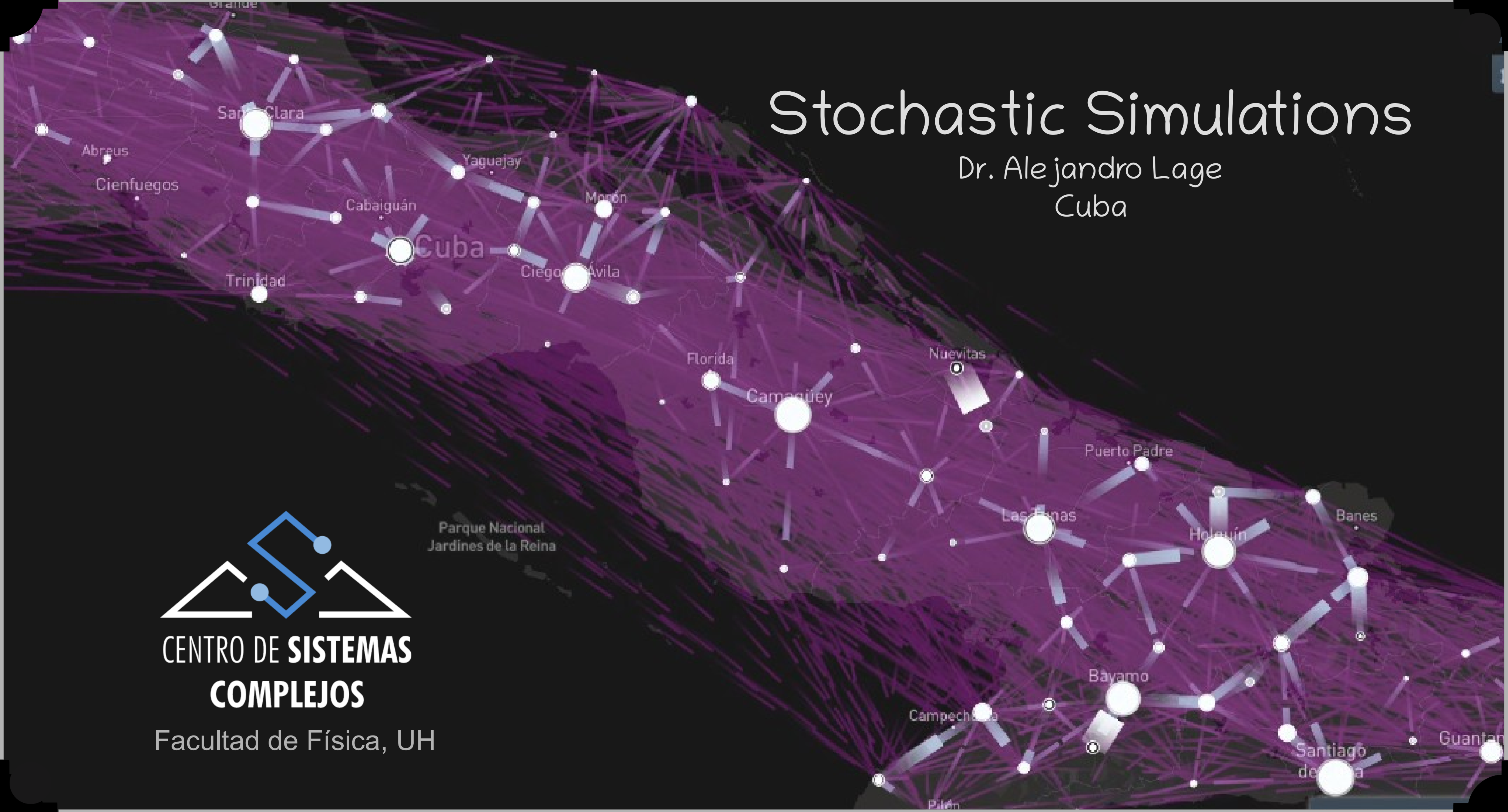
Stochastic Simulations

Dr. Alejandro Lage
Cuba



CENTRO DE **SISTEMAS COMPLEJOS**
Facultad de Física, UH

EPIDEMICS ON NETWORKS

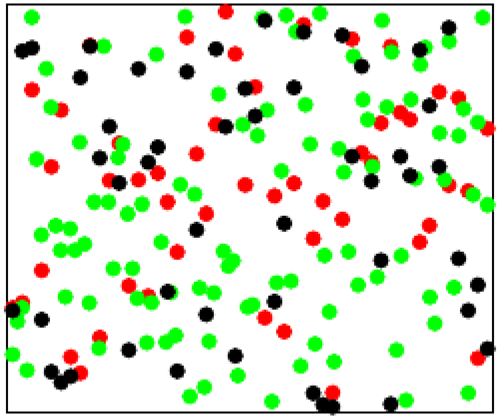
1. Mathematical epidemiology, origins, early results. The compartmental model family.
2. The mean field description of SIR models. Short and long time limits in SIR.
3. **Monte Carlo simulations of epidemics. Gillespie algorithm.**
4. **Monte Carlo simulations Practical Python Class.**
5. Complex networks. Main results. Types and properties. Famous networks. Benchmarks.
6. Playing with networks in Python. Networkx. Plotting. Nice plotting.
7. Master equation of epidemics on networks. The mean field solution and pair based solution.
8. Simulating epidemics on networks. Python libraries.
