Prepared by Julian García, based on material by
David Albrecht and María García de la Banda

Workshop 15:
Stochastic Models

FIT 3139 Computational Modelling and Simulation

MONASH University
Information Technology

Outline

- A stochastic dynamical system.
- Gillespie algorithm.
- Sampling discrete random variables.
- Introduction to (Discrete) Markov Chains

Stochastic model

A model describing how the probability of a system being in different states changes over time.

An experiment takes outcome values in a sample space.

A random variable assigns a unique numerical value to outcomes in an experiment.

Stochastic Process

An *indexed* family of random variables $X(t), t \in T$

Stochastic Process

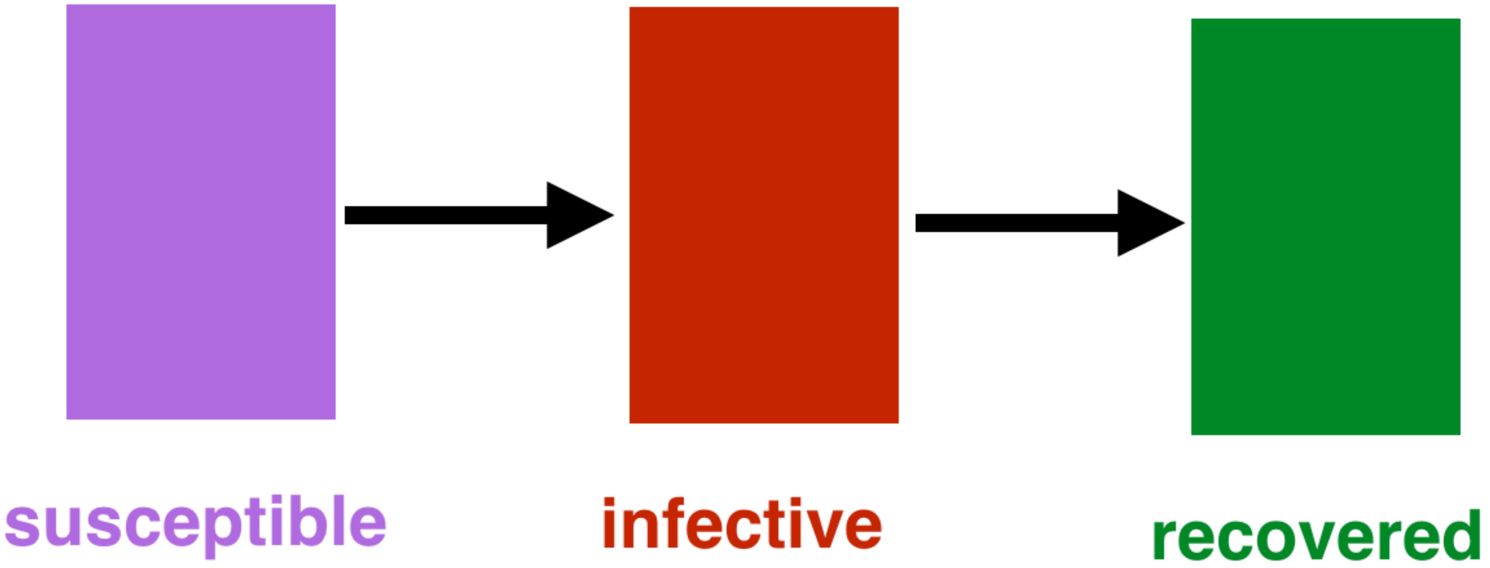
a process where the **rule for making a transition** to a new state of the system at time $t+1$ (or $t+dt$, if time is continuous) from the current state at time t **is a random variable**.

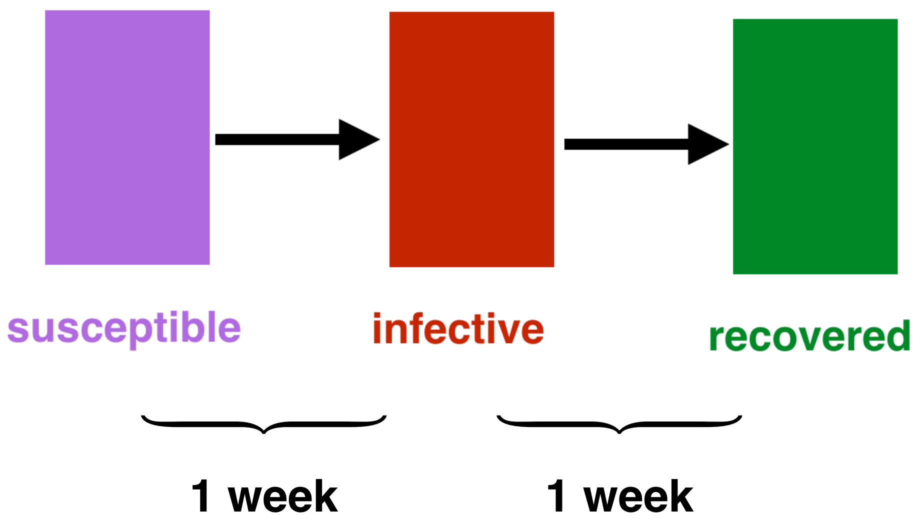
Unlike a deterministic process, only **the probability of being in a given state** n at time t can be specified.

Measles photograph

(trigger warning)

https://www.flickr.com/photos/perpetualplum/3796080398


susceptible
infective
recovered



$S_k \longrightarrow$ *number of susceptibles in week k*

$I_k \longrightarrow$ *number of infective in week k*

$R_k \longrightarrow$ *number of recovered in week k*

$$I_{k+1} = G(S_k, I_k)$$

$$S_{k+1} = F(S_k, I_k)$$

Key Assumptions

- Discrete time
- R compartment , isolated

$\beta \longrightarrow$ *rate of birth*

$\delta \longrightarrow$ *rate of death*

$\alpha \longrightarrow$ *recovery rate*

$$\frac{dS}{dt} = \underbrace{\beta(I + R + S)}_{\text{born into susceptible}} \underbrace{-f * S * I}_{\text{get infected}} \underbrace{-\delta * S}_{\text{die while susceptible}}$$

$$\frac{dI}{dt} = \underbrace{f * S * I}_{\text{get infected}} \underbrace{-\alpha I}_{\text{recover}} \underbrace{-\delta I}_{\text{die while infected}}$$

$$\frac{dR}{dt} = \underbrace{\alpha I}_{\text{recover}} \underbrace{-\delta R}_{\text{die while recovered}}$$

Do try at home (and in the lab)

