Introduction to Numerical Linear Algebra I

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Overview

We assume basic familiarity with linear algebra and will skip much of the preliminary material in this first set of slides.

1. Notation
   - So that we (at least try and) use the same name for the same thing...
   - Almost everything is real (at least in my lectures...)
2. Matrix operations
   - Matrix multiplication is the hardest
3. Basic Matrix Decompositions
   - Main purpose: Linear system solution
4. Determinants
5. Exercises

Notation

Vectors

- $\mathbb{R}$ Set of real numbers (scalars)
- $\mathbb{R}^{17}$ Space of column vectors with 17 real elements

$$\mathsf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{17} \end{pmatrix}$$

- Vectors with all zeros and all ones

$$0 = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \qquad \mathbb{1} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$$

$\mathsf{x} = 0$ *All* elements of x are zero
$\mathsf{x} \neq 0$ *At least* one element of x is non-zero

Matrices

- $\mathbb{R}^{7\times 5}$ Space of 7×5 matrices with real elements

$$A = \begin{pmatrix} a_{11} & \cdots & a_{15} \\ \vdots & & \vdots \\ a_{71} & \cdots & a_{75} \end{pmatrix}$$

- Identity matrix

$$I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} e_1 & e_2 & e_3 \end{pmatrix}$$

Canonical vectors

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Matrix Operations

Transpose

- Transpose of column vector gives row vector

$$\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}^T = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$$

- Transpose of matrix: Columns turn into rows

$$\begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix}^T = \begin{pmatrix} c_1^T \\ c_2^T \\ c_3^T \end{pmatrix}$$

- Transposing twice gives back the original $\quad (A^T)^T = A$

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

Scalar Multiplication

- Every matrix element multiplied by same scalar

$$4 \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix} = \begin{pmatrix} 4\,a_{11} & 4\,a_{12} & 4\,a_{13} \\ 4\,a_{21} & 4\,a_{22} & 4\,a_{23} \end{pmatrix}$$

- Two different zeros

  If $A \in \mathbb{R}^{7\times 5}$ then $\quad 0 \cdot A = 0_{7\times 5}$

- Subtraction: $-A \stackrel{\text{def}}{=} (-1)\,A$

Exercises

1. For $x \in \mathbb{R}^n$ and $\alpha \in \mathbb{R}$ show

$$\alpha x = 0 \quad \iff \quad \alpha = 0 \quad \text{or} \quad x = 0$$

2. For $A \in \mathbb{R}^{m \times n}$ and $\lambda \in \mathbb{R}$ show $\quad (\lambda A)^T = \lambda A^T$

Matrix Addition

- Elements in corresponding positions are added

$$\begin{pmatrix} 1 & 1 & 1 \\ 2 & 2 & 2 \\ 3 & 3 & 3 \end{pmatrix} + I_3 = \begin{pmatrix} 2 & 1 & 1 \\ 2 & 3 & 2 \\ 3 & 3 & 4 \end{pmatrix}$$

- Adding zero changes nothing

  If $A \in \mathbb{R}^{7\times 5}$ then $\qquad A + 0_{7\times 5} = A$

- Distributivity can save work

$$\lambda A + \lambda B = \lambda (A + B)$$

Exercises

1. For $A, B \in \mathbb{R}^{m \times n}$ show $\quad (A + B)^T = A^T + B^T$
2. For $A \in \mathbb{R}^{n \times n}$ show that $A + A^T$ is symmetric

Inner Product

- Row times column (with same # elements) gives scalar

  If $\mathrm{x}, \mathrm{y} \in \mathbb{R}^n$ then

$$\mathrm{x}^T\mathrm{y} = x_1 y_1 + \cdots + x_n y_n = \sum_{j=1}^{n} x_j y_j$$

- Commutative (for real vectors)

$$\mathrm{x}^T\mathrm{y} = \mathrm{y}^T\mathrm{x}$$

- Vectors $\mathrm{x}, \mathrm{y} \in \mathbb{R}^n$ are orthogonal if $\mathrm{x}^T\mathrm{y} = 0$

