Simulation, Analysis, and Validation of Computational Models

— 7.a The SIR model —

— 7.b Dynamics on networks —

Lecturer: Michael Herrmann
School of Informatics, University of Edinburgh
michael.herrmann@ed.ac.uk, +44 131 6 517177

Overview

- Local SI/SIR model
- Graphs and complex networks
- Spreading of diseases, misinformation

Previous lectures

- Lecture 5: Percolation on a regular grid. When modelling disease spreading, percolation with be studied on a graph
- Lecture 6: Non-trivial effects of noise in non-linear systems

- Today: Towards modelling of non-linear dynamics on complex networks
- Simplification of the real world to understand the dynamics of processes such as epidemics
  - Spreading of diseases through air, by water, touch, via parasites, blood etc. is modelled by transmission rates
  - Spatial relations, countermeasures, and many other features can be included into the model in various ways ...
  - Noise, mutation, and external dynamics known to affect the process are not considered now.

Compartmental SIR model

- Consider a small population in a small area during an epidemic.
- People can be Susceptible, Infectious, or Recovered.
- Consider respective fractions of the total population, i.e. normalisation: $S(t) + I(t) + R(t) = 1$.
- Ranges: $0 \leq S(t) \leq 1$, $0 \leq I(t) \leq 1$, $0 \leq R(t) \leq 1$.
- Discrete or continuous time?
  - Incubation period, daily and weekly rhythms suggest discrete time
  - Analytical convenience suggests continuous time.

Simplified discrete model (SIS)

Start with disregarding resistance[1], only susceptible and infectious ($R(t) = 0$, i.e. $S(t) + I(t) = \text{const}$, "endemic" case)

- New infection $S \to I$ prop. to meetings $S(t)\, I(t)$ with rate α
- Recovery $I \to S$ happens individually with rate β

$$\begin{aligned} S(t+1) &= S(t) - \alpha S(t)\, I(t) + \beta I(t) \\ I(t+1) &= I(t) + \alpha S(t)\, I(t) - \beta I(t) \end{aligned}$$

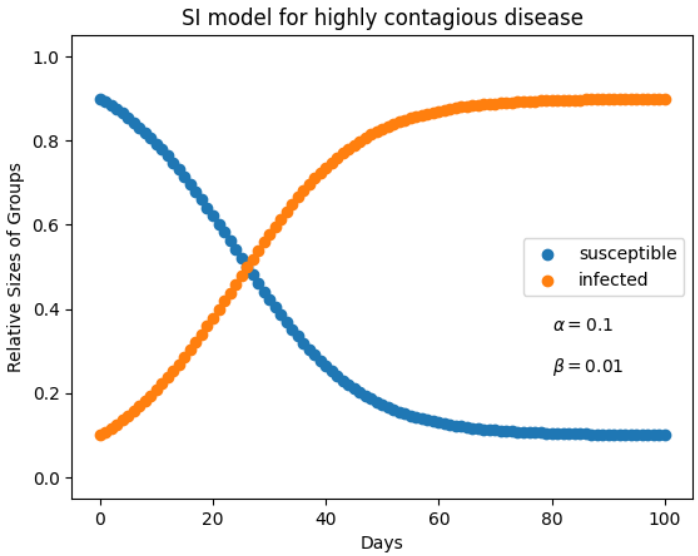
Changes of S and changes of I are[2] opposite $\Rightarrow$
$S(t) + I(t) = \text{const}\ \forall t$

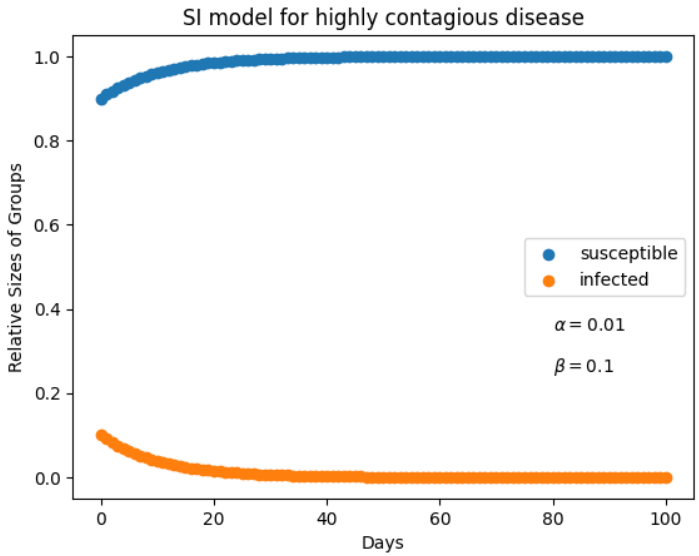
- For stationary state set $S(t+1) = S(t)$, i.e.
  $\alpha S(t)\, I(t) = \beta I(t) \Rightarrow S(\infty) = \beta/\alpha$
  unless $I(t) = 0$, then $S(t) = 1$ (which happens when $\beta \geq \alpha$)
- Rates change: avoiding direct contact (α) and with care (β)