$\beta = \delta = 0.0002$

$f = 0.0005$

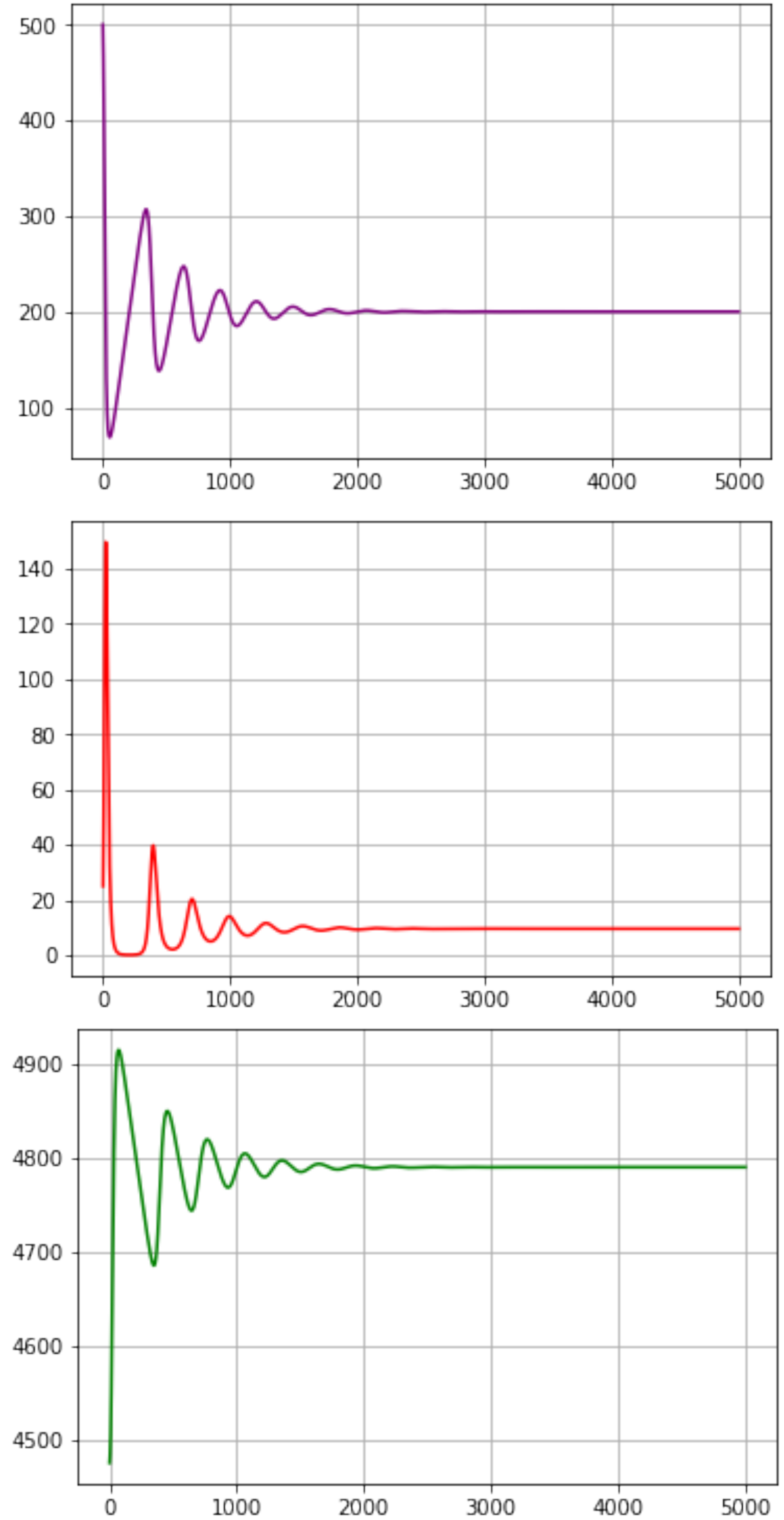
$\alpha = 0.1$

$S_0 = 500, \quad I_0 = 25, \quad R_0 = 4475$

Susceptible

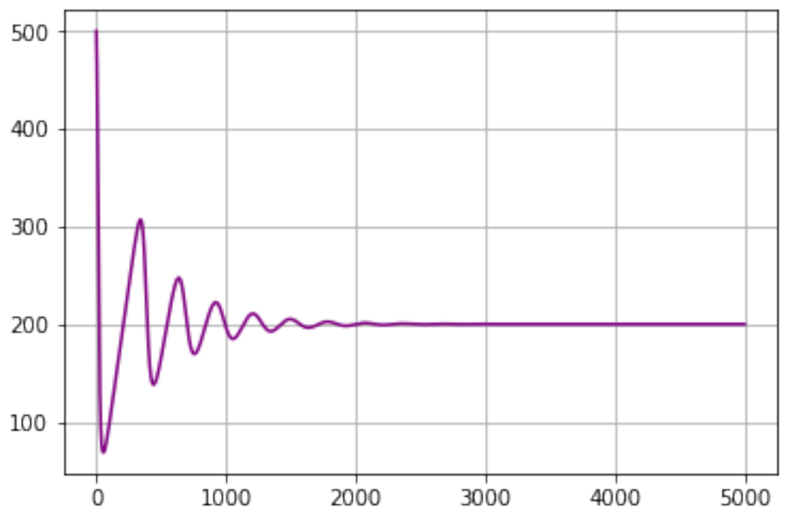
Infected

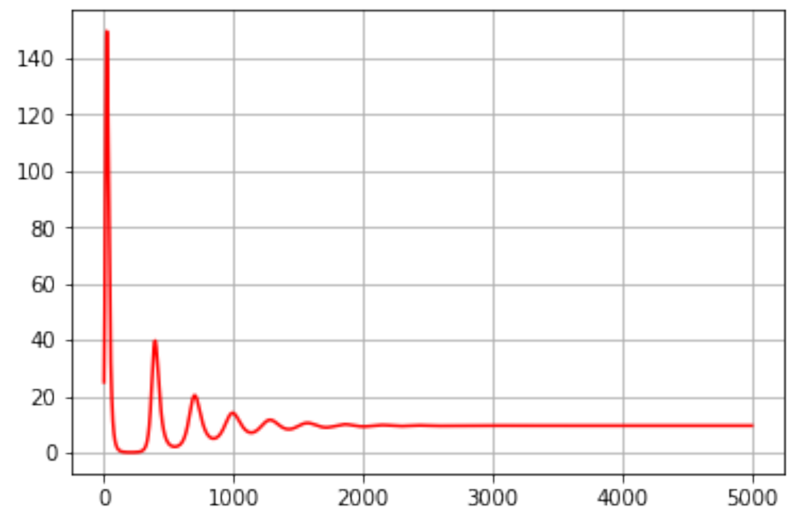
Recovered

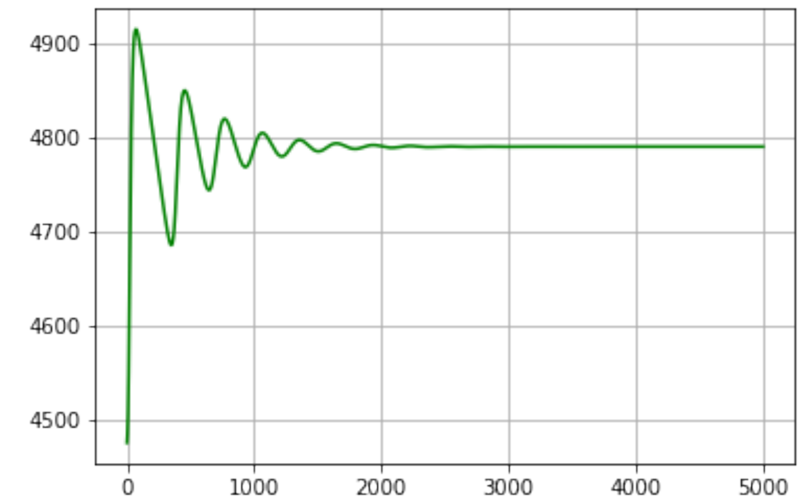


$$\beta = \delta = 0.0002$$
$$f = 0.0005$$
$$\alpha = 0.1$$
$$S_0 = 500, \quad I_0 = 25, \quad R_0 = 4475$$

Is there **randomness** in the system?
Does randomness **matter**?

