Unbiased Statistical Estimators for pathwise FIM and IAT

In both stationary and transient regimes, the numerical computation of the pathwise FIM as well as the variance of the time-averaged observable (IAT) should be performed. For the sake of completeness, we present the statistical estimators of these quantities which require simulations only from the unperturbed process, \( X_t \), i.e., only for the parameter value, \( \theta \). For both regimes, the unnormalized pathwise FIM can be written as (see S1 File)

\[
I(Q^n_{(0,T)}) = E_{Q^n_{(0,T)}} \left[ \int_0^T \sum_{j=1}^J a_j^\theta(X_{t-}) \nabla_\theta \log a_j^\theta(X_{t-}) \nabla_\theta \log a_j^\theta(X_{t-})^T dt \right],
\]

where we assume that both processes started from the same distribution, \( \nu \). Then, the \( n \)-th sample of the unbiased estimator for the pathwise FIM is given by \([1,2]\)

\[
\bar{I}^{(n)} = \frac{1}{N_T} \sum_{i=0}^{N_T} \delta t_i^{(n)} \sum_{j=1}^J a_j^\theta(x_i^{(n)}) \nabla_\theta \log a_j^\theta(x_i^{(n)}) \nabla_\theta \log a_j^\theta(x_i^{(n)})^T + (T - \sum_{i=0}^{N_T} \delta t_i^{(n)}) \sum_{j=1}^J a_j^\theta(x_{N_T}^{(n)}) \nabla_\theta \log a_j^\theta(x_{N_T}^{(n)}) \nabla_\theta \log a_j^\theta(x_{N_T}^{(n)})^T.
\]

where \( \delta t_i^{(n)} \) is an exponential random variable with parameter given by the total rate, \( a_0^\theta(x_i^{(n)}) \), while \( N_T^{(n)} \) is the number of jumps up to time \( T \). The sequence \( \{x_i^{(n)}\}_{i=0}^{N_T^{(n)}} \) is the embedded Markov chain with transition probabilities from state \( x_i^{(n)} \) to state \( x_{i+1}^{(n)} \) given by the ratio \( a_j^\theta(x_i^{(n)}) / a_j^\theta(x_{i+1}^{(n)}) \). The weight \( \delta t_i^{(n)} \), which is the waiting time at state \( x_i^{(n)} \), is necessary for the unbiased estimation of the average value, \([3]\). Notice also that \( \delta t_i^{(n)} \) can be replaced by its average which is the inverse of the total rate, \( a_0^\theta(x_i^{(n)})^{-1} \). Then, assuming that we simulate \( N \) trajectories, the unbiased estimator for the pathwise FIM is simply

\[
\bar{I} = \frac{1}{N_T} \sum_{n=1}^N \bar{I}^{(n)}.
\]

Along the same lines, unbiased estimators for the relative entropy and the relative entropy rate can be obtained, \([1,2]\).

Next, we discuss the computation of the variance of a time-averaged observable function. The unnormalized time-averaged observable for fixed \( T \) is given by

\[
F = E_{Q^n_{(0,T)}} \left[ \int_{t=0}^T f(X_t) dt \right].
\]
The unbiased estimator of $F$ for the $n$–th realization is

$$
\hat{F}^{(n)} = \sum_{i=0}^{N_{T}^{(n)}-1} \delta t_i^{(n)} f(x_i^{(n)}) + (T - \sum_{i=0}^{N_{T}^{(n)}-1} \delta t_i^{(n)}) f(x_{N_{T}^{(n)}}).
$$

Then, the unbiased estimator of the mean of $F$ is given by

$$
\bar{F} = \frac{1}{N} \sum_{n=1}^{N} \hat{F}^{(n)},
$$

while the unbiased estimator of the variance of $F$ is given by

$$
\bar{\sigma}_F^2 = \frac{1}{N-1} \sum_{n=1}^{N} (\hat{F}^{(n)} - \bar{F})^2.
$$

We can obtain a statistical estimator for the sensitivity indices based on the coupling method (see File S3) along the same lines.

**References**

