On the exact analysis of stochastic epidemic processes on networks

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WiN Workshop
28^{th} February 2019, Leeds, UK

Talk based on the manuscripts
López-García M (2016) *Mathematical Biosciences* 271: 42-61.
Economou A, Gómez-Corral A, López-García M (2015) *Physica A: Statistical Mechanics and its Applications* 421: 78-97.

Organization of the talk I

1. Motivation: SIR epidemic model for a small group of heterogeneous individuals
2. Structuring the space of states
3. Stochastic Descriptors / Summary Statistics
4. Numerical Results.

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$$\text{Susceptible } (S) \Rightarrow \text{Infected } (I) \Rightarrow \text{Recovered } (R)$$

for analysing the spread of an epidemic among the members of an heterogeneous population of N individuals. We are interested in the case in which:

1. the population is small (*group* of individuals)
2. the interest is in capturing every heterogeneity among the individuals (families, small group of computer servers, intensive care units,...).

We consider:

1. A susceptible individual $i \in \{1, \dots, N\}$ can become infected due to:
   - An *external* source of infection, which occurs after an exponentially distributed random time with rate $\lambda_i \geq 0$.
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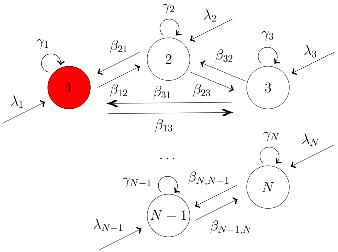
The Network

We model the epidemic with a network. Vertices $\mathcal{N} = \{1, \ldots, N\}$ representing individuals. Edges $(i, j) \in \mathcal{N} \times \mathcal{N}$ representing potential contact between individuals.



Some assumptions:

- In general, we consider the directed case ($\beta_{ij} \neq \beta_{ji}$).
- $\beta_{ij} = 0$ is equivalent to no contact between individuals i and j.
- $\gamma_i > 0$ for all $i \in \mathcal{N}$.

Continuous-time Markov chain (CTMC)

$$\mathcal{X} = \{\mathbf{X}(t) = (X_1(t), X_2(t), \ldots, X_N(t)) : t \geq 0\},$$

$$X_i(t) = \text{“state (S, I or R) of the individual } i \text{ at time } t\text{”},$$

$N = 5, \mathbf{X}(t) = \mathbf{x} = (S, S, I, R, I) \rightarrow$ *Individuals 1 and 2: Susceptible*
Individuals 3 and 5: Infected
Individual 4: Recovered

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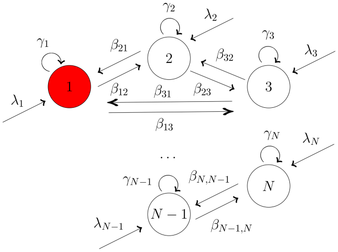

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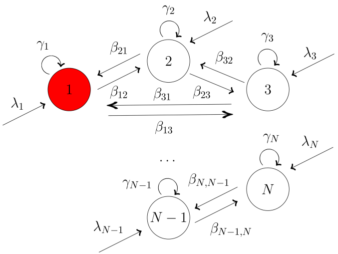

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Space of states of $\mathcal{X}$:

$$\mathcal{S} = \{S, I, R\}^N. \Rightarrow 3^N states \quad \Rightarrow$$

Gillespie Simulations
Mean-field analysis
N-intertwined approximation

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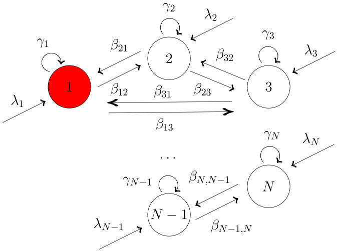

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N-intertwined approximation

The objective

Outbreak: Time interval since the epidemic starts until no infected individual remains.

Stochastic descriptors:

- Population descriptors:
  1. *Length and size of the outbreak*:
     - If every individual is infected during the outbreak: final state $(R, \dots, R)$.
     - Otherwise: how many individuals are recovered at the end of the outbreak?
  2. *Maximum number of individuals simultaneously infected during the outbreak.*
- Individual descriptors:
  3. *Probability of node i being infected, and infection type:*
     - Is the individual N infected during the outbreak? If so, due to an external infection or an individual contact?
  4. *Exact reproduction number of each node*: Random and individual version of the basic reproduction number (Artalejo & Lopez-Herrero (2013), Economou et al (2015)).

$$R_{\mathbf{x}}^{exact}(i) = \text{"}\textit{Number of infections caused directly by individual } i \textit{ until its recovery, given the initial state of the process } \mathbf{x} \in \mathcal{S}\text{"}$$

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The space of states

$$\mathcal{S} \quad = \quad \{S, I, R\}^N \;\approx\; \{0,1,2\}^N$$

$$\mathbf{x} \in \mathcal{S} \quad \Rightarrow \quad \mathbf{x} \;=\; (0,1,0,2,2,1,\dots,1,0)$$

We can *order* the space of states in different manners:

- Option 1: Lexicographically:

$$\begin{array}{r} (0,0,\dots,0,0,0) \\ (0,0,\dots,0,0,1) \\ (0,0,\dots,0,0,2) \\ (0,0,\dots,0,1,0) \\ (0,0,\dots,0,1,1) \\ (0,0,\dots,0,1,2) \\ \dots \end{array}$$

  which does not seem to provide a convenient structure for analysing the stochastic descriptors of interest (Van Mieghem et al. (2009)).

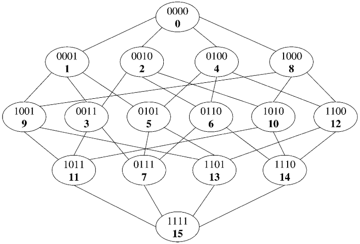

Fig. 1. State diagram in a graph with $N = 4$ nodes and the binary numbering of the states.

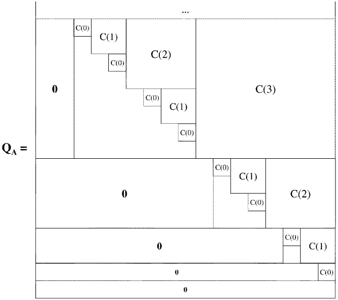

Fig. 3. Upper triangular part Q_A of Q.

VAN MIEGHEM *et al.*: VIRUS SPREAD IN NETWORKS

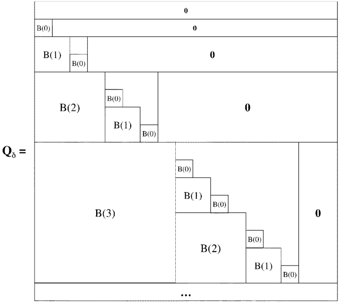

Fig. 2. Lower triangular part Q_δ of the infinitesimal generator Q.

$$Q = Q_\delta + Q_A + Q_{\text{diag}}$$
$$Q_{\text{diag}} = \text{diag}(q_{00}, q_{11}, \ldots, q_{2^{N-1},2^{N-1}})$$

- Option 2: To order the states according the number of susceptible, infected or recovered individuals within each state (Simon et al (2011), Economou et al (2015)):

$$\mathcal{S} = \bigcup_{r=0}^{N} L(r), \quad L(r) = \bigcup_{i=0}^{N-r} l(r;i),$$

where

$$\begin{aligned} L(r) &= \{\mathbf{x} \in \mathcal{S} : \textit{recovered individuals} = r\}, \\ l(r;i) &= \{\mathbf{x} \in \mathcal{S} : \textit{recovered individuals} = r, \textit{infected individuals} = i\}. \end{aligned}$$

