1 Calogero Model

Consider a quantum system of N one-dimensional bosons that are confined in a harmonic oscillator potential and interact via a pair-wise inverse squared potential. The Hamiltonian is given by

$$\hat{H}_{Cal} = \sum_{p=1}^{N} \left(-\frac{1}{2}\frac{\partial^2}{\partial x_p^2} + \frac{1}{2}x_p^2 \right) + \sum_{p<q} \frac{\nu(\nu-1)}{(x_p - x_q)^2}, \tag{1}$$

where $\hbar = m = \omega = 1$ and ν is an interaction parameter. Then the exact ground-state wave function and energy are given by

$$\Psi_{exact}(\vec{x}) = \exp\left(-\frac{1}{2}\sum_{p=1}^{N} x_i^2 \right) \prod_{p<q} |x_p - x_q|^{\nu}, \tag{2}$$

and

$$E_{exact} = \frac{N}{2} + \frac{\nu}{2}N(N-1). \tag{3}$$

Goal: We will compare how two different neural networks, feedforward neural networks (FFNNs) and restricted Boltzmann machines (RBMs), perform as trial wave functions for a variational Monte Carlo calculation. As a benchmark, we will let each network contain only one hidden layer with the same number of hidden neurons. We want to measure how accurately Ψ_{exact} is represented by the optimized networks and how close the final estimation of the ground state energy is to E_{exact}.

2 Variational Monte Carlo

In a variational calculation, we typically define some parametrized wave function Ψ_T, then minimize the expectation value of the energy with respect to the parameters. This involves a very high-dimensional integral, so we use Monte Carlo sampling for computational efficiency. Then the expectation value of the energy can be estimated by

$$E \equiv \frac{\langle \Psi_T | \hat{H} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \approx \frac{1}{n}\sum_{i=1}^{n} E_L(\vec{x}_i) \equiv \langle E_L \rangle, \tag{4}$$

where the positions $\vec{x}_i$ are the sampled from the distribution $|\Psi_T|^2$, n is the number of samples, and the local energy E_L is given by

$$E_L \equiv \frac{1}{\Psi_T}\hat{H}\Psi_T. \tag{5}$$

In order to take samples of positions efficiently, we will use the Metropolis-Hastings algorithm to randomly kick particles into the higher probability regions. To determine the direction of this kick, we will need the quantum force on the pth particle

$$F_p(\vec{x}) = 2\frac{1}{\Psi_T}\frac{\partial}{\partial x_p}\Psi_T. \tag{6}$$

Then the Langevin and Fokker-Planck equations give a new position y from the old position x according to

$$y = x + d\Delta t F(x) + \xi\sqrt{\Delta t}, \tag{7}$$

where $d = 0.5$ is the diffusion constant, ξ is drawn from a normal distribution, and $\Delta t \in [0.001, 0.01]$ is a chosen time step. The transition probability is given by the Green's function

$$G(y, x) = \frac{1}{(4\pi d\Delta t)^{3N/2}} \exp\left(-\frac{(y - x - d\Delta t F(x))^2}{4d\Delta t}\right), \tag{8}$$

so that the Metropolis-Hastings acceptance ratio is

$$A(y, x) = \min\{1, P(y, x)\}, \tag{9}$$

where

$$P(y, x) = \frac{G(x, y)|\Psi_T(y)|^2}{G(y, x)|\Psi_T(x)|^2} = \exp\left(\frac{1}{2}(x - y)(F(y) + F(x)) + \frac{1}{4}d\Delta t(F(x)^2 - F(y)^2)\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2}. \tag{10}$$

