A Gillespie algorithm for simulating interacting non-Markovian point processes

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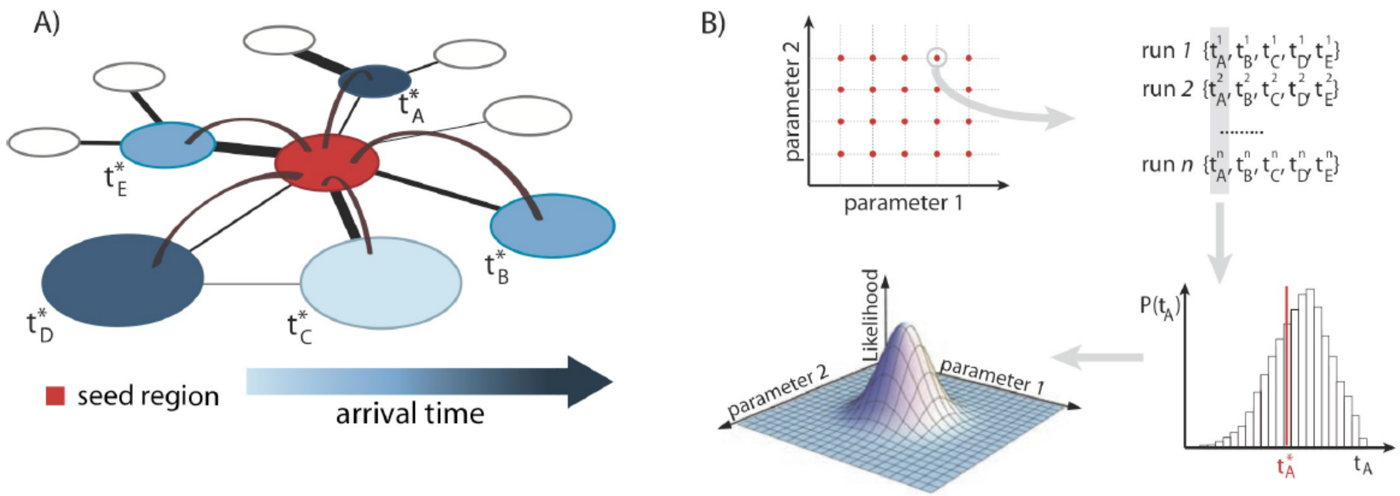
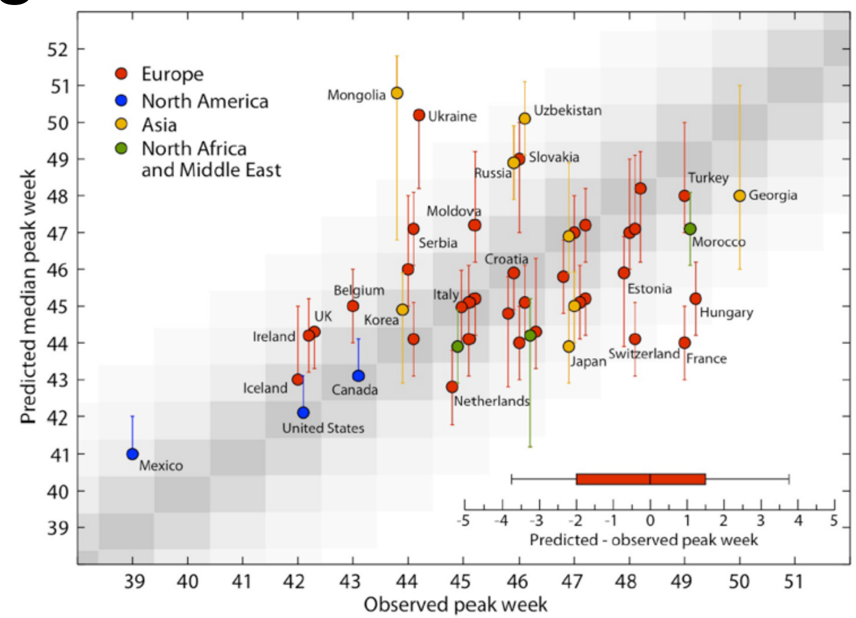
Prediction/retrospective assessment of H1N1 influenza crisis in 2009

Model

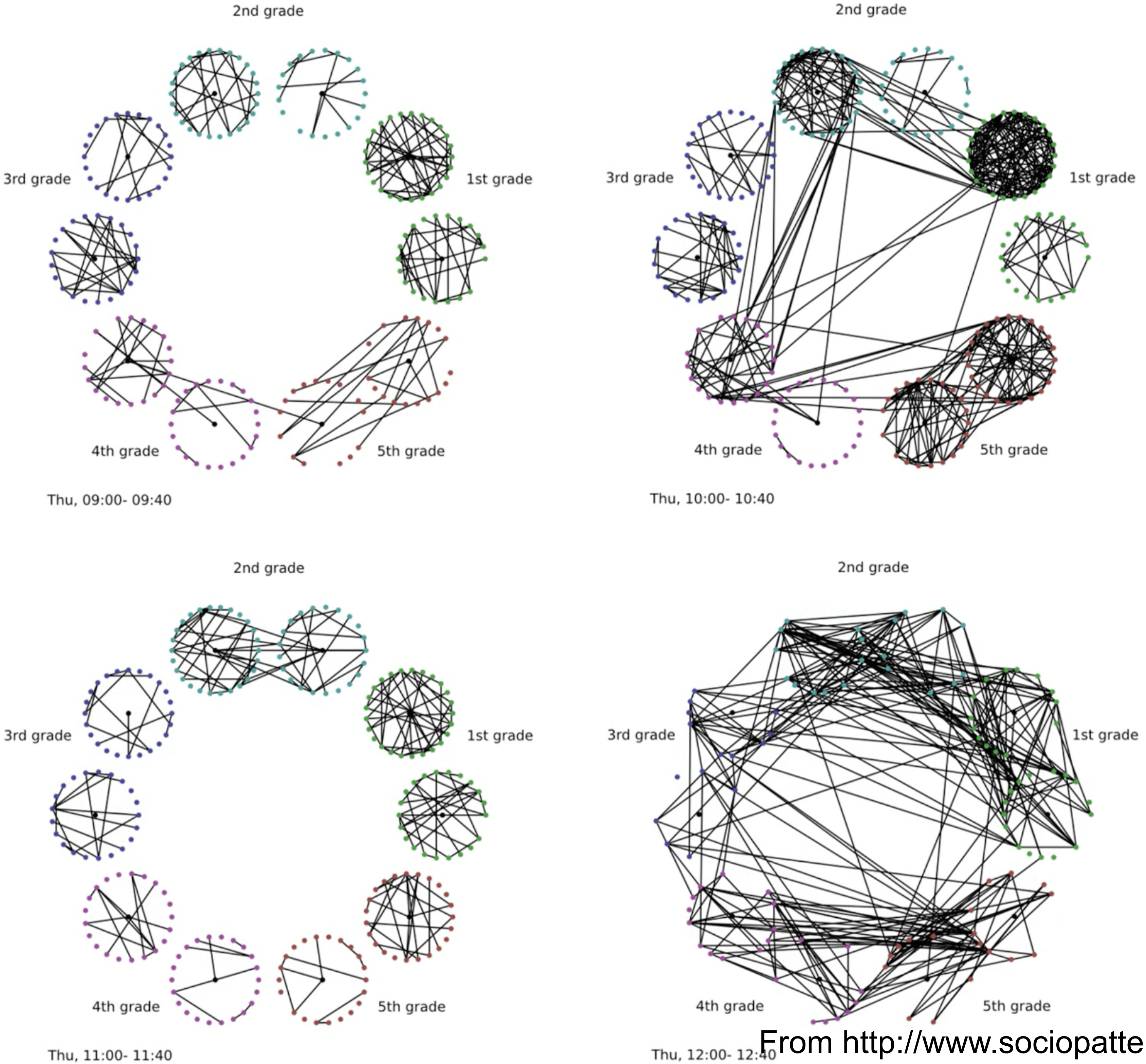


Results



✔ Also effects of vaccination predicted

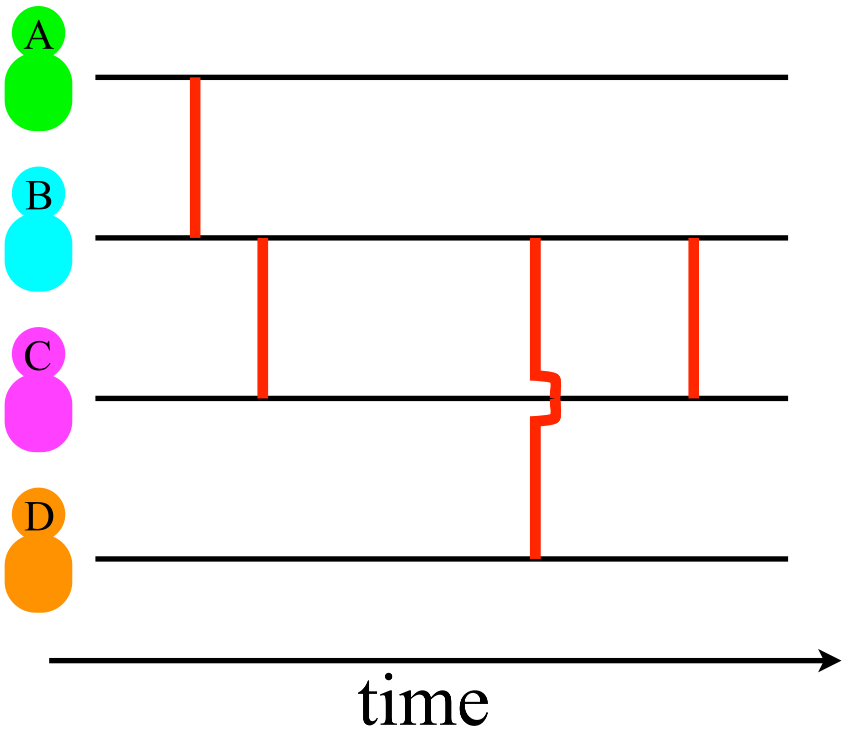
Tizzoni et al., BMC Medicine (2012)



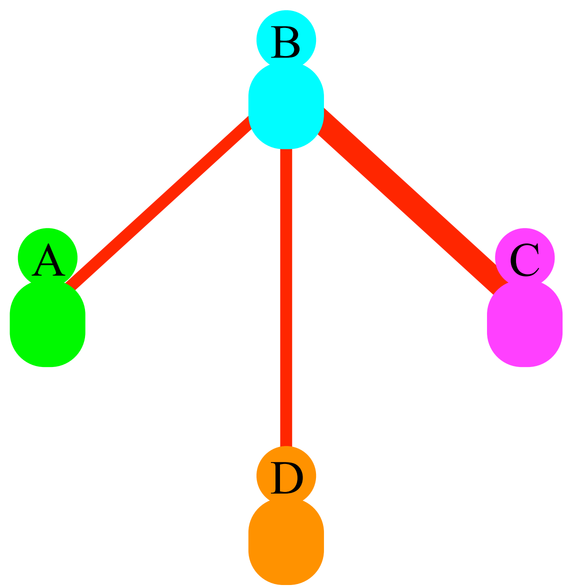
From http://www.sociopatterns.org/gallery/

Why does it matter?

temporal net



aggregate (i.e., static, traditional) net



✓ node A → node D (temporal path)

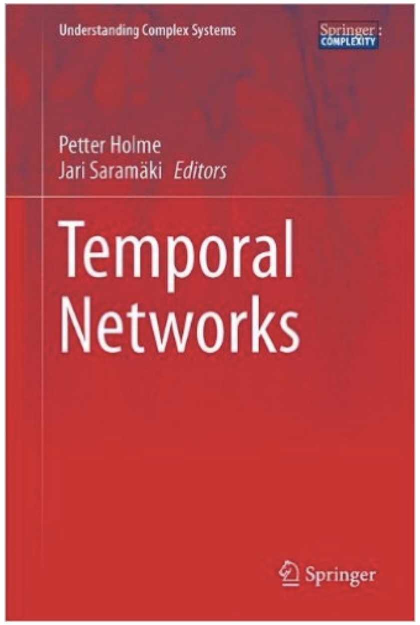
- node D → node A

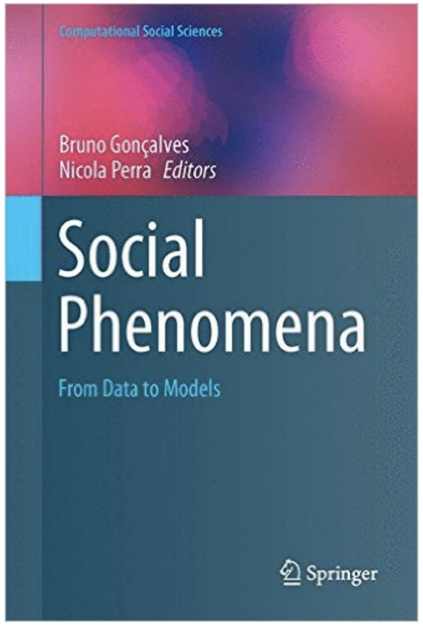
time stamp	ID1	ID2	duration
2009-01-01 14:13	1	3	1 min
2009-01-01 14:15	1	6	4 min
2009-01-01 14:15	5	26	1 min
2009-01-01 14:18	2	5	1 min
2009-01-01 14:19	1	13	4 min
2009-01-01 14:19	3	4	1 min
2009-01-01 14:24	1	22	1 min
2009-01-01 14:26	1	22	7 min
2009-01-01 14:26	3	6	1 min
⋮			

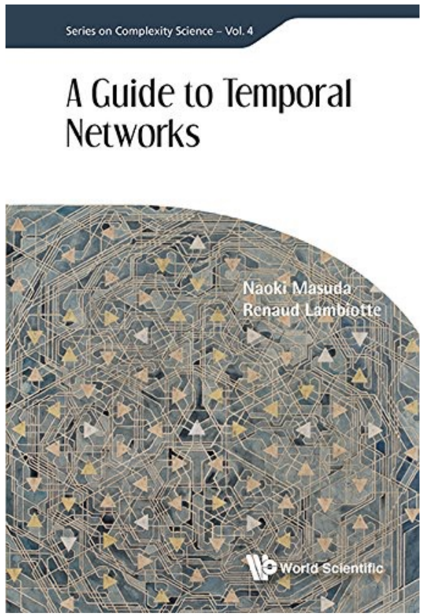
(Takaguchi, Nakamura, Sato, Yano & Masuda, Physical Review X, 2011)

Temporal networks

- Kempe, Kleinberg & Kumar, Proc. STOC'00 (2000)
- Holme and Saramäki, Phys. Rep., 519, 97-125 (2012)
- Holme, Eur. Phys. J. B, 88, 234 (2015).
- Holme & Saramäki, Eds., Temporal networks, Springer (2013).
- Masuda and Holme, F1000Prime Reports, 5, 6 (2013): On epidemics
- Masuda & Lambiotte, A Guide to Temporal Networks, World Scientific (2016): On math and computational tools