9. Inference and belief propagation.
10. The zero patient problem. The contamination source detection problem.
11. The infectious backbone as a cascade process.
12. The effect of contact tracing.

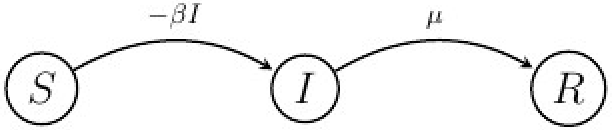
Previously on Epidemics ...

PREVIOUSLY ON EPIDEMICS ...

Epidemics are (matheamtically):

- Stochastic processes
- Discrete states (S,I,R)
- Continuous time
- Good approximation: Markovian





PREVIOUSLY ON EPIDEMICS …

$$\frac{dS}{dt} = -\beta S I$$
$$\frac{dI}{dt} = \beta S I - \mu I$$
$$\frac{dR}{dt} = \mu I$$

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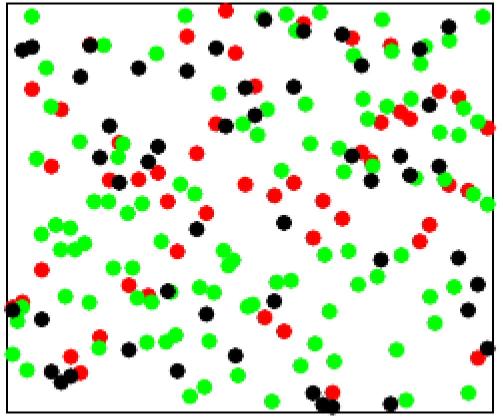


$$S \xrightarrow{-\beta I} I \xrightarrow{\mu} R$$

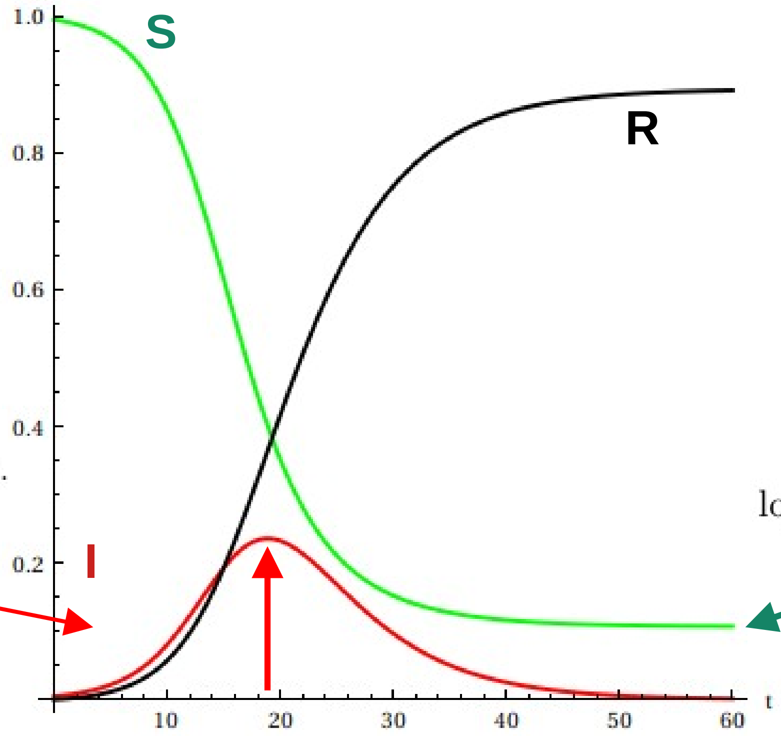
PREVIOUSLY ON EPIDEMICS ...

