All definitions and results

MATH 2740 – Mathematics of Data Science – Lecture 00

Julien Arino

julien.arino@umanitoba.ca

Department of Mathematics @ University of Manitoba

Fall 202X

The University of Manitoba campuses are located on original lands of Anishinaabeg, Ininew, Anisininew, Dakota and Dene peoples, and on the National Homeland of the Red River Métis. We respect the Treaties that were made on these territories, we acknowledge the harms and mistakes of the past, and we dedicate ourselves to move forward in partnership with Indigenous communities in a spirit of Reconciliation and collaboration.

Definitions are colour coded

Memorising the definitions is part of the course. To help, definitions are colour coded

Definition 1 (Definitions)

These definitions are important, you need to know them

Definition 2 (Less important definitions)

These definitions are a little less important, you will not be asked to state them (although it is a good idea to know them anyway)

Results are colour coded

Memorising some of the results is part of the course. To help, results are colour coded

Theorem 3 (Theorems)

Theorems in blue boxes are worth knowing but you will not be asked to reproduce them

Theorem 4 (Important theorems)

Theorems in red boxes are important, you should know them and be able to reproduce them

You must know how to do some proofs

There are a few proofs (not many!) that I want you to know how to do

Such proofs appear on slides like the present one, with a red background

Outline

- Preliminary stuff
- Least squares
- PCA
- Markov chains
- Graph theory

Preliminary stuff

Least squares

PCA

Markov chains

Graph theory

Intersection and union of sets

Let X and Y be two sets

Definition 5 (Intersection)

The intersection of X and Y, $X \cap Y$, is the set of elements that belong to X **and** to Y,

$$X \cap Y = \{x : x \in X \textbf{ and } x \in Y\}$$

Definition 6 (Union)

The union of X and Y, $X \cup Y$, is the set of elements that belong to X **or** to Y,

$$X \cup Y = \{x : x \in X \textbf{ or } x \in Y\}$$

In mathematics, or=and/or in common parlance. We also have an **exclusive or** (xor)

Complex numbers

Definition 7 (Complex numbers)

A **complex number** is an ordered pair (a, b), where $a, b \in \mathbb{R}$. Usually written $a + ib$ or $a + bi$, where $i^2 = -1$ (i.e., $i = \sqrt{-1}$)
The set of all complex numbers is denoted $\mathbb{C}$,

$$\mathbb{C} = \{a + ib : a, b \in \mathbb{R}\}$$

Definition 8 (Addition and multiplication on $\mathbb{C}$)

Letting $a + ib$ and $c + id \in \mathbb{C}$, addition on $\mathbb{C}$ is defined by

$$(a + ib) + (c + id) = (a + c) + i(b + d)$$

and multiplication on $\mathbb{C}$ is defined by

$$(a + ib)(c + id) = (ac - bd) + i(ad + bc)$$

Latter is easy to obtain using regular multiplication and $i^2 = -1$

Definition 9 (Real and imaginary parts)

Let $z = a + ib$. Then $\mathrm{Re}\ z = a$ is **real part** and $\mathrm{Im}\ z = b$ is **imaginary part** of z

If ambiguous, write $\mathrm{Re}\ (z)$ and $\mathrm{Im}\ (z)$

Definition 10 (Conjugate and Modulus)

Let $z = a + ib \in \mathbb{C}$. Then

- **Complex conjugate** of z is
$$\bar{z} = a - ib$$
- **Modulus** (or **absolute value**) of z is
$$|z| = \sqrt{a^2 + b^2} \geq 0$$

$z\bar{z} = |z|^2$ and $\bar{\bar{z}} = z$

Vectors

A **vector** $\boldsymbol{v}$ is an ordered n-tuple of real or complex numbers

Denote $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$ (real or complex numbers). For $v_1, \ldots, v_n \in \mathbb{F}$,

$$\boldsymbol{v} = (v_1, \ldots, v_n) \in \mathbb{F}^n$$

is a vector. $v_1, \ldots, v_n$ are the **components** of $\boldsymbol{v}$

If unambiguous, we write v. Otherwise, $\boldsymbol{v}$ or $\vec{v}$

Vector space

Definition 11 (Vector space)

*A **vector space** over $\mathbb{F}$ is a set V together with two binary operations, **vector addition**, denoted $+$, and **scalar multiplication**, that satisfy the relations:*

1. $\forall \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in V$, $\boldsymbol{u} + (\boldsymbol{v} + \boldsymbol{w}) = (\boldsymbol{u} + \boldsymbol{v}) + \boldsymbol{w}$
2. $\forall \boldsymbol{v}, \boldsymbol{w} \in V$, $\boldsymbol{v} + \boldsymbol{w} = \boldsymbol{w} + \boldsymbol{v}$
3. $\exists \boldsymbol{0} \in V$, *the zero vector, such that* $\boldsymbol{v} + \boldsymbol{0} = \boldsymbol{v}$ *for all* $\boldsymbol{v} \in V$
4. $\forall \boldsymbol{v} \in V$, *there exists an element* $\boldsymbol{w} \in V$, *the additive inverse of* $\boldsymbol{v}$, *such that* $\boldsymbol{v} + \boldsymbol{w} = \boldsymbol{0}$
5. $\forall \alpha \in \mathbb{R}$ *and* $\forall \boldsymbol{v}, \boldsymbol{w} \in V$, $\alpha(\boldsymbol{v} + \boldsymbol{w}) = \alpha\boldsymbol{v} + \alpha\boldsymbol{w}$
6. $\forall \alpha, \beta \in \mathbb{R}$ *and* $\forall \boldsymbol{v} \in V$, $(\alpha + \beta)\boldsymbol{v} = \alpha\boldsymbol{v} + \beta\boldsymbol{v}$
7. $\forall \alpha, \beta \in \mathbb{R}$ *and* $\forall \boldsymbol{v} \in V$, $\alpha(\beta\boldsymbol{v}) = (\alpha\beta)\boldsymbol{v}$
8. $\forall \boldsymbol{v} \in V$, $1\boldsymbol{v} = \boldsymbol{v}$

Norms

Definition 12 (Norm)

Let V be a vector space over $\mathbb{F}$, and $\boldsymbol{v} \in V$ be a vector. The **norm** of $\boldsymbol{v}$, denoted $\|\boldsymbol{v}\|$, is a function from V to $\mathbb{R}_+$ that has the following properties:

1. For all $\boldsymbol{v} \in V$, $\|\boldsymbol{v}\| \geq 0$ with $\|\boldsymbol{v}\| = 0$ iff $\boldsymbol{v} = \mathbf{0}$
2. For all $\alpha \in \mathbb{F}$ and all $\boldsymbol{v} \in V$, $\|\alpha \boldsymbol{v}\| = |\alpha| \, \|\boldsymbol{v}\|$
3. For all $\boldsymbol{u}, \boldsymbol{v} \in V$, $\|\boldsymbol{u} + \boldsymbol{v}\| \leq \|\boldsymbol{u}\| + \|\boldsymbol{v}\|$

Let V be a vector space (for example, $\mathbb{R}^2$ or $\mathbb{R}^3$)

The **zero element** (or **zero vector**) is the vector $\mathbf{0} = (0, \dots, 0)$

The **additive inverse** of $\boldsymbol{v} = (v_1, \dots, v_n)$ is $-\boldsymbol{v} = (-v_1, \dots, -v_n)$

For $\boldsymbol{v} = (v_1, \dots, v_n) \in V$, the length (or Euclidean norm) of $\boldsymbol{v}$ is the **scalar**

$$\|\boldsymbol{v}\| = \sqrt{v_1^2 + \cdots + v_n^2}$$

To **normalize** the vector $\boldsymbol{v}$ consists in considering $\tilde{\boldsymbol{v}} = \boldsymbol{v}/\|\boldsymbol{v}\|$, i.e., the vector in the same direction as $\boldsymbol{v}$ that has unit length

Dot product

Definition 13 (Dot product)

Let $\boldsymbol{a} = (a_1, \ldots, a_n) \in \mathbb{R}^n$, $\boldsymbol{b} = (b_1, \ldots, b_n) \in \mathbb{R}^n$. The **dot product** of $\boldsymbol{a}$ and $\boldsymbol{b}$ is the **scalar**

$$\boldsymbol{a} \bullet \boldsymbol{b} = \sum_{i=1}^{n} a_i b_i = a_1 b_1 + \cdots + a_n b_n$$

Properties of the dot product

Theorem 14

For $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in \mathbb{R}^n$ *and* $\alpha \in \mathbb{R}$,

- $\boldsymbol{a} \bullet \boldsymbol{a} = \|\boldsymbol{a}\|^2$ *(so* $\boldsymbol{a} \bullet \boldsymbol{a} \geq 0$, *with* $\boldsymbol{a} \bullet \boldsymbol{a} = 0$ *iff* $\boldsymbol{a} = \mathbf{0}$*)*
- $\boldsymbol{a} \bullet \boldsymbol{b} = \boldsymbol{b} \bullet \boldsymbol{a}$ *($\bullet$ is commutative)*
- $\boldsymbol{a} \bullet (\boldsymbol{b} + \boldsymbol{c}) = \boldsymbol{a} \bullet \boldsymbol{b} + \boldsymbol{a} \bullet \boldsymbol{c}$ *($\bullet$ distributive over $+$)*
- $(\alpha\boldsymbol{a}) \bullet \boldsymbol{b} = \alpha(\boldsymbol{a} \bullet \boldsymbol{b}) = \boldsymbol{a} \bullet (\alpha\boldsymbol{b})$
- $\mathbf{0} \bullet \boldsymbol{a} = 0$

Some results stemming from the dot product

Theorem 15

If θ is the angle between the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$, then

$$\boldsymbol{a} \bullet \boldsymbol{b} = \|\boldsymbol{a}\| \, \|\boldsymbol{b}\| \, \cos\theta$$

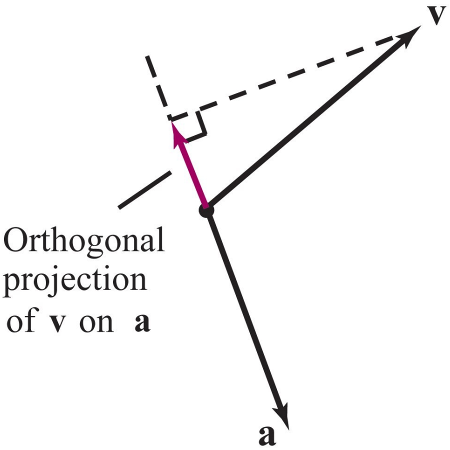
Theorem 16

$\boldsymbol{a}$ and $\boldsymbol{b}$ are orthogonal if and only if $\boldsymbol{a} \bullet \boldsymbol{b} = 0$.

Scalar and vector projections

Scalar projection of $\boldsymbol{v}$ onto $\boldsymbol{a}$ (or component of $\boldsymbol{v}$ along $\boldsymbol{a}$):

$$\mathrm{comp}_{\boldsymbol{a}}\boldsymbol{v} = \frac{\boldsymbol{a} \bullet \boldsymbol{v}}{\|\boldsymbol{a}\|}$$



Vector (or orthogonal) projection of $\boldsymbol{v}$ onto $\boldsymbol{a}$:

$$\mathrm{proj}_{\boldsymbol{a}}\boldsymbol{v} = \left(\frac{\boldsymbol{a} \bullet \boldsymbol{v}}{\|\boldsymbol{a}\|}\right)\frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} = \frac{\boldsymbol{a} \bullet \boldsymbol{v}}{\|\boldsymbol{a}\|^2}\boldsymbol{a}$$

Linear systems

Definition 17 (Linear system)

A **linear system** of m equations in n unknowns takes the form

$$\begin{array}{ccccccccc} a_{11}x_1 & + & a_{12}x_2 & + & \cdots & + & a_{1n}x_n & = & b_1 \\ a_{21}x_1 & + & a_{22}x_2 & + & \cdots & + & a_{2n}x_n & = & b_2 \\ \vdots & & \vdots & & \vdots & & \vdots & & \vdots \\ a_{m1}x_1 & + & a_{m2}x_2 & + & \cdots & + & a_{mn}x_n & = & b_n \end{array} \tag{1}$$

The a_{ij}, x_j and b_j could be in $\mathbb{R}$ or $\mathbb{C}$, although here we typically assume they are in $\mathbb{R}$

The aim is to find $x_1, x_2, \ldots, x_n$ that satisfy all equations simultaneously

Theorem 18 (Nature of solutions to a linear system)

A linear system can have

- *no solution*
- *a unique solution*
- *infinitely many solutions*

Matrices and linear systems

Writing

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}, \quad \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \quad \text{and} \quad \boldsymbol{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

where A is an $m \times n$ **matrix**, $\boldsymbol{x}$ and $\boldsymbol{b}$ are n (column) **vectors** (or $n \times 1$ matrices), then the linear system in the previous slide takes the form

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

If $\boldsymbol{b} = \mathbf{0}$, the system is **homogeneous** and always has the solution $\boldsymbol{x} = 0$ and so the "no solution" option in Theorem 18 goes away

Definition 19 (Matrix)

An m-by-n or $m \times n$ matrix is a rectangular array of elements of $\mathbb{R}$ or $\mathbb{C}$ with m rows and n columns,

$$A = [a_{ij}] = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mn} \end{pmatrix}$$

We always list indices as “row,column”

We denote $\mathcal{M}_{mn}(\mathbb{F})$ or $\mathbb{F}^{mn}$ the set of $m \times n$ matrices with entries in $\mathbb{F} = \{\mathbb{R}, \mathbb{C}\}$. Often, we omit $\mathbb{F}$ in $\mathcal{M}_{mn}$ if the nature of $\mathbb{F}$ is not important

When $m = n$, we usually write $\mathcal{M}_n$

Basic matrix arithmetic

Let $A \in \mathcal{M}_{mn}, B \in \mathcal{M}_{mn}$ be matrices (of the same size) and $c \in \mathbb{F} = \{\mathbb{R}, \mathbb{C}\}$ be a scalar

- **Scalar multiplication**
$$cA = [ca_{ij}]$$
- **Addition**
$$A + B = [a_{ij} + b_{ij}]$$
- **Subtraction** (addition of $-B = (-1)B$ to A)
$$A - B = A + (-1)B = [a_{ij} + (-1)b_{ij}] = [a_{ij} - b_{ij}]$$
- **Transposition** of A gives a matrix $A^T = \mathcal{M}_{nm}$ with
$$A^T = [a_{ji}], \quad j = 1, \ldots, n, \quad i = 1, \ldots, m$$

