Uniformly sampling dimensions in sequence space

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Sampling a single energy dimension

To sample sequences with a uniform distribution of energies, one can do normal MC with a sample probability of $1/\rho(\epsilon(s))$ where $\rho(E)$ is the density of states within $[E, E+dE]$. This can be well estimated using a saddle-point approximation. We start as follows: the number of states within $[E, E+dE]$ is given by

$$\begin{aligned}
\rho(E) &= \sum_s \delta\left(E - \sum_{bj} \epsilon_{bj} s_{bj}\right) & (1)\\
&= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_s \exp\left(i\omega E - i\omega \sum_{bj} \epsilon_{bj} s_{bj}\right) & (2)\\
&= -i \int_{-i\infty}^{i\infty} \frac{d\beta}{2\pi} \prod_j \sum_b \exp\left(\beta E - \beta \epsilon_{bj}\right) & (3)\\
&= -i \int_{-i\infty}^{i\infty} \frac{d\beta}{2\pi} e^{-S_E(\beta)}, & (4)
\end{aligned}$$

where

$$S_E(\beta) = -\beta E - \sum_j \log\left(\sum_b e^{-\beta \epsilon_{bj}}\right). \qquad (5)$$

We proceed with a saddle-point approximation by finding the extremum of $S_E(\beta)$.

$$\begin{aligned}
0 = \partial_\beta S_E &= -E + \sum_j \frac{\sum_b \epsilon_{bj} e^{-\beta\epsilon_{bj}}}{\sum_b e^{-\beta\epsilon_{bj}}} = -E + \langle \epsilon \rangle_\beta & (6)\\
\Rightarrow E(\beta) &\equiv \langle \epsilon \rangle_\beta . & (7)
\end{aligned}$$

Here we've used $\langle f(s) \rangle_\beta$ to denote the expected value of a sequence-dependent function s in the canonical distribution specified by energy $\epsilon(s)$ and inverse temperature β. Indeed, the extremum value for β is simply the inverse temperature at which the expected value of $\epsilon(s)$ in the canonical ensemble is E. Note that β can be negative; this isn't a problem because the number of states is finite and have energies that are bounded above.

As is typical with saddle-point approximations, β is integrated from $-i\infty$ to $+i\infty$. But the integrand exhibits no poles, so we can deform this path into the complex plane however we want. From the form of $E(\beta)$ we see that the minimum of $S_E(\beta)$ obtains at a real value for β. Significant contributions to the integral are most highly localized if the path we choose passes through this extremum in such a way that S_E is minimized at this value for β. How we pass through this point is important, though, because β is a saddle-point of S_E; holomorphic functions don't have internal minima. The function $E(\beta)$ can be numerically inverted to get $\beta(E)$, but keep in mind that the E-domain of this function is limited and depends strongly on the specific energy matrix ϵ_{bj}:

Proceeding, with the calculation, the curvature of the saddle is given by

$$\partial_\beta^2 S_E = -\partial_\beta \langle \epsilon \rangle_\beta = -\left\langle (\delta\epsilon)^2 \right\rangle_\beta \tag{8}$$

From the last relation we see that this curvature is guaranteed negative, indicating a maximum for S_E as one proceeds across $\beta(E)$ along the real β axis. Accordingly, S_E attains a minimum as one crosses the real axis perpendicularly at $\beta(E)$ – making this the direction our path should take. This is typical of paths integrated over when dealing with Lagrange multipliers. [put figure here].

So the saddle-point approximation is

$$\begin{aligned}
\rho(E) &\approx -i \int_{-\infty}^{\infty} \frac{id\Delta}{2\pi} e^{-S_E(\beta) - \frac{1}{2}|\partial_\beta^2 S_E(\beta)|\Delta^2} && (9) \\
&= e^{-S_E(\beta)} \left[2\pi \left|\partial_\beta^2 S_E(\beta)\right|\right]^{-1/2} && (10) \\
&= e^{\beta\langle\epsilon\rangle_\beta} Z_\beta \left[2\pi \left\langle (\delta\epsilon)^2 \right\rangle\right]^{-1/2} && (11)
\end{aligned}$$

where all $\beta = \beta(E)$ and $Z_\beta = \prod_j \sum_b e^{-\epsilon_{bj}}$ is the canonical partition function. A higher-order expansion can be carried out if desired.

