COMMENTS

Comment on "The incomplete beta function law for parallel tempering sampling of classical canonical systems" [J. Chem. Phys. 120, 4119 (2004)]

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Recently, Kofke[1] has derived the following expression for the acceptance probability of swaps between two parallel-tempering replicas of inverse temperatures $\beta' > \beta$ [see Eq. (10) of Ref. 1]:

$$\overline{p}_{\mathrm{acc}}(C) = 4\frac{\Gamma(2C)}{[\Gamma(C)]^2}\frac{2C+1}{C}\int_0^{\beta'/\beta}\frac{\kappa^C}{(1+\kappa)^{2(C+1)}}d\kappa. \tag{1}$$

Equation (1) is derived under the assumption that the heat capacity of the system is almost constant and equal to C (in units of the Boltzmann's constant) on an inverse-temperature interval containing the values β and β'. It is also assumed that the sampled space is the phase space, which contains both the momentum and the position coordinates. If only the (d-dimensional) configuration space is considered, the heat capacity C must be replaced by $C_V = C - d/2$, the potential contribution to the heat capacity.

Standard properties of the Euler's gamma and beta functions together with the substitution $\theta = \kappa/(1+\kappa)$ lead to the following equivalent formulation of Eq. (1):

$$\overline{p}_{\mathrm{acc}}(C) = \frac{2}{B(C+1,C+1)}\int_0^{1/(1+R)}\theta^C(1-\theta)^C d\theta, \tag{2}$$

where $R = \beta'/\beta > 1$ and where $B(C+1,C+1)$ denotes the respective Euler's beta function. Replacing C with $C-1$ in Eq. (2), one obtains the so-called empirical incomplete beta function law, which is Eq. (22) of Ref. 2. Since the replacement $C \mapsto C+1$ does not change the asymptotic properties of Eq. (2) in the limit $C \to \infty$, it follows that Eq. (10) of Ref. 1 correctly predicts the $C^{-1/2}$ loss of efficiency upon the increase of the heat capacity (or dimensionality) of the sampled system. More precisely, to obtain a nonzero and nonunity limiting probability $p \in (0,1)$ in the limit $C \to \infty$, one must decrease the ratio R upon increasing C according to the law $R = 1 + \alpha_C / C^{1/2}$, with α_C chosen such that[2]

$$\alpha \equiv \lim_{C\to\infty} \alpha_C = 2\,\mathrm{erf}^{-1}(1-p). \tag{3}$$

Indeed, since

$$\frac{1}{1+R} = \frac{1}{2}\frac{1}{1+\alpha_C/(2C^{1/2})} \approx \frac{1}{2}\left(1 - \frac{1}{2}\frac{\alpha_C}{C^{1/2}}\right) \tag{4}$$

as $C \to \infty$, Eq. (2) above and Theorem 2 of Ref. 2 give

$$\lim_{C\to\infty}\overline{p}_{\mathrm{acc}}(C) = 1 - \mathrm{erf}\left(\frac{\alpha}{2}\right) = p. \tag{5}$$

In the Introduction of Ref. 2, Predescu, Predescu, and Ciobanu have asserted that Kofke's result does not accurately predict the loss of efficiency in parallel tempering simulations with the increase of the heat capacity or dimensionality. In view of the above-presented analysis, their assertion is incorrect. However, their conclusion has been based on analysis of Eq. (12) of Ref. 1, which, upon setting $B \equiv 1/R \approx 1 - \alpha_C / C^{1/2}$ and letting $C \to \infty$, indicates that $\overline{p}_{\mathrm{acc}}(C)$ diverges to $+\infty$. This improper behavior is largely due to an unfortunate typographical error[3] in the formula as given in Ref. 1. Although correction of this error eliminates the divergence of $\overline{p}_{\mathrm{acc}}(C)$ for $C \to \infty$, the limiting behavior is still not correct. This is because the formula was developed to describe how $\overline{p}_{\mathrm{acc}}$ decreases with increasing dimensionality; accordingly, it is written for a limit taken at constant B. Moreover, it does not attempt to get the behavior correct for B near unity. Therefore it cannot be used to quantify the constant-p loss of efficiency with increasing dimensionality in parallel-tempering simulations. In this regard a more useful asymptotic formula is

$$1 - \overline{p}_{\mathrm{acc}}(C) = \left[\mathrm{erf}\left(\frac{1-B}{1+B}C^{1/2}\right)\right] \times [1 + O(C^{-1})]. \tag{6}$$

This relation is applicable for $C \to \infty$ limits taken either at constant B or constant $\overline{p}_{\mathrm{acc}}$. In the former case, asymptotic expansion of the error function yields Eq. (12) of Ref. 3, while in the latter case the behavior is consistent with Eq. (5) and the limiting law for $B(C)$ given above.

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1 D. A. Kofke, J. Chem. Phys. **117**, 6911 (2002).
2 C. Predescu, M. Predescu, and C. V. Ciobanu, J. Chem. Phys. **120**, 4119 (2004).
3 Erratum to Ref. 1: D. A. Kofke, J. Chem. Phys. **120**, 10852 (2004).