Exercises

1. Sum = inner product with all ones vector

   If $x \in \mathbb{R}^n$ then

$$\sum_{j=1}^{n} x_j = x^T \mathbb{1} = \mathbb{1}^T x$$

2. Given integer $n \geq 1$, represent $n(n+1)/2$ as an inner product

3. Test for zero vector

   For $x \in \mathbb{R}^n$ show $\quad x^T x = 0 \iff x = 0$

Matrix Vector Product

- Matrix times column vector gives column vector

$$A \in \mathbb{R}^{3\times 4} \qquad A = \begin{pmatrix} r_1^T \\ r_2^T \\ r_3^T \end{pmatrix} = \begin{pmatrix} c_1 & c_2 & c_3 & c_4 \end{pmatrix}$$

$x \in \mathbb{R}^4$ (# vector elements = # matrix columns)

- Column vector of inner products

$$Ax = \begin{pmatrix} r_1^T x \\ r_2^T x \\ r_3^T x \end{pmatrix}$$

- Linear combination of columns

$$Ax = c_1 x_1 + c_2 x_2 + c_3 x_3 + c_4 x_4$$

Exercises

1. Show that Ae_j is column j of matrix A
2. Given $A \in \mathbb{R}^{m \times n}$ and $\mathbb{1} \in \mathbb{R}^n$, what does $A\mathbb{1}$ do?
3. For $A, B \in \mathbb{R}^{m \times n}$ show

$$A = B \qquad \Longleftrightarrow \qquad Ax = Bx \quad \text{for all } x \in \mathbb{R}^n$$

Matrix Multiplication

- # columns of A = # rows of B
- A is 2×4 and B is 4×3 $\implies$ AB is 2×3
- Rows of A and columns of B

$$A = \begin{pmatrix} r_1^T \\ r_2^T \end{pmatrix} \qquad B = \begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix}$$

- Matrix of inner products

$$A\,B = \begin{pmatrix} r_1^T c_1 & r_1^T c_2 & r_1^T c_3 \\ r_2^T c_1 & r_2^T c_2 & r_2^T c_3 \end{pmatrix}$$

Other Views of Matrix Multiplication

$$A = \begin{pmatrix} a_1 & a_2 & a_3 & a_4 \end{pmatrix} \qquad B = \begin{pmatrix} b_1^T \\ b_2^T \\ b_3^T \\ b_4^T \end{pmatrix} = \begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix}$$

- Row of matrix vector products

$$AB = \begin{pmatrix} Ac_1 & Ac_2 & Ac_3 \end{pmatrix}$$

- Sum of outer products

$$AB = a_1 b_1^T + a_2 b_2^T + a_3 b_3^T + a_4 b_4^T$$

Properties

- Multiplication by the identity changes nothing

$$A \in \mathbb{R}^{8\times 11} \qquad I_8 A = A = A I_{11}$$

- Associativity $\quad A(BC) = (AB)C$
- Distributivity $\quad A(B + D) = AB + AD$
- No commutativity $\quad AB \neq BA$
- Transpose of product $\quad (AB)^T = B^T A^T$

Exercises

1. More distributivity

   For $A, B \in \mathbb{R}^{m \times n}$, $C \in \mathbb{R}^{n \times k}$ show $\quad (A + B)\, C = AC + BC$

2. Understanding why matrix multiplication is not commutative

   Find simple examples where $AB \neq BA$

3. Understanding the transposition of a product

   Find simple examples where $(AB)^T \neq A^T B^T$

4. For $A \in \mathbb{R}^{m \times n}$ show that AA^T and $A^T A$ are symmetric

Matrix Powers

For $\mathsf{A} \in \mathbb{R}^{n \times n}$ with $\mathsf{A} \neq 0$

$$\begin{aligned} \mathsf{A}^0 &= \mathsf{I}_n \\ \mathsf{A}^k &= \underbrace{\mathsf{A} \cdots \mathsf{A}}_{k} = \mathsf{A}^{k-1}\,\mathsf{A} = \mathsf{A}\,\mathsf{A}^{k-1} \qquad k \geq 1 \end{aligned}$$

