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Advances in the Projective Dynamics Method: A Procedure of Discretizing the Space applied to Markovian Processes

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Abstract

The projection of a continuous space process to a discrete space process via the transition rates between neighboring bins allows us to relate a master equation to a solution of a stochastic differential equation. The presented method is formulated in its general form for the first time and tested with the Brownian Diffusion process of noninteracting particles with white noise in simple one-dimensional potentials. The comparison of the first passage time obtained with Projective Dynamics, Brownian motion simulations and analytical solutions show the accuracy of this method as well as a wide independence of the particular choice of the binning process.

1. Introduction

The Projective Dynamics method [1, 2, 3] was initially formulated for problems with a discrete state space. As a projection process from a continuous to a discrete space, it has already been used for the description of the dynamics of spin systems [4, 5]. By obtaining the transition rates between neighboring states and calculating the residence times, the first passage time and also a free energy landscape can be obtained. Thus far the method has always been limited to an all-spin-up starting configuration.

To be carried forward into a descriptive tool for biophysical phenomena there is a need to generalize the method. Since it is possible to obtain first passage time distributions in single-molecule folding experiments [6], it appears to be crucial for the detailed understanding of the folding dynamics to obtain first passage times for any particular starting configuration of the system.

2. Method: Discretizing the Space, Markovian Procedure

To obtain a description of the trajectory of a Markovian process at discrete values of space, we need first to assign a (discrete) space value to a (continuous) space interval. This can be done by dividing the space coordinate into nonoverlapping bins.

The size of the bin should be chosen to be larger than the maximum possible particle trajectory in a single step. In practice, this can be met for the particular statistics used in the measurement. We now assume that the process probability distribution can be fully recovered from knowing only its transition probabilities between neighboring bins (interpreted as states).

We place the absorbing boundary in bin zero and refer to growing (shrinking) as moving towards (away from) the absorbing state. The growing probability g_k describes then the conditional probability of leaving bin k to $k-1$ given the system being in state k. And the shrinking probability s_k describes the conditional probability of leaving bin k to $k+1$ given the system being in state k.

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We obtain a master equation with nearest-neighbor coupling

$$\frac{\mathrm{d}}{\mathrm{d}t}P(k,t) = g_{k+1}P(k+1,t) - \left[g_k + s_k\right]P(k,t) + s_{k-1}P(k-1,t). \tag{1}$$

Here $P(k,t)$ is the probability of occupation of state k at time t, and the growing and shrinking probabilities represent the transition rates between neighboring states.

By using the fundamental relations [7]

$$\frac{\mathrm{d}}{\mathrm{d}t}P(k,t) = \sum_{k'} W(k,k')P(k',t) \tag{2}$$

and

$$\sum_{k} \tau(k)W(k,k') = -1 \tag{3}$$

the general expression for the first passage time can be written as

$$\tau(S_o) = \sum_{i=1}^{S_o} \frac{1}{g_i} + \sum_{D=1}^{S-1}\left[\sum_{i=1}^{\min(S_o,|S-D|)}\left(\frac{\prod_{j=i}^{i+D-1} s_j}{\prod_{j=i}^{i+D} g_j}\right)\right] \tag{4}$$

where S_o denotes the starting bin and S the total number of bins. The bins are numbered such that bin number 1 lies at the absorbing boundary.

It is important to note that the values of the first passage time obtained from (4) are in the unit of the underlying (continuous) integration step. To obtain a scale free value, one has to multiply the results of (4) with the corresponding time step, $\mathrm{d}t$.

A condition for this method to work is that the binning covers the full trajectory space and that the neighboring states in the underlying dynamics are accessible to each other. The last is fulfilled for the inner bins whenever the time of leaving the domain is finite. If the outer bins (beyond S_o) are empty throughout the whole measurement process one obtains the first passage time by omitting these empty states.

3. Results

The method is tested with the one-dimensional diffusion equation

$$\frac{\partial}{\partial t}x(t) = -\frac{1}{\eta}\frac{\partial}{\partial x}U(x) + \Gamma(t), \tag{5}$$

where the white noise term Γ is given by

$$\langle \Gamma(t)\Gamma(t')\rangle = 2\frac{\mathrm{k}_B T}{\eta}\delta(t-t') \tag{6}$$

with reduced friction constant $\eta = 1.0$ and $\mathrm{k}_B = 1.0$.

The trajectories have been integrated in a simple Euler scheme with a white noise generator [8] along $N = 5000$ paths. In our work the time steps of the Brownian motion ranged from $\mathrm{d}t = 2.5 \times 10^{-6}$ up to 2.0×10^{-5}. The measurements of the growing and shrinking probabilities of the Projective Dynamics method for different bin width have been taken from the same set of trajectories for the same temperatures.

