NUMERICAL LINEAR ALGEBRA

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P1: Preliminaries

Overview

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

1. Notation
2. Matrix operations
3. Basic Matrix Decompositions
4. Determinants

Notation

We (at least try) use the same name for the same thing. Almost everything is in the real vector spaces (at least in my lectures...)

Vectors

$\mathbb{R}$: Set of real numbers (scalars)

$\mathbb{R}^n$: Space of column vectors with n real elements

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix}$$

Vectors with all zeros and all ones

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

Matrices

$\mathbb{R}^{m\times n}$ Space of $m \times n$ matrices with real elements

$$\mathbf{A} = \begin{pmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,n} \\ a_{2,1} & a_{2,2} & \dots & a_{2,n} \\ \vdots & & & \\ a_{m,1} & a_{m,2} & \dots & a_{m,n} \end{pmatrix}$$

Identity matrix $\mathbf{I} \in \mathbb{R}^{n\times n}$

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & & & \\ 0 & 0 & \dots & 1 \end{pmatrix} = (\mathbf{e}_1 \quad \mathbf{e}_2 \quad \mathbf{e}_n)$$

where $\mathbf{e}_i, i = 1,2,\dots,n$ are the canonical vectors

$$\mathbf{e}_i = (0 \quad 0 \quad \dots \quad 1 \quad \dots \quad 0 \quad 0)^T$$

$i-$th entry

Matrix operations

(Assumed that basics matrix operations are known)

Inner products

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

$$\mathbf{x}^T\mathbf{y} = \sum_{i=1,\ldots,n} x_i y_i$$

Commutative (for real vectors)

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

Vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ are orthogonal if

$$\mathbf{x}^T\mathbf{y} = \mathbf{y}^T\mathbf{x} = \mathbf{0}$$

Matrix multiplication - useful properties

1. Multiplication by the identity changes nothing. Example: $A \in \mathbb{R}^{n \times m}$, then $\mathbf{I}_n A = A = A\mathbf{I}_m$
2. Associativity $A(BC) = (AB)C$
3. Distributivity $A(B + D) = AB + AD$
4. No commutativity $AB \neq BA$
5. Transpose of product $(AB)^T = B^T A^T$

Matrix powers

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

$$A^0 = \mathbf{I}_n \qquad A^k = \underbrace{A \cdots A}_{k \text{ times}} = A\,A^{k-1} \qquad k \geq 1$$

2. $A \in \mathbb{R}^{n\times n}$ is
   - idempotent (projector) $A^2 = A$
   - nilpotent $A^k = \mathbf{0}$ for some integer $k \geq 1$

Inverse

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

$$A A^{-1} = \mathbf{I}_n = A^{-1} A$$

- Inverse and transposition interchangeable

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

- Inverse of product. For $A, B \in \mathbb{R}^{n \times n}$

$$(A B)^{-1} = B^{-1} A^{-1}$$

- Remark. If $\mathbf{0} \neq \mathbf{x} \in \mathbb{R}^n$ and $A \mathbf{x} = 0$, then A is singular

Orthogonal matrices

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

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

Triangular matrices

1. Upper triangular matrix ◹

$$\mathbf{U} = \begin{pmatrix} u_{1,1} & a_{1,2} & \dots & u_{1,n} \\ 0 & u_{2,2} & \dots & u_{2,n} \\ \vdots & & & \\ 0 & 0 & \dots & u_{n,n} \end{pmatrix}$$

U is nonsingular if and only if $u_{ii} \neq 0, i = 1, \dots, n$

2. Lower triangular matrix ◺

$$\mathbf{L} = \begin{pmatrix} \ell_{1,1} & 0 & \dots & 0 \\ \ell_{2,1} & \ell_{2,2} & \dots & 0 \\ \vdots & & & \\ \ell_{n,1} & \ell_{n,2} & \dots & \ell_{n,n} \end{pmatrix}$$

L is nonsingular if and only if $\ell_{ii} \neq 0, i = 1, \dots, n$

Unitary triangular matrices

1. Unitary Upper triangular matrix

$$\mathbf{U} = \begin{pmatrix} 1 & a_{1,2} & \dots & u_{1,n} \\ 0 & 1 & \dots & u_{2,n} \\ \vdots & & & \\ 0 & 0 & \dots & 1 \end{pmatrix}$$

