Area maximisation in continuous time

Subhaneil Lahiri

November 8, 2013

Abstract

We try to find the continuous time Markov process that has the maximal area under the signal-to-noise curve.

Contents

1 Continuous time Markov processes

ContMarkov

In this section we'll provide a summary of all the relevant properties of ergodic Markov chains in continuous time. It is a straightforward generalisation of material that can be found in [1] with some ideas from [2].

1.1 Notation

sec:not

For any matrix $\mathbf{A}$, we define matrices $\mathbf{A}^{\mathrm{dg}}$ and $\overline{\mathbf{A}}$ as

$$\mathbf{A}^{\mathrm{dg}}_{ij} \equiv \delta_{ij}\mathbf{A}_{ij}, \qquad \overline{\mathbf{A}} \equiv \mathbf{A} - \mathbf{A}^{\mathrm{dg}}. \tag{1}$$ eq:dgdef

We let $\mathbf{e}$ denote a column-vector of ones and $\mathbf{E} = \mathbf{e}\mathbf{e}^{\mathrm{T}}$ denote a matrix of ones.

A Markov process is described by a matrix of transitions rates, $\mathbf{Q}_{ij}$, from state i to j. The probabilities of being in each state at time t, the row-vector $\mathbf{p}(t)$, evolve according to

$$\frac{\mathrm{d}\mathbf{p}(t)}{\mathrm{d}t} = \mathbf{p}(t)\mathbf{Q}, \qquad \mathbf{p}(t)\mathbf{e} = 1, \qquad \mathbf{Q}\mathbf{e} = 0. \tag{2}$$ eq:rowsum

In Surya's notes, $\mathbf{Q} = r\mathbf{W}^{\mathrm{F}}$.

The equilibrium probabilities, $\mathbf{p}^\infty$, satisfy

$$\mathbf{p}^\infty\mathbf{Q} = 0, \qquad \mathbf{p}^\infty\mathbf{e} = 1. \tag{3}$$ eq:equilibri

As we assume an ergodic process, this eigenvalue is non-degenerate. If all other eigenvalues have strictly negative real parts, the process is regular (aperiodic).

We define additional matrices

$$\boldsymbol{\Lambda} \equiv (-\mathbf{Q}^{\mathrm{dg}})^{-1}, \qquad \mathbf{P} \equiv \mathbf{I} + \boldsymbol{\Lambda}\mathbf{Q}. \tag{4}$$

eq:defDLP

It can be shown that $\boldsymbol{\Lambda}_{ii}$ is the mean time it takes to leave state i and $\mathbf{P}_{ij}$ is the probability the the next transition from state i goes to state j:

$$\boldsymbol{\Lambda}_{ii} = \frac{1}{\sum_{j \neq j} \mathbf{Q}_{ij}}, \qquad \mathbf{P}_{ij} = \begin{cases} 0 & \text{if } i = j, \\ \frac{\mathbf{Q}_{ij}}{\sum_{k \neq j} \mathbf{Q}_{ik}} & \text{otherwise.} \end{cases} \tag{5}$$

eq:LamdaPcmp

Furthermore, we also define

$$\mathbf{D} \equiv \operatorname{diag}(\mathbf{p}^{\infty})^{-1}, \qquad \Longrightarrow \qquad \mathbf{p}^{\infty}\mathbf{D} = \mathbf{e}^{\mathrm{T}}. \tag{6}$$

eq:pdotD

1.2 Fundamental matrix

sec:fund

Definition 1: Fundamental matrix

$$\mathbf{Z} \equiv (-\mathbf{Q} + \mathbf{e}\boldsymbol{\pi})^{-1}, \tag{7}$$

eq:funddef

where $\boldsymbol{\pi}$ is any row-vector with $\boldsymbol{\pi}\mathbf{e} = 1/\tau \neq 0$.

Note that the canonical choice for the discrete time version, $\boldsymbol{\pi} = \mathbf{p}^{\infty}$, is not available here due to problems with units. It will be helpful to choose $\boldsymbol{\pi}$ to be independent of $\mathbf{Q}$, e.g. $\boldsymbol{\pi} = \mathbf{e}^{\mathrm{T}}/(n\tau)$. All quantities that we calculate using $\mathbf{Z}$ below will be independent of this choice.

Theorem 1:
The definition of $\mathbf{Z}$ is valid, i.e. $(-\mathbf{Q} + \mathbf{e}\boldsymbol{\pi})$ is invertible.

Proof. Assume there exists an $\mathbf{x}$ such that

$$(-\mathbf{Q} + \mathbf{e}\boldsymbol{\pi})\mathbf{x} = 0. \tag{8}$$

eq:fundinvke

Multiplying from the left with $\mathbf{p}^{\infty}$ gives

$$\boldsymbol{\pi}\mathbf{x} = 0. \tag{9}$$

eq:fundinvpi

Substituting back into (8) gives

$$\mathbf{Q}\mathbf{x} = 0.$$

As we assume an ergodic process, the zero eigenvalue is non-degenerate. Therefore, $\mathbf{x} = \lambda\mathbf{e}$. Substituting this into (9) gives

$$\lambda\boldsymbol{\pi}\mathbf{e} = \frac{\lambda}{\tau} = 0.$$

As we defined $\boldsymbol{\pi}$ such that $1/\tau \neq 0$, this means $\lambda = 0 \implies \mathbf{x} = 0$. □

Corollary 2:

$$\boldsymbol{\pi}\mathbf{Z} = \mathbf{p}^\infty, \tag{10}$$

eq:fundprob

$$\mathbf{Z}\mathbf{e} = \tau\mathbf{e}, \tag{11}$$

eq:fundrowsu

$$\mathbf{I} + \mathbf{Q}\mathbf{Z} = \mathbf{e}\mathbf{p}^\infty, \tag{12}$$

eq:fundQZ

$$\mathbf{I} + \mathbf{Z}\mathbf{Q} = \tau\mathbf{e}\boldsymbol{\pi}. \tag{13}$$

eq:fundZQ

Proof. We can deduce (10) and (11) be pre/post-multiplying the following equations by $\mathbf{Z}$:

$$\mathbf{p}^\infty(-\mathbf{Q} + \mathbf{e}\boldsymbol{\pi}) = \boldsymbol{\pi},$$
$$(-\mathbf{Q} + \mathbf{e}\boldsymbol{\pi})\mathbf{e} = \frac{\mathbf{e}}{\tau}.$$

We can then deduce (12) and (13) by substituting these into

$$(-\mathbf{Q} + \mathbf{e}\boldsymbol{\pi})\mathbf{Z} = \mathbf{Z}(-\mathbf{Q} + \mathbf{e}\boldsymbol{\pi}) = \mathbf{I}.$$

$\square$

1.3 First passage times

sec:fpt

Definition 2: First passage time matrix
We define $\overline{\mathbf{T}}_{ij}$ as the mean time it takes the process to reach state j for the first time, starting from state i. We also define $\mathbf{T}^{\mathrm{dg}}_{ii}$ as the mean time it takes the process to return to state i. As usual, $\mathbf{T} = \overline{\mathbf{T}} + \mathbf{T}^{\mathrm{dg}}$.

Consider the first time the process leaves state i. On average, this will take time $\boldsymbol{\Lambda}_{ii}$. With probability $\mathbf{P}_{ij}$, it will go directly to j, so the conditional mean time would be $\boldsymbol{\Lambda}_{ii}$. On the other hand, if it goes to some other state, k, with probability $\mathbf{P}_{ik}$, the conditional mean time would be $\overline{\mathbf{T}}_{kj} + \boldsymbol{\Lambda}_{ii}$. Combining these, we get the recursion relation

$$\begin{aligned}
\mathbf{T}_{ij} &= \sum_{k\neq j} \mathbf{P}_{ik}(\overline{\mathbf{T}}_{kj} + \boldsymbol{\Lambda}_{ii}) + \mathbf{P}_{ij}\boldsymbol{\Lambda}_{ii} \\
&= \sum_{k\neq j} \mathbf{P}_{ik}\overline{\mathbf{T}}_{kj} + \sum_{k} \mathbf{P}_{ik}\boldsymbol{\Lambda}_{ii} \\
&= \sum_{k\neq j} \mathbf{P}_{ik}\overline{\mathbf{T}}_{kj} + \boldsymbol{\Lambda}_{ii}, \\
\mathbf{T} &= \mathbf{P}\overline{\mathbf{T}} + \boldsymbol{\Lambda}\mathbf{E},
\end{aligned} \tag{14}$$

eq:fptrecurs

or, using (4),

$$\mathbf{T}^{\mathrm{dg}} = \boldsymbol{\Lambda}\mathbf{Q}\overline{\mathbf{T}} + \boldsymbol{\Lambda}\mathbf{E}. \tag{15}$$

eq:fptrecdg

Theorem 3:
The recurrence times are given by

$$\mathbf{T}^{\mathrm{dg}} = \boldsymbol{\Lambda}\mathbf{D}. \tag{16}$$

eq:recurtime

Proof. Pre-multiply (15) by $\mathbf{p}^\infty \mathbf{\Lambda}^{-1}$:

$$\mathbf{p}^\infty \mathbf{\Lambda}^{-1} \mathbf{T}^{\mathrm{dg}} = \mathbf{e}^{\mathrm{T}},$$

or in component form

$$\mathbf{p}_i^\infty \mathbf{\Lambda}_{ii}^{-1} \mathbf{T}_{ii}^{\mathrm{dg}} = 1.$$

This is the same as (16) in component form: $\mathbf{T}_{ii}^{\mathrm{dg}} = \mathbf{\Lambda}_{ii} / \mathbf{p}_i^\infty$. □

I think the extra factor of $\mathbf{\Lambda}_{ii}$, compared to the discrete case [1, Th.4.4.5], occurs because in this case we are demanding that the process leaves the initial state once before returning, whereas in the discrete case we only measure the time it takes to go to the initial state after the first time-step.

We can substitute this into (15) to get a recursion relation for the off diagonal part:

$$\mathbf{Q}\overline{\mathbf{T}} = \mathbf{D} - \mathbf{E}. \tag{17}$$ eq:fptbrec

Theorem 4:
The off-diagonal solution of (17) is unique.

Proof. Suppose we have two solutions for the off-diagonal part, $\overline{\mathbf{T}}$ and $\overline{\mathbf{T}}'$. Subtracting (17) for these two solutions gives

$$\mathbf{Q}(\overline{\mathbf{T}} - \overline{\mathbf{T}}') = 0.$$

As we are assuming an ergodic process, the zero eigenvalue is non-degenerate. Therefore

$$\overline{\mathbf{T}} - \overline{\mathbf{T}}' = \mathbf{e}\mathbf{y},$$

for some row-vector $\mathbf{y}$. Looking at the diagonal components

$$\mathbf{y}_i = \overline{\mathbf{T}}_{ii} - \overline{\mathbf{T}}'_{ii} = 0,$$

and therefore $\overline{\mathbf{T}} - \overline{\mathbf{T}}' = 0$. □

Theorem 5:
The off-diagonal mean first passage times are given by

$$\overline{\mathbf{T}} = (\mathbf{E}\mathbf{Z}^{\mathrm{dg}} - \mathbf{Z})\mathbf{D}. \tag{18}$$ eq:fptfund

Proof. We just need to show that this satisfies (17) and that the diagonal elements vanish. Premultiply (18) by $\mathbf{Q}$:

$$\begin{aligned} \mathbf{Q}\overline{\mathbf{T}} &= -\mathbf{Q}\mathbf{Z}\mathbf{D} \\ &= (\mathbf{I} - \mathbf{e}\mathbf{p}^\infty)\mathbf{D} \\ &= \mathbf{D} - \mathbf{E}, \end{aligned}$$

where we used (12) and (6). The vanishing of the diagonal elements follows trivially from the component form of (18):

$$\overline{\mathbf{T}}_{ij} = \frac{\mathbf{Z}_{jj} - \mathbf{Z}_{ij}}{\mathbf{p}_j^\infty}. \tag{19}$$ eq:fptfundcm

□

1.4 Mixing time (Kemeny's constant)

ec:mixtime
emenyconst

Theorem 6: The quantity

$$\eta \equiv \sum_j \overline{\mathbf{T}}_{ij}\mathbf{p}^\infty_j \tag{20}$$ eq:mixdef

is independent of i.

