From discrete to continuum time master equation:

Continuous time (CT) discrete state (DS) master equation will prove a useful mathematical tool.

Starting point: $\vec{p}(t_{i+1}) = W(t_i)\vec{p}(t_i)\,\delta t$

$$p_n(t_{i+1}) = \sum_m W_{nm}(t_i)\, p_m(t_i)\,\delta t$$

$$t_i \to t$$
$$t_{i+1} \to t + \delta t$$

(treat δt as infinitesimal, which is a good approx at timescales $\gg \delta t$)

$$p_n(t+\delta t) = \sum_m W_{nm}(t_{\cancel{i}})\, p_m(t_{\cancel{i}})\,\delta t$$

$$\Rightarrow p_n(t) + \frac{dp_n}{dt}(t)\,\delta t = \sum_m W_{nm}(t)\, p_m(t)\,\delta t$$

$$\frac{dp_n}{dt}\,\delta t = \sum_m W_{nm}(t)\, p_m(t)\,\delta t - \underbrace{\left[\sum_m W_{mn}(t)\,\delta t\right]}_{=1}\, p_n(t)$$

so can insert as trick

divide by δt:

$$\frac{dp_n}{dt} = \sum_m \Big[\overbrace{W_{nm}\,p_m - W_{mn}\,p_n}^{\equiv J_{nm}}\Big]$$

gain of prob. from m — loss of prob to m

for now, specialize to case where $W(t) = W$ is time independent

$\cancel{\equiv \sum_m \Omega}$

continuum time master equ:

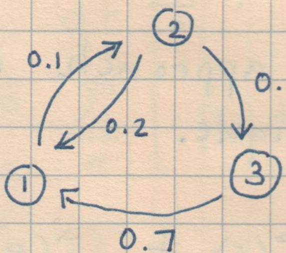
$$\frac{dp_n}{dt} = \sum_m \big[\overbrace{W_{nm}\, p_m - W_{mn}\, p_n}^{J_{nm}}\big]$$

$$= \sum_{m \neq n} \left(W_{nm}\, p_m - W_{mn}\, p_n \right) \quad \text{since } J_{nn} = 0$$

$$= \sum_{m \neq n} W_{nm}\, p_m - p_n \sum_{m' \neq n} W_{m'n} \quad \text{changed } m \to m' \text{ in 2nd sum}$$

define new matrix: $\Omega_{nm} = \begin{cases} W_{nm} & \text{if } n \neq m \\ -\sum_{m' \neq n} W_{m'n} & \text{if } n = m \end{cases}$

then $\dfrac{dp_n}{dt} = \sum_m{}' \, \Omega_{nm}\, p_m \Rightarrow \dfrac{d\vec{p}}{dt} = \Omega \vec{p}$



$\delta t = 1 s^{-1}$

$$W = \begin{pmatrix} 0.9 & 0.2 & 0.7 \\ 0.1 & 0.3 & 0 \\ 0 & 0.5 & 0.3 \end{pmatrix}$$

columns of $W \delta t$ sum to 1

$$\Rightarrow \quad \Omega = \begin{pmatrix} -0.1 & 0.2 & 0.7 \\ 0.1 & -0.7 & 0 \\ 0 & 0.5 & -0.7 \end{pmatrix}$$

columns of Ω sum to zero

$$\Rightarrow \sum_n \Omega_{nm} = 0 \text{ for all } m$$

solution: $\vec{p}(t) = e^{\Omega t}\, \vec{p}(0)$ where

↳ valid when Ω is time-indep.

$$e^{\Omega t} = \mathbb{1} + \Omega t + \frac{t^2}{2!}\Omega^2 + \cdots$$

stat. solution $\vec{p}^s \Rightarrow \quad \frac{d\vec{p}}{dt} = \Omega \vec{p} = 0$

$$\Rightarrow \Omega \vec{p}^s = 0 \quad \text{(right e-vec of } \Omega \text{ w/ e-val } 0\text{)}$$

