1 Matrix exponentials

1.1 SVD for reversible Q

For reversible $\boldsymbol{Q}$, we have

$$\pi_i Q_{ij} = \pi_j Q_{ji}.$$

Thus, $\pi_i Q_{ij}$ is symmetric. Therefore, if we multiply both sides by the symmetric matrix $1/\sqrt{\pi_i \pi_j}$ the result is also symmetric:

$$S_{ij} = \pi_i Q_{ij} \cdot \frac{1}{\sqrt{\pi_i \pi_j}} = Q_{ij}\sqrt{\frac{\pi_i}{\pi_j}}.$$

We define $\Pi_{ij} = \delta_{ij} \cdot \pi_i$ to be the diagonal matrix with the frequencies π_i on the diagonal, where δ is the kronecker δ, indicating the identity matrix. We can then express this as

$$\boldsymbol{S} = \boldsymbol{\Pi}^{\frac{1}{2}} \cdot \boldsymbol{Q} \cdot \boldsymbol{\Pi}^{-\frac{1}{2}}$$

Then we have

$$\begin{aligned} \exp(\boldsymbol{Q}) &= \exp\left(\boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \boldsymbol{S} \cdot \boldsymbol{\Pi}^{\frac{1}{2}}\right) \\ &= \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \exp\left(\boldsymbol{S}\right) \cdot \boldsymbol{\Pi}^{\frac{1}{2}}. \end{aligned}$$

Now, using the SVD we can decompose $\boldsymbol{S}$ as $\boldsymbol{S} = \boldsymbol{O} \cdot \boldsymbol{D} \cdot \boldsymbol{O}^{-1}$, where $\boldsymbol{D}$ is a diagonal matrix (of eigenvalues) that is easy to exponentiate. Since S is a symmetric matrix, the eigenvalues are all real, I think, and also $\boldsymbol{O}^{-1} = \boldsymbol{O}^t$.

$$\begin{aligned} \exp \boldsymbol{Q}t &= \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \exp\left(\boldsymbol{O} \cdot \boldsymbol{D}t \cdot \boldsymbol{O}^{-1}\right) \cdot \boldsymbol{\Pi}^{\frac{1}{2}} \\ &= \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \left[\boldsymbol{O} \cdot \exp \boldsymbol{D}t \cdot \boldsymbol{O}^{-1}\right] \cdot \boldsymbol{\Pi}^{\frac{1}{2}}. \end{aligned}$$

However, this will not yield $\exp \boldsymbol{Q}t = \boldsymbol{I}$ when $t = 0$ because the $\exp D_i t$ terms will be ≈ 1, leading to roundoff errors (on the order of 1e-15) I think. We can instead compute

$$\begin{aligned} \exp \boldsymbol{Q}t - \boldsymbol{I} &= \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \left[\boldsymbol{O} \cdot \exp \boldsymbol{D}t \cdot \boldsymbol{O}^{-1}\right] \cdot \boldsymbol{\Pi}^{\frac{1}{2}} - \boldsymbol{I} \\ &= \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \left[\boldsymbol{O} \cdot \exp \boldsymbol{D}t \cdot \boldsymbol{O}^{-1}\right] \cdot \boldsymbol{\Pi}^{\frac{1}{2}} - \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \boldsymbol{I} \cdot \boldsymbol{\Pi}^{\frac{1}{2}} \\ &= \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \left[\boldsymbol{O} \cdot \exp \boldsymbol{D}t \cdot \boldsymbol{O}^{-1} - \boldsymbol{I}\right] \cdot \boldsymbol{\Pi}^{\frac{1}{2}} \\ &= \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \left[\boldsymbol{O} \cdot \exp \boldsymbol{D}t \cdot \boldsymbol{O}^{-1} - \boldsymbol{O} \cdot \boldsymbol{I} \cdot \boldsymbol{O}^{-1}\right] \cdot \boldsymbol{\Pi}^{\frac{1}{2}} \\ &= \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \left[\boldsymbol{O} \cdot (\exp \boldsymbol{D}t - \boldsymbol{I}) \cdot \boldsymbol{O}^{-1}\right] \cdot \boldsymbol{\Pi}^{\frac{1}{2}}, \end{aligned}$$

leading to the formula

$$\exp \boldsymbol{Q}t = \boldsymbol{I} + \boldsymbol{\Pi}^{-\frac{1}{2}} \cdot \left[\boldsymbol{O} \cdot (\exp \boldsymbol{D}t - I) \cdot \boldsymbol{O}^{-1}\right] \cdot \boldsymbol{\Pi}^{\frac{1}{2}}.$$

where $\exp \boldsymbol{D}t - \boldsymbol{I}$ is computed by applying the expm1 function to the entries of $\boldsymbol{D}$. The benefit of this approach is that when t is close to 0, the expm1 terms will all be proportional to t, thus yielding $\exp \boldsymbol{Q}t = \boldsymbol{I}$ when $t = 0$.