Proof. We use (18), (11) and the transpose of (6):

$$\begin{aligned}
\overline{\mathbf{T}}(\mathbf{p}^\infty)^{\mathrm{T}} &= (\mathbf{E}\mathbf{Z}^{\mathrm{dg}} - \mathbf{Z})\mathbf{D}(\mathbf{p}^\infty)^{\mathrm{T}} \\
&= (\mathbf{e}\mathbf{e}^{\mathrm{T}}\mathbf{Z}^{\mathrm{dg}} - \mathbf{Z})\mathbf{e} \\
&= (\mathbf{e}^{\mathrm{T}}\mathbf{Z}^{\mathrm{dg}}\mathbf{e})\mathbf{e} - \mathbf{Z}\mathbf{e} \\
&= (\operatorname{tr}\mathbf{Z} - \tau)\mathbf{e}.
\end{aligned}$$

which proves (20) with $\eta = \operatorname{tr}\mathbf{Z} - \tau$. □

Note that it is essential that we use $\overline{\mathbf{T}}$ and not $\mathbf{T}$ here, as that would lead to $\eta_i = \eta + \mathbf{\Lambda}_{ii}$, unlike the discrete time version [3] where this would only shift η by 1.

1.5 Sensitivity of equilibrium distribution

ensitivity

Suppose that the Markov process, defined by $\mathbf{Q}$, depends on some parameter α. Differentiating (7) gives

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}\alpha} = \mathbf{Z}\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}\alpha}\mathbf{Z}. \tag{21}$$ eq:diffZ

We can substitute this into the derivative of (10):

$$\frac{\mathrm{d}\mathbf{p}^\infty}{\mathrm{d}\alpha} = \boldsymbol{\pi}\mathbf{Z}\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}\alpha}\mathbf{Z} = \mathbf{p}^\infty\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}\alpha}\mathbf{Z}. \tag{22}$$ eq:diffp

We can rewrite this in component form and use the fact that $\mathbf{Q}_{ii} = -\sum_{i\neq j}\mathbf{Q}_{ij}$:

$$\begin{aligned}
\frac{\mathrm{d}\mathbf{p}^\infty_k}{\mathrm{d}\alpha} &= \sum_{i,j}\mathbf{p}^\infty_i\frac{\mathrm{d}\mathbf{Q}_{ij}}{\mathrm{d}\alpha}\mathbf{Z}_{jk} \\
&= \sum_{i\neq j}\mathbf{p}^\infty_i\frac{\mathrm{d}\mathbf{Q}_{ij}}{\mathrm{d}\alpha}\mathbf{Z}_{jk} + \sum_i \mathbf{p}^\infty_i\frac{\mathrm{d}\mathbf{Q}_{ii}}{\mathrm{d}\alpha}\mathbf{Z}_{ik} \\
&= \sum_{i\neq j}\mathbf{p}^\infty_i\frac{\mathrm{d}\mathbf{Q}_{ij}}{\mathrm{d}\alpha}(\mathbf{Z}_{jk} - \mathbf{Z}_{ik}) \\
&= \sum_{i\neq j}\frac{\mathrm{d}\mathbf{Q}_{ij}}{\mathrm{d}\alpha}\mathbf{p}^\infty_i\mathbf{p}^\infty_k(\overline{\mathbf{T}}_{ik} - \overline{\mathbf{T}}_{jk}),
\end{aligned} \tag{23}$$ eq:diffpT

which is the result of [4] that we need. Note that the summand vanishes for $i = j$, so we can drop the restriction $i \neq j$ from the range of the sum.

1.6 Subsets and flux

ec:subsets

Let us denote the set of states by $\mathcal{S}$. Consider a subset $\mathcal{A} \subset \mathcal{S}$. We can define a projection operator onto this subset:

$$\left(\mathbf{I}^{\mathcal{A}}\right)_{ij} = \begin{cases} 1 & \text{if } i = j \in \mathcal{A}, \\ 0 & \text{otherwise.} \end{cases} \tag{24}$$

eq:proj

We will use superscripts/subscripts to denote projection onto/summation over a subset:

$$\begin{aligned} \boldsymbol{\pi}^{\mathcal{A}} &= \boldsymbol{\pi}\mathbf{I}^{\mathcal{A}}, & \mathbf{M}^{\cdot\mathcal{A}} &= \mathbf{M}\mathbf{I}^{\mathcal{A}}, & \mathbf{M}^{\mathcal{A}\cdot} &= \mathbf{I}^{\mathcal{A}}\mathbf{M}, & \mathbf{x}^{\mathcal{A}} &= \mathbf{I}^{\mathcal{A}}\mathbf{x}, \\ \boldsymbol{\pi}_{\mathcal{A}} &= \boldsymbol{\pi}\mathbf{e}^{\mathcal{A}}, & \mathbf{M}_{\cdot\mathcal{A}} &= \mathbf{M}\mathbf{e}^{\mathcal{A}}, & \mathbf{M}_{\mathcal{A}\cdot} &= \left(\mathbf{e}^{\mathcal{A}}\right)^{\mathrm{T}}\mathbf{M}, & \mathbf{x}_{\mathcal{A}} &= \left(\mathbf{e}^{\mathcal{A}}\right)^{\mathrm{T}}\mathbf{x}, \end{aligned} \tag{25}$$

eq:projsum

where $\boldsymbol{\pi}$ is a row vector, $\mathcal{M}$ is a matrix and $\mathbf{x}$ is a column vector.

We can define a flux matrix, a.k.a. ergodic flow:

$$\boldsymbol{\Phi} = \mathbf{D}^{-1}\mathbf{Q}, \qquad \boldsymbol{\Phi}_{ij} = \mathbf{p}^{\infty}_{i}\mathbf{Q}_{ij}. \tag{26}$$

eq:flux

This measures the flow of probability between states in the equilibrium distribution. Detailed balance, a.k.a. reversibility, is equivalent to $\boldsymbol{\Phi} = \boldsymbol{\Phi}^{\mathrm{T}}$.

The flux between two subsets is a particularly useful quantity:

$$\boldsymbol{\Phi}_{\mathcal{A}\mathcal{B}} = \mathbf{p}^{\infty\mathcal{A}}\mathbf{Q}\mathbf{e}^{\mathcal{B}}. \tag{27}$$

eq:subflux

One can show that

$$\boldsymbol{\Phi}_{\mathcal{A}\mathcal{A}^{\mathrm{c}}} = \boldsymbol{\Phi}_{\mathcal{A}^{\mathrm{c}}\mathcal{A}} = -\boldsymbol{\Phi}_{\mathcal{A}\mathcal{A}} = -\boldsymbol{\Phi}_{\mathcal{A}^{\mathrm{c}}\mathcal{A}^{\mathrm{c}}} \tag{28}$$

eq:compflux

using $\left(\mathbf{p}^{\infty\mathcal{A}} + \mathbf{p}^{\infty\mathcal{A}^{\mathrm{c}}}\right)\mathbf{Q} = 0$ and $\mathbf{Q}\left(\mathbf{e}^{\mathcal{A}} + \mathbf{e}^{\mathcal{A}^{\mathrm{c}}}\right) = 0$.

1.7 Lumpability

sec:lump

Suppose we have partitioned the states into disjoint subsets, $\{\mathcal{A}_\alpha\}$:

$$\bigcup_\alpha \mathcal{A}_\alpha = \mathcal{S}, \qquad \mathcal{A}_\alpha \cap \mathcal{A}_\beta = \delta_{\alpha\beta}\mathcal{A}_\alpha. \tag{29}$$

eq:partition

We will use α instead of $\mathcal{A}_\alpha$ in superscripts and subscripts in the following. The fact that these subsets are disjoint and exhaustive allows us to define the function

$$\sigma(i) = \alpha \qquad \Longleftrightarrow \qquad i \in \mathcal{A}_\alpha. \tag{30}$$

eq:whichsey

We can use this partition to define a new stochastic process associated with the original Markov chain. At time t, if the state of the original process is i, the state of the new process is $\sigma(i)$.

One may ask if this new process is a Markov chain. The answer is yes, if the original Markov chain has a property called lumpability wrt. the partition (see [1, §6.3] for the discrete time version and [5, 6] for continuous time):

$$\sigma(i) = \sigma(j) \quad \Longrightarrow \quad \mathbf{Q}_{i\alpha} = \mathbf{Q}_{j\alpha} \equiv \sum_{k \in \mathcal{A}_\alpha} \mathbf{Q}_{jk}, \tag{31}$$

eq:lump

i.e. the total transition rate from some state to some subset is the same for all starting states within the same subset. This common value is the transition rate for the new lumped Markov chain.

This can be rewritten with the aid of two matrices

$$U_{\alpha i} = \frac{\delta_{\alpha\sigma(i)}}{|\mathcal{A}_\alpha|}, \qquad V_{i\alpha} = \delta_{\sigma(i)\alpha}. \tag{32}$$ eq:lumpmats

Left multiplication by U averages over subsets, right multiplication by V sums over subsets. For U, we chose the uniform measure in each subset. Any measure would work equally well, e.g. one proportional to the equilibrium distribution:

$$U_{\alpha i} = \frac{\mathbf{p}_i^{\infty\alpha}}{\mathbf{p}_\alpha^\infty}. \tag{33}$$ eq:altlumpma

One can show that $(UV)_{\alpha\beta} = \delta_{\alpha\beta}$. The matrix VU is also interesting. It has a block diagonal structure, with each block corresponding to a subset. Each block is a discrete-time ergodic Markov matrix (it is an independent trials process with probabilities given by the measure chosen for U). This means that the right eigenvectors with eigenvalue 1 will be those that are constant in each subset:

$$VU\mathbf{x} = \mathbf{x} \qquad \iff \qquad \mathbf{x} = \sum_\alpha x_\alpha \mathbf{e}^\alpha. \tag{34}$$ eq:setconst

This allows us to write the lumpability condition (31), and the transition matrix for the lumped process compactly:

$$VU\mathbf{Q}V = \mathbf{Q}V, \qquad \widehat{\mathbf{Q}} = U\mathbf{Q}V. \tag{35}$$ eq:lumpcompa

By induction, one can show that similar relations hold for all powers:

$$VU\mathbf{Q}^n V = \mathbf{Q}^n V, \qquad \widehat{\mathbf{Q}}^n = U\mathbf{Q}^n V, \tag{36}$$ eq:lumppower

and, via the Taylor series, for the exponential as well:

$$VU\mathrm{e}^{t\mathbf{Q}}V = \mathrm{e}^{t\mathbf{Q}}V, \qquad \mathrm{e}^{t\widehat{\mathbf{Q}}} = U\mathrm{e}^{t\mathbf{Q}}V. \tag{37}$$ eq:lumpexp

The equilibrium distribution of the lumped process is given by

$$\widehat{\mathbf{p}}^\infty = \mathbf{p}^\infty V. \tag{38}$$ eq:lumpeq

2 Signal-to-Noise ratio (SNR)

sec:SNR

In this section we will look at the signal-to-noise curve, and put an upper bound on its initial value. We will only consider ergodic Markov chains. Transient states would be unoccupied in equilibrium and would not be accessed by the signal creation process, therefore they could be removed from the analysis. Absorbing chains are degenerate cases: they have zero initial signal but infinite decay times, so they can only be approached as the limit of a sequence of ergodic chains.

