

MA933 - Stochastic Modelling and Random Processes

MSc in Mathematics of Systems

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References

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1. Probability

- **sample space** Ω (e.g. $\{H, T\}$, $\{H, T\}^N$, {paths of a stoch. process})
- **events** $A \subseteq \Omega$ (measurable) subsets (e.g. odd numbers on a die)
 $\mathcal{F} \subseteq \mathcal{P}(\Omega)$ is the set of all events (subset of the powerset)

Definition 1.1

A **probability distribution** \mathbb{P} on (Ω, \mathcal{F}) is a function $\mathbb{P} : \mathcal{F} \rightarrow [0, 1]$ which is

- (i) normalized, i.e. $\mathbb{P}[\emptyset] = 0$ and $\mathbb{P}[\Omega] = 1$
- (ii) additive, i.e. $\mathbb{P}[\cup_i A_i] = \sum_i \mathbb{P}[A_i]$,
where A_1, A_2, \dots is a collection of disjoint events, i.e. $A_i \cap A_j = \emptyset$ for all i, j .

The triple $(\Omega, \mathcal{F}, \mathbb{P})$ is called a **probability space**.

- For **discrete** Ω : $\mathcal{F} = \mathcal{P}(\Omega)$ and $\mathbb{P}[A] = \sum_{\omega \in A} \mathbb{P}[\omega]$
e.g. $\mathbb{P}[\text{even number on a die}] = \mathbb{P}[2] + \mathbb{P}[4] + \mathbb{P}[6] = 1/2$
- For **continuous** Ω (e.g. $[0, 1]$): $\mathcal{F} \subsetneq \mathcal{P}(\Omega)$

1. Independence and conditional probability

- Two events $A, B \subseteq \Omega$ are called **independent** if $\mathbb{P}[A \cap B] = \mathbb{P}[A]\mathbb{P}[B]$.

Example. rolling a die repeatedly

- If $\mathbb{P}[B] > 0$ then the **conditional probability** of A given B is

$$\mathbb{P}[A|B] := \mathbb{P}[A \cap B] / \mathbb{P}[B].$$

If A and B are independent, then $\mathbb{P}[A|B] = \mathbb{P}[A]$.

Lemma 1.1 (Law of total probability)

Let B_1, \dots, B_n be a **partition** of Ω such that $\mathbb{P}[B_i] > 0$ for all i . Then

$$\mathbb{P}[A] = \sum_{i=1}^n \mathbb{P}[A \cap B_i] = \sum_{i=1}^n \mathbb{P}[A|B_i] \mathbb{P}[B_i].$$

Note that also $\mathbb{P}[A|C] = \sum_{i=1}^n \mathbb{P}[A|C \cap B_i] \mathbb{P}[B_i|C]$ provided $\mathbb{P}[C] > 0$.

1. Random variables

Definition 1.2

A **random variable** X is a (measurable) function $X : \Omega \rightarrow \mathbb{R}$.

The **distribution function** of the random variable is

$$F(x) = \mathbb{P}[X \leq x] = \mathbb{P}[\{\omega : X(\omega) \leq x\}] .$$

X is called **discrete**, if it only takes values in a countable subset $\Delta = \{x_1, x_2, \dots\} \subseteq \mathbb{R}$, and its distribution is characterized by the **probability mass function**

$$\pi(x) := \mathbb{P}[X = x] , \quad x \in \Delta .$$

X is called **continuous**, if its distribution function is

$$F(x) = \int_{-\infty}^x f(y) dy \quad \text{for all } x \in \mathbb{R} ,$$

where $f : \mathbb{R} \rightarrow [0, \infty)$ is the **probability density function (PDF)** of X .

1. Random variables

- In general, $f = F'$ is given by the derivative (exists for cont. rv's).
For discrete rv's, F is a step function with 'PDF'

$$f(x) = F'(x) = \sum_{y \in \Delta} \pi(y) \delta(x - y).$$

- The **expected value** of X is given by $\mathbb{E}[X] = \begin{cases} \sum_{x \in \Delta} x \pi(x) \\ \int_{\mathbb{R}} x f(x) dx \end{cases}$
- The **variance** is given by $\text{Var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$,
the **covariance** of two r.v.s by $\text{Cov}[X, Y] := \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$.
- Two random variables X, Y are independent if the events $\{X \leq x\}$ and $\{Y \leq y\}$ are independent for all $x, y \in \mathbb{R}$. This implies for **joint distributions**

$$f(x, y) = f^X(x) f^Y(y) \quad \text{or} \quad \pi(x, y) = \pi^X(x) \pi^Y(y)$$

with **marginals** $f^X(x) = \int_{\mathbb{R}} f(x, y) dy$ and $\pi^X(x) = \sum_{y \in \Delta_y} \pi(x, y)$.

- Independence implies $\text{Cov}[X, Y] = 0$, i.e. X and Y are **uncorrelated**.
The inverse is in general false, but holds if X and Y are Gaussian.

1. Simple random walk

Definition 1.3

Let $X_1, X_2, \dots \in \{-1, 1\}$ be a sequence of independent, identically distributed random variables (**iidrv's**) with

$$p = \mathbb{P}[X_i = 1] \quad \text{and} \quad q = \mathbb{P}[X_i = -1] = 1 - p .$$

The sequence Y_0, Y_1, \dots defined as $Y_0 = 0$ and $Y_n = \sum_{k=1}^n X_k$ is called the **simple random walk (SRW)** on \mathbb{Z} .

- for a single **increment** X_k we have

$$\mathbb{E}[X_k] = p - q = 2p - 1 , \quad \text{var}[X_k] = p + q - (p - q)^2 = 4p(1 - p)$$

- $\mathbb{E}[Y_n] = \mathbb{E}\left[\sum_{k=1}^n X_k\right] = \sum_{k=1}^n \mathbb{E}[X_k] = n(2p - 1)$

(expectation is a linear operation)

- $\text{var}[Y_n] = \text{var}\left[\sum_{k=1}^n X_k\right] = \sum_{k=1}^n \text{var}[X_k] = 4np(1 - p)$

(for a sum of **independent** rv's the variance is additive)

1. LLN and CLT

Theorem 1.2 (Weak law of large numbers (LLN))

Let $X_1, X_2, \dots \in \mathbb{R}$ be a sequence of iidrv's with $\mu := \mathbb{E}[X_k] < \infty$ and $\mathbb{E}[|X_k|] < \infty$. Then

$$\frac{1}{n} Y_n = \frac{1}{n} \sum_{k=1}^n X_k \rightarrow \mu \quad \text{as } n \rightarrow \infty$$

in distribution (i.e. the distr. fct. of Y_n converges to $\mathbb{1}_{[\mu, \infty)}(x)$ for $x \neq \mu$).

Theorem 1.3 (Central limit theorem (CLT))

Let $X_1, X_2, \dots \in \mathbb{R}$ be a sequence of iidrv's with $\mu := \mathbb{E}[X_k] < \infty$ and $\sigma^2 := \text{var}[X_k] < \infty$. Then

$$\frac{Y_n - n\mu}{\sigma\sqrt{n}} = \frac{1}{\sigma\sqrt{n}} \sum_{k=1}^n (X_k - \mu) \rightarrow \xi \quad \text{as } n \rightarrow \infty$$

in distr., where $\xi \sim N(0, 1)$ is a **standard Gaussian** with PDF $f(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$.

Expansion. as $n \rightarrow \infty$, $\sum_{k=1}^n X_k = n\mu + \sqrt{n}\sigma\xi + o(\sqrt{n})$, $\xi \sim N(0, 1)$

1. Discrete-time Markov processes

Definition 1.4

A **discrete-time stochastic process** with **state space** S is a sequence $Y_0, Y_1, \dots = (Y_n : n \in \mathbb{N}_0)$ of random variables taking values in S .

The process is called **Markov**, if for all $A \subseteq S$, $n \in \mathbb{N}_0$ and $s_0, \dots, s_n \in S$

$$\mathbb{P}(Y_{n+1} \in A | Y_n = s_n, \dots, Y_0 = s_0) = \mathbb{P}(Y_{n+1} \in A | Y_n = s_n).$$

A Markov process (MP) is called **homogeneous** if for all $A \subseteq S$, $n \in \mathbb{N}_0$ and $s \in S$

$$\mathbb{P}(Y_{n+1} \in A | Y_n = s) = \mathbb{P}(Y_1 \in A | Y_0 = s).$$

If S is discrete, the MP is called a **Markov chain (MC)**.

The generic probability space Ω is the **path space**

$$\Omega = D(\mathbb{N}_0, S) := S^{\mathbb{N}_0} = S \times S \times \dots$$

which is uncountable even when S is finite. For a given $\omega \in \Omega$ the function $n \mapsto Y_n(\omega)$ is called a **sample path**.

Up to finite time N and with finite S , $\Omega_N = S^{N+1}$ is finite.

1. Discrete-time Markov processes

Examples.

- For the simple random walk we have state space $S = \mathbb{Z}$ and $Y_0 = 0$. Up to time N , \mathbb{P} is a distribution on the finite path space Ω_N with

$$\mathbb{P}(\omega) = \begin{cases} p^{\# \text{ of up-steps}} q^{\# \text{ of down-steps}}, & \text{path } \omega \text{ possible} \\ 0 & \text{path } \omega \text{ not possible} \end{cases}$$

There are only 2^N paths in Ω_N with non-zero probability.

For $p = q = 1/2$ they all have the same probability $(1/2)^N$.

- For the generalized random walk with $Y_0 = 0$ and increments $Y_{n+1} - Y_n \in \mathbb{R}$, we have $S = \mathbb{R}$ and $\Omega_N = \mathbb{R}^N$ with an uncountable number of possible paths.
- A sequence $Y_0, Y_1, \dots \in S$ of iidrv's is also a Markov process with state space S .
- Let $S = \{1, \dots, 52\}$ be a deck of cards, and Y_1, \dots, Y_{52} be the cards drawn at random without replacement. Is this a Markov process?

1. Discrete-time Markov chains

Proposition 1.4

Let $(X_n : n \in \mathbb{N}_0)$ be a homogeneous DTMC with **discrete** state space S . Then the **transition function**

$$p_n(x, y) := \mathbb{P}[X_n = y | X_0 = x] = \mathbb{P}[X_{k+n} = y | X_k = x] \quad \text{for all } k \geq 0$$

is well defined and fulfills the **Chapman Kolmogorov equations**

$$p_{k+n}(x, y) = \sum_{z \in S} p_k(x, z) p_n(z, y) \quad \text{for all } k, n \geq 0, x, y \in S.$$

Proof. We use the law of total probability, the Markov property and homogeneity

$$\begin{aligned} \mathbb{P}[X_{k+n} = y | X_0 = x] &= \sum_{z \in S} \mathbb{P}[X_{k+n} = y | X_k = z, X_0 = x] \mathbb{P}[X_k = z | X_0 = x] \\ &= \sum_{z \in S} \mathbb{P}[X_{k+n} = y | X_k = z] \mathbb{P}[X_k = z | X_0 = x] \\ &= \sum_{z \in S} \mathbb{P}[X_n = y | X_0 = z] \mathbb{P}[X_k = z | X_0 = x] \end{aligned}$$

1. Markov chains

- In matrix form with $P_n = (p_n(x, y) : x, y \in S)$ the Chapman Kolmogorov equations read

$$P_{n+k} = P_n P_k \quad \text{and in particular} \quad P_{n+1} = P_n P_1 .$$

With $P_0 = \mathbb{I}$, the obvious solution to this recursion is

$$P_n = P^n \quad \text{where we write} \quad P_1 = P = (p(x, y) : x, y \in S) .$$

- The **transition matrix** P and the initial condition $X_0 \in S$ completely determine a homogeneous DTMC, since for all $k \geq 1$ and all events $A_1, \dots, A_k \subseteq S$

$$\mathbb{P}[X_1 \in A_1, \dots, X_k \in A_k] = \sum_{s_1 \in A_1} \cdots \sum_{s_k \in A_k} p(X_0, s_1) p(s_1, s_2) \cdots p(s_{k-1}, s_k) .$$

- Fixed X_0 can be replaced by an **initial distribution** $\pi_0(x) := \mathbb{P}[X_0 = x]$.

