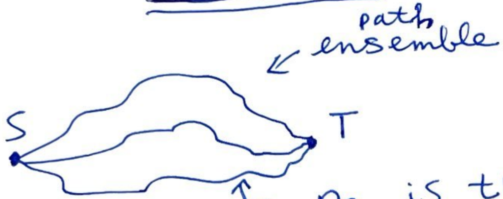
Max Cal



c, p_c is the path prob.

path entropy: $H(\{p_c\}) = -\sum_c p_c \log p_c$

Constraints: $F_j^{\alpha}(\{p_c\}) = 0$

enumerates constraints: $\alpha = 1, \ldots, N_c$

$\downarrow$ narrow to linear constraints

$$\underbrace{\sum_c A_c^{\alpha} p_c}_{\text{average over all paths}} = \bar{A}^{\alpha}, \text{ including } \sum_c p_c = 1$$

Max Cal: maximize H subject to constraints:

$$p_c = \frac{e^{\sum_{\alpha=1}^{N_c} \lambda_\alpha A_c^\alpha}}{\underbrace{\sum_c e^{\sum_\alpha \lambda_\alpha A_c^\alpha}}_{Q(\{\lambda\})}}$$

λ_α – Lagrange multipliers

$Q(\{\lambda\})$ – dynamical part'n f'n

not approx., non-equil., but hard to implement with continuous states (easy with discrete states)

Filyukov & Karpov (1967, 1968)

Discrete time steps: T steps, a path is $\{i_0, \ldots, i_T\}$, where i_x is the system state at time x. $p_c \to p_{i_0 \ldots i_T}$

So, $H(T) = -\sum_{i_0 \ldots i_T} p_{i_0 \ldots i_T} \log p_{i_0 \ldots i_T}$

If we have a 1st order Markov process,

$$p_c = p_{i_0} \underbrace{p_{i_0 \to i_1}}_{\text{transition prob.}} p_{i_1 \to i_2} \dots p_{i_{T-1} \to i_T}$$

Then $H(T) = -\sum_{\{i_0 \dots i_T\}} p_{i_0} p_{i_0 \to i_1} \dots p_{i_{T-1} \to i_T} \times$

$$\times \log(p_{i_0} p_{i_0 \to i_1} \dots) =$$

$$= -\sum_{\{i_0 \dots i_T\}} p_{i_0} \dots p_{i_{T-1} \to i_T} \left\{ \log p_{i_0} + \log p_{i_0 \to i_1} + \dots \right\}$$

Now focus on SS : $\underbrace{\sum_j p_{i \to j} = 1}_{\text{"always jumps"}}$ (1)

$$\sum_i p_i p_{i \to j} = p_j \quad (2)$$

$$\sum_i p_i p_{i \to j} = \sum_i p_j p_{j \to i} = p_j \underbrace{\sum_i p_{j \to i}}_{=1} \Leftarrow \text{"flux in = = flux out"}$$

Detailed balance: $p_i p_{i \to j} = p_j p_{j \to i}$

Then 1st term: $-\sum_{i_0} p_{i_0} \log p_{i_0} \underbrace{\left(\sum_{i_1} p_{i_0 \to i_1} \right)}_{1} \underbrace{(\dots)}_{1} \dots =$

$$= -\sum_i p_i \log p_i$$

2nd term:

$$-\sum_{i_0, i_1} p_{i_0} p_{i_0 \to i_1} \log p_{i_0 \to i_1} \left(\sum_{i_2} p_{i_1 \to i_2} \right) \dots =$$

$$= -\sum_{i,j} p_i p_{i \to j} \log p_{i \to j} .$$

all other terms will be like that too...

