GAUSSIAN-BINARY RESTRICTED BOLTZMANN MACHINES

Notation:

- visible nodes $\vec{x} \in \mathbb{R}^M$ - gaussian units (position coordinates)
- hidden nodes $\vec{h} \in \mathbb{R}^N$ - binary units
- visible biases $\vec{a} \in \mathbb{R}^M$
- hidden biases $\vec{b} \in \mathbb{R}^N$
- interaction weights $\hat{W} \in \mathbb{R}^{M \times N}$
- jth column vector of weight matrix $\vec{W}_j \in \mathbb{R}^M$
- ith row vector of weight matrix $\vec{W}_i^T \in \mathbb{R}^N$
- variational parameters $\vec{\theta} = (a_0, \cdots, a_{M-1}, b_0, \cdots, b_{N-1}, W_{0,0}, \cdots, W_{M-1,N-1})$

Assume that the input $\vec{x}$ is already mean-centered and scaled so that $\sigma = 1$.

"Energy" of a configuration of nodes:

$$
\begin{aligned}
E_{\vec{\theta}}(\vec{x}, \vec{h}) &= \frac{1}{2} \sum_{i=0}^{M-1} (x_i - a_i)^2 - \sum_{j=0}^{N-1} b_j h_j - \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} x_i W_{ij} h_j \\
&= \frac{1}{2} \|\vec{x} - \vec{a}\|^2 - \vec{b}^T \vec{h} - \vec{x}^T \hat{W} \vec{h}
\end{aligned}
$$

Use the marginal probability to represent the wavefunction as a function of the RBM inputs:

$$
\begin{aligned}
\Psi_{\vec{\theta}}(\vec{x}) &= \frac{1}{Z} \sum_{\vec{h}} e^{-E_{\vec{\theta}}(\vec{x}, \vec{h})} \\
&= \frac{1}{Z} \sum_{\{h_j\}} \exp\left(-\frac{1}{2} \sum_{i=0}^{M-1} (x_i - a_i)^2 + \sum_{j=0}^{N-1} b_j h_j + \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} x_i W_{ij} h_j \right) \\
&= \frac{1}{Z} \exp\left(-\frac{1}{2} \sum_{i=0}^{M-1} (x_i - a_i)^2 \right) \sum_{\{h_j\}} \exp\left(\sum_{j=0}^{N-1} b_j h_j + \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} x_i W_{ij} h_j \right) \\
&= \frac{1}{Z} \exp\left(-\frac{1}{2} \sum_{i=0}^{M-1} (x_i - a_i)^2 \right) \prod_{j=0}^{N-1} \sum_{h_j=0}^{1} \exp\left(b_j h_j + \sum_{i=0}^{M-1} x_i W_{ij} h_j \right) \\
&= \frac{1}{Z} \exp\left(-\frac{1}{2} \sum_{i=0}^{M-1} (x_i - a_i)^2 \right) \prod_{j=0}^{N-1} \left(1 + \exp\left(b_j + \sum_{i=0}^{M-1} x_i W_{ij} \right) \right) \\
&= \frac{1}{Z} \exp\left(-\frac{1}{2} \|\vec{x} - \vec{a}\|^2 \right) \prod_{j=0}^{N-1} \left(1 + \exp\left(b_j + \vec{x} \cdot \vec{W}_j \right) \right)
\end{aligned}
$$

Hamiltonian for P D-dimensional particles in a harmonic oscillator:

$$\hat{H} = \frac{1}{2}\sum_{p=0}^{P-1}\left(-\nabla_p^2 + \sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2\right) + \sum_{p<q} V_{int}(r_{pq}), \quad r_{pq} = \sqrt{\sum_{d=0}^{D-1}(r_{p,d} - r_{q,d})^2}$$