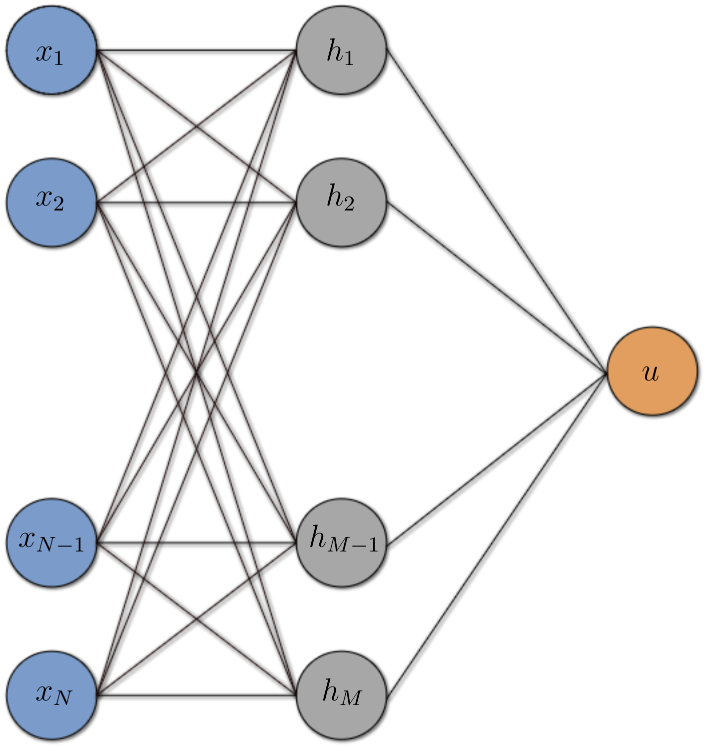
Finally, we need to determine how to change our parameters $\vec{\alpha}$ to give a lower expectation value. Instead of calculating the gradient analytically, we estimate the gradient by taking the following averages

$$\frac{\partial \langle E_L \rangle}{\partial \alpha_k} = 2\left(\left\langle E_L \frac{\partial \ln \Psi_T}{\partial \alpha_k} \right\rangle - \langle E_L \rangle \left\langle \frac{\partial \ln \Psi_T}{\partial \alpha_k} \right\rangle\right). \tag{11}$$

Notation:

$$\begin{aligned} p, q &- \text{visible neurons} \\ i, j &- \text{hidden neurons} \\ k &- \text{variational parameters} \end{aligned}$$

3 Feedforward Neural Networks



The inputs of the feedforward neural network are the positions of the N one-dimensional bosons. They are fully-connected to M hidden neurons by a matrix of weights $W \in \mathbb{R}^{M \times N}$. The hidden neurons also have an associated bias $\vec{b} \in \mathbb{R}^M$ so that

$$\vec{h} = W\vec{x} + \vec{b} \tag{12}$$

The output of the network is given by

$$u = \vec{w}^T \vec{f}(\vec{h}), \tag{13}$$

where f is the activation function and $\vec{w} \in \mathbb{R}^M$ contains the weights connecting the hidden neurons with the single output. Here, we have placed a vector symbol over the activation function f to emphasize that the result is a vector, with the function applied to each element of $\vec{h}$ separately.

Since our system consists of bosons, the total wave function is positive everywhere. Thus, we take the trial wave function to be

$$\Psi_{FFNN}(\vec{x}) = \exp(u) = \exp\left(\vec{w}^T \vec{f}(W\vec{x} + \vec{b})\right) \tag{14}$$

This ansatz depends not only on the positions $\vec{x}$, but on the weights $W, \vec{w}$ and bias $\vec{b}$ as well. These will henceforth be known collectively as the variational parameters $\vec{\alpha} = (W, \vec{b}, \vec{w})$ of our trial wave function. We assume $\vec{\alpha} \in \mathbb{R}^{M(N+2)}$ is the flattened and concatenated form of our parameters.

Now we calculate the local energy (5), quantum force (6), and gradient (11) for $\Psi_T = \Psi_{FFNN}$.
Local energy:

$$
\begin{aligned}
E_L &= \frac{1}{\Psi_T}\hat{H}\Psi_T \\
&= \exp\left(-u\right)\left[\sum_{p=1}^{N}\left(-\frac{1}{2}\frac{\partial^2}{\partial x_p^2}+\frac{1}{2}x_p^2\right)+\sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2}\right]\exp\left(u\right) \\
&= -\frac{1}{2}\sum_{p=1}^{N}\left[\exp\left(-u\right)\frac{\partial^2}{\partial x_p^2}\exp\left(u\right)\right]+\frac{1}{2}\sum_{p=1}^{N}x_p^2+\sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2} \\
&= -\frac{1}{2}\sum_{p=1}^{N}\left[\frac{\partial^2 u}{\partial x_p^2}+\left(\frac{\partial u}{\partial x_p}\right)^2\right]+\frac{1}{2}\sum_{p=1}^{N}x_p^2+\sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2} \\
\frac{\partial u}{\partial x_p} &= \frac{\partial}{\partial x_p}\left[\sum_{i=1}^{M}w_i f(h_i)\right]=\sum_{i=1}^{M}w_i f'(h_i)\frac{\partial h_i}{\partial x_p} \\
&= \sum_{i=1}^{M}w_i f'(h_i)\frac{\partial}{\partial x_p}\left[\sum_{q=1}^{N}W_{iq}x_q+b_i\right]=\sum_{i=1}^{M}w_i W_{ip}f'(h_i) \\
\frac{\partial^2 u}{\partial x_p^2} &= \frac{\partial}{\partial x_p}\left[\sum_{i=1}^{M}w_i W_{ip}f'(h_i)\right]=\sum_{i=1}^{M}w_i W_{ip}f''(h_i)\frac{\partial h_i}{\partial x_p}=\sum_{i=1}^{M}w_i W_{ip}^2 f''(h_i)
\end{aligned}
$$