$$\frac{dS}{dt} = -\beta SI$$
$$\frac{dI}{dt} = \beta SI - \mu I$$
$$\frac{dR}{dt} = \mu I$$

$$\frac{dI}{dt} = \lambda I(t), \qquad \text{where } \lambda = \beta - \mu.$$

$$I(t) = I(0)\exp(\lambda t).$$

$$R_0 = \beta\tau = \beta/\mu$$



$$\log(S_0/S_\infty) = \frac{\beta}{\mu}(1 - S_\infty)$$

STOCHASTIC SIMULATIONS

I. Introduction: Exponential distribution

Rates and exponentials

II. Gillespie Stochastic Simulation Algorithm (SSA)

Derivation

Pseudo code

III. Practical Python Class

10 min Python introduction

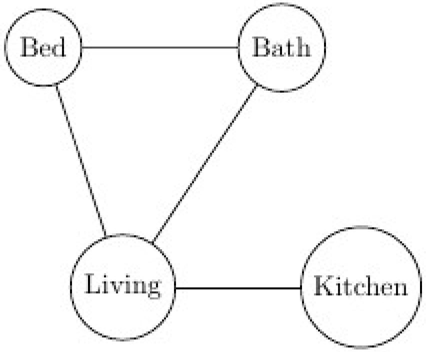
Gillespie algorithm

Drunken man problem

SIR model

SIS model

DRUNKEN MAN PROBLEM



Discrete time $\vec{p}(k+1) = M \cdot \vec{p}(k)$

$$M = \begin{bmatrix} 1-\delta & \delta/2 & \delta/3 & 0 \\ \delta/2 & 1-\delta & \delta/3 & 0 \\ \delta/2 & \delta/2 & 1-\delta & \delta \\ 0 & 0 & \delta/3 & 1-\delta \end{bmatrix}$$

$$\text{Bed} \underset{\delta/2}{\overset{\delta/2}{\rightleftharpoons}} \text{Bath}$$

$$\text{Bed} \underset{\delta/3}{\overset{\delta/2}{\rightleftharpoons}} \text{Living}$$

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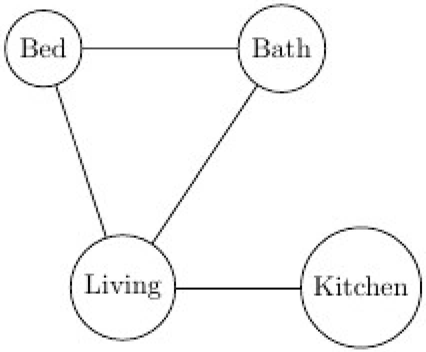

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$$\vec{p}(k) = M^k \vec{p}(0)$$

