PDE LIMIT OF SPREADING PROCESSES ON NETWORKS

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1. Introduction and motivatioan
2. Link to PDEs
3. Summary and future challenges

1. Introduction and motivatioan
   - Why networks?
   - Modelling approaches
   - Formulation of stochastic spreading processes on networks
2. Link to PDEs
3. Summary and future challenges

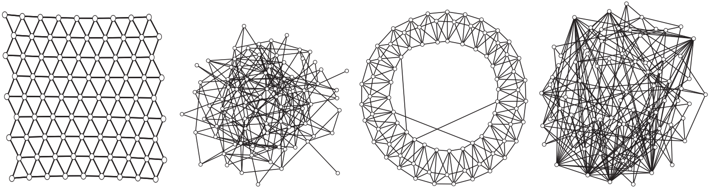

Figure: Individuals interconnected by four networks with very different properties, but with the same average number of contacts per node $\langle k \rangle \simeq 6$. The degree distribution $p(k)$ of these networks changes from almost all nodes having the same number of contacts $p(k) = \delta(k - \langle k \rangle)$ to Poisson with $p(k) = \langle k \rangle^k e^{-\langle k \rangle} / k!$, and finally to scale-free distribution with $p(k) = Ck^{-\gamma}$.

- Networks provide a flexible modelling framework to capture heterogeneities in social or technological interactions,
- Modelling can be more challenging compared to ODE and PDE models.

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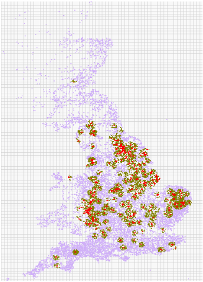

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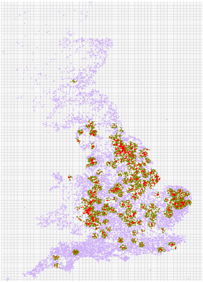

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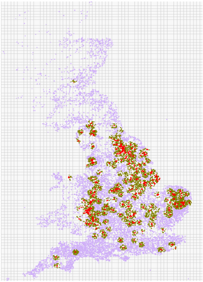
Exact epidemic models on structured populations (graphs/networks) with discrete state space and continuous time: $\dot{X}(t) = PX(t)$, where X is the mapping of the state space ($\mathcal{S}$) onto the probabilities of being in a particular state at time t and P is the transition matrix between states.



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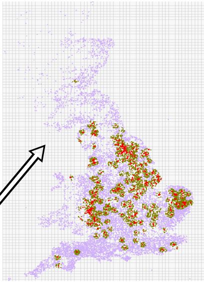

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- Network with N nodes and adjacency matrix $T = (T_{ij})_{i,j=1,2,\dots,N} \in (a,b)^{N^2}$, with $a, b \in \mathbb{R}$ and $T_{ii} = 0 \, \forall i = 1, 2, \dots, N$, weighted, directed network.

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- The forward **Kolmogorov** equation of the stochastic process is

$$\dot{X}(t) = PX,$$

where P is a $2^N \times 2^N$ transition matrix giving the rates of all possible transitions.

- The system can be in $\mathcal{S} = \{SSS, SSI, SIS, ISS, SII, ISI, IIS, III\}$ and the transitions amongst these states need to be described,
- Continuous Time Markov Chain with the following forward Kolmogorov equations:

$$\begin{pmatrix} \dot{x}_{SSS} \\ \dot{x}_{SSI} \\ \dot{x}_{SIS} \\ \dot{x}_{ISS} \\ \dot{x}_{SII} \\ \dot{x}_{ISI} \\ \dot{x}_{IIS} \\ \dot{x}_{III} \end{pmatrix} =$$

$$\begin{pmatrix} 0 & \gamma & \gamma & \gamma & 0 & 0 & 0 & 0 \\ 0 & -2\tau-\gamma & 0 & 0 & \gamma & \gamma & 0 & 0 \\ 0 & 0 & -2\tau-\gamma & 0 & \gamma & 0 & \gamma & 0 \\ 0 & 0 & 0 & -2\tau-\gamma & 0 & \gamma & \gamma & 0 \\ 0 & \tau & \tau & 0 & -2\tau-2\gamma & 0 & 0 & \gamma \\ 0 & \tau & 0 & \tau & 0 & -2\tau-2\gamma & 0 & \gamma \\ 0 & 0 & \tau & \tau & 0 & 0 & -2\tau-2\gamma & \gamma \\ 0 & 0 & 0 & 0 & 2\tau & 2\tau & 2\tau & -3\gamma \end{pmatrix} \begin{pmatrix} x_{SSS} \\ x_{SSI} \\ x_{SIS} \\ x_{ISS} \\ x_{SII} \\ x_{ISI} \\ x_{IIS} \\ x_{III} \end{pmatrix}$$

For full system characterisation $2^3 = 8$ equations are needed.