Imagine we start w/ two diff. initial prob. distributions $\vec{p}(0)$ + $\vec{q}(0)$, leading to two different

solutions: $\quad \vec{p}(t) = e^{\Omega t}\, \vec{p}(0)$

$$\vec{q}(t) = e^{\Omega t}\, \vec{q}(0)$$

For a strongly connected network, we will show that $\vec{p}(t)$ + $\vec{q}(t)$ become the "same" as $t \to \infty$. Since $\vec{p}^s$ exists as a solution, w/

$$\vec{p}^s = e^{\Omega t}\, \vec{p}^s$$

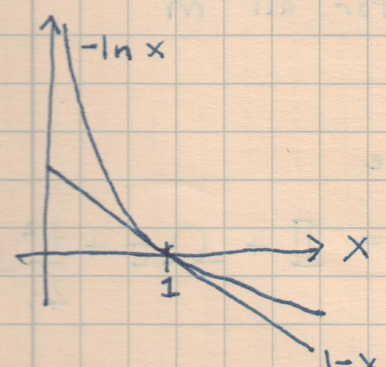
this implies all solutions $\vec{p}(t)$ approach $\vec{p}^s$, as $t \to \infty$. Hence $\vec{p}^s$ must be unique.

First: define "distance" betw. $\vec{p}(t)$ + $\vec{q}(t)$

Kullback-Leibler divergence (KL):

$$D_{KL}(\vec{p} \,||\, \vec{q}) \equiv \sum_n p_n \ln \frac{p_n}{q_n}$$

property: $\quad D_{KL}(\vec{p} \,||\, \vec{q}) = -\sum_n p_n \ln \frac{q_n}{p_n}$



$$\geq \sum_n p_n \left(1 - \frac{q_n}{p_n}\right) \quad \text{since } -\ln x \geq 1-x$$

$$= \sum_n p_n - \sum_n q_n$$

$$= 1 - 1 = 0$$

$$D_{KL}(\vec{p}\,||\,\vec{q}) \geq 0 \quad \text{always}$$
$$= 0 \quad \text{iff} \quad p_n = q_n \text{ for all } n$$
$$(\text{since } -\ln x = 1 - x \text{ iff } x = 0)$$

$\Rightarrow$ thus a valid measure of "distance" betw. $\vec{p}$ + $\vec{q}$, though not a metric

What we will prove: $\frac{d}{dt} D_{KL}(\vec{p}(t)\,||\,\vec{q}(t)) \leq 0$ always

$= 0$ for strongly connected network when $\vec{p}(t) = \vec{q}(t)$

$$\Rightarrow \frac{d}{dt} D_{KL}(\vec{p}(t)\,||\,\vec{q}(t)) \qquad \dot{p}_n \equiv \frac{d}{dt} p_n(t) = \sum_m \Omega_{nm} p_m$$

$$= \frac{d}{dt} \sum_n p_n(t) \ln \frac{p_n(t)}{q_n(t)}$$

$$= \sum_n \left[\dot{p}_n \ln \frac{p_n}{q_n} + p_n \left(\frac{\dot{p}_n}{p_n} - \frac{\dot{q}_n}{q_n} \right) \right]$$

$$= \sum_{n,m} \left[\Omega_{nm} p_m \ln \frac{p_n}{q_n} + p_n \left(\frac{\Omega_{nm} p_m}{p_n} - \frac{\Omega_{nm} q_m}{q_n} \right) \right]$$