We need to vectorize the coordinates of all the particles to input into the RBM:

$$\vec{x} = (r_{0,0}, \cdots, r_{0,D-1}, \cdots, r_{P-1,0}, \cdots, r_{P-1,D-1}) \in \mathbb{R}^M, \;\; M = PD$$

The visible biases and the rows of the weight matrix are organized in the same way. The mapping between coordinates and the visible nodes are:

$$\begin{aligned} r_{p,d} &= x_{Dp+d} \\ x_i &= r_{\text{floor}(i/D), i \text{mod} D} \end{aligned}$$

Now we can write our representation of the wavefunction as a function of all coordinates:

$$\begin{aligned}
\Psi_{\vec{\theta}}(\vec{R}) &= \frac{1}{Z}\exp\left(-\frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}(r_{p,d} - a_{Dp+d})^2\right)\prod_{j=0}^{N-1}\left(1 + \exp\left(b_j + \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d}W_{Dp+d,j}\right)\right) \\
&= \frac{1}{Z}\exp(A(\vec{R}))\prod_{j=0}^{N-1}\exp\left(\ln\left(1 + \exp\left(b_j + \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d}W_{Dp+d,j}\right)\right)\right) \\
&= \frac{1}{Z}\exp(A(\vec{R}))\exp\left(\sum_{j=0}^{N-1}\ln\left(1 + \exp\left(b_j + \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d}W_{Dp+d,j}\right)\right)\right) \\
&= \frac{1}{Z}\exp\left(A(\vec{R}) + B(\vec{R})\right)
\end{aligned}$$

$$\begin{aligned}
A(\vec{R}) &\equiv -\frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}(r_{p,d} - a_{Dp+d})^2 = -\frac{1}{2}\sum_{i=0}^{M-1}(x_i - a_i)^2 = -\frac{1}{2}\|\vec{x} - \vec{a}\|^2 \\
B(\vec{R}) &\equiv \sum_{j=0}^{N-1}\ln\left(1 + \exp\left(B_j(\vec{R})\right)\right) \\
B_j(\vec{R}) &\equiv b_j + \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d}W_{Dp+d,j} = b_j + \sum_{i=0}^{M-1} x_i W_{i,j} = b_j + \vec{x}\cdot\vec{W}_j
\end{aligned}$$

If the particles are bosons with a hard-core interaction:

$$V_{int}(r_{pq}) = \begin{cases} \infty, & r_{pq} \leq a, \\ 0, & r_{pq} > a, \end{cases}$$

and if the particles are electrons (fermions) with a repulsive Coulomb interaction ($e = 1$):

$$V_{int}(r_{pq}) = \frac{1}{r_{pq}}$$

The behaviors due to these interactions are accounted for in the trial wavefunction by a corresponding Jastrow factor so that the full trial wavefunction is

$$\Psi(\vec{R}) = \frac{1}{Z} \exp\Big(A(\vec{R}) + B(\vec{R}) + J(\vec{R}) \Big)$$

For bosons with a hard-core interaction:

$$J(\vec{R}) = \sum_{p<q} \ln\left(1 - \frac{a}{r_{pq}}\right)$$

For electrons with the Coulomb interaction:

$$J(\vec{R}) = \sum_{p<q} \left(\frac{\alpha r_{pq}}{1 + \beta r_{pq}}\right),$$

where β is a variational parameter and α is 1 when the electrons are anti-parallel and $\frac{1}{3}$ when the electrons are parallel.