Matrix Powers

For $A \in \mathbb{R}^{n \times n}$ with $A \neq 0$

$$
\begin{aligned}
A^0 &= I_n \\
A^k &= \underbrace{A \cdots A}_{k} = A^{k-1}A = A\,A^{k-1} \qquad k \geq 1
\end{aligned}
$$

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

- idempotent (projector) $\quad A^2 = A$
- nilpotent $\quad A^k = 0$ for some integer $k \geq 1$

For any $\alpha \in \mathbb{R}$

$$
\begin{pmatrix} 1 & \alpha \\ 0 & 0 \end{pmatrix} \text{ is idempotent} \qquad \begin{pmatrix} 0 & \alpha \\ 0 & 0 \end{pmatrix} \text{ is nilpotent}
$$

Exercises

1. Which matrix is idempotent and nilpotent?
2. If $A \in \mathbb{R}^{n \times n}$ is idempotent then $I_n - A$ is idempotent and $A(I_n - A) = 0$
3. If A and B are idempotent and $AB = BA$ then AB is idempotent

Outer Product

- Column vector times row vector gives matrix

$$\mathrm{x}\,\mathrm{y}^T = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \begin{pmatrix} y_1 & y_2 \end{pmatrix} = \begin{pmatrix} x_1 y_1 & x_1 y_2 \\ x_2 y_1 & x_2 y_2 \\ x_3 y_1 & x_3 y_2 \\ x_4 y_1 & x_4 y_2 \end{pmatrix}$$

- Columns of $\mathrm{x}\,\mathrm{y}^T$ are multiples of x
- Rows of $\mathrm{x}\,\mathrm{y}^T$ are multiples of y^T

Gram Matrix Multiplication

For $A = \begin{pmatrix} a_1 & \cdots & a_n \end{pmatrix} \in \mathbb{R}^{m \times n}$

- Matrix of inner products

$$A^T A = \begin{pmatrix} a_1^T a_1 & \dots & a_1^T a_n \\ \vdots & & \vdots \\ a_n^T a_1 & \cdots & a_n^T a_n \end{pmatrix} \quad \in \mathbb{R}^{n \times n}$$

- Sum of outer products

$$A A^T = a_1 a_1^T + \cdots + a_n a_n^T \quad \in \mathbb{R}^{m \times m}$$

Exercises

1. Write the matrix as an outer product

$$\begin{pmatrix} 4 & 5 \\ 8 & 10 \\ 12 & 15 \end{pmatrix}$$

2. Identity matrix is sum of outer products of canonical vectors

   Show $\quad I_n = e_1 e_1^T + \cdots + e_n e_n^T$

3. Associativity can save work

   For $x \in \mathbb{R}^6$ and $y, z \in \mathbb{R}^4$ compute both sides of

$$(xy^T)\,z = x\,(y^T z)$$

4. For $x, y \in \mathbb{R}^n$ compute $(xy^T)^3\,x$ with inner products and scalar multiplication only

Inverse

- $A \in \mathbb{R}^{n \times n}$ is nonsingular (invertible), if exists A^{-1} with

$$A\,A^{-1} = I_n = A^{-1}\,A$$

- Inverse and transposition interchangeable

$$A^{-T} \stackrel{\text{def}}{=} (A^T)^{-1} = \left(A^{-1}\right)^T$$

- Inverse of product

  For $A, B \in \mathbb{R}^{n \times n}$ nonsingular $\quad (AB)^{-1} = B^{-1}\,A^{-1}$