So, $$H(T) = \underbrace{-\sum_i p_i \log p_i}_{\text{entropy of the initial state}} \underbrace{- T \sum_{i,j} p_i\, p_{i\to j} \log p_{i\to j}}_{H_1\text{, path entropy per step}}$$

Large T: $H(T) \simeq T H_1$

Compare with 0th order Markov chain:

$$H(T) = -(T+1) \sum_i p_i \log p_i$$

So, we assumed 1st order Markov chain →
→ obtained $H(T)$. Can we go backwards?
Data → Markovian (or not)

Start with $H(T) = -\sum_{i_0 \ldots i_T} p_{i_0\ldots i_T} \log p_{i_0 \ldots i_T}$ again,
impose pairwise constraints for each step $n \to m$:

$$\langle N_{n\to m} \rangle = \sum_{i_0 \ldots i_T} p_{i_0 \ldots i_T} \underbrace{N_{m\to n}(i_0 \ldots i_T)}_{\sum_{k=0}^{T-1} \delta_{i_k, m}\, \delta_{i_{k+1}, n} \text{ is the \# } m\to n \text{ transitions}}$$

Indeed, $\sum_{m,n} N_{m\to n} = T$ as expected

Maximize $H(T)$:

$$p_{i_0 \ldots i_T} \sim e^{-\underbrace{\sum_{m,n} \lambda_{mn} N_{m\to n}}_{= \sum_{m,n} \sum_{k=0}^{T-1} \lambda_{mn}\, \delta_{i_k, m}\, \delta_{i_{k+1}, n} = \sum_{k=0}^{T-1} \lambda_{i_k, i_{k+1}}}} = \prod_{k=0}^{T-1} p_{i_k \to i_{k+1}},$$

where
$$p_{i_k \to i_{k+1}} \sim e^{-\lambda_{i_k i_{k+1}}}$$

1st order Markov process

Finally,

$$Q(T) = \sum_{i_0 \dots i_T} e^{-\sum_{k=0}^{T-1} \lambda_{i_k i_{k+1}}}$$

Note that $\langle N_{m\to n}(i_0 \dots i_T)\rangle = -\frac{\partial}{\partial \lambda_{mn}} \log Q(T)$ etc.

Consider both singlet & pairwise constraints:

$$p_{i_0 \dots i_T} \sim e^{-\sum_m \alpha_m \sum_{k=0}^{T} \delta_{i_k, m} - \sum_{m,n} \lambda_{mn} \sum_{k=0}^{T-1} \delta_{i_k, m} \delta_{i_{k+1}, n}}$$

"constraints on energy" "constraints on flux"

Higher-order constraints may be added...

$$Q(T; \{\alpha_m\}, \{\lambda_{nm}\}) = \sum_{i_0 \dots i_T} e^{-\sum_m \alpha_m \dots - \sum_{m,n} \lambda_{mn} \dots} =$$

$$= \sum_{i_0 \dots i_T} e^{-\sum_m \alpha_m \underbrace{N_m(i_0 \dots i_T)}_{\text{total \# of "dwells" in state } m \text{ over } T} - \sum_{m,n} \lambda_{mn} N_{m\to n}(i_0 \dots i_T)}.$$

Q can be found using transfer matrices:

$$Q(T; \{\alpha_m\}, \{\lambda_{nm}\}) = v^+ G^T v$$

$$v_i = e^{-\frac{\alpha_i}{2}} \qquad G_{ij} = e^{-\frac{\alpha_i + \alpha_j}{2} - \lambda_{ij}}$$

Indeed, $Q(T; \{\alpha_m\}, \{\lambda_{nm}\}) = \sum_{i_0 \dots i_T} e^{-\sum_{k=0}^{T} \alpha_{i_k} - \sum_{k=0}^{T-1} \lambda_{i_k, i_{k+1}}}$