The local energy is defined as

$$E_L = \frac{1}{\Psi} \hat{H} \Psi$$

We want an analytical expression for the local energy in terms of our variational parameters $\vec{\theta}$. First, we need the following quantities:

$$\begin{aligned}
\nabla_k\{\Psi\} &= \frac{1}{Z} \nabla_k \Big\{ \exp(A + B + J) \Big\} \\
&= \frac{1}{Z} \exp(A + B + J) \Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\} \Big) \\
&= \Psi \Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\} \Big)
\end{aligned}$$

$$\begin{aligned}
\nabla_k^2\{\Psi\} &= \nabla_k \Big\{ \Psi \Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\} \Big) \Big\} \\
&= \Psi \Big(\nabla_k^2\{A\} + \nabla_k^2\{B\} + \nabla_k^2\{J\} \Big) + \nabla_k\{\Psi\} \Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\} \Big) \\
&= \Psi \left(\nabla_k^2\{A\} + \nabla_k^2\{B\} + \nabla_k^2\{J\} + \Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\} \Big)^2 \right)
\end{aligned}$$

$$\frac{1}{\Psi} \nabla_k^2\{\Psi\} = \nabla_k^2\{A\} + \nabla_k^2\{B\} + \nabla_k^2\{J\} + \Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\} \Big)^2$$

Let $\hat{n}_d$, $d = 0, ..., D-1$, denote the elementary unit vectors in each of the D dimensions. Then,

$$
\begin{aligned}
A(\vec{R}) &\equiv -\frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}(r_{p,d}-a_{Dp+d})^2, \\
\nabla_k\{A\} &= \sum_{d'=0}^{D-1}\frac{\partial A}{\partial r_{k,d'}}\hat{n_{d'}} = \sum_{d'=0}^{D-1}\frac{\partial}{\partial r_{k,d'}}\left\{-\frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}(r_{p,d}-a_{Dp+d})^2\right\}\hat{n_{d'}} \\
&= \sum_{d'=0}^{D-1}\frac{\partial}{\partial r_{k,d'}}\left\{-\frac{1}{2}(r_{k,d'}-a_{Dk+d'})^2\right\}\hat{n_{d'}} = \sum_{d=0}^{D-1}(a_{Dk+d}-r_{k,d})\hat{n_d} \\
\nabla_k^2\{A\} &= \nabla_k\cdot\nabla_k\{A\} = \nabla_k\cdot\sum_{d=0}^{D-1}(a_{Dk+d}-r_{k,d})\hat{n_d} = \sum_{d=0}^{D-1}(-1) = -D
\end{aligned}
$$

$$
\begin{aligned}
B_j(\vec{R}) &\equiv b_j + \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d} W_{Dp+d,j} \\
\nabla_k\{B_j\} &= \sum_{d'=0}^{D-1} \frac{\partial B_j}{\partial r_{k,d'}} \hat{n}_{d'} = \sum_{d'=0}^{D-1} \frac{\partial}{\partial r_{k,d'}} \left\{ b_j + \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d} W_{Dp+d,j} \right\} \hat{n}_{d'} \\
&= \sum_{d'=0}^{D-1} \frac{\partial}{\partial r_{k,d'}} \left[r_{k,d'} W_{Dk+d',j} \right] \hat{n}_{d'} = \sum_{d=0}^{D-1} W_{Dk+d,j} \hat{n}_d \\
\nabla_k^2\{B_j\} &= 0
\end{aligned}
$$