2.1 Framework

:framework

The individual potentiation/depression events will be described by *discrete*-time Markov chains:

$$\mathbf{M}^{\pm} \equiv \mathbf{I} + \mathbf{W}^{\pm}, \qquad \mathbf{M}^{\pm}\mathbf{e} = \mathbf{e}, \qquad \mathbf{M}^{\pm}_{ij} \in [0,1]. \tag{39}$$

eq:MWdef

The initial signal creation event occurs at time $t = 0$, but all subsequent potentiation/depression events occur at random times according to Poisson processes with rates $rf^{\pm}$, where $f^{+}+f^{-} = 1$ are the fraction of plasticity events that are potentiating/depressing respectively. This means that the "forgetting" process will be described by the *continuous*-time Markov chain:

$$\mathbf{Q} = r\mathbf{W}^{\mathrm{F}} \equiv r\left(f^{+}\mathbf{W}^{+} + f^{-}\mathbf{W}^{-}\right). \tag{40}$$

eq:forgettin

We only require that this Markov chain is ergodic. The Markov chains described by $\mathbf{M}^{\pm}$ need not be.

We assume that the probability distribution starts in the equilibrium distribution (3). During the initial signal creation, a fraction f^{+} will change to $\mathbf{p}^{\infty}\mathbf{M}^{+}$ and a fraction f^{-} will change to $\mathbf{p}^{\infty}\mathbf{M}^{-}$. After this, probabilities will evolve according to (2).

2.2 SNR curve

c:SNRcurve

As we ignore correlations between different synapses, the only quantity of interest will be the number of synapses with each strength. The signal can be defined as the increase in synaptic strength due to potentiation plus the decrease in synaptic strength due to depression. If there are N synapses and the strength of the synapse in each state is given by the column vector, $\mathbf{w}$, this is given by

$$S(t) = Nf^{+}[\mathbf{p}(t|+) - \mathbf{p}^{\infty}]\mathbf{w} - Nf^{+}[\mathbf{p}(t|-) - \mathbf{p}^{\infty}]\mathbf{w}, \tag{41}$$

eq:signal

where $\mathbf{p}(t|\pm)$ is the probability of being in each state conditional on potentiation/depression at $t = 0$:

$$\mathbf{p}(t|\pm) = \mathbf{p}^{\infty}\mathbf{M}^{\pm}\mathrm{e}^{rt\mathbf{W}^{\mathrm{F}}}. \tag{42}$$

eq:initprob

We can rewrite the signal as

$$\begin{aligned} S(t) &= N\mathbf{p}^{\infty}(f^{+}\mathbf{W}^{+} - f^{-}\mathbf{W}^{-})\mathrm{e}^{rt\mathbf{W}^{\mathrm{F}}}\mathbf{w} \\ & N(2f^{+}f^{-})\mathbf{p}^{\infty}(\mathbf{W}^{+} - \mathbf{W}^{-})\mathrm{e}^{rt\mathbf{W}^{\mathrm{F}}}\mathbf{w}. \end{aligned} \tag{43}$$

eq:signalr

For the noise, we can use the standard deviation of the synaptic strength:

$$\text{Noise} = \sqrt{N\left(\sum_i \mathbf{p}^{\infty}_i\mathbf{w}^2_i - (\mathbf{p}^{\infty}\mathbf{w})^2\right)}. \tag{44}$$

eq:noise

From now on we shall assume that there are only two possible synaptic strengths, strong and weak, which we will describe by $\mathbf{w}_i = \pm 1$. This splits the set of states into two subsets:

$$+ = \{k|\mathbf{w}_k = +1\}\,, \qquad - = \{k|\mathbf{w}_k = -1\}\,. \tag{45}$$

eq:plusminus

This simplifies the noise:

$$\text{Noise} = \sqrt{N\,(4\mathbf{p}^\infty_+\mathbf{p}^\infty_-)}. \tag{46}$$

eq:noisepm

The factors of $\mathbf{p}^\infty_+\mathbf{p}^\infty_-$ will have little effect on anything that follows, so we will drop them.[1] This leaves the signal-to-noise ratio as

$$\text{SNR}(t) = \sqrt{N}(2f^+f^-)\mathbf{p}^\infty(\mathbf{W}^+ - \mathbf{W}^-)\mathrm{e}^{rt\mathbf{W}^\mathrm{F}}\mathbf{w}. \tag{47}$$

eq:SNRcurve

We can express this in terms of the one parameter family of transition matrices:

$$\mathbf{W}(\alpha) = \alpha\mathbf{W}^+ + (1-\alpha)\mathbf{W}^-, \qquad \Longrightarrow \qquad \begin{aligned} \mathbf{W}^\mathrm{F} &= \mathbf{W}(f^+), \\ \mathbf{W}^+ - \mathbf{W}^- &= \frac{\mathrm{d}\mathbf{W}}{\mathrm{d}\alpha}, \\ \mathbf{p}^\infty\frac{\mathrm{d}\mathbf{W}}{\mathrm{d}\alpha} &= -\frac{\mathrm{d}\mathbf{p}^\infty}{\mathrm{d}\alpha}\mathbf{W}^\mathrm{F}. \end{aligned} \tag{48}$$

eq:Walpha

Then (47) becomes

$$\text{SNR}(t) = \sqrt{N}(2f^+f^-)\frac{\mathrm{d}\mathbf{p}^\infty}{\mathrm{d}\alpha}(-\mathbf{W}^\mathrm{F})\,\mathrm{e}^{rt\mathbf{W}^\mathrm{F}}\mathbf{w}. \tag{49}$$

eq:SNRalpha

2.3 Degrees of freedom and constraints

onstraints

We would like to use the components of $\mathbf{W}^\pm$ as the independent degrees of freedom when we try to maximise quantities associated with the SNR curve (47). However, (39) imposes some restrictions on the space of allowed values. We can solve some of these by setting

$$\mathbf{W}^\pm_{ii} = -\sum_{j\neq i}\mathbf{W}^\pm_{ij}. \tag{50}$$

eq:Wdiag

Then we treat the off-diagonal components as the independent degrees of freedom. These must satisfy the following inequalities:

$$\mathbf{W}^\pm_{ij} \geq 0 \qquad \text{for } i \neq j, \tag{51}$$

eq:Wmin

$$\sum_{j\neq i}\mathbf{W}^\pm_{ij} \leq 1. \tag{52}$$

eq:Wmax

The inequalities $\mathbf{W}^\pm_{ij} \leq 1$, $-1 \leq \mathbf{W}^\pm_{ii} \leq 0$ follow automatically from these.

In §3.2.1, we will see that the area under the SNR curve is invariant under the scaling $\mathbf{W}^\pm \to \lambda\mathbf{W}^\pm$. This means that we can ignore the constraint (52) when maximising the area: after the area has been maximised, we can use this degree of freedom to enforce (52) without changing the area. However, this scaling does change the SNR curve, in particular its initial value, so we can't ignore (52) when maximising that.

[1] They will not affect the optimal transition rates for most quantities, and the optima will correspond to the symmetric case when $\mathbf{p}^\infty_+ = \mathbf{p}^\infty_- = \frac{1}{2}$.

2.4 Lumpability

ec:SNRlump

Suppose that we have a partition such that $\mathbf{W}^+$ and $\mathbf{W}^-$ are simultaneously lumpable, and that all the states in each subset have the same synaptic strength (see §1.7):

$$VU\mathbf{W}^{\pm}V = \mathbf{W}^{\pm}V, \qquad VU\mathbf{w} = \mathbf{w}. \tag{53}$$

eq:lumpables

We can define a new synapse with

$$\widehat{\mathbf{W}}^{\pm} = U\mathbf{W}^{\pm}V, \qquad \hat{\mathbf{w}} = U\mathbf{w}, \qquad \hat{\mathbf{p}}^{\infty} = \mathbf{p}^{\infty}V. \tag{54}$$

eq:lumpedsyn

This synapse has an SNR curve:

$$\begin{aligned}
\frac{\mathrm{SNR}(t)}{\sqrt{N}(2f^+f^-)} &= \hat{\mathbf{p}}^{\infty}(\widehat{\mathbf{W}}^+ - \widehat{\mathbf{W}}^-)\mathrm{e}^{rt\widehat{\mathbf{W}}^F}\hat{\mathbf{w}}. \\
&= \mathbf{p}^{\infty}VU(\mathbf{W}^+ - \mathbf{W}^-)VU\mathrm{e}^{rt\mathbf{W}^\mathrm{F}}VU\mathbf{w}. \\
&= \mathbf{p}^{\infty}(\mathbf{W}^+ - \mathbf{W}^-)VU\mathrm{e}^{rt\mathbf{W}^\mathrm{F}}VU\mathbf{w}. \\
&= \mathbf{p}^{\infty}(\mathbf{W}^+ - \mathbf{W}^-)\mathrm{e}^{rt\mathbf{W}^\mathrm{F}}VU\mathbf{w}. \\
&= \mathbf{p}^{\infty}(\mathbf{W}^+ - \mathbf{W}^-)\mathrm{e}^{rt\mathbf{W}^\mathrm{F}}\mathbf{w}.
\end{aligned} \tag{55}$$

eq:lumpedSNR

i.e. the lumped process has exactly the same SNR as the original one.

2.5 Initial SNR and flux

ec:initflux

Using the first line of (43), we can write the initial SNR as

$$\frac{\mathrm{SNR}(0)}{\sqrt{N}} = I = (\mathbf{p}^{\infty+} + \mathbf{p}^{\infty-})(f^+\mathbf{W}^+ - f^-\mathbf{W}^-)(\mathbf{e}^+ - \mathbf{e}^-). \tag{56}$$

eq:init

Using $\mathbf{W}^{\pm}(\mathbf{e}^+ + \mathbf{e}^-) = 0$ and (28):

$$r\mathbf{p}^{\infty-}(f^+\mathbf{W}^+ + f^-\mathbf{W}^-)\mathbf{e}^+ = \mathbf{\Phi}_{-+} = \mathbf{\Phi}_{+-} = r\mathbf{p}^{\infty+}(f^+\mathbf{W}^+ + f^-\mathbf{W}^-)\mathbf{e}^-,$$

we can rewrite (56) as

$$I = \frac{4\mathbf{\Phi}_{-+}}{r} - 4\mathbf{p}^{\infty+}f^+\mathbf{W}^+\mathbf{e}^- - 4\mathbf{p}^{\infty-}f^-\mathbf{W}^-\mathbf{e}^+. \tag{57}$$

eq:initflux

The last two terms are guaranteed to be negative, as the diagonal parts of $\mathbf{W}^{\pm}$ cannot contribute. Therefore

$$\mathrm{SNR}(0) \leq \frac{4\sqrt{N}\mathbf{\Phi}_{-+}}{r}. \tag{58}$$

eq:initfluxi

This inequality is saturated if potentiation never takes it from a $+$ state to a $-$ state and depression never takes it from a $-$ state to a $+$ state.

2.6 Maximising initial SNR

sec:initmax

The flux will be maximised if potentiation is guaranteed to take it to a + state and depression is guaranteed to take it to a − state:

$$\sum_{j\in +} \mathbf{W}^{+}_{ij} = 1 \quad \forall\, i \in -, \qquad \sum_{j\in -} \mathbf{W}^{-}_{ij} = 1 \quad \forall\, i \in +. \tag{59}$$ eq:guarantee

This implies that the process is lumpable to a two state system (see §1.7 and §2.4):

$$\begin{aligned}\mathbf{W}^{+} &= \begin{pmatrix} -1 & 1 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{W}^{-} = \begin{pmatrix} 0 & 0 \\ 1 & -1 \end{pmatrix}, \quad \mathbf{w} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \\ &\implies \quad \mathbf{W}^{\mathrm{F}} = \begin{pmatrix} -f^{+} & f^{+} \\ f^{-} & -f^{-} \end{pmatrix}, \quad \mathbf{p}^{\infty} = \begin{pmatrix} f^{-} & f^{+} \end{pmatrix}, \end{aligned} \tag{60}$$ eq:binarylum

which leads to the initial SNR [2]

$$\mathrm{SNR}(0) \leq \sqrt{N}(4f^{+}f^{-}). \tag{61}$$ eq:binarySNR

This is maximised at $f^{+} = f^{-} = \frac{1}{2}$:

$$\mathrm{SNR}(0) \leq \sqrt{N}. \tag{62}$$ eq:initmax

3 Area maximisation

sec:areamax

In this section we will find an upper bound on the area under the signal-to-noise curve. As in §2, we will only consider ergodic Markov chains. We will see in §3.4 that the optimal chain is absorbing, so it lies on the boundary of the (open) set of ergodic chains, but it still puts an upper bound on the area.