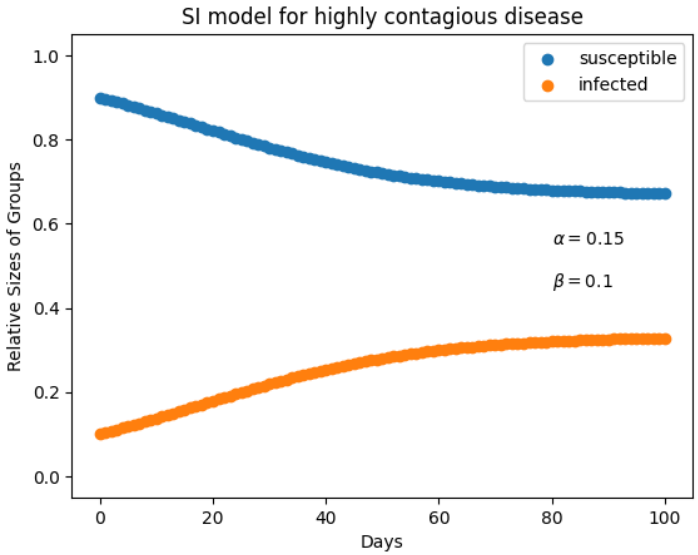
[1] such as by vaccination or immunity after recovery

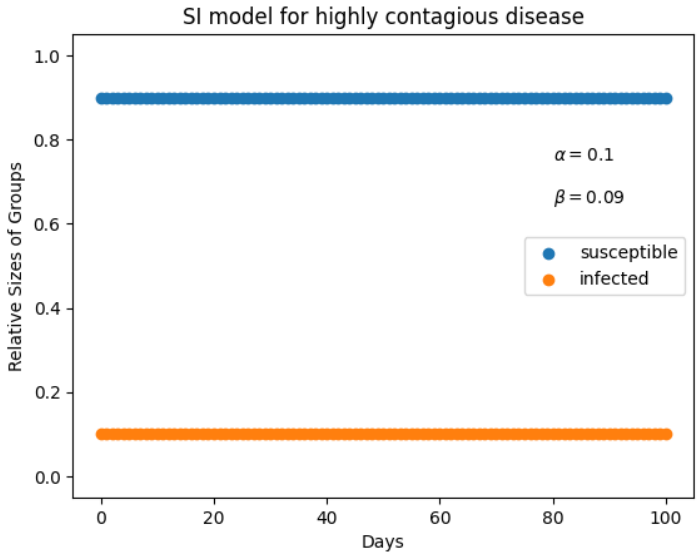
[2] Equation is not correct in Li & Nakano, page 130.

Numerical examples









Provides insight into some aspects, but is far too simple as a model.

SI as a continuous model

Discrete model is difficult to solve and does not work for all parameters $\Rightarrow$ Consider continuous analogue of the previous system

$$\begin{aligned} \frac{dS}{dt} &= -\alpha S(t)\, I(t) + \beta I(t) \\ \frac{dI}{dt} &= \alpha S(t)\, I(t) - \beta I(t) \end{aligned}$$

Solution, e.g. in Maxima:

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ode2(('diff(S,t)=-a*S*I+b*I,'diff(I,t)=a*S*I-b*I),(S,I),t);
```

gives only one solution:

$$I(t) = I_0 \exp\left(\left(\alpha S(t) - \beta\right) t\right)$$

Balanced at $S(t) = \beta/\alpha$, confirms expectation from discrete model, except for shorter time scale.

We could consider instead $\frac{dS}{dt} = -\alpha S(t)\left(1 - S(t)\right) + \beta\left(1 - S(t)\right)$

SIR model

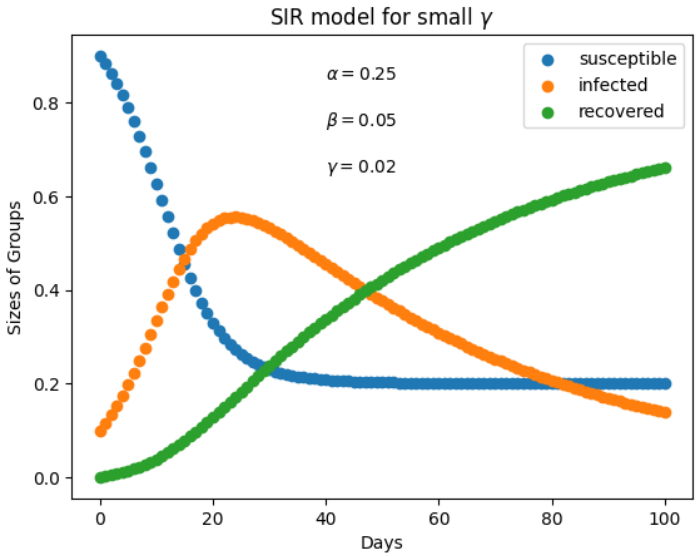
- Susceptible, Infectious, or Recovered (and immune to further infection)
- Recovery rate γ
- Normalisation $R(t) + S(t) + I(t) = 1$ conserved by balanced equations (i.e. already two equation would be sufficient)

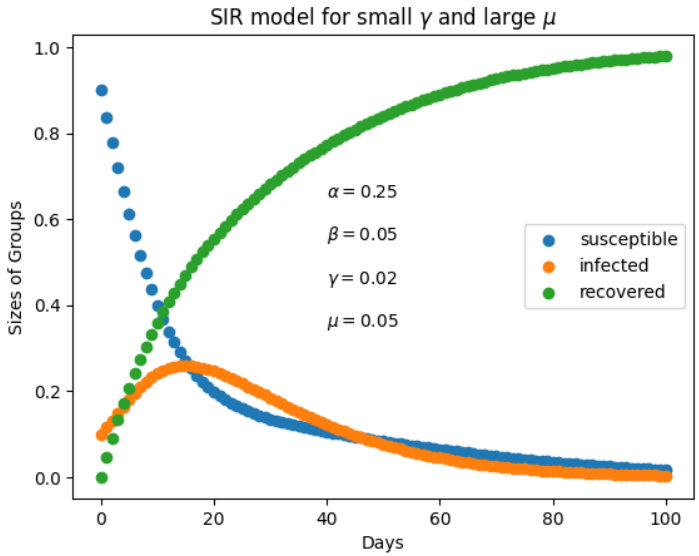
$$\begin{aligned} S(t+1) &= S(t) - \alpha S(t)\, I(t) + \beta I(t) \\ I(t+1) &= I(t) + \alpha S(t)\, I(t) - \beta I(t) - \gamma I(t) \\ R(t+1) &= R(t) + \gamma I(t) \end{aligned}$$

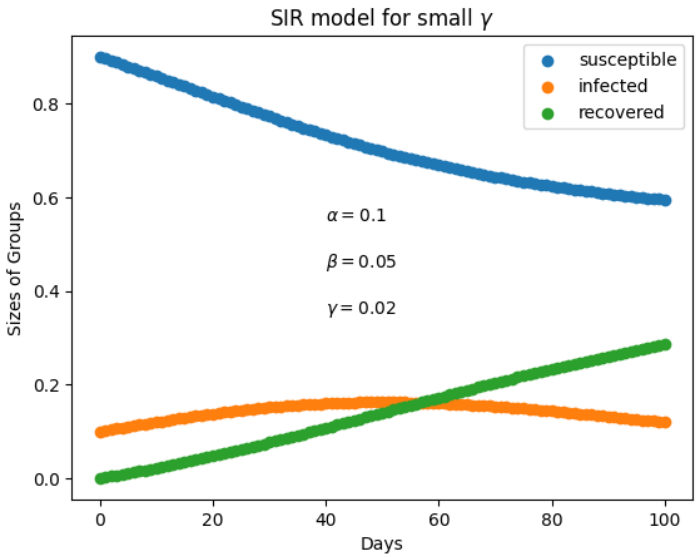
- Include also vaccination rate μ (SIRV)

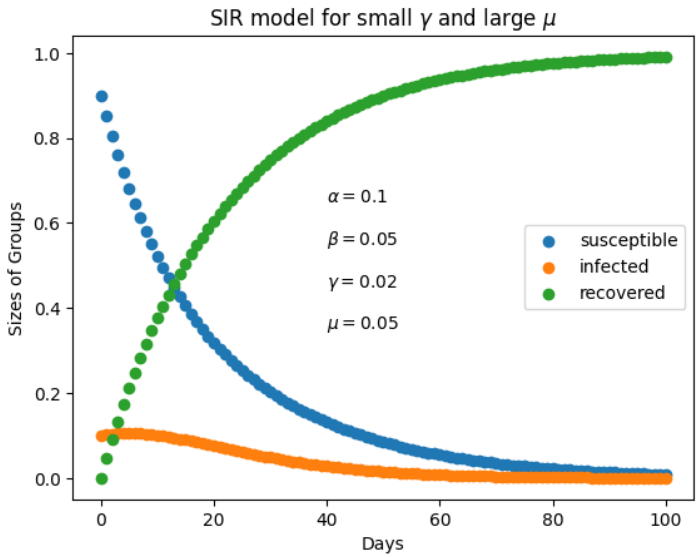
$$\begin{aligned} S(t+1) &= S(t) - \alpha S(t)\, I(t) + \beta I(t) - \mu S(t) \\ I(t+1) &= I(t) + \alpha S(t)\, I(t) - \beta I(t) - \gamma I(t) \\ R(t+1) &= R(t) + \gamma I(t) + \mu S(t) \end{aligned}$$

Numerical examples









Continuous-time SIR model

Susceptible, Infectious, or Recovered (including immunisation, i.e. $\beta = 0$, $\gamma + \beta \to \gamma$)

Continuous system

$$\dot{S} = -\alpha IS$$

$$\dot{I} = \alpha IS - \gamma I$$

$$\dot{R} = \gamma I$$

Semi-analytical solution