The distribution at time n is then

$$\pi_n(x) = \sum_{y \in S} \sum_{s_1 \in S} \cdots \sum_{s_{n-1} \in S} \pi_0(y) p(y, s_1) \cdots p(s_{n-1}, x) \quad \text{or} \quad \langle \pi_n | = \langle \pi_0 | P^n .$$

1. Transition matrices

The transition matrix P is **stochastic**, i.e.

$$p(x,y) \in [0, 1] \quad \text{and} \quad \sum_y p(x,y) = 1 ,$$

or equivalently, the column vector $|1\rangle = (1, \dots, 1)^T$

is **eigenvector** with **eigenvalue** 1: $P|1\rangle = |1\rangle$

Example 1 (Random walk with boundaries)

Let $(X_n : n \in \mathbb{N}_0)$ be a SRW on $S = \{1, \dots, L\}$ with $p(x,y) = p\delta_{y,x+1} + q\delta_{y,x-1}$.

The boundary conditions are

- **periodic** if $p(L, 1) = p$, $p(1, L) = q$,
- **absorbing** if $p(L, L) = 1$, $p(1, 1) = 1$,
- **closed** if $p(1, 1) = q$, $p(L, L) = p$,
- **reflecting** if $p(1, 2) = 1$, $p(L, L-1) = 1$.

1. Stationary distributions

Definition 1.5

Let $(X_n : n \in \mathbb{N}_0)$ be a homogeneous DTMC with state space S . The distribution $\pi(x)$, $x \in S$ is called **stationary** if for all $y \in S$

$$\sum_{x \in S} \pi(x)p(x, y) = \pi(y) \quad \text{or} \quad \langle \pi | P = \langle \pi | .$$

π is called **reversible** if it fulfills the **detailed balance** conditions

$$\pi(x)p(x, y) = \pi(y)p(y, x) \quad \text{for all } x, y \in S .$$

- reversibility implies stationarity, since

$$\sum_{x \in S} \pi(x)p(x, y) = \sum_{x \in S} \pi(y)p(y, x) = \pi(y) .$$

- Stationary distributions as row vectors $\langle \pi | = (\pi(x) : x \in S)$ are **left eigenvectors** with **eigenvalue 1**: $\langle \pi | = \langle \pi | P .$

1. Absorbing states

Definition 1.6

A state $s \in S$ is called **absorbing** for a DTMC with transition matrix $p(x, y)$, if

$$p(s, y) = \delta_{s,y} \quad \text{for all } y \in S .$$

RW with absorbing BC.

Let h_k be the **absorption probability** for $X_0 = k \in S = \{1, \dots, L\}$,

$$h_k = \mathbb{P}[\text{absorption} | X_0 = k] = \mathbb{P}[X_n \in \{1, L\} \text{ for some } n \geq 0 | X_0 = k] .$$

Conditioning on the first jump and using Markov, we have the recursion

$$h_k = ph_{k+1} + qh_{k-1} \quad \text{for } k = 2, \dots, L-1 ; \quad h_1 = h_L = 1 .$$

Ansatz for solution $h_k = \lambda^k$, $\lambda \in \mathbb{C}$:

$$\lambda = p\lambda^2 + q \quad \Rightarrow \quad \lambda_1 = 1, \quad \lambda_2 = q/p$$

General solution of 2nd order linear recursion

$$h_k = a\lambda_1^k + b\lambda_2^k = a + b(q/p)^k, \quad a, b \in \mathbb{R} .$$

Determine coefficients from boundary condition $\Rightarrow h_k \equiv 1$

1. Distribution at time n

Consider a DTMC on a finite state space with $|S| = L$, and let $\lambda_1, \dots, \lambda_L \in \mathbb{C}$ be the **eigenvalues** of the transition matrix P with corresponding

left (row) eigenvectors $\langle u_i |$ and **right (column) eigenvectors** $|v_i\rangle$

in bra-ket notation. Assuming that **all eigenvalues are distinct** we have

$$P = \sum_{i=1}^L \lambda_i |v_i\rangle \langle u_i| \quad \text{and} \quad P^n = \sum_{i=1}^L \lambda_i^n |v_i\rangle \langle u_i|$$

since eigenvectors can be chosen **orthonormal** $\langle u_i | v_j \rangle = \delta_{ij}$.

Since $\langle \pi_n | = \langle \pi_0 | P^n$ we get

$$\langle \pi_n | = \langle \pi_0 | v_1 \rangle \lambda_1^n \langle u_1 | + \dots + \langle \pi_0 | v_L \rangle \lambda_L^n \langle u_L | .$$

- The **Gershgorin theorem** implies that $|\lambda_i| \leq 1$ and contributions with $|\lambda_i| < 1$ decay exponentially (see hand-out 1).
- $\lambda_1 = 1$ corresponds to the **stationary distribution** $\langle \pi | = \langle u_1 |$ and $|v_1\rangle = |1\rangle$.
- Other $\mathbb{C} \ni \lambda_i \neq 1$ with $|\lambda_i| = 1$ correspond to **persistent oscillations**.

1. Lazy Markov chains

Definition 1.7

Let $(X_n : n \in \mathbb{N}_0)$ be a DTMC with transition matrix $p(x, y)$. The DTMC with transition matrix

$$p^\epsilon(x, y) = \epsilon \delta_{x,y} + (1 - \epsilon) p(x, y), \quad \epsilon \in (0, 1)$$

is called a **lazy version** of the original chain.

- P^ϵ has the **same eigenvectors** as P with eigenvalues $\lambda_i^\epsilon = \lambda_i(1-\epsilon) + \epsilon$ since

$$\langle u_i | P^\epsilon = \epsilon \langle u_i | + \lambda_i(1-\epsilon) \langle u_i | \quad (\text{analogously for } |v_i\rangle)$$

- This implies $|\lambda_i^\epsilon| < |\lambda_i| \leq 1$ unless $\lambda_i = 1$.
Such a matrix P^ϵ is called **aperiodic**, and there are no persistent oscillations.
- The stationary distribution is unique if and only if the eigenvalue $\lambda = 1$ is unique (has multiplicity 1), which is independent of laziness (discussed later).

2. Continuous-time Markov chains

Definition 2.1

A **continuous-time stochastic process** with **state space** S is a family $(X_t : t \geq 0)$ of random variables taking values in S . The process is called **Markov**, if for all $A \subseteq S$, $n \in \mathbb{N}$, $t_1 < \dots < t_{n+1} \in [0, \infty)$ and $s_1, \dots, s_n \in S$

$$\mathbb{P}(X_{t_{n+1}} \in A | X_{t_n} = s_n, \dots, X_{t_1} = s_1) = \mathbb{P}(X_{t_{n+1}} \in A | X_{t_n} = s_n).$$

A Markov process (MP) is called **homogeneous** if for all $A \subseteq S$, $t, u > 0$ and $s \in S$

$$\mathbb{P}(X_{t+u} \in A | X_u = s) = \mathbb{P}(X_t \in A | X_0 = s).$$

If S is discrete, the MP is called a continuous-time **Markov chain (CTMC)**.

The generic probability space Ω of a CTMC is the space of **right-continuous paths**

$$\Omega = D([0, \infty), S) := \left\{ X : [0, \infty) \rightarrow S \mid X_t = \lim_{u \searrow t} X_u \right\}$$

\mathbb{P} is a probability distribution on Ω , which by **Kolmogorov's extension theorem** is fully specified by its **finite dimensional distributions (FDDs)** of the form

$$\mathbb{P}[X_{t_1} \in A_1, \dots, X_{t_n} \in A_n], \quad n \in \mathbb{N}, t_i \in [0, \infty), A_i \subseteq S.$$

2. Continuous-time Markov chains

Proposition 2.1

Let $(X_t : t \geq 0)$ be a homogeneous CTMC with state space S . Then for all $t \geq 0$ the **transition function**

$$p_t(x, y) := \mathbb{P}[X_t = y | X_0 = x] = \mathbb{P}[X_{t+u} = y | X_u = x] \quad \text{for all } u \geq 0$$

is well defined and fulfills the **Chapman Kolmogorov equations**

$$p_{t+u}(x, y) = \sum_{z \in S} p_t(x, z) p_u(z, y) \quad \text{for all } t, u \geq 0, x, y \in S.$$

In matrix notation $P_t = (p_t(x, y) : x, y \in S)$ we get

$$P_{t+u} = P_t P_u \quad \text{with} \quad P_0 = \mathbb{I}.$$

In particular $\frac{P_{t+\Delta t} - P_t}{\Delta t} = P_t \frac{P_{\Delta t} - \mathbb{I}}{\Delta t} = \frac{P_{\Delta t} - \mathbb{I}}{\Delta t} P_t,$

taking $\Delta t \searrow 0$ we get the so-called **forward and backward equations**

$$\frac{d}{dt} P_t = P_t G = G P_t, \quad \text{where} \quad G = \left. \frac{dP_t}{dt} \right|_{t=0}$$

is called the **generator** of the process (sometimes also Q -matrix).

2. Continuous-time Markov chains

- The solution is given by the matrix exponential

$$P_t = \exp(tG) = \sum_{k=0}^{\infty} \frac{t^k}{k!} G^k = \mathbb{I} + tG + \frac{t^2}{2} G^2 + \dots \quad (2.1)$$

- The **distribution π_t at time $t > 0$** is then given by

$$\langle \pi_t | = \langle \pi_0 | \exp(tG) \quad \text{which solves} \quad \frac{d}{dt} \langle \pi_t | = \langle \pi_t | G. \quad (2.2)$$

- On a finite state space with $\lambda_1, \dots, \lambda_L \in \mathbb{C}$ eigenvalues of G , P_t **has eigenvalues** $\exp(t\lambda_i)$ with the same eigenvectors $\langle v_i |$, $|u_i\rangle$.

If the λ_i are distinct, we can expand the initial condition in the eigenvector basis

$$\langle \pi_0 | = \alpha_1 \langle v_1 | + \dots + \alpha_L \langle v_L |,$$

where $\alpha_i = \langle \pi_0 | u_i \rangle$. This leads to

$$\langle \pi_t | = \alpha_1 \langle v_1 | e^{\lambda_1 t} + \dots + \alpha_L \langle v_L | e^{\lambda_L t}. \quad (2.3)$$

2. Continuous-time Markov chains

- using (2.1) we have for $G = (g(x, y) : x, y \in S)$

$$p_{\Delta t}(x, y) = g(x, y)\Delta t + o(\Delta t) \quad \text{for all } x \neq y \in S .$$

So $g(x, y) \geq 0$ can be interpreted as **transition rates**.

$$p_{\Delta t}(x, x) = 1 + g(x, x)\Delta t + o(\Delta t) \quad \text{for all } x \in S ,$$

and since $\sum_y p_{\Delta t}(x, y) = 1$ this implies that

$$g(x, x) = - \sum_{y \neq x} g(x, y) \leq 0 \quad \text{for all } x \in S .$$

- (2.2) can then be written intuitively as the **Master equation**

$$\frac{d}{dt} \pi_t(x) = \underbrace{\sum_{y \neq x} \pi_t(y) g(y, x)}_{\text{gain term}} - \underbrace{\sum_{y \neq x} \pi_t(x) g(x, y)}_{\text{loss term}} \quad \text{for all } x \in S .$$

- The Gershgorin theorem now implies that either $\lambda_i = 0$ or $\text{Re}(\lambda_i) < 0$ for the eigenvalues of G , so there are **no persistent oscillations for CTMCs**.

2. Stationary distributions

Definition 2.2

Let $(X_t : t \geq 0)$ be a homogeneous CTMC with state space S . The distribution $\pi(x)$, $x \in S$ is called **stationary** if $\langle \pi | G = \langle 0 |$, or for all $y \in S$

$$\sum_{x \in S} \pi(x)g(x, y) = \sum_{x \neq y} (\pi(x)g(x, y) - \pi(y)g(y, x)) = 0. \quad (2.4)$$

π is called **reversible** if it fulfills the **detailed balance conditions**

$$\pi(x)g(x, y) = \pi(y)g(y, x) \quad \text{for all } x, y \in S. \quad (2.5)$$

- again, **reversibility implies stationarity**, since with (2.5) every single term in the sum (2.4) vanishes
- Stationary distributions are left **eigenvectors** of G with **eigenvalue** 0 .
- $\langle \pi | G = \langle 0 |$ implies $\langle \pi | P_t = \langle \pi | (\mathbb{I} + \sum_{k \geq 1} t^k G^k / k!) = \langle \pi |$ for all $t \geq 0$

2. Stationary distributions

Proposition 2.2 (Existence)

A DTMC or CTMC with **finite** state space S has **at least one** stationary distribution.

