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 $\boldsymbol{x} = [x(t), v(t)]^T$ at our disposal. $(x_1, x_2, ..., x_N)$ are the positions of the particle at times $t = n\Delta t$ where $n = 1, 2, .., N$. Similarly $(v_1, v_2, ..., v_N)$ 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

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

Similarly

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

$$
\boldsymbol{T_3} = \begin{pmatrix} \sum_{n=1}^{N-1} x_n^2 & \sum_{n=1}^{N-1} x_n v_n \\ \sum_{n=1}^{N-1} x_n v_n & \sum_{n=1}^{N-1} v_n^2 \end{pmatrix}
$$

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

$$
\boldsymbol{\lambda}^* = -\frac{1}{\Delta t} \ln(\boldsymbol{T}_2 \boldsymbol{T}_3^{-1}),
$$

$$
\boldsymbol{\Sigma}^* = \frac{1}{N} \left(\boldsymbol{T}_1 - \boldsymbol{T}_2 \boldsymbol{T}_3^{-1} \boldsymbol{T}_2^T \right).
$$

Determination of trap parameters m, k and γ from $\boldsymbol{\lambda}^*$and $\boldsymbol{\Sigma}^*$

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 $\boldsymbol{\Lambda} = \exp(-\boldsymbol{\lambda}\Delta t)$. Using the Onsager relation $\boldsymbol{c}^* = \left[\mathbf{1} - \epsilon_i \epsilon_j e^{-2(\boldsymbol{\lambda}^*)^T \Delta t}\right]^{-1} \boldsymbol{\Sigma}^*$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 $\boldsymbol{\Lambda} = \exp(-\boldsymbol{\lambda}\Delta t)$ is given by

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

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

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

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

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.

Derivation of the linear relation for the diagonal covariance matrix

We have the relation

$$\boldsymbol{\Sigma} \equiv \boldsymbol{c} - \boldsymbol{e}^{-\boldsymbol{\lambda}\boldsymbol{\Delta t}}\boldsymbol{c}\boldsymbol{e}^{-\boldsymbol{\lambda}^{T}\boldsymbol{\Delta t}}$$

Now we assume the covariance matrix to be diagonal at equilibrium, since the cross correlation terms are assumed to decay to zero as $t \to \infty$. Thus for the two dimensional system, we have

$$\boldsymbol{c} = \begin{pmatrix} c_{11} & 0 \\ 0 & c_{22} \end{pmatrix}$$

Using the notation $\boldsymbol{\Lambda} = \exp\left(-\boldsymbol{\lambda}\Delta t\right)$

$$\begin{pmatrix} c_{11} & 0 \\ 0 & c_{22} \end{pmatrix} - \begin{pmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{21} & \Lambda_{22} \end{pmatrix} \begin{pmatrix} c_{11} & 0 \\ 0 & c_{22} \end{pmatrix} \begin{pmatrix} \Lambda_{11} & \Lambda_{21} \\ \Lambda_{12} & \Lambda_{22} \end{pmatrix} = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

Expanding the product

$$\begin{pmatrix} c_{11} & 0 \\ 0 & c_{22} \end{pmatrix} - \begin{pmatrix} c_{11}\Lambda_{11}^2 + c_{22}\Lambda_{12}^2 & M_{12} \\ M_{21} & c_{11}\Lambda_{21}^2 + c_{22}\Lambda_{22}^2 \end{pmatrix} = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

Now we equate the matrix elements on the LHS to the corresponding elements on the RHS. We consider only the diagonal elements, and thus the quantities M_{12} and M_{21}have been ignored. Now, constructing a linear system by taking the diagonal elements of the above matrix equation.

$$c_{11} - \left(c_{11}\Lambda_{11}^2 + c_{22}\Lambda_{12}^2\right) = \Sigma_{11}$$

$$c_{22} - \left(c_{11}\Lambda_{21}^2 + c_{22}\Lambda_{22}^2\right) = \Sigma_{22}$$

Using the vector matrix equation form for the linear system

$$\begin{pmatrix} 1 - \Lambda_{11}^2 & -\Lambda_{12}^2 \\ -\Lambda_{21}^2 & 1 - \Lambda_{22}^2 \end{pmatrix} \begin{pmatrix} c_{11} \\ c_{22} \end{pmatrix} = \begin{pmatrix} \Sigma_{11} \\ \Sigma_{22} \end{pmatrix}$$

Thus we have the elements of the stationary covariance matrix as

$$\begin{pmatrix} c_{11} \\ c_{22} \end{pmatrix} = \begin{pmatrix} 1 - \Lambda_{11}^2 & -\Lambda_{12}^2 \\ -\Lambda_{21}^2 & 1 - \Lambda_{22}^2 \end{pmatrix}^{-1} \begin{pmatrix} \Sigma_{11} \\ \Sigma_{22} \end{pmatrix}$$

Stationary Estimates

The stationary estimates are straightforward and are given by

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