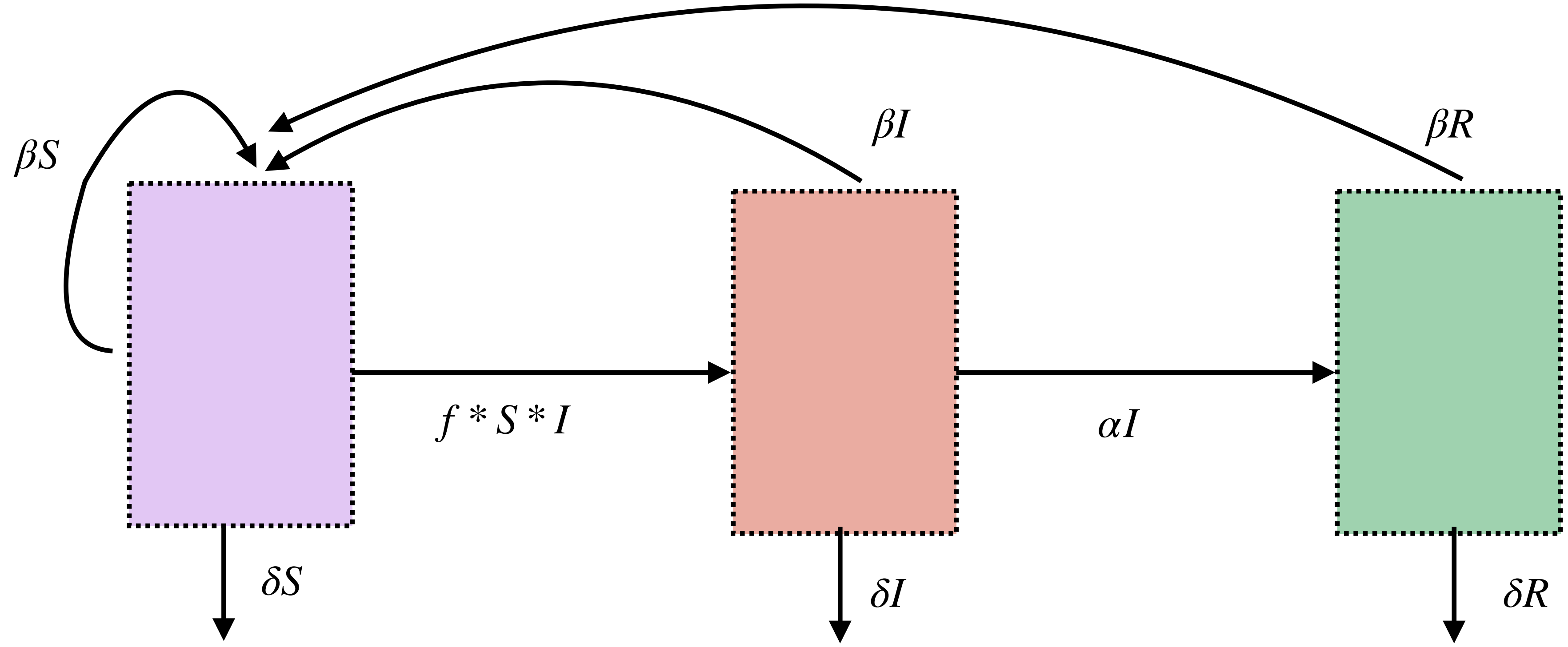






In reality we should observe population fluctuations due to the **random** nature of the events involved.

Even if the **probability** associated with random events is fixed, individuals experience different chances.



$$\frac{dS}{dt} = \underbrace{\beta(I + R + S)}_{\text{1 born into susceptible}} \underbrace{-f * S * I}_{\text{2 get infected}} \underbrace{-\delta * S}_{\text{3 die while susceptible}}$$

$$\frac{dI}{dt} = \underbrace{f * S * I}_{\text{get infected}} \underbrace{-\alpha I}_{\text{4 recover}} \underbrace{-\delta I}_{\text{die while infected 5}}$$

$$\frac{dR}{dt} = \underbrace{\alpha I}_{\text{recover}} \underbrace{-\delta R}_{\text{die while recovered 6}}$$

How many random events?

We have **six stochastic** events… …leading to **updates/actions**

1 a <u>birth</u> happens with propensity: $\beta(I + R + S)$

$$S = S + 1$$

2 an <u>infection</u> happens with propensity: $f * S * I$

$I = I + 1$ and $S = S - 1$

3 a susceptible <u>dies</u> with propensity: $\delta * S$

$$S = S - 1$$

4 an infected <u>recovers</u> with propensity: αI

$R = R + 1$ and $I = I - 1$

5 an infected <u>dies</u> with propensity: δI

$$I = I - 1$$

6 a recovered <u>dies</u> with propensity: δR

$$R = R - 1$$

Gillespie’s general sketch

1. Initialisation step: Set variables to initial values.

2. Montecarlo step: Generate random numbers to determine the next event, as well as time interval.

3. Update: Increase the time according to time generated in step 2. Update the variables affected by event.

4. Iterate: Go back to step 2, and repeat until simulation time has been exceeded.

Remember:

The **Poisson distribution** describes number of events occurring in an interval of time. Rate: λ

The **exponential distribution** describes **time** between independent events that occur at a constant rate.

Density of exponential distribution:

$$f(x \mid \lambda) = \lambda e^{-\lambda x} \qquad x \in [0, \infty]$$

$$F(x \mid \lambda) = \int_0^x f(t \mid \lambda) dt = 1 - e^{-\lambda x}$$

Using inverse transform sampling…

$$x = -\frac{1}{\lambda} \log(1-u)$$

```
def sample(lambda_):
    return -1*np.log(rand())/lambda_
```

Gillespie's algorithm applied to Measles model

1. We have 6 stochastic events $e_1, \ldots, e_6$

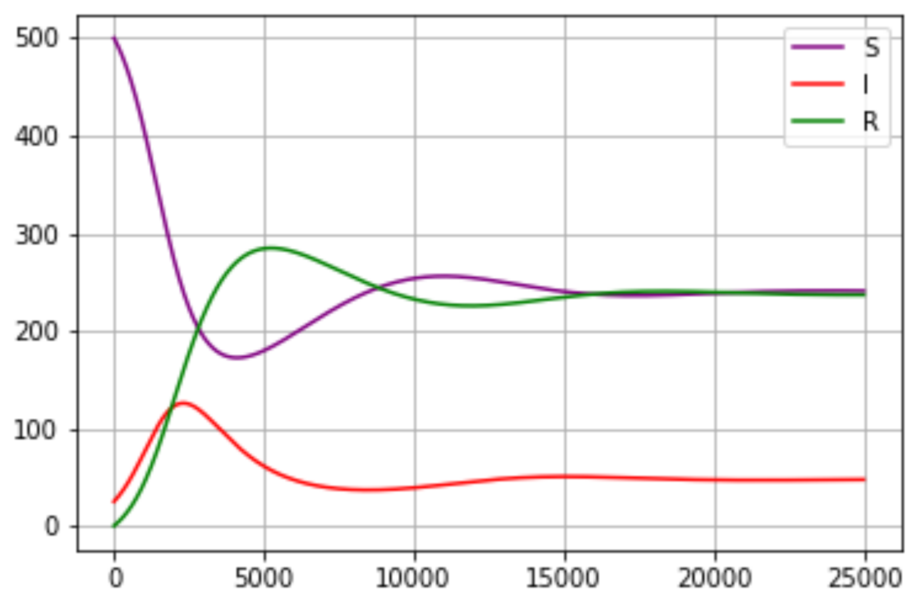
2. For each event determine propensity of occurrence $p_1, \ldots, p_6$

