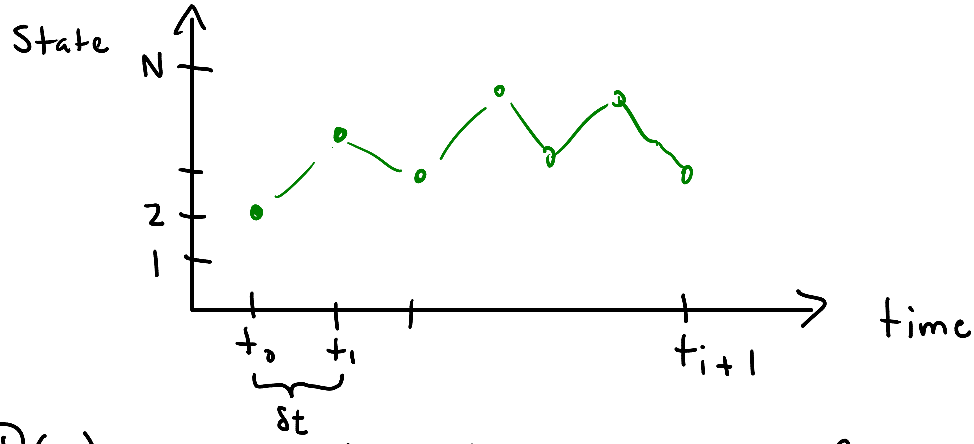
Return to physics: traj. $\nu = (y_0, y_1, \ldots\ldots, y_{i+1})$



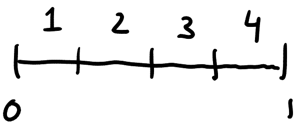
$\mathcal{P}(\nu)$ = prob. to observe a specific ν in ensemble

Key assumption: Markovian dynamics

$$\mathcal{P}(y_{i+1} \mid y_0, y_1, \ldots\ldots, y_i)$$ prob. to be in y_{i+1} given past traj.

$$= \mathcal{P}(y_{i+1} \mid y_i)$$ only depends on immediate past state y_i

example:



states

ran code to gen. a traj:

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

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

$\circ \circ \circ$

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

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

$$\shortparallel$$

$$\frac{\#\text{ traj of form } (*, *, 4, 1, 3)}{\#\text{ traj. of form } (*, *, 4, 1, *)} \overset{?}{=} \frac{\text{"} \quad (*, *, *, 1, 3)}{\text{"} \quad (*, *, *, 1, *)}$$

Why is this assumption useful?

1) Makes calculating $\mathcal{P}(\nu)$ easier:

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

write out LHS of Markov assumption:

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

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

= recursion

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

$$= \ldots$$

$$= \left[\prod_{j=0}^{i} \mathcal{P}(y_{j+1}|y_j)\right] \mathcal{P}(y_0)$$

$\mathcal{P}(y_0)$ ↓ initial distrib.

$y_{j+1} = 1, \ldots, N \qquad y_j = 1, \ldots, N \qquad N = \#$ states

$$\mathcal{P}(y_{j+1} = n \,|\, y_j = m) \equiv W_{nm}(t_j)$$

transition prob. matrix

= prob. of going to n in time step δt if we are currently in m

$W(t_j) = N \times N$ matrix of pos. #'s b/t 0 and 1 (not necessarily symmetric)

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

2) We can find the prob. of being in some state at current time:

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

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

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

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

rewrite in matrix-vector format: $\mathcal{P}(y_i = m) \equiv p_m(t_i)$

$\mathcal{P}(y_{i+1} = n) \equiv p_n(t_{i+1})$

elements of $\vec{p}(t_i), \vec{p}(t_{i+1})$

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

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

discrete-state discrete-time master equation

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