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$$\dot{p}_k = a_{k-1}p_{k-1} - (a_k + c_k)p_k + c_{k+1}p_{k+1}, \quad k = 0, \ldots, N, \quad (1)$$

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- Can we use only N rather than 2^N equations for arbitrary networks?
- If so, what is a_k for an arbitrary network?
- a_k - is in fact a random variable, whose distribution depends on the structure of the network and dynamics.

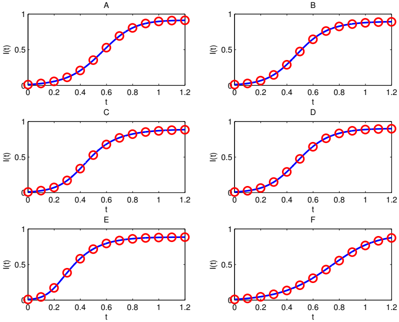

FIGURE: Time evolution of the expected prevalence from simulation (○ markers) and from master equations (1) with a_k taken as an average from simulation (continuous curve) for (A) homogeneous random graph, (B) Erdős-Rényi random graph, (C) bimodal random graph, (D) negative binomial random graph, (E) Barabási-Albert graph, (F) clustered random graph with clustering coefficient 0.4. The parameters are $N = 1000$, $\tau = 2$, $\gamma = 1$, average degree 6, number of initially infected nodes 10. The simulation results were obtained as the average of 250 simulations.

- Can we propose an method to encode the network and dynamics into a_k,

[1] N Nagy, IZ Kiss, and PL Simon. "Approximate Master Equations for Dynamical Processes on Graphs". In: *Mathematical Modelling of Natural Phenomena* 9.02 (2014), pp. 43–57.

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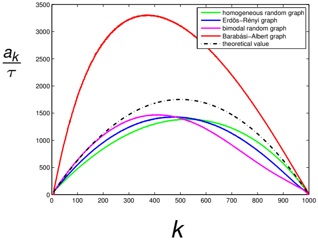

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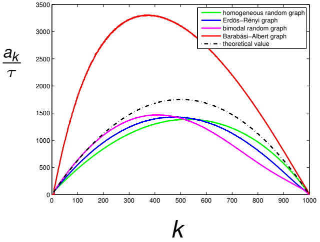

- Work by Nagy et al.[1] showed that approximate master equations can be written down, similar to Eq. (1), but different a_k coefficients:

$$
\begin{aligned}
a_k &= \tau k n \frac{N-k}{N-1}, \\
a_k &= \tau c k^p (N-k)^q, \\
a_k &= \text{numerically inferred.}
\end{aligned}
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1 Introduction and motivatioan

2 Link to PDEs
- Fokker-Planck equation: the basic idea
- Fokker-Planck equation: density dependent case
- Fokker-Planck equation: steady state
- Other potential uses of PDE for dynamics on networks

3 Summary and future challenges

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- The Fokker-Planck equation can be considered as a continuous version of master equation (1) with a discretisation of a continuous function $u(t, z)$ in the interval $[0, 1]$,

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- The PDE is traditionally given in the form

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- The functions g and h will be determined in such a way that the finite difference discretization of this PDE will yield the master equation (1). (In fact, any parabolic type PDE with space dependent coefficients could serve as the continuous version of the master equation.)

- Discretise to relate the PDE and the master equation

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- Using $z = k/n$ and $h = 1/N$ to the partial derivatives of the functions $g(z)u(t,z)$ and $h(z)u(t,z)$ with respect to z leads to

$$\partial_t u\left(t, \frac{k}{N}\right) = \frac{N^2}{2}(g_{k+1}x_{k+1} - 2g_k x_k + g_{k-1}x_{k-1}) - \frac{N}{2}(h_{k+1}x_{k+1} - h_{k-1}x_{k-1}), \quad (4)$$

where the notations $u\left(t, \frac{k}{N}\right) = x_k$, $g_k = g\left(\frac{k}{N}\right)$, $h_k = h\left(\frac{k}{N}\right)$ are used.

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- Applying this at $k = 0$ and $k = N$ requires two artificial mesh points at $z = -1/N$ and at $z = 1/N$. Differentiating (2) with respect to t and using the master equation (1) yields

$$\partial_t u\left(t, \frac{k}{N}\right) = \dot{p}_k = a_{k-1}p_{k-1} - (a_k + c_k)p_k + c_{k+1}p_{k+1}. \quad (5)$$

- Upon substituting p_k by x_k for all k we arrive at the right hand side of (4). Making the coefficients equal leads to

$$a_k = \frac{N}{2} h_k + \frac{N^2}{2} g_k, \quad c_k = \frac{N^2}{2} g_k - \frac{N}{2} h_k. \tag{6}$$

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- Thus g and h are defined so that the two discretisations are equivalent

$$g\left(\frac{k}{N}\right) = g_k = \frac{1}{N^2}(a_k + c_k), \quad h\left(\frac{k}{N}\right) = h_k = \frac{1}{N}(a_k - c_k)$$

hold.

- Assume that a_k and c_k are given by the functions A and C ($\frac{a_k}{N} = A\left(\frac{k}{N}\right)$ and $\frac{c_k}{N} = C\left(\frac{k}{N}\right)$).