$$S(t) = S(0)e^{-Q(t)}$$

$$I(t) = 1 - S(t) - R(t)$$

$$R(t) = R(0) + \frac{\gamma}{\alpha} Q(t)$$

where $Q(t) = \beta \int_0^t I(s)\, ds$ is the part of the solution that requires numerical treatment.

Miller JC (2012) A note on the derivation of epidemic final sizes. Bull. Math Biol. **74**: 2125–2141.

SIR model: Discussion

SIR model can be useful to support an explanation[3]. It flexible to include many other features, such as

- birth and death
- latency period (incubation period)
- passive immunity
- variable transition rates
- heterogeneous population: *ignorant* or *unaware*, *rationally resistant*, and *exhausted*
- social strata (age, living conditions, access to information and vaccination)
- spatial effects (diffusion, travel etc.)

Information from data needed to calibrate models to provide a predictive description

Rahimi e.a. (2023) A review on COVID-19 forecasting models. *Neural Comput. Appl.* **35**, 23671-23681.

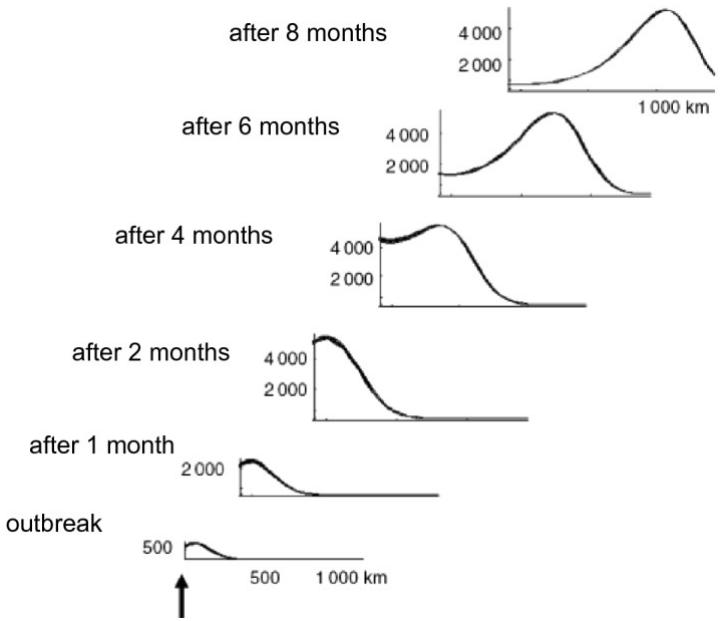
[3] applicable also to other systems, such as short-term synaptic plasticity

Forest fires

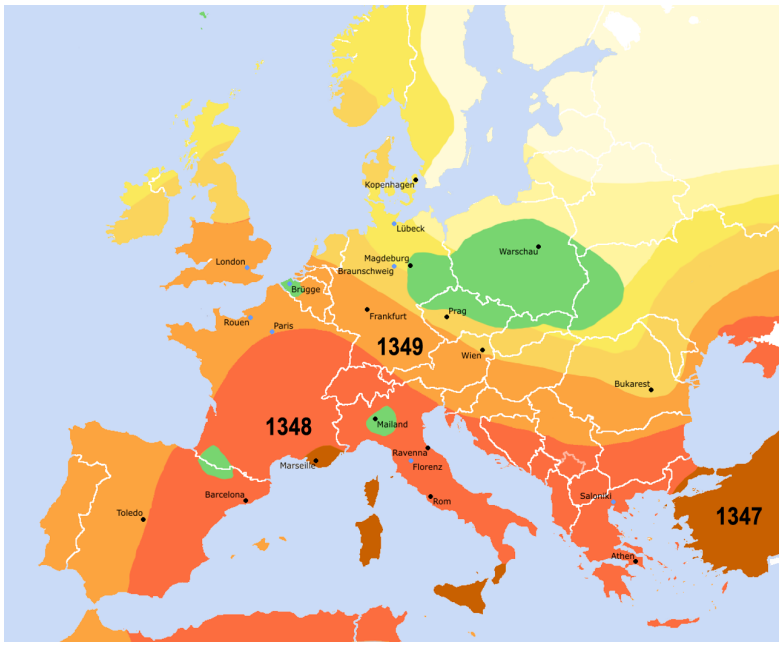
- Fire spreads to the four nearest neighbours, according to our percolation model (hexagonal tessellation is more similar to Euclidean geometry, but forest are often planted on grids).
- If there are enough susceptible tree (i.e. their proportion is high enough), size of the cluster can be "giant" which depends on the total size, but will be a sizeable fraction of the forest.