3.1 Area under signal-to-noise curve

sec:area

The signal-to-noise curve is given by (49). The area is computed by integrating this

$$\begin{aligned} A &= \frac{\sqrt{N}(2f^{+}f^{-})}{r} \frac{\mathrm{d}\mathbf{p}^{\infty}}{\mathrm{d}\alpha} \left[-\mathrm{e}^{rt\mathbf{W}^{\mathrm{F}}} \right]_{0}^{\infty} \mathbf{w} \\ &= \frac{\sqrt{N}(2f^{+}f^{-})}{r} \frac{\mathrm{d}\mathbf{p}^{\infty}}{\mathrm{d}\alpha} (\mathbf{I} - \mathbf{e}\mathbf{p}^{\infty})\mathbf{w} \\ &= \frac{\sqrt{N}(2f^{+}f^{-})}{r} \frac{\mathrm{d}\mathbf{p}^{\infty}}{\mathrm{d}\alpha} \mathbf{w}. \end{aligned} \tag{63}$$ eq:area

[2]Note that including the dropped factors in (46) would only change this to $\mathrm{SNR}(0) \leq \sqrt{N(4f^{+}f^{-})}$, which would have no effect on what follows.

We can rewrite this using (23), with $rA = \sqrt{N}(2f^+f^-)\hat{A}$ and $\mathbf{q}_{ij} \equiv \frac{\mathrm{d}\mathbf{W}^{\mathrm{F}}_{ij}}{\mathrm{d}\alpha} = \mathbf{W}^+_{ij} - \mathbf{W}^-_{ij}$

$$\hat{A} = \sum_{i,j,k} \mathbf{p}^\infty_i \mathbf{q}_{ij} (\overline{\mathbf{T}}_{ik} - \overline{\mathbf{T}}_{jk}) \mathbf{p}^\infty_k \mathbf{w}_k. \tag{64}$$ eq:areaT

Definition 3: Partial mixing times
We define the $\pm$ mixing times as

$$\begin{aligned} \eta^\pm_i &\equiv \sum_k \overline{\mathbf{T}}_{ik} \mathbf{p}^\infty_k \left(\frac{1 \pm \mathbf{w}_k}{2}\right) &&= \sum_{k\in\pm} \overline{\mathbf{T}}_{ik} \mathbf{p}^\infty_k \\ &= \sum_k (\mathbf{Z}_{kk} - \mathbf{Z}_{ik}) \left(\frac{1 \pm \mathbf{w}_k}{2}\right) &&= \sum_{k\in\pm} (\mathbf{Z}_{kk} - \mathbf{Z}_{ik}). \end{aligned} \tag{65}$$ eq:mixingpm

We can think of η^+_i as a measure of the "distance" to the $\mathbf{w}_k = +1$ states and η^-_i as the "distance" to the $\mathbf{w}_k = -1$ states.

Using (20), we can write:

$$\begin{aligned} \eta^+_i + \eta^-_i &= \eta, \\ 2(\eta^+_i - \eta^+_j) &= \sum_k (\overline{\mathbf{T}}_{ik} - \overline{\mathbf{T}}_{jk}) \mathbf{p}^\infty_k \mathbf{w}_k = \sum_k (\mathbf{Z}_{jk} - \mathbf{Z}_{ik}) \mathbf{w}_k. \end{aligned} \tag{66}$$ eq:mixingrel

We could arrange the states in order of decreasing η^+, which is the same as the order of increasing η^-.

We can rewrite (64) as

$$\begin{aligned} \hat{A} &= 2 \sum_{i,j} \mathbf{q}_{ij} \mathbf{p}^\infty_i (\eta^+_i - \eta^+_j) &&= -2 \sum_{i,j} \mathbf{q}_{ij} \mathbf{p}^\infty_i \eta^+_j \\ &= 2 \sum_{i,j} \mathbf{q}_{ij} \mathbf{p}^\infty_i (\eta^-_j - \eta^-_i) &&= 2 \sum_{i,j} \mathbf{q}_{ij} \mathbf{p}^\infty_i \eta^-_j. \end{aligned} \tag{67}$$ eq:areaEta

We can also express it in terms of the fundamental matrix (7) as

$$\hat{A} = \sum_{i,j,k,l} \mathbf{q}_{ij} \boldsymbol{\pi}_l \mathbf{Z}_{li} (\mathbf{Z}_{jk} - \mathbf{Z}_{ik}) \mathbf{w}_k = \boldsymbol{\pi} \mathbf{Z} q \mathbf{Z} \mathbf{w}. \tag{68}$$ eq:areaZ

It is also helpful to define the following quantities:

$$\begin{aligned} c_k &= \frac{\mathrm{d} \ln \mathbf{p}^\infty_k}{\mathrm{d}\alpha} = \sum_{ij} \mathbf{p}^\infty_i \mathbf{q}_{ij} \left(\overline{\mathbf{T}}_{ik} - \overline{\mathbf{T}}_{jk}\right) = -\left(\mathbf{p}^\infty q \overline{\mathbf{T}}\right)_k = \frac{(\mathbf{p}^\infty q \mathbf{Z})_k}{\mathbf{p}^\infty_k}, \\ a_i &= \sum_j \mathbf{q}_{ij} \mathbf{p}^\infty_i (\eta^+_i - \eta^+_j), \\ \implies \hat{A} &= \sum_k c_k \mathbf{p}^\infty_k \mathbf{w}_k = 2 \sum_i a_i. \end{aligned} \tag{69}$$ eq:areacoeff

Note that the optimal choice of $\mathbf{w}$ is $\mathbf{w}_k = \mathrm{sgn}(c_k)$.

3.2 Derivatives wrt. $\mathbf{W}^\pm$

sec:deriv

As discussed in §2.3, we will regard the off-diagonal elements of $\mathbf{W}^\pm_{ij}$ to be the independent variables, with $\mathbf{W}^\pm_{ii} = -\sum_{j\neq i}\mathbf{W}^\pm_{ij}$ imposed by hand. Thus,

$$\frac{\partial \mathbf{W}^{\mathrm{F}}_{ij}}{\partial \mathbf{W}^\pm_{gh}} = f^\pm \delta_{gi}(\delta_{hj}-\delta_{ij}), \qquad \frac{\partial \mathbf{q}_{ij}}{\partial \mathbf{W}^\pm_{gh}} = \pm\delta_{gi}(\delta_{hj}-\delta_{ij}). \tag{70}$$

eq:basicderi

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

In particular, differentiating (7),

$$\frac{\partial \mathbf{Z}_{ij}}{\partial \mathbf{W}^\pm_{gh}} = r f^\pm \mathbf{Z}_{ig}(\mathbf{Z}_{hj}-\mathbf{Z}_{gj}). \tag{71}$$

eq:derivZ

We can then differentiate expression (68) to get

$$\begin{aligned}
\frac{\partial \hat{A}}{\partial \mathbf{W}^\pm_{gh}} &= r f^\pm \sum_{ijkl} \mathbf{q}_{ij}\mathbf{w}_k\boldsymbol{\pi}_l\left[\mathbf{Z}_{lg}(\mathbf{Z}_{hi}-\mathbf{Z}_{gi})(\mathbf{Z}_{jk}-\mathbf{Z}_{ik}) + \mathbf{Z}_{li}(\mathbf{Z}_{jg}-\mathbf{Z}_{ig})(\mathbf{Z}_{hk}-\mathbf{Z}_{gk})\right] \\
&\quad \pm \sum_{kl} \mathbf{w}_k\boldsymbol{\pi}_l\mathbf{Z}_{lg}(\mathbf{Z}_{hk}-\mathbf{Z}_{gk}) \\
&= 2 r f^\pm \sum_{ij} \mathbf{q}_{ij}\mathbf{p}^\infty_i\mathbf{p}^\infty_g\left[(\overline{\mathbf{T}}_{gi}-\overline{\mathbf{T}}_{hi})(\eta^+_i-\eta^+_j) + (\overline{\mathbf{T}}_{ig}-\overline{\mathbf{T}}_{jg})(\eta^+_g-\eta^+_h)\right] \\
&\quad \pm 2\mathbf{p}^\infty_g(\eta^+_g-\eta^+_h) \\
&= 2 r f^\pm \sum_{ij} \mathbf{q}_{ij}\mathbf{p}^\infty_i\mathbf{p}^\infty_g(\overline{\mathbf{T}}_{gi}-\overline{\mathbf{T}}_{hi})(\eta^+_i-\eta^+_j) \pm 2\mathbf{p}^\infty_g(\eta^+_g-\eta^+_h)\left[1+\frac{\partial\ln(\mathbf{p}^\infty_g)}{\partial\ln(f^\pm)}\right] \\
&= 2 r f^\pm \mathbf{p}^\infty_g\left[\sum_i a_i(\overline{\mathbf{T}}_{gi}-\overline{\mathbf{T}}_{hi}) + c_g(\eta^+_g-\eta^+_h)\right] \pm 2\mathbf{p}^\infty_g(\eta^+_g-\eta^+_h).
\end{aligned} \tag{72}$$

eq:derivA

where a_i and c_k were defined in (69).

It is sometimes useful to consider the following derivatives:

$$\frac{\partial}{\partial \mathbf{W}^{\mathrm{F}}_{gh}} \equiv \frac{\partial}{\partial \mathbf{W}^+_{gh}} + \frac{\partial}{\partial \mathbf{W}^-_{gh}}, \qquad \frac{\partial}{\partial \mathbf{q}_{gh}} \equiv f^- \frac{\partial}{\partial \mathbf{W}^+_{gh}} - f^+ \frac{\partial}{\partial \mathbf{W}^-_{gh}}. \tag{73}$$

eq:derivqw

Each of these derivatives behaves as their names suggest:

$$\frac{\partial \mathbf{W}^{\mathrm{F}}_{ij}}{\partial \mathbf{W}^{\mathrm{F}}_{gh}} = \frac{\partial \mathbf{q}_{ij}}{\partial \mathbf{q}_{gh}} = \delta_{gi}(\delta_{hj}-\delta_{ij}), \qquad \frac{\partial \mathbf{q}_{ij}}{\partial \mathbf{W}^{\mathrm{F}}_{gh}} = \frac{\partial \mathbf{W}^{\mathrm{F}}_{ij}}{\partial q_{gh}} = 0. \tag{74}$$

eq:derivqwef

This is because we could treat $\mathbf{W}^{\mathrm{F}}$ and q as the independent variables. However, the boundaries of the allowed region are more easily expressed in terms of $\mathbf{W}^\pm$.

3.2.1 Scaling mode

ec:rescale

Consider the following differential operator:

$$\Delta \equiv \sum_{g,h} \mathbf{W}^+_{gh} \frac{\partial}{\partial \mathbf{W}^+_{gh}} + \mathbf{W}^-_{gh} \frac{\partial}{\partial \mathbf{W}^-_{gh}}. \tag{75}$$

eq:scaleop

This corresponds to the scaling, $\mathbf{W}^\pm \to (1{+}\epsilon)\mathbf{W}^\pm$. Intuitively, this has two effects: it scales up the initial potentiation/depression and it scales down all timescales. This intuition is confirmed by the following results:

$$\begin{aligned} \Delta\mathbf{Z} &= \tau\mathbf{e}\mathbf{p}^\infty - \mathbf{Z}, & \Delta\mathbf{p}^\infty &= 0, & \Delta\mathbf{T} &= -\mathbf{T}, \\ \Delta\eta^\pm_i &= -\eta^\pm_i, & \Delta\mathbf{q}_{ij} &= \mathbf{q}_{ij}, & \Delta\hat{A} &= 0, \end{aligned} \tag{76}$$

eq:scaleeffe

The anomalous bit in the scaling of $\mathbf{Z}$ is due to the lack of dependence of $\boldsymbol{\pi}$ and τ on $\mathbf{W}^\pm$.