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- Summarizing, the Fokker-Plank equation of the one-step-process given by density dependent coefficients is

$$\partial_t u(t,z) = \frac{1}{2N}\partial_{zz}((A(z)+C(z))u(t,z)) - \partial_z((A(z)-C(z))u(t,z)) \tag{7}$$

subject to boundary conditions

$$\delta\partial_z((A+C)u)(-\delta,t) - ((A-C)u)(-\delta,t) = 0, \tag{8}$$

$$\delta\partial_z((A+C)u)(1+\delta,t) - ((A-C)u)(1+\delta,t) = 0, \tag{9}$$

where $\delta = 1/2N$.

- Linear coefficients, $A(z) = a(1-z)$ and $C(z) = cz$, lead to

$$\partial_t u(t,z) = \frac{1}{2N}\partial_{zz}(((c-a)z+a)u(t,z)) - \partial_z((a-(a+c)z)u(t,z)).$$

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- Integrating and using the boundary condition and that the integral of U becomes $1/N$ leads to

$$U(z) = \frac{\sqrt{2}}{\sqrt{\pi N}}\exp\left(-2N(z-\frac{1}{2})^2\right). \tag{10}$$

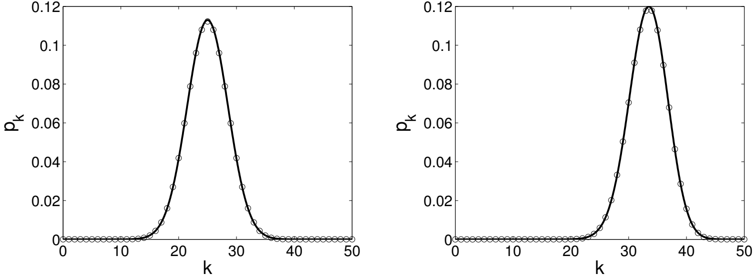

FIGURE: The steady state of the distribution in the linear case, when $A(z) = a(1 - z)$ and $C(z) = cz$ for $N = 50$. The binomial distribution as the exact solution of the master equation (circles) is shown together with U, the solution of the Fokker-Planck equation (continuous curve). In the left panel the case $a = c = 1$ is shown, when U is given by (10). In the right panel the case $a = 2$, $c = 1$ is shown, when U is given by the general case of $a \neq c$.

- Approximate steady state by neglecting the $1/N$ term in the Foker-Planck equation.

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- Use numerical methods.

- Starting from the master equation, use the Probability Generating Formalism $G(t,z)=\sum_{k=0}^{N} z^k p_k(t)$ to store information more effectively, and to develop systematically a series of PDEs for the moments of the distribution.

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- Use the same approach but starting from high-dimensional mean-field models[2].

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$$\begin{aligned}
\frac{dA_{k,l}}{dt} &= \frac{\bar{p}}{2}[kB_{k,l} - lA_{k,l}] \\
&+ \frac{\bar{p}}{2}[(l+1)A_{k-1,l+1} - lA_{k,l}] \\
&+ \frac{\bar{p}}{2}\frac{\sum_{k,l}(k-1)kB_{k,l}}{\sum_{k,l} kB_{k,l}}[(l+1)A_{k-1,l+1} - lA_{k,l}] \\
&+ \frac{\bar{p}}{2}\frac{\sum_{k,l} lkA_{k,l}}{\sum_{k,l} kA_{k,l}}[(k+1)A_{k+1,l-1} - kA_{k,l}] \\
&+ \frac{p}{2}[(l+1)A_{k-1,l+1} - lA_{k,l}] \\
&+ \frac{p}{2}[(l+1)A_{k,l+1} - lA_{k,l}] + \frac{p}{2}\frac{\sum_{k,l} lA_{k,l}}{\sum_{k,l} A_{k,l}}[A_{k-1,l} - A_{k,l}]\dots
\end{aligned}$$

$$Q(t,x,y) = \sum_{k,l} A_{k,l}(t)x^k y^l,$$

$$\begin{aligned}
\frac{\partial Q}{\partial t} &= \frac{\bar{p}}{2}\beta(y-x)\frac{\partial Q}{\partial x} \\
&+ \left[\frac{1+\bar{p}\alpha}{2}(x-y) + \frac{p}{2}(1-y)\right]\frac{\partial Q}{\partial y} \\
&+ \frac{p}{2}\gamma(x-1)Q,
\end{aligned}$$

$$\alpha = \frac{Q_{yy}(t,1,1)}{Q_y(t,1,1)},\ \beta = \frac{Q_{xy}(t,1,1)}{Q_x(t,1,1)}$$

$$\gamma = \frac{Q_y(t,1,1)}{Q(t,1,1)} = \frac{\sum_{k,l} lA_{k,l}}{\sum_{k,l} A_{k,l}}.$$

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1 Introduction and motivatioan

2 Link to PDEs

3 Summary and future challenges

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- Any suggestions/ideas/links to existing results are welcome!

Thank you for your attention!

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