- Test

  If $x \in \mathbb{R}^n$ with $x \neq 0$ and $Ax = 0$, then A is singular

Exercises

1. If $A \in \mathbb{R}^{n \times n}$ with $A + A^2 = I_n$ then A is nonsingular

2. The inverse of a symmetric matrix is symmetric

3. Sherman-Morrison-Woodbury Formula

   For $A \in \mathbb{R}^{n \times n}$ nonsingular, and $U, V \in \mathbb{R}^{m \times n}$ show:
   If $I + VA^{-1}U^T$ nonsingular then

$$\left(A + U^T V\right)^{-1} = A^{-1} - A^{-1}U^T \left(I + VA^{-1}U^T\right)^{-1} VA^{-1}$$

Orthogonal Matrices

$A \in \mathbb{R}^{n \times n}$ is orthogonal matrix if $A^{-1} = A^T$

$$A^T A = I_n = AA^T$$

The meaning of orthogonality depends on who you are

- Two vectors $x, y \in \mathbb{R}^n$ are orthogonal if $x^T y = 0$
- Nonsingular matrix A is orthogonal if $A^{-1} = A^T$

Columns/rows of orthogonal matrix are orthogonal vectors

Examples of Orthogonal Matrices

- Identity I_n

- Permutation matrices (Identity with columns or rows permuted)

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

- 2×2 rotations

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix} \quad \text{for} \quad c^2 + s^2 = 1$$

Exercises

1. If $A \in \mathbb{R}^{n \times n}$ is orthogonal then A^T is orthogonal
2. If $A, B \in \mathbb{R}^{n \times n}$ are orthogonal then AB is orthogonal
3. If $x \in \mathbb{R}^n$ with $x^T x = 1$ then $I_n - 2\,xx^T$ is orthogonal
4. For $A \in \mathbb{R}^{m \times n}$ and permutation $P \in \mathbb{R}^{n \times n}$, describe AP.
5. Let $A = \begin{pmatrix} A_1 & A_2 \end{pmatrix} \in \mathbb{R}^{n \times n}$ where $A_1 \in \mathbb{R}^{n \times k}$
   If A orthogonal then
   $$A_1^T A_1 = I_k \qquad A_2^T A_2 = I_{n-k} \qquad A_1^T A_2 = 0$$
6. If $A^T A = B^T B$ for A, B nonsingular then exists orthogonal matrix Q so that $B = QA$

Triangular Matrices

Upper triangular matrix ◹

$$\mathsf{T} = \begin{pmatrix} t_{11} & \cdots & t_{1n} \\ & \ddots & \vdots \\ & & t_{nn} \end{pmatrix}$$

- ◹ matrix T nonsingular if and only if all $t_{jj} \neq 0$
- Diagonal elements of inverse $(\mathsf{T}^{-1})_{jj} = 1/t_{jj}$

Lower triangular matrix ◺

$$\mathsf{L} = \begin{pmatrix} l_{11} & & \\ \vdots & \ddots & \\ l_{n1} & \cdots & l_{nn} \end{pmatrix}$$

- Transpose: L^T is ◹

Special Triangular Matrices

- Unit triangular: Ones on the diagonal

$$\begin{pmatrix} 1 & * & * \\ 0 & 1 & * \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 \\ * & 1 & 0 \\ * & * & 1 \end{pmatrix}$$

- Strictly triangular: Zeros on the diagonal

$$\begin{pmatrix} 0 & * & * \\ 0 & 0 & * \\ 0 & 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & 0 & 0 \\ * & 0 & 0 \\ * & * & 0 \end{pmatrix}$$

- Diagonal: $\triangledown$ and $\triangle$

$$\begin{pmatrix} d_{11} & & \\ & \ddots & \\ & & d_{nn} \end{pmatrix} = \operatorname{diag}\begin{pmatrix} d_{11} & \cdots & d_{nn} \end{pmatrix}$$

Exercises

1. Sum of ◹ matrices is ◹

   If $A, B \in \mathbb{R}^{n \times n}$ is ◹ then $A + B$ is ◹

2. Product of ◹ matrices is ◹

   If $A, B \in \mathbb{R}^{n \times n}$ is ◹ then AB is ◹
   with diagonal elements $(AB)_{jj} = a_{jj} b_{jj}$ for $1 \leq j \leq n$