For example, for $N = 4$, $r = 2$, $i = 1$:

$$l^{(4)}(2;1) = \{(2,2,1,0),(2,2,0,1),(2,1,2,0),(2,0,2,1),\dots\}$$

Then,

$$\#l(r;i) = \frac{N!}{r!i!(N-r-i)!}, \text{ and } \#L(r) = \sum_{i=0}^{N-r} J(r;i) = \frac{N!}{r!(N-r)!},$$

Given the previous order of states by levels and sub-levels, the infinitesimal generator corresponds to a very particular level-dependent Quasi-birth-and-death (QBD) process:

$$\begin{pmatrix} \mathbf{Q}_{0,0}(N) & \mathbf{Q}_{0,1}(N) & \mathbf{0}_{J^{(N)}(0)\times J^{(N)}(2)} & \cdots & \mathbf{0}_{J^{(N)}(0)\times J^{(N)}(N)} \\ \mathbf{0}_{J^{(N)}(1)\times J^{(N)}(0)} & \mathbf{Q}_{1,1}(N) & \mathbf{Q}_{1,2}(N) & \cdots & \mathbf{0}_{J^{(N)}(1)\times J^{(N)}(N)} \\ \mathbf{0}_{J^{(N)}(2)\times J^{(N)}(0)} & \mathbf{0}_{J^{(N)}(2)\times J^{(N)}(1)} & \mathbf{Q}_{2,2}(N) & \cdots & \mathbf{0}_{J^{(N)}(2)\times J^{(N)}(N)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{J^{(N)}(N-1)\times J^{(N)}(0)} & \mathbf{0}_{J^{(N)}(N-1)\times J^{(N)}(1)} & \mathbf{0}_{J^{(N)}(N-1)\times J^{(N)}(2)} & \cdots & \mathbf{Q}_{N-1,N}(N) \\ \mathbf{0}_{J^{(N)}(N)\times J^{(N)}(0)} & \mathbf{0}_{J^{(N)}(N)\times J^{(N)}(1)} & \mathbf{0}_{J^{(N)}(N)\times J^{(N)}(2)} & \cdots & \mathbf{Q}_{N,N}(N) \end{pmatrix}. \tag{1}$$

$$\mathbf{Q}_{r,r}(N) = \begin{pmatrix} \mathbf{Q}_{r,r}^{0,0}(N) & \mathbf{Q}_{r,r}^{0,1}(N) & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_{r,r}^{1,1}(N) & \mathbf{Q}_{r,r}^{1,2}(N) & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{Q}_{r,r}^{2,2}(N) & \dots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{Q}_{r,r}^{N-r-1,N-r}(N) \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{Q}_{r,r}^{N-r,N-r}(N) \end{pmatrix}, \ 0 \leq r \leq N,$$

$$\mathbf{Q}_{r,r+1}(N) = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{Q}_{r,r+1}^{1,0}(N) & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_{r,r+1}^{2,1}(N) & \dots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{Q}_{r,r+1}^{N-r,N-r-1}(N) \end{pmatrix}, \quad 0 \leq r \leq N-1,$$

Ordering states within sub-levels

- **Order A:** (Economou et al. (2015)) By an algorithm working as a black-box:
  (i) To translate states of $\mathcal{S}^{(N)} = \{S, I, R\}^N$ into states of $\{0, 1, 2\}^N$ with $S \equiv 0$, $I \equiv 1$ and $R \equiv 2$.
  (ii) To order states within $I^{(N)}(r; i)$ in a lexicographical manner.
  (iii) To turn over states $(x_1, \dots, x_N) \in I^{(N)}(r; i) \to (x_N, \dots, x_1) \in I^{(N)}(r; i)$.
  (iv) To translate again states of $\{0, 1, 2\}^N$ into states of $\mathcal{S}^{(N)} = \{S, I, R\}^N$.

$I^{(4)}(2; 1)$

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  - (iii) To turn over states $(x_1, \dots, x_N) \in I^{(N)}(r;i) \longrightarrow (x_N, \dots, x_1) \in I^{(N)}(r;i)$.
  - (iv) To translate again states of $\{0,1,2\}^N$ into states of $\mathcal{S}^{(N)} = \{S, I, R\}^N$.

$I^{(4)}(2;1)$

$$\begin{array}{ccccccccc}
\textit{Unordered States} & & & & & & & & \textit{Ordered States} \\
(R,R,I,S) & & (2,2,1,0) & & (0,1,2,2) & & (2,2,1,0) & & (R,R,I,S) \\
(R,R,S,I) & & (2,2,0,1) & & (0,2,1,2) & & (2,1,2,0) & & (R,I,R,S) \\
(R,I,R,S) & & (2,1,2,0) & & (0,2,2,1) & & (1,2,2,0) & & (I,R,R,S) \\
(R,S,R,I) & & (2,0,2,1) & & (1,0,2,2) & & (2,2,0,1) & & (R,R,S,I) \\
(R,I,S,R) & (i) & (2,1,0,2) & (ii) & (1,2,0,2) & (iii) & (2,0,2,1) & (iv) & (R,S,R,I) \\
(R,S,I,R) & \Rightarrow \; \Rightarrow & (2,0,1,2) & \Rightarrow \; \Rightarrow & (1,2,2,0) & \Rightarrow \; \Rightarrow & (0,2,2,1) & \Rightarrow \; \Rightarrow & (S,R,R,I) \\
(I,R,R,S) & & (1,2,2,0) & & (2,0,1,2) & & (2,1,0,2) & & (R,I,S,R) \\
(S,R,R,I) & & (0,2,2,1) & & (2,0,2,1) & & (1,2,0,2) & & (I,R,S,R) \\
(I,R,S,R) & & (1,2,0,2) & & (2,1,0,2) & & (2,0,1,2) & & (R,S,I,R) \\
(S,R,I,R) & & (0,2,1,2) & & (2,1,2,0) & & (0,2,1,2) & & (S,R,I,R) \\
(I,S,R,R) & & (1,0,2,2) & & (2,2,0,1) & & (1,0,2,2) & & (I,S,R,R) \\
(S,I,R,R) & & (0,1,2,2) & & (2,2,1,0) & & (0,1,2,2) & & (S,I,R,R)
\end{array}$$

$$I^{(N)}(r;i) = \left(I^{(N-1)}(r;i) \times \{S\}\right) \cup \left(I^{(N-1)}(r;i-1) \times \{I\}\right) \cup \left(I^{(N-1)}(r-1;i) \times \{R\}\right),$$

Ordering states within sub-levels

- **Order A:** (Economou et al. (2015)) By an algorithm working as a black-box:
  - (i) To translate states of $\mathcal{S}^{(N)} = \{S, I, R\}^N$ into states of $\{0,1,2\}^N$ with $S \equiv 0$, $I \equiv 1$ and $R \equiv 2$.
  - (ii) To order states within $I^{(N)}(r;i)$ in a lexicographical manner.
  - (iii) To turn over states $(x_1, \ldots, x_N) \in I^{(N)}(r;i) \longrightarrow (x_N, \ldots, x_1) \in I^{(N)}(r;i)$.
  - (iv) To translate again states of $\{0,1,2\}^N$ into states of $\mathcal{S}^{(N)} = \{S, I, R\}^N$.