Matrix multiplication

The (matrix) **product** of A and B, AB, requires the “inner dimensions” to match, i.e., the number of columns in A must equal the number of rows in B

Suppose that is the case, i.e., let $A \in \mathcal{M}_{mn}$, $B \in \mathcal{M}_{np}$. Then the i, j entry in $C := AB$ takes the form

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

Recall that the matrix product is not commutative, i.e., in general, $AB \neq BA$ (when both those products are defined, i.e., when $A, B \in \mathcal{M}_n$)

Special matrices

Definition 20 (Zero and identity matrices)

The **zero** matrix is the matrix 0_{mn} whose entries are all zero. The **identity** matrix is a square $n \times n$ matrix $\mathbb{I}_n$ with all entries on the main diagonal equal to one and all off diagonal entries equal to zero

Definition 21 (Symmetric matrix)

A square matrix $A \in \mathcal{M}_n$ is **symmetric** if $\forall i, j = 1, \ldots, n$, $a_{ij} = a_{ji}$. In other words, $A \in \mathcal{M}_n$ is symmetric if $A = A^T$

Theorem 22

1. *If $A \in \mathcal{M}_n$, then $A + A^T$ is symmetric*
2. *If $A \in \mathcal{M}_{mn}$, then $AA^T \in \mathcal{M}_m$ and $A^TA \in \mathcal{M}_n$ are symmetric*

Proof of Theorem 22

X symmetric $\iff X = X^T$, so use $X =$ the matrix whose symmetric property you want to check

1. True if $A + A^T = (A + A^T)^T$. We have

$$(A + A^T)^T = A^T + (A^T)^T = A^T + A = A + A^T$$

2. AA^T symmetric if $AA^T = (AA^T)^T$. We have

$$(AA^T)^T = (A^T)^T A^T = AA^T$$

$A^T A$ works similarly

Two special matrices and their determinants

Definition 23

$A \in \mathcal{M}_n$ is **upper triangular** if $a_{ij} = 0$ when $i > j$, **lower triangular** if $a_{ij} = 0$ when $j > i$, **triangular** if it is *either* upper or lower triangular and **diagonal** if it is *both* upper and lower triangular

When A diagonal, we often write $A = \operatorname{diag}(a_{11}, a_{22}, \ldots, a_{nn})$

Theorem 24

Let $A \in \mathcal{M}_n$ be triangular or diagonal. Then

$$\det(A) = \prod_{i=1}^{n} a_{ii} = a_{11} a_{22} \cdots a_{nn}$$

Inversion/Singularity

Definition 25 (Matrix inverse)

$A \in \mathcal{M}_n$ is **invertible** (or **nonsingular**) if $\exists A^{-1} \in \mathcal{M}_n$ s.t.

$$AA^{-1} = A^{-1}A = \mathbb{I}$$

A^{-1} is the **inverse** of A. If A^{-1} does not exist, A is **singular**

Eigenvalues / Eigenvectors / Eigenpairs

Definition 26

Let $A \in \mathcal{M}_n$. A vector $\boldsymbol{x} \in \mathbb{F}^n$ such that $\boldsymbol{x} \neq \boldsymbol{0}$ is an **eigenvector** of A if $\exists \lambda \in \mathbb{F}$ called an **eigenvalue**, s.t.

$$A\boldsymbol{x} = \lambda \boldsymbol{x}$$

A couple $(\lambda, \boldsymbol{x})$ with $\boldsymbol{x} \neq \boldsymbol{0}$ s.t. $A\boldsymbol{x} = \lambda \boldsymbol{x}$ is an **eigenpair**

If $(\lambda, \boldsymbol{x})$ eigenpair, then for $c \neq 0$, $(\lambda, c\boldsymbol{x})$ also eigenpair since $A(c\boldsymbol{x}) = cA\boldsymbol{x} = c\lambda \boldsymbol{x}$ and dividing both sides by c..

Similarity

Definition 27 (Similarity)

*$A, B \in \mathcal{M}_n$ are **similar** ($A \sim B$) if $\exists P \in \mathcal{M}_n$ invertible s.t.*

$$P^{-1}AP = B$$

Theorem 28

$A, B \in \mathcal{M}_n$ with $A \sim B$. Then

- $\det A = \det B$
- *A invertible $\iff$ B invertible*
- *A and B have the same eigenvalues*

Diagonalisation

Definition 29 (Diagonalisability)

$A \in \mathcal{M}_n$ is **diagonalisable** if $\exists D \in \mathcal{M}_n$ diagonal s.t. $A \sim D$

In other words, $A \in \mathcal{M}_n$ is diagonalisable if there exists a diagonal matrix $D \in \mathcal{M}_n$ and a nonsingular matrix $P \in \mathcal{M}_n$ s.t. $P^{-1}AP = D$

Could of course write $PAP^{-1} = D$ since P invertible, but $P^{-1}AP$ makes more sense for computations

Theorem 30

$A \in \mathcal{M}_n$ diagonalisable $\iff$ A has n linearly independent eigenvectors

Corollary 31 (Sufficient condition for diagonalisability)

$A \in \mathcal{M}_n$ has all its eigenvalues distinct $\implies$ A diagonalisable

For $P^{-1}AP = D$: in P, put the linearly independent eigenvectors as columns and in D, the corresponding eigenvalues

Linear combination and span

Definition 32 (Linear combination)

Let V be a vector space. A **linear combination** of a set $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$ of vectors in V is a *vector*

$$c_1 \boldsymbol{v}_1 + \cdots + c_k \boldsymbol{v}_k$$

where $c_1, \ldots, c_k \in \mathbb{F}$

Definition 33 (Span)

The set of all linear combinations of a set of vectors $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k$ is the **span** of $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$,

$$\text{span}(\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k) = \{c_1 \boldsymbol{v}_1 + \cdots + c_k \boldsymbol{v}_k : c_1, \ldots, c_k \in \mathbb{F}\}$$

Finite/infinite-dimensional vector spaces

Theorem 34

The span of a set of vectors in V is the smallest subspace of V containing all the vectors in the set

Definition 35 (Set of vectors spanning a space)

If $\text{span}(\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k) = V$, we say $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k$ **spans** V

Definition 36 (Dimension of a vector space)

A vector space V is **finite-dimensional** if some set of vectors in it spans V. A vector space V is **infinite-dimensional** if it is not finite-dimensional

Linear (in)dependence

Definition 37 (Linear independence/Linear dependence)

A set $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$ of vectors in a vector space V is **linearly independent** if

$$(c_1 \boldsymbol{v}_1 + \cdots + c_k \boldsymbol{v}_k = 0) \Leftrightarrow (c_1 = \cdots = c_k = 0)\,,$$

where $c_1, \ldots, c_k \in \mathbb{F}$. A set of vectors is **linearly dependent** if it is not linearly independent.

If linearly dependent, assume w.l.o.g. that $c_1 \neq 0$, then

$$\boldsymbol{v}_1 = -\frac{c_2}{c_1}\boldsymbol{v}_2 - \cdots - \frac{c_k}{c_1}\boldsymbol{v}_k$$

i.e., $\boldsymbol{v}_1$ is a linear combination of the other vectors in the set

Basis

Definition 38 (Basis)

Let V be a vector space. A **basis** of V is a set of vectors in V that is both linearly independent and spanning

Theorem 39 (Criterion for a basis)

A set $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$ of vectors in a vector space V is a basis of $V \iff \forall \boldsymbol{v} \in V$, $\boldsymbol{v}$ can be written uniquely in the form

$$\boldsymbol{v} = c_1 \boldsymbol{v}_1 + \cdots + c_k \boldsymbol{v}_k,$$

where $c_1, \ldots, c_k \in \mathbb{F}$

More on bases

Theorem 40

Any two bases of a finite-dimensional vector space have the same number of vectors

Definition 41 (Dimension)

The **dimension** $\dim V$ of a finite-dimensional vector space V is the number of vectors in any basis of the vector space

Linear algebra in a nutshell

Theorem 42

Let $A \in \mathcal{M}_n$. The following statements are equivalent (TFAE)

1. *The matrix A is invertible*
2. $\forall \boldsymbol{b} \in \mathbb{F}^n$, $A\boldsymbol{x} = \boldsymbol{b}$ *has a unique solution* ($\boldsymbol{x} = A^{-1}\boldsymbol{b}$)
3. *The only solution to* $A\boldsymbol{x} = \mathbf{0}$ *is the trivial solution* $\boldsymbol{x} = \mathbf{0}$
4. $RREF(A) = \mathbb{I}_n$
5. *The matrix A is equal to a product of elementary matrices*
6. $\forall \boldsymbol{b} \in \mathbb{F}^n$, $A\boldsymbol{x} = \boldsymbol{b}$ *has a solution*
7. *There is a matrix* $B \in \mathcal{M}_n$ *such that* $AB = \mathbb{I}_n$
8. *There is an invertible matrix* $B \in \mathcal{M}_n$ *such that* $AB = \mathbb{I}_n$
9. $\det(A) \neq 0$
10. 0 *is not an eigenvalue of* A

The gradient

$f : \mathbb{R}^n \to \mathbb{R}$ function of several variables, $\nabla = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right)$ the gradient operator

Then

$$\nabla f = \left(\frac{\partial}{\partial x_1} f, \ldots, \frac{\partial}{\partial x_n} f\right)$$

So ∇f is a *vector-valued* function, $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$; also written as

$$\nabla f = f_{x_1}(x_1, \ldots, x_n)\boldsymbol{e}_1 + \cdots f_{x_n}(x_1, \ldots, x_n)\boldsymbol{e}_n$$

where f_{x_i} is the partial derivative of f with respect to x_i and $\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n\}$ is the standard basis of $\mathbb{R}^n$

Linearly separable points

Let X_1 and X_2 be two sets of points in $\mathbb{R}^p$

Then X_1 and X_2 are **linearly separable** if there exist $w_1, w_2, .., w_p, k \in \mathbb{R}$ such that

- every point $x \in X_1$ satisfies $\sum_{i=1}^{p} w_i x_i > k$
- every point $x \in X_2$ satisfies $\sum_{i=1}^{p} w_i x_i < k$

where x_i is the ith component of x

Preliminary stuff

Least squares

PCA

Markov chains

Graph theory

Least squares

Least squares problem

Orthogonality and Gram-Schmidt

The QR decomposition

The SVD

The least squares problem

Definition 43 (Least squares solutions)

Consider a collection of points $(x_1, y_1), \dots, (x_n, y_n)$, a matrix $A \in \mathcal{M}_{mn}$, $\boldsymbol{b} \in \mathbb{R}^m$. A **least squares solution** of $A\boldsymbol{x} = \boldsymbol{b}$ is a vector $\tilde{\boldsymbol{x}} \in \mathbb{R}^n$ s.t.

$$\forall \boldsymbol{x} \in \mathbb{R}^n, \quad \|\boldsymbol{b} - A\tilde{\boldsymbol{x}}\| \leq \|\boldsymbol{b} - A\boldsymbol{x}\|$$

Least squares theorem

Theorem 44 (Least squares theorem)

$A \in \mathcal{M}_{mn}$, $\boldsymbol{b} \in \mathbb{R}^m$. Then

1. *$A\boldsymbol{x} = \boldsymbol{b}$ always has at least one least squares solution $\tilde{\boldsymbol{x}}$*
2. *$\tilde{\boldsymbol{x}}$ least squares solution to $A\boldsymbol{x} = \boldsymbol{b} \iff \tilde{\boldsymbol{x}}$ is a solution to the normal equations $A^T A\tilde{\boldsymbol{x}} = A^T\boldsymbol{b}$*
3. *A has linearly independent columns $\iff A^T A$ invertible.*
   In this case, the least squares solution is unique and

$$\tilde{\boldsymbol{x}} = \left(A^T A\right)^{-1} A^T\boldsymbol{b}$$

Fitting an affine function

For a data point $i = 1, \ldots, n$

$$\varepsilon_i = y_i - \tilde{y}_i = y_i - (a + bx_i)$$

So if we write this for all data points,

$$\begin{aligned} \varepsilon_1 &= y_1 - (a + bx_1) \\ &\vdots \\ \varepsilon_n &= y_n - (a + bx_n) \end{aligned}$$

In matrix form

$$\boldsymbol{e} = \boldsymbol{b} - A\boldsymbol{x}$$

with

$$\boldsymbol{e} = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}, A = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \boldsymbol{x} = \begin{pmatrix} a \\ b \end{pmatrix} \text{ and } \boldsymbol{b} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Fitting the quadratic

We have the data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ and want to fit

$$y = a_0 + a_1 x + a_2 x^2$$

At (x_1, y_1),

$$\tilde{y}_1 = a_0 + a_1 x_1 + a_2 x_1^2$$

$\vdots$

At (x_n, y_n),

$$\tilde{y}_n = a_0 + a_1 x_n + a_2 x_n^2$$

In terms of the error

$$
\begin{aligned}
\varepsilon_1 &= y_1 - \tilde{y}_1 = y_1 - (a_0 + a_1 x_1 + a_2 x_1^2) \\
&\vdots \\
\varepsilon_n &= y_n - \tilde{y}_n = y_n - (a_0 + a_1 x_n + a_2 x_n^2)
\end{aligned}
$$

i.e.,

$$\boldsymbol{e} = \boldsymbol{b} - A\boldsymbol{x}$$

where

$$\boldsymbol{e} = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}, A = \begin{pmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix}, \boldsymbol{x} = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} \text{ and } \boldsymbol{b} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Theorem 44 applies, with here $A \in \mathcal{M}_{n3}$ and $\boldsymbol{b} \in \mathbb{R}^n$

Least squares

Least squares problem

Orthogonality and Gram-Schmidt

The QR decomposition

The SVD

Definition 45 (Orthogonal set of vectors)

The set of vectors $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\} \in \mathbb{R}^n$ is an **orthogonal set** if

$$\forall i, j = 1, \ldots, k, \quad i \neq j \implies \boldsymbol{v}_i \bullet \boldsymbol{v}_j = 0$$

Definition 46 (Orthogonal basis)

Let S be a basis of the subspace $W \subset \mathbb{R}^n$ composed of an orthogonal set of vectors. We say S is an **orthogonal basis** of W

