Lecture 11:
Stochastic particle systems

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November 11^{th}, 2021

Plan for today

1. Stochastic particle systems (Section 4 of slides from 2019)
2. Revision the first part of the module

Stochastic particle systems

Stochastic particle systems - introduction

Stochastic particle systems are very useful ways to use Markov chains or Markov processes to simulate real-world scenarios which depend on multiple agents.
Examples include:

- the spread of infections (epidemics)
- opinion dynamics
- some reaction-diffusion processes
- many others

I am used to working with them as systems of stochastic differential equations for different agents (and if you are interested in discussing more about this do let me know!). However, for the purposes of this module, we will work with them with a discrete state space.

Note that: I will often use the term “Interacting particle systems" instead of stochastic, but meaning the same thing.

Stochastic particle systems - definitions

We define stochastic particle systems in a **lattice or population**: $\Lambda = \{1, \dots, L\}$, which is a finite set of points.

Given Λ, the **state space** S of these systems is given by the set of all possible **configurations**:

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

$\eta(i) \in \{0,1\}$ denotes, e.g. the presence of a particle at the location i (reaction-diffusion), or whether an individual i is infected or not (epidemics).

To define the dynamics, we allow for local transitions. This means we can have

- **reaction** $\eta \to \eta^i$ with rate $c(\eta, \eta^i)$, where

$$\eta^i(k) = \begin{cases} \eta(k) & , \; k \neq i \\ 1 - \eta(k) & , \; k = i \end{cases} \qquad \text{a change happens in location } k = i$$

- **transport** $\eta \to \eta^{ij}$ with rate $c(\eta, \eta^{ij})$, where

$$\eta^{ij}(k) = \begin{cases} \eta(k) & , \; k \neq i, j \\ \eta(j) & , \; k = i \\ \eta(i) & , \; k = j \end{cases} \qquad \text{a particle moves from } i \text{ to } j$$

Stochastic particle systems - definitions

Definition

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

$$\mathcal{L}f(\eta) = \sum_{i\in\Lambda} c(\eta,\eta^{i})\left[f(\eta^{i}) - f(\eta)\right] \qquad \text{(reaction)},$$

or

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

And for the rest of today we will see a few examples.

Example 1 - Contact process

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

Definition (Contact process)

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 $\lambda > 0$.

This is a model for contagion without immunity. These days you will have seen many generalisations of this (e.g. SIR, SEIR, etc.).

Contact process - some properties

The CP has one absorbing state $\eta(i) = 0$ for all $i \in \Lambda$, which can be reached from every initial configuration. This means that the process is ergodic and the infection eventually gets **extinct** with probability 1.

$$\pi_t \to \delta_0 \quad \text{as } t \to \infty, \text{ for all } \lambda \geq 0 \text{ and } \pi_0 .$$

We define the **extinction time** by $T := \inf\{t > 0 : \eta_t \equiv 0\}$.
If $q(i,j)$ is irreducible, there exists an **"epidemic threshold"** $\lambda_c > 0$ such that

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

Note that: If $|\Lambda| = \infty$ (e.g. $\Lambda = \mathbb{Z}$), we can have $T = \infty$. In this case, it is possible that

$$\mathbb{P}(T = \infty|\eta_0 = \delta_i) > 0,$$

and there may exist a stationary probability called "**endemic phase**" with $\pi(\eta(j) = 1) = c(\lambda) > 0$.

For more information on this, see extra literature in the last slide on this set.

Example 2 - Voter model

The voter model describes some scenarios in opinion dynamics.
Here we assume that an individual i persuades another individual j to switch his/her opinion with **influence rates** $q(i,j) \geq 0$.

Definition:

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

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

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

Voter model - some properties

Note that: the voter model is **symmetric** under relabelling opinions $0 \leftrightarrow 1$.

If Λ is finite and $q(i,j)$ is irreducible, there are two absorbing states, $\eta \equiv 0, 1$.

- Both states $\eta \equiv 0$ and $\eta \equiv 1$ can be reached from every initial condition. This means that the VM is not ergodic, and **stationary measures** are

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

  pause

- As before, if Λ is not finite, there can be **coexistence** of both opinions (e.g. $\mathbb{Z}^d$ for $d \geq 3$).
- In this case, you can observe “clusters" of opinions which can evolve slowly.

Example 3 - Exclusion process

Our last example is the exclusion process.
It is used to describe the transport (or, probably more accurately, the “exchange") of a conserved quantity (e.g. mass or energy) with **transport rates** $q(i,j) \geq 0$ from site i to j.

Definition:

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

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

- An 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)**.

Exclusion process - some properties

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. In this case, the system is ergodic on S and has a unique stationary distribution.

Click this link for a cool visualisation of TASEP models

Mean-field scaling limits

A common thing to do with large systems is to consider their mean-field limit. Let's see what this means for the contact process.

