

# Area maximisation

Subhaneil Lahiri

December 13, 2011

## Abstract

We extremise the area under the synaptic memory curve

It will be convenient for us to define the diagonal elements of  $\mathbf{T}$  to be zero (it is conventional to define them to be the recurrence times,  $\mathbf{T}_{ii} = 1/\mathbf{p}_i^\infty$ , but that would lead to a lot of extra  $\delta_{ik}$ 's for us). Similarly, we define  $N_{ij}^k = 0$  if  $i = k$  or  $j = k$ .

## 1 Mixing times

Define

$$\eta_i^\pm \equiv \sum_k \mathbf{T}_{ik} \mathbf{p}_k^\infty \left( \frac{1 \pm \mathbf{w}_k}{2} \right). \quad (1) \quad \text{eq:mixingpm}$$

It can be shown that [1]<sup>1</sup>

$$\eta_i^+ + \eta_i^- = \eta \quad (\text{independent of } i). \quad (2) \quad \text{eq:mixing}$$

It would be nice if we could prove (at least for the maximal area) that

$$\mathbf{w}_i = +1 \quad \text{and} \quad \mathbf{w}_j = -1 \quad \implies \quad \eta_i^+ < \eta_j^+ \quad \iff \quad \eta_i^- > \eta_j^- \quad (3) \quad \text{eq:orderingh}$$

then we could use these quantities to order the states.

The area under the memory curve is given by

$$\begin{aligned} A &= \sqrt{N}(4f^+f^-) \sum_{i \neq j} q_{ij} \mathbf{p}_i^\infty (\eta_i^+ - \eta_j^+) = -\sqrt{N}(4f^+f^-) \sum_{i,j} q_{ij} \mathbf{p}_i^\infty \eta_j^+ \\ &= \sqrt{N}(4f^+f^-) \sum_{i \neq j} q_{ij} \mathbf{p}_i^\infty (\eta_j^- - \eta_i^-) = \sqrt{N}(4f^+f^-) \sum_{i,j} q_{ij} \mathbf{p}_i^\infty \eta_j^-. \end{aligned} \quad (4) \quad \text{eq:areamixin}$$

---

<sup>1</sup>Not that their  $\eta$  is equal to our  $\eta + 1$  due to the difference in diagonal elements of  $\mathbf{T}$ .

## 2 Shifting $q_{ij}$

sec:shiftq

Consider the following change

$$\mathbf{M}_{ij}^+ \rightarrow \mathbf{M}_{ij}^+ + f^- \epsilon_{ij}, \quad \mathbf{M}_{ij}^- \rightarrow \mathbf{M}_{ij}^- - f^+ \epsilon_{ij}, \quad \sum_j \epsilon_{ij} = 0. \quad (5) \quad \text{eq:shiftq}$$

This leaves  $\mathbf{M}$  unchanged, and therefore  $\mathbf{p}^\infty$ ,  $\mathbf{T}$ ,  $\eta$ ,  $N_{ik}^j$  and  $H_{ik}^j$  as well. This means

$$A \rightarrow A + \sqrt{N}(4f^+ f^-) \sum_{i \neq j} \epsilon_{ij} \mathbf{p}_i^\infty (\eta_i^+ - \eta_j^+). \quad (6) \quad \text{eq:shiftqare}$$

Suppose  $\eta_i^+ > \eta_j^+$ . We can increase  $A$  by making  $\epsilon_{ij} > 0$ . The only thing that could stop us is if  $\mathbf{M}_{ij}^-$  or  $\mathbf{M}_{ii}^+$  hits zero (which also takes care of the possibility that  $\mathbf{M}_{ij}^+$  hits unity). Similar considerations for  $\eta_i^+ < \eta_j^+$  imply that at the maximum:

$$\begin{aligned} \eta_i^+ > \eta_j^+ &\implies \mathbf{M}_{ij}^- = 0 \quad \text{or} \quad \mathbf{M}_{ii}^+ = 0, \\ \eta_i^+ < \eta_j^+ &\implies \mathbf{M}_{ij}^+ = 0 \quad \text{or} \quad \mathbf{M}_{ii}^- = 0. \end{aligned} \quad (7) \quad \text{eq:shiftqmax}$$

If  $\eta_i^+ = \eta_j^+$ ,  $\epsilon_{ij}$  is a null direction, so we can impose either of the two conditions if we wish. If it weren't for the second possibility in each case, this would imply an upper/lower triangular structure for  $\mathbf{M}^\pm$ .

