix} 1 \\ 3 \\ 5 \\ 7 \end{bmatrix} - 2\begin{bmatrix} -1/2 \\ 1/2 \\ -1/2 \\ 1/2 \end{bmatrix} - 8\begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix} = \begin{bmatrix} -2 \\ -2 \\ 2 \\ 2 \end{bmatrix}$$

- normalize to get

$$R_{33} = \|\tilde{q}_3\| = 4, \qquad q_3 = \frac{1}{R_{33}}\tilde{q}_3 = \begin{bmatrix} -1/2 \\ -1/2 \\ 1/2 \\ 1/2 \end{bmatrix}$$

QR Factorization

Example

Final result

$$
\begin{bmatrix} -1 & -1 & 1 \\ 1 & 3 & 3 \\ -1 & -1 & 5 \\ 1 & 3 & 7 \end{bmatrix} = \begin{bmatrix} q_1 & q_2 & q_3 \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & R_{13} \\ 0 & R_{22} & R_{23} \\ 0 & 0 & R_{33} \end{bmatrix}
$$

$$
= \begin{bmatrix} -1/2 & 1/2 & -1/2 \\ 1/2 & 1/2 & -1/2 \\ -1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & 1/2 \end{bmatrix} \begin{bmatrix} 2 & 4 & 2 \\ 0 & 2 & 8 \\ 0 & 0 & 4 \end{bmatrix}
$$

QR Factorization

Solving Linear Equations

$$Ax = b$$

$$x = A^{-1}b = R^{-1}Q^Tb$$

QR factorization of nonsingular matrix

every nonsingular $A \in \mathbf{R}^{n \times n}$ has a QR factorization

$$A = QR$$

- $Q \in \mathbf{R}^{n \times n}$ is orthogonal ($Q^TQ = QQ^T = I$)
- $R \in \mathbf{R}^{n \times n}$ is upper triangular with positive diagonal elements

Algorithm: to solve $Ax = b$ with nonsingular $A \in \mathbf{R}^{n \times n}$,

1. factor A as $A = QR$
2. compute $y = Q^Tb$
3. solve $Rx = y$ by back substitution

QR Factorization

Solving Linear Equations – Pseudo Inverse

$$Ax = b$$

A is left-invertible
Columns are linear independent

$$A = QR$$

$$A^T A = (QR)^T (QR) = R^T Q^T QR = R^T R,$$

$$A^\dagger = (A^T A)^{-1} A^T = (R^T R)^{-1} (QR)^T = R^{-1} R^{-T} R^T Q^T = R^{-1} Q^T$$

A is right-invertible
rows are linear independent

$$A^T = QR$$

$$AA^T = (QR)^T (QR) = R^T Q^T QR = R^T R$$

$$A^\dagger = A^T (AA^T)^{-1} = QR(R^T R)^{-1} = QRR^{-1} R^{-T} = QR^{-T}$$