$$
\begin{aligned}
B(\vec{R}) &\equiv \sum_{j=0}^{N-1} \ln\left(1 + \exp\left(B_j(\vec{R})\right)\right) \\
\nabla_k\{B\} &= \nabla_k \left\{ \sum_{j=0}^{N-1} \ln\left(1 + \exp\left(B_j\right)\right) \right\} = \sum_{j=0}^{N-1} \nabla_k \left\{ \ln\left(1 + \exp\left(B_j\right)\right) \right\} \\
&= \sum_{j=0}^{N-1} \frac{1}{1+\exp(B_j)} \nabla_k \left\{ 1 + \exp(B_j) \right\} = \sum_{j=0}^{N-1} \frac{\exp(B_j)}{1+\exp(B_j)} \nabla_k\{B_j\} \\
&= \sum_{j=0}^{N-1} \frac{\nabla_k\{B_j\}}{\exp(-B_j)+1} = \sum_{d=0}^{D-1}\sum_{j=0}^{N-1} \frac{W_{Dk+d,j}}{\exp(-B_j)+1} \hat{n}_d \\
\nabla_k^2\{B\} &= \nabla_k \cdot \nabla_k\{B\} = \nabla_k \cdot \left\{ \sum_{j=0}^{N-1} \frac{\nabla_k\{B_j\}}{\exp(-B_j)+1} \right\} \\
&= \sum_{j=0}^{N-1} \left[\nabla_k \left\{ \frac{1}{\exp(-B_j)+1} \right\} \cdot \nabla_k\{B_j\} + \frac{\nabla_k^2\{B_j\}}{\exp(-B_j)+1} \right] \\
&= \sum_{j=0}^{N-1} \frac{\exp(-B_j)}{(\exp(-B_j)+1)^2} \nabla_k\{B_j\} \cdot \nabla_k\{B_j\} \\
&= \sum_{j=0}^{N-1} \frac{\exp(-B_j)}{(\exp(-B_j)+1)^2} \sum_{d=0}^{D-1} W_{Dk+d,j}^2
\end{aligned}
$$

$$
\begin{aligned}
r_{pq} &= \left(\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})^2\right)^{1/2}\\
\nabla_k\{r_{pq}\} &= \frac{1}{2}\left(\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})^2\right)^{-1/2}\nabla_k\Big\{\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})^2\Big\}\\
&= \frac{1}{2r_{pq}}\sum_{d=0}^{D-1}2(r_{p,d}-r_{q,d})(\delta_{k,p}-\delta_{k,q})\hat{n}_d = \frac{1}{r_{pq}}\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})(\delta_{k,p}-\delta_{k,q})\hat{n}_d
\end{aligned}
$$

$$
\begin{aligned}
J(\vec{R}) &= \sum_{p<q}\ln\left(1-\frac{a}{r_{pq}}\right)\\
\nabla_k\{J\} &= \sum_{p<q}\frac{1}{1-\frac{a}{r_{pq}}}\nabla_k\left(1-\frac{a}{r_{pq}}\right) = \sum_{p<q}\frac{r_{pq}}{r_{pq}-a}\frac{a}{r_{pq}^2}\nabla_k\{r_{pq}\}\\
&= \sum_{p<q}\frac{1}{r_{pq}-a}\frac{a}{r_{pq}}\frac{1}{r_{pq}}\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})(\delta_{k,p}-\delta_{k,q})\hat{n}_d\\
&= \sum_{d=0}^{D-1}\frac{1}{2}\sum_{p\neq q}\frac{(r_{p,d}-r_{q,d})(\delta_{k,p}-\delta_{k,q})}{r_{pq}^2(\frac{r_{pq}}{a}-1)}\hat{n}_d\\