If we have a trio  $\eta_i^+ > \eta_j^+ > \eta_k^+$ , two of the transitions can help each other: decreasing  $\mathbf{M}_{jk}^-$  increases  $\mathbf{M}_{jj}^-$ , which allows us to further decrease  $\mathbf{M}_{ji}^+$ . Decreasing  $\mathbf{M}_{ji}^+$  increases  $\mathbf{M}_{jj}^+$ , which allows us to further decrease  $\mathbf{M}_{jk}^-$ . Successful triangulation requires:

$$\begin{aligned} \sum_{\{i|\eta_i^+ > \eta_j^+\}} \mathbf{M}_{ji}^+ &\leq \mathbf{M}_{jj}^- + \sum_{\{i|\eta_i^+ < \eta_j^+\}} \mathbf{M}_{ji}^- &\implies \sum_{\{i|\eta_i^+ > \eta_j^+\}} (\mathbf{M}_{ji}^+ + \mathbf{M}_{ji}^-) &\leq 1, \\ \sum_{\{i|\eta_i^+ < \eta_j^+\}} \mathbf{M}_{ji}^- &\leq \mathbf{M}_{jj}^+ + \sum_{\{i|\eta_i^+ > \eta_j^+\}} \mathbf{M}_{ji}^+ &\implies \sum_{\{i|\eta_i^+ < \eta_j^+\}} (\mathbf{M}_{ji}^+ + \mathbf{M}_{ji}^-) &\leq 1. \end{aligned} \quad (8) \quad \text{eq:triangles}$$

The two left-hand-sides of the final inequalities sum to  $(2 - \mathbf{M}_{jj}^+ - \mathbf{M}_{jj}^-)$ , so they are not quite inconsistent.

## 3 Generalised fundamental matrix

undamental

Define the generalised fundamental matrix as

$$\mathbf{Z} = (\mathbf{I} - \mathbf{M} + \mathbf{c}\boldsymbol{\pi})^{-1}, \quad (9) \quad \text{eq:funddef}$$

where  $\mathbf{c}$  is a row vector of 1's and  $\boldsymbol{\pi}$  is any row vector such that  $\boldsymbol{\pi}\mathbf{c} = 1$ . The usual fundamental matrix has  $\boldsymbol{\pi} = \mathbf{p}^\infty$  [2, §3.2], but it is more convenient to let it be independent of  $\mathbf{M}$  [2, App.VIII], e.g.  $\boldsymbol{\pi} = \mathbf{c}^\text{T}/n$ .

Then we have

$$\begin{aligned}
\mathbf{p}^\infty &= \boldsymbol{\pi} \mathbf{Z}, \\
\mathbf{Z} \mathbf{c} &= \mathbf{c}, \\
\mathbf{T}_{ij} &= \frac{\mathbf{Z}_{jj} - \mathbf{Z}_{ij}}{\mathbf{p}_j^\infty}, \\
\eta_i^+ - \eta_j^+ &= \frac{1}{2} \sum_k (\mathbf{Z}_{jk} - \mathbf{Z}_{ik}) \mathbf{w}_k.
\end{aligned} \tag{10} \quad \text{eq:fromfund}$$

This allows us to write the area as

$$A = \sqrt{N} (2f^+ f^-) \sum_{ijkl} q_{ij} \boldsymbol{\pi}_l \mathbf{Z}_{li} (\mathbf{Z}_{jk} - \mathbf{Z}_{ik}) \mathbf{w}_k. \tag{11} \quad \text{eq:arefund}$$

## 4 Derivatives wrt. $\mathbf{M}_{ij}^\pm$

sec:derivs

We will regard the off-diagonal elements of  $\mathbf{M}_{ij}^\pm$  to be the independent variables, with  $\mathbf{M}_{ii}^\pm = 1 - \sum_{j \neq i} M_{ij}^\pm$ . Thus,

$$\frac{\partial \mathbf{M}_{ij}}{\partial \mathbf{M}_{gh}^\pm} = f^\pm \delta_{gi} (\delta_{hj} - \delta_{ij}), \quad \frac{\partial q_{ij}}{\partial \mathbf{M}_{gh}^\pm} = \pm \delta_{gi} (\delta_{hj} - \delta_{ij}). \tag{12} \quad \text{eq:basicderi}$$

The implicit  $g \neq h$  that comes with all derivatives is unnecessary, as the derivatives above vanish when  $g = h$ .