$$
E_L=\sum_{p=1}^{N}\left[\sum_{i=1}^{M}w_i W_{ip}^2 f''(h_i)-\frac{1}{2}\left(\sum_{i=1}^{M}w_i W_{ip}f'(h_i)\right)^2\right]+\frac{1}{2}\sum_{p=1}^{N}x_p^2+\sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2}
$$

Quantum force on the pth particle:

$$
F_p(\vec{x})=2\frac{1}{\Psi_T}\frac{\partial}{\partial x_p}\Psi_T=2\exp(-u)\frac{\partial}{\partial x_p}\exp(u)=2\frac{\partial u}{\partial x_p}=2\sum_{i=1}^{M}w_i W_{ip}f'(h_i)
$$

Gradient of average local energy with respect to the parameters $\vec{\alpha}$:

$$\begin{aligned}
\frac{\partial \langle E_L \rangle}{\partial \alpha_k} &= 2\left(\left\langle E_L \frac{\partial \ln \Psi_T}{\partial \alpha_k}\right\rangle - \langle E_L \rangle \left\langle \frac{\partial \ln \Psi_T}{\partial \alpha_k}\right\rangle\right) \\
\frac{\partial \ln \Psi_T}{\partial W_{ip}} &= \frac{1}{\Psi_T}\frac{\partial \Psi_T}{\partial W_{ip}} = \exp(-u)\frac{\partial}{\partial W_{ip}}\exp(u) = \frac{\partial u}{\partial W_{ip}} = \frac{\partial}{\partial W_{ip}}\left[\sum_{j=1}^{M} w_j f(h_j)\right] \\
&= \sum_{j=1}^{M} w_j f'(h_j)\frac{\partial h_j}{\partial W_{ip}} = \sum_{j=1}^{M} w_j f'(h_j)\frac{\partial}{\partial W_{ip}}\left[\sum_{q=1}^{N} W_{jq}x_q + b_j\right] \\
&= \sum_{j=1}^{M} w_j f'(h_j) x_p \delta_{ij} = w_i f'(h_i) x_p \\
\frac{\partial \ln \Psi_T}{\partial b_i} &= \frac{\partial u}{\partial b_i} = \frac{\partial}{\partial b_i}\left[\sum_{j=1}^{M} w_j f(h_j)\right] = \sum_{j=1}^{M} w_j f'(h_j)\frac{\partial h_j}{\partial b_i} \\
&= \sum_{j=1}^{M} w_j f'(h_j)\frac{\partial}{\partial b_i}\left[\sum_{q=1}^{N} W_{jq}x_q + b_j\right] = \sum_{j=1}^{M} w_j f'(h_j)\delta_{ij} = w_i f'(h_i) \\
\frac{\partial \ln \Psi_T}{\partial w_i} &= \frac{\partial u}{\partial w_i} = \frac{\partial}{\partial w_i}\left[\sum_{j=1}^{M} w_j f(h_j)\right] = f(h_i)
\end{aligned}$$

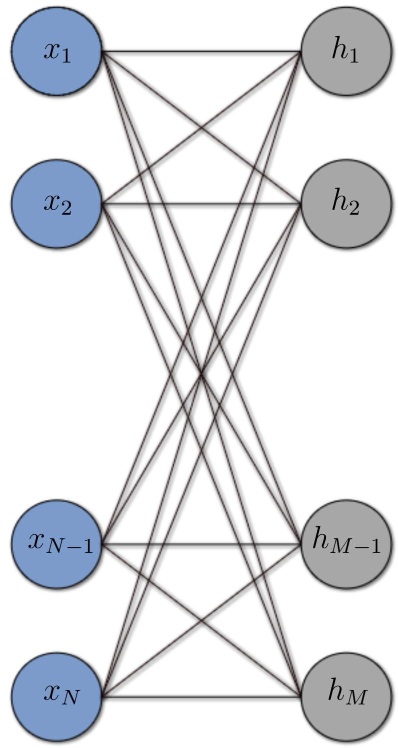
To simplify our calculations, let us define the vector $\vec{g}$ with components given by