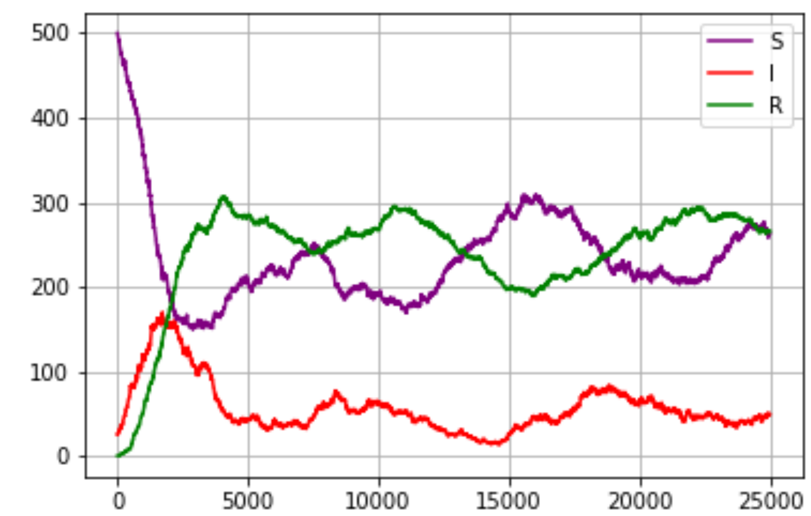
3. Sample time to events: $t_i = -\dfrac{\log u}{p_i}$ $\quad u \sim U(0,1)$

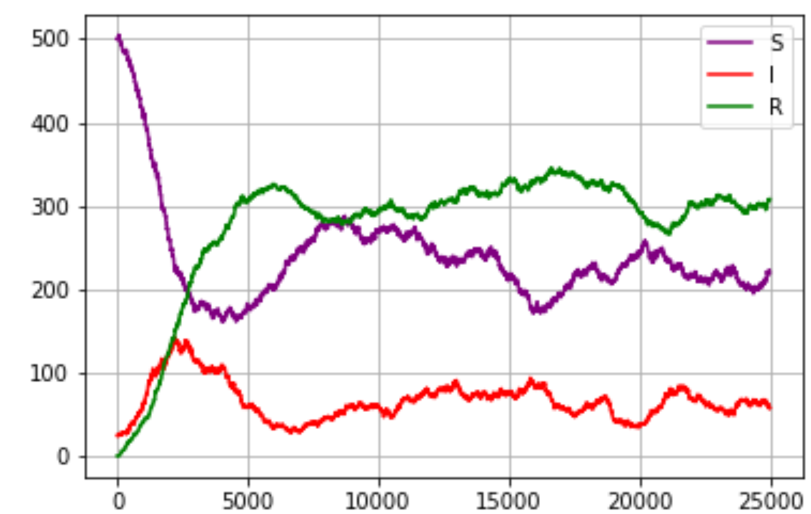
4. Find event that happens earliest $t = \min_{1 \leq i \leq 6} (t_i)$

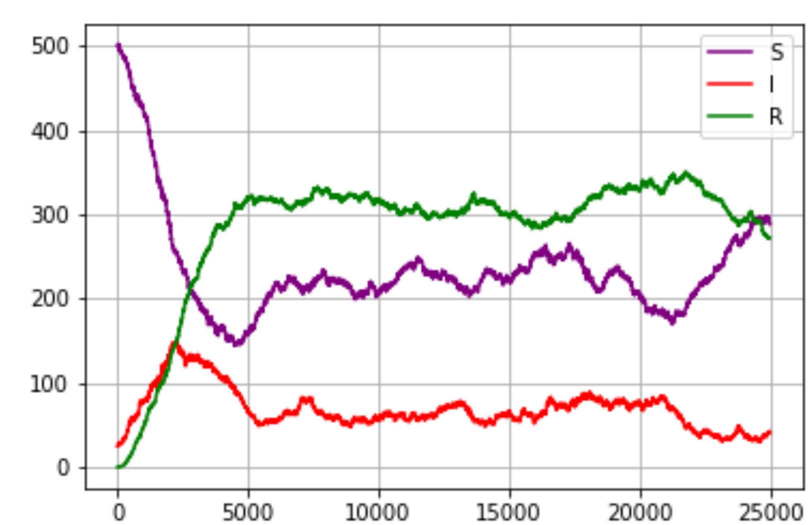
5. Update $t_{curr} = t_{prev} + t$

6. Repeat until the period of the simulation is exceeded.


S
I
R
0
100
200
300
400
500
0
5000
10000
15000
20000
25000


S
I
R
0
100
200
300
400
500
0
5000
10000
15000
20000
25000


S
I
R
0
100
200
300
400
500
0
5000
10000
15000
20000
25000


S
I
R
0
100
200
300
400
500
0
5000
10000
15000
20000
25000

Gillespie’s algorithm

- Due to Gillespie (1977), "Exact Stochastic Simulation of Coupled Chemical Reactions”.
- It is a mechanism to samples a trajectory of the system.
- In general, slow… several variants discuss efficient sampling in specific scenarios.
- Belongs to family of <u>discrete event simulations</u>.

What about generating discrete random variables…

We say a random variable is **discrete**, if it can take a finite (or at most countable) number of values.

$$p(x) = P\{X = x\} \longrightarrow \text{Probability mass function}$$

[for a discrete RV]