Differentiating (9),

$$\frac{\partial \mathbf{Z}_{ij}}{\partial \mathbf{M}_{gh}} = \mathbf{Z}_{ig} (\mathbf{Z}_{hj} - \mathbf{Z}_{gj}). \tag{13} \quad \text{eq:fundderiv}$$

From [3], we have

$$\frac{\partial \mathbf{p}_k^\infty}{\partial \mathbf{M}_{gh}} = \mathbf{p}_k^\infty \mathbf{p}_g^\infty (\mathbf{T}_{gk} - \mathbf{T}_{hk}). \tag{14} \quad \text{eq:pderiv}$$

We can write [4]

$$\mathbf{M}_{ij}^{(k)} = (1 - \delta_{ik})(1 - \delta_{jk}) \mathbf{M}_{ij}, \quad N_{ij}^k = (1 - \delta_{jk})(I - \mathbf{M}^{(k)})_{ij}^{-1}, \quad \mathbf{T}_{ik} = \sum_j N_{ij}^k, \tag{15} \quad \text{eq:NTexpr}$$

with  $i, j \neq k$ . Differentiating,

$$\begin{aligned}
\frac{\partial N_{ij}^k}{\partial \mathbf{M}_{gh}} &= -N_{ig}^k [N_{gj}^k - N_{hj}^k], \\
\frac{\partial \mathbf{T}_{ik}}{\partial \mathbf{M}_{gh}} &= -N_{ig}^k [\mathbf{T}_{gk} - \mathbf{T}_{hk}],
\end{aligned} \tag{16} \quad \text{eq:NTderiv}$$

again with  $i, j \neq k$ .

## 5 Kuhn-Tucker conditions

Consider the Lagrangian

$$\mathcal{L} = \frac{A}{\sqrt{N}(2f^+f^-)} + \sum_{\pm} \sum_{ij} \mu_{ij}^{\pm} \mathbf{M}_{ij}^{\pm}. \quad (17) \quad \text{eq:lagrangian}$$

Necessary conditions for an extremum are

$$\frac{\partial \mathcal{L}}{\partial \mathbf{M}_{gh}^{\pm}} = 0, \quad \mu_{ij}^{\pm} \geq 0, \quad \mathbf{M}_{ij}^{\pm} \geq 0, \quad \mu_{ij}^{\pm} \mathbf{M}_{ij}^{\pm} = 0. \quad (18) \quad \text{eq:extremum}$$

with  $g \neq h$ . We will make statements of the following form repeatedly:

$$A < B \quad \implies \quad A < 0 \quad \text{or} \quad B > 0. \quad (19) \quad \text{eq:ineqstate}$$

Let  $\lambda_{ij}^{\pm} = \mu_{ij}^{\pm} - \mu_{ii}^{\pm}$ . Together with the bounds (18), applying (19) leads to

$$\begin{aligned} \lambda_{ij}^{\pm} > 0 &\implies \mu_{ij}^{\pm} > 0 \implies \mathbf{M}_{ij}^{\pm} = 0, \\ \lambda_{ij}^{\pm} < 0 &\implies \mu_{ii}^{\pm} > 0 \implies \mathbf{M}_{ii}^{\pm} = 0. \end{aligned} \quad (20) \quad \text{eq:lambdaineq}$$

Suppose  $\mathbf{M}_{ii}^+ = 0$ , then for some  $j$ ,  $\mathbf{M}_{ij}^+ \neq 0$  and that  $\lambda_{ij}^+ < 0$ . We can see that

$$\mathbf{M}_{ii}^{\pm} = 0 \quad \iff \quad \min_j \lambda_{ij}^{\pm} < 0. \quad (21) \quad \text{eq:lambdaia}$$