Orthonormal version of things

Definition 47 (Orthonormal set)

The set of vectors $\{\mathbf{v}_1, \dots, \mathbf{v}_k\} \in \mathbb{R}^n$ is an **orthonormal set** if it is an orthogonal set and furthermore

$$\forall i = 1, \dots, k, \quad \|\mathbf{v}_i\| = 1$$

Definition 48 (Orthonormal basis)

A basis of the subspace $W \subset \mathbb{R}^n$ is an **orthonormal basis** if the vectors composing it are an orthonormal set

$\{\mathbf{v}_1, \dots, \mathbf{v}_k\} \in \mathbb{R}^n$ is orthonormal if

$$\mathbf{v}_i \bullet \mathbf{v}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

Projections

Definition 49 (Orthogonal projection onto a subspace)

$W \subset \mathbb{R}^n$ a subspace and $\{\boldsymbol{u}_1, \dots, \boldsymbol{u}_k\}$ an orthogonal basis of W. $\forall \boldsymbol{v} \in \mathbb{R}^n$, the ***orthogonal projection*** *of* $\boldsymbol{v}$ ***onto*** *W is*

$$\mathrm{proj}_W(\boldsymbol{v}) = \frac{\boldsymbol{u}_1 \bullet \boldsymbol{v}}{\|\boldsymbol{u}_1\|^2}\boldsymbol{u}_1 + \cdots + \frac{\boldsymbol{u}_k \bullet \boldsymbol{v}}{\|\boldsymbol{u}_k\|^2}\boldsymbol{u}_k$$

Definition 50 (Component orthogonal to a subspace)

$W \subset \mathbb{R}^n$ a subspace and $\{\boldsymbol{u}_1, \dots, \boldsymbol{u}_k\}$ an orthogonal basis of W. $\forall \boldsymbol{v} \in \mathbb{R}^n$, the ***component*** *of* $\boldsymbol{v}$ ***orthogonal to*** *W is*

$$\mathrm{perp}_W(\boldsymbol{v}) = \boldsymbol{v} - \mathrm{proj}_W(\boldsymbol{v})$$

Gram-Schmidt process

Theorem 51

$W \subset \mathbb{R}^n$ a subset and $\{\boldsymbol{x}_1, \dots, \boldsymbol{x}_k\}$ a basis of W. Let

$$
\begin{aligned}
\boldsymbol{v}_1 &= \boldsymbol{x}_1 \\
\boldsymbol{v}_2 &= \boldsymbol{x}_2 - \frac{\boldsymbol{v}_1 \bullet \boldsymbol{x}_2}{\|\boldsymbol{v}_1\|^2}\boldsymbol{v}_1 \\
\boldsymbol{v}_3 &= \boldsymbol{x}_3 - \frac{\boldsymbol{v}_1 \bullet \boldsymbol{x}_3}{\|\boldsymbol{v}_1\|^2}\boldsymbol{v}_1 - \frac{\boldsymbol{v}_2 \bullet \boldsymbol{x}_3}{\|\boldsymbol{v}_2\|^2}\boldsymbol{v}_2 \\
&\vdots \\
\boldsymbol{v}_k &= \boldsymbol{x}_k - \frac{\boldsymbol{v}_1 \bullet \boldsymbol{x}_k}{\|\boldsymbol{v}_1\|^2}\boldsymbol{v}_1 - \cdots - \frac{\boldsymbol{v}_{k-1} \bullet \boldsymbol{x}_k}{\|\boldsymbol{v}_{k-1}\|^2}\boldsymbol{v}_{k-1}
\end{aligned}
$$

and

$$W_1 = \mathrm{span}(\boldsymbol{x}_1), W_2 = \mathrm{span}(\boldsymbol{x}_1, \boldsymbol{x}_2), \dots, W_k = \mathrm{span}(\boldsymbol{x}_1, \dots, \boldsymbol{x}_k)$$

Then $\forall i = 1, \dots, k$, $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_i\}$ orthogonal basis for W_i

Least squares

Definition 52 (Orthogonal matrix)

$Q \in \mathcal{M}_n$ is an **orthogonal matrix** if its columns form an orthonormal set

So $Q \in \mathcal{M}_n$ orthogonal if $Q^T Q = \mathbb{I}$, i.e., $Q^T = Q^{-1}$

Theorem 53 (NSC for orthogonality)

$Q \in \mathcal{M}_n$ orthogonal $\iff Q^{-1} = Q^T$

Theorem 54 (Orthogonal matrices “encode" isometries)

Let $Q \in \mathcal{M}_n$. TFAE

1. *Q orthogonal*
2. $\forall \boldsymbol{x} \in \mathbb{R}^n$, $\|Q\boldsymbol{x}\| = \|\boldsymbol{x}\|$
3. $\forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$, $Q\boldsymbol{x} \bullet Q\boldsymbol{y} = \boldsymbol{x} \bullet \boldsymbol{y}$

Theorem 55

Let $Q \in \mathcal{M}_n$ be orthogonal. Then

1. *The rows of Q form an orthonormal set*
2. *Q^{-1} orthogonal*
3. $\det Q = \pm 1$
4. $\forall \lambda \in \sigma(Q)$, $|\lambda| = 1$
5. *If $Q_2 \in \mathcal{M}_n$ also orthogonal, then QQ_2 orthogonal*

The QR factorisation

Theorem 56

Let $A \in \mathcal{M}_{mn}$ with LI columns. Then A can be factored as

$$A = QR$$

where $Q \in \mathcal{M}_{mn}$ has orthonormal columns and $R \in \mathcal{M}_n$ is nonsingular upper triangular

Theorem 57 (Least squares with QR factorisation)

$A \in \mathcal{M}_{mn}$ with LI columns, $\boldsymbol{b} \in \mathbb{R}^m$. If $A = QR$ is a QR factorisation of A, then the unique least squares solution $\tilde{\boldsymbol{x}}$ of $A\boldsymbol{x} = \boldsymbol{b}$ is

$$\tilde{\boldsymbol{x}} = R^{-1}Q^T\boldsymbol{b}$$

Least squares

Least squares problem
Orthogonality and Gram-Schmidt
The QR decomposition
The SVD

Singular values

Definition 58 (Singular value)

Let $A \in \mathcal{M}_{mn}(\mathbb{R})$. The **singular values** of A are the real numbers

$$\sigma_1 \geq \sigma_2 \geq \cdots \sigma_n \geq 0$$

that are the square roots of the eigenvalues of $A^T A$

Singular values are real and nonnegative?

Recall that $\forall A \in \mathcal{M}_{mn}$, $A^T A$ is symmetric

Claim 1. Real symmetric matrices have real eigenvalues

Claim 2. For $A \in \mathcal{M}_{mn}(\mathbb{R})$, the eigenvalues of $A^T A$ are real and nonnegative

Claim 3. For $A \in \mathcal{M}_{mn}(\mathbb{R})$, the nonzero eigenvalues of $A^T A$ and AA^T are the same

Claim 2. For $A \in \mathcal{M}_{mn}(\mathbb{R})$, the eigenvalues of $A^T A$ are real and nonnegative

Proof. We know that for $A \in \mathcal{M}_{mn}$, $A^T A$ symmetric and from previous claim, if $A \in \mathcal{M}_{mn}(\mathbb{R})$, then $A^T A$ is symmetric and real and with real eigenvalues

Let $(\lambda, \boldsymbol{v})$ be an eigenpair of $A^T A$, with $\boldsymbol{v}$ chosen so that $\|\boldsymbol{v}\| = 1$

Norms are functions $V \to \mathbb{R}_+$, so $\|A\boldsymbol{v}\|$ and $\|A\boldsymbol{v}\|^2$ are ≥ 0 and thus

$$\begin{aligned} 0 \leq \|A\boldsymbol{v}\|^2 &= (A\boldsymbol{v}) \bullet (A\boldsymbol{v}) = (A\boldsymbol{v})^T(A\boldsymbol{v}) \\ &= \boldsymbol{v}^T A^T A\boldsymbol{v} = \boldsymbol{v}^T(A^T A\boldsymbol{v}) = \boldsymbol{v}^T(\lambda\boldsymbol{v}) \\ &= \lambda(\boldsymbol{v}^T\boldsymbol{v}) = \lambda(\boldsymbol{v} \bullet \boldsymbol{v}) = \lambda\|\boldsymbol{v}\|^2 \\ &= \lambda \end{aligned}$$

The singular value decomposition (SVD)

Theorem 59 (SVD)

$A \in \mathcal{M}_{mn}$ with singular values $\sigma_1 \geq \cdots \geq \sigma_r > 0$ and $\sigma_{r+1} = \cdots = \sigma_n = 0$

Then there exists $U \in \mathcal{M}_m$ orthogonal, $V \in \mathcal{M}_n$ orthogonal and a block matrix $\Sigma \in \mathcal{M}_{mn}$ taking the form

$$\Sigma = \begin{pmatrix} D & 0_{r,n-r} \\ 0_{m-r,r} & 0_{m-r,n-r} \end{pmatrix}$$

where

$$D = \mathrm{diag}(\sigma_1, \ldots, \sigma_r) \in \mathcal{M}_r$$

such that

$$A = U \Sigma V^T$$

Definition 60

We call a factorisation as in Theorem 59 the **singular value decomposition** of A. The columns of U and V are, respectively, the **left** and **right singular vectors** of A

U and V^T are *rotation* or *reflection* matrices, Σ is a *scaling* matrix

$U \in \mathcal{M}_m$ orthogonal matrix with columns the eigenvectors of AA^T

$V \in \mathcal{M}_n$ orthogonal matrix with columns the eigenvectors of $A^T A$

Outer product form of the SVD

Theorem 61 (Outer product form of the SVD)

$A \in \mathcal{M}_{mn}$ with singular values $\sigma_1 \geq \cdots \geq \sigma_r > 0$ and $\sigma_{r+1} = \cdots = \sigma_n = 0$, $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_r$ and $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_r$, respectively, left and right singular vectors of A corresponding to these singular values

Then

$$A = \sigma_1 \boldsymbol{u}_1 \boldsymbol{v}_1^T + \cdots + \sigma_r \boldsymbol{u}_r \boldsymbol{v}_r^T \tag{2}$$

Computing the SVD (case of $\neq$ eigenvalues)

To compute the SVD, we use the following result

Theorem 62

Let $A \in \mathcal{M}_n$ symmetric, $(\lambda_1, \boldsymbol{u}_1)$ and $(\lambda_2, \boldsymbol{u}_2)$ be eigenpairs, $\lambda_1 \neq \lambda_2$. Then $\boldsymbol{u}_1 \bullet \boldsymbol{u}_2 = 0$

Proof of Theorem 62

$A \in \mathcal{M}_n$ symmetric, $(\lambda_1, \boldsymbol{u}_1)$ and $(\lambda_2, \boldsymbol{u}_2)$ eigenpairs with $\lambda_1 \neq \lambda_2$

$$\begin{aligned}
\lambda_1(\boldsymbol{v}_1 \bullet \boldsymbol{v}_2) &= (\lambda_1 \boldsymbol{v}_1) \bullet \boldsymbol{v}_2 \\
&= A\boldsymbol{v}_1 \bullet \boldsymbol{v}_2 \\
&= (A\boldsymbol{v}_1)^T \boldsymbol{v}_2 \\
&= \boldsymbol{v}_1^T A^T \boldsymbol{v}_2 \\
&= \boldsymbol{v}_1^T (A\boldsymbol{v}_2) \qquad [A \text{ symmetric so } A^T = A] \\
&= \boldsymbol{v}_1^T (\lambda_2 \boldsymbol{v}_2) \\
&= \lambda_2(\boldsymbol{v}_1^T \boldsymbol{v}_2) \\
&= \lambda_2(\boldsymbol{v}_1 \bullet \boldsymbol{v}_2)
\end{aligned}$$

So $(\lambda_1 - \lambda_2)(\boldsymbol{v}_1 \bullet \boldsymbol{v}_2) = 0$. But $\lambda_1 \neq \lambda_2$, so $\boldsymbol{v}_1 \bullet \boldsymbol{v}_2 = 0$ $\square$

Pseudoinverse of a matrix

Definition 63 (Pseudoinverse)

$A = U\Sigma V^T$ an SVD for $A \in \mathcal{M}_{mn}$, where

$$\Sigma = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix}, \text{ with } D = \text{diag}(\sigma_1, \ldots, \sigma_r)$$

(D contains the nonzero singular values of A ordered as usual)

The **pseudoinverse** (or **Moore-Penrose inverse**) of A is $A^+ \in \mathcal{M}_{nm}$ given by

$$A^+ = V\Sigma^+ U^T$$

with

$$\Sigma^+ = \begin{pmatrix} D^{-1} & 0 \\ 0 & 0 \end{pmatrix} \in \mathcal{M}_{nm}$$

Least squares revisited

Theorem 64

Let $A \in \mathcal{M}_{mn}$, $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{b} \in \mathbb{R}^m$. The least squares problem $A\boldsymbol{x} = \boldsymbol{b}$ has a unique least squares solution $\tilde{\boldsymbol{x}}$ of minimal length (closest to the origin) given by

$$\tilde{\boldsymbol{x}} = A^+\boldsymbol{b}$$

where A^+ is the pseudoinverse of A

Preliminary stuff

Least squares

PCA

Markov chains

Graph theory

Change of basis

Definition 65 (Change of basis matrix)

$\mathcal{B} = \{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n\}$ and $\mathcal{C} = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n\}$ bases of vector space V
The **change of basis matrix** $P_{\mathcal{C} \leftarrow \mathcal{B}} \in \mathcal{M}_n$,

$$P_{\mathcal{C} \leftarrow \mathcal{B}} = [[\boldsymbol{u}_1]_{\mathcal{C}} \cdots [\boldsymbol{u}_n]_{\mathcal{C}}]$$

has columns the coordinate vectors $[\boldsymbol{u}_1]_{\mathcal{C}}, \ldots, [\boldsymbol{u}_n]_{\mathcal{C}}$ of vectors in $\mathcal{B}$ with respect to $\mathcal{C}$

Theorem 66

$\mathcal{B} = \{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n\}$ and $\mathcal{C} = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n\}$ bases of vector space V and $P_{\mathcal{C} \leftarrow \mathcal{B}}$ a change of basis matrix from $\mathcal{B}$ to $\mathcal{C}$