$$g_i = w_i f'(h_i) \tag{15}$$

Then we have

$$\begin{aligned}
E_L &= \sum_{p=1}^{N}\left[\sum_{i=1}^{M} w_i W_{ip}^2 f''(h_i) - \frac{1}{2}\left(\vec{g}^T \vec{W}_p\right)^2\right] + \frac{1}{2}\sum_{p=1}^{N} x_p^2 + \sum_{p<q}\frac{\nu(\nu-1)}{(x_p - x_q)^2} \\
F_p(\vec{x}) &= 2\vec{g}^T \vec{W}_p \\
\frac{\partial \ln \Psi_T}{\partial W} &= \vec{g}\vec{x}^T \\
\frac{\partial \ln \Psi_T}{\partial \vec{b}} &= \vec{g} \\
\frac{\partial \ln \Psi_T}{\partial \vec{w}} &= \vec{f}(\vec{h})
\end{aligned}$$

4 Restricted Boltzmann Machines



On the surface, restricted Boltzmann machines look very similar to feedforward neural networks like the one above. However, instead of learning a mapping between the inputs $\vec{x}$ and the desired output (the many-body wave function), RBMs learn the probability distribution over its inputs $P(\vec{x})$. Since wave functions are related to probability distributions, we can approach the same problem in a different way. First, let us define the energy of a configuration of nodes for real visible nodes and binary hidden nodes:

$$E_{RBM}(\vec{x},\vec{h}) = \frac{1}{2\sigma^2}\sum_{p=1}^{N}(x_p - a_p)^2 - \sum_{i=1}^{M} b_i h_i - \frac{1}{\sigma^2}\sum_{p=1}^{N}\sum_{i=1}^{M} h_i W_{ip} x_p \tag{16}$$

$$= \frac{1}{2\sigma^2}\|\vec{x}-\vec{a}\|^2 - \vec{b}^T\vec{h} - \frac{1}{\sigma^2}\vec{h}^T W\vec{x} \tag{17}$$

Here, $\vec{a} \in \mathbb{R}^N$ is the visible bias, $\vec{b} \in \mathbb{R}^M$ is the hidden bias, and $W \in \mathbb{R}^{M\times N}$ is the matrix of weights connecting the visible nodes with the hidden nodes. From this energy expression, we can define the probability of a certain configuration occurring:

$$P(\vec{x},\vec{h}) = \frac{1}{Z}\exp\left(-E_{RBM}(\vec{x},\vec{h})\right)$$

If we integrate over the hidden nodes, we obtain a marginal probability distribution that depends only on the positions $\vec{x}$. Let the square root of this marginal probability be our representation of the wave function for our system of bosons:

$$
\begin{aligned}
\Psi_{RBM}(\vec{x}) &= \sqrt{P(\vec{x})} = \sqrt{\sum_{\vec{h}} P(\vec{x}, \vec{h})} \\
&= \sqrt{\sum_{\vec{h}} \frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2}\|\vec{x}-\vec{a}\|^2 + \vec{b}^T\vec{h} + \frac{1}{\sigma^2}\vec{h}^T W \vec{x}\right)} \\
&= \sqrt{\frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2}\|\vec{x}-\vec{a}\|^2\right) \prod_{i=1}^{M} \sum_{h_i=0}^{1} \exp\left(b_i h_i + \frac{1}{\sigma^2}\sum_{p=1}^{N} h_i W_{ip} x_p\right)} \\
&= \sqrt{\frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2}\|\vec{x}-\vec{a}\|^2\right) \prod_{i=1}^{M} \sum_{h_i=0}^{1} \exp\left(b_i h_i + \frac{1}{\sigma^2}\sum_{p=1}^{N} h_i W_{ip} x_p\right)} \\
&= \frac{1}{Z^{1/2}} \exp\left(-\frac{1}{4\sigma^2}\|\vec{x}-\vec{a}\|^2\right) \prod_{i=1}^{M} \left(1 + \exp\left(b_i + \frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\right)^{1/2} \\
&= \frac{1}{Z^{1/2}} \exp\left(-\frac{1}{4\sigma^2}\|\vec{x}-\vec{a}\|^2\right) \prod_{i=1}^{M} \exp\left(\frac{1}{2}\ln\left(1 + \exp\left(b_i + \frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\right)\right) \\
&= \frac{1}{Z^{1/2}} \exp\left(-\frac{1}{4\sigma^2}\|\vec{x}-\vec{a}\|^2\right) \exp\left(\frac{1}{2}\sum_{i=1}^{M}\ln\left(1 + \exp\left(b_i + \frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\right)\right)
\end{aligned}
$$