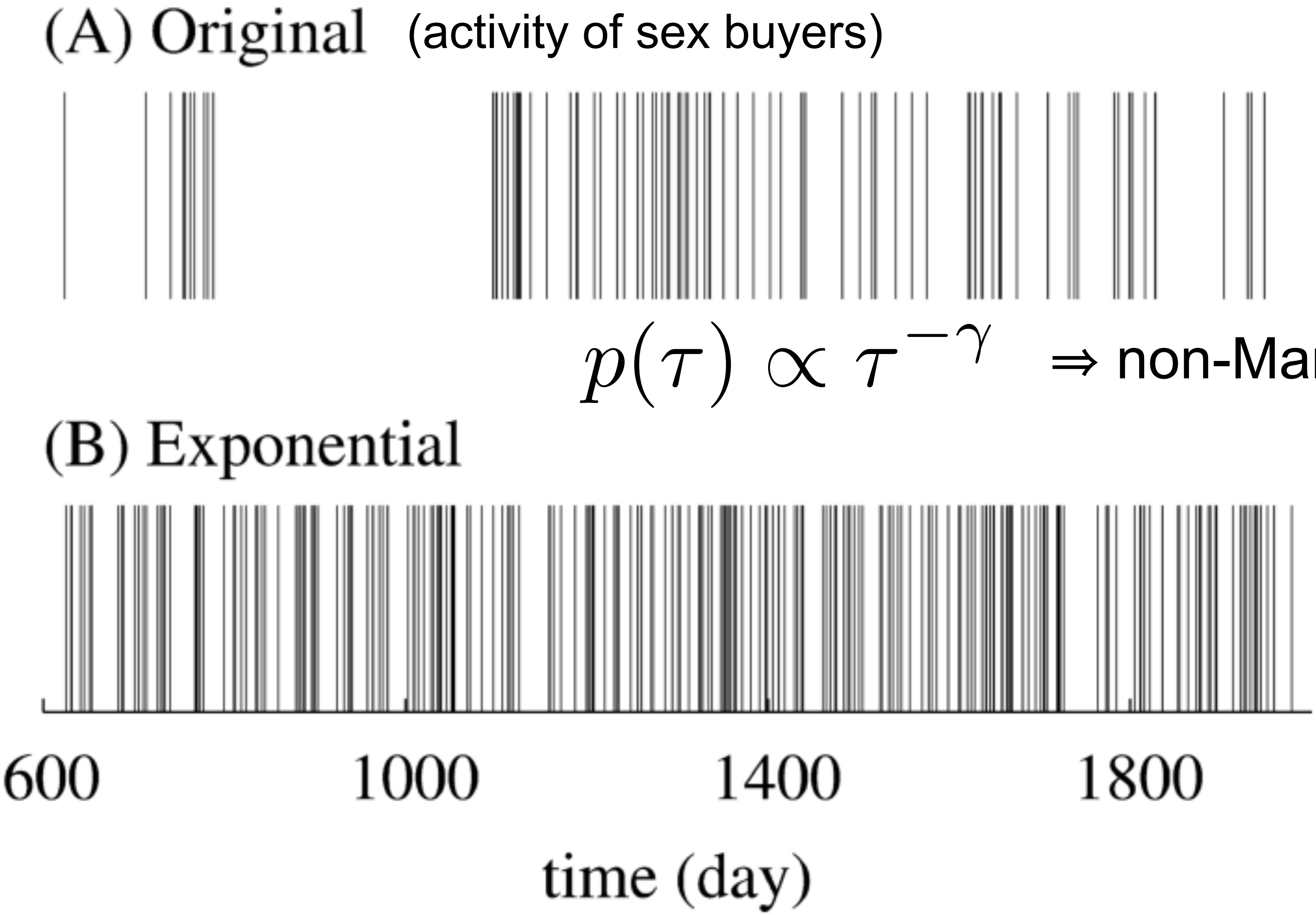






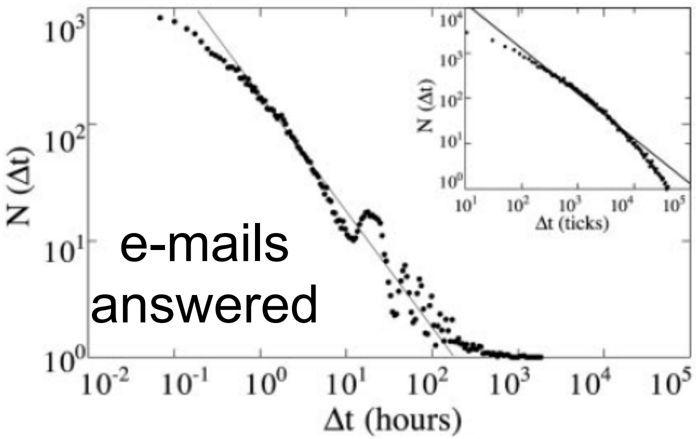
1. Long-tailed distributions of inter-event times

(activity of sex buyers)

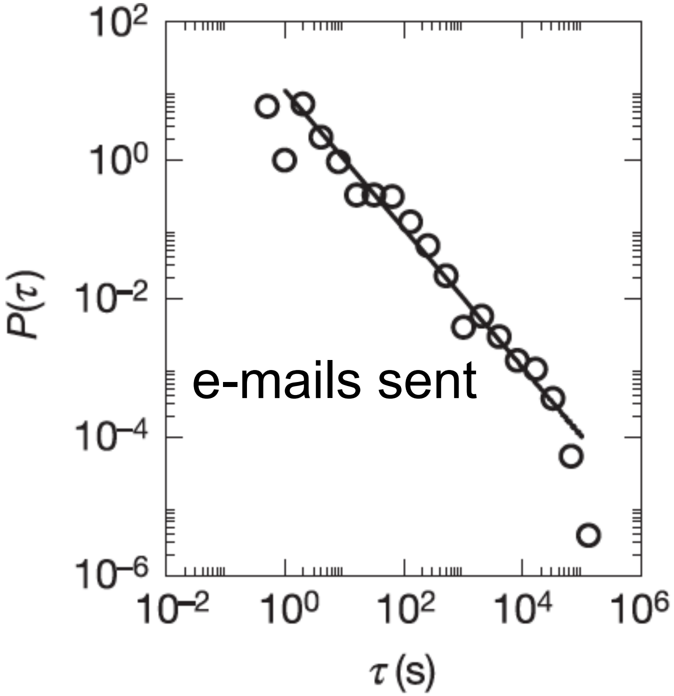


$p(\tau) \propto \tau^{-\gamma}$ ⇒ non-Markovian

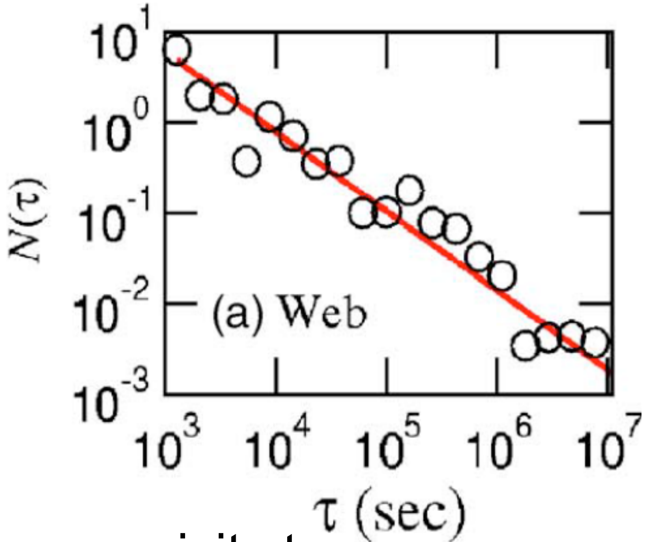
(Masuda & Holme, F1000Prime Rep. 2013)



(Eckmann et al., PNAS 2004)

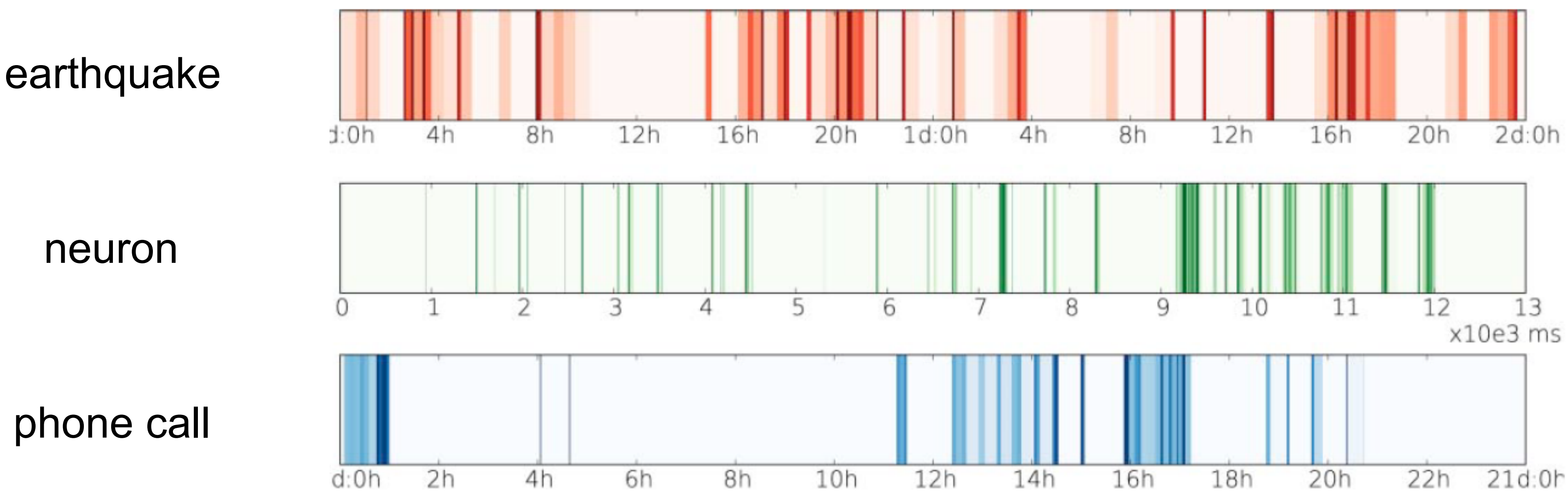


(Barabási, Nature 2005)



visits to a
web portal

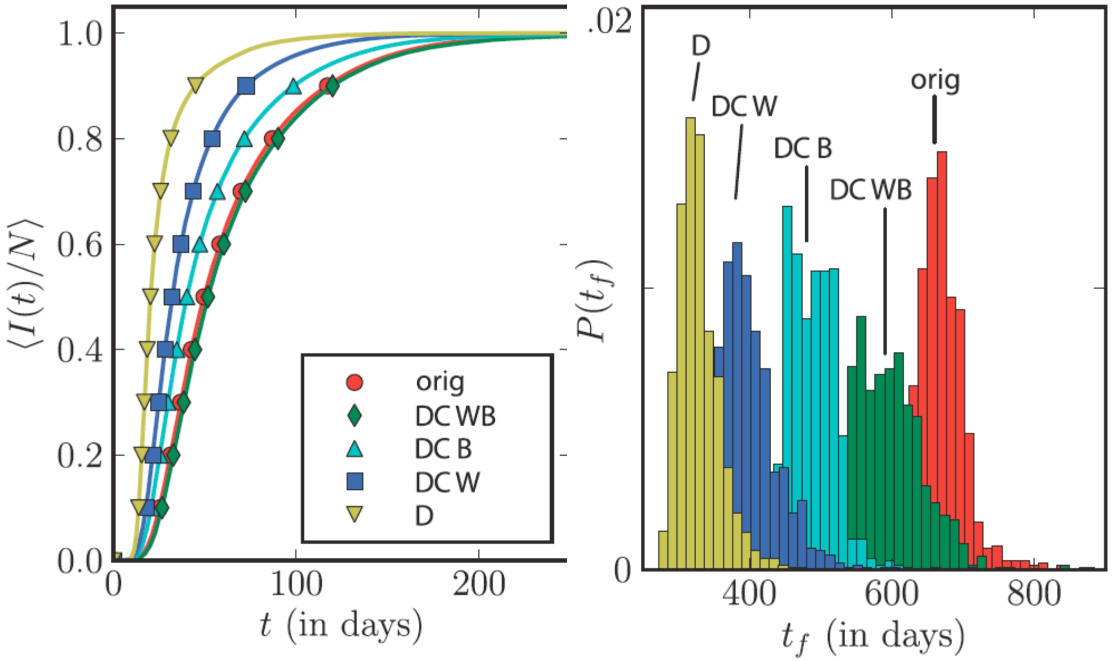
(Vázquez et al., PRE 2006)



(Karsai et al., Sci. Rep. 2012)

Less spreading on empirical temporal networks

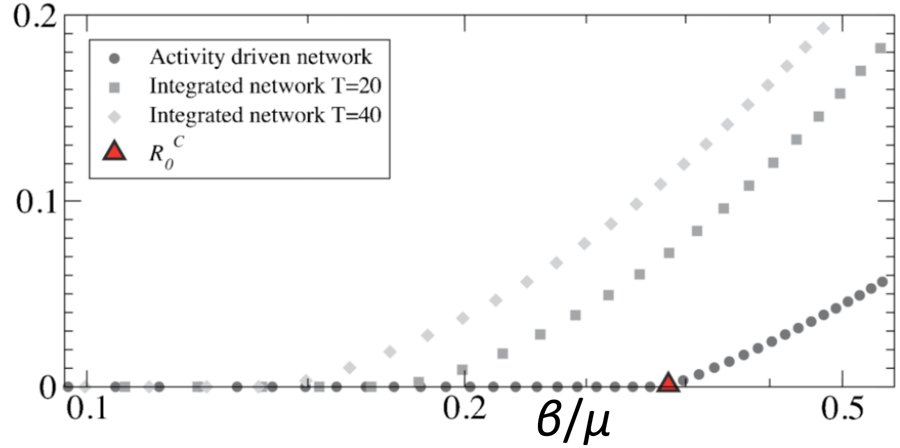
- Deterministic SI
  - Mobile phone data with 4.5M nodes, 9M links, 31M contacts (phone calls), and two other data sets



(Karsai et al., PRE 2011)

- SIS
  - the activity driven network model

%I @ stationarity



(Perra et al., Sci. Rep. 2012)

- Results depend on
  - data sets
  - disease dynamics models
  - parameters

Outstanding questions

- How does temporal information on networks change epidemic dynamics?
    - Data analysis
    - Theory
    - Numerical analysis
        - on empirical data (and their randomisations)
        - on models
- Can we make use of temporal information to better inform prediction and intervention methods?