Proof. Since P and G have row sum 1 and 0 we have $P|\mathbf{1}\rangle = |\mathbf{1}\rangle$ and $G|\mathbf{1}\rangle = |\mathbf{0}\rangle$. So 1 and 0 are eigenvalues, and left eigenvectors can be shown to have non-negative entries and thus can be normalized to be stationary distributions $\langle \pi |$. \square

Remark. If S is countably infinite, stationary distributions may not exist, as for example for the SRW on \mathbb{Z} or the Poisson process on \mathbb{N} (see later).

Definition 2.3

A CTMC (or DTMC) is called **irreducible**, if for all $x, y \in S$

$$p_t(x, y) > 0 \text{ for some } t > 0 \quad (p_n(x, y) > 0 \text{ for some } n \in \mathbb{N}).$$

Remark. For continuous time irreducibility implies $p_t(x, y) > 0$ for **all** $t > 0$.

2. Stationary distributions

Proposition 2.3 (Uniqueness)

An **irreducible** Markov chain has **at most one** stationary distribution.

Proof. Follows from the **Perron Frobenius theorem**:

Let P be a stochastic matrix ($P = P_t$ for any $t \geq 0$ for CTMCs). Then

- 1 $\lambda_1 = 1$ is an eigenvalue of P , it is singular if and only if the chain is irreducible. Corresponding left and right eigenvectors have non-negative entries.
- 2 if the chain is continuous-time or discrete-time aperiodic, all remaining eigenvalues $\lambda_i \in \mathbb{C}$, $i \neq 1$ satisfy $\text{Re}(\lambda_i) < 0$ or $|\lambda_i| < 1$, respectively

The second part of the Perron Frobenius theorem also implies convergence of the transition functions to the stationary distribution, since

$$p_t(x, y) = \sum_{i=1}^{|S|} \langle \delta_x | u_i \rangle \langle v_i | e^{\lambda_i t} \rightarrow \langle v_1 | = \langle \pi | \quad \text{as } t \rightarrow \infty .$$

2. Sample paths

Sample paths $t \mapsto X_t(\omega)$ are piecewise constant and right-continuous by convention.

For $X_0 = x$, define the **holding time** $W_x := \inf\{t > 0 : X_t \neq x\}$.

Proposition 2.4

$W_x \sim \text{Exp}(|g(x, x)|)$, i.e. it is **exponentially distributed** with mean $1/|g(x, x)|$, and if $|g(x, x)| > 0$ the chain jumps to $y \neq x$ after time W_x with probability $g(x, y)/|g(x, x)|$.

Proof. W_x has the **memoryless property**, i.e. for all $t, u > 0$

$$\mathbb{P}(W_x > t + u | W_x > t) = \mathbb{P}(W_x > t + u | X_t = x) = \mathbb{P}(W_x > u)$$

where we used the Markov property and homogeneity. Therefore

$$\mathbb{P}(W_x > t + u) = \mathbb{P}(W_x > u)\mathbb{P}(W_x > t) \quad \Rightarrow \quad \mathbb{P}(W_x > t) = e^{\gamma t}$$

where $\gamma = \left. \frac{d}{dt} \mathbb{P}(W_x > t) \right|_{t=0} = \lim_{\Delta t \searrow 0} \frac{p_{\Delta t}(x, x) + o(\Delta t) - 1}{\Delta t} = g(x, x) \leq 0$.

Conditioned on leaving the current state shortly, the probability to jump to y is

$$\lim_{\Delta t \searrow 0} \frac{p_{\Delta t}(x, y)}{1 - p_{\Delta t}(x, x)} = \lim_{\Delta t \searrow 0} \frac{\Delta t g(x, y)}{1 - 1 - \Delta t g(x, x)} = \frac{g(x, y)}{-g(x, x)}.$$

2. Sample paths

- the **jump times** J_0, J_1, \dots are defined recursively as

$$J_0 = 0 \quad \text{and} \quad J_{n+1} = \inf\{t > J_n : X_t \neq X_{J_n}\}.$$

- due to right-continuous paths, jump times are **stopping times**, i.e. for all $t \geq 0$, the event $\{J_n \leq t\}$ depends only on $(X_s : 0 \leq s \leq t)$.
- By the **strong Markov property** (allows conditioning on state at stopping time), subsequent holding times and jump probabilities are all independent.
- The **jump chain** $(Y_n : n \in \mathbb{N}_0)$ with $Y_n := X_{J_n}$ is then a discrete-time Markov chain with transition matrix

$$p^Y(x, y) = \begin{cases} 0 & , x = y \\ g(x, y)/|g(x, x)| & , x \neq y \end{cases} \text{ if } g(x, x) < 0 \quad \text{and}$$
$$p^Y(x, y) = \delta_{x,y} \text{ if } g(x, x) = 0 \quad (\text{by convention}).$$

- A **sample path** is constructed by simulating the jump chain $(Y_n : n \in \mathbb{N}_0)$ together with independent **holding times** $(W_{Y_n} : n \in \mathbb{N}_0)$, so that $J_n = \sum_{k=0}^{n-1} W_{Y_k}$

2. Examples

- A **Poisson process** with **rate** λ (short $\text{PP}(\lambda)$) is a CTMC with

$$S = \mathbb{N}_0, X_0 = 0 \quad \text{and} \quad g(x, y) = \lambda \delta_{x+1, y} - \lambda \delta_{x, y} .$$

The $\text{PP}(\lambda)$ has **stationary and independent increments** with

$$\mathbb{P}[X_{t+u} = n + k | X_u = n] = p_t(0, k) = \frac{(\lambda t)^k}{k!} e^{-\lambda t} \quad \text{for all } u, t > 0, k, n \in \mathbb{N}_0$$

since $\pi_t(k) = p_t(0, k)$ solves the Master equation $\frac{d}{dt} \pi_t(k) = (\pi_t G)(k)$.

- A **birth-death chain** with **birth rates** α_x and **death rates** β_x is a CTMC with

$$S = \mathbb{N}_0 \quad \text{and} \quad g(x, y) = \alpha_x \delta_{x+1, y} + \beta_x \delta_{x-1, y} - (\alpha_x + \beta_x) \delta_{x, y} ,$$

where $\beta_0 = 0$.

Special cases include

- ▶ **M/M/1 server queues:** $\alpha_x \equiv \alpha > 0, \beta_x \equiv \beta > 0$ for $x > 1$
- ▶ **M/M/ ∞ server queues:** $\alpha_x \equiv \alpha > 0, \beta_x = x\beta$
- ▶ **population growth model:** $\alpha_x = x\alpha, \beta_x = x\beta$

2. Ergodicity

Definition 2.4

A Markov process is called **ergodic** if it has a unique stationary distribution π and

$$p_t(x, y) = \mathbb{P}[X_t = y | X_0 = x] \rightarrow \pi(y) \quad \text{as } t \rightarrow \infty, \quad \text{for all } x, y \in S.$$

Theorem 2.5

An **irreducible** (aperiodic) MC with finite state space is **ergodic**.

Theorem 2.6 (Ergodic Theorem)

Consider an **ergodic Markov chain** with unique stationary distribution π . Then for every bounded function $f : S \rightarrow \mathbb{R}$ we have with probability 1

$$\frac{1}{T} \int_0^T f(X_t) dt \quad \text{or} \quad \frac{1}{N} \sum_{n=1}^N f(X_n) \rightarrow \mathbb{E}_\pi[f] \quad \text{as } T, N \rightarrow \infty.$$

- for a proof see e.g. [GS], chapter 9.5
- in practice, use relaxation/burn-in time before computing time averages

2. Markov Chain Monte Carlo (MCMC)

Typical problems related to sampling from π on a very large state space S

- Compute **expectations** $\mathbb{E}_{\pi}[f] = \sum_{x \in S} f(x) \pi(x)$
- for **Gibbs measures** $\pi(x) = \frac{1}{Z(\beta)} e^{-\beta H(x)}$ (stoch. mech. problems),
compute **partition function** $Z(\beta) = \sum_{x \in S} e^{-\beta H(x)}$

Use the **ergodic theorem** to estimate expectations by time averages

- assume $\pi(x) > 0$ for all $x \in S$ (otherwise restrict S)
- invent CTMC/DTMC such that π is stationary, e.g. via **detailed balance**

$$\pi(x)g(x, y) = \pi(y)g(y, x) \quad \text{or} \quad \pi(x)p(x, y) = \pi(y)p(y, x)$$

for Gibbs measures $e^{-\beta H(x)} g(x, y) = e^{-\beta H(y)} g(y, x)$

Typically $g(x, y) = q(x, y) a(x, y)$, i.e. **propose move** from x to y with rate $q(x, y) = q(y, x)$ (irreducible on S but 'local'), **accept** with probability $a(x, y)$

- **Heat bath algorithm:** $a(x, y) = \frac{e^{-\beta H(y)}}{e^{-\beta H(x)} + e^{-\beta H(y)}}$
- **Metropolis-Hastings:** $a(x, y) = \begin{cases} 1 & , \text{ if } H(y) \leq H(x) \\ e^{\beta(H(x)-H(y))} & , \text{ if } H(y) > H(x) \end{cases}$

2. Reversibility

Proposition 2.7 (Time reversal)

Let $(X_t : t \in [0, T])$ be a finite state, irreducible CTMC with generator G^X on a compact time interval which is **stationary**, i.e. $X_t \sim \pi$ for $t \in [0, T]$. Then the **time reversed chain**

$$(Y_t : t \in [0, T]) \quad \text{with} \quad Y_t := X_{T-t}$$

is a stationary CTMC with generator $g^Y(x, y) = \frac{\pi(y)}{\pi(x)} g^X(y, x)$ and stat. prob. π .

- An analogous statement holds for stationary, finite state, irreducible DTMCs

$$\text{with} \quad p^Y(x, y) = \frac{\pi(y)}{\pi(x)} p^X(y, x).$$

- Stationary chains with reversible π are **time-reversible**, $g^Y(x, y) = g^X(x, y)$.
- The definition of stationary chains can be extended to negative times, $(X_t : t \in \mathbb{R})$, with the time reversed chain given by $Y_t := X_{-t}$.
- The time reversal of non-stationary MCs is in general **not** a homogeneous MC, for DTMCs using Bayes' Theorem we get $p^Y(x, y; n) = \frac{\pi_{N-n-1}(y)}{\pi_{N-n}(x)} p^X(y, x)$

2. Countably infinite state space

For infinite state space, Markov chains can get 'lost at infinity' and have no stationary distribution. Let $T_x := \inf\{t > J_1 : X_t = x\}$ be the first **return time** to a state x .

(For DTMCs return times are defined as $T_x := \inf\{n \geq 1 : X_n = x\}$)

Definition 2.5

A state $x \in S$ is called

- **transient**, if $\mathbb{P}[T_x = \infty | X_0 = x] > 0$
- **null recurrent**, if $\mathbb{P}[T_x < \infty | X_0 = x] = 1$ and $\mathbb{E}[T_x | X_0 = x] = \infty$
- **positive recurrent**, if $\mathbb{P}[T_x < \infty | X_0 = x] = 1$ and $\mathbb{E}[T_x | X_0 = x] < \infty$

and these properties partition S into **communicating classes**.

- For an irreducible MC all states are either transient, null or positive recurrent.
- A MC has a **unique stationary distribution if and only if it is positive recurrent**

and in this case
$$\pi(x) = \frac{1}{\mathbb{E}[T_x | X_0 = x]} \mathbb{E} \left[\int_0^{T_x} \mathbb{1}_x(X_s) ds | X_0 = x \right].$$

2. Countably infinite state space

A CTMC with an infinite transient component in S can exhibit **explosion**.

Definition 2.6

For a CTMC define the **explosion time**

$$J_\infty := \lim_{n \rightarrow \infty} J_n \in (0, \infty] \quad \text{where } J_n \text{ are the jump times of the chain.}$$

The chain is called **non-explosive** if $\mathbb{P}[J_\infty = \infty] = 1$, otherwise it is **explosive**.

- If the exit rates are uniformly bounded, i.e. $\sup_{x \in S} |g(x, x)| < \infty$, then the chain is non-explosive, which is always the case if S is finite.
- As an example, consider a **pure birth chain** with $X_0 = 1$ and rates

$$g(x, y) = \alpha_x \delta_{y, x+1} - \alpha_x \delta_{y, x}, \quad x, y \in S = \mathbb{N}_0.$$

If $\alpha_x \rightarrow \infty$ fast enough (e.g. $\alpha_x = x^2$) we get

$$\mathbb{E}[J_\infty] = \sum_{x=1}^{\infty} \mathbb{E}[W_x] = \sum_{x=1}^{\infty} \frac{1}{\alpha_x} < \infty$$

since holding times $W_x \sim \text{Exp}(\alpha_x)$. This implies $\mathbb{P}[J_\infty = \infty] = 0 < 1$.