- Disconnected forests are more save, however, wildlife prefers connected habitats.
- What effects may "bridges" have? Or any other type of (non-local) connections?

Spread of diseases depends on mobility

The Black Death was a pandemic occurring in Europe 1346-1353.



Vogl, G. (2019) The Diffusion of the Black Death and Today's Global Epidemics. Adventure Diffusion, Springer, p. 97-110.



Roger_Zenner, 2005 (wikipedia CC)

Today, network properties are more critical than geographic distance:

Hufnagel e a. (2004) Forecast and control of epidemics in a globalized world. PNAS 101, 15124-15129.

Graphs

- A graph represents relations between discrete elements.
- A graph is a pair $G = (V, E)$, where V is a set of vertices, and E is a set of edges, i.e. pairs $\{v_1, v_2\}$, $v_i \in V$.
- Edges can be ordered pairs (directed graph) or unordered pairs (undirected graph).
- Connected components define reachability in undirected graphs. In directed graph, reachability requires to find a path from one vertex to the other one which can be done quite quickly.
- Adjacency matrix $A = \{a_{ij}\}$ with $a_{ij} = 1$ if $\{v_i, v_j\} \in E$, and $a_{ij} = 0$ otherwise.

Graphs as complex networks: Small-worldness

- Distance from v_i and v_j: $L_{ij} = n$ if $(A^m)_{ij} = 0$, $\forall m < n$ and $(A^n)_{ij} > 0$
- Local clustering coefficient locally for node i (with k_i neighbours)

$$C_i = \frac{\#\{j,k : L_{ij} = 1 \wedge L_{ik} = 1 \Rightarrow L_{jk} = 1\}}{k_i(k_i-1)/2}$$

or with the respective elements of the adjacency matrix