3.1. Absorption Process in Square Potential

The potential is

$$U(x) = \begin{cases} \infty & \text{if } x < 0, \\ 0 & \text{if } 0 \le x \le 1, \\ -\infty & \text{if } x > 1. \end{cases} \tag{7}$$

Defining the domain as the interval $x \epsilon [0, 1]$ we tested the method for $S = 5, 10$ and 20 bins of equal length. The trajectories are started at the origin, which corresponds to bin $S_o = 5, 10$ and 20. First passage times have been obtained at the temperatures $T = 0.1, 0.075, 0.05$ and 0.025.

Our results show that the numerical values of the mean first passage time from Projective Dynamics deviates less than 1% from the analytical solutions. Furthermore, our work appears to suggest that for a fixed computational effort the Projective Dynamics (for this simple potential) provides a more accurate statistical estimate of the mean first passage time than does Brownian motion at low temperatures. The values of the mean first passage time are presented in Table (1). Our results indicate a wide independence with the number of bins, which provides a freedom in the choice of the particular binning procedure.

3.2. Absorption Process in Kramers Potential

In this example free particles are subject to the potential

$$U(x) = -\frac{a}{2}x^2 + \frac{b}{4}x^4, \tag{8}$$

where $a = 1.0$ and $b = 1.25$.

The domain is defined as the interval $x \epsilon [-\infty, 0]$. First passage times have been obtained at the temperatures $T = 0.1, 0.075$ and 0.05. The trajectories are started as a delta function at $x = -0.9$, which corresponds to the initial states $S_o = 3$ (for $S = 5$ total bins), $S_o = 9$ ($S = 10$) and $S_o = 10$ ($S = 20$). The space intervals are of equal length covering the interval $x \epsilon [-2.0, 0.0]$.

Here we compared the results of the Projective Dynamics method to those of a Brownian motion simulation and of a semi-analytic Riemann integration. The values of the mean first passage time are presented in Table (2). The Projective Dynamics method is stable within a 3% deviation at different time steps and also these results are in good agreement with both the Brownian motion measurement and the Riemann integration. Furthermore, our results indicate that the values of the mean first passage time obtained with Projective Dynamics are stable (within the statistical deviation) against the chosen binning procedure.

4. Conclusions

We have applied a generalized Projective Dynamics method to obtain the mean [1] first passage time for two simple potentials. Our study suggests that the method correctly reproduces the values of the mean first passage time compared to analytical and semi-analytical solutions [see Fig. (1)]. We have analyzed the behavior of the first passage time for different time steps of the underlying dynamics and demonstrated that the method itself is stable within 1% (square potential) and 3% (Kramer's potential) deviation for our statistics in measuring g_k and s_k. A comparison with Brownian motion shows a better prediction of the mean first passage times at the temperatures $T = 0.05, 0.025$ (square potential) and $T = 0.075$ (Kramer's potential) with Projective Dynamics than with simple measurements with the same statistics.

The values for the mean first passage time where obtained with three different numbers of bins (of fixed length). The comparison of results for $S = 5, 10$ and 20 showed no difference for the square potential and a difference within the statistical error for the Kramers potential.

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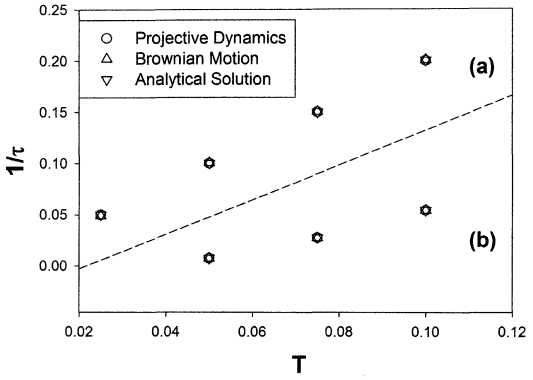

Figure 1: Reciprocal mean first passage times τ at different temperatures. Comparison of Projective Dynamics with Brownian motion simulation and analytical solutions for square potential (a) and Kramer's potential (b). The dashed line only separates (a) and (b) portions of the graph.

Table 1: First passage times, square potential

	Projective	Dynamics		Brownian	analytical
T	$S = 5$	$S = 10$	$S = 20$	motion	solution
0.1	5.01(±0.03)	5.01(±0.03)	5.01(±0.03)	4.99(±0.04)	5.00
0.075	6.68(±0.04)	6.68(±0.04)	6.68(±0.04)	6.66(±0.04)	6.67
0.05	10.01(±0.06)	10.01(±0.06)	10.01(±0.06)	9.96(±0.07)	10.00
0.025	20.0(±0.1)	20.0(±0.1)	20.0(±0.1)	20.3(±0.1)	20.00

Table 2: First passage times, Kramers potential

	Projective	Dynamics		Brownian	Riemann
T	$S = 5$	$S = 10$	$S = 20$	motion	integration
0.1	18.5(±0.2)	18.5(±0.2)	18.5(±0.2)	18.4(±0.2)	18.44
0.075	36.7(±0.4)	36.7(±0.4)	36.7(±0.4)	36.9(±0.4)	36.46
0.05	135(±3)	136(±3)	136(±3)	136(±3)	135.8