$$I^{(4)}(2;1)$$

$$
\begin{array}{ccccccccc}
\textit{Unordered States} & & & & & & & & \textit{Ordered States} \\
(R,R,I,S) & & (2,2,1,0) & & (0,1,2,2) & & (2,2,1,0) & & (R,R,I,S) \\
(R,R,S,I) & & (2,2,0,1) & & (0,2,1,2) & & (2,1,2,0) & & (R,I,R,S) \\
(R,I,R,S) & & (2,1,2,0) & & (0,2,2,1) & & (1,2,2,0) & & (I,R,R,S) \\
(R,S,R,I) & & (2,0,2,1) & & (1,0,2,2) & & (2,2,0,1) & & (R,R,S,I) \\
(R,I,S,R) & (i) & (2,1,0,2) & (ii) & (1,2,0,2) & (iii) & (2,0,2,1) & (iv) & (R,S,R,I) \\
(R,S,I,R) & \Rightarrow \;\; \Rightarrow & (2,0,1,2) & \Rightarrow \;\; \Rightarrow & (1,2,2,0) & \Rightarrow \;\; \Rightarrow & (0,2,2,1) & \Rightarrow \;\; \Rightarrow & (S,R,R,I) \\
(I,R,R,S) & & (1,2,2,0) & & (2,0,1,2) & & (2,1,0,2) & & (R,I,S,R) \\
(S,R,R,I) & & (0,2,2,1) & & (2,0,2,1) & & (1,2,0,2) & & (I,R,S,R) \\
(I,R,S,R) & & (1,2,0,2) & & (2,1,0,2) & & (2,0,1,2) & & (R,S,I,R) \\
(S,R,I,R) & & (0,2,1,2) & & (2,1,2,0) & & (0,2,1,2) & & (S,R,I,R) \\
(I,S,R,R) & & (1,0,2,2) & & (2,2,0,1) & & (1,0,2,2) & & (I,S,R,R) \\
(S,I,R,R) & & (0,1,2,2) & & (2,2,1,0) & & (0,1,2,2) & & (S,I,R,R)
\end{array}
$$

$$I^{(N)}(r;i) \quad = \quad \left(I^{(N-1)}(r;i) \times \{S\}\right) \cup \left(I^{(N-1)}(r;i-1) \times \{I\}\right) \cup \left(I^{(N-1)}(r-1;i) \times \{R\}\right),$$

- **Order B:** Lexicographic order within each sub-level.

Position	*State* $\mathbf{x}$											
in $I^{(N)}(r;i)$	x_1	$\dots$	x_{N-r-i}	$x_{N-r-i+1}$	$\dots$	x_{N-r-1}	x_{N-r}	x_{N-r+1}	x_{N-r+2}	$\dots$	x_{N-1}	x_N
0	0	$\dots$	0	1	$\dots$	1	1	2	2	$\dots$	2	2
1	0	$\dots$	0	1	$\dots$	1	2	1	2	$\dots$	2	2
2	0	$\dots$	0	1	$\dots$	1	2	2	1	$\dots$	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
r	0	$\dots$	0	1	$\dots$	1	2	2	2	$\dots$	2	1
$r+1$	0	$\dots$	0	1	$\dots$	2	1	1	2	$\dots$	2	2
$r+2$	0	$\dots$	0	1	$\dots$	2	1	2	1	$\dots$	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Given a state $\mathbf{x} = (0,1,1,2,0,1,1,2,2,1) \in I^{(10)}(3;5)$, which is its position within $I^{(10)}(3;5)$? $\#I^{(10)}(3;5) = 2520$ states.
We reexpress $\mathbf{x} = \{(a_1,\dots,a_i),(b_1,\dots,b_r)\} = \{(2,3,6,7,10),(4,8,9)\}$ and

$$Pos_r^i(\mathbf{x}) = \sum_{k=0}^{r}\left(\sum_{l=j_k}^{j_{k+1}-1}\binom{N-a_l}{r-k|i-l+1}\right)+\sum_{k=1}^{r}\left(\binom{N-b_k}{r-k+1|i-(j_k-1)}\right.$$
$$\left.+\binom{N-b_k}{r-k+1|i-j_k}\right), \Rightarrow \; Pos_3^5(\mathbf{x}) = 173$$

- **Order B:** Lexicographic order within each sub-level.

Position in $I^{(N)}(r;i)$	x_1	$\dots$	x_{N-r-i}	$x_{N-r-i+1}$	$\dots$	x_{N-r-1}	x_{N-r}	x_{N-r+1}	x_{N-r+2}	$\dots$	x_{N-1}	x_N
0	0	$\dots$	0	1	$\dots$	1	1	2	2	$\dots$	2	2
1	0	$\dots$	0	1	$\dots$	1	2	1	2	$\dots$	2	2
2	0	$\dots$	0	1	$\dots$	1	2	2	1	$\dots$	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
r	0	$\dots$	0	1	$\dots$	1	2	2	2	$\dots$	2	1
$r+1$	0	$\dots$	0	1	$\dots$	2	1	1	2	$\dots$	2	2
$r+2$	0	$\dots$	0	1	$\dots$	2	1	2	1	$\dots$	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

State $\mathbf{x}$

Given a state $\mathbf{x} = (0,1,1,2,0,1,1,2,2,1) \in I^{(10)}(3;5)$, which is its position within $I^{(10)}(3;5)$? $\# I^{(10)}(3;5) = 2520$ states.

We reexpress $\mathbf{x} = \{(a_1,\dots,a_i),(b_1,\dots,b_r)\} = \{(2,3,6,7,10),(4,8,9)\}$ and

$$Pos^i_r(\mathbf{x}) = \sum_{k=0}^{r}\left(\sum_{l=j_k}^{j_{k+1}-1}\binom{N-a_l}{r-k|i-l+1}\right) + \sum_{k=1}^{r}\left(\binom{N-b_k}{r-k+1|i-(j_k-1)}\right.$$

$$\left. + \binom{N-b_k}{r-k+1|i-j_k}\right), \Rightarrow Pos^5_3(\mathbf{x}) = 173$$

- **Order B:** Lexicographic order within each sub-level.

Position in $I^{(N)}(r;i)$	x_1	$\dots$	x_{N-r-i}	$x_{N-r-i+1}$	$\dots$	x_{N-r-1}	x_{N-r}	x_{N-r+1}	x_{N-r+2}	$\dots$	x_{N-1}	x_N
0	0	$\dots$	0	1	$\dots$	1	1	2	2	$\dots$	2	2
1	0	$\dots$	0	1	$\dots$	1	2	1	2	$\dots$	2	2
2	0	$\dots$	0	1	$\dots$	1	2	2	1	$\dots$	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
r	0	$\dots$	0	1	$\dots$	1	2	2	2	$\dots$	2	1
$r+1$	0	$\dots$	0	1	$\dots$	2	1	1	2	$\dots$	2	2
$r+2$	0	$\dots$	0	1	$\dots$	2	1	2	1	$\dots$	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Given a state $\mathbf{x} = (0,1,1,2,0,1,1,2,2,1) \in I^{(10)}(3;5)$, which is its position within $I^{(10)}(3;5)$? $\#I^{(10)}(3;5) = 2520$ states.
We reexpress $\mathbf{x} = \{(a_1,\dots,a_i),(b_1,\dots,b_r)\} = \{(2,3,6,7,10),(4,8,9)\}$ and

$$Pos_r^i(\mathbf{x}) = \sum_{k=0}^{r}\left(\sum_{l=j_k}^{j_{k+1}-1}\binom{N-a_l}{r-k|i-l+1}\right)+\sum_{k=1}^{r}\left(\binom{N-b_k}{r-k+1|i-(j_k-1)}\right.$$
$$\left.+\binom{N-b_k}{r-k+1|i-j_k}\right), \Rightarrow Pos_3^5(\mathbf{x}) = 173$$

- **Order B:** Lexicographic order within each sub-level.