1. $\forall \boldsymbol{x} \in V$, $P_{\mathcal{C} \leftarrow \mathcal{B}}[\boldsymbol{x}]_{\mathcal{B}} = [\boldsymbol{x}]_{\mathcal{C}}$
2. $P_{\mathcal{C} \leftarrow \mathcal{B}}$ *s.t.* $\forall \boldsymbol{x} \in V$, $P_{\mathcal{C} \leftarrow \mathcal{B}}[\boldsymbol{x}]_{\mathcal{B}} = [\boldsymbol{x}]_{\mathcal{C}}$ *is* ***unique***
3. $P_{\mathcal{C} \leftarrow \mathcal{B}}$ *invertible and* $P_{\mathcal{C} \leftarrow \mathcal{B}}^{-1} = P_{\mathcal{B} \leftarrow \mathcal{C}}$

Row-reduction method for changing bases

Theorem 67

$\mathcal{B} = \{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n\}$ and $\mathcal{C} = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n\}$ bases of vector space V. Let $\mathcal{E}$ be any basis for V,

$$B = [[\boldsymbol{u}_1]_{\mathcal{E}}, \ldots, [\boldsymbol{u}_n]_{\mathcal{E}}] \text{ and } C = [[\boldsymbol{v}_1]_{\mathcal{E}}, \ldots, [\boldsymbol{v}_n]_{\mathcal{E}}]$$

and let $[C|B]$ be the augmented matrix constructed using C and B. Then

$$RREF\left([C|B]\right) = [\mathbb{I}|P_{\mathcal{C}\leftarrow\mathcal{B}}]$$

If working in $\mathbb{R}^n$, this is quite useful with $\mathcal{E}$ the standard basis of $\mathbb{R}^n$ (it does not matter if $\mathcal{B} = \mathcal{E}$)

Definition 68 (Variance)

Let X be a random variable. The **variance** of X is given by

$$\operatorname{Var} X = E\left[(X - E(X))^2\right]$$

where E is the expected value

Definition 69 (Covariance)

Let X, Y be jointly distributed random variables. The **covariance** of X and Y is given by

$$\operatorname{cov}(X, Y) = E\left[(X - E(X))\,(Y - E(Y))\right]$$

Note that $\operatorname{cov}(X, X) = E\left[(X - E(X))^2\right] = \operatorname{Var} X$

Definition 70 (Unbiased estimators of the mean and variance)

Let $x_1, \ldots, x_n$ be data points (the *sample*) and

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

be the **mean** of the data. An unbiased estimator of the variance of the sample is

$$\sigma^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

Definition 71 (Unbiased estimator of the covariance)

Let $(x_1, y_1), \ldots, (x_n, y_n)$ be data points,

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \text{ and } \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

be the means of the data. An estimator of the covariance of the sample is

$$\operatorname{cov}(x, y) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

The covariance matrix (we usually have more than 2 variables)

Definition 72

Suppose p random variables $X_1, \dots, X_p$. Then the covariance matrix is the symmetric matrix

$$\begin{pmatrix} \operatorname{Var} X_1 & \operatorname{cov}(X_1, X_2) & \cdots & \operatorname{cov}(X_1, X_p) \\ \operatorname{cov}(X_1, X_2) & \operatorname{Var} X_2 & \cdots & \operatorname{cov}(X_2, X_p) \\ \vdots & \vdots & & \vdots \\ \operatorname{cov}(X_1, X_p) & \operatorname{cov}(X_2, X_p) & \cdots & \operatorname{Var} X_p \end{pmatrix}$$

Picking the right eigenvalue

$(\lambda, \boldsymbol{\alpha}_1)$ eigenpair of Σ, with $\boldsymbol{\alpha}_1$ having unit length

But which λ to choose?

Recall that we want Var $\boldsymbol{\alpha}_1^T \boldsymbol{x} = \boldsymbol{\alpha}_1^T \Sigma \boldsymbol{\alpha}_1$ maximal

We have

$$\text{Var } \boldsymbol{\alpha}_1^T \boldsymbol{x} = \boldsymbol{\alpha}_1^T \Sigma \boldsymbol{\alpha}_1 = \boldsymbol{\alpha}_1^T (\Sigma \boldsymbol{\alpha}_1) = \boldsymbol{\alpha}_1^T (\lambda \boldsymbol{\alpha}_1) = \lambda (\boldsymbol{\alpha}_1^T \boldsymbol{\alpha}_1) = \lambda$$

$\Longrightarrow$ we pick $\lambda = \lambda_1$, the largest eigenvalue (covariance matrix symmetric so eigenvalues real)

What we have this far..

The first principal component is $\alpha_1^T \boldsymbol{x}$ and has variance λ_1, where λ_1 the largest eigenvalue of Σ and α_1 an associated eigenvector with $\|\alpha_1\| = 1$

We want the second principal component to be *uncorrelated* with $\alpha_1^T \boldsymbol{x}$ and to have maximum variance Var $\alpha_2^T \boldsymbol{x} = \alpha_2^T \Sigma \alpha_2$, under the constraint that $\|\alpha_2\| = 1$

$\alpha_2^T \boldsymbol{x}$ uncorrelated to $\alpha_1^T \boldsymbol{x}$ if $\mathrm{cov}(\alpha_1^T \boldsymbol{x}, \alpha_2^T \boldsymbol{x}) = 0$

We have

$$\begin{aligned}
\text{cov}(\boldsymbol{\alpha}_1^T \boldsymbol{x}, \boldsymbol{\alpha}_2^T \boldsymbol{x}) &= \boldsymbol{\alpha}_1^T \Sigma \boldsymbol{\alpha}_2 \\
&= \boldsymbol{\alpha}_2^T \Sigma^T \boldsymbol{\alpha}_1 \\
&= \boldsymbol{\alpha}_2^T \Sigma \boldsymbol{\alpha}_1 \quad [\Sigma \text{ symmetric}] \\
&= \boldsymbol{\alpha}_2^T (\lambda_1 \boldsymbol{\alpha}_1) \\
&= \lambda \boldsymbol{\alpha}_2^T \boldsymbol{\alpha}_1
\end{aligned}$$

So $\boldsymbol{\alpha}_2^T \boldsymbol{x}$ uncorrelated to $\boldsymbol{\alpha}_1^T \boldsymbol{x}$ if $\boldsymbol{\alpha}_1 \perp \boldsymbol{\alpha}_2$

This is beginning to sound a lot like Gram-Schmidt, no?

In short

Take whatever covariance matrix is available to you (known Σ or sample S_X) – assume sample from now on for simplicity

For $i = 1, \ldots, p$, the ith principal component is

$$z_i = \boldsymbol{v}_i^T \boldsymbol{x}$$

where $\boldsymbol{v}_i$ eigenvector of S_X associated to the ith largest eigenvalue λ_i

If $\boldsymbol{v}_i$ is normalised, then $\lambda_i = \text{Var } z_k$

Covariance matrix

Σ the covariance matrix of the random variable, S_X the sample covariance matrix

$X \in \mathcal{M}_{mp}$ the data, then the (sample) covariance matrix S_X takes the form

$$S_X = \frac{1}{n-1} X^T X$$

where the data is centred!

Sometimes you will see $S_X = 1/(n-1)XX^T$. This is for matrices with observations in columns and variables in rows. Just remember that you want the covariance matrix to have size the number of variables, not observations, this will give you the order in which to take the product

Preliminary stuff

Least squares

PCA

Markov chains

Graph theory

Definition 73 (Markov chain)

An experiment with finite number of possible outcomes $S_1, \ldots, S_n$ is repeated. The sequence of outcomes is a **Markov chain** if there is a set of n^2 numbers $\{p_{ij}\}$ such that the conditional probability of outcome S_i on any experiment given outcome S_j on the previous experiment is p_{ij}, i.e., for $1 \leq i, j \leq n$, $t = 1, \ldots$,

$$p_{ij} = \mathbb{P}(S_i \text{ on experiment } t+1 \mid S_j \text{ on experiment } t)$$

Outcomes $S_1, \ldots, S_n$ are **states** and p_{ij} are **transition probabilities**. $P = [p_{ij}]$ the **transition matrix**

In the following, we often write

$$\mathbb{P}(S_i \text{ on experiment } t+1 \mid S_j \text{ on experiment } t) \text{ as } \mathbb{P}(S_i(t+1) \mid S_j(t))$$

The matrix

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1r} \\ p_{21} & p_{22} & \cdots & p_{2r} \\ \\ p_{r1} & p_{r2} & \cdots & p_{rr} \end{pmatrix}$$

has

- entries that are probabilities, i.e., $0 \leq p_{ij} \leq 1$
- column sum 1, which we write

$$\sum_{i=1}^{n} p_{ij} = 1, \quad j = 1, \ldots, n$$

  or, using the notation $\mathbb{1}^T = (1, \ldots, 1)$,

$$\mathbb{1}^T P = \mathbb{1}^T$$

In matrix form

$$p(t+1) = Pp(t), \quad n = 1, 2, 3, \ldots$$

where $p(t) = (p_1(t), p_2(t), \ldots, p_n(t))^T$ is a probability vector and $P = (p_{ij})$ is an $n \times n$ *transition matrix*,

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1r} \\ p_{21} & p_{22} & \cdots & p_{2r} \\ & & & \\ p_{r1} & p_{r2} & \cdots & p_{rr} \end{pmatrix}$$

Stochastic matrices

Definition 74 (Stochastic matrix)

The nonnegative $n \times n$ matrix M is **row-stochastic** (resp. **column-stochastic**) if $\sum_{j=1}^{n} a_{ij} = 1$ for all $i = 1, \ldots, n$ (resp. $\sum_{i=1}^{n} a_{ij} = 1$ for all $j = 1, \ldots, n$)

We often say **stochastic** and let the context determine whether we mean row- or column-stochastic

If it is both row- and column-stochastic, the matrix is **doubly stochastic**

Theorem 75

Let $M \in \mathcal{M}_n$ be a stochastic matrix. Then all eigenvalues λ of M are such that $|\lambda| \leq 1$.

Theorem 76

Let $M \in \mathcal{M}_n$ be a stochastic matrix. $\lambda = 1$ is an eigenvalue of M. If M is row-stochastic, the eigenvalue 1 is associated to the column vector of ones (a right eigenvector of M); if M is column-stochastic, the eigenvalue 1 is associated to the row vector of ones (a left eigenvector of M)

Proof of Theorem 76

Suppose $M \in \mathcal{M}_n$ is row-stochastic. One way to write the requirement that each row sum equals 1 is as

$$M\mathbf{1} = \mathbf{1} \tag{3}$$

where $\mathbf{1} = (1, \ldots, 1) \in \mathbb{C}^n$ is a column vector

If $M \in \mathcal{M}_n$, then the eigenpair equation takes the form

$$M\boldsymbol{v} = \lambda\boldsymbol{v}, \quad \boldsymbol{v} \neq \mathbf{0}$$

So, in (3), $\boldsymbol{v} = \mathbf{1}$ and $\lambda = 1$

This works the same way for a column-stochastic matrix, except that here the relation is $\mathbf{1}M = \mathbf{1}$ with $\mathbf{1}$ a row vector and the (left)eigenpair relation is $\boldsymbol{v}^T M = \lambda\boldsymbol{v}^T$ with $\boldsymbol{v}^T$ a row vector

Long time behaviour

Let $p(0)$ be the initial distribution vector. Then

$$\begin{aligned} p(1) &= Pp(0) \\ p(2) &= Pp(1) \\ &= P\left(Pp(0)\right) \\ &= P^2 p(0) \end{aligned}$$

Continuing, we get, for any t,

$$p(t) = P^t p(0)$$

Therefore,

$$\lim_{t \to +\infty} p(t) = \lim_{t \to +\infty} P^t p(0) = \left(\lim_{t \to +\infty} P^t\right) p(0)$$

if this limit exists

The matrix P^t

Theorem 77

If M, N are nonsingular stochastic matrices, then MN is a stochastic matrix

Corollary 78

If M is a nonsingular stochastic matrix, then for any $k \in \mathbb{N}$, M^k is a stochastic matrix

So P^t is stochastic

Regular Markov chains

Definition 79 (Regular Markov chain)

A **regular** Markov chain has P^k (entry-wise) positive for some integer $k > 0$, i.e., P^k has only positive entries

Definition 80 (Primitive matrix)

A nonnegative matrix M is **primitive** if, and only if, there is an integer $k > 0$ such that M^k is positive.

Theorem 81

Markov chain regular $\iff$ *transition matrix* P *primitive*

What is a directed graph?