We should carry this expansion out to higher order. Let $s = S_E/L$, evaluate all derivatives at β^*, and let $i\Delta = (\beta - \beta^*)/\sqrt{L}$.

$$\begin{aligned}
\rho(E) &= \sqrt{L} \int_{-\infty}^{\infty} \frac{d\Delta}{2\pi} \exp\left[-Ls + \frac{1}{2}s''\Delta^2 + \frac{i}{3!\sqrt{L}} s'''\Delta^3 - \frac{1}{4!L} s''''\Delta^4 + o(L^{-3/2}\Delta^5)\right] && (12) \\
&\approx \exp\left[\frac{i}{3!\sqrt{L}} s'''\partial_J^3 - \frac{1}{4!L} s''''\partial_J^4\right] \sqrt{L} \int_{-\infty}^{\infty} \frac{d\Delta}{2\pi} \exp\left[-Ls - \frac{1}{2}|s''|\Delta^2 + J\Delta\right]_{J=0} && (13) \\
&= \sqrt{\frac{L}{2\pi|s''|}} e^{-Ls} \exp\left[\frac{i}{3!\sqrt{L}} s^{(3)}\partial_J^3 - \frac{1}{4!L} s^{(4)}\partial_J^4\right] \exp\left[-\frac{1}{2}|s''|^{-1}J^2\right]_{J=0} && (14) \\
&= \sqrt{\frac{L}{2\pi|s''|}} e^{-Ls} \left[1 + \frac{is^{(3)}\partial_J^3}{3!\sqrt{L}} - \frac{s^{(4)}\partial_J^4}{4!L} - \frac{[s^{(3)}]^2\partial_J^6}{2(3!)^2 L}\right] \exp\left[-\frac{1}{2}|s''|^{-1}J^2\right]_{J=0} && (15)
\end{aligned}$$

$$= \sqrt{\frac{L}{2\pi|s''|}} e^{-Ls} \left[1 - \frac{1}{L}\left(\frac{s^{(4)}}{24}|s''|^{-2} + \frac{[s^{(3)}]^2}{72}|s''|^{-3}\right) + o(L^{-2})\right] \tag{16}$$

$$\tag{17}$$

Here

$$Ls' = -\beta E + \sum_j \frac{\sum_b \epsilon_{bj} e^{-\beta\epsilon_{bj}}}{Z_j} \tag{18}$$

$$Ls'' = \sum_j \left[-\frac{\sum_b \epsilon_{bj}^2 e^{-\beta\epsilon_{bj}}}{Z_j} + \frac{\left(\sum_b \epsilon_{bj} e^{-\beta\epsilon_{bj}}\right)^2}{Z_j^2}\right] \tag{19}$$

$$Ls^{(3)} = \sum_j \left[\frac{\sum_b \epsilon_{bj}^3 e^{-\beta\epsilon_{bj}}}{Z_j} + 3\frac{\left(\sum_b \epsilon_{bj} e^{-\beta\epsilon_{bj}}\right)\left(\sum_b \epsilon_{bj}^2 e^{-\beta\epsilon_{bj}}\right)^2}{Z_j^2}\right] \tag{20}$$

Cumulant expansion

$$\kappa_1 = \langle\epsilon\rangle \tag{21}$$

$$\kappa_2 = \left\langle\epsilon^2\right\rangle - \langle\epsilon\rangle^2 \tag{22}$$

$$\kappa_3 = \left\langle\epsilon^3\right\rangle - 3\left\langle\epsilon^2\right\rangle\langle\epsilon\rangle + 2\langle\epsilon\rangle^3 \tag{23}$$

$$\kappa_4 = \left\langle\epsilon^4\right\rangle - 4\left\langle\epsilon^3\right\rangle\langle\epsilon\rangle - 3\left\langle\epsilon^2\right\rangle^2 + 12\left\langle\epsilon^2\right\rangle\langle\epsilon\rangle^2 - 6\langle\epsilon\rangle^4 \tag{24}$$

