CHAPTER 7

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1. Constrained Langevin dynamics

Recall in the deterministic case, the constrained dynamics equations are

$$\begin{aligned} d\boldsymbol{q} &= \boldsymbol{M}^{-1}\boldsymbol{p}dt, \\ d\boldsymbol{p} &= -\nabla U(\boldsymbol{q})dt - \boldsymbol{g}'(\boldsymbol{q})^T\boldsymbol{\lambda}dt, \\ \boldsymbol{0} &= \boldsymbol{g}(\boldsymbol{q}). \end{aligned}$$

Analogously, the constrained Langevin dynamics equations are

$$\begin{aligned} d\boldsymbol{q} &= \boldsymbol{M}^{-1}\boldsymbol{p}dt, \\ d\boldsymbol{p} &= -\nabla U(\boldsymbol{q})dt - \gamma\boldsymbol{p}dt + \sqrt{2\gamma k_B T\boldsymbol{M}}d\mathbf{W} - \boldsymbol{g}'(\boldsymbol{q})^T\boldsymbol{\lambda}dt, \\ \boldsymbol{0} &= \boldsymbol{g}(\boldsymbol{q}). \end{aligned}$$

where the equations of constraint and hidden constraint are

$$\boldsymbol{g}(\boldsymbol{q}) = \boldsymbol{0}, \qquad \boldsymbol{g}'(\boldsymbol{q})\boldsymbol{M}^{-1}\boldsymbol{p} = 0.$$

In the infinite time limit, solutions $\boldsymbol{q}$ and $\boldsymbol{p}$ sample $\tilde{\rho}_\beta$ ergodically, such that

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \phi(\boldsymbol{q}(t),\boldsymbol{p}(t))dt = \int_{\mathcal{D}} \phi(\boldsymbol{q},\boldsymbol{p})d\omega.$$

Interpretation. The right-hand-side of the equation is, by definition, the expectation $\mathbb{E}\phi(\boldsymbol{q},\boldsymbol{p})$, where $\boldsymbol{q},\boldsymbol{p} \sim \tilde{\rho}_\beta$. We can also approximate the left-hand-side by

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \phi(\boldsymbol{q}(t),\boldsymbol{p}(t))dt \approx \frac{1}{N}\sum_{i=0}^{N}\phi(\boldsymbol{q}(t_i),\boldsymbol{p}(t_i)).$$

As N increases, the large time-limit components outweigh the initial condition components. Therefore, it is reasonable to believe that this integral samples the expectation $\mathbb{E}\phi(\boldsymbol{q},\boldsymbol{p})$.

$\tilde{\rho}_\beta$ is the normalized constrained canonical distribution,

$$\tilde{\rho}_\beta = Z^{-1}\exp(-\beta H(\boldsymbol{q},\boldsymbol{p}))\delta[\boldsymbol{g}(\boldsymbol{q})]\delta[\boldsymbol{g}'(\boldsymbol{q})\boldsymbol{M}^{-1}\boldsymbol{p}],$$

where $\delta[\boldsymbol{z}] = \prod_i \delta[z_i]$.

Interpretation. The constraint factors are $\delta[\boldsymbol{g}(\boldsymbol{q})]\delta[\boldsymbol{g}'(\boldsymbol{q})\boldsymbol{M}^{-1}\boldsymbol{p}]$. For non-permissible points, these constraint factors equal zero, and they will not be sampled from the constrained distribution.

(Discussion on the SHAKE method deferred until read chap 4.)