As the area is invariant under this scaling, we can consider the $\mathbf{W}^\pm$ to be projective coordinates. Therefore we don't need to enforce the constraint (52) while looking for the maximum area, as we can use this null-mode to enforce it afterwards without changing the area. We also don't have to worry about the boundary at infinity, as sending some of them to infinity is equivalent to sending the rest to zero.

3.3 Kuhn-Tucker conditions

kuhntucker

Consider the Lagrangian

$$\mathcal{L} = \hat{A} + \sum_\pm \sum_{i\neq j} \mu^\pm_{ij} \mathbf{W}^\pm_{ij} + \lambda \mathbf{p}^\infty \mathbf{w}. \tag{77}$$

eq:lagrangia

The last term ensures that we hold $\mathbf{p}^\infty_\pm$ fixed during this extremisation, so that we can safely ignore the factors that we dropped from the noise in (46). Necessary conditions for an extremum are

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^\pm_{gh}} = 0, \qquad \mu^\pm_{gh} \geq 0, \quad \mathbf{W}^\pm_{gh} \geq 0, \quad \mu^\pm_{gh} \mathbf{W}^\pm_{gh} = 0. \tag{78}$$

eq:extremum

with $g \neq h$. This enforces the constraints (51), but not (52). As discussed in §2.3 and §3.2.1, that can be enforced after finding the maximum with the null scaling degree of freedom.

3.3.1 Triangularity

triangular

Consider

$$\frac{\partial \mathcal{L}}{\partial \mathbf{q}_{gh}} = f^- \frac{\partial \mathcal{L}}{\partial \mathbf{W}^+_{gh}} - f^+ \frac{\partial \mathcal{L}}{\partial \mathbf{W}^-_{gh}} = (f^- \mu^+_{gh} - f^+ \mu^-_{gh}) + 2\mathbf{p}^\infty_g (\eta^+_g - \eta^+_h) = 0. \tag{79}$$

eq:shiftqder

This corresponds to the shift

$$\mathbf{W}^{+}_{ij} \to \mathbf{W}^{+}_{ij} + f^{-}\epsilon_{ij}, \qquad \mathbf{W}^{-}_{ij} \to \mathbf{W}^{-}_{ij} - f^{+}\epsilon_{ij}, \qquad \sum_j \epsilon_{ij} = 0, \tag{80}$$

eq:shiftq

which leaves $\mathbf{W}^{\mathrm{F}}$ unchanged, and therefore $\mathbf{p}^{\infty}$, $\mathbf{T}$ and $\eta^{\pm}$ as well.

Assume $\eta^{+}_{g} > \eta^{+}_{h}$. Then

$$f^{-}\mu^{+}_{gh} - f^{+}\mu^{-}_{gh} < 0 \qquad \Longrightarrow \qquad \mu^{-}_{gh} > 0 \qquad \Longrightarrow \qquad \mathbf{W}^{-}_{gh} = 0. \tag{81}$$

eq:lowertria

Similarly, if $\eta^{+}_{g} < \eta^{+}_{h}$, then

$$f^{-}\mu^{+}_{gh} - f^{+}\mu^{-}_{gh} > 0 \qquad \Longrightarrow \qquad \mu^{+}_{gh} > 0 \qquad \Longrightarrow \qquad \mathbf{W}^{+}_{gh} = 0. \tag{82}$$

eq:uppertria

Thus, if we arrange the states in order of decreasing η^{+}, $\mathbf{W}^{+}$ is upper-triangular and $\mathbf{W}^{-}$ is lower triangular.

We have ignored the possibility that $\mathbf{p}^{\infty}_{g} = 0$, as this would imply that $\mathbf{T}_{ig} = \infty$, which would in turn imply that the Markov process is not ergodic.

3.3.2 Increasing c_k

acoeffincr

Consider the following combinations of derivatives:

$$\Delta_{gh} \equiv \frac{1}{\mathbf{p}^{\infty}_{g}} \left(\frac{\partial}{\partial \mathbf{W}^{\mathrm{F}}_{gh}} \right) + \frac{1}{\mathbf{p}^{\infty}_{h}} \left(\frac{\partial}{\partial \mathbf{W}^{\mathrm{F}}_{hg}} \right), \tag{83}$$

$$\tag{84}$$

eq:areacoeff

Note that they are only well defined if all the states have non-zero equilibrium probabilities (see the comment in §3.3.1 about this being satisfied for ergodic chains).

One can show that the equilibrium probabilities, $\mathbf{p}^{\infty}$, are invariant under these operators:

$$\Delta_{gh} \mathbf{p}^{\infty}_{i} = 0, \tag{85}$$

eq:sareacoef

which makes it possible to integrate the perturbation:

$$\mathbf{W}^{\pm} \to \mathbf{W}^{\pm} + \mathbf{D}\boldsymbol{\epsilon}, \qquad \begin{aligned} \boldsymbol{\epsilon} &= \boldsymbol{\epsilon}^{\mathrm{T}}, \\ \boldsymbol{\epsilon}\mathbf{e} &= 0. \end{aligned} \tag{86}$$

eq:areacoeff

But more interestingly:

$$\Delta_{gh} \mathcal{L} = \frac{\mu^{+}_{gh} + \mu^{-}_{gh}}{\mathbf{p}^{\infty}_{g}} + \frac{\mu^{+}_{hg} + \mu^{-}_{hg}}{\mathbf{p}^{\infty}_{h}} + 2r\left(c_g - c_h\right)\left(\eta^{+}_{g} - \eta^{+}_{h}\right), \tag{87}$$

$$\tag{88}$$

eq:areacoeff

where c_k were defined in (69).

Using the non-negativity of the Kuhn-Tucker multipliers, $\mu^{\pm}_{ij}$, (87) tells us that if we arrange the states in order of decreasing η^{+}_{i}, the optimal process will have non-decreasing c_k (if any of the η^{+}_{k} are degenerate, we can choose their order to ensure this).

Note that, according to §3.3.1, either $\mathbf{W}^{+}_{gh}$ or $\mathbf{W}^{-}_{gh}$ will be zero at the maximum, therefore we can expect one of $\mu^{+}_{gh} + \mu^{-}_{gh}$ to be non-zero. This would rule out degeneracy of the c_k or η^{+}_{k}. Looking at (79) closely, the only way $\mu^{+}_{gh} + \mu^{-}_{gh}$ could be zero is if $\eta^{+}_{g} = \eta^{+}_{h}$ or $\mathbf{p}^{\infty}_{g} = 0$.

3.3.3 Shortcuts

:shortcuts

Now consider the following combinations of derivatives for $m > 1$:

$$\widetilde{\Delta}^{\pm}_{g,m} \equiv \left[\sum_{k=0}^{m-1} \frac{1}{\mathbf{p}^{\infty}_{g\pm k}} \left(\frac{\partial}{\partial \mathbf{W}^{\pm}_{g\pm k, g\pm(k+1)}}\right)\right] - \frac{1}{\mathbf{p}^{\infty}_{g}} \left(\frac{\partial}{\partial \mathbf{W}^{\pm}_{g,g\pm m}}\right). \tag{89}$$

eq:shortcutd

Once again, they are only well defined if all the states have non-zero equilibrium probabilities (see the comment in §3.3.1 about this being satisfied for ergodic chains).

One can show that the equilibrium probabilities, $\mathbf{p}^{\infty}$, are invariant under these operators:

$$\widetilde{\Delta}^{\pm}_{g,m} \mathbf{p}^{\infty}_{i} = 0, \tag{90}$$

eq:shortcutp

which makes it possible to integrate the perturbation:

$$\mathbf{W}^{\pm} \to \mathbf{W}^{\pm} + \mathbf{D}\boldsymbol{\epsilon}^{\pm(g,m)}, \qquad \begin{aligned} \left(\boldsymbol{\epsilon}^{\pm(g,m)}\right)_{g,g\pm m} &= -\epsilon, \\ \left(\boldsymbol{\epsilon}^{\pm(g,m)}\right)_{g\pm k, g\pm(k+1)} &= \epsilon \qquad \forall\, k \in [0, m-1], \\ \left(\boldsymbol{\epsilon}^{\pm(g,m)}\right)_{g\pm k, g\pm k} &= -\epsilon \qquad \forall\, k \in [1, m-1]. \end{aligned} \tag{91}$$

eq:shortcutf

But more interestingly for our purposes:

$$\widetilde{\Delta}^{\pm}_{g,m} \mathcal{L} = \left[\sum_{k=0}^{m-1} \frac{\mu^{\pm}_{g\pm k, g\pm(k+1)}}{\mathbf{p}^{\infty}_{g\pm k}} - \frac{\mu^{\pm}_{g,g\pm m}}{\mathbf{p}^{\infty}_{g}}\right] + 2rf^{\pm} \sum_{k=0}^{m-1} \left(\eta^{+}_{g\pm k} - \eta^{+}_{g\pm(k+1)}\right) \left(c_{g\pm k} - c_{g}\right), \tag{92}$$

eq:shortcuta

If we put the states in order of decreasing η^{+}_{k}, the results of the §3.3.2 tell us that the c_k are non-decreasing. This implies that the last term of the final expression in (92) is non-negative. If it is non-zero (there would need to be a lot of degeneracy for it to be zero), this would imply that $\mu^{\pm}_{g,g\pm m} > 0$, which in turn implies that $\mathbf{W}^{\pm}_{g,g\pm m} = 0$. This would tell us that the process with the maximal area has to have a multi-state topology.

3.3.4 Summary

:KTsummary

Using the Kuhn-Tucker formalism, we have shown that, with the states arranged in order of non-increasing η^{+}_{i}:

- There can be no ergodic maximum for which $\mathbf{W}^+$ contains backwards transitions or $\mathbf{W}^-$ contains forwards transitions.
- There can be no ergodic maximum with the c_k decreasing.
- The c_k may only be degenerate at an ergodic maximum if the corresponding η_k^+ are also degenerate.
- If the c_k increase and the η_i^+ decrease, there can be no ergodic maximum with shortcuts.

These were shown by finding allowed perturbations that increase the area.

This leaves two possibilities for the maximum area Markov chain. Either there is no degeneracy and no shortcuts, which implies the Multi-state topology that we'll discuss in §3.4, or there is some degeneracy, which would allow shortcuts provided that they do not bypass an entire degenerate set (see (92)).

Degeneracy tends to be very delicate. It is usually hard to arrange without some symmetry relating degenerate states. Such a symmetry would imply lumpability (see §1.7). The lumped chain would not have any shortcuts, as an entire degenerate set cannot be bypassed. As this lumped chain has the same area (see §2.4), we would need only consider the multi-state topology.

3.4 Multi-state topology

multistate

The multi-state topology is defined by (see [7, 8]):

$$\mathbf{W}^+_{ij} = q_i^+ \delta_{i+1,j}, \qquad \mathbf{W}^-_{ij} = q_j^- \delta_{i,j+1}. \tag{93}$$

eq:multistat

It saturates various inequalities:

$$\begin{aligned} \overline{\mathbf{T}}_{ik} - \overline{\mathbf{T}}_{jk} &= \begin{cases} \overline{\mathbf{T}}_{ij}, & \text{if} \quad i \leq j \leq k \quad \text{or} \quad i \geq j \geq k, \\ -\overline{\mathbf{T}}_{ji}, & \text{if} \quad j \leq i \leq k \quad \text{or} \quad j \geq i \geq k, \end{cases} \\ r\mathbf{p}_i^\infty \mathbf{W}^{\mathrm{F}}_{ij} \left(\overline{\mathbf{T}}_{ij} + \overline{\mathbf{T}}_{ji} \right) &= 1 \quad \text{if} \quad i = j \pm 1, \end{aligned} \tag{94}$$

eq:multistat

and it satisfies detailed balance (a.k.a. reversibility a.k.a. $\mathcal{L}^2_{\mathbf{p}^\infty}$ self-adjointness):

$$f^+ q_i^+ \mathbf{p}_i^\infty = f^- q_i^- \mathbf{p}_{i+1}^\infty, \tag{95}$$

eq:multistat

which means we can always choose the transition rates, $q_i^\pm$, to give any desired equilibrium probabilities, $\mathbf{p}_i^\infty$.