Two-state example $e^{-\alpha_1}+e^{-\alpha_2}$

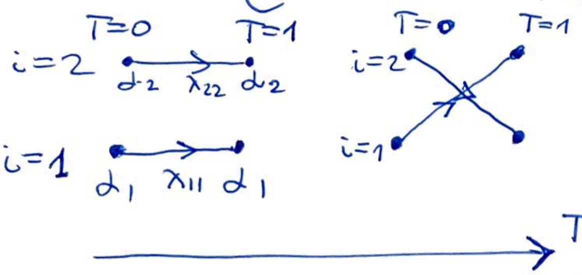
$T=0$: $\overline{v_1 v_2}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} =$ as expected

$$T=1:\quad \overline{v_1 v_2}\begin{pmatrix} e^{-\alpha_1-\lambda_{11}} & e^{-\frac{\alpha_1+\alpha_2}{2}-\lambda_{12}} \\ e^{-\frac{\alpha_1+\alpha_2}{2}-\lambda_{21}} & e^{-\alpha_2-\lambda_{22}} \end{pmatrix}\begin{pmatrix} e^{-\frac{\alpha_1}{2}} \\ e^{-\frac{\alpha_2}{2}} \end{pmatrix} =$$

$$= \overline{e^{-\frac{\alpha_1}{2}}e^{-\frac{\alpha_2}{2}}}\begin{pmatrix} e^{-\frac{3}{2}\alpha_1-\lambda_{11}} + e^{-\frac{\alpha_1}{2}-\alpha_2-\lambda_{12}} \\ e^{-\alpha_1-\frac{\alpha_2}{2}-\lambda_{21}} + e^{-\frac{3}{2}\alpha_2-\lambda_{22}} \end{pmatrix} =$$

$$= e^{-2\alpha_1-\lambda_{11}} + e^{-\alpha_1-\alpha_2-\lambda_{12}} +$$

$$+ e^{-\alpha_1-\alpha_2-\lambda_{21}} + e^{-2\alpha_2-\lambda_{22}}$$



Specify an initial condition:

$$Q(T; \{\alpha_m\}, \{\lambda_{nm}\}) = a^{+} G^{T} \cdot v$$

Final cond'n:

$$Q = v^{+} \cdot G^{T} \cdot b$$

Note that

$$\begin{cases} \langle N_m^k(i_0 \dots i_T)\rangle_c = (-1)^k \dfrac{\partial^k}{\partial \alpha_m^k} \log Q \\ \langle N_{m\to n}^k(i_0 \dots i_T)\rangle_c = (-1)^k \dfrac{\partial^k}{\partial \lambda_{nm}^k} \log Q \end{cases}$$

$T \to \infty$: expect only first-order constraints to contribute (such as $\langle J \rangle$, the average flux)

[Master eq'n can be obtained from Max Cal:]

In general, both $p_{i_k \to i_{k+1}}$ & p_{i_k} are time-dependent. Consider the case when transition probs are t-indep., but single-state probs are time-dep.

Start with

$$p_{i_0 \dots i_T} = \frac{\vartheta(i_0) G(i_0, i_1) \dots G(i_{T-1}, i_T) \vartheta(i_T)}{\underbrace{\vartheta^+ G^T \vartheta}_{Q}}$$

Then

$$p(a_1 \dots a_m; t) = \sum_{i_0 \dots i_{t-m};\, i_{t+1} \dots i_T} p(i_0, i_1 \dots i_{t-m}, \overbrace{a_1 \dots a_m}^{m \text{ consecutive points}}, i_{t+1} \dots i_T) =$$

$$= \frac{[\vartheta^+ G^{t-m}](a_1) \overbrace{G(a_1, a_2) \dots G(a_{m-1}, m)}^{m-1 \text{ factors}} [G^{T-t+1} \vartheta](a_m)}{\vartheta^+ G^T \vartheta}$$

Note that

$$p(a_1 \dots a_m; t)\, p(a_1 \dots a_m \to a_{m+1}; t) =$$
$$= p(a_1 \dots a_{m+1}; t+1)$$