Definition 82 (Digraph)

A **directed graph** (or **digraph**) G is a pair (V, A) where:

- V is a finite set of elements called **vertices** or **nodes**
- $A \subseteq V \times V$ is a set of ordered pairs of vertices called **arcs** or **directed edges**

Definition 83 (Arc)

An **arc** $a = (u, v) \in A$ represents a connection **from** vertex u **to** vertex v

- u is the **tail** of the arc
- v is the **head** of the arc

Definition 84 (Reducible/irrecible matrix)

A matrix $M \in \mathcal{M}_n$ is **reducible** if there exists a permutation matrix P such that

$$P^T MP = \begin{pmatrix} P & Q \\ \mathbf{0} & R \end{pmatrix},$$

i.e., M is similar to a block upper triangular matrix. The matrix M is **irreducible** if no such matrix exists

Definition 85 (Strongly connected digraph)

A digraph $\mathcal{G} = (V, A)$ is **strongly connected** if for any pair of vertices $u, v \in V$, there is a directed path from u to v

Theorem 86

$P \in \mathcal{M}_n$ *irreducible* $\iff$ $\mathcal{G}(P)$ *strongly connected*

A sufficient condition for primitivity

Theorem 87

Let $M \in \mathcal{M}_n$ be a nonnegative matrix. If $\mathcal{G}(M)$ is strongly connected and at least one of the diagonal entries m_{ii} of M is positive, then M is primitive

Behaviour of a regular MC

Theorem 88

If P is the transition matrix of a regular Markov chain, then

1. *the powers P^t approach a stochastic matrix W*
2. *each column of W is the same (column) vector $w = (w_1, \ldots, w_n)^T$*
3. *the components of w are positive*

So if the Markov chain is regular

$$\lim_{t \to +\infty} p(t) = \lim_{t \to +\infty} P^t p(0) = Wp(0)$$

Computing W

Recall that since P is a stochastic matrix, 1 is an eigenvalue of P. As P is column stochastic, 1 is associated to the left (row) eigenvector $\mathbb{1}$

Now, if $\boldsymbol{p}(t)$ converges, then $\boldsymbol{p}(t+1) = P\boldsymbol{p}(t)$ at the limit, so $\boldsymbol{w} = \lim_{t\to\infty} \boldsymbol{p}(t)$ is a **fixed point** of the system. Replacing $\boldsymbol{p}$ with its limit, we have

$$\boldsymbol{w} = P\boldsymbol{w}$$

Solving for $\boldsymbol{w}$ thus amounts to finding $\boldsymbol{w}$ as a (right) eigenvector corresponding to the eigenvalue 1

Remember to normalise

$\boldsymbol{w}$ might have to be normalized since you want a probability vector

Check that the norm $\|\boldsymbol{w}\|_1$ defined by

$$\|\boldsymbol{w}\|_1 = |w_1| + \cdots + |w_n| = w_1 + \cdots + w_n$$

(since $\boldsymbol{w} \geq \mathbf{0}$) is equal to one

If not, use

$$\tilde{\boldsymbol{w}} = \frac{\boldsymbol{w}}{\|\boldsymbol{w}\|_1}$$

Absorbing Markov chains

Definition 89 (Absorbing state)

A state S_i in a Markov chain is **absorbing** if whenever it occurs on the t^{th} generation of the experiment, it then occurs on every subsequent step. In other words, S_i is absorbing if $p_{ii} = 1$ and $p_{ij} = 0$ for $i \neq j$

Definition 90 (Absorbing chain)

A Markov chain is **absorbing** if it has at least one absorbing state, and if from every state it is possible to go to an absorbing state. In an absorbing Markov chain, a state that is not absorbing is called **transient**

Questions about absorbing chains

1. Does the process eventually reach an absorbing state?
2. What is the average number of steps spent in a transient state, if starting in a transient state?
3. What is the average number of steps before entering an absorbing state?
4. What is the probability of being absorbed by a given absorbing state, when there are more than one, when starting in a given transient state?

The answer to the first question ("Does the process eventually reach an absorbing state?") is given by the following result

Theorem 91

In an absorbing Markov chain, the probability of reaching an absorbing state is 1

To answer the other questions, write the transition matrix in **standard** form

For an absorbing chain with k absorbing states and $r-k$ transient states, write transition matrix as

$$P = \begin{pmatrix} \mathbb{I}_k & R \\ \mathbf{0} & Q \end{pmatrix}$$

with following meaning

	Absorbing states	Transient states
Absorbing states	$\mathbb{I}_k$	R
Transient states	$\mathbf{0}$	Q

with $\mathbb{I}_k$ the $k \times k$ identity matrix, $\mathbf{0}$ an $(r-k) \times k$ matrix of zeros, R an $k \times (r-k)$ matrix and Q an $(r-k) \times (r-k)$ matrix. The matrix $\mathbb{I}_{r-k} - Q$ is invertible. Let

- $N = (\mathbb{I}_{r-k} - Q)^{-1}$ the **fundamental matrix** of the MC
- T_i sum of the entries on column i of N
- $B = RN$

Answers to our remaining questions:

2. N_{ij} average number of times the process is in the ith transient state if it starts in the jth transient state

3. T_i average number of steps before the process enters an absorbing state if it starts in the ith transient state

4. B_{ij} probability of eventually entering the ith absorbing state if the process starts in the jth transient state

Preliminary stuff

Least squares

PCA

Markov chains

Graph theory

Binary relation

Definition 92 (Binary relation)

- A **binary relation** is an arbitrary association of elements of one set with elements of another (maybe the same) set
- A binary relation over the sets X and Y is defined as a subset of the Cartesian product $X \times Y = \{(x, y) | x \in X, y \in Y\}$
- $(x, y) \in R$ is read "x is R-related to y" and is denoted xRy
- If $(x, y) \notin R$, we write "not xRy" or $x \not R y$

Definition 93 (Properties of binary relations)

A binary relation R over a set X is

- **Reflexive** if $\forall x \in X$, xRx
- **Irreflexive** if there does not exist $x \in X$ such that xRx
- **Symmetric** if $xRy \Rightarrow yRx$
- **Asymmetric** if $xRy \Rightarrow y \not R x$
- **Antisymmetric** if xRy and $yRx \Rightarrow x = y$
- **Transitive** if xRy and $yRz \Rightarrow xRz$
- **Total** (or **complete**) if $\forall x, y \in X$, xRy or yRx

Definition 94 (Equivalence relation)

A relation that is reflexive ($\forall x \in X$, xRx), symmetric ($xRy \Rightarrow yRx$) and transitive (xRy and $yRz \Rightarrow xRz$) is an **equivalence relation**

Definition 95 (Partial order)

A relation that is reflexive ($\forall x \in X$, xRx), antisymmetric (xRy and $yRx \Rightarrow x = y$) and transitive (xRy and $yRz \Rightarrow xRz$) is a ***partial order***

Definition 96 (Total order)

A partial order that is total ($\forall x, y \in X$, xRy or yRx) is a ***total order***

Graph, vertex and edge

Definition 97 (Graph)

An **undirected graph** is a pair $G = (V, E)$ of sets such that

- V is a set of points: $V = \{v_1, \dots, v_p\}$
- E is a set of 2-element subsets of V: $E = \{\{v_i, v_j\}, \{v_i, v_k\}, \dots, \{v_n, v_p\}\}$ or $E = \{v_i v_j, v_i v_k, \dots, v_n v_p\}$

Definition 98 (Vertex)

The elements of V are the **vertices** (or nodes, or points) of the graph G. V (or $V(G)$) is the vertex set of the graph G

Definition 99 (Edge)

The elements of E are the **edges** (or lines) of the graph G. E (or $E(G)$) is the edge set of the graph G

Order and Size

Definition 100 (Order of a graph)

The number of vertices in G is the **order** of G. Using the notation $|V(G)|$ for the *cardinality* of $V(G)$,

$$|V(G)| = \text{order of G}$$

Definition 101 (Size of a graph)

The number of edges in G is the **size** of G,

$$|E(G)| = \text{size of G}$$

- A graph having order p and size q is called a $(p, q)-$graph
- A graph is finite if $|V(G)| < \infty$

Incident – Adjacent

Definition 102 (Incident)

- A vertex v is **incident** with an edge e if $v \in e$; then e is an edge at v
- If $e = uv \in E(G)$, then u and v are each incident with e
- The two vertices incident with an edge are its ends
- An edge $e = uv$ is incident with both vertices u and v

Definition 103 (Adjacent)

- Two vertices u and v are **adjacent** in a graph G if $uv \in E(G)$
- If uv and uw are distinct edges (i.e. $v \neq w$) of a graph G, then uv and uw are adjacent edges

Definition 104 (Multiple edge)

Multiple edges are two or more edges connecting the same two vertices within a multigraph

Definition 105 (Loop)

A **loop** is an edge with both the same ends; *e.g.* $\{u, u\}$ is a loop

Definition 106 (Simple graph)

A **simple graph** is a graph which contains no loops or multiple edges

Definition 107 (Multigraph)

A **multigraph** is a graph which can contain multiple edges or loops

Definition 108 (Degree of a vertex)

Let v be a vertex of $G = (V, E)$.

- The number of edges of G incident with v is the **degree** of v in G
- The degree of v in G is noted $d_G(v)$ or $deg_G(v)$

Theorem 109

Let G be a $(p, q)-$graph with vertices $v_1, \ldots, v_p$, then

$$\sum_{i=1}^{p} d_G(v_i) = 2q$$

Definition 110 (Odd vertex)

A vertex is an **odd vertex** if its degree is odd

Theorem 111

Every graph contains an even number of odd vertices

Isomorphic graphs

Definition 112 (Isomorphic graphs)

*Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$ be two graphs. G_1 and G_2 are **isomorphic** if there exists an isomorphism ϕ from G_1 to G_2, that is defined as an injective mapping $\phi : V(G_1) \rightarrow V(G_2)$ such that two vertices u_1 and v_1 are adjacent in $G_1 \iff$ the vertices $\phi(u_1)$ and $\phi(v_1)$ are adjacent in G_2*

If ϕ is an isomorphism from G_1 to G_2, then the inverse mapping ϕ^{-1} from $V(G_2)$ to $V(G_1)$ also satisfies the definition of an isomorphism. As a consequence, if G_1 and G_2 are isomorphic graphs, then

- G_1 is isomorphic to G_2
- G_2 is isomorphic to G_1

Theorem 113

The relation "is isomorphic to" is an equivalence relation on the set of all graphs

Theorem 114

If G_1 and G_2 are isomorphic graphs, then the degrees of vertices of G_1 are exactly the degrees of vertices of G_2

Subgraph

Definition 115 (Subgraph)

Let $G = (V, E)$ be a graph. A graph $H = (V(H), E(H))$ is a **subgraph** of G if $V(H) \subseteq V$ and $E(H) \subseteq E$

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs

Definition 116 (Union of G_1 and G_2)

$G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$

Definition 117 (Intersection of G_1 and G_2)

$G_1 \cap G_2 = (V_1 \cap V_2, E_1 \cap E_2)$

Definition 118 (Disjoint graphs)

If $G_1 \cap G_2 = (\emptyset, \emptyset) = \emptyset$ (empty graph) then G_1 and G_2 are **disjoint**

Definition 119 (Complement of G_1)

The **complement** $\bar{G}_1$ of G_1 is the graph on V_1, with the edge set
$E(\bar{G}_1) = [V_1]^2 \setminus E_1$ ($e \in E(\bar{G}_1) \iff e \notin E_1$)

Graph theory

Undirected graphs

Walks, trails, paths

Complete, bipartite and other notable graphs

Planar graphs

Graph colouring

Directed graphs

Directed graphs

Walks, paths, etc.

Connectivity in digraphs

Orientable graphs

Matrices associated to a graph/digraph

Adjacency matrices

Other matrices associated to a graph/digraph

Linking graphs and linear algebra

Characterisation of graphs

Connected vertices and graph, components

Definition 120 (Connected vertices)

Two vertices u and v in a graph G are **connected** if $u = v$, or if $u \neq v$ and there exists a path in G that links u and v

(For *path*, see Definition 133 later)

Definition 121 (Connected graph)

A graph is **connected** if every two vertices of G are connected; otherwise, G is **disconnected**

A necessary condition for connectedness

Theorem 122

A connected graph on p vertices has at least $p - 1$ edges

In other words, a connected graph G of order p has size$(G) \geq p - 1$

Connectedness is an equivalence relation

Denote $x \equiv y$ the relation "$x = y$, or $x \neq y$ and there exists a path in G connecting x and y". $\equiv$ is an equivalence relation since

1. $x \equiv y$ [reflexivity]
2. $x \equiv y \implies y \equiv x$ [symmetry]
3. $x \equiv y, y \equiv z \implies x \equiv z$ [transitivity]

Definition 123 (Connected component of a graph)

The classes of the equivalence relation $\equiv$ partition V into connected sub-graphs of G called **connected components** (or **components** for short) of G

A connected subgraph H of a graph G is a component of G if H is not contained in any connected subgraph of G having more vertices or edges than H

Vertex deletion & cut vertices

Definition 124 (Vertex deletion)

If $v \in V(G)$ is a vertex of G, the graph $G - v$ is the graph formed from G by removing v and all edges incident with v

Definition 125 (Cut-vertices)

Let G be a connected graph. Then v is a **cut-vertex** G if $G - v$ is disconnected

Edge deletion & bridges

Definition 126 (Edge deletion)

If e is an edge of G, the graph $G - e$ is the graph formed from G by removing e from G

Definition 127 (Bridge)

An edge e in a connected graph G is a **bridge** if $G - e$ is disconnected

Theorem 128

Let G be a connected graph. An edge e of G is a bridge of G $\iff$ e does not lie on any cycle of G

(For *cycle*, see Definition 136 later)

Graph theory

- Undirected graphs
- **Walks, trails, paths**
- Complete, bipartite and other notable graphs
- Planar graphs
- Graph colouring
- Directed graphs
- Directed graphs
- Walks, paths, etc.
- Connectivity in digraphs
- Orientable graphs
- Matrices associated to a graph/digraph
- Adjacency matrices
- Other matrices associated to a graph/digraph
- Linking graphs and linear algebra
- Characterisation of graphs

Walk

Definition 129 (Walk)

A **walk** in a graph $G = (V, E)$ is a non-empty alternating sequence $v_0 e_0 v_1 e_1 v_2 \dots e_{k-1} v_k$ of vertices and edges in G such that $e_i = \{v_i, v_{i+1}\}$ for all $i < k$. This walk begins with v_0 and ends with v_k

Definition 130 (Length of a walk)

The **length** of a walk is equal to the number of edges in the walk

Definition 131 (Closed walk)

If $v_0 = v_k$, the walk is **closed**

Trail and path

Definition 132 (Trail)

If the edges in the walk are all distinct, it defines a **trail** in $G = (V, E)$

Definition 133 (Path)

If the vertices in the walk are all distinct, it defines a **path** in G

The sets of vertices and edges determined by a trail is a subgraph

Distance between two vertices

Definition 134 (Distance between two vertices)

The (**geodesic**) **distance** $d(u, v)$ in $G = (V, E)$ between two vertices u and v is the length of the shortest path linking u and v in G

If no such path exists, we assume $d(u, v) = \infty$

Circuit and cycle

Definition 135 (Circuit)

A trail linking u to v, containing at least 3 edges and in which $u = v$, is a **circuit**

Definition 136 (Cycle)

A circuit which does not repeat any vertices (except the first and the last) is a **cycle** (or **simple circuit**)

Definition 137 (Length of a cycle)

The **length of a cycle** is its number of edges

Eulerian and Hamiltonian trails and circuits

Eulerian	Hamiltonian
A walk in an undirected multigraph M that uses each edge **exactly once** is a **Eulerian trail** of M	A path containing all vertices of a graph G is a **Hamiltonian path** of G
If a graph G has a Eulerian trail, then G is a **traversable graph**	If a graph G has an Hamiltonian path, then G is a **traceable graph**
A circuit containing all the vertices and edges of a multigraph M is a **Eulerian circuit** of M	A cycle containing all vertices of a graph G is a **Hamiltonian cycle** of G
A graph (resp. multigraph) containing an Eulerian circuit is a **Eulerian graph** (resp. **Eulerian multigraph**)	A graph containing a Hamiltonian cycle is a **Hamiltonian graph**