This allows us to calculate the c_k's:

$$\begin{aligned}
c_k &= \sum_{i<k} \mathbf{T}_{i,i+1} \left(\mathbf{p}^\infty_i q^+_i + \mathbf{p}^\infty_{i+1} q^-_i\right) - \sum_{i\geq k} \mathbf{T}_{i+1,i} \left(\mathbf{p}^\infty_i q^+_i + \mathbf{p}^\infty_{i+1} q^-_i\right), \\
c_{k+1} - c_k &= \left(\mathbf{T}_{k,k+1} + \mathbf{T}_{k+1,k}\right) \left(\frac{\mathbf{p}^\infty_k \mathbf{W}^\mathrm{F}_{k,k+1}}{f^+} + \frac{\mathbf{p}^\infty_{k+1} \mathbf{W}^\mathrm{F}_{k+1,k}}{f^-} \right) = \frac{1}{rf^+f^-}, \\
\sum_k c_k \mathbf{p}^\infty_k &= \sum_{ij} \mathbf{p}^\infty_i \mathbf{q}_{ij} (\eta - \eta) = 0, \\
\implies c_k &= \frac{k - \sum_j j \mathbf{p}^\infty_j}{rf^+f^-},
\end{aligned} \tag{96}$$

eq:areacoeff

where we used (94) to derive the first two equations respectively and Th.6 to derive the third. This allows us to write the area as

$$A = \frac{2\sqrt{N}}{r} \sum_k \left[k - \sum_j j \mathbf{p}^\infty_j \right] \mathbf{p}^\infty_k \mathbf{w}_k = \frac{2\sqrt{N}}{r} \sum_k \left| k - \sum_j j \mathbf{p}^\infty_j \right| \mathbf{p}^\infty_k, \tag{97}$$

eq:multistat

where we used $\mathbf{w}_k = \mathrm{sgn}(c_k)$, as discussed after (69).

First let us maximise (97) at fixed $\mathbf{p}^\infty_\pm = \sum_k \mathbf{p}^\infty_k \left(\frac{1\pm\mathbf{w}_k}{2}\right)$. Clearly this will happen when we put all of the probability at the ends: $\mathbf{p}^\infty_1 = \mathbf{p}^\infty_-$ and $\mathbf{p}^\infty_n = \mathbf{p}^\infty_+$ are the only non-zero $\mathbf{p}^\infty_k$. This gives an area of [3]

$$A \leq \frac{\sqrt{N}}{r} (n-1) \left(4 \mathbf{p}^\infty_+ \mathbf{p}^\infty_-\right). \tag{98}$$

eq:multistat

This is maximised at $\mathbf{p}^\infty_+ = \mathbf{p}^\infty_- = \frac{1}{2}$:

$$A \leq \frac{\sqrt{N}}{r} (n-1). \tag{99}$$

eq:maxarea

Note that the chain that achieves this is not ergodic, the two states at each end are absorbing. This is similar to the results found numerically in [9] in a slightly different situation.

4 Finite time SNR

finitetime

The SNR at time t was given in (47) as

$$\mathrm{SNR}(t) = \sqrt{N} (2f^+f^-) \mathbf{p}^\infty \mathbf{q}\, \mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w}.$$

[3] Note that including the dropped factors in (46) would only change this to $A \leq \sqrt{N(4\mathbf{p}^\infty_+\mathbf{p}^\infty_-)}(n-1)/r$, which would have no effect on what follows.

Let us try to maximise this at time t only. We will consider the independent parameters to be the off-diagonal elements of $\mathbf{M}^\pm$, with the diagonal elements determined via $\mathbf{M}^\pm_{ii} = \sum_{j\neq i} \mathbf{M}^\pm_{ij}$. Consider the Lagrangian

$$\mathcal{L} = \mathbf{p}^\infty \mathbf{q} \mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} + \sum_\pm \sum_{ij} \mu^\pm_{ij} \mathbf{M}^\pm_{ij}. \tag{100}$$

eq:finlagran

Necessary conditions for an extremum are

$$\frac{\partial \mathcal{L}}{\partial \mathbf{M}^\pm_{gh}} = 0, \qquad \mu^\pm_{gh} \geq 0, \quad \mathbf{M}^\pm_{gh} \geq 0, \quad \mu^\pm_{gh} \mathbf{M}^\pm_{gh} = 0.$$

We can use the results of [10] to write down the shift of this Lagrangian under an infinitesimal perturbation

$$\begin{aligned} \delta\mathcal{L} = {} & \mathbf{p}^\infty \delta\mathbf{W}^\mathrm{F} \mathbf{Z}\, \mathbf{q}\, \mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} + \mathbf{p}^\infty \delta\mathbf{q}\, \mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} + r \int_0^t \mathrm{d}\tau\, \mathbf{p}^\infty \mathbf{q}\, \mathrm{e}^{r\tau\mathbf{W}^\mathrm{F}} \delta\mathbf{W}^\mathrm{F} \mathrm{e}^{r(t-\tau)\mathbf{W}^\mathrm{F}} \mathbf{w} \\ & + \sum_\pm \sum_{ij} \mu^\pm_{ij} \delta\mathbf{M}^\pm_{ij} \end{aligned} \tag{101}$$

eq:finpert

This can be rewritten using the eigenvector decomposition of $\mathbf{W}^\mathrm{F}$.

$$\mathbf{W}^\mathrm{F} = \sum_a -q_a \mathbf{u}^a \mathbf{v}^a, \quad \mathbf{v}^a \mathbf{u}^b = \delta_{ab}, \quad \mathbf{W}^\mathrm{F} \mathbf{u}^a = -q_a \mathbf{u}^a, \quad \mathbf{v}^a \mathbf{W}^\mathrm{F} = -q_a \mathbf{v}^a. \tag{102}$$

eq:eigendeco

People often write $\mathbf{v}$ as $\mathbf{v}^\mathrm{T}$, presumably because they find the concept of row vectors too difficult to handle. We're better than that. We can choose $q_1 = 0$, $\mathbf{u}^1 = \mathbf{e}$ and $\mathbf{v}^1 = \mathbf{p}^\infty$.

Then, defining

$$F_{ab} = \begin{cases} rt\, \mathrm{e}^{-q_a rt}, & \text{if } q_a = q_b, \\ \dfrac{\mathrm{e}^{-q_a rt} - \mathrm{e}^{-q_b rt}}{q_b - q_a}, & \text{otherwise}, \end{cases} \tag{103}$$

eq:eigdiff

we get

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{M}^\pm_{gh}} = {} & f^\pm \mathbf{p}^\infty_g \left(\left[\mathbf{Z}\, \mathbf{q}\, \mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} \right]_h - \left[\mathbf{Z}\, \mathbf{q}\, \mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} \right]_g \right) \\ & \pm \mathbf{p}^\infty_g \left(\left[\mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} \right]_h - \left[\mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} \right]_g \right) \\ & + \sum_{ab} F_{ab} (\mathbf{p}^\infty \mathbf{q} \mathbf{u}^a) \mathbf{v}^a_g (\mathbf{u}^b_h - \mathbf{u}^b_g)(\mathbf{v}^a \mathbf{w}) \\ & + \mu^\pm_{gh} - \mu^\pm_{gg}. \end{aligned} \tag{104}$$

findiff

Consider

$$\begin{aligned} f^- \frac{\partial \mathcal{L}}{\partial \mathbf{M}^+_{gh}} - f^+ \frac{\partial \mathcal{L}}{\partial \mathbf{M}^-_{gh}} = {} & \mathbf{p}^\infty_g \left(\left[\mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} \right]_h - \left[\mathrm{e}^{rt\mathbf{W}^\mathrm{F}} \mathbf{w} \right]_g \right) \\ & + f^- \mu^+_{gh} + f^+ \mu^-_{gg} - f^+ \mu^-_{gh} - f^- \mu^+_{gg} \\ = {} & 0, \end{aligned} \tag{105}$$

eq:finshiftq

which corresponds to the shift considered in §3.3.1. We can see that

$$\begin{aligned}
\left[\mathrm{e}^{rt\mathbf{W}^{\mathrm{F}}}\mathbf{w}\right]_g < \left[\mathrm{e}^{rt\mathbf{W}^{\mathrm{F}}}\mathbf{w}\right]_h \qquad &\Longrightarrow \qquad \mu^-_{gh} > 0 \qquad \text{or} \qquad \mu^+_{gg} > 0\\
&\Longrightarrow \qquad \mathbf{M}^-_{gh} = 0 \qquad \text{or} \qquad \mathbf{M}^+_{gg} = 0,\\
\left[\mathrm{e}^{rt\mathbf{W}^{\mathrm{F}}}\mathbf{w}\right]_g > \left[\mathrm{e}^{rt\mathbf{W}^{\mathrm{F}}}\mathbf{w}\right]_h \qquad &\Longrightarrow \qquad \mu^+_{gh} > 0 \qquad \text{or} \qquad \mu^-_{gg} > 0\\
&\Longrightarrow \qquad \mathbf{M}^+_{gh} = 0 \qquad \text{or} \qquad \mathbf{M}^-_{gg} = 0.
\end{aligned} \tag{106}$$

eq:etalambda

5 Laplace transform

sec:laplace

5.1 Fundamental matrix etc.

sec:lfund

In analogy to (7), define

$$\mathbf{Z}(s) = (s\mathbf{I} + \mathbf{e}\boldsymbol{\pi} - \mathbf{Q})^{-1}. \tag{107}$$

eq:lfund

This reduces to the fundamental matrix at $s = 0$. The analogous result to (11) is

$$\mathbf{Z}(s)\mathbf{e} = \frac{\tau}{1 + s\tau}\mathbf{e}. \tag{108}$$

eq:lfundrows

The analogues of (10), (12) and (13) are much uglier, but luckily we won't need them. Supose we have some row vector $\mathbf{a}$ such that $\mathbf{ae} = 0$. Then $\mathbf{aZ}(s)$ is independent of $\boldsymbol{\pi}$:

$$\frac{\partial(\mathbf{aZ}(s))_i}{\partial\boldsymbol{\pi}_k} = (\mathbf{aZ}(s)\mathbf{e})\mathbf{Z}_{ki}(s) = \frac{\tau}{1 + s\tau}(\mathbf{ae})\mathbf{Z}_{ki}(s) = 0. \tag{109}$$

eq:alfund

Then we also define

$$\overline{\mathbf{T}}(s) = (\mathbf{EZ}^{\mathrm{dg}}(s) - \mathbf{Z}(s))\mathbf{D}, \qquad \overline{\mathbf{T}}_{ij}(s) = \frac{\mathbf{Z}_{jj}(s) - \mathbf{Z}_{ij}(s)}{\mathbf{p}^\infty_j}. \tag{110}$$

eq:lfptb

This reduces to the first passage time matrix at $s = 0$, but at other s there is (probably) no relation.

Using the exact same proof as Theorem 6, we see that the quantity

$$\eta(s) = \sum_j \overline{\mathbf{T}}_{ij}(s)\mathbf{p}^\infty_j \tag{111}$$

eq:lkemeny

is independent of the starting state i, but now $\eta(s) = \operatorname{tr}\mathbf{Z}(s) - \frac{\tau}{1+s\tau}$. We can the define

$$\eta^\pm_i(s) = \sum_j \overline{\mathbf{T}}_{ij}(s)\mathbf{p}^\infty_j\left(\frac{1 \pm \mathbf{w}_j}{2}\right) = \sum_{j\in\pm} \overline{\mathbf{T}}_{ij}(s)\mathbf{p}^\infty_j. \tag{112}$$

eq:lpmixtime

We can arrange the states in order of decreasing $\eta^+_i(s)$ or increasing $\eta^-_i(s)$.