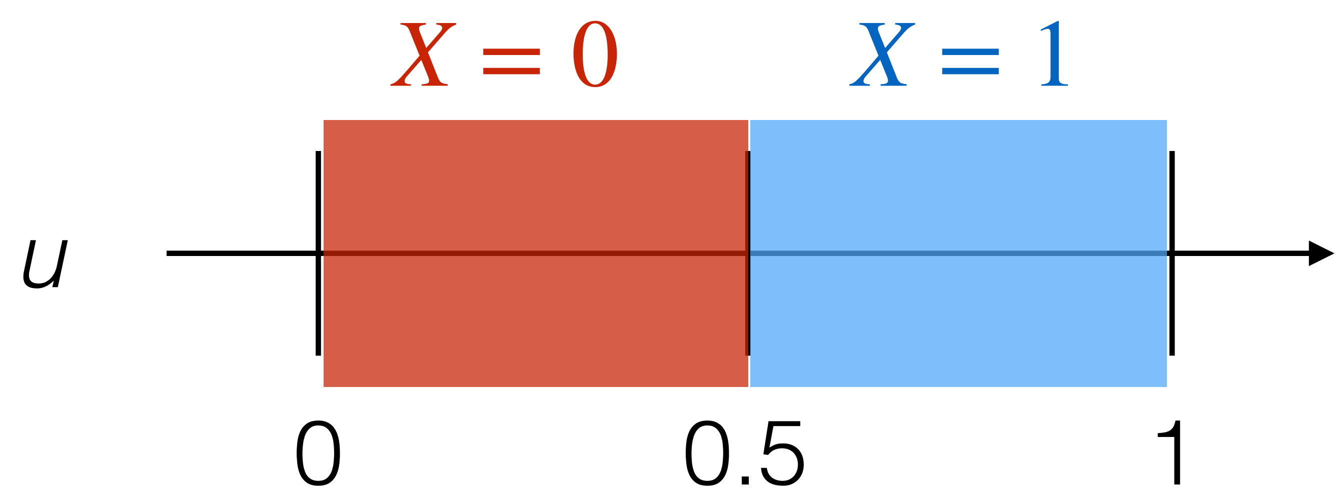
Example:

$$S = \{0,1\}$$

$$P\{X = 0\} = \frac{1}{2} \qquad P\{X = 1\} = \frac{1}{2}$$

Example:

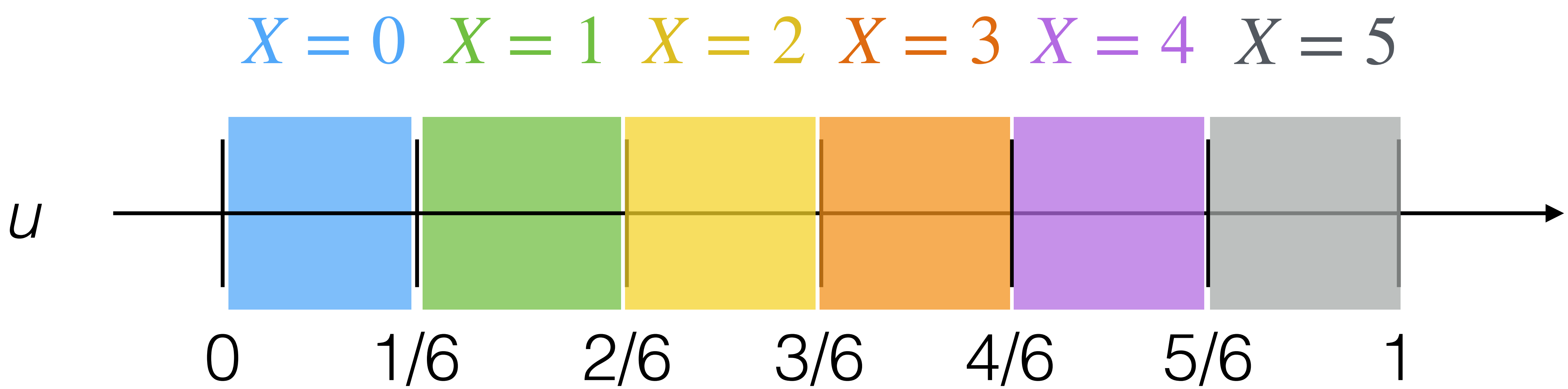
$$S = \{0,1\} \qquad P\{X=0\} = \frac{1}{2} \qquad P\{X=1\} = \frac{1}{2}$$




```python
def coin():
    if rand() < 0.5:
        return 0
    else:
        return 1
```

Example:

$$S = \{0,1,\ldots,5\} \qquad P\{X = i\} = \frac{1}{6} \forall i \in S$$




```python
def dice():
    u = rand()
    for i in range(0, 6):
        if i/6 < u < (i+1)/6:
            return i
```

For a discrete random variable, with mass given by

$$P\{X = x_j\} = p_j \qquad j = 0, 1, \ldots \sum_j p_j = 1$$

Inverse transform

$$X = \begin{cases} x_0 & \text{if } U < p_0 \\ x_1 & \text{if } p_0 \leq U < p_0 + p_1 \\ & \vdots \\ x_j & \text{if } \sum_{i=0}^{j-1} p_i \leq U < \sum_{i=0}^{j} p_i \\ & \vdots \end{cases}$$

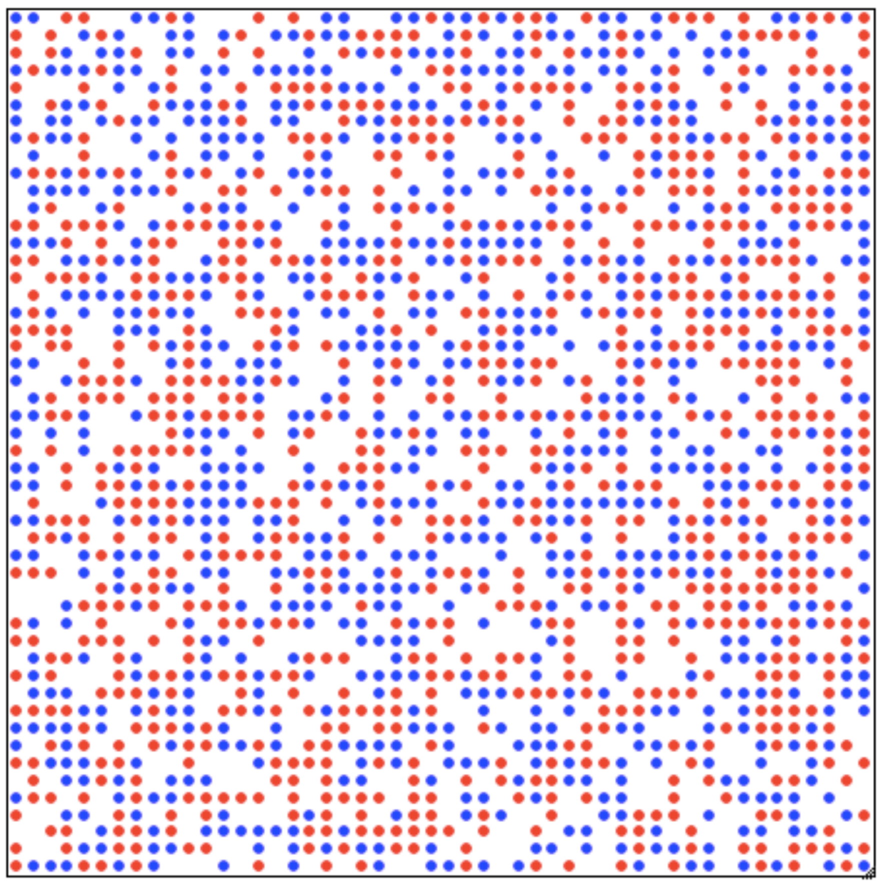
with U, uniformly distributed on (0,1)

