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An Introduction to Markov State Models and Their Application to Long Timescale Molecular Simulation

Springer

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Acronyms

ESR	Electron spin resonance
MD	Molecular dynamics (simulation)
MSM	Markov state model
PCCA	Perron cluster cluster analysis
TPT	Transition path theory
TPS	Transition path sampling

Mathematical Symbols

$\mathbf{T}(\tau)$ A transition probability matrix (row-stochastic) in $\mathbb{R}^{n\times n}$ describing the probabilities of hopping amongst a discrete set of states. The elements $T_{ij}(\tau)$ give the probability of an $i \to j$ transition during a time interval τ.

$\hat{\mathbf{T}}(\tau)$ An estimate of $\mathbf{T}(\tau)$ from trajectory data.

$\mathbf{C}(\tau)$ A transition count matrix (row-dominant) in $\mathbb{R}^{n\times n}$ describing the number of transitions observed amongst a discrete set of states. The elements $c_{ij}(\tau)$ count the number of $i \to j$ transitions observed, each of which occurred during a time interval τ.

τ The time resolution (or lag time) of a model.

n The number of discrete states.

$\mathbf{p}(t)$ A (column) vector in $\mathbb{R}^n$ where the entry $\mathbf{p}_i(t)$ specifies the probability of being in state i at time t.

$\boldsymbol{\pi}$ A (column) vector in $\mathbb{R}^n$ where the entry $\boldsymbol{\pi}_i$ specifies the equilibrium probability of being in state i.

λ_i The i'th largest eigenvalue of a transition probability matrix T. The largest eigenvalue is λ_1 and eigenvalues are ordered such that $1 = \lambda_1 > \lambda_2 > \lambda_3$.

$\boldsymbol{\psi}_i$ The i'th right eigenvector of a transition probability matrix T in $\mathbb{R}^n$. The first right eigenvector is $\boldsymbol{\psi}_1$.

$\boldsymbol{\phi}_i$ The i'th left eigenvector of a transition probability matrix T in $\mathbb{R}^n$. The first left eigenvector is $\boldsymbol{\phi}_1$.

χ_i An indicator function for state i that is 1 within state i and 0 elsewhere. It may also refer to the degree of membership in state i.

$\boldsymbol{\theta}_i$ An experimental observable characteristic of sate i.

q_i The commitor probability for state i. That is, the probability of reaching some predefined set of final states from state i before reaching some predefined set of initial states.

Ω A continuous state space (including positions and momenta).

$\mathbf{x}(t)$ A state in Ω (including positions and momenta) at time t.

$\mu(\mathbf{x})$ The stationary density of $\mathbf{x}$.

$p(\mathbf{x}, \mathbf{y}; \tau)$ The transition probability density to $\mathbf{y} \in \Omega$ after time τ given the system is in $\mathbf{x} \in \Omega$.

$\mathcal{T}(\tau)$	A transfer operator that propagates the continuous dynamics for a time τ.
m	The number of dominant eigenfunctions/eigenvalues considered.
$S_1, \ldots, S_n$	Discrete sets which partition the state space Ω.
$\mu_i(\mathbf{x})$	The local stationary density restricted to a discrete state i.
$\langle f, g\rangle$	The scalar product $\langle f, g\rangle = \int f(\mathbf{x})g(\mathbf{x})\,d\mathbf{x}$.
$\langle f, g\rangle_\mu$	The weighted scalar product $\langle f, g\rangle_\mu = \int \mu(\mathbf{x})f(\mathbf{x})g(\mathbf{x})\,d\mathbf{x}$.