2. Unitary Lower triangular matrix

$$\mathbf{L} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ \ell_{2,n} & 1 & \dots & 0 \\ \vdots & & & \\ \ell_{n,1} & \ell_{n,2} & \dots & 1 \end{pmatrix}$$

Basic matrix decompositions

LU factorisation with (partial) pivoting

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

$$PA = LU$$

- P is a permutation matrix
- L is unit lower triangular
- U is upper triangular

Linear system solution

$$A\mathbf{x} = \mathbf{b}$$

1. Factor $PA = LU$ (Expensive part: $O(n^3)$ flops)
2. Solve $L\mathbf{y} = P\mathbf{b}$ (◺ system, $O(n^2)$ flops)
3. Solve $U\mathbf{x} = \mathbf{y}$ (◹ system, $O(n^2)$ flops)

Cholesky decomposition

If $A \in \mathbb{R}^{n\times n}$ is symmetric ($A^T = A$) and positive definite, i.e.

$$\mathbf{z}^T A \mathbf{z} > 0 \text{ for all } \mathbf{z} \neq \mathbf{0}$$

then

$$A = L^T L$$

- L is lower triangular (with positive entries on the diagonal)

Linear system solution

$$A\mathbf{x} = \mathbf{b}$$

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

QR decomposition

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

$$A = QR$$

- Q is an orthogonal
- R is upper triangular

Linear system solution

$$A\mathbf{x} = \mathbf{b}$$

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

Determinants

Some properties

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

$$\det(T) = \prod_{i=1}^{n} t_{i,i}$$

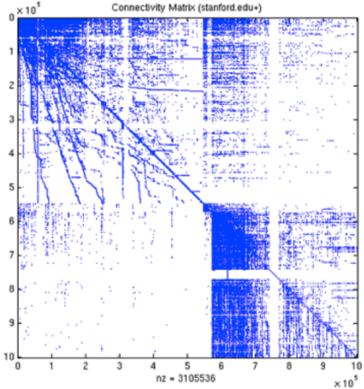
2. Let $A, B \in \mathbb{R}^{n \times n}$ then $\det(AB) = \det(A)\det(B)$
3. Let $A \in \mathbb{R}^{n \times n}$, then $\det(A^T) = \det(A)$
4. Let $A \in \mathbb{R}^{n \times n}$, $\det(A) \neq 0 \iff A$ is non singular
5. Computation. Let $A \in \mathbb{R}^{n \times n}$ be non singular.
   A. Factor $PA = LU$
   B. $\det(A) = \pm \det(U) = \pm u_{1,1} \dots u_{n,n}$

Sparse matrices

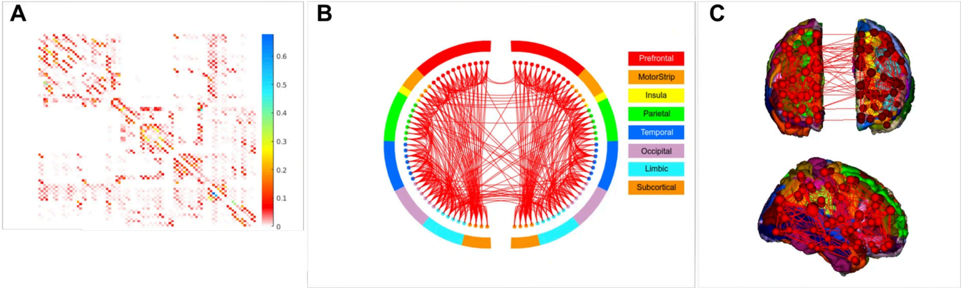
Definition

A sparse matrix is a matrix in which most elements are zero, roughly speaking, given $A \in \mathbb{R}^{n \times n}$ the number of non-zero entries of A, nnz(A), is $O(n)$ we say that A is sparse.
Many matrices arising from real applications are sparse.