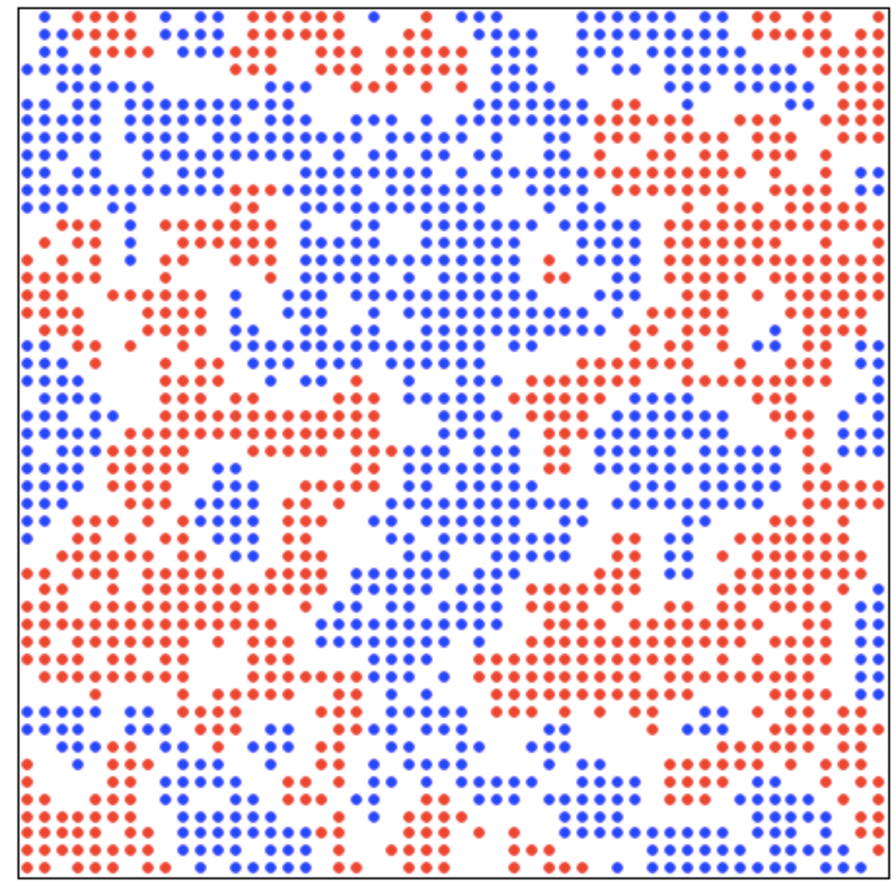
Follows from:

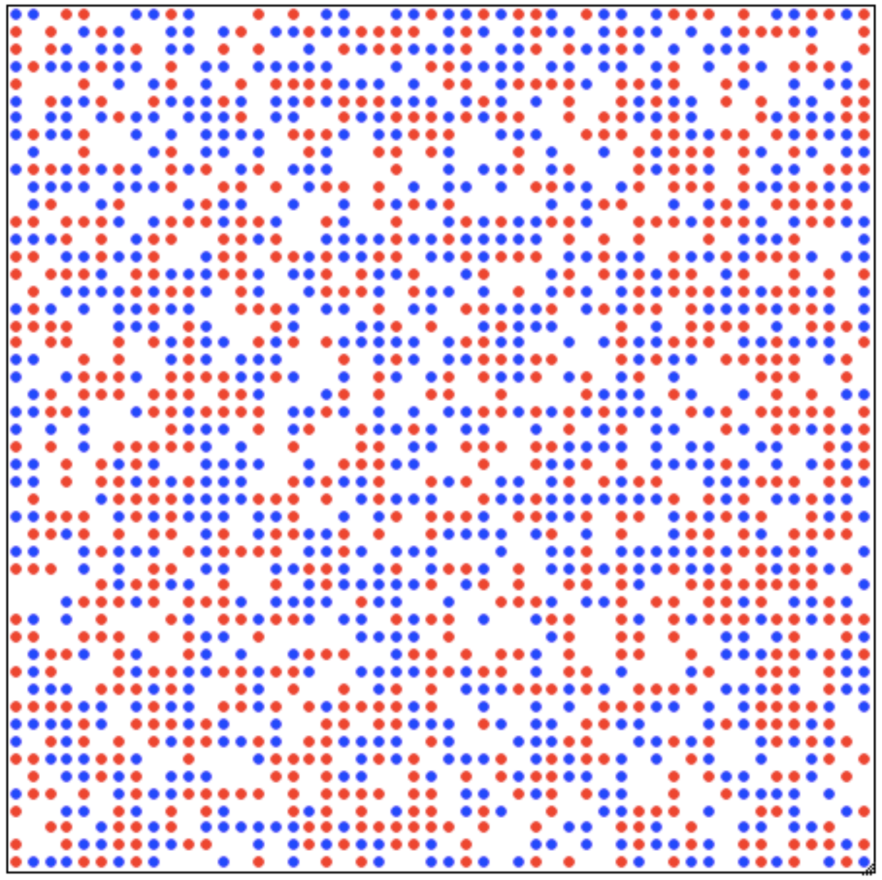
$$0 < a < b < 1, P\{a \leq U < b\} = b - a$$

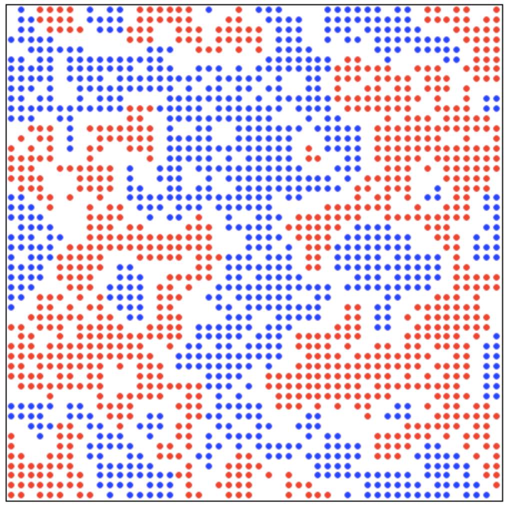
Gillespie was continuous time…

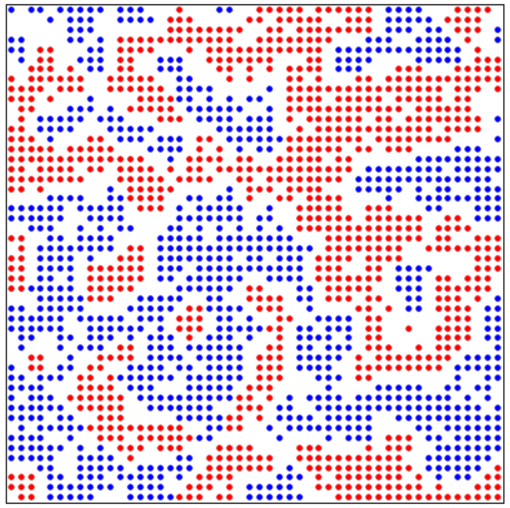
what about discrete time?