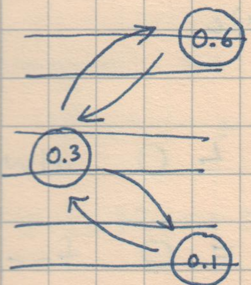
$$= \sum_{n,m} \Omega_{nm} p_m \left(\ln \frac{p_n}{q_n} + 1 - \frac{p_n q_m}{p_m q_m} \right)$$

$$= \sum_{\substack{n,m \\ n \neq m}} \Omega_{nm} p_m \left(\ln \frac{p_n}{q_n} + 1 - \frac{p_n q_m}{p_m q_m} \right) + \sum_m \underbrace{\Omega_{mm}}_{= -\sum_{n\neq m} \Omega_{nm}} p_m \ln \frac{p_m}{q_m}$$

$$= \sum_{\substack{n,m \\ n \neq m}} \underbrace{\Omega_{nm} p_m}_{\geq 0} \underbrace{\left(\ln \frac{p_n q_m}{q_n p_m} + 1 - \frac{p_n q_m}{q_n p_m} \right)}_{\substack{= 1 - x - (-\ln x) \\ \leq 0}} \quad \text{where } x = \frac{p_n q_m}{q_n p_m}$$

Hence $\frac{d}{dt} D_{KL}(\vec{p}(t) \| \vec{q}(t)) \leq 0$

Equality to zero $\Rightarrow$ requires $x = \frac{p_n q_m}{q_n p_m} = 1$



for every pair (n, m)
connected by arrows
(where $\Omega_{nm} \neq 0$)

$\Rightarrow \frac{p_n}{p_m} = \frac{q_n}{q_m}$ for every connected (n,m)

since network is strongly connected

Since both $\vec{p}$ + $\vec{q}$ sum to 1, the only way this is possible is if $\vec{p} = \vec{q}$.

Summary : $D_{KL}(\vec{p}(t) \| \vec{q}(t)) \geq 0$
$= 0$ iff $\vec{p}(t) = \vec{q}(t)$

$\frac{d}{dt} D_{KL}(\vec{p}(t) \| \vec{q}(t)) \leq 0$
(*) for ergodic network: $= 0$ iff $\vec{p}(t) = \vec{q}(t)$

If two stat. states existed, $\vec{p}(t) = \vec{p}^{\,s}_A$, $\vec{q}(t) = \vec{p}^{\,s}_B$
with $\vec{p}^{\,s}_A \neq \vec{p}^{\,s}_B \Rightarrow D_{KL}(\vec{p}^{\,s}_A \| \vec{p}^{\,s}_B) > 0$

$\frac{d}{dt} D_{KL}(\vec{p}^{\,s}_A \| \vec{p}^{\,s}_B) = 0$

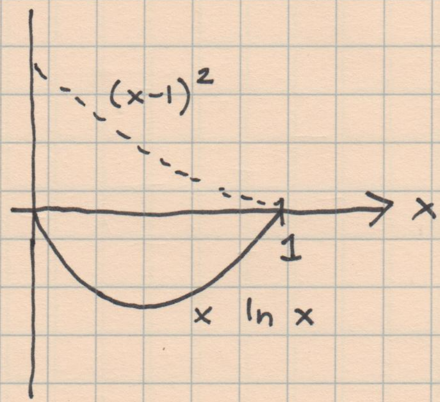
contradicts (*) above
$\Rightarrow$ cannot be ergodic netw.

Hence ergodic netw (strongly connected) must have <u>unique</u> stat. state.

Can readily generalize this theorem beyond KL divergence. Define <u>f-divergence</u>

$$D_f(\vec{p} \,\|\, \vec{q}) \equiv \sum_n q_n f\left(\frac{p_n}{q_n}\right)$$

f is any function which is convex $[f''(x) > 0]$ and $f(1) = 0$



examples:

$f(x) = x \ln x$: KL diverg.

$f(x) = (x-1)^2$: χ^2- diverg.

$f(x) = (\sqrt{x}-1)^2$: Hellinger div.

$$D_f(\vec{p} \,\|\, \vec{q}) = \begin{cases} 0 & \text{iff } \vec{p} = \vec{q} \\ >0 & \text{if } \vec{p} \neq \vec{q} \end{cases}$$

can prove: $\frac{d}{dt} D_f(\vec{p}(t) \,\|\, \vec{p}^s) \leq 0$ for ergodic Markovian net

$= 0$ iff $\vec{p}(t) = \vec{p}^s$

converges to stat. state