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Approaching a parameter-free metadynamics

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We present a unique derivation of metadynamics. This work leads to a more robust understanding of the error in the computed free energy than what has been obtained previously. Moreover, a formula for the exact free energy is introduced. The formula can be used to post-process any existing well-tempered metadynamics data allowing one, in principle, to obtain an exact free energy regardless the metadynamics parameters.

The last decade has seen the introduction of a number of adaptive biasing techniques developed for free energy computation.[1–4] In practice, these techniques accumulate a biasing potential or a biasing force during trajectory evolution. The goal is to specify a biasing force or potential that will effectively flatten the free energy landscape and enhance sampling. Here we focus on a particular adaptive biasing potential (ABP) method called metadynamics, introduced in references 5 and 6. Metadynamics is an ABP method that has been widely used for chemical, solid state and biological systems.[7]

One area of metadynamics that can still be improved upon is that of the dependence of the error in the computed free energy on the metadynamics parameters.[8–10] Metadynamics requires one to specify several system dependent parameters. The parameters are the energy rate, which is the product of the Gaussian height and the deposition period, and the Gaussian width.[8] The error associated with these is mostly well understood, with one exception: The Gaussian width. At present, the analytic error estimates suggest that, for fixed computational time, the error decreases as the Gaussian width increases[8,9] while numerical experiments reveal that the error will actually increase in the limit of large Gaussian widths and that the empirically derived error estimate will break down[8].

Below, we derive metadynamics in a novel way. Originally, the goal was to propose an adaptive biasing scheme with on-the-fly reweighting (as in references 3,4) and then, by an approximation, show that the reweighting factors could be removed. The problem with the on-the-fly reweighting methods is that they are difficult to study formally because of the time-dependent reweighting. The hope was to introduce an ABP method that was free from these reweighting factors, allowing it to be studied rigorously like metadynamics and adaptive biasing force methods.[11] However, this process leads one directly to metadynamics, both the well-tempered and standard forms. This derivation accentuates an interpretation that leads to an understanding of the error incurred by choosing a finite Gaussian width and ultimately affords an exact expression for the free energy, independent of the Gaussian width. In other words, a formula follows from this interpretation that is exact even for finite Gaussian width. This formula could be used to post-process any existing well-tempered metadynamics data. We also stress that the biased dynamics can be cast in a form consistent with the dynamics studied in reference 11; The biasing force can be expressed as an average taken over replicas of the system rather than an average over time. It is expected that because of this, it will be possible to obtain convergence results for the well-tempered metadynamics without assuming "instantaneous equilibration" of the dynamics. Convergence results have already been obtained for the standard metadynamics without this assumption.[11]

Below we present the derivation by first introducing the on-the-fly reweighting strategy and then introducing our approximations. Once metadynamics is recovered we present an error estimate and an exact formula for free energy.

Let $\boldsymbol{x}$ be a single configuration in the n-dimensional configuration space $\mathcal{X}$ of some interesting dynamical system. For this system, assume N collective variables (CVs) have been specified and further suppose that the CVs are good descriptors of the interesting features of $\mathcal{X}$. The CV space is Ω. Let $\boldsymbol{\xi}$ denote a point in Ω. Following reference 4, let us define the mollified free energy (up to an arbitrary constant ζ)

$$\zeta e^{-\beta A_\alpha(\boldsymbol{\xi})} = Z^{-1}\int_{\mathcal{X}} \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x})-\boldsymbol{\xi})\, e^{-\beta V(\boldsymbol{x})}\, d\boldsymbol{x}, \tag{1}$$

where

$$\delta_\alpha(\boldsymbol{\xi}) = \exp\left(-\frac{|\boldsymbol{\xi}|^2}{\alpha^2}\right). \tag{2}$$

Let Z absorb the normalization of δ_α. In the limit $\alpha \to 0$ this is the exact free energy. When α is finite, the exact free energy can in principal be recovered via deconvolution[4] and we will later make use of this.

In practice, (1) would be computed via trajectory averages. Let $\boldsymbol{x}_t$ be a trajectory solving the following Langevin equation,

$$d\dot{\boldsymbol{x}}_t = -f\dot{\boldsymbol{x}}_t dt - \nabla V(\boldsymbol{x}_t)dt + \sqrt{2f\beta^{-1}}d\boldsymbol{B}_t$$

where we assume it to be ergodic with respect to the Boltzmann density on $\mathcal{X}$, f is the Langevin friction coefficient and β is the inverse temperature. The random force $d\boldsymbol{B}_t$ is given by the increments of a Brownian motion.