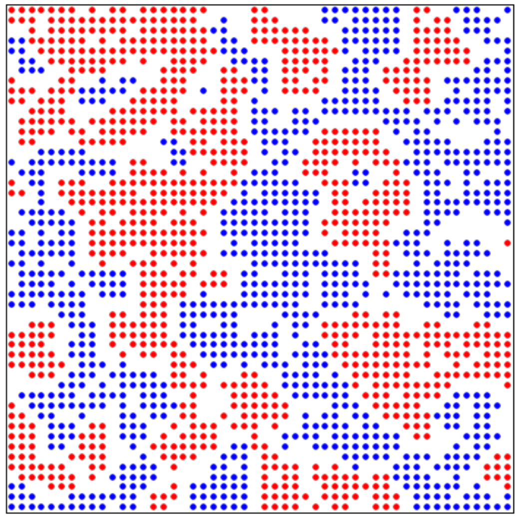












Markov chain

- Set of states $S = \{s_1, s_2, s_3, ..., s_r\}$
- Probability of going from s_i to s_j is given by p_{ij} (transition probability)
- For each i $\sum_j p_{ij} = 1$
- Transition matrix, $A = \{p_{ij}\}$
- Initial distribution **u**, probability vector of size r

conditional probability distribution of future states depends only on the present state

The Land of Oz is blessed by many things, but not by good weather.

They ***never have two nice days in a row****.*
If they ***have a nice day, they are just as likely to have snow as rain the next day.***

If they have snow or rain, they have an even chance of having the same the next day.

If there is change from snow or rain, only half of the time is this a change to a nice day.

$$\mathbf{P} = \begin{array}{c c} & \begin{array}{ccc} R & N & S \end{array} \\ \begin{array}{c} R \\ N \\ S \end{array} & \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{pmatrix} \end{array}$$

Simulation

- At every time step there is a discrete random variable that needs to be sampled.
- While stopping criteria is not met, decide what is the next state.

If transitions are explicit....

$$P\{X = x_j\} = p_j \qquad j = 0, 1, \ldots \sum_j p_j = 1$$

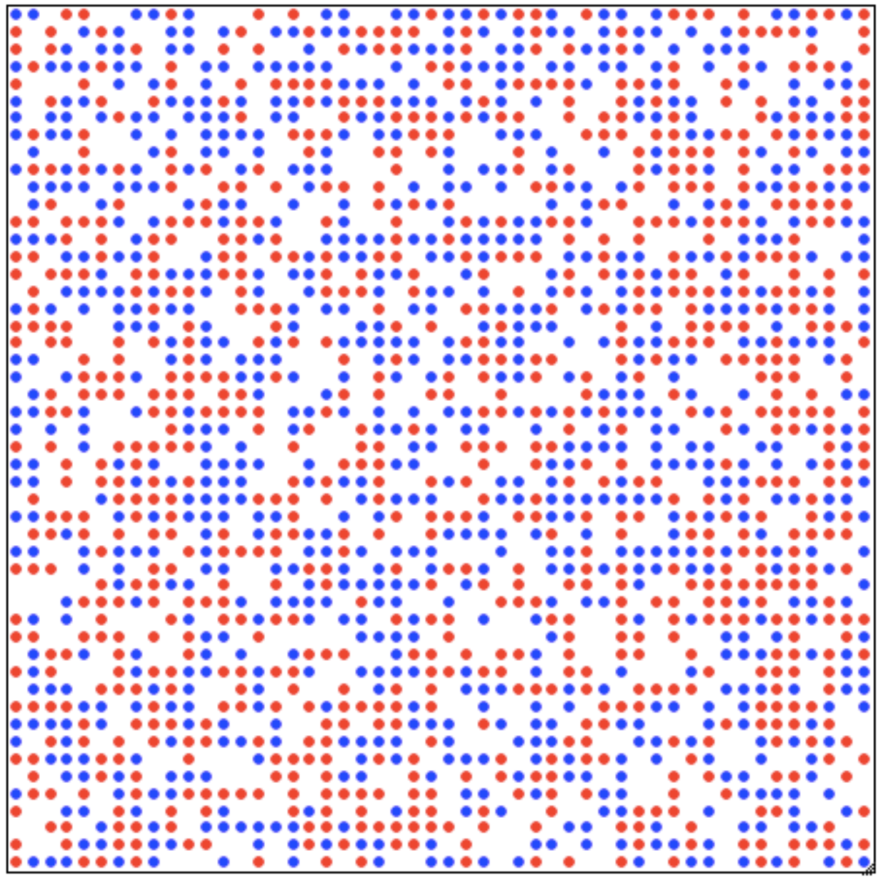
$$X = \begin{cases} x_0 & \text{if } U < p_0 \\ x_1 & \text{if } p_0 \leq U < p_0 + p_1 \\ & \vdots \\ x_j & \text{if } \sum_{i=0}^{j-1} p_i \leq U < \sum_{i=0}^{j} p_i \\ & \vdots \end{cases}$$

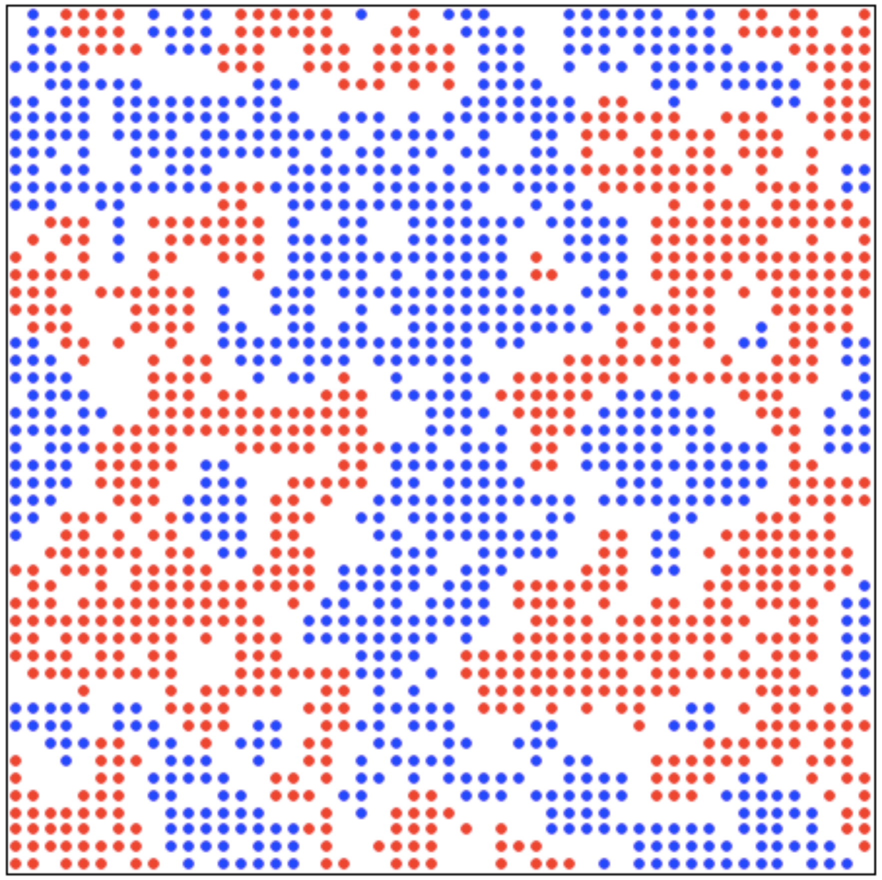
with U, uniformly distributed on (0,1)