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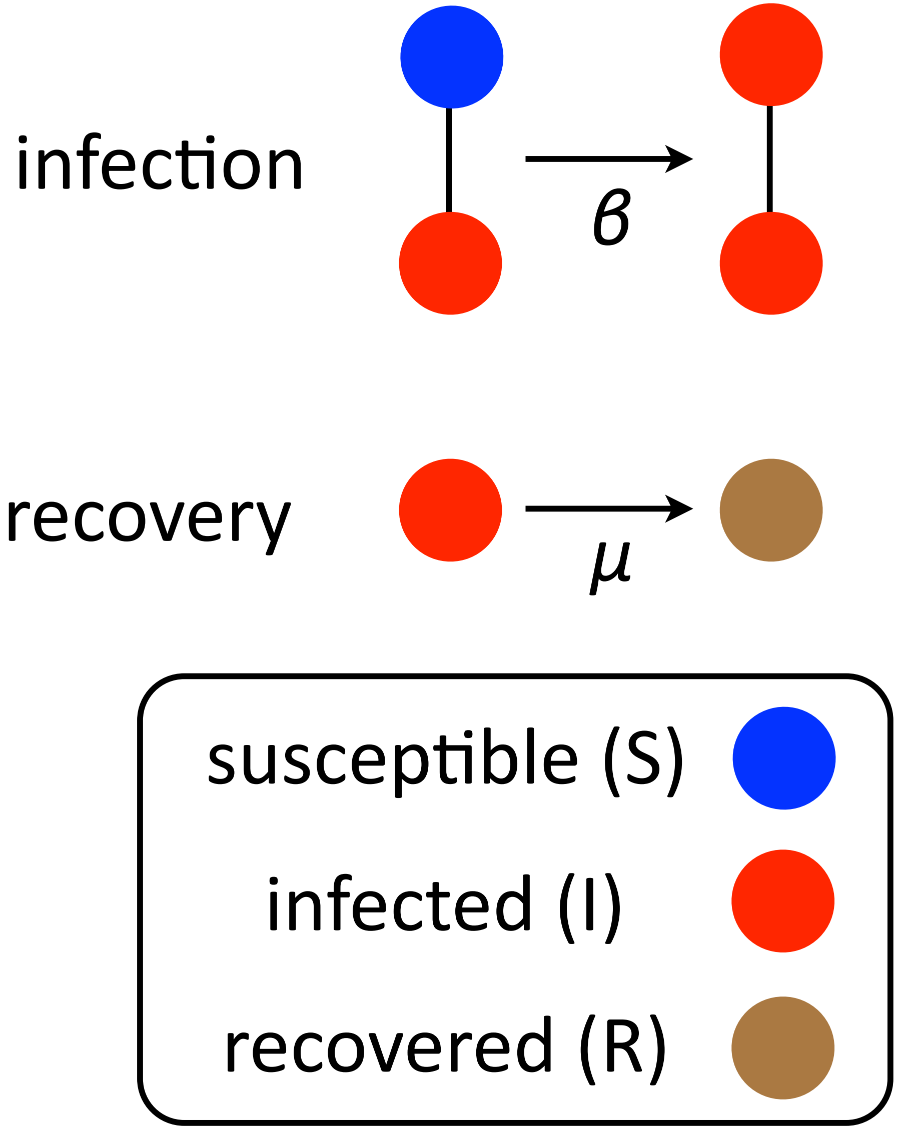
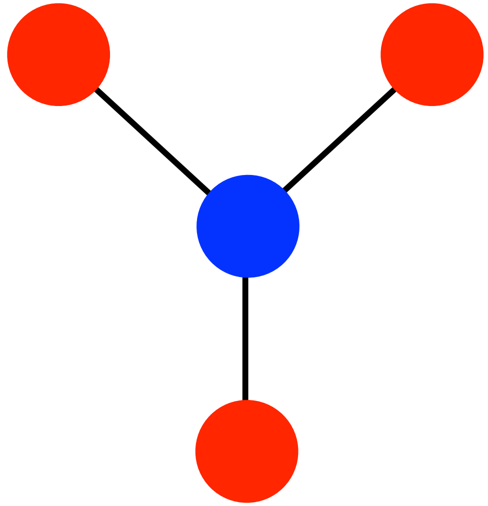
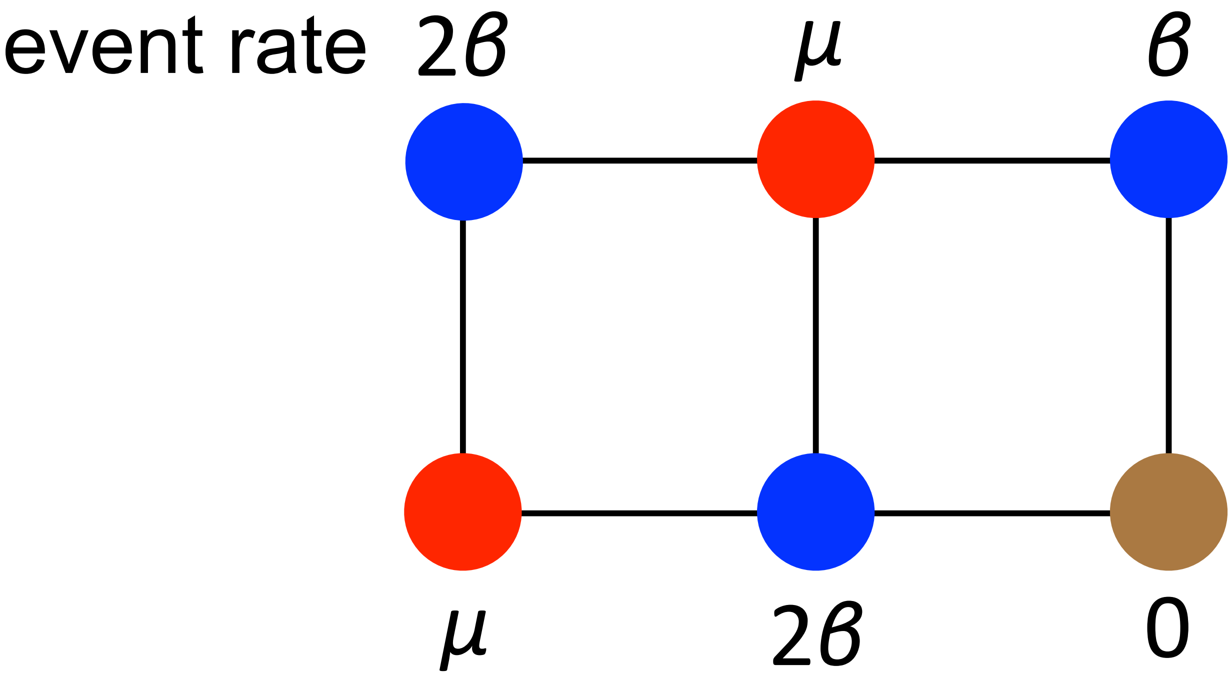
SIR model

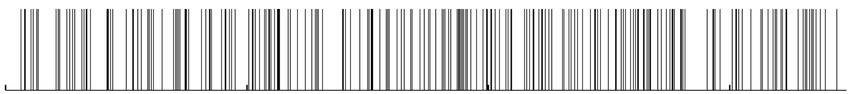




measles, HIV/
AIDS, SARS etc.

Stochastic SIR dynamics





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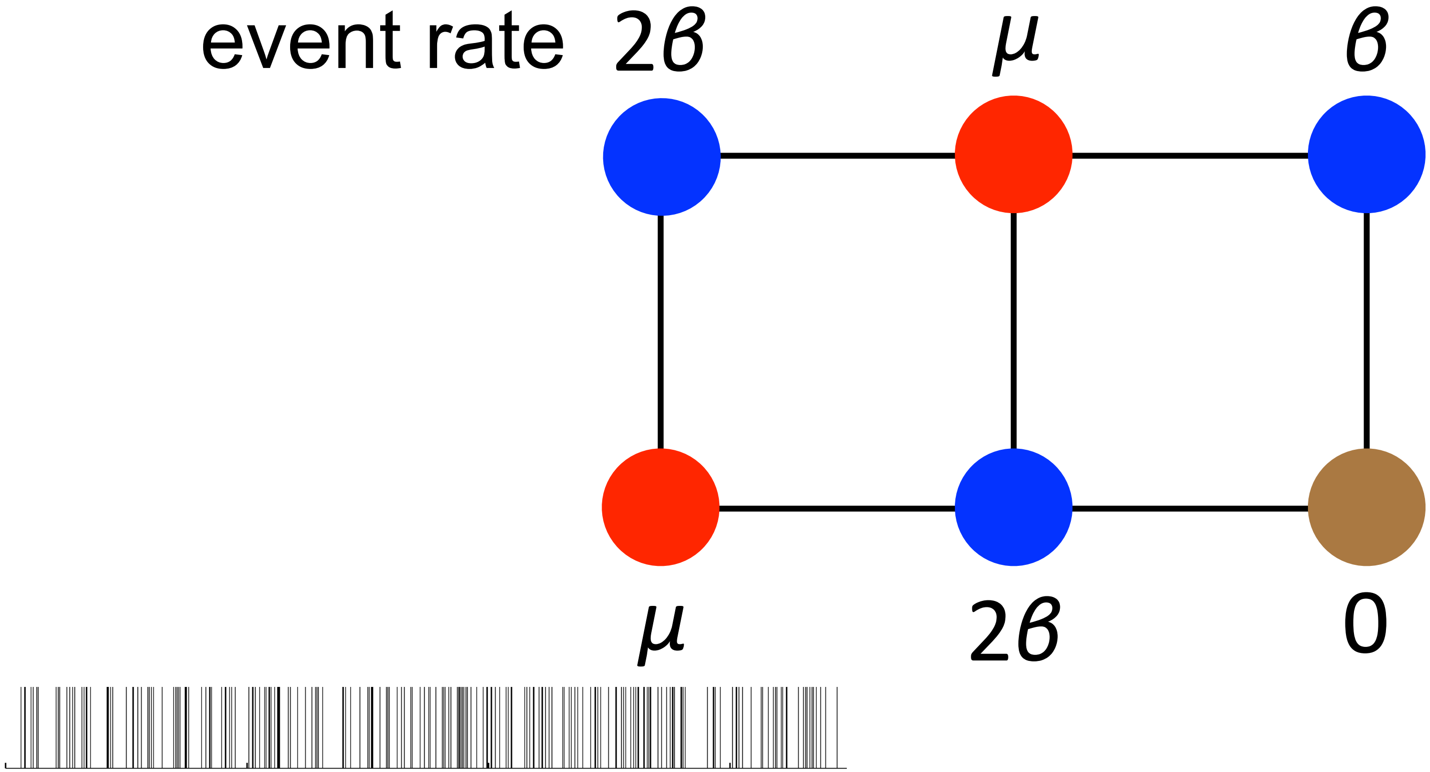

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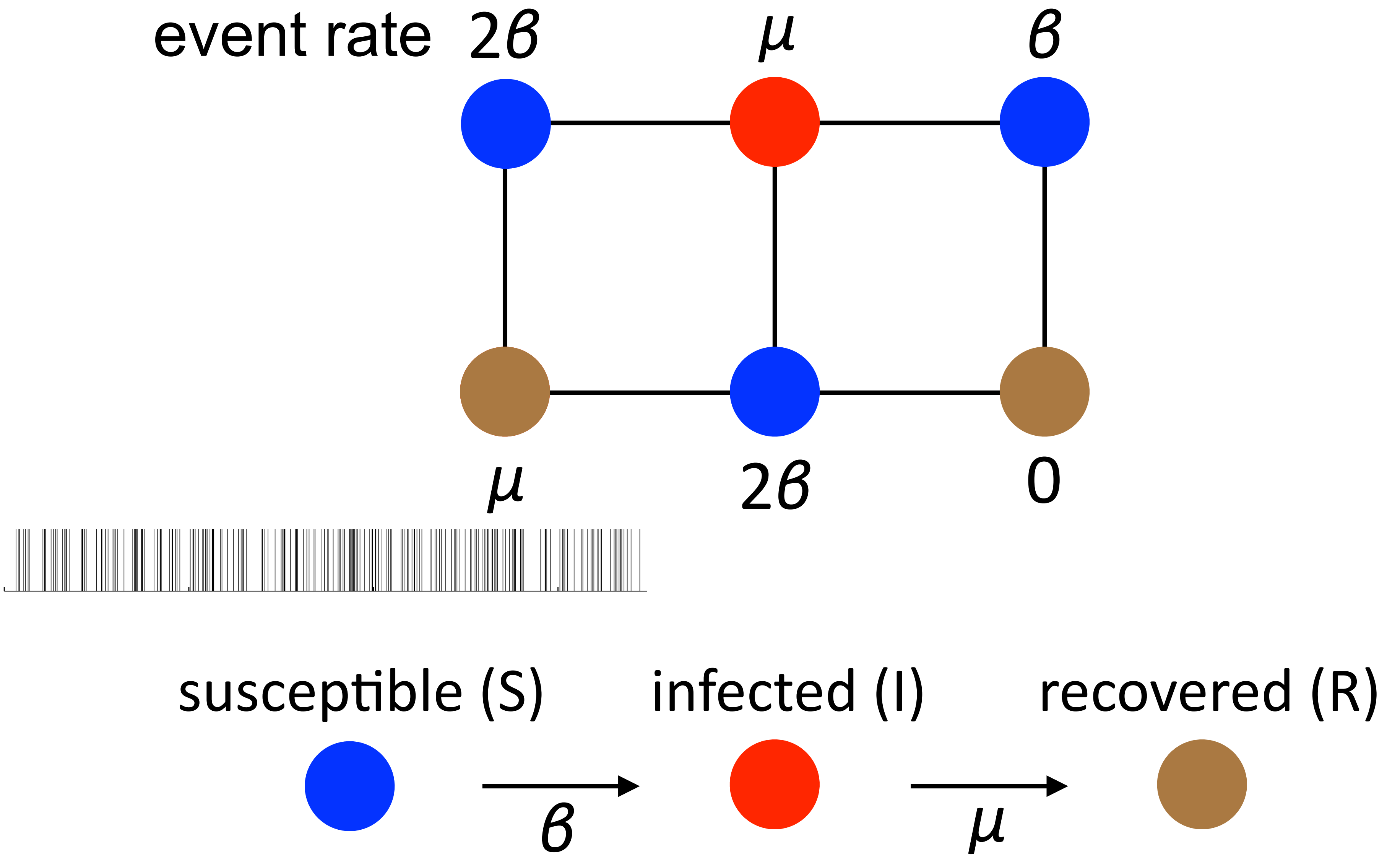

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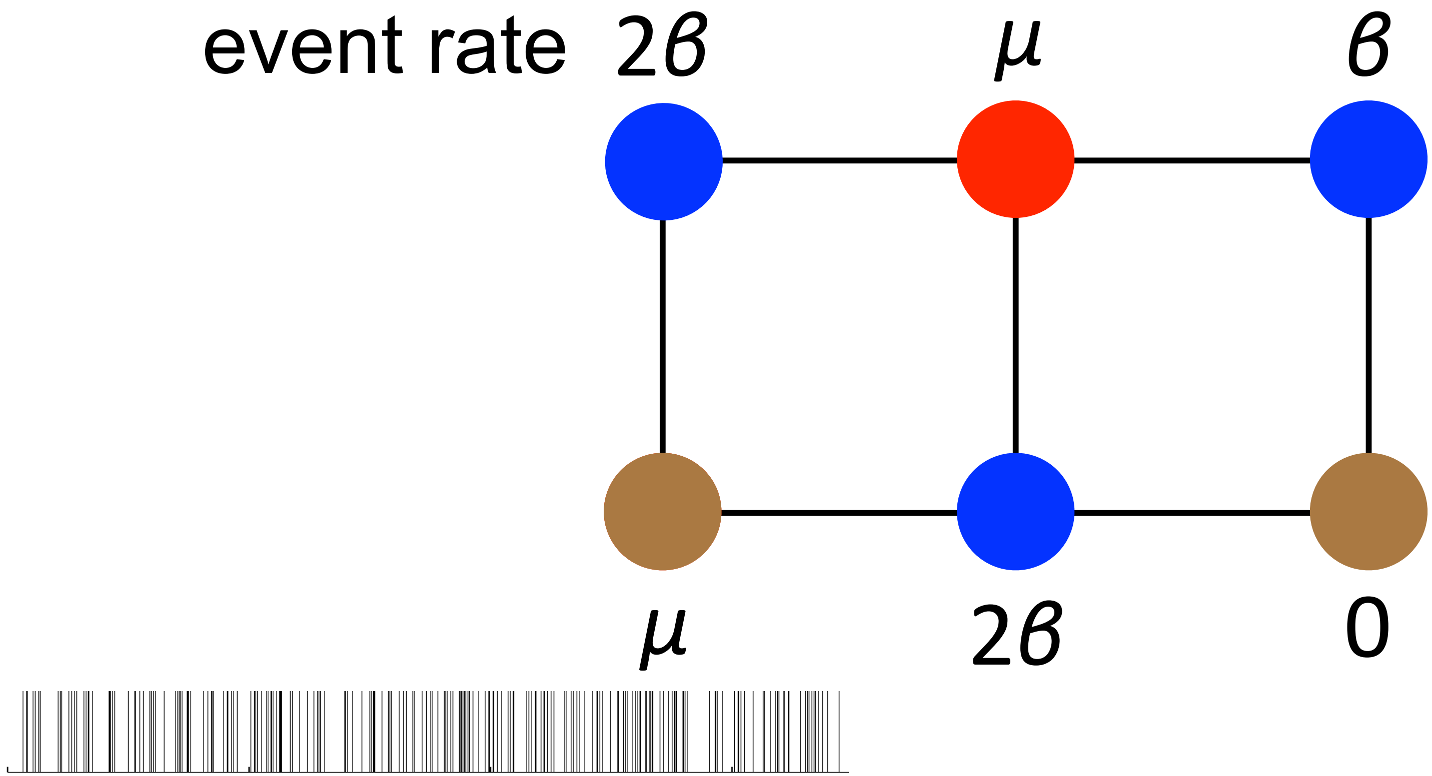

