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

$W_{nm}(t_i)$ = prob. to go to state n
if starting in state m
over time step δt at time t_i

Properties of W matrix:

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

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

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

each column sums to 1

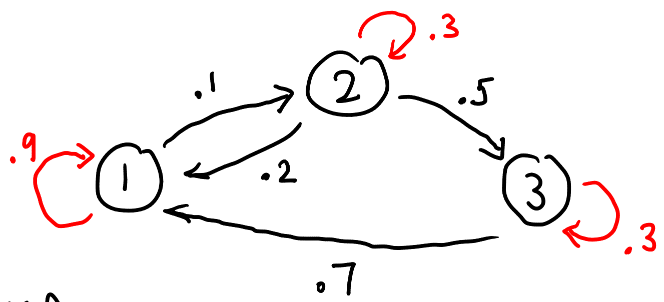
example:

$N=3$

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

every comp. is b/t 0 and 1

graph:



$= W$

time-independ.

note: typically simplify
by not drawing self arrows (red)
but they are implicitly there

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

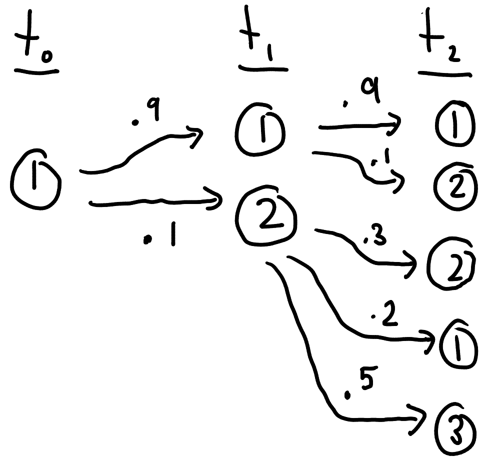
all possible three state trajectories:

in our example

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

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

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



v	prob
1 1 1	.81
1 1 2	.09
1 2 2	.03
1 2 1	.02
1 2 3	.05

sum to 1

$$P(v) = W_{n_2 n_1} W_{n_1 n_0} \cdot p_{n_0}(t_0)$$

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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 equation

generalizations: continuous time (CT) $t_i \to t$

and/or continuous state (CS) $n \to x$ (i.e. position)

	DT	CT
DS	DTDS master equ. / simulate trans. graph	CTDS master equ. / kinetic Monte Carlo (Gillespie)
CS	numerical simulations	Fokker-Planck equ. / Langevin equ.

keep track of states (blue)

keep track of trajectories (red)

Focus initially: DTDS b/c it's easiest to derive proofs initially time-independent environmental 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?

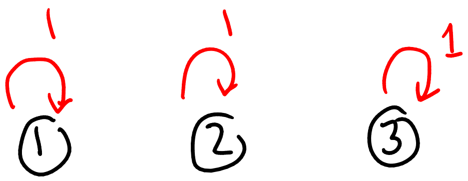
$$W^n \xrightarrow[n\to\infty]{} \text{const. matrix indep. of } n$$

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

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

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

formally: there exists a vector $\vec{p}^{\,s}$ such that $\vec{p}^{\,s} = W \vec{p}^{\,s}$



$\vec{p}^{\,s}$ is called a <u>stationary probability</u>

$\Rightarrow$

1) does it always exist?

2) is it unique?

3) $W^n \vec{p}(t_0)$ is this guaranteed approach $\vec{p}^{\,s}$ as $n \to \infty$?