Follows from:

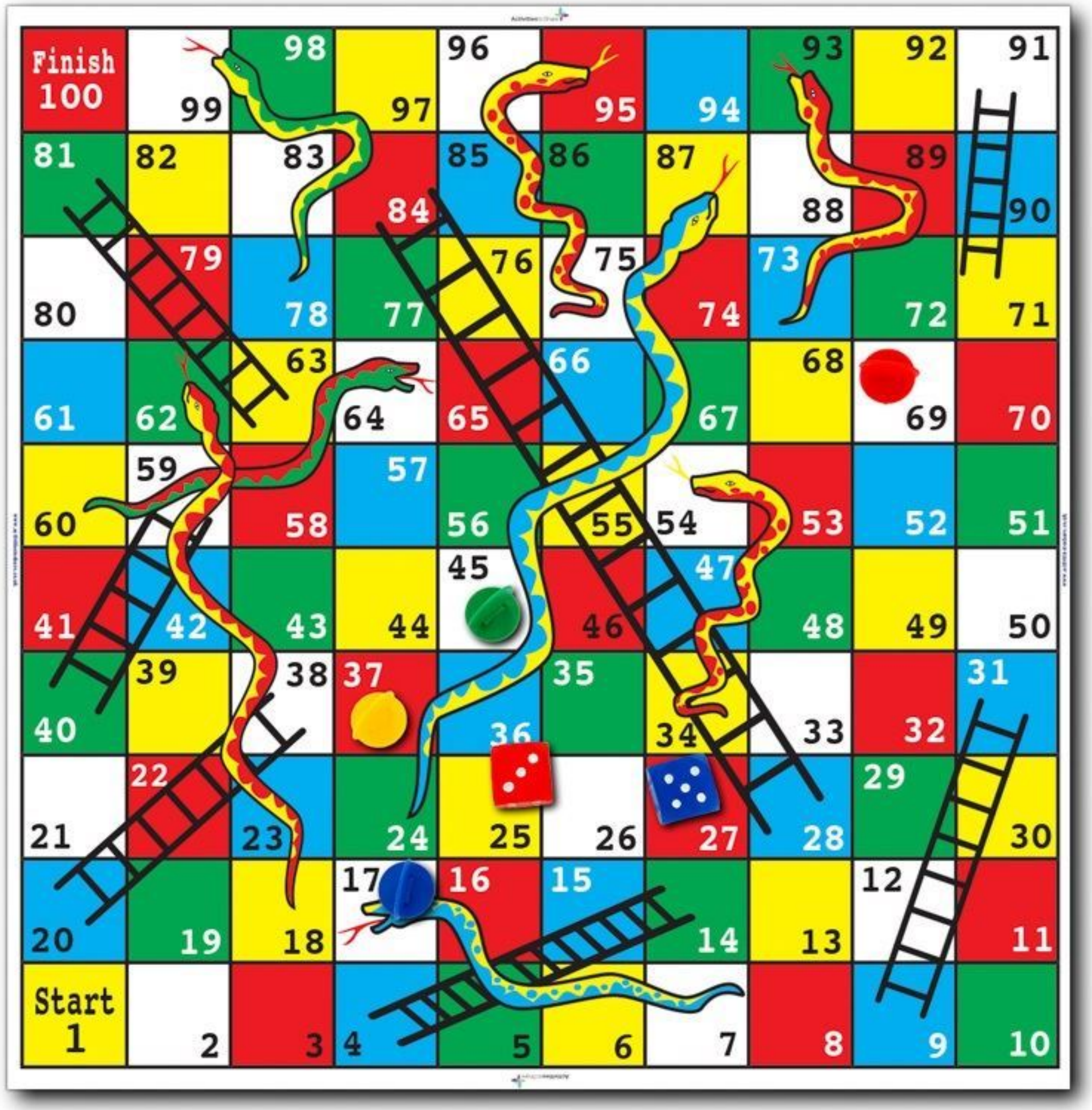
$$0 < a < b < 1, P\{a \leq U < b\} = b - a$$

Examples of Markov Chains





Examples of Markov Chains



Some simple Markov chains with explicit transitions…

$$\mathbf{P} = \begin{array}{c c} & \begin{array}{ccc} R & N & S \end{array} \\ \begin{array}{c} R \\ N \\ S \end{array} & \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{pmatrix} \end{array}$$

If it is raining today, what is the probability that it will be snowing in two days?

$$\mathbf{P} = \begin{array}{c c} & \begin{array}{ccc} R & N & S \end{array} \\ \begin{array}{c} R \\ N \\ S \end{array} & \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{pmatrix} \end{array}$$

Given that today we are in state i, what's the chance that we are in state j in two steps...

$$p_{ij}^{(2)} = \sum_k p_{ik} p_{kj}$$

for a Markov chain given by transition matrix $\mathbf{P}$

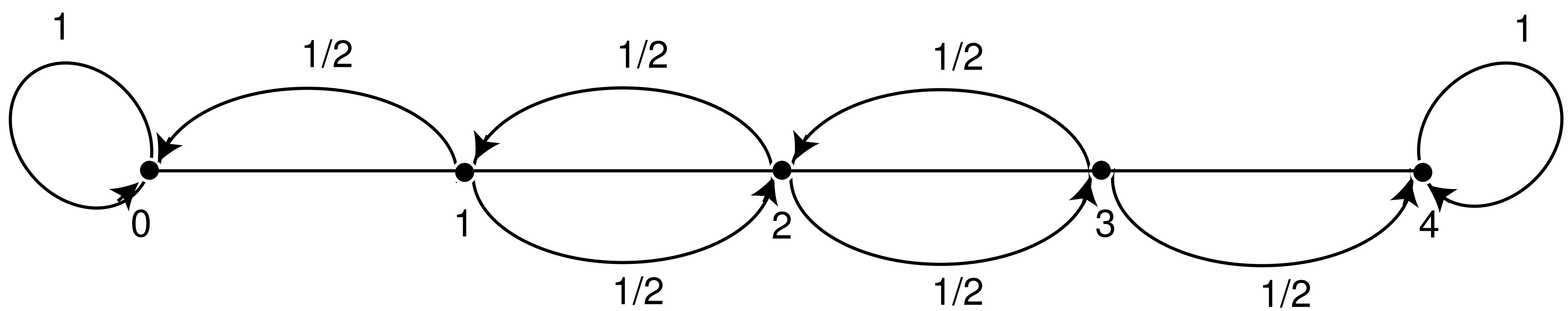
$p_{ij}^{(n)}$ the probability to go from state s_i to state s_j

in *n* steps, is given by the *ij-th entry of* $\mathbf{P}^n$

Long-term behaviour:

$$\mathbf{P}^* = \lim_{k\to\infty} \mathbf{P}^k$$

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 & 0 \\ 0 & 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0.5 & 0 & 0.5 \\ 0 & 0 & 0 & 0 & 1.0 \end{pmatrix}$$



What happens in the long term...

$$\mathbf{P} = \begin{array}{c c} & \begin{array}{ccc} R & N & S \end{array} \\ \begin{array}{c} R \\ N \\ S \end{array} & \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{pmatrix} \end{array}$$

What happens in the long term...

Next up:

Useful markov chain theory