Graph theory

- Undirected graphs
- Walks, trails, paths
- **Complete, bipartite and other notable graphs**
- Planar graphs
- Graph colouring
- Directed graphs
- Directed graphs
- Walks, paths, etc.
- Connectivity in digraphs
- Orientable graphs
- Matrices associated to a graph/digraph
- Adjacency matrices
- Other matrices associated to a graph/digraph
- Linking graphs and linear algebra
- Characterisation of graphs

Definition 138 (Complete graph)

A graph is complete if every two of its vertices are adjacent

Definition 139 (n-clique)

A simple, complete graph on n vertices is called an n-**clique** and is often denoted K_n

Note that a complete graph of order p is $(p-1)$-regular

Bipartite graph

Definition 140 (Bipartite graph)

A graph is **bipartite** if its vertices can be partitioned into two sets V_1 and V_2, such that no two vertices in the same set are adjacent. This graph may be written $G = (V_1, V_2, E)$

Definition 141 (Complete bipartite graph)

A bipartite graph in which every two vertices from the 2 different partitions are adjacent is called a **complete bipartite graph**

We often denote $K_{p,q}$ a simple, complete bipartite graph with $|V_1| = p$ and $|V_2| = q$

Some specific graphs

Definition 142 (Tree)

Any connected graph that has no cycles is a **tree**

Definition 143 (Cycle C_n)

For $n \geq 3$, the **cycle** C_n is a connected graph of order n that is a cycle on n vertices

Definition 144 (Path P_n)

The **path** P_n is a connected graph that consists of $n \geq 2$ vertices and $n - 1$ edges. Two vertices of P_n have degree 1 and the rest are of degree 2

Definition 145 (Star S_n)

The **star** of order n is the complete bipartite graph $K_{1,n-1}$ (1 vertex of degree $n - 1$ and $n - 1$ vertices of degree 1)

Graph theory

- Undirected graphs
- Walks, trails, paths
- Complete, bipartite and other notable graphs
- **Planar graphs**
- Graph colouring
- Directed graphs
- Directed graphs
- Walks, paths, etc.
- Connectivity in digraphs
- Orientable graphs
- Matrices associated to a graph/digraph
- Adjacency matrices
- Other matrices associated to a graph/digraph
- Linking graphs and linear algebra
- Characterisation of graphs

Planar graph

Definition 146 (Planar graph)

A graph is **planar** if it *can be* drawn in the plane with no crossing edges (except at the vertices). Otherwise, it is **nonplanar**

Definition 147 (Plane graph)

A **plane graph** is a graph *that is drawn* in the plane with no crossing edges. (This is only possible if the graph is planar)

(To see the difference, have you ever played this game?)

Let G be a plane graph

- the connected parts of the plane are called **regions**
- vertices and edges that are incident with a region R make up a **boundary** of R

Theorem 148 (Euler's formula)

Let G be a connected plane graph with p vertices, q edges, and r regions, then

$$p - q + r = 2$$

Corollary 149

Let G be a plane graph with p vertices, q edges, r regions, and k connected components, then

$$p - q + r = k + 1$$

Two well-known non-planar graphs

$K_{3,3}$ and K_5 are nonplanar

Theorem 150 (Kuratowski Theorem)

A graph G is planar $\iff$ it contains no subgraph isomorphic to K_5 or $K_{3,3}$ or any subdivision of K_5 or $K_{3,3}$

Note: If a graph G is nonplanar and G is a subgraph of G', then G' is also nonplanar

Graph theory

Undirected graphs
Walks, trails, paths
Complete, bipartite and other notable graphs
Planar graphs
Graph colouring
Directed graphs
Directed graphs
Walks, paths, etc.
Connectivity in digraphs
Orientable graphs
Matrices associated to a graph/digraph
Adjacency matrices
Other matrices associated to a graph/digraph
Linking graphs and linear algebra
Characterisation of graphs

Definition 151 (Colouring of a graph G)

A **colouring** of a graph G is an assignment of colours to the vertices of G such that adjacent vertices have different colours

Definition 152 (n-colouring of G)

A **n-colouring** is a colouring of G using n colours

Definition 153 (n-colourable)

G is **n-colourable** if there exists a colouring of G that uses n colours

Definition 154 (Chromatic number)

The **chromatic number** $\chi(G)$ of a graph G is the minimal value n for which an n-colouring of G exists

Property 155

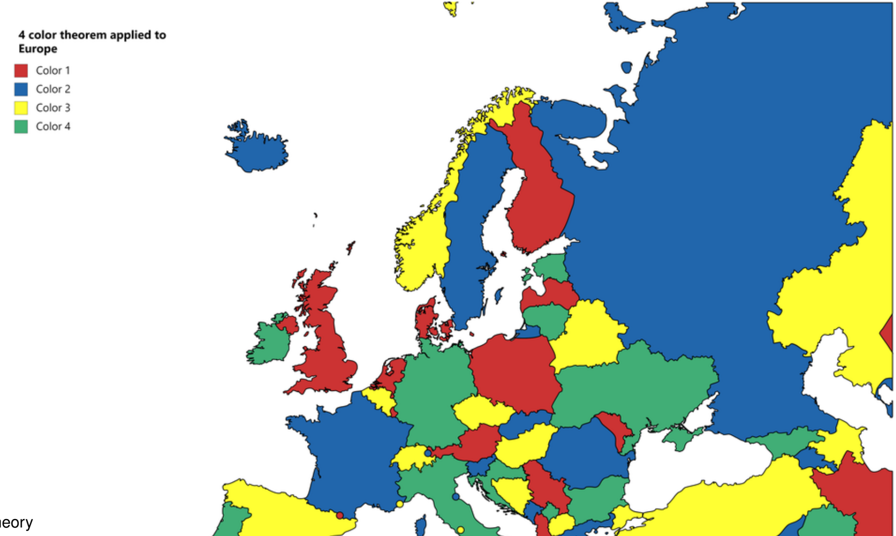
- $\chi(G) = 1 \iff$ *G have no edges*
- *If* $G = K_{n,m}$, *then* $\chi(G) = 2$
- *If* $G = K_n$, *then* $\chi(G) = n$
- *For any graph G,*

  $$\chi(G) \leq 1 + \Delta(G)$$

  where $\Delta(G)$ *is the maximum degree of G*
- *If G is a planar graph, then* $\chi(G) \leq 4$

“Real life” problem

What is the minimal number of colours to colour all states in the map so that two adjacent states have different colours?



Graph theory

Undirected graphs
Walks, trails, paths
Complete, bipartite and other notable graphs
Planar graphs
Graph colouring
Directed graphs
Directed graphs
Walks, paths, etc.
Connectivity in digraphs
Orientable graphs
Matrices associated to a graph/digraph
Adjacency matrices
Other matrices associated to a graph/digraph
Linking graphs and linear algebra
Characterisation of graphs

Definitions

Definition 156 (Digraph)

A directed graph (or **digraph**) is a pair $G = (V, A)$ of sets such that

- V is a set of points: $V = \{v_1, v_2, v_3, .., v_p\}$
- A is a set of ordered pairs of V: $A = \{(v_i, v_j), (v_i, v_k), \dots, (v_n, v_p)\}$ or $A = \{v_i v_j, v_i v_k, \dots, v_n v_p\}$

Definition 157 (Vertex)

The elements of V are the vertices of the digraph G. V or $V(G)$ is the vertex set of the digraph G

Definition 158 (Arc)

The elements of A are the **arcs** (directed edges) of the digraph G. A or $A(G)$ is the arc set of the digraph G

Directed network/weighted (di)graph

Definition 159 (Directed network)

A directed network is a digraph together with a function f,

$$f : A \to \mathbb{R},$$

which maps the arc set A into the set of real number. The value of the arc $uv \in A$ is $f(uv)$

Another name is **weighted** (di)graph

Loops & Multiple arcs

Definition 160 (Loop)

A **loop** is an arc with both the same ends; *e.g.* (u, u) is a loop

Definition 161 (Multiple arcs)

Multiple arcs (or multi-arcs) are two or more arcs connecting the same two vertices

Multidigraph/Digraph

Definition 162 (Multidigraph)

A **multidigraph** is a digraph which allows repetition of arcs or loops

Definition 163 (Digraph)

In a digraph, no more than one arc can join any pair of vertices

Let $G = (V, A)$ be a digraph

Definition 164 (Arc endpoints)

For an arc $u = (x, y)$, vertex x is the **initial endpoint**, and vertex y is the **terminal endpoint**

Definition 165 (Predecessor - Successor)

If $(u, v) \in A(G)$ is an arc of G, then

- u is a **predecessor** of v
- v is a **successor** of u

Definition 166 (Neighbours of a vertex)

Let $x \in V$ be a vertex. The **neighbours** of x is the set $\Gamma(x) = \Gamma^+_G(x) \cup \Gamma^-_G(x)$, where $\Gamma^+_G(x)$ and $\Gamma^-_G(x)$ are, respectively, the set of successors and predecessors of v

Sources and sinks

Definition 167 (Directed away - Directed towards)

If $a = (u, v) \in A(G)$ is an arc of G, then

- *the arc a is said to be **directed away** from u*
- *the arc a is said to be **directed towards** v*

Definition 168 (Source - Sink)

- *Any vertex which has no arcs directed towards it is a **source***
- *Any vertex which has no arcs directed away from it is a **sink***

Adjacent arcs

Definition 169 (Adjacent arcs)

Two arcs are **adjacent** if they have at least one endpoint in common

Arcs incident to a subset of arcs

Definition 170 (Arc incident out of $X \subset A(G)$)

If the initial endpoint of an arc u belongs to $X \subset A(G)$ and if the terminal endpoint of arc u does not belong to X, then u is said to be **incident out of** X; we write $u \in \omega^+(X)$

Similarly, we define an **arc incident into** X and the set $\omega^-(X)$

Finally, the set of arcs **incident to** X is denoted

$$\omega(X) = \omega^+(X) \cup \omega^-(X)$$

Definition 171 (Subgraph of G generated by $A \subset V$)

The **subgraph** of G generated by A is the graph with A as its vertex set and with all the arcs in G that have both their endpoints in A. If $G = (V, \Gamma)$ is a 1-graph, then the subgraph generated by A is the 1-graph $G_A = (A, \Gamma_A)$ where

$$\Gamma_A(x) = \Gamma(x) \cap A \qquad (x \in A)$$

Definition 172 (Partial graph of G generated by $V \subset U$)

The graph (X, V) whose vertex set is X and whose arc set is V. In other words, it is graph G without the arcs $U - V$

Definition 173 (Partial subgraph of G)

A partial subgraph of G is the subgraph of a partial graph of G

Graph theory

- Undirected graphs
- Walks, trails, paths
- Complete, bipartite and other notable graphs
- Planar graphs
- Graph colouring
- Directed graphs
- **Directed graphs**
- Walks, paths, etc.
- Connectivity in digraphs
- Orientable graphs
- Matrices associated to a graph/digraph
- Adjacency matrices
- Other matrices associated to a graph/digraph
- Linking graphs and linear algebra
- Characterisation of graphs

Degree

Let v be a vertex of a digraph $G = (V, A)$

Definition 174 (Outdegree of a vertex)

The number of arcs directed away from a vertex v, in a digraph is called the **outdegree** of v and is written $d_G^+(v)$

Definition 175 (Indegree of a vertex)

The number of arcs directed towards a vertex v, in a digraph is called the **indegree** of v and is written $d_G^-(v)$

Definition 176 (Degree)

For any vertex v in a digraph, the **degree** of v is defined as

$$d_G(v) = d_G^+(v) + d_G^-(v)$$

Theorem 177

For any (di)graph, the sum of the degrees of the vertices equals twice the number of edges (arcs)

Corollary 178

In any (di)graph, the sum of the degrees of the vertices is a nonnegative even integer

Theorem 179

If G is a digraph with vertex set $V(G) = \{v_1, \dots, v_p\}$ and q arcs, then

$$\sum_{i=1}^{p} d_G^+(v_i) = \sum_{i=1}^{p} d_G^-(v_i) = q$$

Definition 180 (Regular digraph)

A digraph G is r-regular if $d_G^+(v) = d_G^-(v) = r$ for all $v \in V(G)$

Symmetric/antisymmetric digraphs

Definition 181 (Symmetric digraph)

Let $G = (V, A)$ be a digraph with associated binary relation R. If R is *symmetric*, the digraph is symmetric

Definition 182 (Anti-symmetric digraph)

Let $G = (V, A)$ be a digraph with associated binary relation R. The digraph G is **anti-symmetric** if

$$xRy \implies y \not R x$$

Definition 183 (Symmetric multidigraph)

Let $G = (V, A)$ be a multidigraph. G is symmetric if $\forall x, y \in V(G)$, the number of arcs from x to y equals the number of arcs from y to x

Graph theory

Undirected graphs
Walks, trails, paths
Complete, bipartite and other notable graphs
Planar graphs
Graph colouring
Directed graphs
Directed graphs
Walks, paths, etc.
Connectivity in digraphs
Orientable graphs
Matrices associated to a graph/digraph
Adjacency matrices
Other matrices associated to a graph/digraph
Linking graphs and linear algebra
Characterisation of graphs

Walks

Let $G = (V, A)$ be a digraph.

Definition 184 (Directed walk)

A **directed walk** in a digraph G is a non-empty alternating sequence $v_0 a_0 v_1 a_1 v_2 \dots a_{k-1} v_k$ of vertices and arcs in G such that $a_i = (v_i, v_{i+1})$ for all $i < k$. This walk begins with v_0 and ends with v_k

Definition 185 (Length of a directed walk)

The length of a directed walk is equal to the number of arcs in the directed walk

Definition 186 (Closed walk)

If $v_0 = v_k$, the walk is closed

Trails

Let $G = (V, A)$ be a digraph.