Stationary state

$$\vec{p}_\infty = M \cdot \vec{p}_\infty$$

$$\boxed{\vec{p}_\infty = (2,2,3,1)/8}$$

Continuous time limit

$$\vec{p}(k+1) - \vec{p}(k) = (M(\delta/T) - \mathbb{I}) \cdot \vec{p}(k)$$

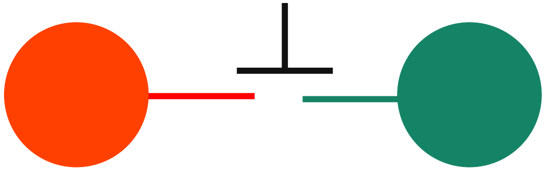
Exponential solutions

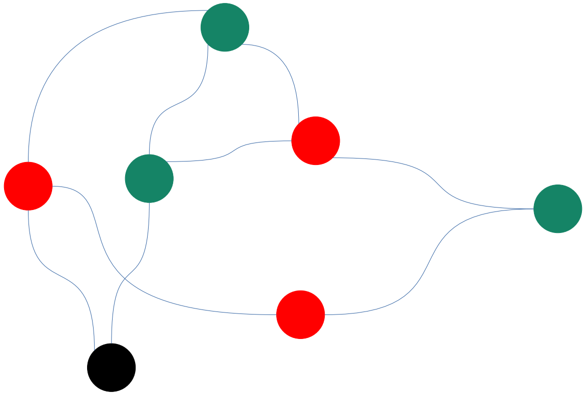
$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = (M(\delta) - \mathbb{I}) \cdot \vec{p}$$

Eigenvalue problem:

$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = 0 \quad \Rightarrow (M(\delta) - \mathbb{I}) \cdot \vec{p} = 0$$

RATES AND EXPONENTIALS





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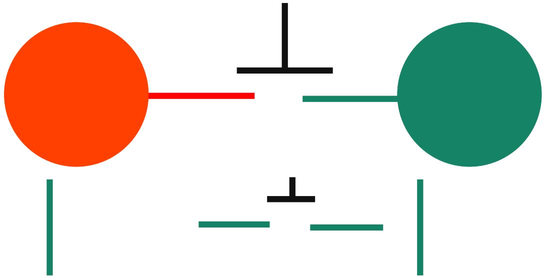

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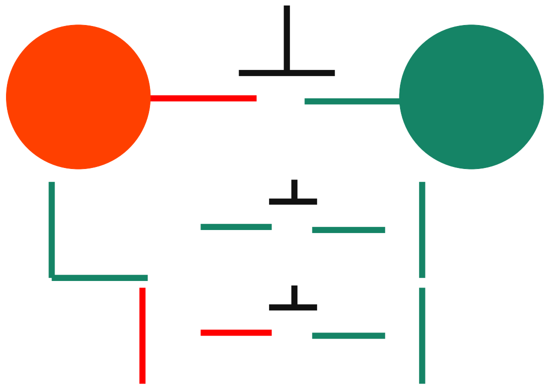

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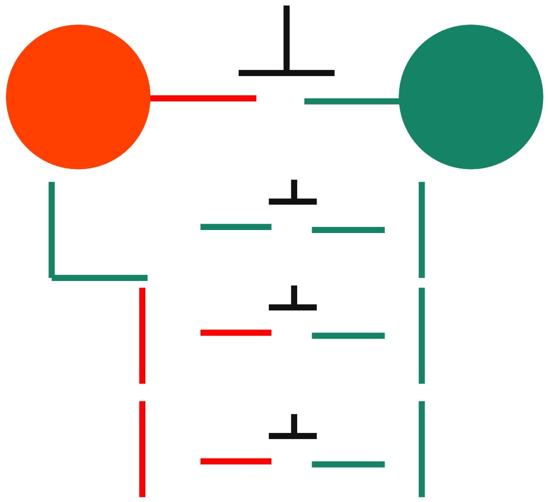

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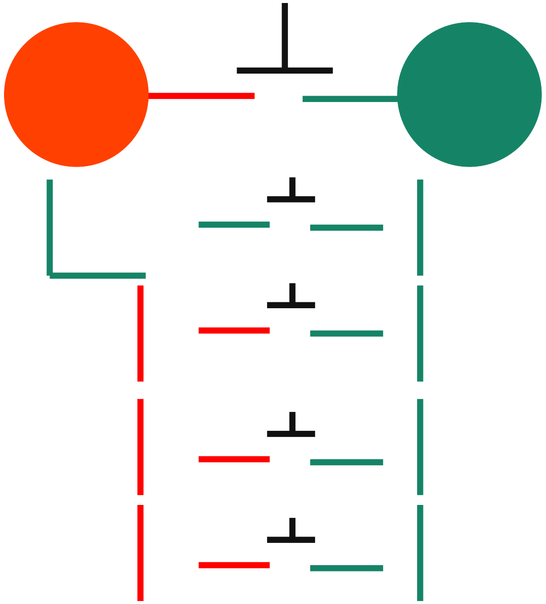