Defining the population at $\boldsymbol{\xi}$

$$g(\boldsymbol{\xi},t)=\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})\,ds \tag{3}$$

and

$$Z_t=\int_\Omega g(\boldsymbol{\xi},t)d\boldsymbol{\xi}, \tag{4}$$

the free energy may be computed from a long trajectory $\boldsymbol{x}_t$ as

$$\zeta\, e^{-\beta A_\alpha(\boldsymbol{\xi},t)}=Z_t^{-1}g(\boldsymbol{\xi},t), \tag{5}$$

where at $t=0$

$$Z_0^{-1}g(\boldsymbol{\xi},0)=\frac{\delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_0)-\boldsymbol{\xi})}{\alpha\sqrt{\pi}}. \tag{6}$$

Now, we propose the following on-the-fly reweighting scheme to compute (5) via an adaptive biasing potential. In this case we propose the biasing potential

$$e^{\beta V_b(\boldsymbol{\xi},t)}=(cg(\boldsymbol{\xi},t)+1)^b \tag{7}$$

where b and c are scalars. b controls the strength of the bias and c is a coupling parameter with units of inverse time. With the bias defined this way, the initial conditions for the biased dynamics reduce to those of the unbiased case and $0\le V_b$.

Using this bias potential, one can write the mollified free energy as time averages over Langevin trajectories driven by $V+V_b$ with on-the-fly reweighting,

$$\zeta e^{-\beta A_\alpha(\boldsymbol{\xi},t)}=Z_t^{-1}g(\boldsymbol{\xi},t), \tag{8}$$

where

$$g(\boldsymbol{\xi},t)=\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})e^{\beta V_b(\boldsymbol{\xi}(\boldsymbol{x}_s),s)}\,ds \tag{9}$$

and

$$Z_t=\int_\Omega g(\boldsymbol{\xi},t)d\boldsymbol{\xi}. \tag{10}$$

It is natural for the development of the ABP method to terminate here; these equations could be implemented as-is. See reference 4 for example.

In this case one can go a bit further, however, by introducing an approximation to (9). The idea behind the following manipulations is to derive an expression for $g(\boldsymbol{\xi},t)$ in which the factor $\exp[\beta V_b]$ does not appear. Once obtained, we recover metadynamics. Using a first-order expansion $V_b(\boldsymbol{\xi}(\boldsymbol{x}_t),t)\approx V_b(\boldsymbol{\xi},t)+V_b'(\boldsymbol{\xi},t)\cdot(\boldsymbol{\xi}(\boldsymbol{x}_t)-\boldsymbol{\xi})$ and an expansion of e^y, we obtain

$$\begin{aligned}g(\boldsymbol{\xi},t)&\approx\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})e^{\beta V_b(\boldsymbol{\xi},s)}e^{\beta V_b'(\boldsymbol{\xi},s)\cdot(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})}\,ds\\ &\approx\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})e^{\beta V_b(\boldsymbol{\xi},s)}(1+\beta V_b'(\boldsymbol{\xi},s)\cdot(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi}))\,ds\\ &=\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})e^{\beta V_b(\boldsymbol{\xi},s)}ds+\Delta(\alpha).\end{aligned} \tag{11}$$

The last term is roughly the error between the populations computed by (9) and the population computed with the first term in the last line of (11) where,

$$\Delta(\alpha)=\frac{\alpha^2\,\beta}{2}\int_0^t \delta_\alpha'(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})\cdot V_b'(\boldsymbol{\xi},s)e^{\beta V_b(\boldsymbol{\xi},s)}ds. \tag{12}$$

Ignoring $\Delta(\alpha)$, the final line in (11) can be seen as an integral solution to the differential equation

$$\frac{dg(\boldsymbol{\xi},t)}{dt}=\delta_\alpha(\boldsymbol{\xi}(x_t))-\boldsymbol{\xi})e^{\beta V_b(\boldsymbol{\xi},t)},$$

which can be solved via separation of variables

$$g(\boldsymbol{\xi},t)=\frac{1}{c}\left(\left(c(1-b)\int_0^t \delta_\alpha(\boldsymbol{\xi}(x_s)-\boldsymbol{\xi})ds+1\right)^{\frac{1}{1-b}}-1\right). \tag{13}$$

To avoid the possibility of complex valued g, we restrict $c\ge 0$ and $b\le 1$. We can now express g without evaluating $\exp[\beta V_b]$.

