Thermostat-assisted Continuous-tempered Hamiltonian Monte Carlo for Multimodal Posterior Sampling

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Motivation & Solution

1. To sample multimodal posterior

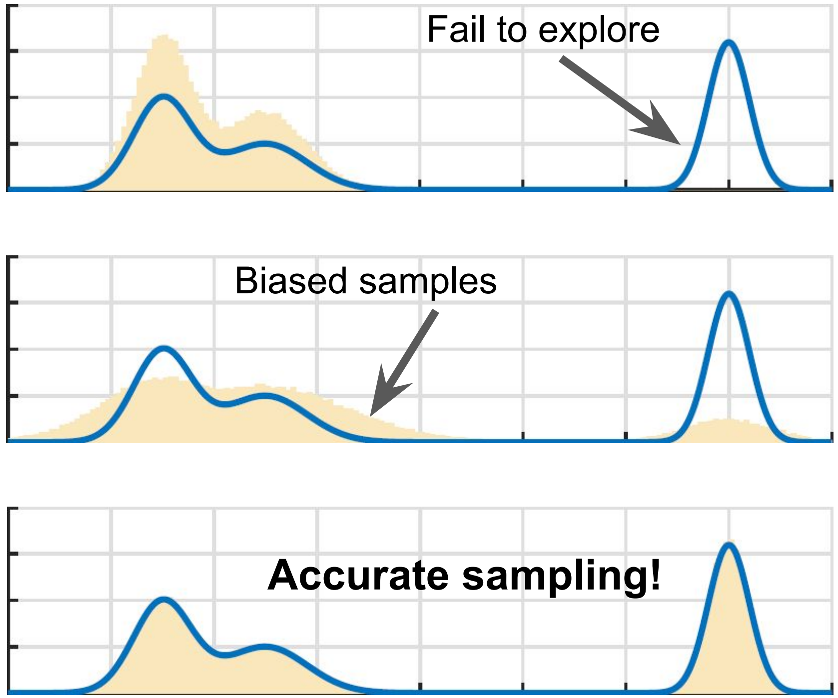
   Continous tempering

2. To leverage minibatches

   Nose-Hoover thermostat

3. To establish a systematic integration

   Fokker-Plank equation



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Formulation & Simulation

$$
\begin{aligned}
\frac{\mathrm{d}\boldsymbol{\theta}}{\mathrm{d}t} &= \boldsymbol{M}_\theta^{-1}\boldsymbol{p}_\theta, &
\frac{\mathrm{d}\boldsymbol{p}_\theta}{\mathrm{d}t} &= \frac{\tilde{\boldsymbol{f}}(\boldsymbol{\theta})}{\lambda(\xi)} - \frac{\boldsymbol{S}_\theta\boldsymbol{p}_\theta}{\lambda^2(\xi)}, &
\frac{\mathrm{d}s_\theta^{\langle i,j\rangle}}{\mathrm{d}t} &= \frac{Q_\theta^{\langle i,j\rangle}}{\lambda^2(\xi)}\left[\frac{p_{\theta_i}p_{\theta_j}}{m_{\theta_i}} - T\delta_{ij}\right], \\
\frac{\mathrm{d}\xi}{\mathrm{d}t} &= \frac{p_\xi}{m_\xi}, &
\frac{\mathrm{d}p_\xi}{\mathrm{d}t} &= \frac{\lambda'(\xi)}{\lambda^2(\xi)}\tilde{U}(\boldsymbol{\theta}) - W'(\xi) - \left[\frac{\lambda'(\xi)}{\lambda^2(\xi)}\right]^2 s_\xi p_\xi, &
\frac{\mathrm{d}s_\xi}{\mathrm{d}t} &= \left[\frac{\lambda'(\xi)}{\lambda^2(\xi)}\right]^2 Q_\xi\left[\frac{p_\xi^2}{m_\xi} - T\right].
\end{aligned}
$$