3. Markov processes with $S = \mathbb{R}$

Proposition 3.1

Let $(X_t : t \geq 0)$ be a homogeneous MP as in Definition 18 with state space $S = \mathbb{R}$. Then for all $t \geq 0$ and (measurable) $A \subseteq \mathbb{R}$ the **transition kernel** for all $x \in \mathbb{R}$

$$P_t(x, A) := \mathbb{P}[X_t \in A | X_0 = x] = \mathbb{P}[X_{t+u} \in A | X_u = x] \quad \text{for all } u \geq 0$$

is well defined. If it is absolutely continuous the **transition density** p_t with

$$P_t(x, A) = \int_A p_t(x, y) dy$$

exists and fulfills the **Chapman Kolmogorov equations**

$$p_{t+u}(x, y) = \int_{\mathbb{R}} p_t(x, z) p_u(z, y) dz \quad \text{for all } t, u \geq 0, x, y \in \mathbb{R}.$$

As for CTMCs, the transition densities and the initial distribution $p_0(x)$ describe all **finite dimensional distributions (fdds)**

$$\mathbb{P}[X_{t_1} \leq x_1, \dots, X_{t_n} \leq x_n] = \int_{\mathbb{R}} dz_0 p_0(z_0) \int_{-\infty}^{x_1} dz_1 p_{t_1}(z_0, z_1) \cdots \int_{-\infty}^{x_n} dz_n p_{t_n - t_{n-1}}(z_{n-1}, z_n)$$

3. Jump processes

$(X_t : t \geq 0)$ is a **jump process** with state space $S = \mathbb{R}$ characterized by a **jump rate density** $r(x, y) \geq 0$ with a uniformly bounded **total exit rate** $R(x) = \int_{\mathbb{R}} r(x, y) dy < \bar{R} < \infty$ for all $x \in \mathbb{R}$.

Ansatz for transition function as $\Delta t \rightarrow 0$:

$$p_{\Delta t}(z, y) = r(z, y)\Delta t + (1 - R(z)\Delta t)\delta(y - z)$$

Then use the Chapman Kolmogorov equations

$$\begin{aligned} p_{t+\Delta t}(x, y) - p_t(x, y) &= \int_{\mathbb{R}} p_t(x, z) p_{\Delta t}(z, y) dz - p_t(x, y) = \\ &= \int_{\mathbb{R}} p_t(x, z) r(z, y) \Delta t dz + \int_{\mathbb{R}} (1 - R(z)\Delta t - 1) p_t(x, z) \delta(y - z) dz \end{aligned}$$

to get the **Kolmogorov-Feller equation** (x is a fixed initial condition)

$$\frac{\partial}{\partial t} p_t(x, y) = \int_{\mathbb{R}} \left(p_t(x, z) r(z, y) - p_t(x, y) r(y, z) \right) dz .$$

As for CTMC sample paths $t \mapsto X_t(\omega)$ are piecewise constant and right-continuous.

3. Gaussian processes

$\mathbf{X} = (X_1, \dots, X_n) \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$ is a **multivariate Gaussian** in \mathbb{R}^n if it has PDF

$$f(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n \det \Sigma}} \exp\left(-\frac{1}{2} \langle \mathbf{x} - \boldsymbol{\mu} | \Sigma^{-1} | \mathbf{x} - \boldsymbol{\mu} \rangle\right),$$

with **mean** $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n) \in \mathbb{R}^n$ and **covariance matrix**

$$\Sigma = (\sigma_{ij} : i, j = 1, \dots, n), \quad \sigma_{ij} = \text{Cov}[X_i, X_j] = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)].$$

Definition 3.1

A stochastic process $(X_t : t \geq 0)$ with state space $S = \mathbb{R}$ is a **Gaussian process** if for all $n \in \mathbb{N}$, $0 \leq t_1 < \dots < t_n$ the vector $(X_{t_1}, \dots, X_{t_n})$ is a multivariate Gaussian.

Proposition 3.2

All fdds of a Gaussian process $(X_t : t \geq 0)$ are fully characterized by the **mean** and the **covariance function**

$$m(t) := \mathbb{E}[X_t] \quad \text{and} \quad \sigma(s, t) := \text{Cov}[X_s, X_t].$$

3. Stationary independent increments

Definition 3.2

A stochastic process $(X_t : t \geq 0)$ has **stationary increments** if

$$X_t - X_s \sim X_{t-s} - X_0 \quad \text{for all } 0 \leq s \leq t.$$

It has **independent increments** if for all $n \geq 1$ and $0 \leq t_1 < \dots < t_n$

$$\{X_{t_{k+1}} - X_{t_k} : 1 \leq k < n\} \quad \text{are independent.}$$

Example. The Poisson process $(N_t : t \geq 0) \sim PP(\lambda)$ has stationary independent increments with $N_t - N_s \sim \text{Poi}(\lambda(t-s))$.

Proposition 3.3

The following two statements are equivalent for a stochastic process $(X_t : t \geq 0)$:

- X_t has stationary independent increments and $X_t \sim \mathcal{N}(0, t)$ for all $t \geq 0$.
- X_t is a Gaussian process with $m(t) = 0$ and $\sigma(s, t) = \min\{s, t\}$.

Stationary independent incr. have **stable distributions** such as Gaussian or Poisson.

3. Brownian motion

Definition 3.3

Standard Brownian motion $(B_t : t \geq 0)$ is a stochastic process that satisfies either of the two equivalent properties in Proposition 3.3 and has **continuous paths**, i.e.

$$\mathbb{P}[\{\omega : t \mapsto B_t(\omega) \text{ is continuous in } t \geq 0\}] = 1 .$$

Theorem 3.4 (Wiener 1923)

There exists a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ on which standard Brownian motion exists.

Proof idea.* Construction on $\Omega = \mathbb{R}^{[0, \infty)}$, using **Kolmogorov's extension theorem**:

For every 'consistent' description of finite dimensional distributions (fdds) there exists a 'canonical' process $X_t[\omega] = \omega(t)$ characterized by a law \mathbb{P} on Ω .

The main problem is to show that there exists a 'version' of the process that has continuous paths, i.e. \mathbb{P} can be chosen to concentrate on continuous paths ω .

Remark.* Construction of $(N_t : t \geq 0) \sim PP(\lambda)$ is

$$N_t := \max \{k \geq 1 : \tau_1 + \dots + \tau_k \leq t\}, \quad \tau_1, \tau_2, \dots \sim \text{Exp}(\lambda) \text{ iidrvs}$$

3. Properties of Brownian motion

- SBM is a time-homogeneous MP with $B_0 = 0$.
- $\sigma B_t + x$ with $\sigma > 0$ is a (general) BM with $B_t \sim \mathcal{N}(x, \sigma^2 t)$.
The transition density is given by a Gaussian PDF

$$p_t(x, y) = \frac{1}{\sqrt{2\pi\sigma^2 t}} \exp\left(-\frac{(y-x)^2}{2\sigma^2 t}\right)$$

This is also called the **heat kernel**, since it solves the **heat/diffusion equation**

$$\frac{\partial}{\partial t} p_t(x, y) = \frac{\sigma^2}{2} \frac{\partial^2}{\partial y^2} p_t(x, y) \quad \text{with} \quad p_0(x, y) = \delta(y - x).$$

- SBM is **self-similar** with **Hurst exponent** $H = 1/2$, i.e.

$$(B_{\lambda t} : t \geq 0) \sim \lambda^H (B_t : t \geq 0) \quad \text{for all } \lambda > 0.$$

- $t \mapsto B_t$ is $\mathbb{P} - a.s.$ **not differentiable** at t for all $t \geq 0$.

For fixed $h > 0$ define $\xi_t^h := (B_{t+h} - B_t)/h \sim \mathcal{N}(0, 1/h)$, which is a mean-0

Gaussian process with covariance $\sigma(s, t) = \begin{cases} 0 & , |t - s| > h \\ (h - |t - s|)/h^2 & , |t - s| < h \end{cases}$.

The (non-existent) derivative $\xi_t := \lim_{h \rightarrow 0} \xi_t^h$ is called **white noise** and is formally a mean-0 Gaussian process with covariance $\sigma(s, t) = \delta(t - s)$.

3. Generators as operators

For a **CTMC** $(X_t : t \geq 0)$ with discrete state space S we have for $f : S \rightarrow \mathbb{R}$

$$\mathbb{E}[f(X_t)] = \sum_{x \in S} \pi_t(x) f(x) = \langle \pi_t | f \rangle \quad \text{and} \quad \underbrace{\frac{d}{dt} \langle \pi_t |}_{\text{master equation}} = \langle \pi_t | G$$

Therefore $\frac{d}{dt} \mathbb{E}[f(X_t)] = \frac{d}{dt} \langle \pi_t | f \rangle = \langle \pi_t | G f \rangle = \mathbb{E}[(Gf)(X_t)]$.

The **generator** G can be defined as an operator G acting on functions $f : S \rightarrow \mathbb{R}$

$$G|f\rangle(x) = (Gf)(x) = \sum_{y \neq x} g(x, y) [f(y) - f(x)].$$

For **Brownian motion** use the **heat eq.** and integration by parts for $f \in C^2(\mathbb{R})$

$$\frac{d}{dt} \mathbb{E}_x[f(X_t)] = \int_{\mathbb{R}} \partial_t p_t(x, y) f(y) dy = \frac{\sigma^2}{2} \int_{\mathbb{R}} \partial_y^2 p_t(x, y) f(y) dy = \mathbb{E}_x[(\mathcal{L}f)(X_t)]$$

where the **generator of BM** is $(\mathcal{L}f)(x) = \frac{\sigma^2}{2} \Delta f(x)$ (or $\frac{\sigma^2}{2} f''(x)$).

For **jump processes** with $S = \mathbb{R}$ and rate density $r(x, y)$ the generator is

$$(\mathcal{L}f)(x) = \int_{\mathbb{R}} r(x, y) [f(y) - f(x)] dy.$$

3. Brownian motion as scaling limit

Proposition 3.5

Let $(X_t : t \geq 0)$ be a jump process on \mathbb{R} with **translation invariant rates** $r(x, y) = q(y - x)$ which have

$$\text{mean zero} \quad \int_{\mathbb{R}} q(z) z \, dz = 0 \quad \text{and}$$

$$\text{finite second moment} \quad \sigma^2 := \int_{\mathbb{R}} q(z) z^2 \, dz < \infty .$$

Then for all $T > 0$ the rescaled process

$$(\epsilon \mathbf{X}_{t/\epsilon^2} : t \in [0, T]) \quad \Rightarrow \quad (\mathbf{B}_t : t \in [0, T]) \quad \text{as } \epsilon \rightarrow 0$$

converges in distribution to a BM with generator $\mathcal{L} = \frac{1}{2}\sigma^2\Delta$ for all $T > 0$.

Proof. Taylor expansion of the generator for test functions $f \in C^3(\mathbb{R})$, and tightness argument for continuity of paths (requires fixed interval $[0, T]$).

3. Diffusion processes

Definition 3.4

A **diffusion process** with **drift** $a(x, t) \in \mathbb{R}$ and **diffusion** $\sigma(x, t) > 0$ is a real-valued process with continuous paths and generator

$$(\mathcal{L}f)(x) = a(x, t)f'(x) + \frac{1}{2}\sigma^2(x, t)f''(x) .$$

Examples.

- The **Ornstein-Uhlenbeck process** is a diffusion process with generator

$$(\mathcal{L}f)(x) = -\alpha xf'(x) + \frac{1}{2}\sigma^2 f''(x) , \quad \alpha, \sigma^2 > 0 .$$

It has a Gaussian stationary distribution $\mathcal{N}(0, \sigma^2/(2\alpha))$.

If the initial distribution π_0 is Gaussian, this is a **Gaussian process**.

- The **Brownian bridge** is a Gaussian diffusion with $X_0 = 0$ and generator

$$(\mathcal{L}f)(x) = -\frac{x}{1-t}f'(x) + \frac{1}{2}f''(x) .$$

Equivalently, it can be characterized as a SBM conditioned on $B_1 = 0$.