$$C_i = \frac{1}{k_i(k_i-1)} \sum_{j,k} A_{ij} A_{jk} A_{ki}$$

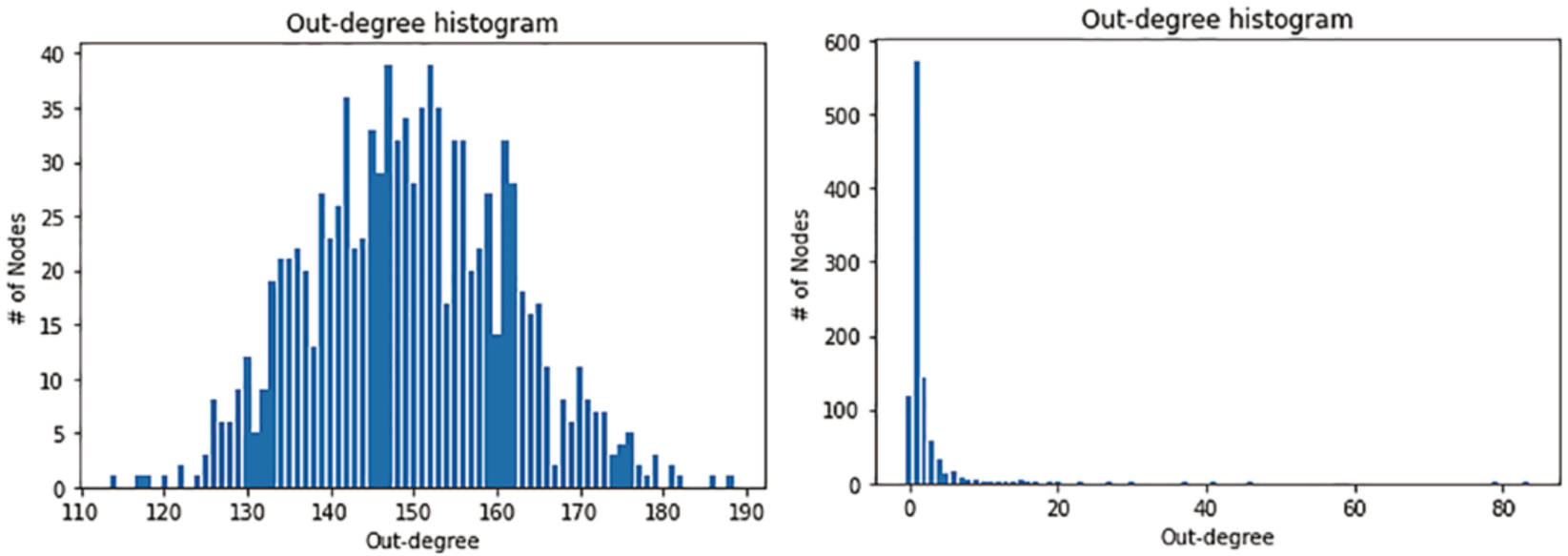
or the relative number of triangles in the graph.

- Small-world network: high clustering coefficient and quick reachability, i.e. $\langle L_{ij} \rangle \propto \log N$ for a graph with Nvertices.
- Generation: Start with a locally connected graph (high $\langle C_i \rangle$) and replace some connections by random links (low $\langle L_{ij} \rangle$)

Watts & Strogatz (1998) Collective dynamics of 'small-world' networks" Nature. 393 (6684): 440–442.

Graphs as complex networks: Degree distribution

- In-degree the number of incoming edges of a vertex: $k_i^{\text{in}} = \#\{j : L_{ij} = 1\}$
- Out-degree the number of outgoing edges of a vertex: $k_i^{\text{out}} = \#\{j : L_{ji} = 1\}$
- Degree distribution: $p_{\text{in/out}}(m) = \text{Prob}\left(k^{\text{in/out}} = m\right)$



(left) random graph (right), power-law (scale free) graph. N=1000, (Li & Nakano)

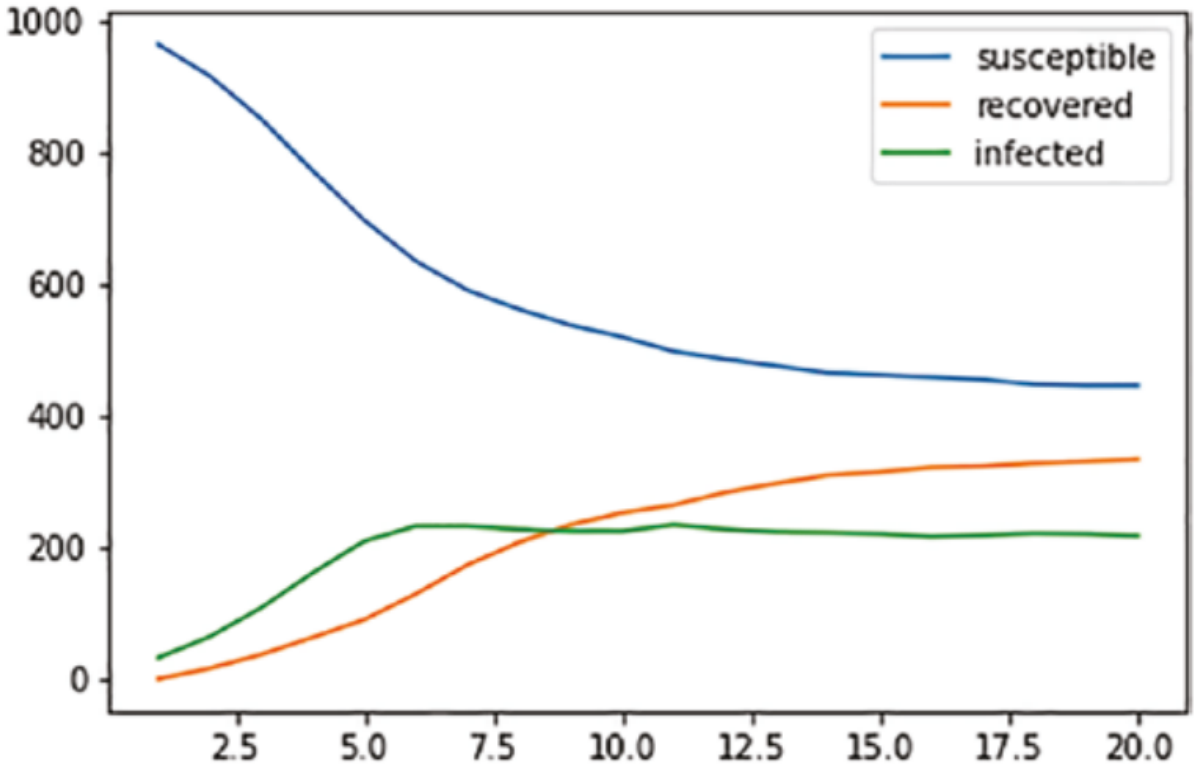
Graphs vs. continuous systems*

- Spectral graph theory studies eigenvalues and eigenvectors of the adjacency matrix and other graph-related matrices, so one can study dynamical systems characterised by these matrices.
- In complex systems, we have connections between nodes (fixed points), e.g. two saddle nodes can be connected be a directed flow line, or some of the flow lines from an unstable fixed point can connect to a stable fixed point, however the embedding space affects some dynamical properties as well.