Definition 187 (Directed trail)

A directed walk in G in which all arcs are distinct is a **directed trail** in G

Definition 188 (Directed path)

A directed walk in G in which all vertices are distinct is a **directed path** in G

Definition 189 (Directed cycle)

A closed walk is a **directed cycle** if it contains at least three vertices and all its vertices are distinct except for $v_0 = v_k$

Graph theory

Undirected graphs
Walks, trails, paths
Complete, bipartite and other notable graphs
Planar graphs
Graph colouring
Directed graphs
Directed graphs
Walks, paths, etc.
Connectivity in digraphs
Orientable graphs
Matrices associated to a graph/digraph
Adjacency matrices
Other matrices associated to a graph/digraph
Linking graphs and linear algebra
Characterisation of graphs

Definitions

Definition 190 (Underlying graph)

Given a digraph, the undirected graph with each arc replaced by an edge is called the ***underlying graph***

Definition 191 (Weakly connected digraph)

If the underlying graph is a connected graph, then the digraph is **weakly connected**

Definition 192 (Strongly connected digraph)

A digraph G is **strongly connected** if for every two distinct vertices u and v of G, there exists a directed path from u to v

Definition 193 (Disconnected digraph)

A digraph is said to be **disconnected** if it is not weakly connected

Strong connectedness is an equivalence relation

Denote $x \equiv y$ the relation "$x = y$, or $x \neq y$ and there exists a directed path in G from x to y". $\equiv$ is an equivalence relation since

1. $x \equiv y$ [reflexivity]
2. $x \equiv y \implies y \equiv x$ [symmetry]
3. $x \equiv y, y \equiv z \implies x \equiv z$ [transitivity]

Definition 194 (Connected component of a graph)

Sets of the form

$$A(x_0) = \{x : x \in V, x \equiv x_0\}$$

are equivalence classes. They partition V into strongly connected sub-digraphs of G called **strongly connected components** (or **strong components**) of G

A strong component in G is a maximal strongly connected subdigraph of G

Theorem 195 (Properties)

Let $G = (V, A)$ be a digraph

- *If G is strongly connected, it has only one strongly connected component*
- *The strongly connected components partition the vertices $V(G)$, with every vertex in exactly one strongly connected component*

Condensation of a digraph

Definition 196 (Condensation of a digraph)

The condensation G^* of a digraph G is a digraph having as vertices the strongly connected components (SCC) of G and such that there exists an arc in G^* from a SCC C_i to another SCC C_j if there is an arc in G from some vertex of S_i to a vertex of S_j

Definition 197 (Articulation set)

For a connected graph, a set X of vertices is called an ***articulation set*** *(or a* ***cutset****) if the subgraph of G generated by $V - X$ is not connected*

Definition 198 (Stable set)

A set S of vertices is called a ***stable set*** *if no arc joins two distinct vertices in S*

Graph theory

- Undirected graphs
- Walks, trails, paths
- Complete, bipartite and other notable graphs
- Planar graphs
- Graph colouring
- Directed graphs
- Directed graphs
- Walks, paths, etc.
- Connectivity in digraphs
- **Orientable graphs**
- Matrices associated to a graph/digraph
- Adjacency matrices
- Other matrices associated to a graph/digraph
- Linking graphs and linear algebra
- Characterisation of graphs

Orientation

Definition 199 (Orienting a graph)

Given a connected *graph*, we describe the act of assigning a direction to each edge (edge $\rightarrow$ arc) as **orienting the graph**

Definition 200 (Strong orientation)

If the digraph resulting from orienting a graph is strongly connected, the orientation is a **strong orientation**

Orientable graph

Definition 201 (Orientable graph)

A connected graph G is **orientable** if it admits a strong orientation

Theorem 202

A connected graph $G = (V, E)$ is orientable $\iff$ G contains no bridges

(in other words, iff every edge is contained in a cycle)

Graph theory

Undirected graphs
Walks, trails, paths
Complete, bipartite and other notable graphs
Planar graphs
Graph colouring
Directed graphs
Directed graphs
Walks, paths, etc.
Connectivity in digraphs
Orientable graphs
Matrices associated to a graph/digraph
Adjacency matrices
Other matrices associated to a graph/digraph
Linking graphs and linear algebra
Characterisation of graphs

Matrices associated to a graph/digraph

There are multiple matrices associated to a graph/digraph

The branch of graph theory that studies the properties of matrices derived from graphs and uses of these matrices in determining graph properties is *spectral graph theory*

Graphs greatly simplify some problems in linear algebra and vice versa

Graph theory

- Undirected graphs
- Walks, trails, paths
- Complete, bipartite and other notable graphs
- Planar graphs
- Graph colouring
- Directed graphs
- Directed graphs
- Walks, paths, etc.
- Connectivity in digraphs
- Orientable graphs
- Matrices associated to a graph/digraph
- **Adjacency matrices**
- Other matrices associated to a graph/digraph
- Linking graphs and linear algebra
- Characterisation of graphs

Adjacency matrix (undirected case)

Let $G = (V, E)$ be a graph of order p and size q, with vertices $v_1, \ldots, v_p$ and edges $e_1, \ldots, e_q$

Definition 203 (Adjacency matrix)

The **adjacency matrix** is

$$M_A = M_A(G) = [m_{ij}]$$

is a $p \times p$ matrix in which

$$m_{ij} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

Theorem 204 (Adjacency matrix and degree)

The sum of the entries in row i of the adjacency matrix is the degree of v_i in the graph

We often write $A(G)$ and, reciprocally, if A is an adjacency matrix, $G(A)$ the corresponding graph

G undirected $\implies$ $A(G)$ symmetric

$A(G)$ has nonzero diagonal entries if G is not simple

Adjacency matrix (directed case)

Let $G = (V, A)$ be a digraph of order p with vertices $v_1, \ldots, v_p$

Definition 205 (Adjacency matrix)

The **adjacency matrix** $M = M(G) = [m_{ij}]$ is a $p \times p$ matrix in which

$$m_{ij} = \begin{cases} 1 & \text{if arc } v_i v_j \in A \\ 0 & \text{otherwise} \end{cases}$$

Theorem 206 (Properties of the adjacency matrix)

Let M be the adjacency matrix of a digraph G

- *M is not necessarily symmetric*
- *The sum of any column of M is equal to the number of arcs directed towards v_j*
- *The sum of the entries in row i is equal to the number of arcs directed away from vertex v_i*
- *The $(i, j)-$entry of M^n is equal to the number of walks of length n from vertex v_i to v_j*

```r
# Adjacency matrix (directed)
M <- as.matrix(as_adjacency_matrix(G, sparse = FALSE))

## Error in h(simpleError(msg, call)):  error in evaluating the
argument 'x' in selecting a method for function 'as.matrix':  object
'G' not found

# Column sums = indegrees, row sums = outdegrees (directed case)
all.equal(rowSums(M), degree(G, mode = "out"))

## Error in h(simpleError(msg, call)):  error in evaluating the
argument 'target' in selecting a method for function 'all.equal':
error in evaluating the argument 'x' in selecting a method for
function 'rowSums':  object 'M' not found

all.equal(colSums(M), degree(G, mode = "in"))

## Error in h(simpleError(msg, call)):  error in evaluating the
argument 'target' in selecting a method for function 'all.equal':
```

```
error in evaluating the argument 'x' in selecting a method for
function 'colSums':  object 'M' not found

# Walks of length 3 from 1 to 15 via M^3
M3 <- M %*% M %*% M

## Error:  object 'M' not found

M3[1, 15]

## Error:  object 'M3' not found
```

Definition 207 (Multiplicity of a pair)

*The **multiplicity** of a pair x, y is the number $m_G^+(x, y)$ of arcs with initial endpoint x and terminal endpoint y. Let*

$$
\begin{aligned}
m_G^-(x, y) &= m_G^+(y, x) \\
m_G(x, y) &= m_G^+(x, y) + m_G^-(x, y)
\end{aligned}
$$

If $x \neq y$, then $m_G(x, y)$ is number of arcs with both x and y as endpoints. If $x = y$, then $m_G(x, y)$ equals twice the number of loops attached to vertex x. If $A, B \subset V$, $A \neq B$, let

$$
\begin{aligned}
m_G^+(A, B) &= \{u : u \in U, u = (x, y), x \in A, y \in B\} \\
m_G(A, B) &= m_G^+(A, B) + m_G^+(A, B)
\end{aligned}
$$

Adjacency matrix (multigraph case)

Definition 208 (Adjacency matrix of a multigraph)

G an ℓ-graph, then the adjacency matrix $M_A = [m_{ij}]$ is defined as follows

$$m_{ij} = \begin{cases} k & \text{if arc there are } k \text{ arcs } (i, j) \in U \\ 0 & \text{otherwise} \end{cases}$$

with $k \leq \ell$

G undirected $\implies M_A(G)$ symmetric

$M_A(G)$ has nonzero diagonal entries if G is not simple.

Weighted adjacency matrices

Sometimes, adjacency matrices (typically for 1-graphs) have real entries, usually positive

This means that the arcs/edges have been given a weight

Theorem 209 (Number of walks of length n)

Let A be the adjacency matrix of a graph $G = (V(G), E(G))$, where $V(G) = \{v_1, v_2, \ldots, v_p\}$. Then the $(i,j)-$entry of A^n, $n \geq 1$, is the number of different walks linking v_i to v_j of length n in G.

(two walks of the same length are equal if their edges occur in exactly the same order)

Example: let A be the adjacency matrix of a graph $G = (V(G), E(G))$.

- the $(i,i)-$entry of A^2 is equal to the degree of v_i.
- the $(i,i)-$entry of A^3 is equal to twice the number of C_3 containing v_i.

Graph theory

Undirected graphs
Walks, trails, paths
Complete, bipartite and other notable graphs
Planar graphs
Graph colouring
Directed graphs
Directed graphs
Walks, paths, etc.
Connectivity in digraphs
Orientable graphs
Matrices associated to a graph/digraph
Adjacency matrices
Other matrices associated to a graph/digraph
Linking graphs and linear algebra
Characterisation of graphs

Incidence matrix (undirected case)

Let $G = (V, E)$ be a graph of order p, and size q, with vertices $v_1, \ldots, v_p$, and edges $e_1, \ldots, e_q$

Definition 210 (Incidence matrix)

The incidence matrix is

$$B = B(G) = [b_{ij}]$$

is that $p \times q$ matrix in which

$$b_{ij} = \begin{cases} 1 & \text{if } v_i \text{ is incident with } e_j \\ 0 & \text{otherwise} \end{cases}$$

Theorem 211 (Incidence matrix and degrees)

The sum of the entries in row i of the incidence matrix is the degree of v_i in the graph

Incidence matrix (directed case)

Let $G = (V, A)$ be a digraph of order p and size q, with vertices $v_1, \ldots, v_p$ and arcs $a_1, \ldots, a_q$

Definition 212 (Incidence matrix)

The **incidence matrix** $B = B(G) = [b_{ij}]$ is a $p \times q$ matrix in which

$$b_{ij} = \begin{cases} 1 & \text{if arc } a_j \text{ is directed away from a vertex } v_i \\ -1 & \text{if arc } a_j \text{ is directed towards a vertex } v_i \\ 0 & \text{otherwise} \end{cases}$$

Spectrum of a graph

We will come back to this later, but for now..

Definition 213 (Spectrum of a graph)

The **spectrum** of a graph G is the spectrum (set of eigenvalues) of its associated adjacency matrix $M(G)$

This is regardless of the type of adjacency matrix or graph

Distance matrix

Let G be a graph of order p with vertices $v_1, \ldots, v_p$

Definition 214 (Distance matrix)

The distance matrix $\Delta(G) = [d_{ij}]$ is a $p \times p$ matrix in which

$$\delta_{ij} = d_G(v_i, v_j)$$

Note $\delta_{ii} = 0$ for $i = 1, \ldots, p$

Property 215

- *M is not necessarily symmetric*
- *The sum of any column of M is equal to the number of arcs directed towards v_j*
- *The sum of the entries in row i is equal to the number of arcs directed away from vertex v_i*
- *The $(i,j)-$entry of M^n is equal to the number of walks of length n from vertex v_i to v_j*

Graph theory

- Undirected graphs
- Walks, trails, paths
- Complete, bipartite and other notable graphs
- Planar graphs
- Graph colouring
- Directed graphs
- Directed graphs
- Walks, paths, etc.
- Connectivity in digraphs
- Orientable graphs
- Matrices associated to a graph/digraph
- Adjacency matrices
- Other matrices associated to a graph/digraph
- **Linking graphs and linear algebra**
- Characterisation of graphs

Counting paths

Theorem 216

G a digraph and $M_A(G)$ its adjacency matrix. Denote $P = [p_{ij}]$ the matrix $P = M_A^k$. Then p_{ij} is the number of distinct paths of length k from i to j in G

Definition 217 (Irreducible matrix)

A matrix $A \in \mathcal{M}_n$ is **reducible** if $\exists P \in \mathcal{M}_n$, permutation matrix, s.t. $P^T AP$ can be written in block triangular form. If no such P exists, A is **irreducible**

Theorem 218

A irreducible $\iff$ $G(A)$ strongly connected

Theorem 219

Let A be the adjacency matrix of a graph G on p vertices. A graph G on p vertices is connected $\iff$

$$I + A + A^2 + \cdots + A^{p-1} = C$$

has no zero entries

Theorem 220

Let M be the adjacency matrix of a digraph D on p vertices. A digraph D on p vertices is strongly connected $\iff$

$$I + M + M^2 + \cdots + M^{p-1} = C$$

has no zero entries

Nonnegative matrix

$A = [a_{ij}] \in \mathcal{M}_n(\mathbb{R})$ **nonnegative** if $a_{ij} \geq 0$ $\forall i, j = 1, \ldots, n$; $\boldsymbol{v} \in \mathbb{R}^n$ nonnegative if $v_i \geq 0$ $\forall i = 1, \ldots, n$. **Spectral radius** of A

$$\rho(A) = \max_{\lambda \in \mathrm{Sp}(A)} \{|\lambda|\}$$

$\mathrm{Sp}(A)$ the **spectrum** of A

Perron-Frobenius (PF) theorem

Theorem 221 (PF – Nonnegative case)

$0 \leq A \in \mathcal{M}_n(\mathbb{R})$. *Then* $\exists \mathbf{v} \geq \mathbf{0}$ *s.t.*

$$A\mathbf{v} = \rho(A)\mathbf{v}$$

Theorem 222 (PF – Irreducible case)