3. Diffusion processes

Time evolution of the mean. Use $\frac{d}{dt}\mathbb{E}[f(X_t)] = \mathbb{E}[(\mathcal{L}f)(x_t)]$ with $f(x) = x$

$$\frac{d}{dt}\mathbb{E}[X_t] = \mathbb{E}[a(X_t, t)]$$

Time evolution of the transition density. With $X_0 = x$ we have for $p_t(x, y)$

$$\int_{\mathbb{R}} \frac{\partial}{\partial t} p_t(x, y) f(y) dy = \frac{d}{dt} \mathbb{E}[f(X_t)] = \int_{\mathbb{R}} p_t(x, y) \mathcal{L}f(y) dy \quad \text{for any } f.$$

Use integration by parts to get the **Fokker-Planck equation**

$$\frac{\partial}{\partial t} p_t(x, y) = -\frac{\partial}{\partial y} (a(y, t) p_t(x, y)) + \frac{1}{2} \frac{\partial^2}{\partial y^2} (\sigma^2(y, t) p_t(x, y)).$$

Stationary distributions for time-independent $a(y) \in \mathbb{R}$ and $\sigma^2(y) > 0$

$$\frac{d}{dy} (a(y) p^*(y)) = \frac{1}{2} \frac{d^2}{dy^2} (\sigma^2(y) p^*(y)),$$

leads to a stationary density (modulo normalization fixing $p^*(0)$)

$$p^*(x) = p^*(0) \exp\left(\int_0^x \frac{2a(y) - (\sigma^2)'(y)}{\sigma^2(y)} dy\right).$$

3. Beyond diffusion

Definition 3.5

A **Lévy process** $(X_t : t \geq 0)$ is a real-valued process with right-continuous paths and stationary, independent increments.

The generator has a part with **constant drift** $a \in \mathbb{R}$ and **diffusion** $\sigma^2 \geq 0$

$$\mathcal{L}f(x) = af'(x) + \frac{\sigma^2}{2}f''(x) + \int_{\mathbb{R}} \left(f(x+z) - f(x) - zf'(x)\mathbb{1}_{(0,1)}(|z|) \right) q(z) dz,$$

and a translation invariant **jump part** with density $q(z)$ (or measure $\nu(dz)$)

and fulfills $\int_{|z|>1} q(z) dz < \infty$ and $\int_{0<|z|<1} z^2 q(z) dz < \infty$.

- Diffusion processes, in particular **BM** with $a = 0$, $\sigma^2 > 0$ and $q(z) \equiv 0$, or jump processes, in particular **Poisson** with $a = \sigma = 0$ and $q(z) = \lambda\delta(z-1)$.
- For $a = \sigma = 0$ and heavy-tailed jump distribution

$$q(z) = \frac{C}{|z|^{1+\alpha}} \quad \text{with } C > 0 \text{ and } \alpha \in (0, 2]$$

the process is called **α -stable symmetric Lévy process** or **Lévy flight**.

self-similar $(X_{\lambda t} : t \geq 0) \sim \lambda^H (X_t : t \geq 0)$, $\lambda > 0$ with $H = 1/\alpha$

\Rightarrow **super-diffusive behaviour** with $\mathbb{E}[X_t^2] \propto t^{2/\alpha}$

3. Beyond diffusion

In general, a process $(X_t : t \geq 0)$ is said to exhibit **anomalous diffusion** if

$$\text{Var}[X_t]/t \rightarrow \begin{cases} 0 & , \text{ sub-diffusive} \\ \infty & , \text{ super-diffusive} \end{cases} \quad \text{as } t \rightarrow \infty .$$

Definition 3.6

A **fractional Brownian motion (fBM)** $(B_t^H : t \geq 0)$ with **Hurst index** $H \in (0, 1)$ is a **mean-zero Gaussian process** with continuous paths, $B_0^H = 0$ and **covariances**

$$\mathbb{E}[B_t^H B_s^H] = \frac{1}{2} \left(t^{2H} + s^{2H} - |t - s|^{2H} \right) \quad \text{for all } s, t \geq 0 .$$

- For $H = 1/2$, fBM is standard Brownian motion.
- fBM has stationary Gaussian increments where for all $t > s \geq 0$

$$B_t^H - B_s^H \sim B_{t-s}^H \sim \mathcal{N}(0, (t-s)^{2H}) ,$$

which for $H \neq 1/2$ are **not** independent and the process is **non-Markov**.

- fBM is **self-similar**, i.e. $(B_{\lambda t}^H : t \geq 0) \sim \lambda^H (B_t^H : t \geq 0)$ for all $\lambda > 0$.

3. Fractional BM and noise

- fBM exhibits **anomalous diffusion** with $\text{Var}[B_t^H] = t^{2H}$
- $H > 1/2$: super-diffusive with positively correlated increments
- $H < 1/2$: sub-diffusive with negatively correlated increments

$$\mathbb{E}[B_1^H (B_{t+1}^H - B_t^H)] = \frac{(t+1)^{2H} - 2t^{2H} + (t-1)^{2H}}{2} \underset{t \rightarrow \infty}{\simeq} H(2H-1)t^{2(H-1)}$$

For a **stationary process** $(X_t : t \geq 0)$ on \mathbb{R} define the **autocorrelation/covariance fct**

$$c(t) := \text{Cov}[X_s, X_{s+t}] \quad \text{for all } s, t \in \mathbb{R}.$$

Its Fourier transform is the **spectral density** $S(\omega) := \int_{\mathbb{R}} c(t) e^{-i\omega t} dt$

- **white noise** $(\xi_t : t \geq 0)$, stationary GP with mean zero and

$$c(t) = \delta(t) \quad \Rightarrow \quad S(\omega) \equiv 1.$$

- **fractional or 1/f noise** $(\xi_t^H : t \geq 0)$, stationary GP with mean zero and

$$c(t) = \frac{2H(2H-1)}{|t|^{2(1-H)}} \quad \Rightarrow \quad S(\omega) \propto |\omega|^{2(1-H)-1} = \frac{1}{\omega^{2H-1}}$$

3. SDEs and Itô's formula

Let $(B_t : t \geq 0)$ be a standard BM. Then a diffusion process with drift $a(x, t)$ and diffusion $\sigma(x, t)$ solves the **Stochastic differential equation (SDE)**

$$dX_t = a(X_t, t)dt + \sigma(X_t, t)dB_t .$$

Here dB_t is white noise, interpreted in integrated form as

$$X_t - X_0 = \int_0^t a(X_s, s)ds + \int_0^t \sigma(X_s, s)dB_s .$$

Theorem 3.6 (Itô's formula for diffusions)

Let $(X_t : t \geq 0)$ be a diffusion with generator \mathcal{L} and $f : \mathbb{R} \rightarrow \mathbb{R}$ a smooth. Then

$$f(X_t) - f(X_0) = \int_0^t (\mathcal{L}f)(X_s)ds + \int_0^t \sigma(X_s, s)f'(X_s)dB_s .$$

or, equivalently in terms of SDEs

$$df(X_t) = a(X_t, t)f'(X_t)dt + \frac{1}{2}\sigma^2(X_t, t)f''(X_t)dt + \sigma(X_t, t)f'(X_t)dB_t .$$

3. SDEs and Itô's formula

Itô's formula for diffusions implies the following.

Proposition 3.7

Let $(X_t : t \geq 0)$ be a diffusion process with drift $a(x, t)$ and diffusion $\sigma(x, t)$, and $f : \mathbb{R} \rightarrow \mathbb{R}$ a smooth invertible function. Then $(Y_t : t \geq 0)$ with $Y_t = f(X_t)$ is a diffusion process with $(x = f^{-1}(y))$

$$\mathbf{drift} \quad a(x, t)f'(x) + \frac{1}{2}\sigma^2(x, t)f''(x) \quad \text{and} \quad \mathbf{diffusion} \quad \sigma(x, t)f'(x) .$$

Geometric BM. $Y_t := e^{\theta B_t}$, so $f(x) = e^{\theta x}$ with $f'(x) = \theta f(x)$ and $f''(x) = \theta^2 f(x)$, where $(B_t : t \geq 0)$ is standard BM with $a \equiv 0$, $\sigma^2 \equiv 1$ and $\theta \in \mathbb{R}$.

Then $(Y_t : t \geq 0)$ is a diffusion process with SDE $dY_t = \frac{\theta}{2}Y_t dt + \theta Y_t dB_t$.

Exponential martingale.

$Z_t := e^{\theta B_t - \theta^2 t/2}$, so $f(x, t) = e^{\theta x - \theta^2 t/2}$ and $\partial_t f(x, t) = -\frac{\theta^2}{2}f(x, t)$

Then $dZ_t = \frac{\theta}{2}Z_t dt - \frac{\theta}{2}Z_t dt + \theta Z_t dB_t = \theta Z_t dB_t$

and $(Z_t : t \geq 0)$ is a **martingale** (see next slide) with $\mathbb{E}[Z_t] \equiv Z_0 = 1$.

3. Fluctuations and martingales

Definition 3.7

A real-valued stochastic process $(M_t : t \geq 0)$ is a **martingale** w.r.t. the process $(X_t : t \geq 0)$ if for all $t \geq 0$ we have $\mathbb{E}[|M_t|] < \infty$ and

$$\mathbb{E}[M_t | \{X_u : 0 \leq u \leq s\}] = M_s \quad \text{a.s. for all } s \leq t.$$

If in addition $\mathbb{E}[M_t^2] < \infty$, there exists a unique increasing process $([M]_t : t \geq 0)$ called the **quadratic variation**, with $[M]_0 = 0$ and such that $M_t^2 - [M]_t$ is martingale.

Theorem 3.8 (Itô's formula)

Let $(X_t : t \geq 0)$ be a Markov process on state space S with generator \mathcal{L} . Then for any smooth enough $f : S \times [0, \infty) \rightarrow \mathbb{R}$

$$f(X_t, t) - f(X_0, 0) = \int_0^t (\mathcal{L}f)(X_s, s) ds + \int_0^t \partial_s f(X_s, s) ds + M_t^f,$$

where $(M_t^f : t \geq 0)$ is a martingale w.r.t. $(X_t : t \geq 0)$ with $M_0^f = 0$ and

$$\text{quadratic variation} \quad [M^f]_t = \int_0^t ((\mathcal{L}f^2)(X_s, s) - 2(f\mathcal{L}f)(X_s, s)) ds.$$

3. Fluctuations and martingales

- For a **Poisson process** $(N_t : t \geq 0)$ with rate $\lambda > 0$ Itô's formula implies that

$$M_t := N_t - \lambda t \quad \text{is a martingale with quadr. variation} \quad [M]_t = \lambda t .$$

- **Watanabe's characterization of PP:** Let $(N_t : t \geq 0)$ be a **counting process**, i.e. a jump process on $S = \mathbb{N}$ with jump size $+1$ only. If $M_t = N_t - \lambda t$ is a martingale, then $(N_t : t \geq 0) \sim PP(\lambda)$.
- For a **diffusion process**, choosing $f(X_t, t) = X_t$ in Itô's formula leads to

$$X_t - X_0 = \int_0^t a(X_s, s) ds + M_t \quad \text{with} \quad [M]_t = \int_0^t \sigma^2(X_s, s) ds .$$

In particular for BM with $a(x, t) \equiv 0$ and $\sigma^2(x, t) \equiv \sigma^2$ we have

$$(B_t : t \geq 0) \text{ is a martingale with quadratic variation} \quad [B]_t = t .$$

- **Lévy's characterization of BM:** Any continuous martingale $(M_t : t \geq 0)$ on \mathbb{R} with $M_0 = 0$ and quadratic variation $[M]_t = t$ is standard Brownian motion.

Furthermore, **any continuous martingale** $(M_t : t \geq 0)$ **on** \mathbb{R} **with** $M_0 = 0$ **is a continuous (random) time-change of a standard BM**, i.e.

$$(M_t : t \geq 0) \sim (B_{[M]_t} : t \geq 0) \quad \text{for SBM} \quad (B_t : t \geq 0) .$$

3. Fluctuations and martingales

- For a **diffusion process** $(X_t : t \geq 0)$ we have

$$X_t - X_0 = \int_0^t a(X_s, s) ds + M_t \quad \text{with} \quad [M]_t = \int_0^t \sigma^2(X_s, s) ds .$$

with M_t a continuous martingale $\Rightarrow (M_t : t \geq 0) \sim (B_{[M]_t} : t \geq 0)$

- Related time-changed BMs can be written as **stochastic Itô integrals**

$$M_t = \int_0^t \sigma(X_s, s) dB_s := B_{[M]_t} .$$

Therefore $\sigma \equiv 0$ implies **deterministic dynamics** with $M_t \equiv 0$,
(also because $\mathcal{L}f^2 = 2ff'a = 2f\mathcal{L}f$ for all f , so $[M^f]_t \equiv 0$ in Itô's formula)
and the corresponding SDE is an ODE $dX_t/dt = a(X_t, t)$.