&= \sum_{d=0}^{D-1}\frac{1}{2}\left[\sum_{q\neq k}\frac{r_{k,d}-r_{q,d}}{r_{kq}^2\left(\frac{r_{kq}}{a}-1\right)}-\sum_{k\neq k}\frac{r_{p,d}-r_{k,d}}{r_{pk}^2\left(\frac{r_{pk}}{a}-1\right)}\right]\hat{n}_d\\
&= \sum_{d=0}^{D-1}\frac{1}{2}\left[2\sum_{p\neq k}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right]\hat{n}_d = \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\hat{n}_d\\
\nabla_k^2\{J\} &= \sum_{d'=0}^{D-1}\hat{n}_{d'}\frac{\partial}{\partial r_{k,d'}}\cdot\left\{\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\hat{n}_d\right\}\\
&= \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{\partial}{\partial r_{k,d}}\left\{\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right\}\\
&= \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\left[(r_{k,d}-r_{p,d})\frac{\partial}{\partial r_{k,d}}\left\{r_{kp}^{-2}\left(\frac{r_{kp}}{a}-1\right)^{-1}\right\}+\frac{\partial}{\partial r_{k,d}}\Big\{r_{k,d}-r_{p,d}\Big\}\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right]\\
&= \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\left[(r_{k,d}-r_{p,d})\left[r_{kp}^{-2}\frac{\partial}{\partial r_{k,d}}\left\{\left(\frac{r_{kp}}{a}-1\right)^{-1}\right\}+\frac{\partial}{\partial r_{k,d}}\Big\{r_{kp}^{-2}\Big\}\left(\frac{r_{kp}}{a}-1\right)^{-1}\right]+\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right]\\
&= \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\Bigg[(r_{k,d}-r_{p,d})\left[\frac{-1}{ar_{kp}^2}\left(\frac{r_{kp}}{a}-1\right)^{-2}\frac{\partial}{\partial r_{k,d}}\Big\{r_{kp}\Big\}+\frac{-2}{r_{kp}^3}\frac{\partial}{\partial r_{k,d}}\Big\{r_{kp}\Big\}\left(\frac{r_{kp}}{a}-1\right)^{-1}\right]\\
&\qquad +\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\Bigg]\\
&= \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\left[-\frac{(r_{k,d}-r_{p,d})}{r_{kp}^2}\left(\frac{r_{kp}}{a}-1\right)^{-1}\frac{\partial}{\partial r_{k,d}}\Big\{r_{kp}\Big\}\left[\frac{1}{a}\left(\frac{r_{kp}}{a}-1\right)^{-1}+\frac{2}{r_{kp}}\right]+\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right]
\end{aligned}
$$

