

# 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  $\hat{W} \in \mathbb{R}^{M \times N}$
- $j$ th column vector of weight matrix  $\vec{W}_j \in \mathbb{R}^M$
- variational parameters  $\vec{\theta} = (a_0, \dots, a_{M-1}, b_0, \dots, b_{N-1}, W_{0,0}, \dots, W_{M-1,N-1})$

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 bosons in a harmonic oscillator:

$$\hat{H} = \frac{1}{2} \sum_{p=0}^{P-1} \left( -\nabla_p^2 + \sum_{d=0}^{D-1} \omega_d^2 r_{p,d}^2 \right)$$

This is also the Hamiltonian for non-interacting fermions.

Q: How do we deal with the hard-core interaction?

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

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

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:

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

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

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

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:

$$\begin{aligned}
\nabla_k \Psi_{\vec{\theta}}(\vec{R}) &= \frac{1}{Z} \nabla_k [\exp(A) B] = \frac{1}{Z} (\exp(A) \nabla_k [B] + \nabla_k [\exp(A)] B) \\
&= \frac{1}{Z} \exp(A) (\nabla_k [B] + \nabla_k [A] B)
\end{aligned}$$

$$\begin{aligned}
\nabla_k^2 \Psi_{\vec{\theta}}(\vec{R}) &= \frac{1}{Z} \nabla_k [\exp(A) (\nabla_k [B] + \nabla_k [A] B)] \\
&= \frac{1}{Z} (\exp(A) \nabla_k [\nabla_k [B] + \nabla_k [A] B] + \nabla_k [\exp(A)] (\nabla_k [B] + \nabla_k [A] B)) \\
&= \frac{1}{Z} (\exp(A) (\nabla_k^2 [B] + \nabla_k [A] \nabla_k [B] + \nabla_k^2 [A] B) + \exp(A) \nabla_k [A] (\nabla_k [B] + \nabla_k [A] B)) \\
&= \frac{1}{Z} \exp(A) (\nabla_k^2 [B] + \nabla_k [A] \nabla_k [B] + \nabla_k^2 [A] B + \nabla_k [A] \nabla_k [B] + (\nabla_k [A])^2 B) \\
&= \frac{1}{Z} \exp(A) (\nabla_k^2 [B] + 2 \nabla_k [A] \nabla_k [B] + \nabla_k^2 [A] B + (\nabla_k [A])^2 B)
\end{aligned}$$

$$\begin{aligned}
\frac{1}{\Psi_{\vec{\theta}}(\vec{R})} \nabla_k^2 \Psi_{\vec{\theta}}(\vec{R}) &= \frac{Z \exp(-A)}{B} \frac{1}{Z} \exp(A) (\nabla_k^2 [B] + 2 \nabla_k [A] \nabla_k [B] + \nabla_k^2 [A] B + (\nabla_k [A])^2 B) \\
&= \frac{\nabla_k^2 [B]}{B} + 2 \frac{\nabla_k [A] \nabla_k [B]}{B} + \nabla_k^2 [A] + (\nabla_k [A])^2
\end{aligned}$$