Vanishing drift $a \equiv 0$ implies $X_t - X_0 = M_t$ or $dX_t = \sigma(X_t, t)dB_t$
and the process $(X_t : t \geq 0)$ is a **martingale**.

- Recall the **exponential martingale** $e^{\theta B_t - \theta^2 t/2}$ as a non-trivial example.

3. Martingales and conservation laws

Consider a **CTMP** $(X_t : t \geq 0)$ on state space S with **generator** \mathcal{L} , and an **observable** $f : S \rightarrow \mathbb{R}$ such that $\mathcal{L}f : S \rightarrow \mathbb{R}$ is well defined (e.g. $f \in C^2(S, \mathbb{R})$ for diffusions).

Proposition 3.9

If $\mathcal{L}f(x) = 0$ for all $x \in S$, then $f(X_t)$ is a **martingale**, and is **conserved in expectation**, i.e. (for any initial condition X_0)

$$E[f(X_t)] = \mathbb{E}[f(X_0)] \quad \text{for all } t \geq 0 .$$

If in addition $\mathcal{L}f^2(x) = 0$ for all $x \in S$, then $f(X_t)$ is **conserved** (or a **conserved quantity**), i.e. (for any initial condition X_0)

$$f(X_t) = f(X_0) \quad \text{almost surely for all } t \geq 0 .$$

Proof. The first claim follows directly from Itô's formula (Theorem 3.8).

For the second claim, we have $f(X_t) = f(X_0) + M_t^f$ and M_t^f has quadratic variation

$$[M^f]_t = \int_0^t ((\mathcal{L}f^2)(X_s, s) - 2(f\mathcal{L}f)(X_s, s)) ds = 0 ,$$

for all $t \geq 0$, which implies $M_t^f \equiv 0$ almost surely. □

4. Stochastic particle systems

- **lattice/population:** $\Lambda = \{1, \dots, L\}$, finite set of points
- **state space** S is given by the set of all **configurations**

$$\eta = (\eta(i) : i \in \Lambda) \in S = \{0, 1\}^L \quad (\text{often also written } \{0, 1\}^\Lambda).$$

$\eta(i) \in \{0, 1\}$ signifies the presence of a particle/infection at site/individual i .

- Only local transitions are allowed with rates

$$\eta \rightarrow \eta^i \quad \text{with rate} \quad c(\eta, \eta^i) \quad \textbf{(reaction)}$$

$$\eta \rightarrow \eta^{ij} \quad \text{with rate} \quad c(\eta, \eta^{ij}) \quad \textbf{(transport)}$$

$$\text{where } \eta^i(k) = \begin{cases} \eta(k) & , k \neq i \\ 1 - \eta(k) & , k = i \end{cases} \quad \text{and} \quad \eta^{ij}(k) = \begin{cases} \eta(k) & , k \neq i, j \\ \eta(j) & , k = i \\ \eta(i) & , k = j \end{cases}$$

Definition 4.1

A **stochastic particle system** is a CTMC with state space $S = \{0, 1\}^\Lambda$ and generator

$$\mathcal{L}f(\eta) = \sum_{i \in \Lambda} c(\eta, \eta^i) [f(\eta^i) - f(\eta)] \quad \text{or} \quad \mathcal{L}f(\eta) = \sum_{i, j \in \Lambda} c(\eta, \eta^{ij}) [f(\eta^{ij}) - f(\eta)].$$

4. Contact process

The contact process is a simple stochastic model for the **SI epidemic** with **infection rates** $q(i, j) \geq 0$ and uniform **recovery rate** 1.

Definition 4.2

The **contact process (CP)** $(\eta_t : t \geq 0)$ is an IPS with rates

$$c(\eta, \eta^i) = \underbrace{1 \cdot \delta_{\eta(i), 1}}_{\text{recovery}} + \underbrace{\delta_{\eta(i), 0} \sum_{j \neq i} q(j, i) \delta_{\eta(j), 1}}_{\text{infection}} \quad \text{for all } i \in \Lambda .$$

Usually, $q(i, j) = q(j, i) \in \{0, \lambda\}$, i.e. connected individuals infect each other with fixed rate $\lambda > 0$.

- The CP has one absorbing state $\eta(i) = 0$ for all $i \in \Lambda$, which can be reached from every initial configuration. Therefore the process is ergodic and the infection eventually gets **extinct** with probability 1.
- Let $T := \inf\{t > 0 : \eta_t \equiv 0\}$ be the **extinction time**. Then there exists a **critical value (epidemic threshold)** $\lambda_c > 0$ such that (for irreducible $q(i, j)$)

$$\mathbb{E}[T | \eta_0 \equiv 1] \propto \log L \quad \text{for } \lambda < \lambda_c \quad \text{and} \quad \mathbb{E}[T | \eta_0 \equiv 1] \propto e^{cL} \quad \text{for } \lambda > \lambda_c .$$

4. Voter model

The voter model describes opinion dynamics with **influence rates** $q(i, j) \geq 0$ at which individual i persuades j to switch to her/his opinion.

Definition 4.3

The **linear voter model (VM)** $(\eta_t : t \geq 0)$ is an IPS with rates

$$c(\eta, \eta^i) = \sum_{j \neq i} \underbrace{q(j, i) (\delta_{\eta(i), 1} \delta_{\eta(j), 0} + \delta_{\eta(i), 0} \delta_{\eta(j), 1})}_{j \text{ influences } i \text{ if opinions differ}} \quad \text{for all } i \in \Lambda .$$

In non-linear versions the rates can be replaced by general (symmetric) functions.

- The VM is **symmetric** under relabelling opinions $0 \leftrightarrow 1$.
- If $q(i, j)$ is irreducible there are two absorbing states, $\eta \equiv 0, 1$, both of which can be reached from every initial condition. Therefore the VM is not ergodic, and **stationary measures** are

$$\alpha \delta_0 + (1 - \alpha) \delta_1 \quad \text{with } \alpha \in [0, 1] \text{ depending on the initial condition .}$$

- **Coexistence** of both opinions can occur on infinite lattices (e.g. \mathbb{Z}^d for $d \geq 3$).

4. Exclusion process

The exclusion process describes transport of a conserved quantity (e.g. mass or energy) with **transport rates** $q(i,j) \geq 0$ site i to j .

Definition 4.4

The **exclusion process (EP)** $(\eta_t : t \geq 0)$ is an IPS with rates

$$c(\eta, \eta^{ij}) = q(i,j) \delta_{\eta(i),1} \delta_{\eta(j),0} \quad \text{for all } i,j \in \Lambda .$$

The EP is called **simple (SEP)** if jumps occur only between nearest neighbours on Λ . The SEP is **symmetric (SSEP)** if $q(i,j) = q(j,i)$, otherwise **asymmetric (ASEP)**.

- The SEP is mostly studied in a 1D geometry with periodic or open boundaries.
- For periodic boundary conditions the total number of particles $N = \sum_i \eta(i)$ is **conserved**. The process is ergodic on the sub-state space

$$S_N = \left\{ \eta \in \{0, 1\}^L : \sum_i \eta(i) = N \right\}$$

for each value $N = 0, \dots, L$, and has a unique stationary distribution.

- For open boundaries particles can be created and destroyed at the boundary, the system is ergodic on S and has a unique stationary distribution.

4. Mean-field scaling limits

Consider the contact process $(\eta_t : t \geq 0)$ on a **complete graph**, using $\eta(i) \in \{0, 1\}$ we can write the generator as

$$\mathcal{L}f(\eta) = \sum_{i \in \Lambda} \left(\eta(i) + \lambda(1 - \eta(i)) \sum_{j \in \Lambda} \eta(j) \right) [f(\eta^i) - f(\eta)] .$$

For **mean-field observables** such as $N(\eta) := \sum_{i \in \Lambda} \eta(i)$ one can compute for $f : \mathbb{N}_0 \rightarrow \mathbb{R}$ (see problem sheet 3)

$$\mathcal{L}(f \circ N)(\eta) = \lambda(L - N)N[f(N + 1) - f(N)] + N[f(N - 1) - f(N)] ,$$

which shows that $t \mapsto N_t := N(\eta_t)$ is a Markov process with above generator for all L .

Mean-field scaling limit. $L \rightarrow \infty$ with $\lambda L \rightarrow \hat{\lambda}$

then $N_t/L \rightarrow X_t$, which is a **diffusion process** on $[0, 1]$ with generator

$$\mathcal{L}f(x) = (\hat{\lambda}x(1 - x) - x)f'(x) + \frac{1}{2L}(\hat{\lambda}x(1 - x) + x)f''(x)$$

In the limit the diffusion coefficient vanishes and the process is **deterministic** (blue) with leading order diffusive correction (red) and corresponding SDE

$$dX_t = (\hat{\lambda}X_t(1 - X_t) - X_t)dt + \sqrt{\frac{1}{L}(\hat{\lambda}X_t(1 - X_t) + X_t)}dB_t$$

5. Graphs - definition

Definition 5.1

A **graph** (or **network**) $G = (V, E)$ consists of a finite set $V = \{1, \dots, N\}$ of **vertices** (or **nodes, points**), and a set $E \subseteq V \times V$ of **edges** (or **links, lines**).

The graph is called **undirected** if $(i, j) \in E$ implies $(j, i) \in E$, otherwise **directed**.

The structure of the graph is encoded in the **adjacency** (or **connectivity**) **matrix**

$$A = (a_{ij} : i, j \in V) \quad \text{where} \quad a_{ij} = \begin{cases} 1, & (i, j) \in E \\ 0, & (i, j) \notin E \end{cases}.$$

We denote the number of edges by $K = |E|$ for directed, or $K = |E|/2$ for undirected graphs.

- Graphs we consider do not have self edges, i.e. $(i, i) \notin E$ for all $i \in V$, or multiple edges, since edges (i, j) are unique elements of E .
- **Weighted graphs** with edge weights $w_{ij} \in \mathbb{R}$ can be used to represent continuous- or discrete-time Markov chains.
- In general graphs can also be infinite, but we will focus on finite graphs. Many of the following graph characteristics only make sense in the finite case.

5. Graphs - paths and connectivity

Definition 5.2

A **path** γ_{ij} of length $l = |\gamma_{ij}|$ from vertex i to j is sequence of vertices

$$\gamma_{ij} = (v_1 = i, v_2, \dots, v_{l+1} = j) \quad \text{with} \quad (v_k, v_{k+1}) \in E \text{ for all } k = 1, \dots, l,$$

and $v_k \neq v_{k'}$ for all $k \neq k' \in \{1, \dots, l\}$ (i.e. each vertex is visited only once).

If such a path exists, we say that vertex i is **connected** to j (write $i \rightarrow j$).

Shortest paths between vertices i, j are called **geodesics** (not necessarily unique) and their length d_{ij} is called the **distance** from i to j . If $i \not\rightarrow j$ we set $d_{ij} = \infty$.

A graph is **connected** if $d_{ij} < \infty$ for all $i, j \in V$.

The **diameter** and the **characteristic path length** of the graph G are given by

$$\begin{aligned} \text{diam}(G) &:= \max\{d_{ij} : i, j \in V\} \in \mathbb{N}_0 \cup \{\infty\}, \\ L = L(G) &:= \frac{1}{N(N-1)} \sum_{i, j \in V} d_{ij} \in [0, \infty]. \end{aligned}$$

For undirected graphs we have $d_{ij} = d_{ji}$ which is finite if $i \leftrightarrow j$, and they can be decomposed into **connected components**, where we write

$$C_i = \{j \in V : j \leftrightarrow i\} \quad \text{for the component containing vertex } i.$$

5. Graphs - degrees

Definition 5.3

The **in-** and **out-degree** of a node $i \in V$ is defined as

$$k_i^{\text{in}} = \sum_{j \in V} a_{ji} \quad \text{and} \quad k_i^{\text{out}} = \sum_{j \in V} a_{ij} .$$

$k_1^{\text{in}}, \dots, k_N^{\text{in}}$ is called the **in-degree sequence** and the **in-degree distribution** is

$$(p^{\text{in}}(k) : k \in \{0, \dots, K\}) \quad \text{with} \quad p^{\text{in}}(k) = \frac{1}{N} \sum_{i \in V} \delta_{k, k_i^{\text{in}}}$$

giving the fraction of vertices with in-degree k . The same holds for out-degrees, and in undirected networks we simply write $k_i = k_i^{\text{in}} = k_i^{\text{out}}$ and $p(k)$.