5.2 Laplace transform of SNR curve

laplaceSNR

Consider the Laplace transform of the evolution operator:

$$\mathbf{G}(s) = \int_0^\infty \mathrm{d}t \, \mathrm{e}^{(\mathbf{Q}-s)t}. \tag{113}$$

eq:levol

For $\mathfrak{Re}\, s > 0$, we have

$$(s-\mathbf{Q})\mathbf{G}(s) = \int_0^\infty \mathrm{d}t \, (s-\mathbf{Q})\mathrm{e}^{(\mathbf{Q}-s)t} = \left[-\mathrm{e}^{(\mathbf{Q}-s)t}\right]_0^\infty = \mathbf{I}. \tag{114}$$

eq:levolcalc

As $(s-\mathbf{Q})$ is invertible for $\mathfrak{Re}\, s > 0$, because all eigenvalues of $\mathbf{Q}$ are nonpositive, we have

$$\mathbf{G}(s) = (s-\mathbf{Q})^{-1}. \tag{115}$$

eq:levolres

For $s = 0$, we can avoid our problems by replacing $\mathbf{G}(s) \to \mathbf{Z}(s)$.

Now consider the Laplace transform of the SNR curve (47)

$$\begin{aligned} A(s) &= \int_0^\infty \mathrm{d}t \mathrm{e}^{-st}\, \mathrm{SNR}(t) \\ &= \int_0^\infty \mathrm{d}t \, \sqrt{N}(2f^+f^-)\mathbf{p}^\infty \mathbf{q} \mathrm{e}^{(r\mathbf{W}^{\mathrm{F}}-s)t}\mathbf{w} \\ &= \frac{\sqrt{N}(2f^+f^-)}{r} \mathbf{p}^\infty \mathbf{q} \left(s - r\mathbf{W}^{\mathrm{F}}\right)^{-1} \mathbf{w}. \end{aligned} \tag{116}$$

eq:lsnr

This expression is ill-behaved at $s = 0$. Thanks to (109), we can solve this by the replacement $\mathbf{G}(s) \to \mathbf{Z}(s)$, as $\mathbf{qe} = 0$.

$$\begin{aligned} \hat{A}(s) = \frac{rA(s)}{\sqrt{N}(2f^+f^-)} &= \mathbf{p}^\infty \mathbf{q} \mathbf{Z}(s) \mathbf{w} \\ &= \sum_{ijk} \mathbf{p}_i^\infty \mathbf{q}_{ij} \left(\overline{\mathbf{T}}_{ik}(s) - \overline{\mathbf{T}}_{jk}(s)\right) \mathbf{p}_k^\infty \mathbf{w}_k \\ &= 2\sum_{ij} \mathbf{p}_i^\infty \mathbf{q}_{ij} (\eta_i^+(s) - \eta_j^+(s)). \end{aligned} \tag{117}$$

eq:larea

Note that $A(0) = A$, the area, and $\lim_{s\to\infty}\{sA(s)\} = \mathrm{SNR}(0)$, the initial SNR.

In analogy with (69), we define

$$\begin{aligned} c_k(s) &= \sum_{ij} \mathbf{p}_i^\infty \mathbf{q}_{ij} \left(\overline{\mathbf{T}}_{ik}(s) - \overline{\mathbf{T}}_{jk}(s)\right) \\ a_i(s) &= \sum_j \mathbf{p}_i^\infty \mathbf{q}_{ij} (\eta_i^+(s) - \eta_j^+(s)), \\ \implies \hat{A}(s) &= \sum_k c_k(s) \mathbf{p}_k^\infty \mathbf{w}_k = 2\sum_i a_i(s). \end{aligned} \tag{118}$$

eq:lareacoef

5.3 Perturbation analysis

sec:lpert

Using the same approach as the area bound, we find that the derivatives are

$$\begin{aligned}\frac{\partial \hat{A}(s)}{\partial \mathbf{W}^{\pm}_{gh}} &= 2rf^{\pm}\mathbf{p}^{\infty}_{g}\left[\sum_i a_i(s)(\overline{\mathbf{T}}_{gi}(0) - \overline{\mathbf{T}}_{hi}(0)) + c_g(s)(\eta^{+}_{g}(s) - \eta^{+}_{h}(s))\right] \\ &\quad \pm 2\mathbf{p}^{\infty}_{g}(\eta^{+}_{g}(s) - \eta^{+}_{h}(s)).\end{aligned} \tag{119}$$

eq:lAdiff

This is exactly the same as (72). It follows that, using exactly the same perturbations, that the Laplace transform of the SNR curve for *any* model is lower than that of a certain model with the serial topology having the same equilibrium distribution.

5.4 Envelope

sec:env

Hopefully we can prove an upper bound on the Laplace transform of the memory curve:

$$A(s) \leq \sqrt{N}B(s) = \frac{\sqrt{N}}{C(s)}. \tag{120}$$

eq:lbound

We will assume that $C(s)$ is a concave function. We already know that $C(0) = \frac{1}{M-1}$ and $C(s) \to s$ as $s \to \infty$.

In the eigenmode decomposition, this reads

$$\sum_a \frac{\mathcal{I}_a}{q_a + s} \leq B(s). \tag{121}$$

eq:lboundeig

Now let's maximise $\mathrm{SNR}(t_0)$ with respect to $\{\mathcal{I}_a, q_a\}$. Consider the Lagrangian

$$\mathcal{L} = \sum_a \mathcal{I}_a \mathrm{e}^{-q_a t_0} + \int_0^\infty \mathrm{d}s\, \mu(s)\left[B(s) - \sum_a \frac{\mathcal{I}_a}{q_a + s}\right]. \tag{122}$$

eq:envlagran

Necessary conditions for a maximum are

$$\frac{\partial \mathcal{L}}{\partial \mathcal{I}_a} = \mathrm{e}^{-q_a t_0} - \int \mathrm{d}s\, \frac{\mu(s)}{q_a + s} = 0, \tag{123}$$

eq:envI

$$\frac{\partial \mathcal{L}}{\partial q_a} = \mathcal{I}_a\left[-t_0 \mathrm{e}^{-q_a t_0} + \int \mathrm{d}s\, \frac{\mu(s)}{(q_a + s)^2}\right] = 0, \tag{124}$$

eq:envq

$$\mu(s)\frac{\delta \mathcal{L}}{\delta \mu(s)} = \mu(s)\left[B(s) - \sum_a \frac{\mathcal{I}_a}{q_a + s}\right] = 0, \tag{125}$$

eq:envKT

$$\mu(s) \geq 0, \tag{126}$$

eq:envKTm

$$\frac{\delta \mathcal{L}}{\delta \mu(s)} = B(s) - \sum_a \frac{\mathcal{I}_a}{q_a + s} \geq 0. \tag{127}$$

eq:envKTbnd

If we assume $\mathcal{I}_a \neq 0$ for some a, then (123) and (124) read

$$\begin{aligned} \mathrm{e}^{-q_a t_0} &= \int \mathrm{d}s \, \frac{\mu(s)}{q_a + s}, \\ t_0 \mathrm{e}^{-q_a t_0} &= \int \mathrm{d}s \, \frac{\mu(s)}{(q_a + s)^2}. \end{aligned} \tag{128}$$

eq:envnumexp

The second of these is the derivative of the first with respect to q, therefore the two curves in the first must touch each other tangentially at q_a. As both curves are decreasing convex functions, it seems unlikely that this could happen at multiple values of q. We will assume that there is a single non-zero $\mathcal{I}_a = \mathcal{I}$, with the corresponding $q_a = q$, in the following.

For (123) to have a solution, $\mu(s)$ must be nonzero for at least one value of s. Then, by (125), we must saturate (127) at those values of s. If there were more than two such values, $\mathcal{I}$ and q would be overconstrained. Assume there are two such values, $s = s_0$ and $s = s_1$.

$$\mathcal{I} = B(s_0)(q + s_0) = B(s_1)(q + s_1) \qquad \Longrightarrow \quad q = \frac{s_0 B(s_0) - s_1 B(s_1)}{B(s_1) - B(s_0)}. \tag{129}$$

eq:sattwice

Now the bound (127) reads

$$\begin{aligned} B(s) \geq \frac{B(s_0)(q + s_0)}{q + s} &= \frac{s_0 - s_1}{(s - s_1)C(s_0) + (s_0 - s)C(s_1)}, \\ xC(s_0) + (1 - x)C(s_1) &\geq C(xs_0 + (1 - x)s_1), \end{aligned} \tag{130}$$

eq:satwicebn

where we substituted $s = xs_0 + (1 - x)s_1$. As we assumed that $C(s)$ is concave, this is impossible.

Therefore the bound must be saturated exactly once and $\mu(s) = \mu_0 \delta(s - s_0)$. Now (123), (124) and (125) read

$$\mu_0 = (q + s_0)\mathrm{e}^{-qt_0}, \qquad (q + s_0)t_0 = 1, \qquad \mathcal{I} = \frac{B(s_0)}{t_0}. \tag{131}$$

eq:satonce

This satisfies (126). Now (127) tells us

$$B(s) \geq \frac{B(s_0)}{(q + s)t_0}, \qquad \text{or} \qquad 1 + (s - s_0)t_0 \geq \frac{C(s)}{C(s_0)}. \tag{132}$$

eq:satoncebn

As the two sides are equal at $s = s_0$, it is necessary that they touch tangentially for this bound to be true elsewhere. The linearity of the LHS and concavity of the RHS ensure that this is sufficient for the bound to be satisfied for all s. This condition is

$$t_0 = \frac{C'(s_0)}{C(s_0)}. \tag{133}$$

eq:envs0t0

The resulting SNR curve and envelope are

$$\mathrm{SNR}(t) = \frac{\mathrm{e}^{(s_0 - 1/t_0)t}}{C'(s_0)}, \qquad \mathrm{SNR}(t_0) = \frac{\mathrm{e}^{s_0 t_0 - 1}}{C'(s_0)}, \tag{134}$$

eq:env

where s_0 is determined as a function of t_0 by (133).

A Other quantities

Here we collect useless facts.

A.1 Differences in c_k's

eacoeffdiff

In the general case, making full use of [1, Cor.6.2.7], we can show that:

$$\begin{aligned}
c_{k+1} - c_k &= \frac{N^{k+1}_{kk}}{\mathbf{p}^\infty_k} \left[\sum_{i<j} \mathbf{p}^\infty_i \frac{\mathbf{W}^{\mathrm{F}}_{ij}}{f^+} \left(H^{k+1}_{i,k} + H^{k}_{j,k+1} - 1 \right) \right. \\
&\qquad\qquad\qquad\qquad \left. + \sum_{i>j} \mathbf{p}^\infty_i \frac{\mathbf{W}^{\mathrm{F}}_{ij}}{f^+} \left(H^{k+1}_{j,k} + H^{k}_{i,k+1} - 1 \right) \right] \\
&= \frac{N^{k+1}_{kk}}{\mathbf{p}^\infty_k} \left[\sum_{i<j} \mathbf{p}^\infty_i \frac{\mathbf{W}^{\mathrm{F}}_{ij}}{f^+} \left(1 - H^{k+1}_{j,k} + H^{k}_{i,k+1} \right) \right. \\
&\qquad\qquad\qquad\qquad \left. + \sum_{i>j} \mathbf{p}^\infty_i \frac{\mathbf{W}^{\mathrm{F}}_{ij}}{f^+} \left(1 - H^{k+1}_{i,k} + H^{k}_{j,k+1} \right) \right], \qquad (135) \\
\eta^+_k - \eta^+_{k+1} &= \mathbf{T}_{k,k+1} \mathbf{p}^\infty_+ - \sum_{\{i|\mathbf{w}_i>0\}} N^{k+1}_{ii} \left(1 - H^{i}_{k,k+1} \right) \\
&= \sum_{\{i|\mathbf{w}_i>0\}} N^{k}_{ii} \left(1 - H^{i}_{k+1,k} \right) - \mathbf{T}_{k+1,k} \mathbf{p}^\infty_+ \\
= \eta^-_{k+1} - \eta^-_k &= \mathbf{T}_{k+1,k} \mathbf{p}^\infty_- - \sum_{\{i|\mathbf{w}_i<0\}} N^{k}_{ii} \left(1 - H^{i}_{k+1,k} \right) \\
&= \sum_{\{i|\mathbf{w}_i<0\}} N^{k+1}_{ii} \left(1 - H^{i}_{k,k+1} \right) - \mathbf{T}_{k,k+1} \mathbf{p}^\infty_- .
\end{aligned}$$

eq:areacoeff

We need to show that the positivity of one ($\forall k$) implies that the positivity of the other.