Consider the contact process $(\eta_t : t \geq 0)$ on a **complete graph** (meaning, every agent in the graph is connected to everybody else).
Recall that the CP with $q(i,j) = \lambda$ has rates

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

Using $\eta(i) \in \{0,1\}$ we can write the generator as

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

Mean-field observables

We can define **mean-field observables** such as the current number of “infected agents":

$$N(\eta) := \sum_{i \in \Lambda} \eta(i).$$

Using this, together with the generator, we can compute for a given function $f : \mathbb{N}_0 \to \mathbb{R}$

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

This expression depends on η only through N, so now we have that the random variable $t \mapsto N_t := N(\eta_t)$ is a Markov process with above generator for all L.

Mean-field scaling limit

If we now let $L \to \infty$, we can define the **mean-field scaling limit.**
This involves defining the right scaling, and for the CP this means we define a new rate $\hat{\lambda}$: $\lambda L \to \hat{\lambda}$.
We can then see that $N_t/L \to X_t$, which is a **diffusion process** on $[0, 1]$ with generator

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

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

$$dX_t = \big(\hat{\lambda}X_t(1-X_t) - X_t\big)dt + \sqrt{\tfrac{1}{L}\big(\hat{\lambda}X_t(1-X_t) + X_t\big)}\,dB_t.$$

This means that we can simulate what happens to this system by solving this SDE instead!

Some literature on this

If you want to read more about stochastic particle systems, here are some references that are available via the library:

- Stochastic Interacting Systems: Contact, Voter and Exclusion Processes, T.M. Liggett, 1999. Check here for the link
- Lecture Notes on Particle Systems and Percolation, R. Durrett, 1988. The non-French text in this link ;)
- Warwick lecture notes on complexity science, 2014 (edited by lots of previous lecturers in Complexity/MathSys). See this link. Chapter 3 is in stochastic particle systems, and the chapters written by R. MacKay are related to this too.
- Nice review-like paper about the TASEP model paper by Blythe et al

Lecture 12:
Networks - basic definitions

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November 12^{th}, 2021

Plan for today

1. Graphs and some initial examples
2. Chat about assignment 2.

Networks - basic definitions and characteristics

Graphs - definition

Everything we will learn about networks is based on a concept which most of you have probably seen before - a graph. Today we will review basic definitions and concepts of graph theory which will be useful in the next few weeks.

Definition:

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

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

Two nodes $i, j \in V$ are **adjacent** or **neighbouring** if $(i, j) \in E$.

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

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

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

Some space for examples

Some things to note about graphs

The definition of a graph is quite general, and with the way it is written in the previous slide we could allow for *self-edges*, i.e., edges like (i, i), or *multiple edges* (multiple instances of (i, j). We do not allow for this in this module.

One can also consider **weighted graphs**, which are graphs with edge weights $w_{ij} \in \mathbb{R}$. These 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.

Graphs - paths and shortest paths

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

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

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

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

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

Shortest paths between vertices i, j are called **geodesics**. They are not necessarily unique, and their length d_{ij} is called the **distance** from i to j.

If $i \not\to j$ we set $d_{ij} = \infty$.

Graphs - connectivity

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

We can define the **diameter** of the graph G by

$$\mathrm{diam}(G) := \max\{d_{ij} : i, j \in V\} \in \mathbb{N}_0 \cup \{\infty\},$$

and the **characteristic path length** of the graph G by

$$L = L(G) := \frac{1}{N(N-1)} \sum_{i,j \in V} d_{ij} \in [0, \infty].$$

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

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

Graphs - degrees

An important characteristic of any graph is the degree.

Definition:

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

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

$k_1^{\text{in}}, \ldots k_N^{\text{in}}$ is called the **in-degree sequence**. With it, we can define the **in-degree distribution**:

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

which gives the fraction of vertices with in-degree k. The same holds for out-degrees.

In undirected networks, we simply write $k_i = k_i^{\text{in}} = k_i^{\text{out}}$ and $p(k)$.

Some properties of the degree

Here are some things to note about the degree of a graph:

- We have that, for an undirected graph, $\sum_{i \in V} k_i = \sum_{i,j \in V} a_{ij} = |E|$ (but this is also true for directed graphs)
- It is common to compute the average degree and the variance, which are given by

$$\langle k \rangle = \frac{1}{N} \sum_{i \in V} k_i = \frac{|E|}{N} = \sum_k kp(k), \qquad \text{and} \qquad \sigma^2 = \langle k^2 \rangle - \langle k \rangle^2.$$

- If a graph is such that each vertex has the same degree $k_i \equiv k$, we call it a **regular graph** (and it is usually undirected).
- Graphs where the degree distribution $p(k)$ 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 $\alpha \approx 3$.

Graphs - first examples

Here are some examples of 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 $k = 2d$.

A special example

A particularly useful example of a graph is a tree:

Definition:

A **tree** is an undirected graph where any two vertices are connected by exactly one path.

In a tree, vertices with degree 1 are called **leaves**.

A **rooted tree** is a tree in which one vertex $i \in V$ is the designated **root**.

Then the graph can be directed, where all vertices point towards or away from the root.

Trees and cycles

Recall that a **cycle** is a closed path γ_{ii} of length $|\gamma_{ii}| > 2$. Using this, we can see that G is a tree if and only if

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