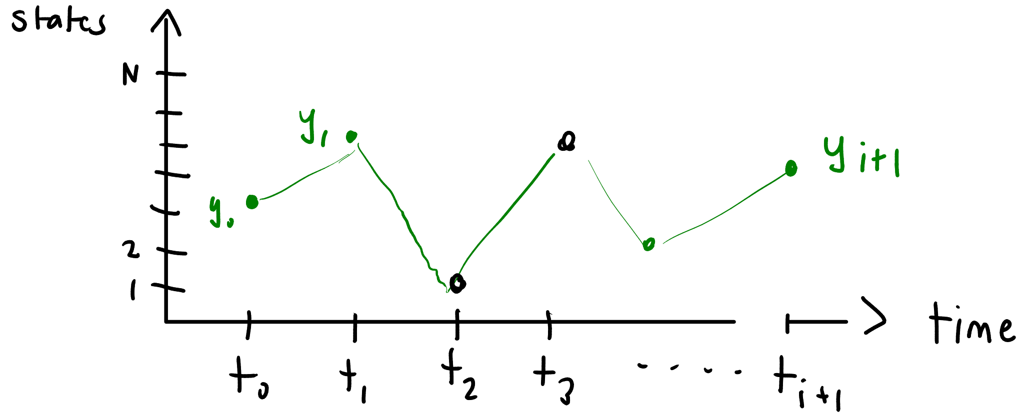
recall : trajectory $\nu = (y_0, y_1, y_2, \ldots)$



$\mathcal{P}(\nu)$ = prob. to observe ν in ensemble

Key assumption: Markovian dynamics

$$\mathcal{P}(y_{i+1} | y_0, y_1, \ldots, y_i)$$

prob. of y_{i+1} given all past history $y_0, \ldots, y_i$

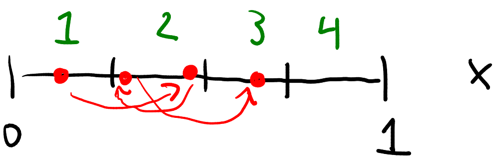
$$= \mathcal{P}(y_{i+1} | y_i)$$

only depends on immediate past y_i

$$\frac{\partial \psi}{\partial t} \approx \frac{\psi(t+\Delta t) - \psi(t)}{\Delta t} \Rightarrow \psi(t+\Delta t) \approx \psi(t) + \Delta t \, (\overset{\text{RHS}}{\cdots\cdots})$$

example from HW #1

PS #1



run simulations

traj: $(1, 1, 2, 1, 3)$

$(1, 2, 3, 4, 2)$

$\ldots$

$$(y_0, y_1, y_2, y_3, y_4)$$

$$\mathcal{P}(y_4 = 3 \mid y_2 = 4, y_3 = 1) \underset{\text{check}}{\overset{?}{=}} \mathcal{P}(y_4 = 3 \mid y_3 = 1)$$

$$\frac{\#\text{ traj. of form } (*, *, 4, 1, 3)}{\#\text{ traj. of form } (*, *, 4, 1, *)} \approx \frac{(*, *, *, 1, 3)}{(*, *, *, 1, *)}$$

Why is Markovianity useful?

1) makes calc: $\mathcal{P}(v)$ easier;

$$\mathcal{P}(A \mid B) = \frac{\mathcal{P}(A, B)}{\mathcal{P}(B)}$$

LHS: $$\frac{\mathcal{P}(y_0, y_1, \dots, y_{i+1})}{\mathcal{P}(y_0, y_1, \dots, y_i)} \underset{\text{Markov}}{=} \mathcal{P}(y_{i+1} \mid y_i)$$

$$\underbrace{\mathcal{P}(y_0, \dots, y_{i+1})}_{\mathcal{P}(v)} = \mathcal{P}(y_{i+1} \mid y_i)\, \mathcal{P}(y_0, \dots, y_i)$$

$$= \text{recursion}$$

$$= \mathcal{P}(y_{i+1} \mid y_i)\, \mathcal{P}(y_i \mid y_{i-1}) \cdots \mathcal{P}(y_0)$$

$$= \left[\prod_{j=0}^{i} \mathcal{P}(y_{j+1} \mid y_j) \right] \underset{\substack{\downarrow \\ \text{initial dist.}}}{\mathcal{P}(y_0)}$$

$$y_{j+1} = 1, \dots, \overset{\substack{\#\text{ states} \\ \downarrow}}{N} \qquad y_j = 1, \dots, N$$

define $\mathcal{P}(y_{j+1} = n \mid y_j = m) = W_{nm}(t_j)$

end   start   "transition" probability

given m prob. of going to n

$W(t_j) = N \times N$ matrix of prob.