Using the formulae of §4,

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{M}_{gh}^{\pm}} &= \lambda_{gh}^{\pm} \pm \sum_k \mathbf{p}_g^{\infty} \mathbf{p}_k^{\infty} \mathbf{w}_k (\mathbf{T}_{gk} - \mathbf{T}_{hk}) \\ &\quad + f^{\pm} \sum_k \sum_{i \neq j} q_{ij} \mathbf{p}_i^{\infty} \mathbf{p}_k^{\infty} \mathbf{w}_k \mathbf{p}_g^{\infty} (\mathbf{T}_{ik} - \mathbf{T}_{jk}) (\mathbf{T}_{gi} - \mathbf{T}_{hi} + \mathbf{T}_{gk} - \mathbf{T}_{hk}) \\ &\quad - f^{\pm} \sum_k \sum_{i \neq j} q_{ij} \mathbf{p}_i^{\infty} \mathbf{p}_k^{\infty} \mathbf{w}_k (N_{ig}^k - N_{jg}^k) (\mathbf{T}_{gk} - \mathbf{T}_{hk}) \\ &= \lambda_{gh}^{\pm} \pm \sum_{kl} \mathbf{w}_k \boldsymbol{\pi}_l \mathbf{Z}_{lg} (\mathbf{Z}_{hk} - \mathbf{Z}_{gk}) \\ &\quad + f^{\pm} \sum_{ijkl} q_{ij} \mathbf{w}_k \boldsymbol{\pi}_l [\mathbf{Z}_{lg} (\mathbf{Z}_{hi} - \mathbf{Z}_{gi}) (\mathbf{Z}_{jk} - \mathbf{Z}_{ik}) + \mathbf{Z}_{li} (\mathbf{Z}_{jg} - \mathbf{Z}_{ig}) (\mathbf{Z}_{hk} - \mathbf{Z}_{gk})] \\ &= \lambda_{gh}^{\pm} \pm 2 \mathbf{p}_g^{\infty} (\eta_g^+ - \eta_h^+) \\ &\quad + 2 f^{\pm} \sum_{ij} q_{ij} \mathbf{p}_i^{\infty} \mathbf{p}_g^{\infty} [(\mathbf{T}_{gi} - \mathbf{T}_{hi}) (\eta_i^+ - \eta_j^+) + (\mathbf{T}_{ig} - \mathbf{T}_{jg}) (\eta_g^+ - \eta_h^+)] \\ &= 0. \end{aligned} \quad (22) \quad \text{eq:lagrange}$$

Consider

$$f^- \frac{\partial \mathcal{L}}{\partial \mathbf{M}_{gh}^+} - f^+ \frac{\partial \mathcal{L}}{\partial \mathbf{M}_{gh}^-} = (f^- \lambda_{gh}^+ - f^+ \lambda_{gh}^-) + 2\mathbf{p}_g^\infty (\eta_g^+ - \eta_h^+) = 0, \quad (23) \quad \text{eq:derivsshi}$$

which corresponds to the shift considered in §2. We can see that

$$\begin{aligned} \eta_g^+ > \eta_h^+ &\implies f^+ \lambda_{gh}^- > f^- \lambda_{gh}^+ \implies \lambda_{gh}^- > 0 \quad \text{or} \quad \lambda_{gh}^+ < 0 \\ &\implies \mathbf{M}_{gh}^- = 0 \quad \text{or} \quad \mathbf{M}_{gg}^+ = 0, \\ \eta_g^+ < \eta_h^+ &\implies f^- \lambda_{gh}^+ > f^+ \lambda_{gh}^- \implies \lambda_{gh}^+ > 0 \quad \text{or} \quad \lambda_{gh}^- < 0 \\ &\implies \mathbf{M}_{gh}^+ = 0 \quad \text{or} \quad \mathbf{M}_{gg}^- = 0, \end{aligned} \quad (24) \quad \text{eq:etalambda}$$

which we've already seen in §2.

Consider

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{M}_{gh}^+} + \frac{\partial \mathcal{L}}{\partial \mathbf{M}_{gh}^-} &= (\lambda_{gh}^+ + \lambda_{gh}^-) + 2 \sum_{ij} q_{ij} \mathbf{p}_i^\infty \mathbf{p}_j^\infty [(\mathbf{T}_{gi} - \mathbf{T}_{hi})(\eta_i^+ - \eta_j^+) + (\mathbf{T}_{ig} - \mathbf{T}_{jg})(\eta_g^+ - \eta_h^+)] \\ &= 0. \end{aligned} \quad (25) \quad \text{eq:derivsove}$$

If we could argue that  $\lambda_{gh}^+ + \lambda_{gh}^- > 0$ , this would imply that  $\mathbf{M}_{gh}^+ \mathbf{M}_{gh}^- = 0$ .

## References

- [1] J. Hunter, “Mixing times with applications to perturbed Markov chains,” *Linear algebra and its applications* **417** (2006) no. 1, 108–123. 2006mixing
- [2] J. Kemeny and J. Snell, *Finite markov chains*. Springer, 1960. 1960finite
- [3] G. Cho and C. Meyer, “Markov chain sensitivity measured by mean first passage times,” *Linear Algebra and its Applications* **316** (2000) no. 1-3, 21–28. [http://meyer.math.ncsu.edu/Meyer/PS\\_Files/SensitivityByMFP.pdf](http://meyer.math.ncsu.edu/Meyer/PS_Files/SensitivityByMFP.pdf). 2000markov
- [4] C. Grinstead and J. Snell, *Introduction to probability*. Amer Mathematical Society, 1997. <http://math.dartmouth.edu/~prob/prob/prob.pdf>. troduction