

MAP Estimates of trap parameters from position velocity data

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Sufficient Statistic Matrices and MAP estimate matrices

We have position velocity data $\mathbf{x} = [x(t), v(t)]^T$ at our disposal. (x_1, x_2, \dots, x_N) are the positions of the particle at times $t = n\Delta t$ where $n = 1, 2, \dots, N$. Similarly (v_1, v_2, \dots, v_N) are observed velocities of the particles at corresponding times. Hence the position velocity data matrix is a $N \times 2$ matrix, where N is the number of observations. Our first objective is to evaluate the sufficient matrices T_1, T_2 and T_3

$$\begin{aligned} T_1 &= \sum \mathbf{x}_{n+1} \mathbf{x}_{n+1}^T \\ &= \sum_{n=1}^{N-1} \begin{pmatrix} x_{n+1} \\ v_{n+1} \end{pmatrix} \begin{pmatrix} x_{n+1} & v_{n+1} \end{pmatrix} \\ &= \begin{pmatrix} \sum_{n=1}^{N-1} x_{n+1}^2 & \sum_{n=1}^{N-1} x_{n+1} v_{n+1} \\ \sum_{n=1}^{N-1} x_{n+1} v_{n+1} & \sum_{n=1}^{N-1} v_{n+1}^2 \end{pmatrix} \end{aligned}$$

Similarly

$$\begin{aligned} T_2 &= \begin{pmatrix} \sum_{n=1}^{N-1} x_{n+1} x_n & \sum_{n=1}^{N-1} x_{n+1} v_n \\ \sum_{n=1}^{N-1} x_n v_{n+1} & \sum_{n=1}^{N-1} v_{n+1} v_n \end{pmatrix} \\ T_3 &= \begin{pmatrix} \sum_{n=1}^{N-1} x_n^2 & \sum_{n=1}^{N-1} x_n v_n \\ \sum_{n=1}^{N-1} x_n v_n & \sum_{n=1}^{N-1} v_n^2 \end{pmatrix} \end{aligned}$$

Now, we have to estimate the $\boldsymbol{\lambda}^*$ and $\boldsymbol{\Sigma}^*$ matrices using the results from equations 12(a) and 12(b) from our paper

$$\boldsymbol{\lambda}^* = -\frac{1}{\Delta t} \ln(T_2 T_3^{-1}),$$

$$\boldsymbol{\Sigma}^* = \frac{1}{N} \left(T_1 - T_2 T_3^{-1} T_2^T \right).$$

Determination of trap parameters m , k and γ from λ^* and Σ^*

We know that the covariance matrix c at equilibrium is given by

$$c = \begin{pmatrix} \frac{k_B T}{k} & 0 \\ 0 & \frac{k_B T}{m} \end{pmatrix}$$

We denote $\Lambda = \exp(-\lambda \Delta t)$. Using the Onsager relation $c^* = \left[\mathbf{1} - \epsilon_i \epsilon_j e^{-2(\lambda^*)^T \Delta t} \right]^{-1} \Sigma^*$ or using the following linear system

$$\begin{pmatrix} \frac{k_B T}{k^*} \\ \frac{k_B T}{m^*} \end{pmatrix} = \begin{pmatrix} 1 - \Lambda_{11}^{*2} & -\Lambda_{12}^{*2} \\ -\Lambda_{21}^{*2} & 1 - \Lambda_{22}^{*2} \end{pmatrix}^{-1} \begin{pmatrix} \Sigma_{11}^* \\ \Sigma_{22}^* \end{pmatrix}$$

we can get the estimates for m^* and k^* , the mass of the particle and the trap stiffness respectively. Now, the explicit form of the matrix exponential $\Lambda = \exp(-\lambda \Delta t)$ is given by

$$\Lambda = \exp(-\lambda \Delta t) = \exp\left(-\frac{\Delta t}{2\tau}\right) \left[\cos(\omega \Delta t) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sin(\omega \Delta t) \begin{pmatrix} \frac{1}{2\omega\tau} & \frac{1}{\omega} \\ -\frac{\omega_0^2}{\omega} & -\frac{1}{2\omega\tau} \end{pmatrix} \right]$$

Similarly, the diagonal element of the variance covariance matrix $\langle xv \rangle$ is given by

$$\Sigma_{12} = \sigma_{xv}^2 = \frac{D}{\omega^2 \tau^2} \exp\left(\frac{-\Delta t}{\tau}\right) \sin^2(\omega \Delta t)$$

$$\text{Now } \Lambda_{12} = \exp\left(-\frac{\Delta t}{2\tau}\right) \frac{\sin(\omega \Delta t)}{\omega}$$

Thus, using the relations $D = \frac{k_B T}{\gamma}$ and $\tau = \frac{m}{\gamma}$, it is easy to see that

$$\gamma^* = \frac{m^{*2} \Sigma_{12}^*}{k_B T \Lambda_{12}^{*2}}$$

where m^* has been estimated in the previous step.

Stationary Estimates

The stationary estimates are straightforward and are given by

$$\frac{k^*}{k_B T} = \frac{N}{\sum_{n=1}^N x_n^2}, \quad \frac{m^*}{k_B T} = \frac{N}{\sum_{n=1}^N v_n^2}.$$