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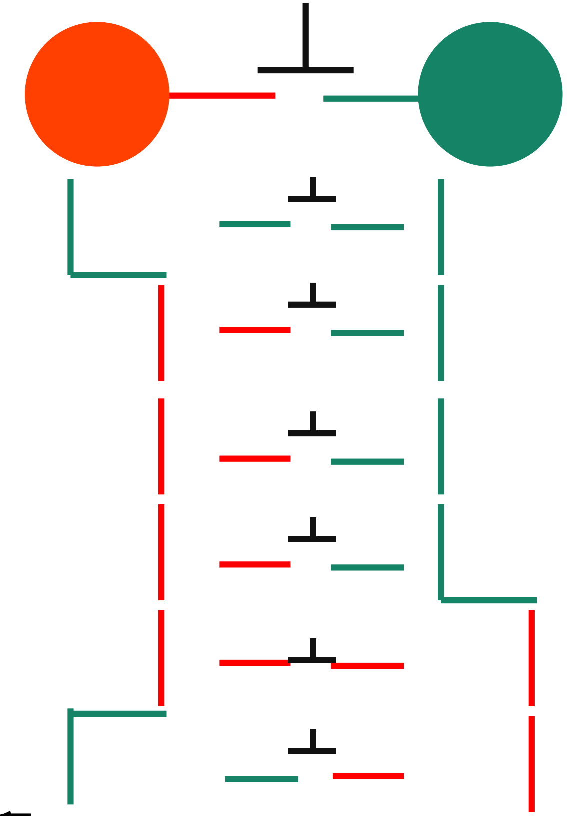

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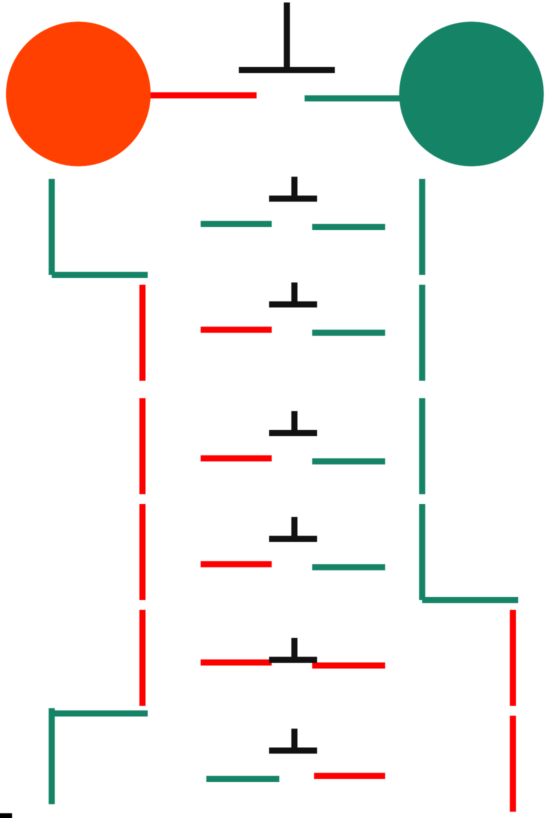