$$
\begin{aligned}
\nabla_k^2\{J\} &= \sum_{d=0}^{D-1} \sum_{p=0,\ p\neq k}^{P-1} \left[-\frac{(r_{k,d}-r_{p,d})}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)} \left(\frac{r_{k,d}-r_{p,d}}{r_{kp}}\right) \left[\frac{1}{r_{kp}-a}+\frac{2}{r_{kp}}\right] + \frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)} \right] \\
&= \sum_{d=0}^{D-1} \sum_{p=0,\ p\neq k}^{P-1} \frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)} \left[-\frac{(r_{k,d}-r_{p,d})^2}{r_{kp}} \left[\frac{3r_{kp}-2a}{r_{kp}(r_{kp}-a)}\right] + 1 \right] \\
&= \sum_{d=0}^{D-1} \sum_{p=0,\ p\neq k}^{P-1} \frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)} \left[\left(\frac{r_{k,d}-r_{p,d}}{r_{kp}}\right)^2 \frac{2a-3r_{kp}}{r_{kp}-a} + 1 \right]
\end{aligned}
$$

Putting all this together...

$$
\begin{aligned}
E_L &= \frac{1}{\Psi}\left[\frac{1}{2}\sum_{p=0}^{P-1} -\nabla_p^2 + \frac{1}{2}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2\right]\Psi \\
&= -\frac{1}{2}\sum_{k=0}^{P-1}\frac{1}{\Psi}\nabla_k^2\Psi + \frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2 \\
&= -\frac{1}{2}\sum_{k=0}^{P-1}\left(\nabla_k^2\{A\} + \nabla_k^2\{B\} + \nabla_k^2\{J\} + \Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\}\Big)^2\right) + \frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2 \\
&= -\frac{1}{2}\sum_{k=0}^{P-1}\left(- D + \sum_{j=0}^{N-1}\frac{\exp(-B_j)}{(\exp(-B_j)+1)^2}\sum_{d=0}^{D-1}W_{Dk+d,j}^2\right. \\
&\qquad\qquad + \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\left[\left(\frac{r_{k,d}-r_{p,d}}{r_{kp}}\right)^2\frac{2a-3r_{kp}}{r_{kp}-a}+1\right] \\
&\qquad\qquad \left. + \left(\sum_{d=0}^{D-1}(a_{Dk+d}-r_{k,d})\hat{n_d} + \sum_{d=0}^{D-1}\sum_{j=0}^{N-1}\frac{W_{Dk+d,j}}{\exp(-B_j)+1}\hat{n}_d + \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\hat{n}_d\right)^2\right) \\
&\quad + \frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2 \\
&= -\frac{1}{2}\sum_{k=0}^{P-1}\left(\sum_{d=0}^{D-1}\left[\sum_{j=0}^{N-1}\frac{\exp(-B_j)W_{Dk+d,j}^2}{(\exp(-B_j)+1)^2} + \sum_{p=0,\ p\neq k}^{P-1}\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\left[\left(\frac{r_{k,d}-r_{p,d}}{r_{kp}}\right)^2\frac{2a-3r_{kp}}{r_{kp}-a}+1\right]\right]\right. \\
&\qquad\qquad \left. + \left(\sum_{d=0}^{D-1}\left[(a_{Dk+d}-r_{k,d}) + \sum_{j=0}^{N-1}\frac{W_{Dk+d,j}}{\exp(-B_j)+1} + \sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right]\hat{n_d}\right)^2\right) \\
&\quad + \frac{PD}{2} + \frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2 \\
&= -\frac{1}{2}\sum_{k=0}^{P-1}\sum_{d=0}^{D-1}\left[\sum_{j=0}^{N-1}\frac{\exp(-B_j)W_{Dk+d,j}^2}{(\exp(-B_j)+1)^2} + \sum_{p=0,\ p\neq k}^{P-1}\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\left[\left(\frac{r_{k,d}-r_{p,d}}{r_{kp}}\right)^2\frac{2a-3r_{kp}}{r_{kp}-a}+1\right]\right. \\
&\qquad\qquad \left. + \left((a_{Dk+d}-r_{k,d}) + \sum_{j=0}^{N-1}\frac{W_{Dk+d,j}}{\exp(-B_j)+1} + \sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right)^2\right] \\
&\quad + \frac{PD}{2} + \frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2
\end{aligned}
$$

To write E_L in terms of the inputs x_i, we define the distance between the kth and pth particle as

$$\begin{aligned} R_i(p) \equiv r_{kp} &= \left(\sum_{d=0}^{D-1} (r_{k,d} - r_{p,d})^2 \right)^{1/2} \\ &= r_{(\mathrm{floor}(i/D))p} = \left(\sum_{d=0}^{D-1} (x_{D(\mathrm{floor}(i/D))+d} - x_{Dp+d})^2 \right)^{1/2} \end{aligned}$$

Then,

$$
\begin{aligned}
E_L = -\frac{1}{2}\sum_{i=0}^{M-1}\Bigg[\sum_{j=0}^{N-1}\frac{\exp(-B_j)W_{i,j}^2}{(\exp(-B_j)+1)^2} \\
&+ a \sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{1}{R_i(p)^2\big(R_i(p)-a\big)}\bigg[\Big(\frac{x_i - x_{Dp+(i\mathrm{mod}D)}}{R_i(p)}\Big)^2\frac{2a-3R_i(p)}{R_i(p)-a}+1\bigg] \\
&+ \Bigg((a_i - x_i) + \sum_{j=0}^{N-1}\frac{W_{i,j}}{\exp(-B_j)+1} + a\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{x_i - x_{Dp+(i\mathrm{mod}D)}}{R_i(p)^2\left(R_i(p)-a\right)}\Bigg)^2\Bigg] \\
&+ \frac{M}{2} + \frac{1}{2}\sum_{i=0}^{M-1}\omega_{i\mathrm{mod}D}^2 x_i^2
\end{aligned}
$$