- Graphs can be embedded in a 2D surface of suitable topology. Hypergraphs may need more complex embeddings. See also *simplicial complex*.

Misinformation spreading on a Graph

- Disinformation: Wrong on purpose.
- Misinformation: Does not care about evidence or is incomplete or biased
- Either may pose as or use the other
- Are the rates and frequencies more important for spreading or the structure of the graph?

Misinformation spreading on a Graph



Spreading of misinformation in an $N = 1000$ random graph (Li & Nakano).

Applications of network dynamics

Relevant application domains include

- Spreading of misinformation on social media,
- Spreading of diseases in RW social networks
- Failures in communications networks
- Equity in financial networks
- Superposition in acoustic networks
- Transport in logistic systems
- Activation in neural networks
- Transcription regulation in genetic networks
- Ideas in academic networks.

The predictive power of network theory varies across domains.

Misinformation spreading on a Graph

- Similar to SIR: Source, susceptible, follower, resistant
- Also dynamics is similar, if we maintain:
  - List of neighbours
  - State of neighbours
  - Direction of links is important here
  - Different information spreads differently

Conclusion

- Simulation on a graph go beyond the neighbourhood-based simulation in extended systems.
- Different types of graphs differ in their support for dynamic phenomena

Next topics

- Multi-agent systems (MAS)
- Case studies
- Simulation, verification etc.