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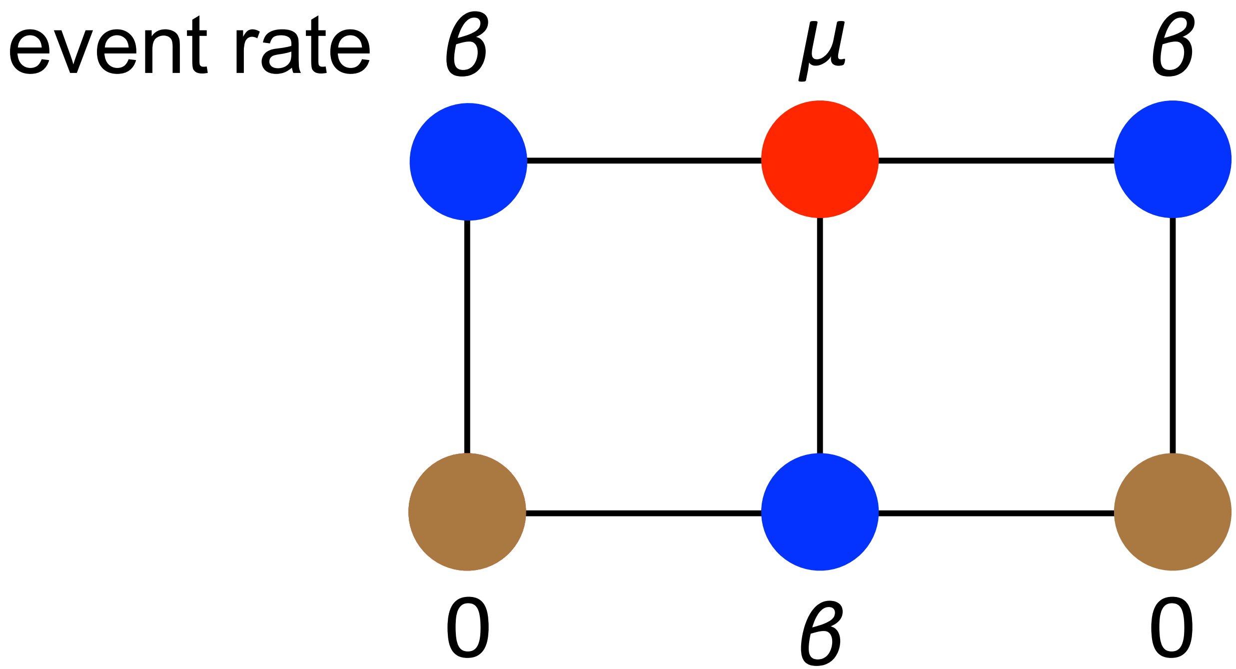
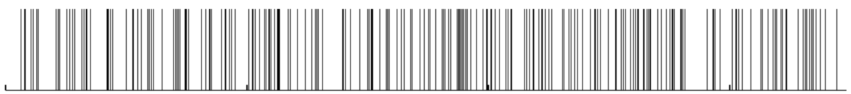
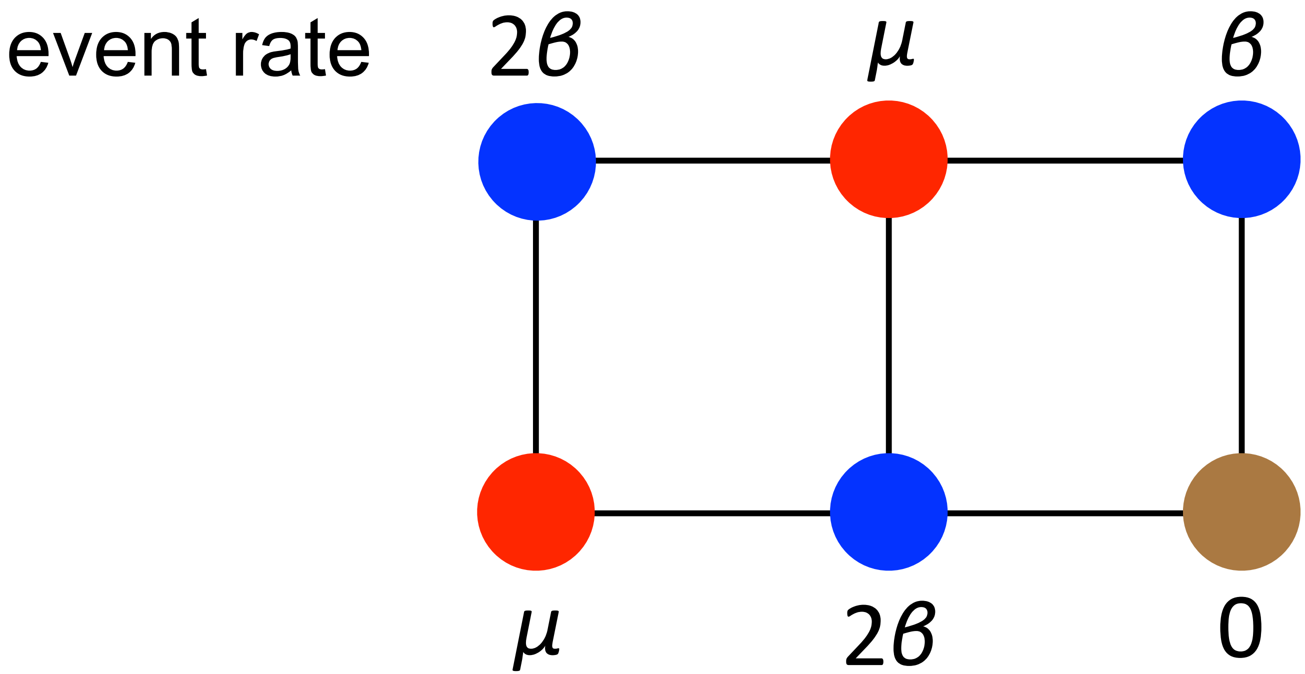




Rejection method



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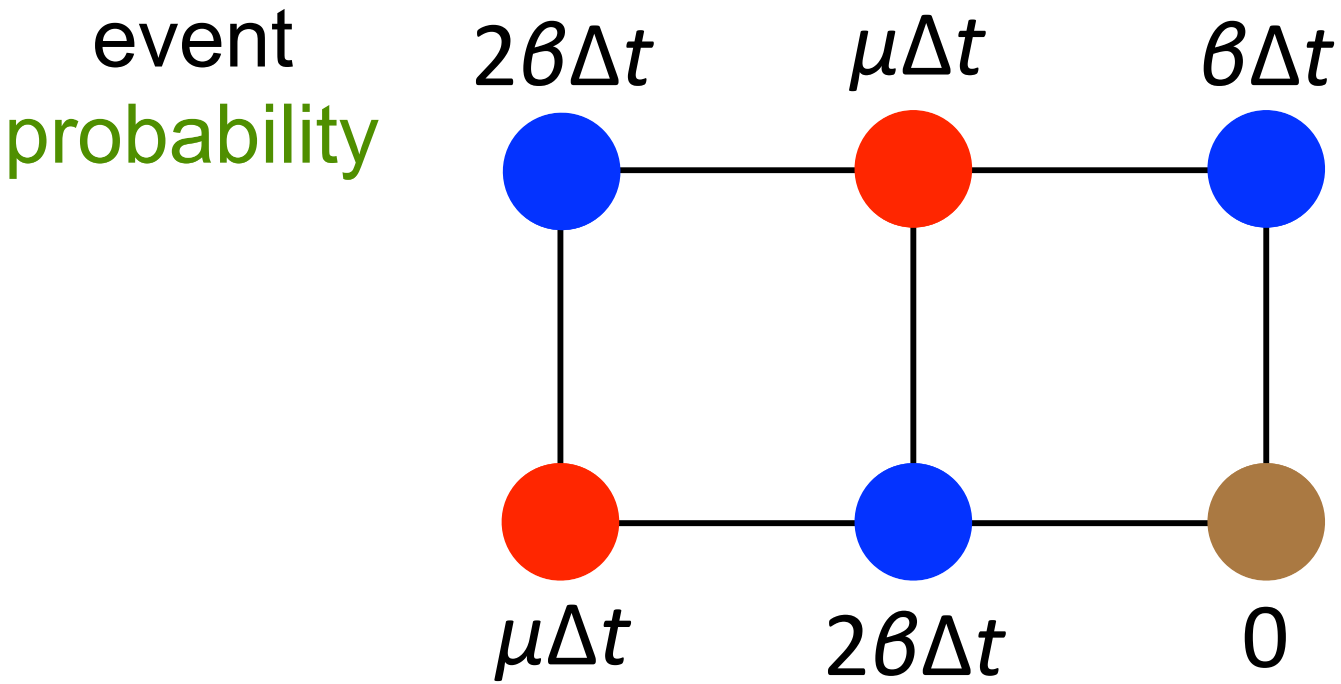
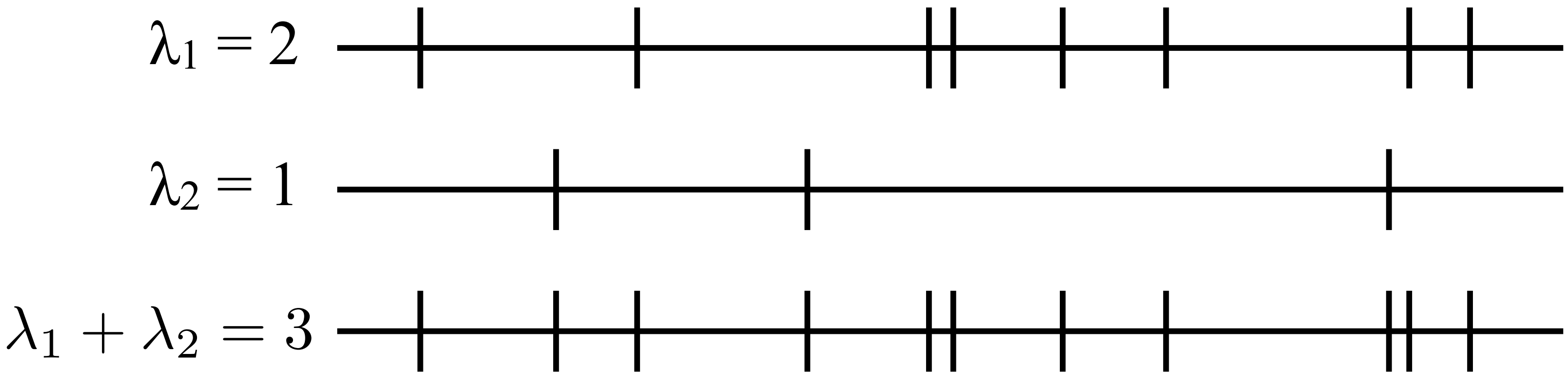
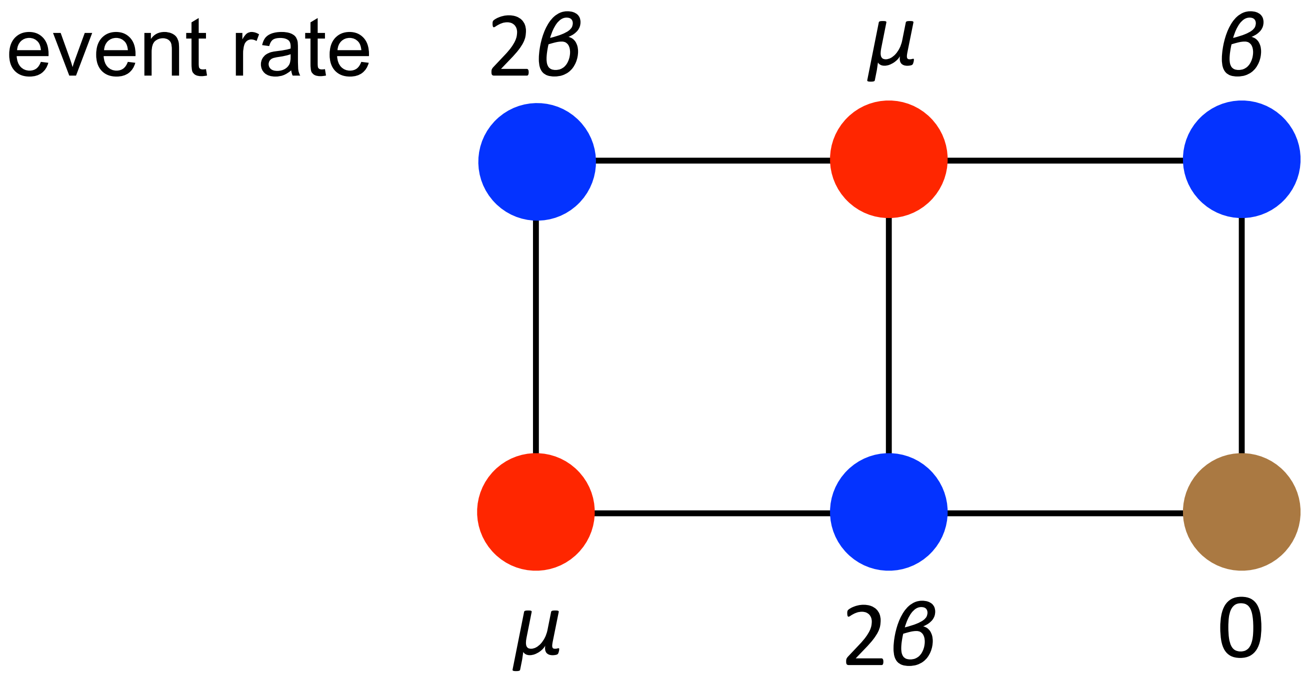


- Δt has to be small
- Should avoid multiple events to occur in a single time window
- Huge computation time, yet non-exact

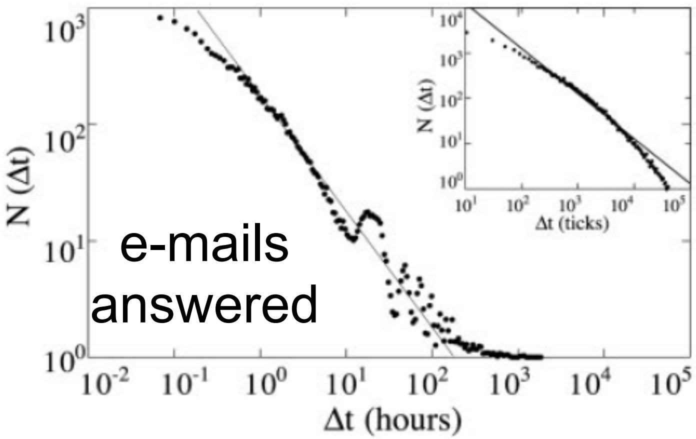
Superposition of Poisson processes is a Poisson process



Gillespie algorithm (1976)



- total event rate = $5\beta + 2\mu$
- τ: time to the next event
- pdf $\psi(\tau) = (5\beta + 2\mu)e^{-(5\beta+2\mu)\tau} \quad \rightarrow \quad \tau = -\ln u/(5\beta + 2\mu)$
- Node 1 produced the event with prob $2\beta/(5\beta+2\mu)$ etc.