$$
\begin{aligned}
&= -\frac{1}{2}\sum_{j=0}^{N-1}\frac{\exp(-B_j)}{(\exp(-B_j)+1)^2}\sum_{i=0}^{M-1}W_{i,j}^2 \\
&- \frac{a}{2}\sum_{i=0}^{M-1}\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{1}{R_i(p)^2\big(R_i(p)-a\big)}\bigg[\Big(\frac{x_i - x_{Dp+(i\mathrm{mod}D)}}{R_i(p)}\Big)^2\frac{2a-3R_i(p)}{R_i(p)-a}+1\bigg] \\
&- \frac{1}{2}\sum_{i=0}^{M-1}\Bigg((a_i - x_i) + \sum_{j=0}^{N-1}\frac{W_{i,j}}{\exp(-B_j)+1} + a\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{x_i - x_{Dp+(i\mathrm{mod}D)}}{R_i(p)^2\left(R_i(p)-a\right)}\Bigg)^2 \\
&+ \frac{M}{2} + \frac{1}{2}\sum_{i=0}^{M-1}\omega_{i\mathrm{mod}D}^2 x_i^2
\end{aligned}
$$

$$
\begin{aligned}
&= -\frac{1}{2}\sum_{j=0}^{N-1}\frac{\exp(-B_j)}{(\exp(-B_j)+1)^2}\vec{W}_j\cdot\vec{W}_j \\
&- \frac{a}{2}\sum_{i=0}^{M-1}\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{1}{R_i(p)^2\big(R_i(p)-a\big)}\bigg[\Big(\frac{x_i - x_{Dp+(i\mathrm{mod}D)}}{R_i(p)}\Big)^2\frac{2a-3R_i(p)}{R_i(p)-a}+1\bigg] \\
&- \frac{1}{2}\sum_{i=0}^{M-1}\Bigg((a_i - x_i) + \sum_{j=0}^{N-1}\frac{W_{i,j}}{\exp(-B_j)+1} + a\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{x_i - x_{Dp+(i\mathrm{mod}D)}}{R_i(p)^2\left(R_i(p)-a\right)}\Bigg)^2 \\
&+ \frac{M}{2} + \frac{1}{2}(\Omega\%\Omega)\cdot(\vec{x}\%\vec{x})
\end{aligned}
$$

In the last line, we have defined a vector $\vec{\Omega}$ with elements $\Omega_i = \omega_{i\mathrm{mod}D}$. To increase the computational speed, we will precalculate and store the values B_j in a vector $\vec{B}$ and store the following factors in a vector $\vec{f} \in \mathbb{R}^N$:

$$
f_j \equiv \frac{1}{\exp(-B_j)+1}
$$

Then, the local energy becomes

$$
\begin{aligned}
E_L = &-\frac{1}{2}\sum_{j=0}^{N-1}\exp(-B_j)\|f_j\vec{W}_j\|^2 + \frac{M}{2} + \frac{1}{2}(\Omega\%\Omega)\cdot(\vec{x}\%\vec{x}) \\
&-\frac{a}{2}\sum_{i=0}^{M-1}\sum_{p=0,\ p\neq \text{floor}(i/D)}^{P-1}\frac{1}{R_i(p)^2\big(R_i(p)-a\big)}\left[\left(\frac{x_i - x_{Dp+(i\text{mod}D)}}{R_i(p)}\right)^2\frac{2a-3R_i(p)}{R_i(p)-a}+1\right] \\
&-\frac{1}{2}\sum_{i=0}^{M-1}\left((a_i - x_i) + \vec{W}_i^T\vec{f} + a\sum_{p=0,\ p\neq \text{floor}(i/D)}^{P-1}\frac{x_i - x_{Dp+(i\text{mod}D)}}{R_i(p)^2\left(R_i(p)-a\right)}\right)^2
\end{aligned}
$$

For stochastic gradient descent, we will also need the gradient of the local energy with respect to the RBM parameters $\vec{\theta} = (\vec{a}, \vec{b}, \hat{W})$:

$$
G_k = \frac{\partial\langle E_L\rangle}{\partial\theta_k} = 2\left(\left\langle E_L\frac{1}{\Psi}\frac{\partial\Psi}{\partial\theta_k}\right\rangle - \langle E_L\rangle\left\langle\frac{1}{\Psi}\frac{\partial\Psi}{\partial\theta_k}\right\rangle\right)
$$