Equations (7) and (13) combine to give the bias potential

$$V_b(\boldsymbol{\xi},t)=\beta^{-1}\frac{b}{1-b}\ln[c\,(1-b)\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})ds+1]. \tag{14}$$

In the limit $b\to 1$ the bias reduces to

$$V_b(\boldsymbol{\xi},t)=\beta^{-1}c\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})ds. \tag{15}$$

These bias potentials are the well-tempered[1] and standard metadynamics[5] bias potentials, respectively. Indeed, making the substitutions $\omega=\beta^{-1}c\,b$ and $\Delta T=\beta^{-1}b/(1-b)$ in (14), we find the well-tempered metadynamics,

$$V_b(\boldsymbol{\xi},t)=\Delta T\ln\left(\frac{\omega}{\Delta T}\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})ds+1\right). \tag{16}$$

(15) is the standard metadynamics with an energy rate of $\beta^{-1}c$. We have derived metadynamics via the approximations in (11) having started with an on-the-fly reweighting scheme.

To derive an exact expression for the free energy when $0\le b<1$, it will be useful to work with the biasing force and with averages taken over independent replicas of the dynamics, rather than averages in time. The gradient of (14) is

$$\frac{\partial V_b(\boldsymbol{\xi},t)}{\partial\xi_i}=\frac{c\,b\,\beta^{-1}\int_0^t \partial_{\xi_i}\delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})\,ds}{1+c\,(1-b)\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})\,ds}, \tag{17}$$

where

$$\partial_{\xi_i}\delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_t)-\boldsymbol{\xi})=\frac{2(\xi_i(\boldsymbol{x}_t)-\xi_i)}{\alpha^2}\delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_t)-\boldsymbol{\xi}). \tag{18}$$

In the long-time limit,

$$\frac{\partial V_b(\boldsymbol{\xi},t)}{\partial \xi_i} = \frac{b\,\beta^{-1}\displaystyle\int_0^t \partial_{\xi_i}\delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})\,ds}{(1-b)\displaystyle\int_0^t \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x}_s)-\boldsymbol{\xi})\,ds}. \tag{19}$$

Notice that in the long-time limit c vanishes. This implies that for well-tempered metadynamics the Gaussian height will not impact the long-time accuracy of the computation.

Noting the $i-$th replica of the biased dynamics with $\boldsymbol{x}_t(i)$, the replica density can be defined

$$\psi(\boldsymbol{x},t) = \lim_{M\to\infty}\frac{1}{M}\sum_{i=1}^{M} 1_{[\boldsymbol{x}_t(i)=\boldsymbol{x}]}.$$

Each replica is an independent solution to the biased Langevin-equation

$$d\dot{\boldsymbol{x}}_t = -f\dot{\boldsymbol{x}}_t dt - \nabla(V(\boldsymbol{x}_t)+V_b(\boldsymbol{\xi}(\boldsymbol{x}_t)))dt + \sqrt{2f\beta^{-1}}d\boldsymbol{B}_t. \tag{20}$$

Equation (19) can be cast as the following replica average

$$\frac{\partial V_b(\boldsymbol{\xi},t)}{\partial \xi_i} = \frac{\beta^{-1}b\displaystyle\int_{\mathcal{X}} \partial_{\xi_i}\delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x})-\boldsymbol{\xi})\psi(\boldsymbol{x},t)d\boldsymbol{x}}{(1-b)\displaystyle\int_{\mathcal{X}} \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x})-\boldsymbol{\xi})\psi(\boldsymbol{x},t)d\boldsymbol{x}}. \tag{21}$$