Position in $I^{(N)}(r;i)$	*State* $\mathbf{x}$: x_1	$\dots$	x_{N-r-i}	$x_{N-r-i+1}$	$\dots$	x_{N-r-1}	x_{N-r}	x_{N-r+1}	x_{N-r+2}	$\dots$	x_{N-1}	x_N
0	0	$\dots$	0	1	$\dots$	1	1	2	2	$\dots$	2	2
1	0	$\dots$	0	1	$\dots$	1	2	1	2	$\dots$	2	2
2	0	$\dots$	0	1	$\dots$	1	2	2	1	$\dots$	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
r	0	$\dots$	0	1	$\dots$	1	2	2	2	$\dots$	2	1
$r+1$	0	$\dots$	0	1	$\dots$	2	1	1	2	$\dots$	2	2
$r+2$	0	$\dots$	0	1	$\dots$	2	1	2	1	$\dots$	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Given a state $\mathbf{x} = (0,1,1,2,0,1,1,2,2,1) \in I^{(10)}(3;5)$, which is its position within $I^{(10)}(3;5)$? $\#I^{(10)}(3;5) = 2520$ states.
We reexpress $\mathbf{x} = \{(a_1,\dots,a_i),(b_1,\dots,b_r)\} = \{(2,3,6,7,10),(4,8,9)\}$ and

$$
\begin{aligned}
Pos_r^i(\mathbf{x}) \quad &= \quad \sum_{k=0}^{r}\left(\sum_{l=j_k}^{j_{k+1}-1}\binom{N-a_l}{r-k \mid i-l+1}\right) + \sum_{k=1}^{r}\left(\binom{N-b_k}{r-k+1 \mid i-(j_k-1)}\right. \\
&\quad \left. + \binom{N-b_k}{r-k+1 \mid i-j_k}\right), \Rightarrow \; Pos_3^5(\mathbf{x}) = 173
\end{aligned}
$$

Organization of the talk I

1. Motivation: SIR epidemic model for a small group of heterogeneous individuals
2. Structuring the space of states
3. Stochastic Descriptors / Summary Statistics
4. Numerical Results.

Analysing Population Stochastic Descriptors

- Length and size of an outbreak:
- Maximum number of simultaneously infected individuals during the outbreak:

$$\begin{aligned} I_{\mathbf{x}}^{max} &= \text{“}\textit{Maximum number of individuals simultaneously infected during} \\ &\quad \textit{the outbreak, given that the current state of } \mathcal{X} \textit{ is } \mathbf{x}\text{''}, \\ T_{\mathbf{x}}^{I} &= \text{“}\textit{Time until reaching an exact number } I \textit{ of individuals simultaneously} \\ &\quad \textit{infected during the outbreak, given that the current state of } \mathcal{X} \textit{ is } \mathbf{x}\text{''}. \end{aligned}$$

We work with the Laplace-Stieltjes transforms of $T_{\mathbf{x}}^{I}$,

$$\varphi_{\mathbf{x}}(I;z) \quad = \quad E\left[e^{-zT_{\mathbf{x}}^{I}} 1_{\{T_{\mathbf{x}}^{I}<\infty\}}\right], \quad \Re(z) \geq 0,$$

the probability mass function of the *peak of infection*, $I_{\mathbf{x}}^{max}$, can be computed in terms of $\mathbb{P}(I_{\mathbf{x}}^{max} \geq I) = \varphi_{\mathbf{x}}(I;0)$. Moreover, the restricted lth order moments

$$n_{\mathbf{x}}^{(l)}(I) \quad = \quad E\left[\left(T_{\mathbf{x}}^{I}\right)^{l} 1_{\{T_{\mathbf{x}}^{I}<\infty\}}\right] \quad = \quad \frac{d^{l}}{dz^{l}}\varphi_{\mathbf{x}}(I;z)\bigg|_{z=0}, \quad l \geq 1, \quad \mathbf{x} \in \mathcal{C},$$

allow us to analyse the speed at which this peak of infection is reached.

The restricted Laplace-Stieltjes transforms and moments of $T_{\mathbf{x}}^{I}$ are derived by a first-step argument. In particular, we have

$$\varphi_{\mathbf{x}}(I;z) = \sum_{j\in S(\mathbf{x})} \frac{\lambda_j + \sum_{k\in I(\mathbf{x})} \beta_{kj}}{z+q_{\mathbf{x}}} \varphi_{I_j(\mathbf{x})}(I;z) + \sum_{k\in I(\mathbf{x})} \frac{\gamma_k}{z+q_{\mathbf{x}}} \varphi_{R_k(\mathbf{x})}(I;z),$$

where

- $S(\mathbf{x})$ and $I(\mathbf{x})$ are the sub-sets of individuals susceptible and infected, respectively, according to $\mathbf{x}$.
- $I_j(\mathbf{x})$ and $R_j(\mathbf{x})$ are new states obtained from $\mathbf{x}$ by replacing $\mathbf{x}_j$ by I and R, respectively, for any $j \in \{1,\dots,N\}$.

Moments are obtained by successive differentiation of previous expression:

$$\begin{aligned} n_{\mathbf{x}}^{(l)}(I) &= \sum_{j\in S(\mathbf{x})} \frac{\lambda_j + \sum_{k\in I(\mathbf{x})} \beta_{kj}}{q_{\mathbf{x}}} n_{I_j(\mathbf{x})}^{(l)}(I) + \sum_{k\in I(\mathbf{x})} \frac{\gamma_k}{q_{\mathbf{x}}} n_{R_k(\mathbf{x})}^{(l)}(I) \\ &\quad + \frac{l}{q_{\mathbf{x}}} n_{\mathbf{x}}^{(l-1)}(I), \quad l \geq 1, \end{aligned}$$

Order A

Algorithm 1M (Laplace-Stieltjes transforms of $T_{\mathbf{x}}^{I}$, $I \geq \# I(\mathbf{x})$. Order A)

For $I = 1, \dots, N$*:*

PART 1

$\mathbf{h}_{N-I}^{I-1}(I;z) = \mathbf{A}_{N-I,N-I}^{I-1,I}(z)\mathbf{e}_{J(N-I;I)}$;

For $i = I-2, \dots, 1$*:*

$\mathbf{h}_{N-I}^{i}(I;z) = \mathbf{A}_{N-I,N-I}^{i,i+1}(z)\mathbf{h}_{N-I}^{i+1}(I;z)$;

For $r = N-I-1, \dots, 0$*:*

$\mathbf{h}_{r}^{I-1}(I;z) = \mathbf{A}_{r,r+1}^{I-1,I-2}(z)\mathbf{h}_{r+1}^{I-2}(I;z) + \mathbf{A}_{r,r}^{I-1,I}(z)\mathbf{e}_{J(r;I)}$;

For $i = I-2, \dots, 2$*:*

$\mathbf{h}_{r}^{i}(I;z) = \mathbf{A}_{r,r+1}^{i,i-1}(z)\mathbf{h}_{r+1}^{i-1}(I;z) + \mathbf{A}_{r,r}^{i,i+1}(z)\mathbf{h}_{r}^{i+1}(I;z)$;