Then $p(a_1 \dots a_m \to a_{m+1}; t) =$

$$= \frac{[\vartheta^+ G^{t-m}](a_1) G(a_1, a_2) \dots G(a_m, a_{m+1}) [G^{T-t} \vartheta](a_{m+1})}{[\vartheta^+ G^{t-m}](a_1) G(a_1, a_2) \dots G(a_{m-1}, a_m) [G^{T-t+1} \vartheta](a_m)} =$$

$$= \frac{G(a_m, a_{m+1}) [G^{T-t} \vartheta](a_{m+1})}{[G^{T-t+1} \vartheta(a_m)]} \equiv p(a_m \to a_{m+1}; t)$$

1st order Markov process

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Finally, note that

1) $\langle y | G = r \langle y | r$, $y_i > 0 \;\; \forall i$

$r > 0$ is the largest eigenvalue

2) $G | z \rangle = r | z \rangle$, $z_i > 0 \;\; \forall i$

3) Then $\langle y | G | z \rangle = r \langle y | z \rangle = r y^+ z$,

$\langle y | G^2 | z \rangle = r^2 \langle y | z \rangle = r^2 y^+ z$, etc.

In general, $\lim_{T\to\infty} \frac{G^T}{r^T} = z y^+$

Then
$$\begin{cases} \lim_{T\to\infty} \dfrac{G^T \vartheta}{r^T} = \underbrace{z}_{\text{vector}} \underbrace{(y^+ \vartheta)}_{\#} \\ \\ \lim_{T\to\infty} \dfrac{\vartheta^+ G^T}{r^T} = \underbrace{(\vartheta^+ z)}_{\#} \underbrace{y^+}_{\substack{\text{vector}\\ \text{transpose}}} \end{cases}$$

So, as $T \to \infty$, $p(a \to b) = \dfrac{G(a,b) \, \cancel{(y^+\vartheta)} \, z(b) \, r^T}{\cancel{(y^+\vartheta)} \, z(a) \, r^{T+1}} =$

$$= \frac{G(a,b) \, z(b)}{r \, z(a)} \quad \text{time-indep.}$$

However,

$$p(a;t) = \frac{[\vartheta^+ G^{t-1}](a) \, [G^{T-t+1} \vartheta](a)}{\vartheta^+ G^T \vartheta} =$$

$$= \frac{[\vartheta^+ G^{t-1}](a) * z(a) \, \cancel{(y^+\vartheta)} \, r^{T-t+1}}{(\vartheta^+ z) \, r^T \, \cancel{(y^+\vartheta)}} =$$

$$= \frac{[\vartheta^+ G^{t-1}](a) \, z(a)}{(\vartheta^+ z) \, r^{t-1}} \quad \text{time-dependent}$$

Note that

$$\sum_b p(b;t)\,p(b\to a) = \sum_b \frac{[v^+ G^{t-1}](b)\,\cancel{z(b)}}{(v^+ z)\, r^{t-1}}\;\frac{G(b,a)\,z(a)}{r\,\cancel{z(b)}} =$$

$$= \frac{z(a)}{r^t\,(v^+ z)} \underbrace{\sum_b [v^+ G^{t-1}](b)\; G(b,a)}_{[v^+ G^t](a)} = p(a;t+1)$$

Then $p(a;t+1) - p(a;t) = \sum_b p(b;t)\,p(b\to a) - p(a;t) =$

$$= \sum_b \Big[p(b;t)\,p(b\to a) - p(a;t)\,p(a\to b) \Big]$$

$\sum_b p(a\to b) = 1$

Cont. limit:

$$\frac{p(a;t+\Delta t) - p(a;t)}{\Delta t} = \sum_b \Big[p(b;t) \underbrace{\frac{p(b\to a)}{\Delta t}}_{k_{b\to a}} - p(a;t) \underbrace{\frac{p(a\to b)}{\Delta t}}_{k_{a\to b}} \Big],$$

$$\dot p(a;t) = \sum_b \Big[p(b;t)\,k_{b\to a} - p(a;t)\,k_{a\to b} \Big]$$