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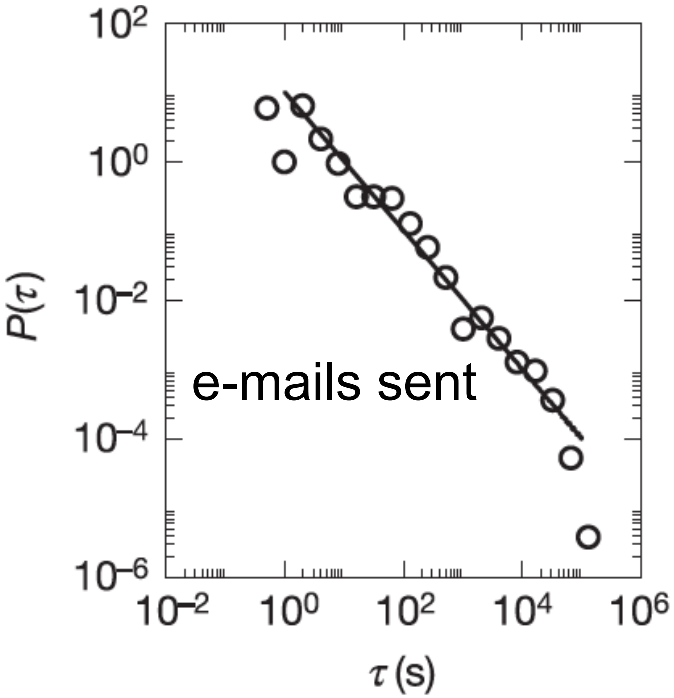

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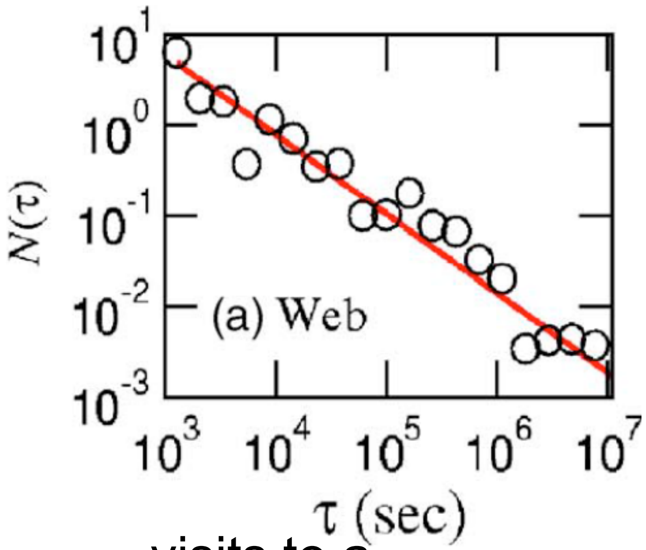

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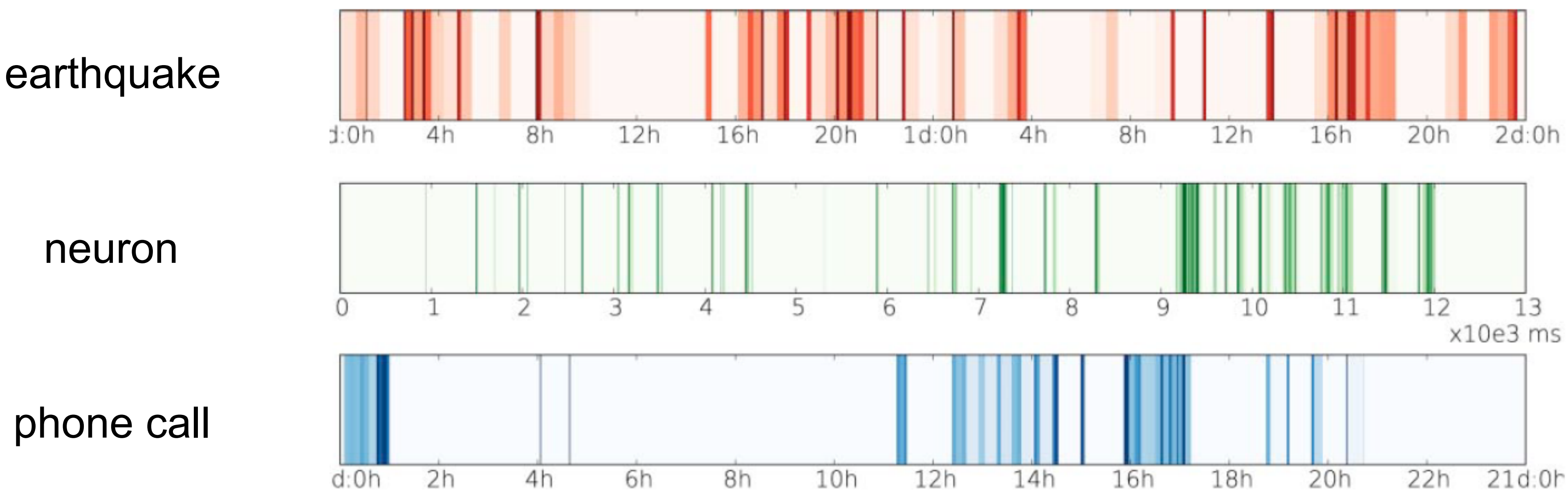
(Vázquez et al., PRE 2006)

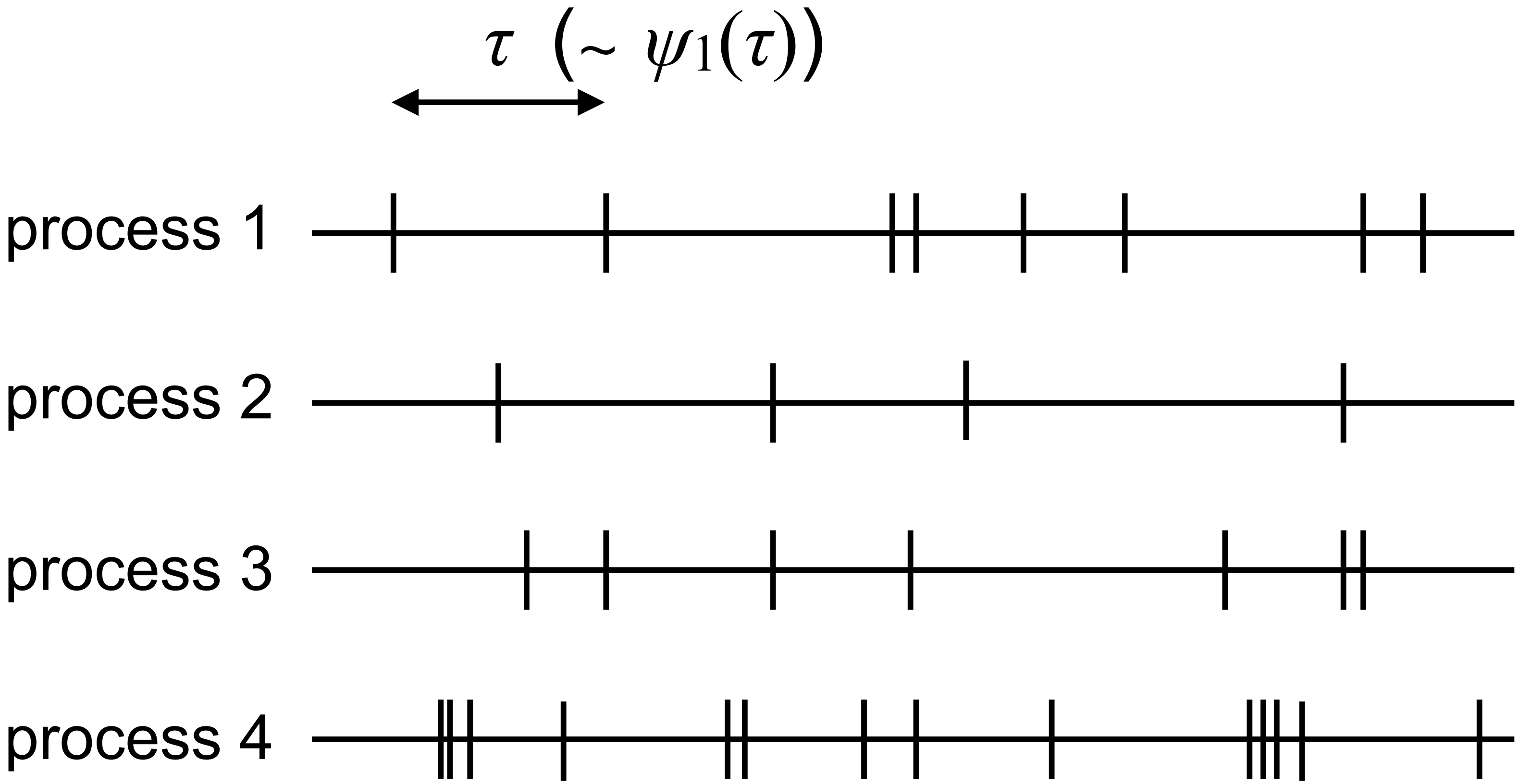


(Karsai et al., Sci. Rep. 2012)

Simulations with renewal processes

- Consider a renewal process where inter-event times (IETs) are distributed according to $\psi_i(\tau)$ for the *i*th process.
- Poisson processes if $\psi_i(\tau)$ is exponential
- Independence between different IETs assumed
- Not just for epidemic processes:
    - Interacting earthquakes
    - Neuronal networks
    - Financial transactions
    - Crimes

Aim



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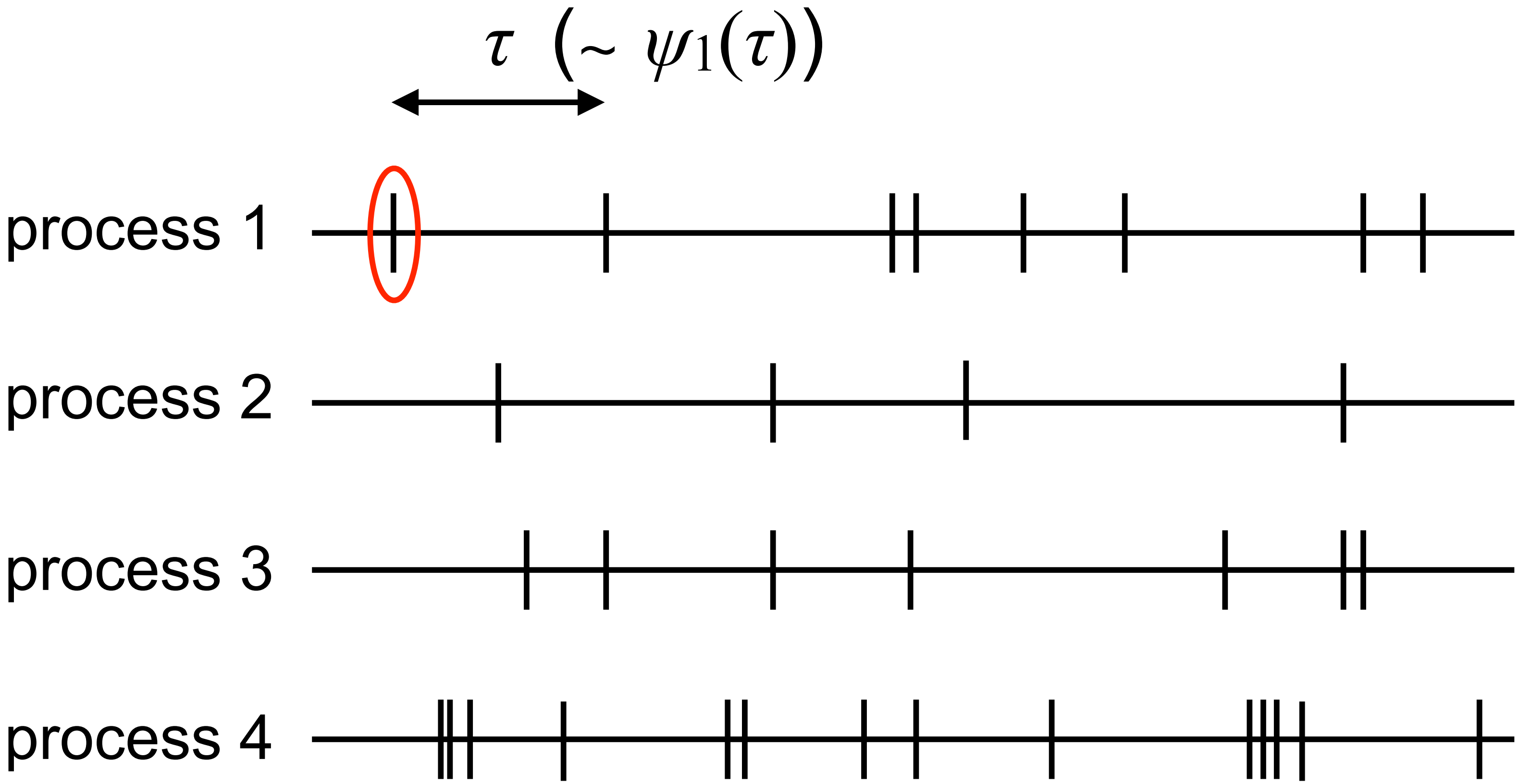

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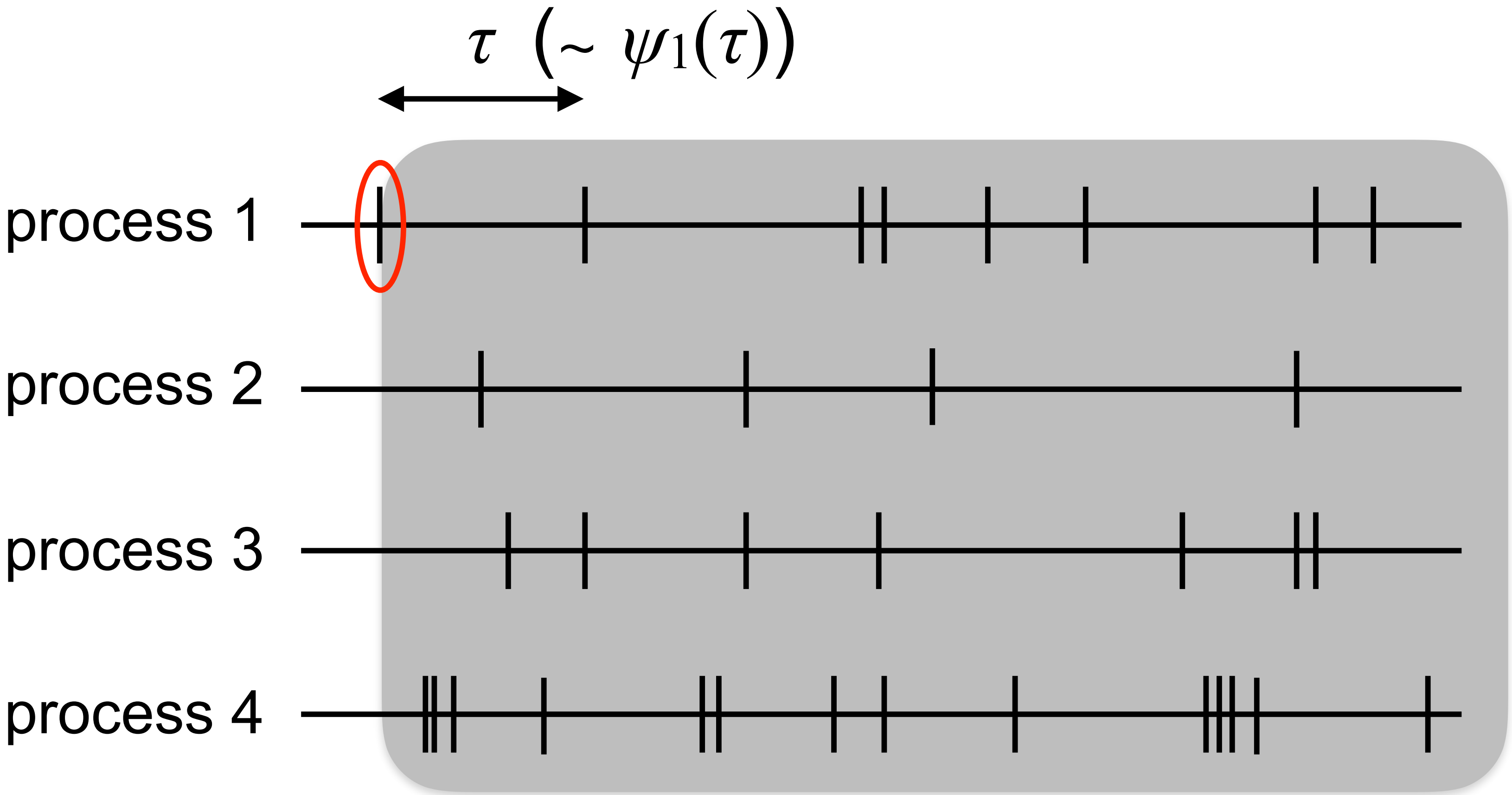


non-Markovian Gillespie algorithm (Boguñá et al. PRE 2014)