A.2 Derivatives wrt. $\overline{\mathbf{T}}$

sec:derivT

The Markov chain, $\mathbf{W}^{\mathrm{F}}$, is completely determined by the off-diagonal mean first passage times, $\overline{\mathbf{T}}$, [1, Th.4.4.12]:

$$\begin{aligned}
\mathbf{p}^\infty &= \eta \left(\overline{\mathbf{T}}^{-1} \mathbf{e} \right)^{\mathrm{T}}, \\
r\mathbf{W}^{\mathrm{F}} &= \mathbf{Q} = (\mathbf{D} - \mathbf{E}) \overline{\mathbf{T}}^{-1}.
\end{aligned} \qquad (136)$$

eq:fptdet

where η can be determined by normalising $\mathbf{p}^\infty$ and $\mathbf{D}$ is determined by $\mathbf{p}^\infty$, (6). Clearly q will be undetermined.

We can then define derivatives wrt. $\overline{\mathbf{T}}$:

$$\frac{\partial}{\partial \overline{\mathbf{T}}_{gh}} = \sum_{ij} \left(\frac{\partial \mathbf{W}^{\mathrm{F}}_{ij}}{\partial \overline{\mathbf{T}}_{gh}} \right) \frac{\partial}{\partial \mathbf{W}^{\mathrm{F}}_{ij}}, \qquad (137)$$

eq:derivTdef

where

$$\frac{\partial \mathbf{W}^{\mathrm{F}}_{ij}}{\partial \overline{\mathbf{T}}_{gh}} = r\mathbf{p}^{\infty}_{h}\mathbf{W}^{\mathrm{F}}_{ig}\left(\mathbf{W}^{\mathrm{F}}_{ij} - \mathbf{W}^{\mathrm{F}}_{hj}\right), \qquad \frac{\partial \mathbf{p}^{\infty}_{i}}{\partial \overline{\mathbf{T}}_{gh}} = -r\mathbf{p}^{\infty}_{h}\mathbf{p}^{\infty}_{i}\mathbf{W}^{\mathrm{F}}_{ig}. \tag{138}$$

eq:derivTWp

These derivatives of q will vanish.

This means that the derivatives of the area are:

$$\frac{\partial \hat{A}}{\partial \overline{\mathbf{T}}_{gh}} = -\mathbf{p}^{\infty}_{h}\left[\sum_{i}\mathbf{p}^{\infty}_{i}\mathbf{q}_{ig}\mathbf{w}_{h} + r\sum_{ijk}\left(\mathbf{W}^{\mathrm{F}}_{ig} + \mathbf{W}^{\mathrm{F}}_{kg}\right)\mathbf{p}^{\infty}_{i}\mathbf{q}_{ij}\left(\overline{\mathbf{T}}_{ik} - \overline{\mathbf{T}}_{jk}\right)\mathbf{p}^{\infty}_{k}\mathbf{w}_{k}\right]. \tag{139}$$

eq:derivTare

A.3 Initial SNR

sec:initSNR

Let us write $\mathrm{SNR}(0) = \sqrt{N}(2f^{+}f^{-})\hat{I}$. Using (47), we can write

$$\begin{aligned}
\hat{I} &= \frac{\mathrm{d}\mathbf{p}^{\infty}}{\mathrm{d}\alpha}(-\mathbf{W}^{\mathrm{F}})\mathbf{w} && = -\boldsymbol{\pi}\mathbf{Z}\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}\alpha}\mathbf{Z}\mathbf{W}^{\mathrm{F}}\mathbf{w} && = -\boldsymbol{\pi}\mathbf{Z}\frac{\mathrm{d}\mathbf{W}^{\mathrm{F}}}{\mathrm{d}\alpha}\mathbf{Z}\mathbf{Q}\mathbf{w} \\
&= \boldsymbol{\pi}\mathbf{Z}\frac{\mathrm{d}\mathbf{W}^{\mathrm{F}}}{\mathrm{d}\alpha}(\mathbf{I} - \tau\mathbf{e}\boldsymbol{\pi})\mathbf{w} && = \boldsymbol{\pi}\mathbf{Z}\frac{\mathrm{d}\mathbf{W}^{\mathrm{F}}}{\mathrm{d}\alpha}\mathbf{w} && = \mathbf{p}^{\infty}\frac{\mathrm{d}\mathbf{W}^{\mathrm{F}}}{\mathrm{d}\alpha}\mathbf{w}.
\end{aligned} \tag{140}$$

eq:initSNR

We can also write this in component form

$$\begin{aligned}
\hat{I} &= \sum_{i,j}\mathbf{p}^{\infty}_{i}\mathbf{q}_{ij}\mathbf{w}_{j} \\
&= \sum_{i\neq j}\mathbf{p}^{\infty}_{i}\mathbf{q}_{ij}\mathbf{w}_{j} + \sum_{i}\mathbf{p}^{\infty}_{i}\mathbf{q}_{ii}\mathbf{w}_{i} \\
&= \sum_{i\neq j}\mathbf{q}_{ij}\mathbf{p}^{\infty}_{i}(\mathbf{w}_{j} - \mathbf{w}_{i}).
\end{aligned} \tag{141}$$

eq:initSNRcm

We can differentiate the expression in terms of $\mathbf{Z}$ to get

$$\begin{aligned}
\frac{\partial \hat{I}}{\partial \mathbf{W}^{\pm}_{gh}} &= rf^{\pm}\sum_{ijk}\boldsymbol{\pi}_{k}\mathbf{Z}_{kg}(\mathbf{Z}_{hi} - \mathbf{Z}_{gi})\mathbf{q}_{ij}\mathbf{w}_{j} \pm \sum_{k}\boldsymbol{\pi}_{k}\mathbf{Z}_{kg}(\mathbf{w}_{h} - \mathbf{w}_{g}) \\
&= rf^{\pm}\sum_{ij}\mathbf{p}^{\infty}_{g}\mathbf{q}_{ij}(\overline{\mathbf{T}}_{gi} - \overline{\mathbf{T}}_{hi})\mathbf{p}^{\infty}_{i}\mathbf{w}_{j} \pm \mathbf{p}^{\infty}_{g}(\mathbf{w}_{h} - \mathbf{w}_{g}).
\end{aligned} \tag{142}$$

eq:initSNRdi

If we wished to maximise the area with fixed initial SNR, $\hat{I} = I_0$, we would add $\beta(\hat{I} - I_0)$ to the Lagrangian (77) and extremise wrt β.

A.4 Fixing mixing time (Kemeny's constant)

sec:fixmix

The mixing time, η (20), can be thought of as the mean time to pass between two states drawn from the equilibrium distribution [3, 11]. It should be a measure of the time it takes to reach equilibrium, and therefore related to the time it takes the SNR to decay. It could be interesting to hold it fixed while maximising the area, as this could help prevent degenerate solutions with very low initial SNR but long decay time. This can be done by adding $\gamma(\eta - \eta_0)$ to the Lagrangian (77) and extremising wrt γ.

It would help to calculate its derivatives.

$$\begin{aligned} \frac{\partial \eta}{\partial \mathbf{W}^{\pm}_{gh}} &= \frac{\partial}{\partial \mathbf{W}^{\pm}_{gh}} \left[\sum_i \mathbf{Z}_{ii} - \tau \right] \\ &= r f^{\pm} \sum_i \mathbf{Z}_{ig} (\mathbf{Z}_{hi} - \mathbf{Z}_{gi}) \\ &= r f^{\pm} (\mathbf{Z}^2_{hg} - \mathbf{Z}^2_{gg}). \end{aligned} \tag{143}$$

eq:mixingdif

A.5 Scaling mode

scaleconstr

Consider the following differential operator:

$$\Delta \equiv \sum_{g,h} \mathbf{W}^{+}_{gh} \frac{\partial}{\partial \mathbf{W}^{+}_{gh}} + \mathbf{W}^{-}_{gh} \frac{\partial}{\partial \mathbf{W}^{-}_{gh}}. \tag{144}$$

eq:scaleopap

This corresponds to the scaling, $\mathbf{W}^{\pm} \to (1+\epsilon)\mathbf{W}^{\pm}$. Intuitively, this has two effects: it scales up the initial potentiation/depression and it scales down all timescales. This intuition is confirmed by the following results:

$$\begin{gathered} \Delta \mathbf{Z} = \tau \mathbf{e} \mathbf{p}^{\infty} - \mathbf{Z}, \quad \Delta \mathbf{p}^{\infty} = 0, \quad \Delta \mathbf{T} = -\mathbf{T}, \quad \Delta \eta^{\pm}_i = -\eta^{\pm}_i, \quad \Delta \mathbf{q}_{ij} = \mathbf{q}_{ij}, \\ \Delta \hat{A} = 0, \quad \Delta \hat{I} = \hat{I}, \qquad \Delta \eta = -\eta. \end{gathered} \tag{145}$$

eq:scaleeffe

The anomalous bit in the scaling of $\mathbf{Z}$ is due to the lack of dependence of $\boldsymbol{\pi}$ and τ on $\mathbf{W}^{\pm}$.

Suppose we don't hold anything fixed when maximising the area. Then we'd have

$$\Delta \mathcal{L} = 0,$$

i.e. this scaling is a null direction. Area maximisation can only determine the ratios of transition rates, not their absolute values.

Now suppose we only fix $\hat{I}$ when maximising the area. Then we'd have

$$\Delta \mathcal{L} = \beta \hat{I} = \beta I_0 = 0.$$

As the Lagrange multiplier is zero, the constraint doesn't change the derivatives of the Lagrangian wrt $\mathbf{W}^{\pm}$. The sole effect of the constraint would be to fix the scaling mode. It wouldn't change the ratios of transition rates, topology, etc.

Exactly the same conclusions would follow if we only fixed η when maximising the area. This would also only fix the scaling mode. However, if we held them both fixed, it would have more of an effect:

$$\Delta \mathcal{L} = \beta \hat{I} - \gamma \eta = \beta I_0 - \gamma \eta_0 = 0. \tag{146}$$

eq:scalecons

The Lagrange multipliers are non-zero, so this could affect the topology of the optimal Markov chain.

References

r1960finite [1] J. Kemeny and J. Snell, *Finite markov chains.* Springer, 1960.

r2000survey [2] J. Hunter, "A survey of generalized inverses and their use in stochastic modelling," *Research Letters in the Information and Mathematical Sciences* **1** (2000) no. 1, 25–36.

r2006mixing [3] J. Hunter, "Mixing times with applications to perturbed Markov chains," *Linear algebra and its applications* **417** (2006) no. 1, 108–123.

2000markov [4] 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.

8markovian [5] C. Burke and M. Rosenblatt, "A Markovian function of a Markov chain," *The Annals of Mathematical Statistics* **29** (1958) no. 4, 1112–1122.

umpability [6] F. Ball and G. F. Yeo, "Lumpability and Marginalisability for Continuous-Time Markov Chains," *Journal of Applied Probability* **30** (1993) no. 3, 518–528.

94learning [7] D. J. Amit and S. Fusi, "Learning in neural networks with material synapses," *Neural Computation* **6** (1994) no. 5, 957–982.

multistate [8] S. Fusi and L. F. Abbott, "Limits on the memory storage capacity of bounded synapses," *Nat. Neurosci.* **10** (Apr, 2007) 485–493.

08discrete [9] A. B. Barrett and M. C. van Rossum, "Optimal learning rules for discrete synapses," *PLoS Comput. Biol.* **4** (Nov, 2008) e1000230.

diffmatexp [10] M. Ortiz, R. A. Radovitzky, and E. A. Repetto, "The computation of the exponential and logarithmic mappings and their first and second linearizations," *International Journal for Numerical Methods in Engineering* **52** (2001) no. 12, 1431–1441.

2002kemeny [11] M. Levene and G. Loizou, "Kemeny's constant and the random surfer," *The American mathematical monthly* **109** (2002) no. 8, 741–745.