$\mathbf{h}_{r}^{1}(I;z) = \mathbf{A}_{r,r}^{1,2}(z)\mathbf{h}_{r}^{2}(I;z)$;

$$I^{(N)}(r;i) = \left(I^{(N-1)}(r;i) \times \{S\}\right) \cup \left(I^{(N-1)}(r;i-1) \times \{I\}\right) \cup \left(I^{(N-1)}(r-1;i) \times \{R\}\right),$$

Order A

Algorithm 1M (Laplace-Stieltjes transforms of $T_{\mathbf{x}}^{I}$, $I \geq \#I(\mathbf{x})$. Order A)

For $I = 1, \dots, N$*:*

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$\mathbf{h}_{N-I}^{I-1}(I;z) = \mathbf{A}_{N-I,N-I}^{I-1,I}(z)\mathbf{e}_{J(N-I;I)}$;

For $i = I-2, \dots, 1$*:*

$\mathbf{h}_{N-I}^{i}(I;z) = \mathbf{A}_{N-I,N-I}^{i,i+1}(z)\mathbf{h}_{N-I}^{i+1}(I;z)$;

For $r = N-I-1, \dots, 0$*:*

$\mathbf{h}_{r}^{I-1}(I;z) = \mathbf{A}_{r,r+1}^{I-1,I-2}(z)\mathbf{h}_{r+1}^{I-2}(I;z) + \mathbf{A}_{r,r}^{I-1,I}(z)\mathbf{e}_{J(r;I)}$;

For $i = I-2, \dots, 2$*:*

$\mathbf{h}_{r}^{i}(I;z) = \mathbf{A}_{r,r+1}^{i,i-1}(z)\mathbf{h}_{r+1}^{i-1}(I;z) + \mathbf{A}_{r,r}^{i,i+1}(z)\mathbf{h}_{r}^{i+1}(I;z)$;

$\mathbf{h}_{r}^{1}(I;z) = \mathbf{A}_{r,r}^{1,2}(z)\mathbf{h}_{r}^{2}(I;z)$;

$$I^{(N)}(r;i) \quad = \quad \left(I^{(N-1)}(r;i) \times \{S\}\right) \cup \left(I^{(N-1)}(r;i-1) \times \{I\}\right) \cup \left(I^{(N-1)}(r-1;i) \times \{R\}\right),$$

The restricted Laplace-Stieltjes transforms and moments of $T_{\mathbf{x}}^{I}$ are derived by a first-step argument. In particular, we have

$$\varphi_{\mathbf{x}}(I;z) \quad = \quad \sum_{j\in S(\mathbf{x})} \frac{\lambda_j + \sum\limits_{k\in I(\mathbf{x})} \beta_{kj}}{z+q_{\mathbf{x}}} \varphi_{I_j(\mathbf{x})}(I;z) + \sum_{k\in I(\mathbf{x})} \frac{\gamma_k}{z+q_{\mathbf{x}}} \varphi_{R_k(\mathbf{x})}(I;z),$$

Moments are obtained by successive differentiation of previous expression:

$$\begin{aligned} n_{\mathbf{x}}^{(l)}(I) \quad &= \quad \sum_{j\in S(\mathbf{x})} \frac{\lambda_j + \sum\limits_{k\in I(\mathbf{x})} \beta_{kj}}{q_{\mathbf{x}}} n_{I_j(\mathbf{x})}^{(l)}(I) + \sum_{k\in I(\mathbf{x})} \frac{\gamma_k}{q_{\mathbf{x}}} n_{R_k(\mathbf{x})}^{(l)}(I) \\ &\quad + \frac{l}{q_{\mathbf{x}}} n_{\mathbf{x}}^{(l-1)}(I), \quad l \geq 1, \end{aligned}$$

The restricted Laplace-Stieltjes transforms and moments of $T_{\mathbf{x}}^{I}$ are derived by a first-step argument. In particular, we have

$$\varphi_{(b_1,\ldots,b_r)}^{(a_1,\ldots,a_i)}(I;z) = \sum_{\substack{j \in \{1,\ldots,N\} \\ j \notin \{a_1,\ldots,a_i\} \\ j \notin \{b_1,\ldots,b_r\}}} \frac{\lambda_j + \sum_{i'=1}^{i} \beta_{a_{i'}j}}{z + q_{(b_1,\ldots,b_r)}^{(a_1,\ldots,a_i)}} \varphi_{(b_1,\ldots,b_r)}^{(a_1,\ldots,j,\ldots,a_i)}(I;z) + \sum_{i'=1}^{i} \frac{\gamma_{a_{i'}}}{z + q_{(b_1,\ldots,b_r)}^{(a_1,\ldots,a_i)}} \varphi_{(b_1,\ldots,a_{i'},\ldots,b_r)}^{(a_1,\ldots,a_{i'-1},a_{i'+1},\ldots,a_i)}(I;z).$$

Moments are obtained by successive differentiation of previous expression:

$$n_{\mathbf{x}}^{(l)}(I) = \sum_{j \in S(\mathbf{x})} \frac{\lambda_j + \sum_{k \in I(\mathbf{x})} \beta_{kj}}{q_{\mathbf{x}}} n_{I_j(\mathbf{x})}^{(l)}(I) + \sum_{k \in I(\mathbf{x})} \frac{\gamma_k}{q_{\mathbf{x}}} n_{R_k(\mathbf{x})}^{(l)}(I) + \frac{l}{q_{\mathbf{x}}} n_{\mathbf{x}}^{(l-1)}(I), \quad l \geq 1,$$

The restricted Laplace-Stieltjes transforms and moments of $T_{\mathbf{x}}^{I}$ are derived by a first-step argument. In particular, we have

$$\begin{aligned}\varphi_{(b_1,\dots,b_r)}^{(a_1,\dots,a_i)}(I;z) &= \sum_{\substack{j \in \{1,\dots,N\} \\ j \notin \{a_1,\dots,a_i\} \\ j \notin \{b_1,\dots,b_r\}}} \frac{\lambda_j + \sum_{i'=1}^{i} \beta_{a_{i'}j}}{z + q_{(b_1,\dots,b_r)}^{(a_1,\dots,a_i)}} \varphi_{(b_1,\dots,b_r)}^{(a_1,\dots,j,\dots,a_i)}(I;z) \\ &\quad + \sum_{i'=1}^{i} \frac{\gamma_{a_{i'}}}{z + q_{(b_1,\dots,b_r)}^{(a_1,\dots,a_i)}} \varphi_{(b_1,\dots,a_{i'},\dots,b_r)}^{(a_1,\dots,a_{i'-1},a_{i'+1},\dots,a_i)}(I;z).\end{aligned}$$

Moments are obtained by successive differentiation of previous expression:

$$\begin{aligned}n_{(b_1,\dots,b_r)}^{(a_1,\dots,a_i),(l)}(I) &= \sum_{\substack{j \in \{1,\dots,N\} \\ j \notin \{a_1,\dots,a_i\} \\ j \notin \{b_1,\dots,b_r\}}} \frac{\lambda_j + \sum_{i'=1}^{i} \beta_{a_{i'}j}}{q_{(b_1,\dots,b_r)}^{(a_1,\dots,a_i)}} n_{(b_1,\dots,b_r)}^{(a_1,\dots,j,\dots,a_i),(l)}(I) + \sum_{i'=1}^{i} \frac{\gamma_{a_{i'}}}{q_{(b_1,\dots,b_r)}^{(a_1,\dots,a_i)}} \\ &\quad \times n_{(b_1,\dots,a_{i'},\dots,b_r)}^{(a_1,\dots,a_{i'-1},a_{i'+1},\dots,a_i),(l)}(I) + \frac{l}{q_{(b_1,\dots,b_r)}^{(a_1,\dots,a_i)}} n_{(b_1,\dots,b_r)}^{(a_1,\dots,a_i),(l-1)}(I),\end{aligned}$$

