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

$P_n(t_{i+1})$ = prob. to observe state n at time t_{i+1}

$W_{nm}(t_i)$ = prob. to go to state n, given start at state m over time step δt

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

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

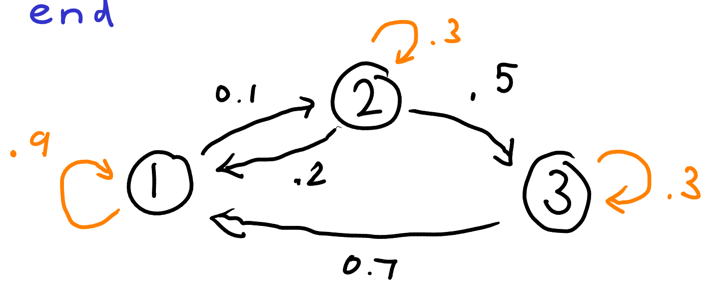
each column sums to 1 $$\boxed{\sum_n W_{nm}(t_i) = 1}$$

example:

$N = 3$

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

graph:

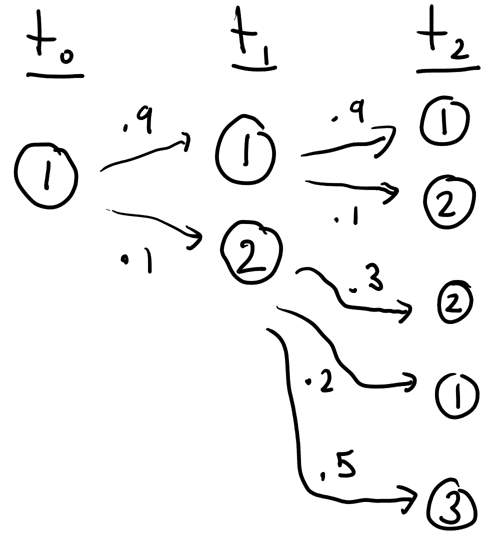


most of the time leave self arrows out (can work out values b/c columns sum to 1)

recall $$\mathcal{P}(\nu) = W_{n_i n_{i-1}}(t_{i-1}) \cdots W_{n_1 n_0}(t_0)\, p_{n_0}(t_0)$$
ν " $(n_0, n_1, \ldots, n_{t_{i+1}})$

all possible 3 time step trajectories:

state prob's at each time step



v	$P(v)$
1 1 1	.81
1 1 2	.09
1 2 2	.03
1 2 1	.02
1 2 3	.05

sum to 1

$$\sum_v P(v) = 1$$

$$\vec{p}(t_0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\vec{p}(t_1) = W\vec{p}(t_0) = \begin{pmatrix} .9 \\ .1 \\ 0 \end{pmatrix}$$

$$\vec{p}(t_2) = W\vec{p}(t_1) = \begin{pmatrix} .83 \\ .12 \\ .05 \end{pmatrix}$$

so far: $p_n(t_i)$

n: discrete state (DS)

t_i: discrete time (DT)

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

DSDT master equ.

generalizations: continuous time CT

$t_i \to t$

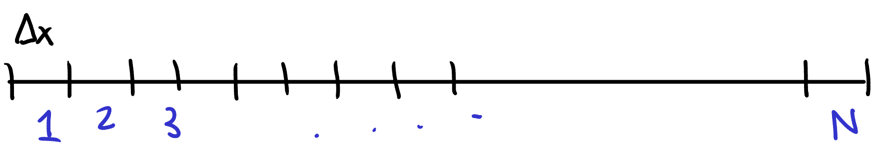
$\delta t \to 0$

continuous state CS

$n \to x$

	DT	CT
DS	DTDS master equ. simulate trans. graph	CT DS master equ. Kinetic Monte Carlo (gillespie)
CS	numerical simulations	Fokker-Planck eqn. Langevin equ.

initial focus: DTDS



$\Delta x \to 0$: keep track of pos. x

$$\rightsquigarrow \quad \frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2}$$

assume: time-independent envir. conditions

$$W(t_i) = W$$

$$\vec{p}(t_n) = W^n \vec{p}(t_0)$$

observation: W^n seems to converge as $n \to \infty$

Why?

$$W^n \xrightarrow[n\to\infty]{} \text{const. matrix indep. of } n$$

$$\vec{p}(t_{n+2}) = W \underbrace{W^{n+1} \vec{p}(t_0)}_{\vec{p}(t_{n+1})} \quad \text{for large } n$$

$$\tilde{\vec{p}}(t_{n+2}) \approx \vec{p}(t_{n+1}) \approx \vec{p}(t_n)$$

$$\approx \vec{p}^{\,s} \quad \text{for large } n$$

stationary probability

$$\Rightarrow \quad \vec{p}^{\,s} = W \vec{p}^{\,s}$$

right e-vec of W w/ e-val 1

$\Rightarrow$
1) does it always exist?
2) is it unique?
3) $W^n \vec{p}(t_0)$ is this guaranteed to approach $\vec{p}^{\,s}$ as $n \to \infty$?

Question #1: does W always have at least one e-vec w/ e-val 1?

quick lemma: matrix M

right e-vec: $M\vec{v} = \lambda \vec{v}$

$\Leftrightarrow$ λ is a sol'n of $\det(M - \lambda I) = 0$

left e-vec: $\vec{u}^T M = \sigma \vec{u}^T$

transpose: $M^T \vec{u} = \sigma \vec{u}$

$\Rightarrow$ σ is a sol'n of

$\det(M^T - \sigma I) = 0$

$\det A^T = \det A$ $\qquad$ $\det((M - \sigma I)^T) = 0$

$\det(M - \sigma I) = 0$

$\Rightarrow$ left e-vals σ are <u>same</u> as right e-vals

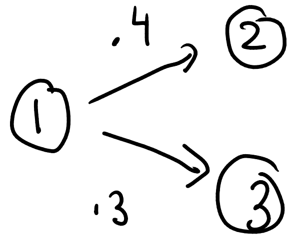
$\Rightarrow$ if we know a left e-val σ exists $\Rightarrow$ there must exist a right e-vec $\vec{v}$ w/ $M\vec{v} = \sigma \vec{v}$

$M = W$ $\Rightarrow$ claim there always exists a left e-vec $\vec{u}^T = (1\ 1\ 1 \dots 1)$ w/ e-val 1

$$(1\ 1\ 1)\begin{pmatrix} .1 & .2 & .1 \\ .3 & .5 & .1 \\ .6 & .3 & .8 \end{pmatrix} = (1\ 1\ 1)$$

$\Rightarrow$ works b/c cols sum to 1

$\Rightarrow$ there exists a right e-vec $\vec{p}^{\,s}$ w/ e-val 1 (not necessarily unique) example:



$$W = \begin{array}{cc} & \begin{array}{ccc} 1 & 2 & 3 \end{array} \ \text{start} \\ \begin{array}{c} 1 \\ 2 \\ 3 \end{array} & \begin{pmatrix} .3 & 0 & 0 \\ .4 & 1 & 0 \\ .3 & 0 & 1 \end{pmatrix} \\ \text{end} & \end{array}$$

$$P_A^S = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad P_B^S = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$P_C^S = \alpha \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + (1-\alpha) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$0 \le \alpha \le 1$$

∞ of possible stationary states