Assuming that when $t\to\infty$ the method converges and $\psi(\boldsymbol{x},\infty)\propto\exp[-\beta(V(\boldsymbol{x})+V_b(\boldsymbol{\xi}(\boldsymbol{x}),\infty))]$, we find that

$$\begin{aligned}
&\frac{\beta^{-1}\displaystyle\int_{\mathcal{X}} \partial_{\xi_i}\delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x})-\boldsymbol{\xi})e^{-\beta(V(\boldsymbol{x})+V_b(\boldsymbol{\xi}(\boldsymbol{x}),\infty))}d\boldsymbol{x}}{\displaystyle\int_{\mathcal{X}} \delta_\alpha(\boldsymbol{\xi}(\boldsymbol{x})-\boldsymbol{\xi})e^{-\beta(V(\boldsymbol{x})+V_b(\boldsymbol{\xi}(\boldsymbol{x}),\infty))}d\boldsymbol{x}}\\
&= \frac{\beta^{-1}\displaystyle\int_{\Omega} \partial_{\xi_i}\delta_\alpha(\bar{\boldsymbol{\xi}}-\boldsymbol{\xi})e^{-\beta(A(\bar{\boldsymbol{\xi}})+V_b(\bar{\boldsymbol{\xi}},\infty))}d\bar{\boldsymbol{\xi}}}{\displaystyle\int_{\Omega} \delta_\alpha(\bar{\boldsymbol{\xi}}-\boldsymbol{\xi})e^{-\beta(A(\bar{\boldsymbol{\xi}})+V_b(\bar{\boldsymbol{\xi}},\infty))}d\bar{\boldsymbol{\xi}}}\\
&= -\frac{\partial\mu_\alpha(\boldsymbol{\xi},\infty)}{\partial\xi_i},
\end{aligned} \tag{22}$$

where we have defined the mollified free energy in the biased ensemble μ_α. For finite α, the biasing force is thus a rescaling of the mollified mean force in the biased ensemble and $V_b = -b\,\mu_\alpha/(1-b)$ up to an additive constant. This interpretation of the biasing force in well-tempered metadynamics leads directly to an exact expression for the free energy.

Consider the exact mean force in the biased ensemble,

$$\begin{aligned}
&-\frac{\partial\mu(\boldsymbol{\xi},\infty)}{\partial\xi_i} = \frac{\beta^{-1}\displaystyle\int_{\Omega} \partial_{\xi_i}\delta(\bar{\boldsymbol{\xi}}-\boldsymbol{\xi})e^{-\beta(A(\bar{\boldsymbol{\xi}})+V_b(\bar{\boldsymbol{\xi}},\infty))}d\bar{\boldsymbol{\xi}}}{\displaystyle\int_{\Omega} \delta(\bar{\boldsymbol{\xi}}-\boldsymbol{\xi})e^{-\beta(A(\bar{\boldsymbol{\xi}})+V_b(\bar{\boldsymbol{\xi}},\infty))}d\bar{\boldsymbol{\xi}}}\\
&= -(\partial_{\xi_i}A(\boldsymbol{\xi})+\partial_{\xi_i}V_b(\boldsymbol{\xi},\infty))\\
&= -\partial_{\xi_i}A(\boldsymbol{\xi}) + \frac{b}{1-b}\partial_{\xi_i}\mu_\alpha(\boldsymbol{\xi},\infty).
\end{aligned} \tag{23}$$

The exact free energy to an unimportant constant is therefore,

$$A(\boldsymbol{\xi}) = \mu(\boldsymbol{\xi},\infty) + \frac{b}{1-b}\mu_\alpha(\boldsymbol{\xi},\infty). \tag{24}$$

What makes this expression useful is that μ can be obtained by a deconvolution of μ_α and the known Gaussian δ_α.

If one ignores the deconvolution and assumes $\mu\approx\mu_\alpha$,

$$A(\boldsymbol{\xi}) \approx -\frac{1}{b}V_b(\boldsymbol{\xi},\infty) \tag{25}$$

where the error associated with this approximation is roughly,

$$\beta^{-1}\ln\left(1+\frac{\alpha^2}{4}\left[(\beta|\mu'(\boldsymbol{\xi},\infty)|)^2\right]\right). \tag{26}$$

We have used $V_b = -b\,\mu_\alpha/(1-b)$ in (25). This error estimate was also given in reference 4 (see equation (21) there). This estimate is found by making a Taylor series expansion of $\exp[-\beta\mu(\boldsymbol{\xi},\infty)]$ in

$$e^{-\beta\mu_\alpha(\boldsymbol{\xi}^*,\infty)} = \int_\Omega \delta_\alpha(\boldsymbol{\xi}-\boldsymbol{\xi}^*)e^{-\beta\mu(\boldsymbol{\xi},\infty)}d\boldsymbol{\xi} \tag{27}$$

and keeping terms up to the first moment of δ_α. Notice that the error in well-tempered metadynamics is related to a convolution of the configurational density in the biased ensemble. In reference 4 the error was due to a convolution of the configurational density in the unbiased ensemble.