Order B

Algorithm 1S (Laplace-Stieltjes transforms of $T^l_{\mathbf{x}}$, $l \geq \#I(\mathbf{x})$. Order B)

For $l = 1, \ldots, N$*:*

PART 1

For $r = N - l, \ldots, 0$*:*

For $i = l - 1, \ldots, 1$*:*

For any $\mathbf{x} = \{(a_1, \ldots, a_i), (b_1, \ldots, b_r)\}$*:*

Compute $\varphi^{(a_1,\ldots,a_i)}_{(b_1,\ldots,b_r)}(l; z)$ *from the first-step scalar equation and store it in position* $Pos^i_r(\mathbf{x})$ *of vector* $\mathbf{h}^i_r(l; z)$*;*

$$Pos^i_r(\mathbf{x}) = \sum_{k=0}^{r}\left(\sum_{l=j_k}^{j_{k+1}-1}\binom{N-a_l}{r-k|i-l+1}\right) + \sum_{k=1}^{r}\left(\binom{N-b_k}{r-k+1|i-(j_k-1)} + \binom{N-b_k}{r-k+1|i-j_k}\right),$$

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$$Pos_r^i(\mathbf{x}) = \sum_{k=0}^{r} \left(\sum_{l=j_k}^{j_{k+1}-1} \binom{N - a_l}{r - k | i - l + 1} \right) + \sum_{k=1}^{r} \left(\binom{N - b_k}{r - k + 1 | i - (j_k - 1)} + \binom{N - b_k}{r - k + 1 | i - j_k} \right),$$

The objective

Stochastic descriptors:

- Population descriptors:
    1. *Length and size of the outbreak*
    2. *Maximum number of individuals simultaneously infected during the outbreak*
- Individual descriptors:
    3. *Probability of node i being infected, and infection type*
    4. *Exact reproduction number of each node*.

Organization of the talk I

1. Motivation: SIR epidemic model for a small group of heterogeneous individuals
2. Structuring the space of states
3. Stochastic Descriptors / Summary Statistics
4. Numerical Results.

Spread of MRSA in Intensive Care Units

Spread of the nosocomial pathogen *Methicillin-resistant Staphylococcus Aureus* (MRSA) among the patients within an intensive care unit (ICU).

- Methicillin-resistant Staphylococcus aureus (MRSA) is a bacterium responsible for several difficult-to-treat infections in humans. In particular, is any strain of Staphylococcus aureus resistant to beta-lactam antibiotics.
- It is a hospital-acquire infection, since hospital patients with open wounds or weakened immune system are at special risk of becoming infected.
- Treatment depends on many factors, as the severity of the symptoms and the localization of the infection (nasal, skin...). In most of the cases usual treatments range between 5-10 days.

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Spread of MRSA in Intensive Care Units

- Analysis of **different types of patients** or of several control strategies (**Isolation**, **Room configuration**,...) ⇒ Non-homogeneous
- Small group of individuals ⇒ Convenience of considering the whole complexity given by an heterogeneous network.

- ICU of 9 beds, and patient 1 starting an outbreak.
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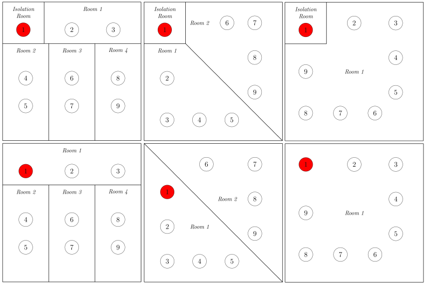

- Same room: $\beta = \beta_{ij} = 0.329/9$ (Cooper et al. (2004))
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- Different rooms: $\beta_{ij} = 0.65\beta$ (intermediate case)
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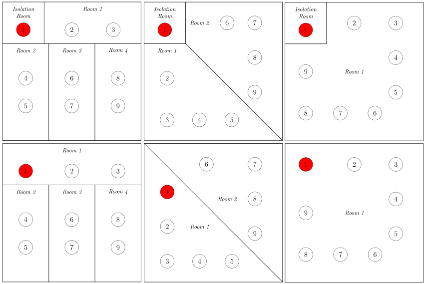

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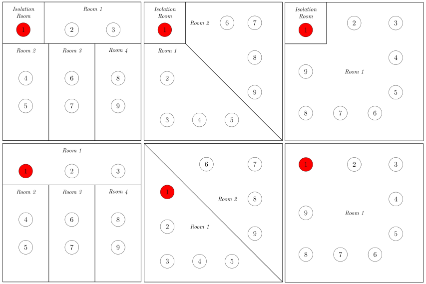

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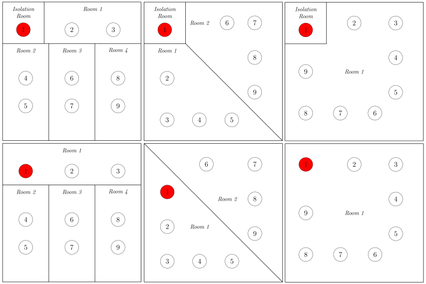

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Length and size of the outbreak

$$
\begin{aligned}
T &= \text{“\textit{Time duration of the outbreak (in days)}”}, \\
R &= \text{“\textit{Number of recovered individuals at the end of the outbreak}”}
\end{aligned}
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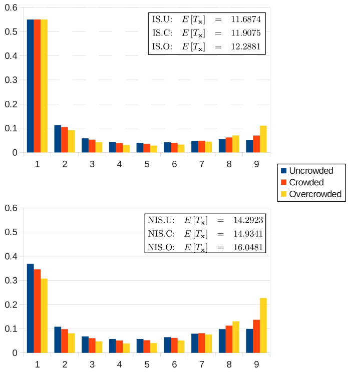

- Bimodal shape = two-output situation:
  1. Final number of infected individuals equals 1 if epidemic does not escape the isolation room.
  2. Once it escapes, it will reach a size of the outbreak near the larger mode.
- Room configuration becomes more important when no isolation measures are taken.
- Preventive measures can result in reductions of up to 35% for avoiding infection of any other patient, and of up to 28% in the length of the outbreak (in *days*).