Waiting-time distribution for an isolated renewal process:

$$\psi_i^{\mathrm{w}}(\tau|t_i) = \frac{\psi_i(t_i+\tau)}{\Psi_i(t_i)} \equiv \frac{\psi_i(t_i+\tau)}{\int_{t_i}^{\infty}\psi_i(\tau')\mathrm{d}\tau'}$$

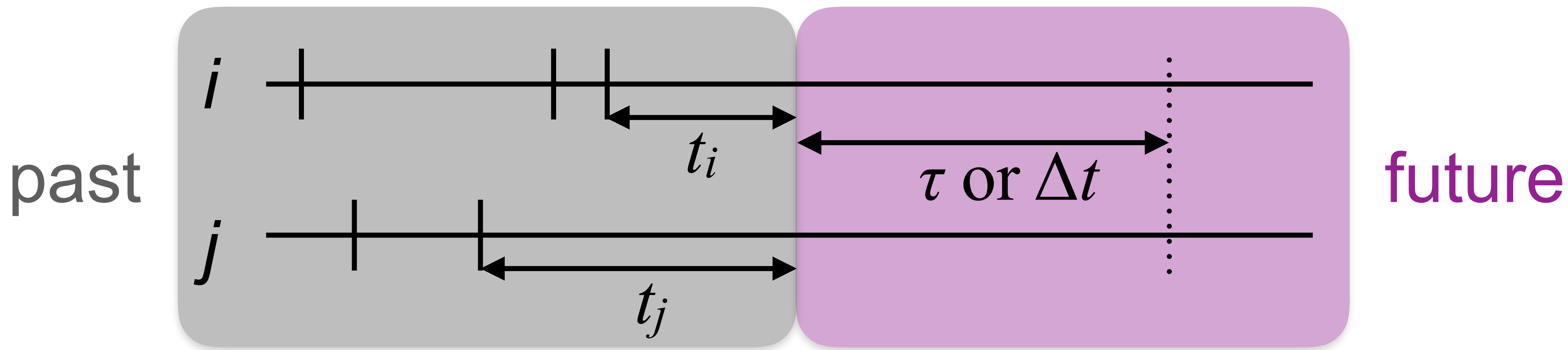
survival probability

PDF with which the *i*th process fires after Δt:

$$\phi(\Delta t, i|\{t_j\}) = \psi_i^{\mathrm{w}}(\Delta t|t_i)\prod_{j=1;j\neq i}^{N}\Psi_j(\Delta t|t_j) = \frac{\psi_i(t_i+\Delta t)}{\Psi_i(t_i+\Delta t)}\prod_{j=1}^{N}\frac{\Psi_j(t_j+\Delta t)}{\Psi_j(t_j)}$$

event rate $\equiv \lambda_i(t_i+\Delta t)$

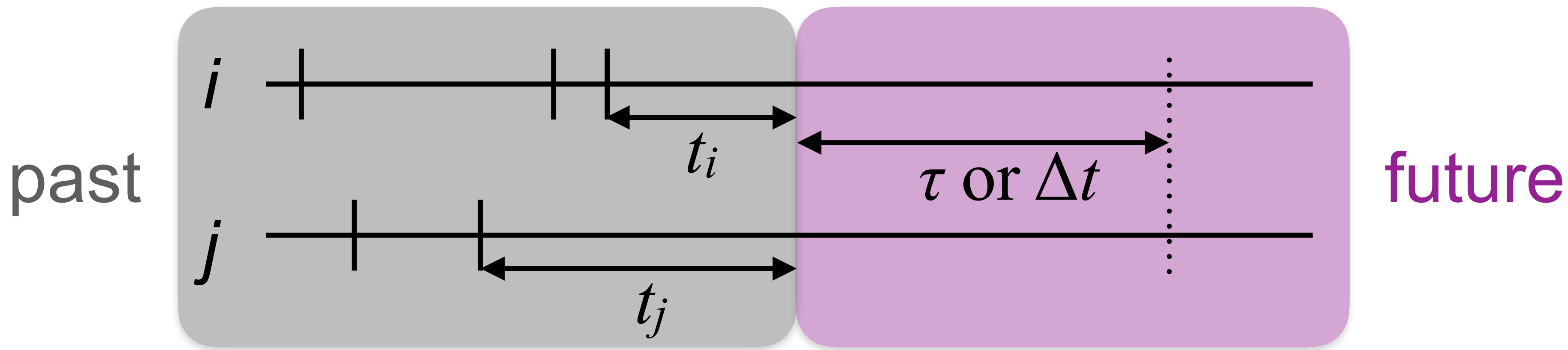
no event for Δt



So, an extended Gillespie algorithm consists in:

1. Draw Δt by solving $\prod_{j=1}^{N} \frac{\Psi_j(t_j + \Delta t)}{\Psi_j(t_j)} = u$

2. Select *i* with prob $\Pi_i = \frac{\lambda_i(t_i + \Delta t)}{\sum_{j=1}^{N} \lambda_j(t_j + \Delta t)}$



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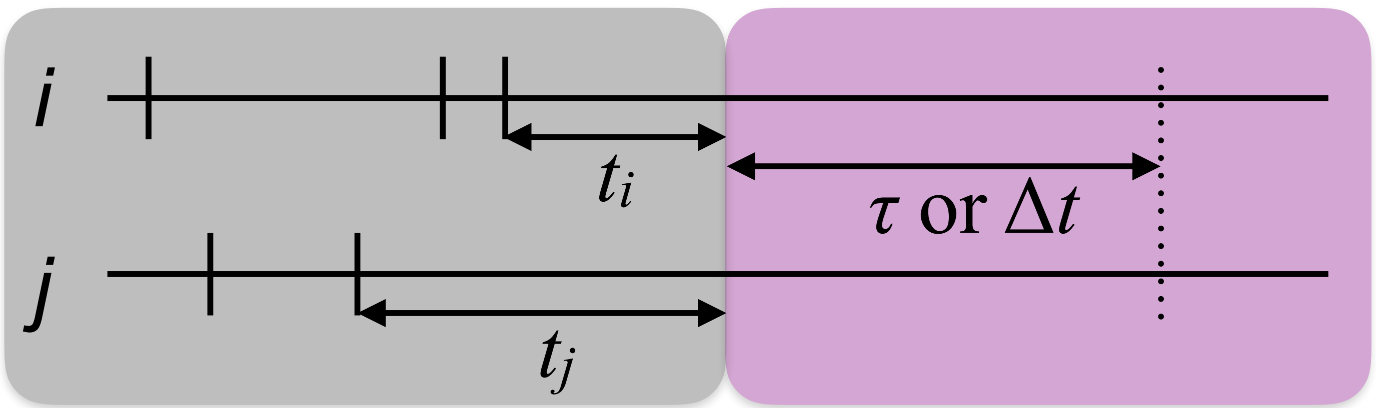
past



future

So, an extended Gillespie algorithm consists in:

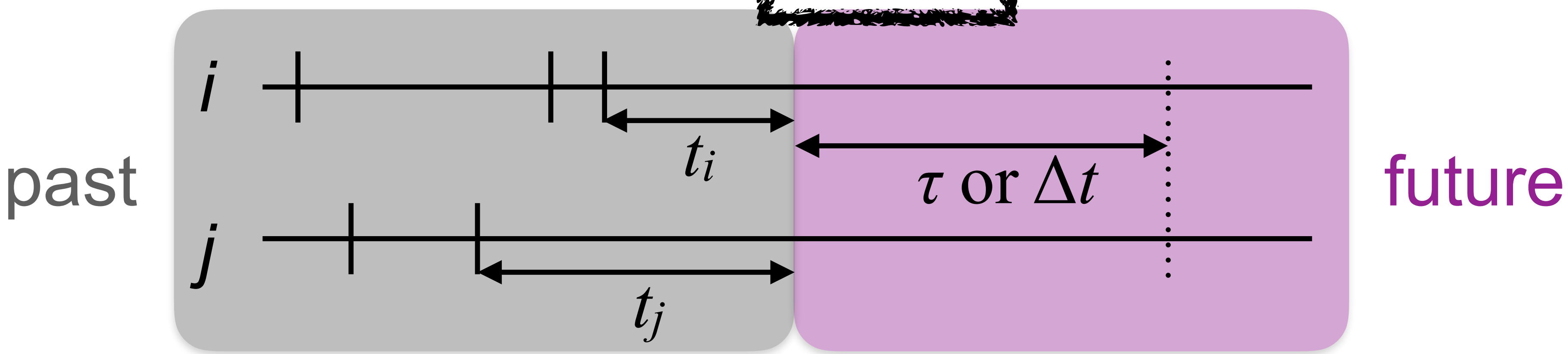
1. Draw Δt by solving $\prod_{j=1}^{N} \frac{\Psi_j(t_j+\Delta t)}{\Psi_j(t_j)} = u$

2. Select *i* with prob $\Pi_i = \frac{\lambda_i(t_i+\Delta t)}{\sum_{j=1}^{N} \lambda_j(t_j+\Delta t)}$

Taylor expansion: $\prod_{j=1}^{N} \frac{\Psi_j(t_j+\Delta t)}{\Psi_j(t_j)} \approx \exp\left[-\Delta t N \overline{\lambda}(\{t_j\})\right]$

where $\overline{\lambda}(\{t_j\}) = \frac{\sum_{j=1}^{N} \lambda_j(t_j)}{N} = \frac{1}{N}\sum_{j=1}^{N} \frac{\psi_j(t_j)}{\Psi_j(t_j)}$

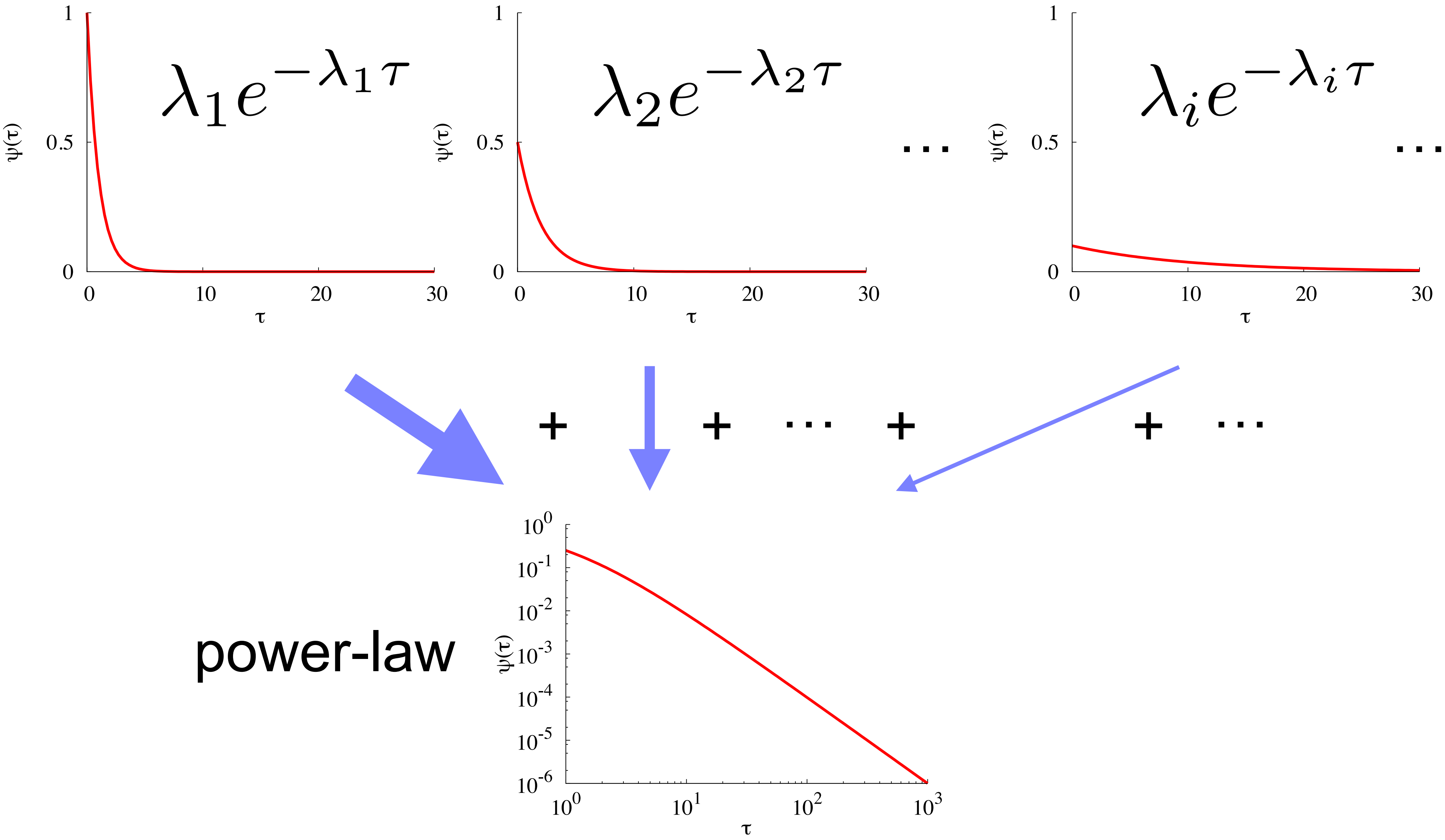
Use $\Delta t = -\ln u / N\overline{\lambda}(\{t_j\})$ nMGA



nMGA

- Exact for large *N*
- Still time-consuming to update the instantaneous event rate upon each event