- Note that $\sum_{i \in V} k_i = \sum_{i, j \in V} a_{ij} = |E|$ (also for directed), average and variance are

$$\langle k \rangle = \frac{1}{N} \sum_{i \in V} k_i = |E|/N = \sum_k k p(k), \quad \sigma^2 = \langle k^2 \rangle - \langle k \rangle^2 .$$

- In a **regular graph** (usually undirected) all vertices have equal degree $k_i \equiv k$.
- Graphs where the degree distribution shows a power law decay, i.e. $p(k) \propto k^{-\alpha}$ for large k , are often called **scale-free**.

Real-world networks are often scale-free with exponent around $\alpha \approx 3$.

5. Graphs - first examples

Example 2 (Some graphs)

The **complete graph** K_N with N vertices is an undirected graph where all $N(N - 1)/2$ vertices $E = ((i, j) : i \neq j \in V)$ are present.

Regular lattices \mathbb{Z}^d with edges between nearest neighbours are examples of regular graphs with degree $k = 2d$.

Definition 5.4

A **tree** is an undirected graph where any two vertices are connected by exactly one path. Vertices with degree 1 are called **leaves**.

In a **rooted tree** one vertex $i \in V$ is the designated **root**, and the graph can be directed, where all vertices point towards or away from the root.

A **cycle** is a closed path γ_{ii} of length $|\gamma_{ii}| > 2$. G is a tree if and only if

- it is connected and has no cycles;
- it is connected but is not connected if a single edge is removed;
- it has no cycles but a cycle is formed if any edge is added.

5. Graphs - degree correlations

Definition 5.5

For undirected graphs, the **joint degree distribution** of nodes linked by an edge is

$$q(k, k') = \frac{1}{|E|} \sum_{(i,j) \in E} \delta_{k_i, k} \delta_{k_j, k'} = \frac{\sum_{i,j \in V} a_{ij} \delta_{k_i, k} \delta_{k_j, k'}}{\sum_{i,j \in V} a_{ij}} = q(k', k).$$

With the marginal $q(k') = \sum_k q(k, k')$ we have the **conditional degree distribution**

$$q(k|k') = q(k, k')/q(k') \quad \text{with average} \quad k_{nn}(k') := \sum_k k q(k|k').$$

The network is called **uncorrelated** if $k_{nn}(k')$ is independent of k' , **assortative** if $k_{nn}(k') \nearrow$ in k' and **disassortative** if $k_{nn}(k') \searrow$ in k' .

- The marginal $q(k)$ corresponds to **edge biased degree sampling**, i.e.

$$q(k) = \sum_{k'} q(k, k') = \frac{1}{|E|} \sum_{i,j \in V} a_{ij} \delta_{k_i, k} = \frac{N}{|E|} \frac{1}{N} \sum_{i \in V} k_i \delta_{k_i, k} = \frac{kp(k)}{\langle k \rangle}.$$

For uncorrelated networks $q(k|k') = q(k)$ and thus $k_{nn}(k') = \langle k^2 \rangle / \langle k \rangle$.

5. Subgraphs

- The degree of correlation can be quantified by the **correlation coefficient**

$$\chi := \frac{\langle kk' \rangle_q - \langle k \rangle_q^2}{\langle k^2 \rangle_q - \langle k \rangle_q^2} = \frac{\sum_{k,k'} kk' (q(k, k') - q(k)q(k'))}{\sum_k k^2 q(k) - (\sum_k k q(k))^2} \in [-1, 1].$$

Definition 5.6

A **subgraph** $G' = (V', E')$ of $G = (V, E)$ is a graph such that $V' \subseteq V$ and $E' \subseteq E$.

- Small connected subgraphs are also called **motifs**, the simplest non-trivial examples in undirected graphs are connected triples and triangles.
- Fully connected (complete) subgraphs which are maximal with respect to connectedness are called **cliques**.
- A **spanning tree** is a tree subgraph that contains all vertices of the graph.
- A subgraph G' is called a **community**, if (for example)

$$\sum_{i,j \in V'} a_{ij} > \sum_{i \in V', j \notin V'} a_{ij} \quad (\text{there are also other definitions}).$$

5. Clustering

Clustering aims to quantify the probability that two neighbours of a given vertex are themselves neighbours. Two different definitions are used in the literature.

Definition 5.7

The **global clustering coefficient** for an undirected graph is defined as

$$C = \frac{3 \times \# \text{ of (connected) triangles}}{\# \text{ of (connected) triples}} = \frac{3 \sum_{i < j < l} a_{ij} a_{jl} a_{li}}{\sum_{i < j < l} (a_{ij} a_{il} + a_{ji} a_{jl} + a_{li} a_{lj})} \in [0, 1].$$

Alternatively, one can define a **local clustering coefficient**

$$C_i = \frac{\# \text{ of triangles containing vertex } i}{\# \text{ of triples centered on vertex } i} = \frac{\sum_{j < l} a_{ij} a_{jl} a_{li}}{\sum_{j < l} a_{ij} a_{il}} \in [0, 1],$$

and use the average $\langle C_i \rangle = \frac{1}{N} \sum_i C_i$ to quantify clustering.

- For a tree we have $C = \langle C_i \rangle = 0$ and for the complete graph $C = \langle C_i \rangle = 1$.
- Higher-order clustering coefficients can be defined similarly, using different subgraphs as basis.

5. Graph spectra

Definition 5.8

The **spectral density** of a graph $G = (V, E)$ is

$$\rho(\lambda) := \frac{1}{N} \sum_{i \in V} \delta(\lambda - \lambda_i) \quad \text{where } \lambda_1, \dots, \lambda_N \in \mathbb{C}$$

are the eigenvalues of the adjacency matrix A .

- **Perron-Frobenius:** A has a real eigenvalue $\lambda_1 > 0$ with maximal modulus and real, non-negative eigenvector(s). If the graph is connected, it has multiplicity 1 and $|\lambda_j| < \lambda_1$ for all other eigenvalues with $j \neq 1$.
- For undirected graphs, $(A^n)_{ij}$ is equal to the **number of walks** (paths which allow repeated vertices) from i to j of length n . We also have

$$\text{Tr}(A^n) = \sum_{i=1}^N \lambda_i^n \quad \text{and} \quad (\text{Tr}(A))^n = 0,$$

which can be used to derive statements like:

$$\sum_{i < j} \lambda_i \lambda_j = -|E|, \quad \sum_{i < j < l} \lambda_i \lambda_j \lambda_l = 2 \cdot \# \text{ of triangles in } G.$$

5. Graph Laplacian

Definition 5.9

The **Graph Laplacian** for a graph (V, E) with adjacency matrix A is defined as

$$Q := A - D \quad \text{where} \quad D = \left(\delta_{ij} \sum_{l \neq i} a_{il} : i, j \in V \right).$$

- Q has eigenvalues in \mathbb{C} with real part $\text{Re}(\lambda) < 0$ except for $\lambda_1 = 0$, which follows directly from the Gershgorin theorem and vanishing row sums. The **multiplicity of λ_1 equals the number of connected components** in undirected graphs. Properly chosen orthogonal eigenvectors to λ_1 have non-zero entries on the individual connected components. The smaller the second largest real part of an eigenvalue, the harder it is to cut G into separated components by removing edges.
- Q defines a generator matrix of a continuous-time random walk on V with transition rates a_{ij} . Using weighted graphs, any finite state CTMC can be represented in this way.
- The Laplacian determines the first order linearized dynamics of many complex processes on graphs and is therefore of particular importance.

5. The Wigner semi-circle law

Theorem 5.1 (Wigner semi-circle law)

Let $A = (a_{ij} : i, j = 1, \dots, N)$ be a real, symmetric matrix with iid entries a_{ij} for $i \leq j$ with finite moments, and $\mathbb{E}[a_{ij}] = 0$, $\text{var}[a_{ij}] = \sigma^2$ (called a **Wigner matrix**). Then the spectral density ρ_N of the matrix A/\sqrt{N} converges in distribution to

$$\rho_N(\lambda) \rightarrow \rho_{sc}(\lambda) := \begin{cases} (2\pi\sigma^2)^{-1} \sqrt{4\sigma^2 - \lambda^2}, & \text{if } |\lambda| < 2\sigma \\ 0, & \text{otherwise} \end{cases}.$$

- The bulk of eigenvalues of unscaled Wigner matrices typically lies in the interval $[-2\sqrt{N}\sigma, 2\sqrt{N}\sigma]$.
- Adjacency matrices A of $\mathcal{G}_{N,p}$ **random graphs** are symmetric with iid $\text{Be}(p)$ entries with $\mathbb{E}[a_{ij}] = p$ and $\text{var}[a_{ij}] = p(1-p)$, so are not Wigner matrices. A has a maximal **Perron-Frobenius eigenvalue** of order pN , but all other eigenvalues have modulus of order \sqrt{N} .
For fixed $p > 0$ or scaled $p = p_N \gg p_c = 1/N$ the Wigner semi-circle law holds for $N \rightarrow \infty$ with support width $4\sqrt{N}\sigma_N$.
For $p = p_N \ll p_c = 1/N$ the asymptotic spectral density deviates from ρ_{sc} .
- There is a related **circular law** for **non-symmetric Wigner matrices**.

5. More general graphs and networks

- For **multigraphs**, multiple edges between nodes and loops ($a_{ii} > 0$) are allowed.
- **Hypergraphs** (V, E) are generalizations in which an edge can connect any number of vertices. Formally, the set of **hyperedges** $E \subseteq \mathcal{P}(V)$ is a set of non-empty subsets of V .
- In **bipartite graphs** the edge set can be partitioned into two sets $V_1, V_2 \subseteq V$ each non-empty, with no connections within themselves, i.e. $a_{ij} = a_{ji} = 0$ for all $i, j \in V_1$ and also for all $i, j \in V_2$.

Simple undirected examples include regular lattices \mathbb{Z}^d for $d \geq 1$ which are partitioned into sites with even and odd parity. Feed-forward neural networks are examples of directed graphs with bipartite or multi-partite structure.

- **Multilayer networks** $M = (\mathbf{G}, \mathbf{C})$ consist of a family of m (weighted or unweighted) graphs $G_\alpha = (V_\alpha, E_\alpha)$ (called **layers** of M), and the set of interconnections between nodes of different layers

$$\mathbf{C} = \{c_{\alpha,\beta} \subseteq V_\alpha \times V_\beta : \alpha, \beta \in \{1, \dots, m\}, \alpha \neq \beta\}.$$

Real examples include transportation networks or social networks with different types of connections.

6. E-R Random graphs

Definition 6.1

An **(Erdős-Rényi, short E-R) random graph** $G \sim \mathcal{G}_{N,K}$ has uniform distribution on the set of all undirected graphs with N vertices and $K = |E|/2$ edges, i.e.

$$\mathbb{P}_{N,K}[G = (V, E)] = 1 / \binom{N(N-1)/2}{K}.$$

An **(E-R) random graph** $G \sim \mathcal{G}_{N,p}$ has N vertices and each (undirected) edge is present independently with probability $p \in [0, 1]$, i.e.

$$\mathbb{P}_{N,p}[G = (V, E)] = p^{|E|/2} (1-p)^{N(N-1)/2 - |E|/2}.$$

- The ensemble $\mathcal{G}_{N,p}$ is easier to work with and is mostly used in practice, and for N, K large, $\mathcal{G}_{N,K}$ is largely equivalent to $\mathcal{G}_{N,p}$ with $p = 2K/(N(N-1))$.
- Since edges are present independently, graphs $G \in \mathcal{G}_{N,p}$ should typically be uncorrelated. Indeed, one can show that $\chi(G), \mathbb{E}[\chi] \rightarrow 0$ as $N \rightarrow \infty$.

6. E-R Random graphs - properties

- The number of undirected edges for $G \sim \mathcal{G}_{N,p}$ is **random**, $K \sim \text{Bi}\left(\frac{N(N-1)}{2}, p\right)$. For all i by homogeneity, $k_i \sim \text{Bi}(N-1, p)$ and $\mathbb{E}[\langle k \rangle] = \mathbb{E}[k_i] = (N-1)p$.
- The expected number of triangles in a $\mathcal{G}_{N,p}$ graph is $\binom{N}{3}p^3$, and the number of triples is $\binom{N}{3}3p^2$.