Waiting times: geometric distribution

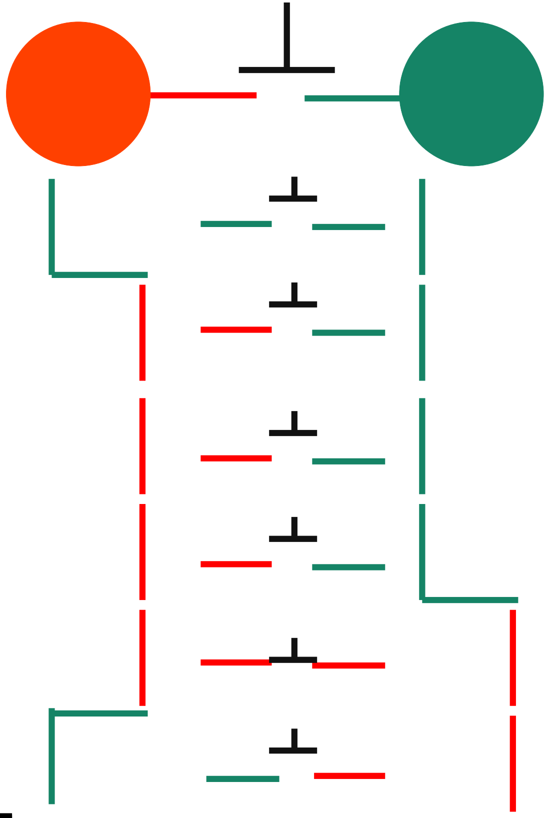
$$P(K=k) = (1-q)^{k-1}q$$

Continuous time limit $q = q'/N$

$$\begin{aligned} P(X=k/N) &= P(K=k) = (1-q)^{k-1}q \\ &= (1-\frac{q'}{N})^{Nx-1}\frac{q'}{N} \end{aligned}$$

$$f(x) = \lim_{N\to\infty}\frac{P(X=k/N)}{1/N} = q'e^{-xq'}$$

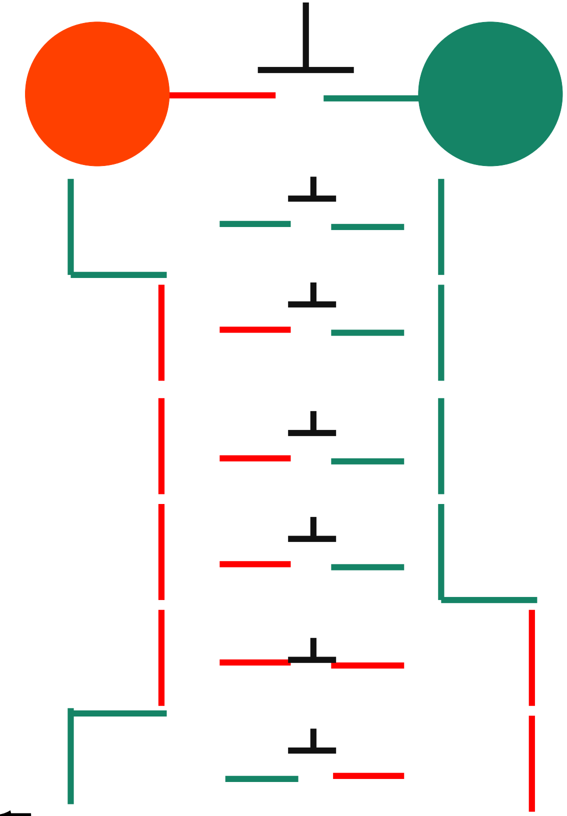
RATES AND EXPONENTIALS



When something **happens at a rate**:
It will happen in **exponential time**

$$f(x) = \lim_{N\to\infty} \frac{P(X = k/N)}{1/N} = q' e^{-xq'}$$

RATES AND EXPONENTIALS



Properties of exponential distributions $f(x) = \lambda e^{-\lambda x}$

Mean $\langle X \rangle = \frac{1}{\lambda}$.

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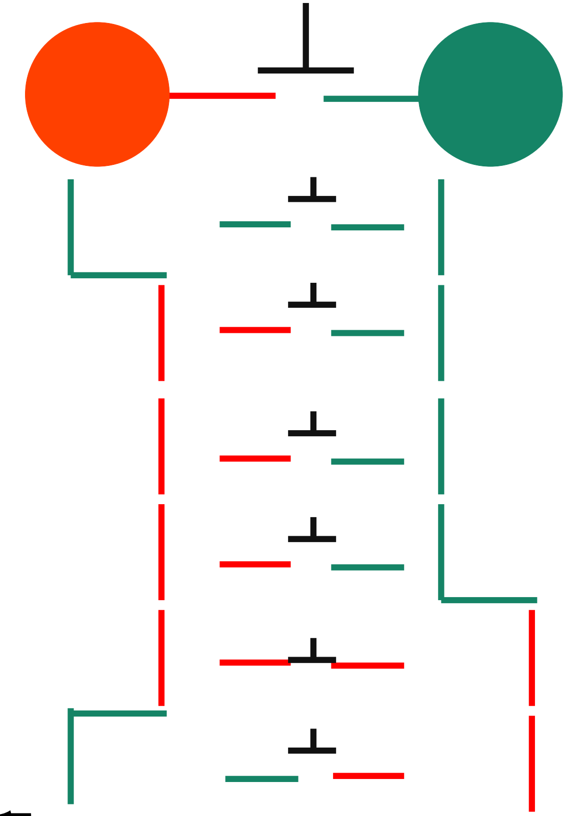