Idea



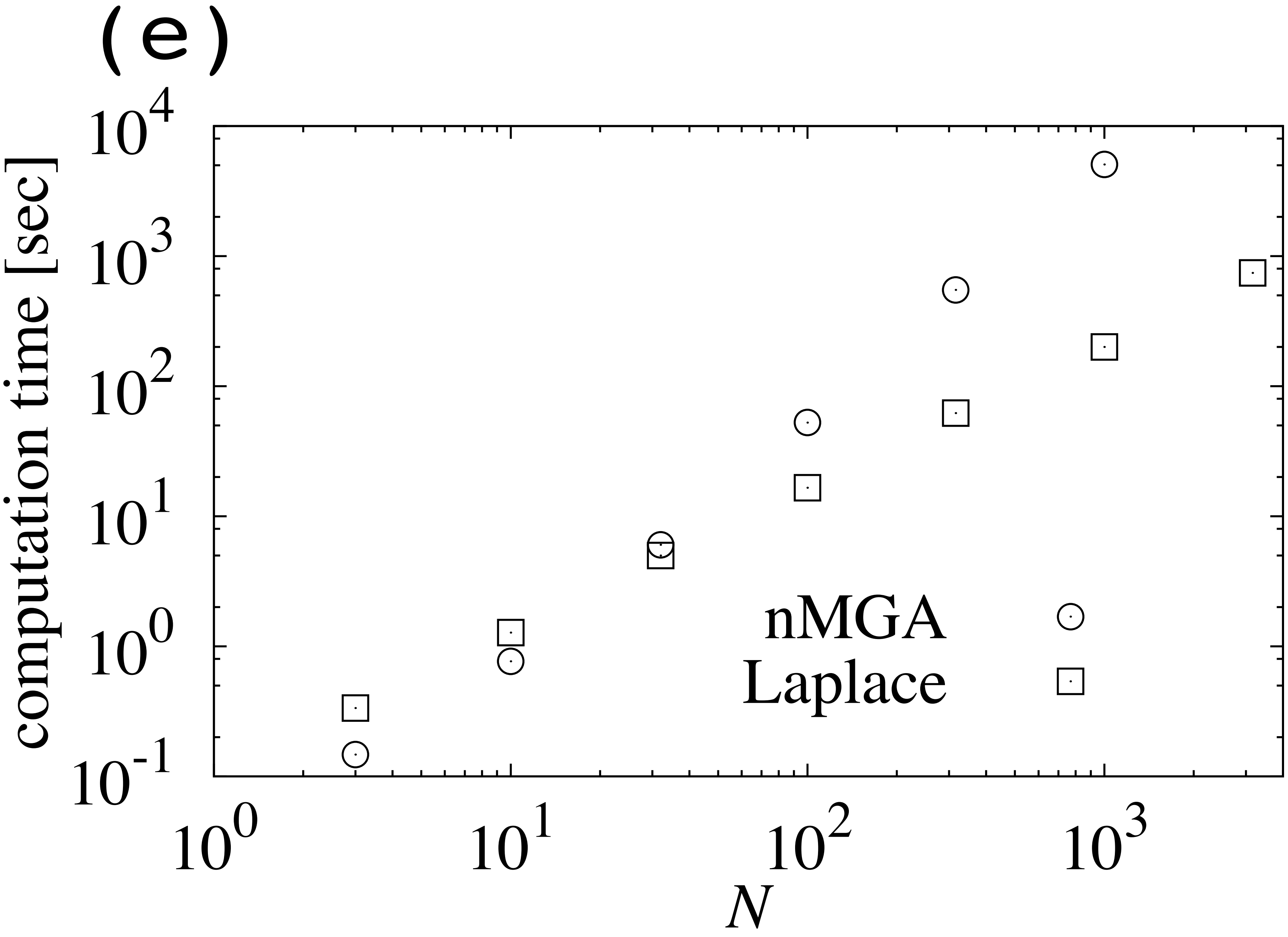
$\lambda_1 e^{-\lambda_1 \tau}$
$\lambda_2 e^{-\lambda_2 \tau}$
$\lambda_i e^{-\lambda_i \tau}$
ψ(τ)
τ
+ + ⋯ + + ⋯
power-law

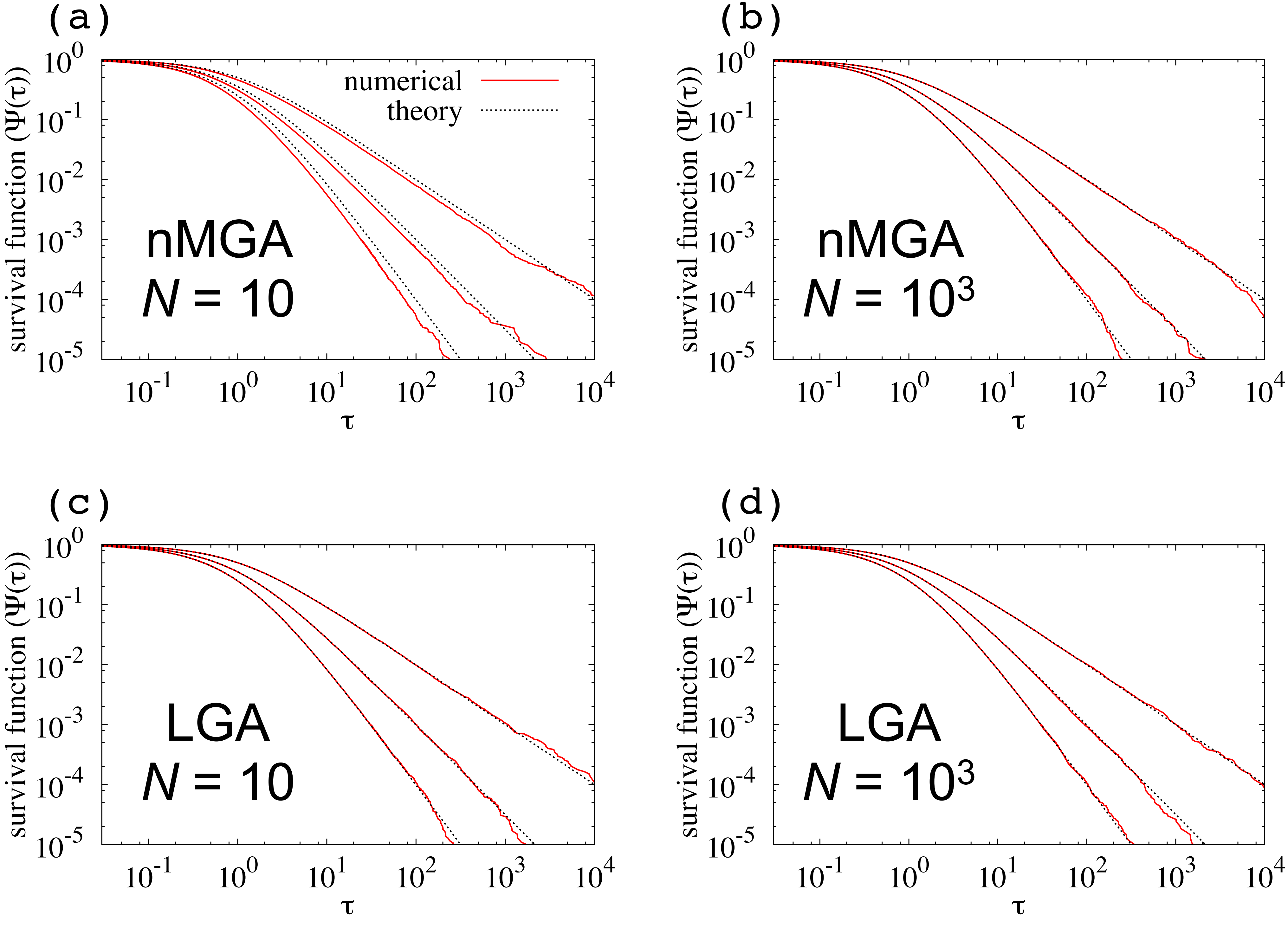
Laplace Gillespie algorithm

1. Given $\psi_i(\tau)$, determine the distribution of the Poisson rate $p_i(\lambda_i)$
2. Pick the Poisson rate λ_i from $p_i(\lambda_i)$
3. Draw the time to the next event $\Delta t = -\ln u / \sum_{j=1}^{N} \lambda_j$
4. Select i with probability $\Pi_i = \frac{\lambda_i}{\sum_{j=1}^{N} \lambda_j}$
5. Draw a new rate λ_i according to $p_i(\lambda_i)$. Also update other p_j and λ_j as necessary
6. Repeat steps 3-5

Advantages

- Exact for any *N*.
  - Important for stochastic processes in a population/network because the number of active processes is often small near the beginning/end of dynamics.
- Faster computation
  - No need to recalculate the instantaneous rate of each process.


(e)
computation time [sec]
10^4
10^3
10^2
10^1
10^0
10^{-1}
10^0
10^1
10^2
10^3
N
nMGA
Laplace


(a)
(b)
(c)
(d)
numerical
theory
nMGA
N = 10
nMGA
N = 10^3
LGA
N = 10
LGA
N = 10^3
survival function (Ψ(τ))
τ

Theory

Distribution of inter-event times:

$$\psi(\tau) = \int_0^\infty p(\lambda)\lambda e^{-\lambda\tau}\mathrm{d}\lambda$$

Survival probability:

$$\Psi(\tau) = \int_\tau^\infty \psi(\tau')\mathrm{d}\tau' = \int_0^\infty p(\lambda)e^{-\lambda\tau}\mathrm{d}\lambda$$

Laplace transform!

Bernstein's theorem (1929)

A function is the Laplace transform of a pdf (on $\lambda \geq 0$) iff

1. $\Psi(0) = 1 \leftarrow$ trivially satisfied

and

2. Ψ is completely monotone, i.e.,

$$(-1)^n \frac{\mathrm{d}^n \Psi(\tau)}{\mathrm{d}\tau^n} \geq 0 \quad (\tau \geq 0, n = 0, 1, \ldots)$$

$\leftarrow$ nontrivial for $n \geq 2$

$$n = 0: \quad \Psi(\tau) \geq 0$$

$$n = 1: \quad \psi(\tau) \geq 0$$

$$n = 2: \quad \psi'(\tau) \leq 0$$

Examples

Exponential distribution (Poisson process)

$$\psi(\tau) = \lambda_0 e^{-\lambda_0 \tau}$$

$$p(\lambda) = \delta(\lambda - \lambda_0)$$

Power-law distributions

$$\psi(\tau) = \frac{\kappa}{(1+\kappa\tau)^{\alpha+1}}$$

$$p(\lambda) = \frac{\lambda^{\alpha-1} e^{-\lambda/\kappa}}{\Gamma(\alpha)\kappa^{\alpha}}$$

exponential $p(\lambda)$ with α=1

With an exponential tail

$$\psi(\tau) = \frac{e^{-\lambda_0 \tau}}{(1+\kappa\tau)^{\alpha}} \left(\lambda_0 + \frac{\kappa\alpha}{1+\kappa\tau}\right)$$

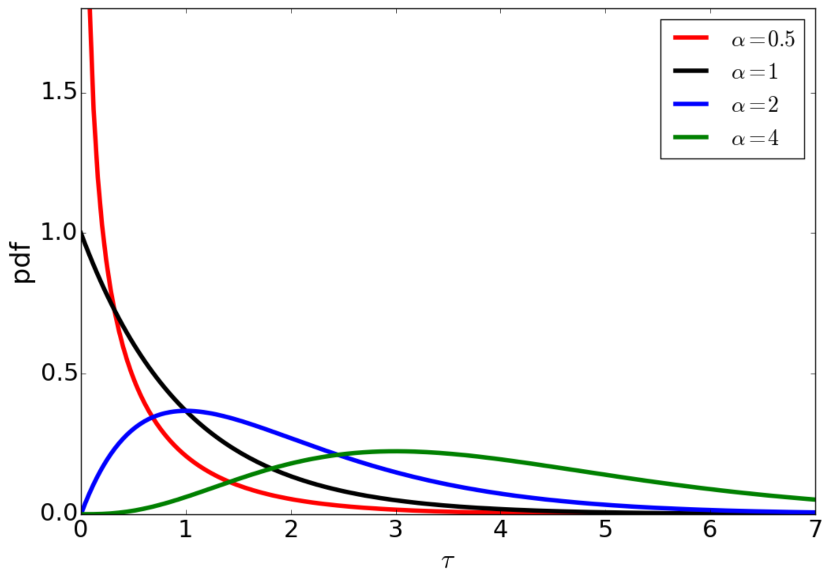
$$\Psi(\tau) = \frac{e^{-\lambda_0 \tau}}{(1+\kappa\tau)^{\alpha}}$$

$$p(\lambda) = \begin{cases} \frac{(\lambda-\lambda_0)^{\alpha-1} e^{-(\lambda-\lambda_0)/\kappa}}{\Gamma(\alpha)} & (\lambda \geq \lambda_0) \\ 0 & (0 < \lambda < \lambda_0) \end{cases}$$

Gamma distribution

$$\psi(\tau) = \frac{\tau^{\alpha-1} e^{-\tau/\kappa}}{\Gamma(\alpha)\kappa^{\alpha}}$$

$$p(\lambda) = \begin{cases} 0 & (0 < \lambda < \kappa^{-1}) \\ \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)\lambda(\kappa\lambda-1)^{\alpha}} & (\lambda \geq \kappa^{-1}) \end{cases}$$



Note: $0 < \alpha \leq 1$ only

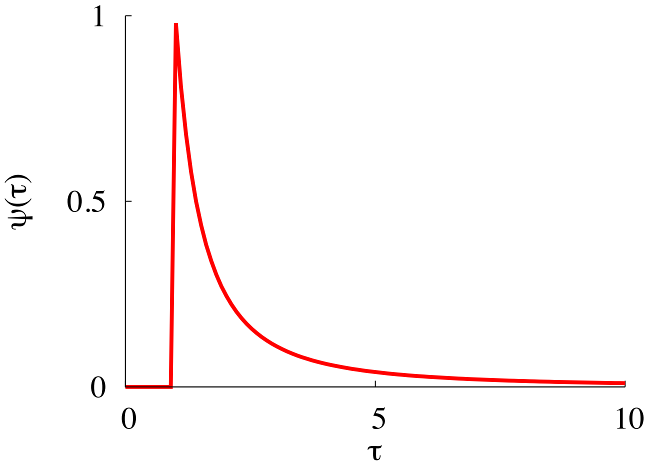
Other examples

- Special cases of the Weibull distribution
- Mittag-Leffler distribution
- Survival function obtained as
  - integral of a valid survival function
  - product of survival functions

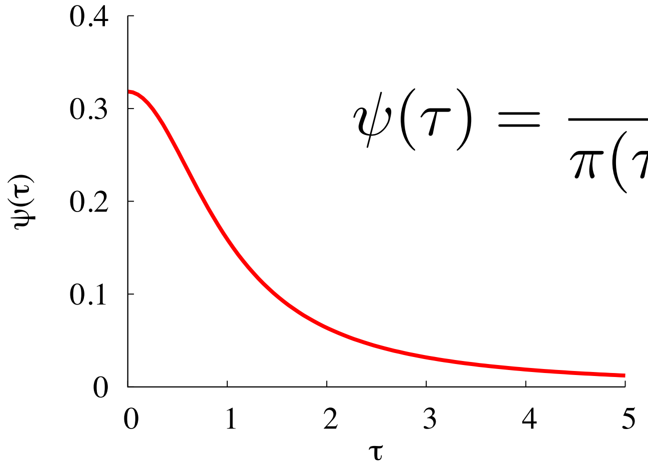
Limitations

- Complete monotoneness
  - Coefficient of Variation ≥ 1 only (Yannaros, Ann. Inst. Stat. Math. 1994)
  - Invalid examples: Pareto, one-sided Cauchy, two-peak distributions