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

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

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

$$\begin{aligned}
\nabla_k^2[B] &= \nabla_k \cdot \nabla_k[B] \\
&= \left( \sum_{d'=0}^{D-1} \hat{n}_{d'} \frac{\partial}{\partial r_{k,d'}} \right) \cdot \left[ \sum_{d=0}^{D-1} \left( \sum_{j=0}^{N-1} W_{Dk+d,j} \exp(B_j) \prod_{j' \neq j} (1 + \exp(B_{j'})) \right) \hat{n}_d \right] \\
&= \sum_{d=0}^{D-1} \frac{\partial}{\partial r_{k,d}} \left[ \sum_{j=0}^{N-1} W_{Dk+d,j} \exp(B_j) \prod_{j' \neq j} (1 + \exp(B_{j'})) \right] \\
&= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dk+d,j} \frac{\partial}{\partial r_{k,d}} \left[ \exp(B_j) \prod_{j' \neq j} (1 + \exp(B_{j'})) \right] \\
&= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dk+d,j} \left( \exp(B_j) \frac{\partial}{\partial r_{k,d}} \left[ \prod_{j' \neq j} (1 + \exp(B_{j'})) \right] + \frac{\partial}{\partial r_{k,d}} [\exp(B_j)] \prod_{j' \neq j} (1 + \exp(B_{j'})) \right) \\
&= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dk+d,j} \left( \exp(B_j) \sum_{j'=0, j' \neq j}^{N-1} \frac{\partial}{\partial r_{k,d}} [1 + \exp(B_{j'})] \prod_{j'' \neq j, j'} (1 + \exp(B_{j''})) \right. \\
&\quad \left. + \exp(B_j) \frac{\partial}{\partial r_{k,d}} [B_j] \prod_{j' \neq j} (1 + \exp(B_{j'})) \right) \\
&= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dk+d,j} \exp(B_j) \left( \sum_{j'=0, j' \neq j}^{N-1} \exp(B_{j'}) \frac{\partial}{\partial r_{k,d}} [B_{j'}] \prod_{j'' \neq j, j'} (1 + \exp(B_{j''})) \right. \\
&\quad \left. + \frac{\partial}{\partial r_{k,d}} [B_j] \prod_{j' \neq j} (1 + \exp(B_{j'})) \right) \\
&= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dk+d,j} \exp(B_j) \left( \sum_{j'=0, j' \neq j}^{N-1} \exp(B_{j'}) W_{Dk+d,j'} \prod_{j'' \neq j, j'} (1 + \exp(B_{j''})) \right. \\
&\quad \left. + W_{Dk+d,j} \prod_{j' \neq j} (1 + \exp(B_{j'})) \right) \\
\frac{\nabla_k^2[B]}{B} &= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dk+d,j} \exp(B_j) \left( \sum_{j'=0, j' \neq j}^{N-1} \exp(B_{j'}) W_{Dk+d,j'} \frac{\prod_{j'' \neq j, j'} (1 + \exp(B_{j''}))}{\prod_{j''=0}^{N-1} (1 + \exp(B_{j''}))} \right. \\
&\quad \left. + W_{Dk+d,j} \frac{\prod_{j' \neq j} (1 + \exp(B_{j'}))}{\prod_{j'=0}^{N-1} (1 + \exp(B_{j'}))} \right) \\
&= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dk+d,j} \exp(B_j) \left( \sum_{j'=0, j' \neq j}^{N-1} \exp(B_{j'}) W_{Dk+d,j'} \frac{1}{(1 + \exp(B_j))(1 + \exp(B_{j'}))} \right. \\
&\quad \left. + W_{Dk+d,j} \frac{1}{1 + \exp(B_j)} \right) \\
&= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dk+d,j} \frac{\exp(B_j)}{1 + \exp(B_j)} \left( \sum_{j'=0, j' \neq j}^{N-1} W_{Dk+d,j'} \frac{\exp(B_{j'})}{1 + \exp(B_{j'})} + W_{Dk+d,j} \right) \\
&= \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} \frac{W_{Dk+d,j}}{\exp(-B_j) + 1} \left( \sum_{j'=0, j' \neq j}^{N-1} \frac{W_{Dk+d,j'}}{\exp(-B_{j'}) + 1} + W_{Dk+d,j} \right)
\end{aligned}$$

Putting all this together...

$$\begin{aligned}
E_L &= \frac{1}{\Psi_{\vec{\theta}}(\vec{R})} \left[ \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) \right] \Psi_{\vec{\theta}}(\vec{R}) \\
&= \sum_{p=0}^{P-1} \left[ -\frac{1}{2} \left( \frac{\nabla_p^2[B]}{B} + 2 \frac{\nabla_p[A] \nabla_p[B]}{B} + \nabla_p^2[A] + (\nabla_p[A])^2 \right) + \sum_{d=0}^{D-1} \frac{1}{2} \omega_d^2 r_{p,d}^2 \right] \\
&= \sum_{p=0}^{P-1} \left[ -\frac{1}{2} \frac{\nabla_p^2[B]}{B} - \frac{\nabla_p[A] \nabla_p[B]}{B} - \frac{1}{2} \nabla_p^2[A] - \frac{1}{2} (\nabla_p[A])^2 + \sum_{d=0}^{D-1} \frac{1}{2} \omega_d^2 r_{p,d}^2 \right] \\
&= \sum_{p=0}^{P-1} \left[ -\frac{1}{2} \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} \frac{W_{Dp+d,j}}{\exp(-B_j) + 1} \left( \sum_{j'=0, j' \neq j}^{N-1} \frac{W_{Dp+d,j'}}{\exp(-B_{j'}) + 1} + W_{Dp+d,j} \right) \right. \\
&\quad \left. - \left( \sum_{d'=0}^{D-1} (a_{Dp+d'} - r_{p,d'}) \hat{n}_{d'} \right) \cdot \left( \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} \frac{W_{Dp+d,j}}{\exp(-B_j) + 1} \hat{n}_d \right) \right. \\
&\quad \left. - \frac{1}{2}(-D) - \frac{1}{2} \sum_{d=0}^{D-1} (a_{Dp+d} - r_{p,d})^2 + \sum_{d=0}^{D-1} \frac{1}{2} \omega_d^2 r_{p,d}^2 \right] \\
&= \sum_{p=0}^{P-1} \left[ -\frac{1}{2} \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} \frac{W_{Dp+d,j}}{\exp(-B_j) + 1} \left( \sum_{j'=0, j' \neq j}^{N-1} \frac{W_{Dp+d,j'}}{\exp(-B_{j'}) + 1} + W_{Dp+d,j} \right) \right. \\
&\quad \left. - \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} \frac{(a_{Dp+d} - r_{p,d}) W_{Dp+d,j}}{\exp(-B_j) + 1} + \frac{D}{2} - \frac{1}{2} \sum_{d=0}^{D-1} (a_{Dp+d} - r_{p,d})^2 + \sum_{d=0}^{D-1} \frac{1}{2} \omega_d^2 r_{p,d}^2 \right] \\
&= \frac{PD}{2} + \sum_{p=0}^{P-1} \sum_{d=0}^{D-1} \left[ -\frac{1}{2} \sum_{j=0}^{N-1} \sum_{j'=0, j' \neq j}^{N-1} \frac{W_{Dp+d,j} W_{Dp+d,j'}}{(\exp(-B_j) + 1)(\exp(-B_{j'}) + 1)} - \frac{1}{2} \sum_{j=0}^{N-1} \frac{W_{Dp+d,j}^2}{\exp(-B_j) + 1} \right. \\
&\quad \left. - \sum_{j=0}^{N-1} \frac{(a_{Dp+d} - r_{p,d}) W_{Dp+d,j}}{\exp(-B_j) + 1} - \frac{1}{2} (a_{Dp+d} - r_{p,d})^2 + \frac{1}{2} \omega_d^2 r_{p,d}^2 \right]
\end{aligned}$$