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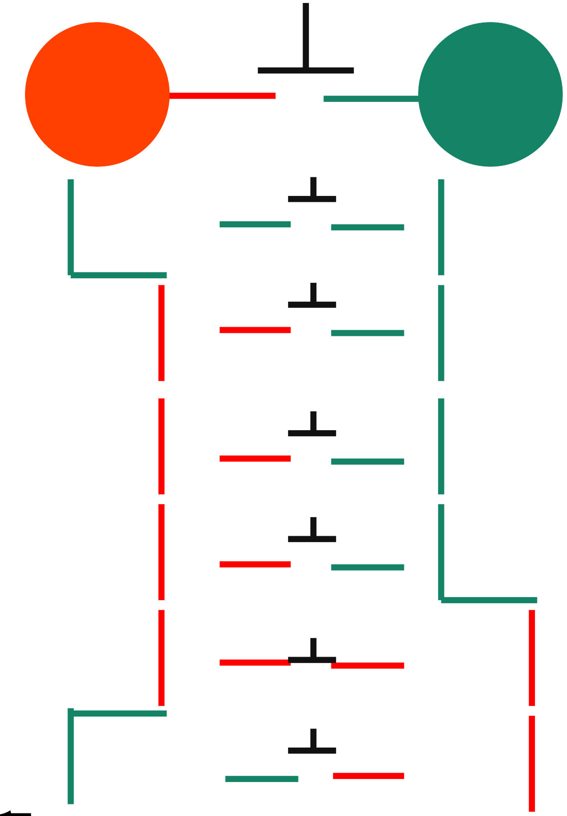

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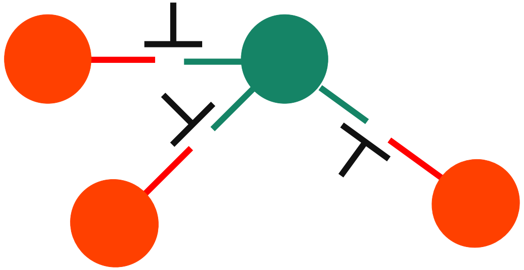
Memorylessness

$$P(X > s+t | X > s) = \frac{P(X > s+t)}{P(X > s)} = \frac{e^{-\lambda(s+t)}}{e^{-\lambda s}} = e^{-\lambda t}$$

$$= 1 - F(t) = P(X > t)$$

RATES AND EXPONENTIALS



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Law of the minimum

$$\begin{cases} X_i \sim \mathcal{E}xp(\lambda_i), \\ Y_i = \min_i X_i, \\ Z_i = \text{argmin}_i X_i \end{cases} \Rightarrow \begin{cases} Y \sim \mathcal{E}xp(\sum_i \lambda_i) \\ \mathbb{P}(Z = i) = \frac{\lambda_i}{\sum_j \lambda_j} \end{cases}$$

CHEMICAL REACTIONS

Drunken man

$$\mathrm{Bed} \underset{\delta/2}{\overset{\delta/2}{\rightleftharpoons}} \mathrm{Bath}$$
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SIR

$$\begin{aligned} S + I &\xrightarrow{\beta} 2I \\ I &\xrightarrow{\mu} R \end{aligned}$$

SIRS

$$\begin{aligned} S + I &\xrightarrow{\beta} 2I \\ I &\xrightarrow{\mu} R \\ R &\xrightarrow{\eta} S \end{aligned}$$

Any chemical reaction

$$A + B \xrightarrow{k_1} C + B$$
$$C \xrightarrow{k_2} 2D$$
$$2D + B \xrightarrow{k_3} A$$