Pareto



One-sided Cauchy



$$\psi(\tau) = \frac{1}{\pi(\tau^2 + 1)}$$

Applications

1. IET sequences with positive correlations
2. A stochastic epidemic process model

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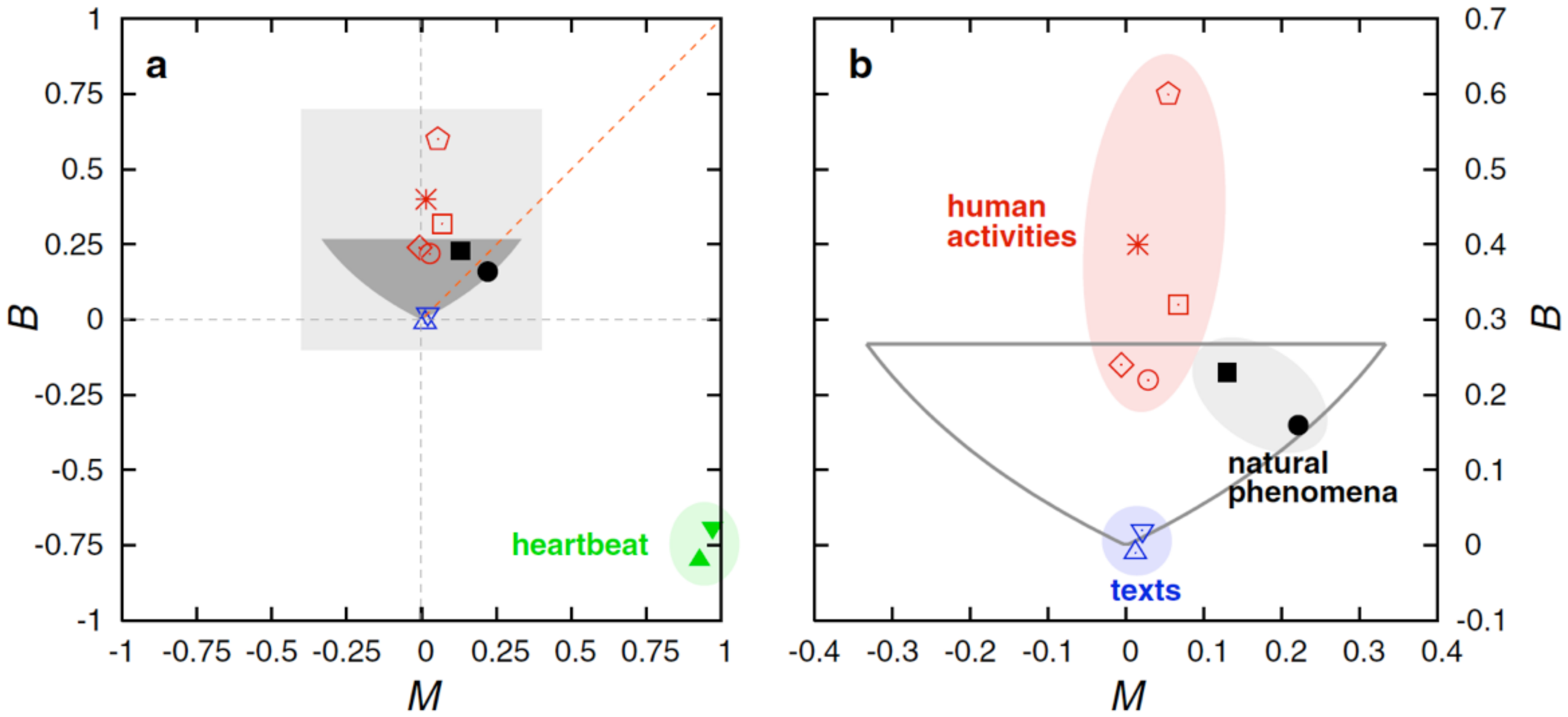
2. A stochastic epidemic process model

memory coefficient: $M \equiv \frac{1}{n_\tau - 1} \sum_{i=1}^{n_\tau - 1} \frac{(\tau_i - m_1)(\tau_{i+1} - m_2)}{\sigma_1 \sigma_2}$,

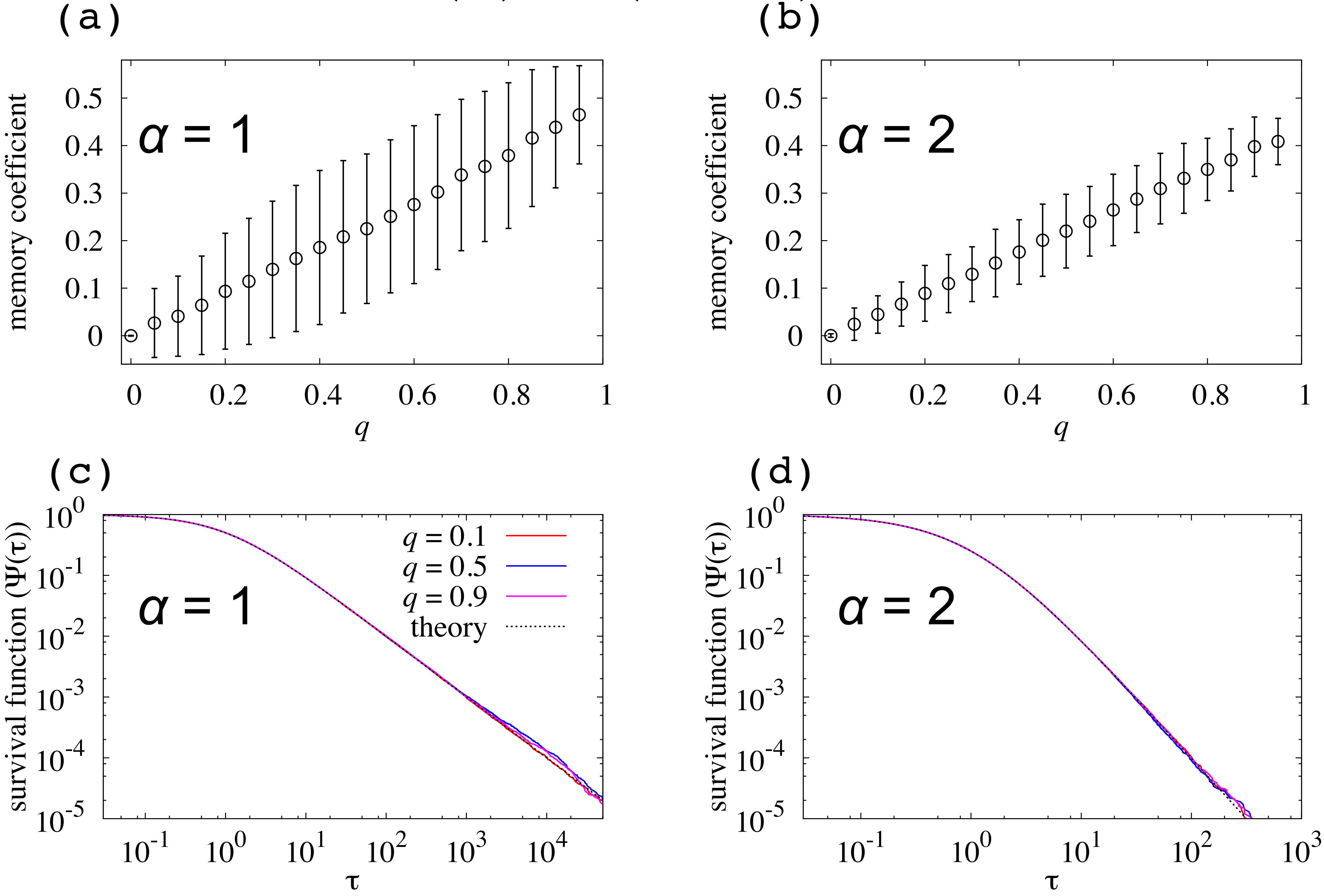


(Goh & Barabási, EPL, 2008)

Laplace Gillespie algorithm

1. Given $\psi_i(\tau)$, determine the distribution of the Poisson rate $p_i(\lambda_i)$
2. Pick the Poisson rate λ_i from $p_i(\lambda_i)$
3. Draw the time to the next event $\Delta t = -\ln u / \sum_{j=1}^{N} \lambda_j$
4. Select i with probability $\Pi_i = \frac{\lambda_i}{\sum_{j=1}^{N} \lambda_j}$
5. Draw a new rate λ_i according to $p_i(\lambda_i)$ with probability 1-q. Also update other p_j and λ_j as necessary
6. Repeat steps 3-5

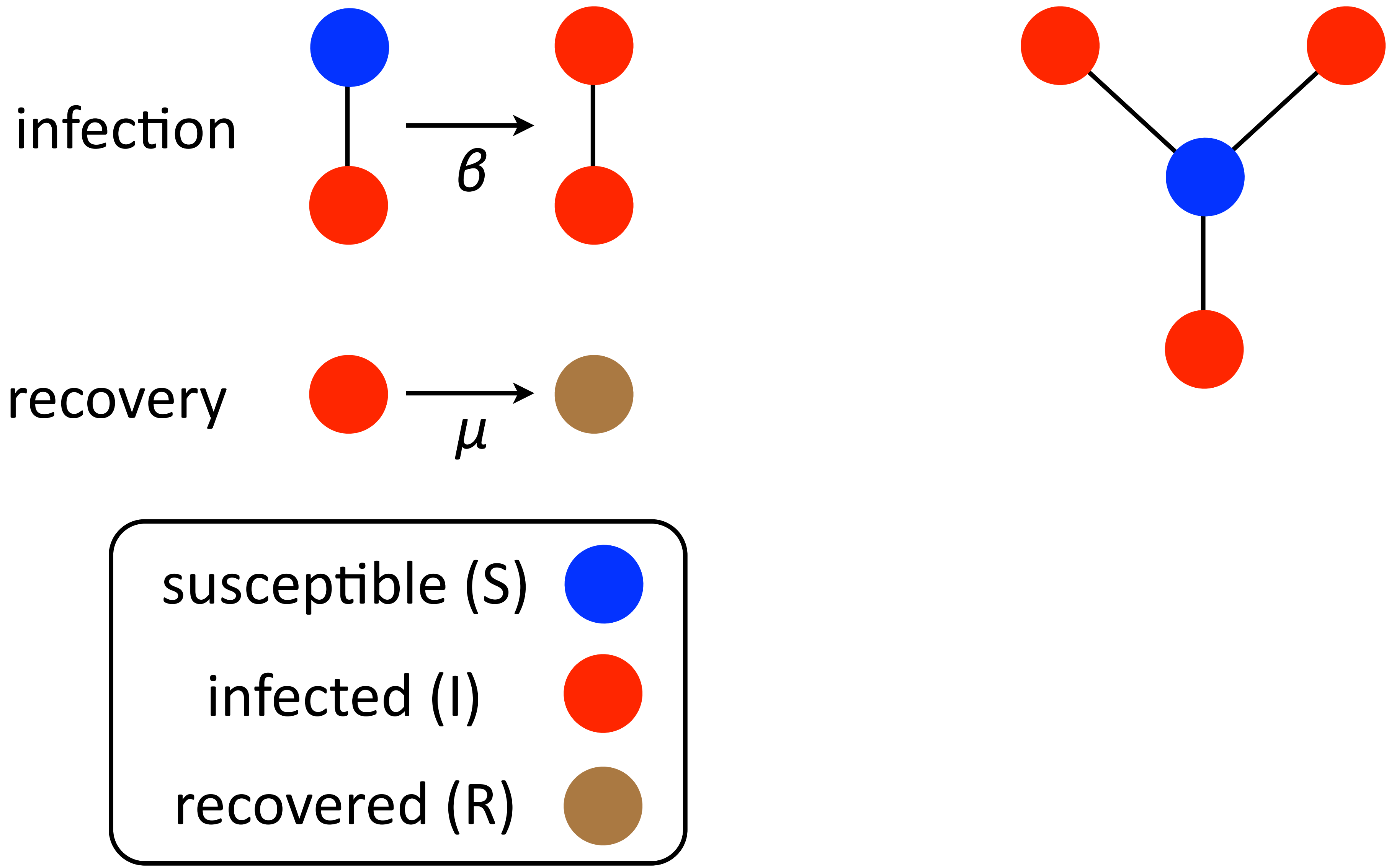
$$\psi(\tau) = (1+\tau)^{-(\alpha+1)}$$



Applications

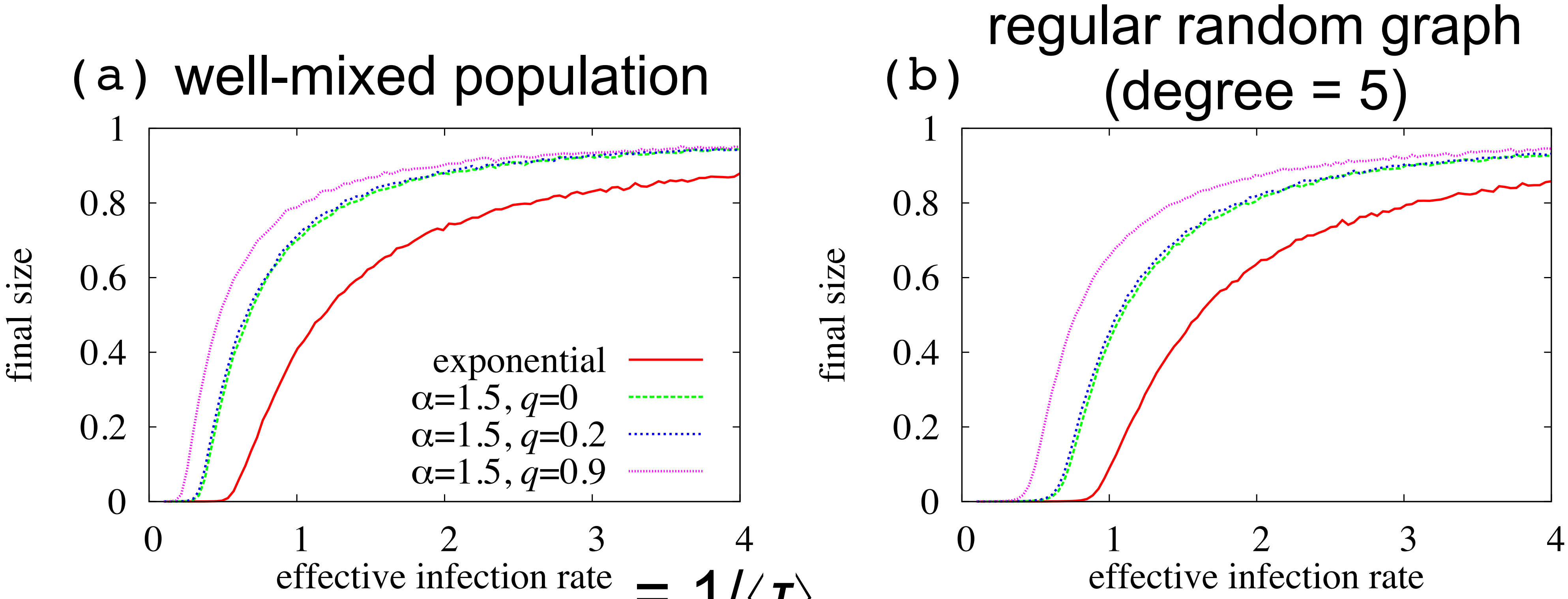
1. IET sequences with positive correlations
2. A stochastic epidemic process model

SIR model


infection
β
recovery
μ
susceptible (S)
infected (I)
recovered (R)

An SIR model

- Poissonian recovery at rate 1
- Power-law renewal process on each node (same pdf)
- An activated node selects a neighbour with the uniform probability and infects it (when it can)
- Equilibrium renewal process



$= 1/\langle \tau \rangle$

Use $\psi(\tau) = (1+\tau)^{-(\alpha+1)}$

Observations:

- Power-law IET enhances the outbreak size
- Positive IET corr enhances the outbreak size

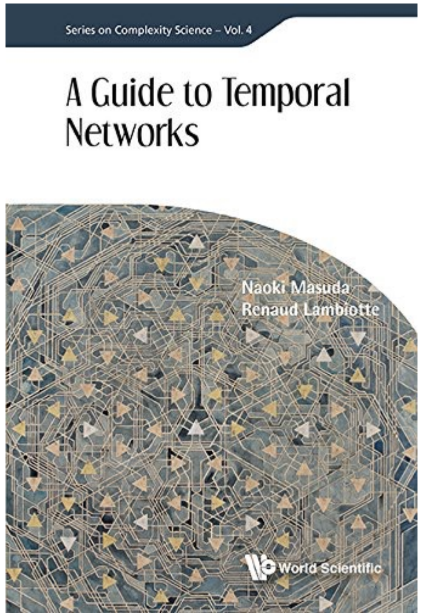
Conclusions

- Laplace Gillespie algorithm
  - Can treat renewal processes
  - Faster than previous algorithms
  - Can produce positive correlation
  - Completely monotonicity condition
    - Explicit expression for $p(\lambda)$ in various examples
    - No short-tail distributions, no Pareto
- Issues
  - Somehow treat short-tailed distributions (e.g., recovery events in epidemic processes)
  - Applications?
    - Probably not chemical reaction systems?
    - Other social processes, earthquakes, operations research?

Acknowledgments

- Luis E. C. Rocha (Karolinska, Sweden & Namur, Belgium)

Also in



- Masuda and Rocha, SIAM Review, in press (2017). Preprint arxiv:1601.01490