In practice one needs the histograms

$$\begin{aligned}
h(\boldsymbol{\xi},t) &= \int_0^t \delta_\alpha(\boldsymbol{\xi}(x_s)-\boldsymbol{\xi})\,ds\\
h_b(\boldsymbol{\xi},t) &= h(\boldsymbol{\xi},t)^{\frac{b}{1-b}}
\end{aligned} \tag{28}$$

and the exact free energy can be computed with

$$A(\boldsymbol{\xi},t) = -\beta^{-1}\ln\left[(\delta_\alpha^{-1}*h(\boldsymbol{\xi},t))h_b(\boldsymbol{\xi},t)\right] \tag{29}$$

where we use $\delta_\alpha^{-1}*h$ to indicate a deconvolution.

By now it has been demonstrated that metadynamics is a powerful computational tool[7], so we use a very simple model here to demonstrate that the formula given in (29) can be used to compute an accurate free energy even for large α. The Richardson-Lucy scheme[12,13] was used for the deconvolution, as described in reference 4.

We apply the method with $\xi(x) = x$ and $A(x) = V(x) = x^4 - x^2 + 0.25$. The dynamics are given by (20) where $f = 1/2dt$, $k_BT = .25/10$ (one tenth of the barrier height), the particle mass is unity. The Langevin integrator from reference 14 was used to evolve the trajectory. The coordinate x is discretized from $x = -2$ to $x = 2$ into 400 bins. At $t = 0$ the initial phase point is $(x,\dot{x}) = (\sqrt{0.5},0)$.

Here we implement the above stated grid-based metadynamics for a single trajectory with $b = 0.8$ and $c =$

$1/dt$. The histogram $h(\xi,t)$ defined above and its derivative

$$h'(\xi,t) = \int_0^t \partial_\xi \delta_\alpha(\xi(x_s) - \xi)\, ds \tag{30}$$

are computed on the grid of values ξ, where at each timestep the trajectory makes a contribution to all grid points. The gradient of the bias potential is given by (17). At the end of the simulation we apply (29) to remove the impact of finite α.

We evolve for 10^7 dynamical steps and compute the error $\epsilon = \sum_i |A(\xi_i) - \hat{A}(\xi_i,t)| d\xi/4$ where i runs over all bins such that $A(\xi_i) < \beta^{-1}$ and 4 is the length of the grid. We adopt this condition from reference 8. The error is shown in figure 1 where $\hat{A}$ is either the estimate of A with or without deconvolution. The two are clearly labeled in figure 1 and we find that the deconvolution makes a significant improvement to the computed free energy. The grid spacing should satisfy $d\xi << \alpha$ so that the δ_α are well represented on the grid. If the grid is too coarse, one can expect an increase in error as α decreases.

In conclusion, we have presented a derivation of metadynamics that leads to an understanding of the error associated with finite α and a formula for removing this error. We have demonstrated that the formula in (29) can indeed be used to correct the computed free energy even when α is large. Equation (29) can be used to post process any existing well-tempered metadynamics data to remove the blurring related to using a finite α. In hindsight, it appears that both (29) and the error in (26) should follow straight from the presentation of metadynamics in reference 1. One only needs to notice that the biasing force is related to the mollified mean force in the biased ensemble.

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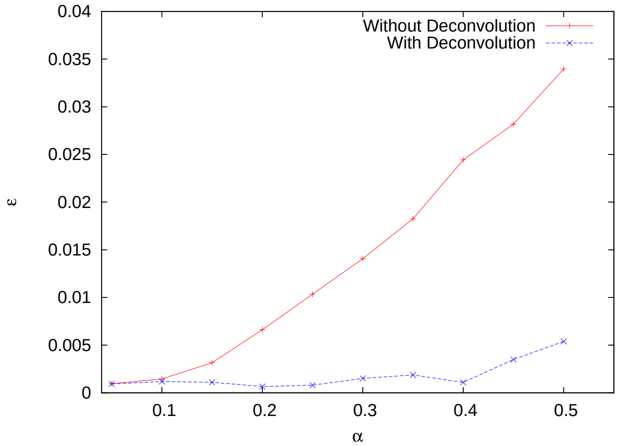

FIG. 1: (Color online) Error as a function of α with and without deconvolution.