$$\kappa_5 = \left\langle\epsilon^5\right\rangle - 5\left\langle\epsilon^4\right\rangle\langle\epsilon\rangle - 10\left\langle\epsilon^3\right\rangle\left\langle\epsilon^2\right\rangle + 20\left\langle\epsilon^3\right\rangle\langle\epsilon\rangle^2 + \tag{25}$$

$$30\left\langle\epsilon^2\right\rangle^2\langle\epsilon\rangle - 60\left\langle\epsilon^2\right\rangle\langle\epsilon\rangle^3 + 24\left\langle\epsilon^5\right\rangle \tag{26}$$

$$\kappa_6 = \left\langle\epsilon^6\right\rangle - 6\left\langle\epsilon^5\right\rangle\langle\epsilon\rangle - 15\left\langle\epsilon^4\right\rangle\left\langle\epsilon^2\right\rangle + 30\left\langle\epsilon^4\right\rangle\langle\epsilon\rangle^2 - 10\left\langle\epsilon^3\right\rangle^2 + 120\left\langle\epsilon^3\right\rangle\left\langle\epsilon^2\right\rangle\langle\epsilon\rangle \tag{27}$$

$$-120\left\langle\epsilon^3\right\rangle\langle\epsilon\rangle^3 + 30\left\langle\epsilon^2\right\rangle^3 - 270\left\langle\epsilon^2\right\rangle^2\langle\epsilon\rangle^2 + 360\left\langle\epsilon^2\right\rangle\langle\epsilon\rangle^4 - 120\langle\epsilon\rangle^6 \tag{28}$$

$$\rho(E) = \sqrt{\frac{L}{2\pi|\kappa_2|}} Z e^{\kappa_1} \left[1 - \frac{1}{L}\left(\frac{\kappa_4|\kappa_2|^{-2}}{24} + \frac{\kappa_3^2|\kappa_2|^{-3}}{72}\right)\right] \tag{29}$$

Sampling multiple energy dimensions

$$\rho(\vec{E}) = \sum_s \prod_n \delta\left(E_n - \sum_{bj} \epsilon_{bj}^n s_{bj}\right) = (-i)^N \int \frac{d^N\vec{\beta}}{(2\pi)^N} e^{-S_{\vec{E}}(\vec{\beta})} \tag{30}$$

where all integrals are taken from $-i\infty$ to $i\infty$, and

$$S_{\vec{E}}(\vec{\beta}) = -\sum_n \beta_n E_n - \log Z_{\vec{\beta}} \tag{31}$$

$$Z_{\vec{\beta}} = \prod_j \sum_b e^{-\sum_n \beta_n \epsilon_{bj}^n} \tag{32}$$

The saddle-point is found via

$$\frac{\partial S_{\vec{E}}}{\partial \beta_n} = -E_n + \langle \epsilon_n \rangle_{\vec{\beta}} \;\Rightarrow\; \vec{E} = \langle \vec{\epsilon} \rangle_{\vec{\beta}} \tag{33}$$

and the corresponding Hessian is

$$\frac{\partial S_{\vec{E}}}{\partial \beta_n \partial \beta_m} = -\langle (\delta \epsilon_n)(\delta \epsilon_m) \rangle_{\beta}\,. \tag{34}$$

Given $\vec{E}$ one can solve for $\vec{\beta}$ using Newton's method. I expect this should be fast and robust, especially if E doesn't change all that much, perhaps provably so. With $\vec{\beta}$ in hand, one can carry out the expansion as far as one wants. At second-order,

$$\rho(\vec{E}) \approx (2\pi)^{-N/2} \exp\left[\sum_n \beta_n \langle \epsilon_n \rangle_{\vec{\beta}}\right] Z_{\vec{\beta}} \det\left(\left\langle \vec{\delta\epsilon}\ \vec{\delta\epsilon}^T \right\rangle_{\vec{\beta}}\right)^{-1/2}. \tag{35}$$

Should try to carry this out to fourth order.