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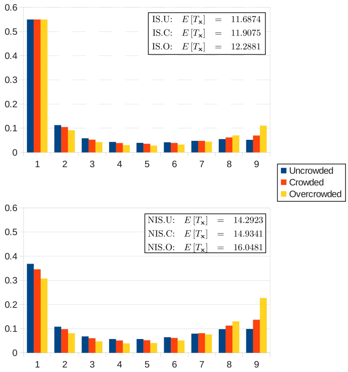

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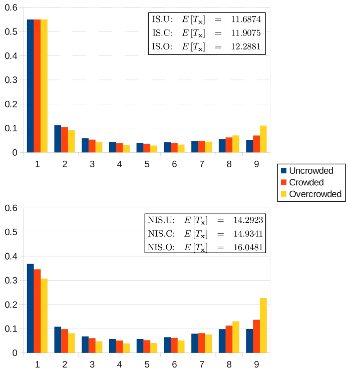

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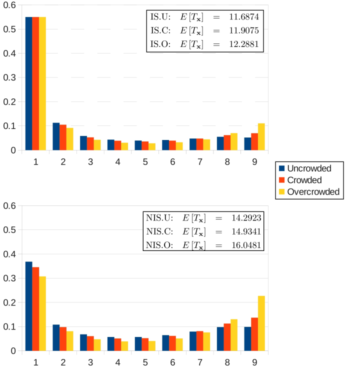

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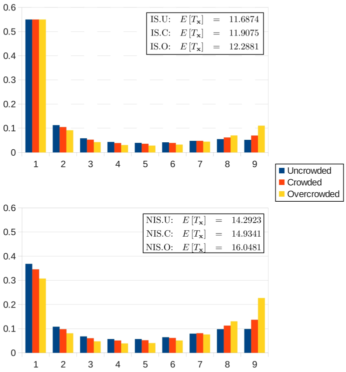

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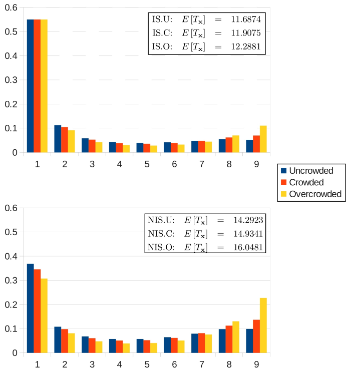

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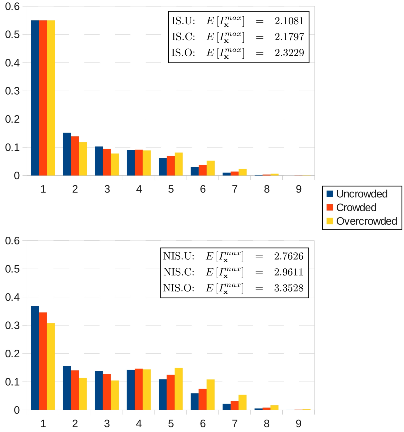
Maximum number of individuals simultaneously infected

$$I^{max} \quad = \quad \text{“Maximum number of individuals simultaneously infected during the outbreak”}$$



Individual fate

$$A = \text{"}\textit{The particular individual does not become infected}\text{"},$$
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Fate of Patient i	$i \in \mathcal{N}$	$i \in \mathcal{N}$	$i \in \mathcal{N}$
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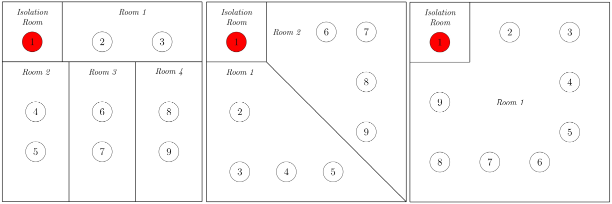
$\mathbb{P}(B)$	0.0282	0.0277	0.0265
$\mathbb{P}(C)$	0.1984	0.2151	0.2464
$E[T_{\mathbf{x}}^B 1_{\{T_{\mathbf{x}}^B < \infty\}}]$	0.2285	0.2182	0.1970
$E[T_{\mathbf{x}}^C 1_{\{T_{\mathbf{x}}^C < \infty\}}]$	2.0602	2.2205	2.4832
$E[T_{\mathbf{x}}^{B\vee C} 1_{\{T_{\mathbf{x}}^{B\vee C} < \infty\}}]$	2.2887	2.4387	2.6802
$E[T_{\mathbf{x}}^{B\vee C} \mid \{T_{\mathbf{x}}^{B\vee C} < \infty\}]$	10.1005	10.0467	9.8192



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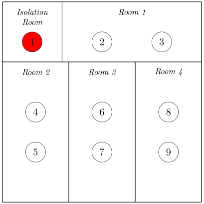

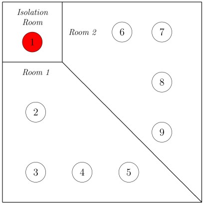

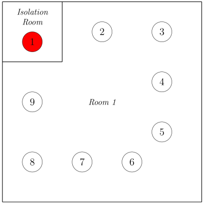

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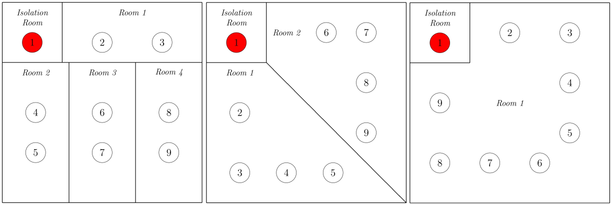

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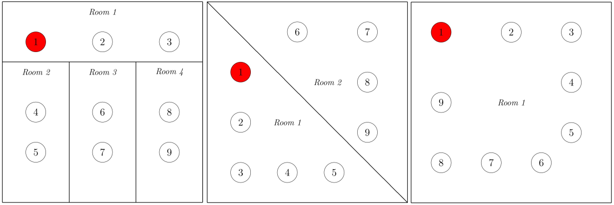
Fate of Patient i	$i \in \{2,3\}$	$i \in \{4,\dots,9\}$	$i \in \{2,\dots,5\}$	$i \in \{6,\dots,9\}$	$i \in \mathcal{N}$
$\mathbb{P}(A)$	0.6110	0.6426	0.5774	0.6074	0.5132
$\mathbb{P}(B)$	0.0265	0.0287	0.0261	0.0284	0.0251
$\mathbb{P}(C)$	0.3625	0.3286	0.3965	0.3643	0.4617
$E[T_{\mathbf{x}}^{B} 1_{\{T_{\mathbf{x}}^{B}<\infty\}}]$	0.2062	0.2355	0.1977	0.2264	0.1777
$E[T_{\mathbf{x}}^{C} 1_{\{T_{\mathbf{x}}^{C}<\infty\}}]$	2.8283	2.8899	3.0782	3.1733	3.4914
$E[T_{\mathbf{x}}^{B\vee C} 1_{\{T_{\mathbf{x}}^{B\vee C}<\infty\}}]$	3.0345	3.1254	3.2759	3.3997	3.6692
$E[T_{\mathbf{x}}^{B\vee C} \mid \{T_{\mathbf{x}}^{B\vee C}<\infty\}]$	7.8008	8.7452	7.7510	8.6586	7.5368



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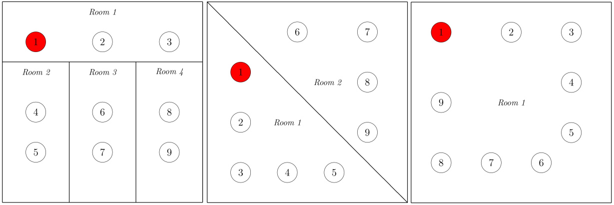
$\mathbb{P}(C)$	0.3625	0.3286	0.3965	0.3643	0.4617
$E[T_{\mathbf{x}}^{B} 1_{\{T_{\mathbf{x}}^{B}<\infty\}}]$	0.2062	0.2355	0.1977	0.2264	0.1777
$E[T_{\mathbf{x}}^{C} 1_{\{T_{\mathbf{x}}^{C}<\infty\}}]$	2.8283	2.8899	3.0782	3.1733	3.4914
$E[T_{\mathbf{x}}^{B\vee C} 1_{\{T_{\mathbf{x}}^{B\vee C}<\infty\}}]$	3.0345	3.1254	3.2759	3.3997	3.6692
$E[T_{\mathbf{x}}^{B\vee C} \mid \{T_{\mathbf{x}}^{B\vee C}<\infty\}]$	7.8008	8.7452	7.7510	8.6586	7.5368