Since fluctuations are of lower order, this implies for all $G_N \sim \mathcal{G}_{N,p}$

$$C(G_N) = \frac{3\binom{N}{3}p^3(1+o(1))}{\binom{N}{3}3p^2(1+o(1))} \rightarrow p \quad \text{as } N \rightarrow \infty.$$

- The **expected** degree distribution for $G_N \sim \mathcal{G}_{N,p}$ is $\text{Bi}(N-1, p)$. In the limit $N \rightarrow \infty$ with $p = p_N = z/(N-1)$ keeping $z = \mathbb{E}[\langle k \rangle]$ fixed we have

$$\mathbb{E}[p(k)] = \mathbb{P}[k_i = k] = \binom{N-1}{k} p_N^k (1-p_N)^{N-1-k} \rightarrow \frac{z^k}{k!} e^{-z}.$$

Therefore, E-R $\mathcal{G}_{N,p}$ graphs are sometimes called **Poisson random graphs**.

- In this scaling limit E-R graphs are **locally tree-like**, i.e. connected components

$$C_i^n := \{j \in V : j \leftrightarrow i, d_{ij} \leq n\}, \quad n \text{ fixed}$$

are tree subgraphs as $N \rightarrow \infty$ with probability 1.

Vertex degrees are $k_i \sim \text{Poi}(z)$ and iid $k_j \sim \text{Poi}(z) + 1$.

6. Percolation

Percolation studies robustness of connectivity properties of graphs under deletion of edges or vertices (e.g. random attacks or immunization).

Definition 6.2

Consider a connected, undirected graph $G = (V, E)$. **Bond percolation** is a static probabilistic model with state space

$$S = \Omega = \{0, 1\}^E = \{e_{ij} \in \{0, 1\} : (i, j) \in E\},$$

and distribution $p = \mathbb{P}[e_{ij} = 1] = 1 - \mathbb{P}[e_{ij} = 0]$, i.e. $e_{ij} \sim \text{Be}(p)$ iid with $p \in [0, 1]$. Edges $(i, j) \in E$ are called **open** if $e_{ij} = 1$ and **closed** if $e_{ij} = 0$, and we denote by

$$G^o = (V, E^o) \quad \text{with} \quad E^o = \{(i, j) \in E : e_{ij} = 1\} \subseteq E$$

the (random) subgraph containing only open edges. A sequence of connected graphs G_N of increasing size $|V_N| = N$ exhibits **percolation with parameter p** if

$$|\bar{C}_N^o|/N \geq c > 0 \quad \text{as } N \rightarrow \infty \quad \text{with probability 1,}$$

where $|\bar{C}_N^o| = \max_{i \in V_N} |C_i^o|$ is the size of the largest connected component \bar{C}_N^o of G_N^o .

6. Percolation and E-R graphs

- Alternatively, percolation can be defined on an infinite graph G (e.g. \mathbb{Z}^d) with

$$\text{percolation probability } \theta(p) = \mathbb{P}[|C_0| = \infty] \begin{cases} = 0, & \text{for } p < p_c \\ > 0, & \text{for } p > p_c \end{cases},$$

changing behaviour at a **critical value** $p_c \in [0, 1]$.

- In **site percolation** vertices and their adjacent edges are deleted.
- E-R random graphs $\mathcal{G}_{N,p}$ have the same distribution as open subgraphs $(G^o, E^o) \subseteq K_N$ under **percolation on the complete graph** K_N with parameter p .

Theorem 6.1 (Giant component for E-R graphs)

Consider $G_{N,p} \sim \mathcal{G}_{N,p}$ with $p = z/N$ and **maximal connected component** $\bar{C}_{N,p}$. Then

$$|\bar{C}_{N,p}| = \begin{cases} O(\log N), & \text{for } z < 1 \\ O(N^{2/3}), & \text{for } z = 1 \\ O(N), & \text{for } z > 1 \end{cases} \quad \text{and} \quad \theta(z) = \begin{cases} 0, & \text{for } z \leq 1 \\ > 0, & \text{for } z > 1 \\ \rightarrow 1, & \text{for } z \rightarrow \infty \end{cases}$$

where $\theta(z) := \lim_{N \rightarrow \infty} |\bar{C}_{N,p}|/N$ is a continuous, monotone increasing function of z . For $z > 1$, $\bar{C}_{N,p}$ is the only **giant component**, and the second largest is $O(\log N)$.

Local trees with $1 + \text{Poi}(z)$ degrees die out with probability 1 if and only if $z \leq 1$.

6. Preferential attachment

The prevalence of power-law degree distributions in real complex networks can be attributed to growth mechanisms subject to **preferential attachment**.

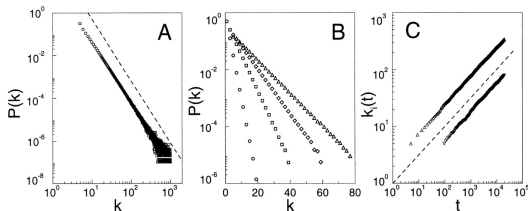
Definition 6.3

Starting with a complete graph (V_0, E_0) of $|V_0| = m_0$ nodes, at each time step $t = 1, \dots, N - m_0$ a new node $j = t + m_0$ is added. It forms $m \leq m_0$ undirected edges with existing nodes $i \in V_{t-1}$ with a probability proportional to their degree $\pi_{j \leftrightarrow i} = k_i / \sum_{l \in V_t} k_l$ (preferential attachment).

The resulting, undirected graph with N nodes and $K = m_0(m_0 - 1)/2 + m(N - m_0)$ is called a **Barabási-Albert** random graph, denoted by $\mathcal{G}_{N,K}^{\text{BA}}$.

- As $N \rightarrow \infty$, the average degree is $\langle k \rangle = 2m$ and the degree distribution $p_N(k)$ converges to a distribution $p(k)$ with **power law tail**, i.e. $p(k) = Ck^{-\alpha}$ for large k where $\alpha = 3$, which is close to exponents observed for real-world networks. This is independent of the parameters m_0 and m .
- Characteristic path length and clustering coefficient typically behave like $L = O(\log N)$ and $C = O(N^{-0.75})$ for $\mathcal{G}_{N,K}^{\text{BA}}$ graphs, and they are **uncorrelated**.
- They are **not homogeneous**, the expected degree of nodes increases with age.

6. Preferential attachment



(A) power law for $\gamma = 1$, $m_0 = m = 5$, $N = 200K$, (B) exponential tail for $\gamma = 0$, $m_0 = m = 1, 3, 5, 7$,
(C) degree increasing with time for $t_1 = 5$, $t_2 = 95$

taken from [A.-L. Barabási, R. Albert, Science **286**(5439), 509-512 (1999)]

- Variations of the model connecting to vertices i with probability proportional to $k_i + k_0$ lead to power law degree distributions with $\alpha = 3 + k_0/m$.
- For **non-linear preferential attachment** proportional to k_i^γ we get
 $\gamma \in [0, 1)$: $p(k)$ has a **stretched exponential tail** $\exp(-Ck^{1-\gamma})$
and the graph is **assortative**
 $\gamma > 1$: all vertices connect to m **super vertices** and the graph is **disassortative**

6. Small-world networks

Definition 6.4

A sequence of connected graphs G_N with increasing size $|V_N| = N$ exhibits the **small-world property**, if the characteristic path length $L(G_N) = O(\log N)$.

Examples include trees with degrees $k_i \geq 3$ and also the giant or largest component in E-R random graphs. In most graph models small-worldness is paired with low clustering coefficients, e.g. 0 for trees and p for $\mathcal{G}_{N,p}$ graphs. However, many real examples of small world networks exhibit also **large clustering coefficients**, such as networks of social contacts.

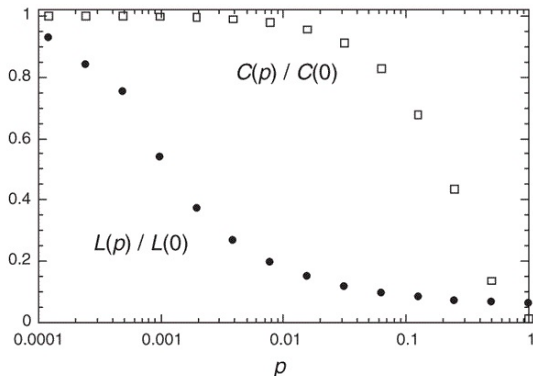
Definition 6.5

Consider a $2m$ -regular ring graph with adjacency matrix $a_{ij} = \begin{cases} 1, & |i-j| \leq m \\ 0, & \text{otherwise} \end{cases}$ of size N with a total number of $K = mN$ undirected edges.

For all i , each edge (i, j) with a clockwise neighbour with $j > i$ is **rewired** with probability $p \in [0, 1]$, i.e. replaced by an edge (i, l) where l is chosen uniformly among vertices not adjacent to i . The resulting graph is a **Watts-Strogatz random graph**, denoted by $\mathcal{G}_{N,K}^{\text{WS}}$.

6. Watts-Strogatz model

- W-S random graphs interpolate between a regular lattice for $p = 0$ and a $\mathcal{G}_{N,K}$ E-R random graph conditioned on the event that all vertices have degree $k_i \geq m$.
- Expected clustering coefficient $\mathbb{E}[C(p)]$ and characteristic path length $\mathbb{E}[L(p)]$ are monotone decreasing functions of p and show the following behaviour.



$N = 1000$ and $m = 5$, taken from [D.J. Watts, S.H. Strogatz, Nature **393**, 440-442 (1998)]

6. Configuration model

Definition 6.6

The **configuration model** $\mathcal{G}_{N,D}^{\text{conf}}$ is defined as the uniform distribution among all undirected graphs with N vertices with a given degree sequence $D = (k_1, \dots, k_N)$, such that $\sum_{i \in V} k_i = 2K$.

- Not all sequences D that sum to an even number are **graphical**.
- Sampling is usually done by attaching k_i half edges to each vertex i and matching them randomly. This can lead to self loops and rejections.
- General **randomized graphs** with given degree distribution $p(k)$ can be sampled in the same way. If $k_{\max} = \max_i k_i$ is bounded, one can show that these graphs exhibit a giant (connected) component of size $O(N)$ if

$$Q := \sum_{k \geq 0} k(k-2)p(k) > 0,$$

and if $Q < 0$ the largest component is of size $O(k_{\max}^2 \log N)$.

- For directed versions with D^{in} and D^{out} we need $\sum_{i \in V} k_i^{\text{in}} = \sum_{i \in V} k_i^{\text{out}}$.

6. Planar graphs and spatial point processes

Definition 6.7

A **planar graph** is an undirected graph that can be embedded in the plane, i.e. it can be drawn in such a way that no edges cross each other. The edges of a particular embedding partition the plane into **faces**. A connected planar graph G has a **dual graph** G^* , which has one vertex in each face of G , and a unique edge crossing each edge of G . G^* may be a multigraph with self-loops.

A **maximal planar graph** is called a **triangulation**.

- Every planar graph is 4-partite or 4-colourable.
- In a triangulation each face is bounded by three edges. By induction, every triangulation with $N > 2$ nodes has $K = 3N - 6$ undirected edges and $2N - 4$ faces.

Definition 6.8

A random countable set $\Pi \subseteq \mathbb{R}^d$ is called a **spatial point process**.

$\Pi \subseteq \mathbb{R}^d$ is called a homogeneous **Poisson point process PPP(λ)** with rate $\lambda > 0$ if

- for all $A \subseteq \mathbb{R}^d$ we have $N(A) := |\Pi \cap A| \sim \text{Poi}(\lambda|A|)$,
- for all disjoint $A_1, \dots, A_n \subseteq \mathbb{R}^d$, $N(A_1), \dots, N(A_n)$ are independent.

6. Planar graphs and spatial point processes

- To sample from a PPP(λ) e.g. in a box $A = [0, L]^d$, pick $N(A) \sim \text{Poi}(\lambda L^d)$, then place $N(A)$ particles independently in A each with uniform distribution, i.e. pick the d coordinates uniformly in $[0, L]$.
- A Poisson process PP(λ) is equivalent to a PPP(λ) on $[0, \infty)$.

Definition 6.9

Let $\Pi = \{x_1, x_2, \dots\}$ be a countable subset of \mathbb{R}^d , endowed with a distance function $d(x, y)$. A **Voronoi tessellation (or diagram)** is given by the family of **Voronoi cells** $\{A_1, A_2, \dots\} \subseteq \mathbb{R}^d$ where

$$A_i = \{x \in \mathbb{R}^d : d(x, x_i) \leq d(x, x_j) \text{ for all } j \neq i\}$$

is the set of points closest to x_i .

Properties in 2 dimensions.

- The shape of Voronoi cells depends on the distance function, for Euclidean distance $d(x, y) = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}$ they are convex polygons, and boundaries between adjacent cells are straight lines.
- The dual graph of a Voronoi diagram of a set Π is called **Delaunay triangulation**, which is not unique if 4 or more cells intersect in a point.