Let $0 \leq A \in \mathcal{M}_n(\mathbb{R})$ *irreducible. Then* $\exists \mathbf{v} > \mathbf{0}$ *s.t.*

$$A\mathbf{v} = \rho(A)\mathbf{v}$$

$\rho(A) > 0$ *and with algebraic multiplicity 1. No nonnegative eigenvector is associated to any other eigenvalue of* A

Primitive matrices

Definition 223

$0 \leq A \in \mathcal{M}_n(\mathbb{R})$ **primitive** (with **primitivity index** $k \in \mathbb{N}_+^*$) if $\exists k \in \mathbb{N}_+^*$ s.t.

$$A^k > 0,$$

with k the smallest integer for which this is true. A **imprimitive** if it is not primitive

A primitive $\implies$ A irreducible; the converse is false

Theorem 224

$A \in \mathcal{M}_n(\mathbb{R})$ irreducible and $\exists i = 1, \ldots, n$ s.t. $a_{ii} > 0 \implies$ A primitive

Here d is the index of imprimitivity (i.e., the number of eigenvalues that have the same modulus as $\lambda_p = \rho(A)$). If $d = 1$, then A is primitive. We have that $d = \mathrm{gcd}$ of all the lengths of closed walks in $G(A)$

Theorem 225

$\mathbf{0} \leq A \in \mathcal{M}_n$, $\lambda_P = \rho(A)$ the Perron root of A, $\boldsymbol{v}_P$ and $\boldsymbol{w}_P$ the corresponding right and left Perron vectors of A, respectively, d the index of imprimitivity of A (with $d = 1$ when A is primitive) and $\lambda_j \in \sigma(A)$ the spectrum of A, with $j = 2, \ldots, n$ unless otherwise specified (assuming $\lambda_1 = \lambda_P$)

NONNEGATIVE → REDUCIBLE, IRREDUCIBLE

IRREDUCIBLE → IMPRIMITIVE, PRIMITIVE

REDUCIBLE

- $\lambda_P \geq 0$
- $\boldsymbol{w}_P \geq 0$
- $\boldsymbol{v}_P \geq 0$
- $\lambda_P \geq |\lambda_j|$

IMPRIMITIVE

- $\lambda_P > 0$
- $\boldsymbol{w}_P > 0$
- $\boldsymbol{v}_P > 0$
- $\lambda_P = |\lambda_j|$, $j = 2, \ldots, d$
- $\lambda_P > |\lambda_j|$, $j > d$

PRIMITIVE

- $\lambda_P > 0$
- $\boldsymbol{w}_P > 0$
- $\boldsymbol{v}_P > 0$
- $\lambda_P > |\lambda_j|$, $j \neq P$

Definition 226 (Minimally connected graph)

G is **minimally connected** if it is strongly connected and removal of any arc destroys strong-connectedness

A minimally connected graph is 1-graph without loops

Definition 227 (Contraction)

$G = (V, U)$. The **contraction** of the set $A \subset V$ of vertices consists in replacing A by a single vertex a and replacing each arc into (resp. out of) A by an arc with same index into (resp. out of) a

Theorem 228

G minimally connected, $A \subset V$ generating a strongly connected subgraph of G. Then the contraction of A gives a minimally connected graph

Arborescences

Definition 229 (Root)

Vertex $a \in V$ in $G = (V, U)$ is a **root** if all vertices of G can be reached by paths *starting* from a

Not all graphs have roots

Definition 230 (Quasi-strong connectedness)

G is **quasi-strongly connected** if $\forall x, y \in V$, exists $z \in V$ (denoted $z(x, y)$ to emphasize dependence on x, y) from which there is a path to x and a path to y

Strongly connected $\implies$ quasi-strongly connected (take $z(x, y) = x$); converse not true
Quasi-strongly connected $\implies$ connected

Graph theory

- Undirected graphs
- Walks, trails, paths
- Complete, bipartite and other notable graphs
- Planar graphs
- Graph colouring
- Directed graphs
- Directed graphs
- Walks, paths, etc.
- Connectivity in digraphs
- Orientable graphs
- Matrices associated to a graph/digraph
- Adjacency matrices
- Other matrices associated to a graph/digraph
- Linking graphs and linear algebra
- **Characterisation of graphs**

Geodesic distance

Definition 231 (Geodesic distance)

For $x, y \in V$, the **geodesic distance** $d(x, y)$ is the length of the shortest path from x to y, with $d(x, y) = \infty$ if no such path exists

Eccentricity

Definition 232 (Vertex eccentricity)

The **eccentricity** $e(x)$ of vertex $x \in V$ is

$$e(x) = \max_{\substack{y \in V \\ y \neq x}} d(x, y)$$

Central points, radius and centre

Definition 233 (Central point)

A **central point** of G is a vertex x_0 with smallest eccentricity

Definition 234 (Radius)

The **radius** of G is $\rho(G) = e(x_0)$, where x_0 is a centre of G In other words,

$$\rho(G) = \min_{x \in V} e(x)$$

Definition 235 (Centre)

The **centre** of G is the set of vertices that are central points of G, i.e.,

$$\{x \in V : e(x) = \rho(G)\}$$

Betweenness

Definition 236 (Betweenness)

$G = (V, A)$ a (di)graph. The **betweenness** of $v \in V$ is

$$b_{\mathcal{D}}(v) = \sum_{s \neq t \neq v \in V} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

where

- σ_{st} is number of shortest geodesic paths from s to t
- $\sigma_{st}(v)$ is number of shortest geodesic paths from s to t through v

In other words

- For each pair of vertices (s, t), compute the shortest paths between them
- For each pair of vertices (s, t), determine the fraction of shortest paths that pass through vertex v
- Sum this fraction over all pairs of vertices (s, t)

Closeness

Definition 237

$G = (V, A)$. The **closeness** of $v \in V$ is

$$c_{\mathcal{D}}(v) = \frac{1}{n-1} \sum_{t \in V \setminus \{v\}} d_{\mathcal{D}}(v, t)$$

i.e., mean geodesic distance between a vertex v and all other vertices it has access to

Another definition is

$$c_{\mathcal{D}}(v) = \frac{1}{\displaystyle\sum_{t \in V \setminus \{v\}} d_{\mathcal{D}}(v, t)}$$

Diametre and periphery of a graph

Definition 238 (Diametre of a graph)

The **diametre** of G is

$$\delta(G) = \max_{\substack{x,y \in V \\ x \neq y}} d(x,y) = \max_{x \in V} e(x)$$

$\delta(G) < \infty \iff G$ strongly connected

Definition 239 (Periphery)

The **periphery** of a graph is the set of vertices whose eccentricity achieves the diametre, i.e.,

$$\{x \in V : e(x) = \delta(G)\}$$

Definition 240 (Antipodal vertices)

Vertices $x, y \in V$ are **antipodal** if $d(x,y) = \delta(G)$

Degree distribution

Definition 241 (Arc incident to a vertex)

If a vertex x is the initial endpoint of an arc u, which is not a loop, the arc u is **incident out of vertex** x

The number of arcs incident out of x plus the number of loops attached to x is denoted $d_G^+(x)$ and is the **outer demi-degree** of x

An arc **incident into vertex** x and the **inner demi-degree** $d_G^-(x)$ are defined similarly

Definition 242 (Degree)

The **degree** of vertex x is the number of arcs with x as an endpoint, each loop being counted twice. The degree of x is denoted $d_G(x) = d_G^+(x) + d_G^-(x)$

If each vertex has the same degree, the graph is **regular**

Definition 243 (Isolated vertex)

A vertex of degree 0 is **isolated**.

Definition 244 (Average degree of G)

$d(G) = \frac{1}{|V|} \sum_{v \in V} deg_G(v)$.

Definition 245 (Minimum degree of G)

$\delta(G) = \min\{deg_G(v) | v \in V\}$.

Definition 246 (Maximum degree of G)

$\Delta(G) = \max\{deg_G(v) | v \in V\}$.

- Average (nearest) neighbour degree, to encode for *preferential attachment* (one prefers to hang out with popular people)

$$k_i^{nn} = \frac{1}{k(i)} \sum_{j \in \mathcal{N}(i)} k(j)$$

or, in terms of the adjacency matrix $A = [a_{ij}]$,

$$k_i^{nn} = \frac{1}{k(i)} \sum_j a_{ij} k(j)$$

- *Excess degree*: take nearest neighbour degree but do not consider the edge/arc followed to get to the neighbour
- Degree, nearest neighbour and excess degree distributions

Degree from adjacency matrix

Suppose adjacency matrix take the form $A = [a_{ij}]$ with $a_{ij} = 1$ if there is an arc from the vertex indexed i to the vertex indexed j and 0 otherwise. (Could be the other way round, using A^T, just make sure)

Let $\boldsymbol{e} = (1, \ldots, 1)^T$ be the vector of all ones

$A\boldsymbol{e} = (d_G^+(1), \ldots, d_G^+(1))^T$ (out-degree)

$\boldsymbol{e}^T A = (d_G^-(1), \ldots, d_G^-(1))$ (in-degree)

Circumference

Definition 247 (Circumference)

In an undirected (resp. directed) graph, the total number of edges (resp. arcs) in the longest cycle of graph G is the **circumference** of G

Girth

Definition 248 (Girth)

The total number of edges in the shortest cycle of graph G is the **girth** $g(G)$

Completeness

Definition 249 (Complete undirected graph)

An undirected graph is complete if every two of its vertices are adjacent.

Definition 250 (Complete digraph)

A digraph $D(V, A)$ is complete if $\forall u, v \in V$, $uv \in A$.

In case of simple graphs, completeness effectively means that "information" can be transmitted from every vertex to every other vertex quickly (1 step)

It can be useful to know how far away we are from being complete

Number of edges/arcs in a complete graph

$G = (V, E)$ undirected and simple of order n has at most

$$\frac{n(n-1)}{2}$$

edges, while $G = (V, A)$ directed and simple of order n has at most

$$n(n-1)$$

arcs

Density of a graph

Definition 251 (Density)

The fraction of maximum number of edges or arcs present in the graph is the **density** of the graph.

If the graph has p edges or arcs, then its density is, respectively,

$$\frac{2p}{n(n-1)}$$

or

$$\frac{p}{n(n-1)}$$

Connectedness

We have already seen connectedness (quasi- or strong in the oriented case)

Connectedness is important in terms of characteristing graph properties, as it shows the capacity of the graph to convey information to all the members of the graph (the vertices)

Definition 252 (Connected graph)

A **connected graph** is a graph that contains a chain $\mu[x, y]$ for each pair x, y of distinct vertices

Denote $x \equiv y$ the relation "$x = y$, or $x \neq y$ and there exists a chain in G connecting x and y". $\equiv$ is an equivalence relation since

1. $x \equiv y$ [reflexivity]
2. $x \equiv y \implies y \equiv x$ [symmetry]
3. $x \equiv y, y \equiv z \implies x \equiv z$ [transitivity]

Definition 253 (Connected component of a graph)

The classes of the equivalence relation $\equiv$ partition V into connected sub-graphs of G called **connected components**

Articulation set

Definition 254 (Articulation set)

For a connected graph, a set A of vertices is called an **articulation set** (or a **cutset**) if the subgraph of G generated by $V - A$ is not connected

`articulation_points(G)` in `igraph` (assumes the graph is undirected, makes it so if not)

Strongly connected graphs

$G = (V, U)$ connected. A **path of length 0** is any sequence $\{x\}$ consisting of a single vertex $x \in V$

For $x, y \in V$, let $x \equiv y$ be the relation "there is a path $\mu_1[x, y]$ from x to y as well as a path $\mu_2[y, x]$ from y to x". This is an equivalence relation (it is reflexive, symmetric and transitive)

Definition 255 (Strong components)

Sets of the form

$$A(x_0) = \{x : x \in V, x \equiv x_0\}$$

are equivalence classes; they partition V and are the **strongly connected components** of G

Definition 256 (Strongly connected graph)

G **strongly connected** if it has a single strong component

Definition 257 (Minimally connected graph)

G is **minimally connected** if it is strongly connected and removal of any arc destroys strong-connectedness

Definition 258 (Contraction)

$G = (V, U)$. The **contraction** of the set $A \subset V$ of vertices consists in replacing A by a single vertex a and replacing each arc into (resp. out of) A by an arc with same index into (resp. out of) a

Quasi-strong connectedness

Definition 259 (Quasi-strong connectedness)

G **quasi-strongly connected** if $\forall x, y \in V$, exists $z \in V$ (denoted $z(x, y)$ to emphasize dependence on x, y) from which there is a path to x and a path to y

Strongly connected $\implies$ quasi-strongly connected (take $z(x, y) = x$); converse not true

Quasi-strongly connected $\implies$ connected

Lemma 260

$G = (V, U)$ has a root $\iff$ G quasi-strongly connected

Weak-connectedness

Definition 261 (Weakly connected graph)

$G = (V, U)$ **weakly connected** if $G = (V, E)$ connected, where E is obtained from U by ignoring the direction of arcs

Weak components

Define for $x, y \in V$ the relation $x \equiv y$ as "$x = y$ or $x \neq y$ and there is a chain in G connecting x and y" [like for components in an undirected graph, except the graph is directed here]

This defines an equivalence relation

Definition 262 (Weak components)

Sets of the form

$$A(x_0) = \{x : x \in V, x \equiv x_0\}$$

are equivalence classes partitioning V into the **weakly connected components** of G

$G = (V, U)$ is weakly connected if there is a single weak component

Cliques

Definition 263 (Clique in undirected graphs)

$G = (V, E)$ a simple undirected graph. A **clique** is a subgraph G' of G such that all vertices in G' are adjacent

Definition 264 (n-clique)

A simple, complete graph on n vertices is called an n-**clique** and is often denoted K_n

Definition 265 (Clique in directed graphs)

$G = (V, U)$ a simple directed graph. A **clique** is a subgraph G' of G such that all vertices in G' are mutually adjacent

Definition 266 (Maximal clique)

A **maximal clique** is a clique that cannot be extended by adding another adjacent vertex

k-core

Definition 267 (k-core of a graph)

$G = (V, U)$ a graph. The **k-core** of G is a maximal subgraph in which each vertex has degree at least k

Definition 268 (Coreness of a vertex)

$G = (V, U)$ a graph, $x \in V$. The **coreness** of x is k if x belongs to the k-core of G but not to the $k + 1$ core of G

For directed graphs, in-cores or out-cores depending on whether in-degree or out-degree is used