Individual fate

$$A = \text{"The particular individual does not become infected"},$$
$$B = \text{"The particular individual becomes infected due to external reasons"},$$
$$C = \text{"The particular individual becomes infected due to a within-network contact"}$$

Non-isolated	NIS.U		NIS.C		NIS.O
Fate of Patient i	$i \in \{2,3\}$	$i \in \{4,\ldots,9\}$	$i \in \{2,\ldots,5\}$	$i \in \{6,\ldots,9\}$	$i \in \mathcal{N}$
$\mathbb{P}(A)$	0.6110	0.6426	0.5774	0.6074	0.5132
$\mathbb{P}(B)$	0.0265	0.0287	0.0261	0.0284	0.0251
$\mathbb{P}(C)$	0.3625	0.3286	0.3965	0.3643	0.4617
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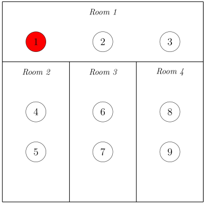
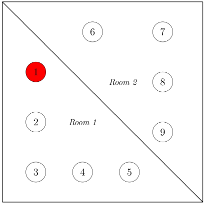
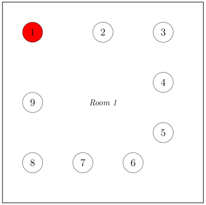
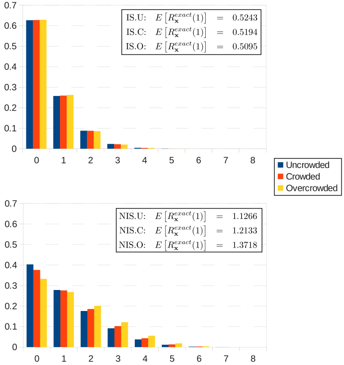






$R^{exact}(1) =$ *"Number of infections caused by patient 1 until he recovers"*



- When patient 1 is isolated, he directly infects an average of 0.51 individuals until he recovers.
- *Paradoxically*, under more crowded situations, patient 1 plays a bit less important role in the infectious process.
- Isolation of patient 1 can reduce its infectiousness, in terms of $E[R^{exact}(1)]$, up to more than a 50%.
- Under no isolation, room configuration becomes more important.

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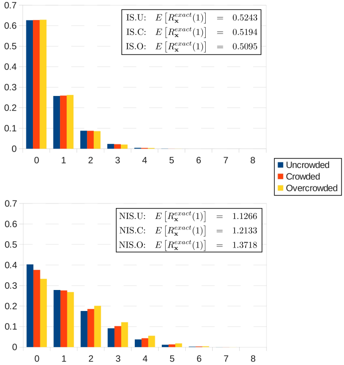

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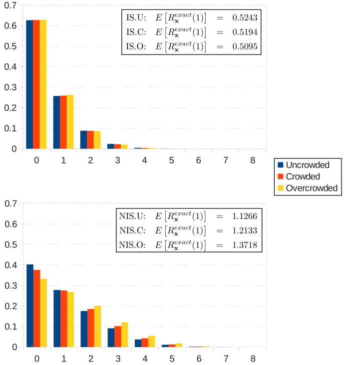

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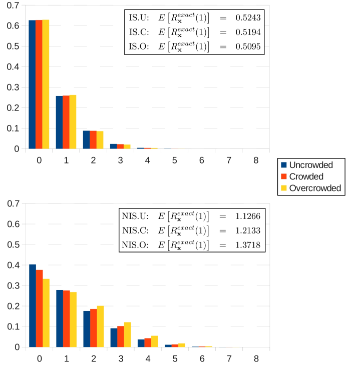

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Conclusions

- We focus here in the SIR epidemic model among an heterogeneous population of N individuals, which is model by a network.
- Under highly heterogeneous conditions, the heterogeneity at the individual level can only be addressed by means of analysing in an exact way the continuous-time Markov chain representing the spread of the epidemic within the directed network.
- Since this yields the space of states $\mathcal{S} = \{S, I, R\}^N$, it is crucial to make some decisions on how to order the states within $\mathcal{S}$, and to make focus on the algorithmic issue.
- We have presented two orders, Order A and B, which permit to work with a matrix and a scalar formalism, respectively.

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Conclusions

- By following this orders, we present four stochastic descriptors that permit to analyse the spread dynamics of the disease from the population and the individual perspective.
- This descriptors have been analysed in an algorithmic manner, by means of first-step arguments, Laplace-Stieltjes transforms, auxiliary absorbing Markov chains and probability generating functions.
- We illustrate our approach by studying the spread of a nosocomial pathogen among the patients within an intensive care unit. Control strategies (isolation of the initially infected patient, room crowding) are analysed by means of our approach and our stochastic descriptors. Isolation remains as the most effective strategy.

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Thank you very much for your attention.

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Computational Comparison

Table: Computational comparison (time, in *seconds*, and memory usage, in *megabytes*) between Algorithm 1S and 1M. Homogeneous population with N individuals. $\lambda_i = 1$, $\gamma_i = 3$ for all $i \in \mathcal{N}$, $\beta_{ij} = 2$ for all $(i,j) \in \mathcal{L}$

	N	4	5	6	7	8
$E\left[I^{max}_{(I,S,S,\dots,S)}\right]$		2.5090	3.1029	3.7490	4.4414	5.1729
Time	*Alg. 2S*	0.08	0.44	2.41	11.64	52.49
	Alg. 2M	0.01	0.1	0.71	5.66	49.06
Memory Usage	*Alg. 2S*	< 15	18.29	18.36	18.59	19.20
	Alg. 2M	< 15	< 15	19.01	28.48	107.04
	N	9	10	11	12	13
$E\left[I^{max}_{(I,S,S,\dots,S)}\right]$		5.9368	6.7272	7.5393	8.3695	9.2146
Time	*Alg. 2S*	201.78	834.78	3647.25	13102.28	49655.32
	Alg. 2M	330.39	2783.13	–	–	–
Memory Usage	*Alg. 2S*	21.02	25.33	38.23	77.23	200.29
	Alg. 2M	701.48	5653	$> 32GB$	$> 32GB$	$> 32GB$

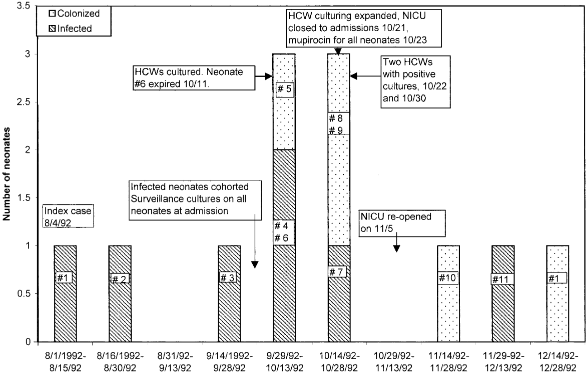

Figure: Outbreak data from a neonatal intensive care unit (Childrens National Medical Center, District of Columbia). Figure from Sumathi Nambiar et al. (2003)