The derivatives of our new wavefunction with respect to the variational parameters are given by:

$$
\begin{aligned}
\frac{\partial\Psi}{\partial\vec{a}} &= \Psi\frac{\partial A(\vec{a})}{\partial\vec{a}} = \Psi(\vec{x}-\vec{a}) \\
\frac{\partial\Psi}{\partial\vec{b}} &= \Psi\frac{\partial B(\vec{b},\hat{W})}{\partial\vec{b}} = \Psi\vec{f} \\
\frac{\partial\Psi}{\partial\hat{W}} &= \Psi\frac{\partial B(\vec{b},\hat{W})}{\partial\hat{W}} = \Psi\vec{x}\vec{f}^T
\end{aligned}
$$

The quantum force on the kth particle is defined as

$$
\vec{F}_k(\vec{R}) = 2\frac{1}{\Psi}\nabla_k\Psi. \tag{1}
$$

Using the derivatives we have already calculated, we have

$$
\begin{aligned}
\vec{F}_k(\vec{R}) &= 2\Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\}\Big) \\
&= 2\left(\sum_{d=0}^{D-1}(a_{Dk+d} - r_{k,d})\hat{n}_d + \sum_{d=0}^{D-1}\sum_{j=0}^{N-1}\frac{W_{Dk+d,j}}{\exp(-B_j)+1}\hat{n}_d + \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\hat{n}_d\right) \\
&= 2\sum_{d=0}^{D-1}\left[(a_{Dk+d} - r_{k,d}) + \vec{W}_{Dk+d}^T\vec{f} + a\sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(r_{kp}-a\right)}\right]\hat{n}_d
\end{aligned}
$$

The Langevin and Fokker-Planck equations give a new position y from the old position x:

$$
y = x + d\Delta t F(x) + \xi\sqrt{\Delta t}, \tag{2}
$$

where $d = 0.5$ is the diffusion constant and $\Delta t \in [0.001, 0.01]$ is a chosen time step.

The transition probability is given by the Green's function

$$G(y,x) = \frac{1}{(4\pi d\Delta t)^{3N/2}} \exp\left(-\frac{(y-x-d\Delta t F(x))^2}{4d\Delta t}\right), \tag{3}$$

so that the Metropolis-Hastings acceptance ratio is

$$A(y,x) = \min\{1, P(y,x)\}, \tag{4}$$

where

$$\begin{aligned}
P(y,x) &= \frac{G(x,y)|\Psi_T(y)|^2}{G(y,x)|\Psi_T(x)|^2} \\
&= \exp\left(-\frac{(x-y-d\Delta t F(y))^2}{4d\Delta t}\right) \exp\left(\frac{(y-x-d\Delta t F(x))^2}{4d\Delta t}\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2} \\
&= \exp\left(-\frac{(x-y)^2 - 2(x-y)d\Delta t F(y) + d^2\Delta t^2 F(y)^2}{4d\Delta t}\right) \\
&\quad \times \exp\left(\frac{(y-x)^2 - 2(y-x)d\Delta t F(x) + d^2\Delta t^2 F(x)^2}{4d\Delta t}\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2} \\
&= \exp\left(\frac{2(x-y)d\Delta t(F(y)+F(x)) + d^2\Delta t^2(F(x)^2 - F(y)^2)}{4d\Delta t}\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2} \\
&= \exp\left(\frac{2(x-y)(F(y)+F(x)) + d\Delta t(F(x)^2 - F(y)^2)}{4}\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2} \\
&= \exp\left(\frac{1}{2}(x-y)(F(y)+F(x)) + \frac{1}{4}d\Delta t(F(x)^2 - F(y)^2)\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2}
\end{aligned}$$