3. Diagonal matrices commute

   If $A, B \in \mathbb{R}^{n \times n}$ is diagonal then $AB = BA$ is diagonal

4. Let $A = I_n - \alpha\, e_i e_j$ for some $1 \leq i, j \leq n$ and scalar α.
   When is A ◹? When is A nonsingular?

5. If $D \in \mathbb{R}^{n \times n}$ is diagonal and $D = (I + A)^{-1} A$ for some A then A is diagonal

Basic Matrix Decompositions

Gaussian Elimination (LU) with partial pivoting

If $A \in \mathbb{R}^{n \times n}$ nonsingular then

$$PA = LU$$

P is permutation, L is unit ◺, U is ◹

Linear system solution $Ax = b$

1. Factor $PA = LU$ {Expensive part: $\mathcal{O}(n^3)$ flops}
2. Solve $Ly = Pb$ {◺ system}
3. Solve $Ux = y$ {◹ system}

QR Decomposition

If $A \in \mathbb{R}^{n \times n}$ nonsingular then

$$A = Q\,R$$

Q is orthogonal matrix, R is ◹

Linear system solution $A\,x = b$

1. Factor $A = Q\,R$ $\{$Expensive part: $\mathcal{O}(n^3)$ flops$\}$
2. Multiply $c = Q^T\,b$ $\{\mathcal{O}(n^2)$ flops$\}$
3. Solve $R\,x = c$ $\{$◹ system$\}$

Cholesky Decomposition

Symmetric $A \in \mathbb{R}^{n \times n}$ is positive definite (spd) if

$$x^T A x > 0 \qquad \text{for all } x \neq 0$$

If $A \in \mathbb{R}^{n \times n}$ spd then $A = L L^T$ where L is ◺

Linear system solution $A x = b$

1. Factor $A = L L^T$ {Expensive part: $\mathcal{O}(n^3)$ flops}
2. Solve $L y = b$ {◺ system}
3. Solve $L^T x = y$ {◹ system}

Determinants

A Simple Characterization

1. If $T \in \mathbb{R}^{n \times n}$ is $\triangledown$ or $\triangle$ then

$$\det(T) = \prod_{j=1}^{n} t_{jj}$$

2. If $A, B \in \mathbb{R}^{n \times n}$ then

$$\det(AB) = \det(A)\,\det(B)$$

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

- Transpose: $\det(A^T) = \det(A)$
- Singularity: $\det(A) \neq 0 \iff A$ nonsingular

Laplace Expansions

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

A_{ij} is $(n-1)\times(n-1)$ submatrix of A
obtained by deleting row i and column j of A

- Expansion is along row i

$$\det(A) = \sum_{k=1}^{n} (-1)^{i+k}\, a_{ik}\, \det(A_{ik}) \qquad 1 \le i \le n$$

- Expansion along column j

$$\det(A) = \sum_{k=1}^{n} (-1)^{k+j}\, a_{kj}\, \det(A_{kj}) \qquad 1 \le j \le n$$

Computation

If $A \in \mathbb{R}^{n \times n}$ nonsingular

1. Factor $PA = LU$
2. $\det(A) = \pm \det(U) = \pm u_{11} \cdots u_{nn}$

Exercises

Assume: $A, B \in \mathbb{R}^{n \times n}$

1. Triangular matrices

   If A is unit $\triangledown$ or $\triangle$ then $\det(A) = 1$

   If A is strictly $\triangledown$ or $\triangle$ then $\det(A) = 0$

2. If $A, B \in \mathbb{R}^{n \times n}$ then $\det(AB) = \det(BA)$

3. Scalar multiplication

   $\det(\alpha A) = \alpha^n \det(A)$ for any $\alpha \in \mathbb{R}$

4. If A nonsingular then $\det(A^{-1}) = 1/\det(A)$

5. If $A \in \mathbb{R}^{n \times n}$ is orthogonal then $|\det(A)| = 1$