In terms of the inputs  $x_i$ ,  $i = 0, \dots, M-1$ ,

$$\begin{aligned}
E_L &= \frac{M}{2} + \sum_{i=0}^{M-1} \left[ - \sum_{j=0}^{N-1} \sum_{j' < j} \frac{W_{i,j} W_{i,j'}}{(\exp(-B_j) + 1)(\exp(-B_{j'}) + 1)} - \frac{1}{2} \sum_{j=0}^{N-1} \frac{W_{i,j}^2}{\exp(-B_j) + 1} \right. \\
&\quad \left. - \sum_{j=0}^{N-1} \frac{(a_i - x_i) W_{i,j}}{\exp(-B_j) + 1} - \frac{1}{2} (a_i - x_i)^2 + \frac{1}{2} \omega_{i \bmod D}^2 x_i^2 \right] \\
&= \frac{M}{2} + \sum_{j=0}^{N-1} \left[ - \sum_{j' < j} \sum_{i=0}^{M-1} \frac{W_{i,j} W_{i,j'}}{(\exp(-B_j) + 1)(\exp(-B_{j'}) + 1)} - \frac{1}{2} \sum_{i=0}^{M-1} \frac{W_{i,j}^2}{\exp(-B_j) + 1} - \sum_{i=0}^{M-1} \frac{(a_i - x_i) W_{i,j}}{\exp(-B_j) + 1} \right] \\
&\quad + \sum_{i=0}^{M-1} \left[ - \frac{1}{2} (a_i - x_i)^2 + \frac{1}{2} \omega_{i \bmod D}^2 x_i^2 \right] \\
&= \frac{M}{2} + \sum_{j=0}^{N-1} \left[ - \sum_{j' < j} \frac{\vec{W}_j \cdot \vec{W}_{j'}}{(\exp(-B_j) + 1)(\exp(-B_{j'}) + 1)} - \frac{1}{2} \frac{\vec{W}_j \cdot \vec{W}_j}{\exp(-B_j) + 1} - \frac{(\vec{a} - \vec{x}) \cdot \vec{W}_j}{\exp(-B_j) + 1} \right] \\
&\quad - \frac{1}{2} (\vec{a} - \vec{x}) \cdot (\vec{a} - \vec{x}) + \frac{1}{2} \sum_{i=0}^{M-1} \omega_{i \bmod D}^2 x_i^2 \\
&= \frac{M}{2} - \sum_{j=0}^{N-1} \left[ \frac{\vec{W}_j}{\exp(-B_j) + 1} \cdot \left( \sum_{j' < j} \frac{\vec{W}_{j'}}{\exp(-B_{j'}) + 1} + \frac{1}{2} \vec{W}_j + (\vec{a} - \vec{x}) \right) \right] - \frac{1}{2} \|\vec{a} - \vec{x}\|^2 + \frac{1}{2} (\Omega \% \Omega) \cdot (\vec{x} \% \vec{x})
\end{aligned}$$

In the last line, we have defined a vector  $\vec{\Omega}$  with elements  $\Omega_i = \omega_{i \bmod D}$ . For more efficient computation of  $E_L$  I will store the factors  $f_j \equiv \frac{1}{\exp(-B_j) + 1}$  in a vector  $\vec{f}$  so that

$$E_L = \frac{M}{2} - \sum_{j=0}^{N-1} \left[ f_j \vec{W}_j \cdot \left( \sum_{j' < j} f_{j'} \vec{W}_{j'} + \frac{1}{2} \vec{W}_j + (\vec{a} - \vec{x}) \right) \right] - \frac{1}{2} \|\vec{a} - \vec{x}\|^2 + \frac{1}{2} (\Omega \% \Omega) \cdot (\vec{x} \% \vec{x})$$