Example: A 1M-by-1M submatrix of the web connectivity graph (archive at the Stanford WebBase).
The picture shows the nonzero structure of the matrix



More examples: Connectivity Matrices and Brain Graphs

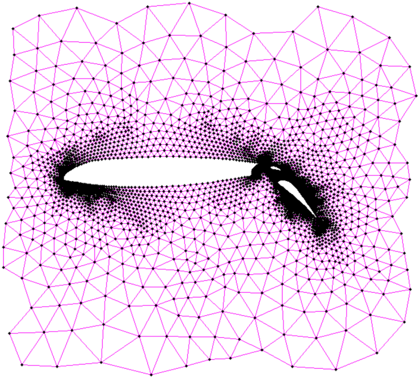


Average structural connectivity. (A) The adjacency matrix of the average structural connectivity (up). (B) Network representation of structural connectivity. (C) Connectivity is mapped on the brain surface.

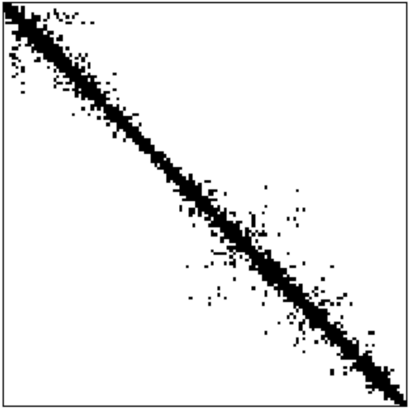
Figure re-adapted from: Škoch, A., Rehák Bučková, B., Mareš, J. *et al.* Human brain structural connectivity matrices–ready for modelling. *Sci Data* **9**, 486 (2022).

More examples

Examples from Tim Davis's Sparse Matrix Collection, http://www.cise.ufl.edu/research/sparse/matrices/



2D airfoil profile



Sparse numerical linear algebra: motivation

We wish to solve

$$A\mathbf{x} = \mathbf{b}$$

where A is sparse (often it comes from the discretisation of partial differential equations)

Important points

- Iterative methods only use A in context of matrix-vector product.
- You only need to provide matrix-vector product to solvers.
- If storing A , exploit sparse structure.

Storage schemes

- Rather than storing a dense array (with many zeros), store only the non-zero entries, plus their locations.
- Data size becomes $O(\text{nnz})$ rather than $O(n^2)$.
- For finite stencils (as from mesh-based discretisations) asymptotically save $O(n)$.
- Common sparse storage types

Name	Easy insertion	Fast $A\mathbf{x}$
Coordinate (COO)	Yes	No
CSR	No	Yes
CSC	No	Yes
ELLPACK	No	Yes

[Saad 2003, § 3.4]

Coordinate format (COO)

The data structure consists of three arrays (of length nnz(A):

- AA: all the values of the nonzero elements of A in any order
- JR: integer array containing their row indices;
- JC: integer array containing their column indices.

$$A = \begin{pmatrix} 1. & 0. & 0. & 2. & 0. \\ 3. & 4. & 0. & 5. & 0. \\ 6. & 0. & 7. & 8. & 9. \\ 0. & 0. & 10. & 11. & 0. \\ 0. & 0. & 0. & 0. & 12. \end{pmatrix}$$

AA	12.	9.	7.	5.	1.	2.	11.	3.	6.	4.	8.	10.
JR	5	3	3	2	1	1	4	2	3	2	3	4
JC	5	5	3	4	1	4	4	1	1	2	4	3

Coordinate Compressed Sparse Row (CSR) format

If the elements of A are listed by row, the array JC might be replaced by an array that points to the beginning of each row.

- AA: all the values of the nonzero elements of A, stored row by row from $1,\ldots,n$
- JA: contains the column indices
- IA: contains the pointers to the beginning of each row in the arrays A and JA. Thus $IA(i)$ contains the position in the arrays AA and JA where the $i-$th row starts. The length of IA is $n+1$, with IA$(n+1)$ containing the number A(1)+ nnz(A).

$$A = \begin{pmatrix} 1. & 0. & 0. & 2. & 0. \\ 3. & 4. & 0. & 5. & 0. \\ 6. & 0. & 7. & 8. & 9. \\ 0. & 0. & 10. & 11. & 0. \\ 0. & 0. & 0. & 0. & 12. \end{pmatrix}$$

AA	1.	2.	3.	4.	5.	6.	7.	8.	9.	10.	11.	12.
JA	1	4	1	2	4	1	3	4	5	3	4	5
IA	1	3	6	10	12	13						