How do the rates depend on the state?

$$\begin{aligned} a_1 &= k_1[A][B] \\ a_2 &= k_2[C] \\ a_3 &= k_3[D]^2[B] \end{aligned}$$

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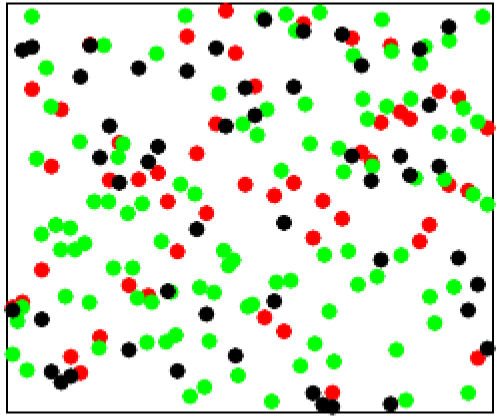

State of the system

$$X = (n_A, n_B, n_C, n_D)$$

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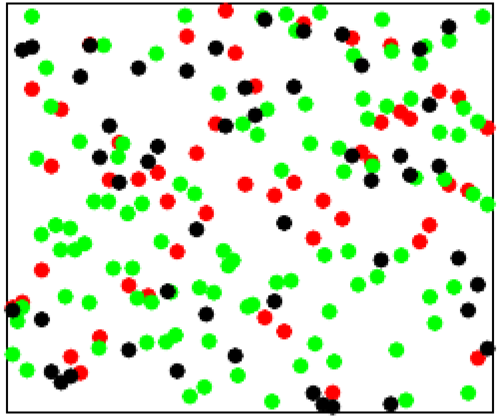

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Remains unchanged until
one of this take place

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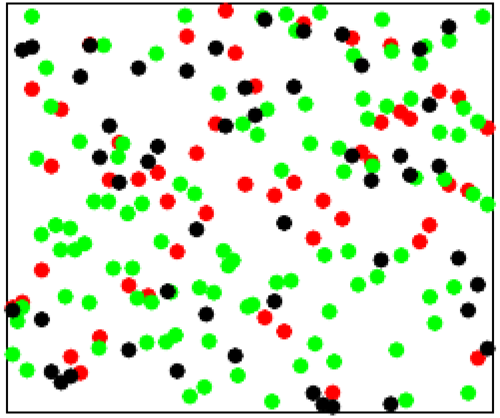
One occurrence is defined by

$$\mathcal{P} = \{(t_1, r_1), (t_2, r_2)..\}$$

Two random values:

- Time for jumping
- Reaction to use

CHEMICAL REACTIONS



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$$X(t) = X(t_{k-1}) + \Delta X_{r_k}$$

Stoichiometric matrix

$$\Delta X_1 = \begin{pmatrix} -1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \Delta X_2 = \begin{pmatrix} 0 \\ 0 \\ -1 \\ 2 \end{pmatrix} \quad \Delta X_3 = \begin{pmatrix} 1 \\ -1 \\ 0 \\ -2 \end{pmatrix}$$

GILLESPIE SSA

Total rate

$$a_0 = \sum_i a_i$$

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Minimum i.i.d exponentials,
Jumping time:

$$\tau = \frac{1}{a_0} \ln \frac{1}{r_1}$$

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Next reaction:

$$P_i = \frac{a_i}{\sum_j a_j}$$

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Algorithm 1

Gillespie SSA

$t = 0$
$X(0) = X_0$
while $t < t_{end}$ **do**
    Update(a_i)
    $a_0 = \sum_i a_i$
    for $i = 1 \ldots K$ **do**
        $P_i = \frac{a_i}{a_0}$
    $r_1 \sim U(0,1)$
    $r_2 \sim U(0,1)$
    $\tau = \frac{1}{a_0} \ln \frac{1}{r_1}$
    $k = i | P_{i-1} < r_2 < P_i$
    $X(t+\tau) = X(t) + \Delta X_k$
    Set $t = t + \tau$

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PRACTICAL PYTHON CLASS

Algorithm 1

Gillespie SSA

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  $a_0 = \sum_i a_i$
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你好

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