(all real, b/t 0 + 1)

[not necessarily symm.]

$$\boxed{\begin{array}{l} \mathcal{P}(\nu) = W_{n_{i+1} n_i}(t_i)\, W_{n_i n_{i-1}}(t_{i-1}) \cdots W_{n_1 n_0}(t_0)\, \mathcal{P}(n_0) \\ \parallel \\ (n_0, n_1, \ldots, n_{i+1}) \end{array}}$$

2) we can find prob. of being in some state at curr. time

$$\mathcal{P}(y_{i+1}) = \sum_{y_0=1}^{N} \cdots \sum_{y_i=1}^{N} \mathcal{P}(y_0, y_1, \ldots, y_{i+1})$$

$$\overset{\text{Markov}}{=} \sum_{y_0} \cdots \sum_{y_{i-1}} \sum_{y_i} \mathcal{P}(y_{i+1} \mid y_i)\, \mathcal{P}(y_0, \ldots, y_i)$$

$$= \sum_{y_i} \mathcal{P}(y_{i+1} \mid y_i)\, \mathcal{P}(y_i)$$

rewrite :

$$\left.\begin{array}{l} \mathcal{P}(y_i = m) = p_m(t_i) \\ \mathcal{P}(y_{i+1} = n) = p_n(t_{i+1}) \end{array}\right\} \quad \begin{array}{l} \text{elements of} \\ \vec{p}(t_i) \\ \vec{p}(t_{i+1}) \end{array}$$

$$p_n(t_{i+1}) = \sum_{m=1}^{N} W_{nm}(t_i)\, p_m(t_i)$$

(DTDS)
discrete
state
discrete
time
master eq.

$$\boxed{\vec{p}(t_{i+1}) = W(t_i)\,\vec{p}(t_i)}$$

$$\boxed{\vec{p}(t_{i+1}) = W(t_i)\cdots W(t_1)W(t_0)\,\vec{p}(t_0)}$$

solution: chain of matrix multiplications

$$\boxed{\begin{array}{l} \mathcal{P}(\underset{\parallel}{\nu}) = W_{n_{i+1}n_i}(t_i)\, W_{n_i n_{i-1}}(t_{i-1}) \cdots W_{n_1 n_0}(t_0)\, \mathcal{P}(n_0) \\ (n_0, n_1, \ldots, n_{i+1}) \end{array}}$$

chain of matrix <u>elements</u>
multiplied

recall $$\sum_A \mathcal{P}(A \mid B) = 1$$

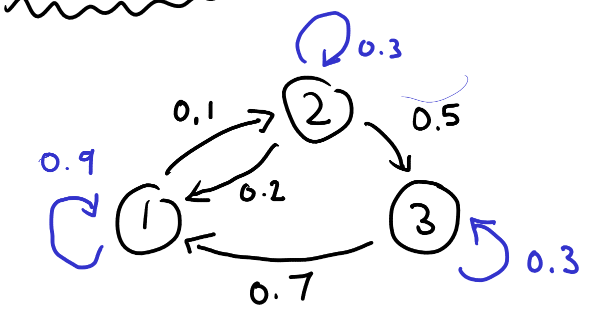
$$\sum_{y_{i+1}} \mathcal{P}(y_{i+1} \mid y_i) = \underline{1}$$

$$\sum_n W_{nm}(t_i) = 1$$

sum of
each
column of
W is $\underline{1}$

example:

N = 3



start

$$W = \begin{array}{cc} & \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \end{array} & \begin{pmatrix} 0.9 & 0.2 & 0.7 \\ 0.1 & 0.3 & 0 \\ 0 & 0.5 & 0.3 \end{pmatrix} \end{array}$$

end

mostly leave self arrows out
b/c we can deduce them from

col. summing to 1