Define the following to simplify our expression for the wave function:

$$A(\vec{x}) \equiv -\frac{1}{4\sigma^2}\|\vec{x}-\vec{a}\|^2 \tag{18}$$

$$B(\vec{x}) \equiv \frac{1}{2}\sum_{i=1}^{M}\ln\left(1 + \exp\left(b_i + \frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\right) \tag{19}$$

$$\Psi_{RBM}(\vec{x}) = \frac{1}{Z^{1/2}} \exp\left(A(\vec{x}) + B(\vec{x})\right) \tag{20}$$

Then the local energy becomes:

$$
\begin{aligned}
E_L &= \frac{1}{\Psi_T}\hat{H}\Psi_T \\
&= \exp(-A-B)\left[\sum_{p=1}^{N}\left(-\frac{1}{2}\frac{\partial^2}{\partial x_p^2} + \frac{1}{2}x_p^2\right) + \sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2}\right]\exp(A+B) \\
&= -\frac{1}{2}\sum_{p=1}^{N}\left[\exp(-A-B)\frac{\partial^2}{\partial x_p^2}\exp(A+B)\right] + \frac{1}{2}\sum_{p=1}^{N}x_p^2 + \sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2} \\
&= -\frac{1}{2}\sum_{p=1}^{N}\left[\frac{\partial^2 A}{\partial x_p^2} + \frac{\partial^2 B}{\partial x_p^2} + \left(\frac{\partial A}{\partial x_p} + \frac{\partial B}{\partial x_p}\right)^2\right] + \frac{1}{2}\sum_{p=1}^{N}x_p^2 + \sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2}
\end{aligned}
$$

Take derivatives to get the full form of the local energy:

$$\begin{aligned}
A(\vec{x}) &\equiv -\frac{1}{4\sigma^2}\|\vec{x}-\vec{a}\|^2 = -\frac{1}{4\sigma^2}\sum_{q=1}^{N}(x_q-a_q)^2 \\
\frac{\partial A}{\partial x_p} &= -\frac{1}{4\sigma^2}\sum_{q=1}^{N}2(x_q-a_q)\delta_{pq} = \frac{1}{2\sigma^2}(a_p-x_p) \\
\frac{\partial^2 A}{\partial x_p^2} &= -\frac{1}{2\sigma^2}
\end{aligned}$$

$$\begin{aligned}
B(\vec{x}) &\equiv \frac{1}{2}\sum_{i=1}^{M}\ln\left(1+\exp\left(b_i+\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\right) \\
\frac{\partial B}{\partial x_p} &= \frac{1}{2}\sum_{i=1}^{M}\left(1+\exp\left(b_i+\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\right)^{-1}\exp\left(b_i+\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\frac{\partial}{\partial x_p}\left[\frac{1}{\sigma^2}\sum_{q=1}^{N}W_{iq}x_q\right] \\
&= \frac{1}{2\sigma^2}\sum_{i=1}^{M}W_{ip}\left(\exp\left(-b_i-\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)+1\right)^{-1} \\
\frac{\partial^2 B}{\partial x_p^2} &= -\frac{1}{2\sigma^2}\sum_{i=1}^{M}W_{ip}\left(\exp\left(-b_i-\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)+1\right)^{-2}\exp\left(-b_i-\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\frac{\partial}{\partial x_p}\left[-\frac{1}{\sigma^2}\sum_{q=1}^{N}W_{iq}x_q\right] \\
&= \frac{1}{2\sigma^4}\sum_{i=1}^{M}W_{ip}^2\left(\exp\left(-b_i-\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)+1\right)^{-2}\exp\left(-b_i-\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)
\end{aligned}$$

Quantum force on the pth particle:

$$\begin{aligned}
F_p(\vec{x}) &= 2\frac{1}{\Psi_T}\frac{\partial}{\partial x_p}\Psi_T = 2\exp(-A-B)\frac{\partial}{\partial x_p}\exp(A+B) \\
&= 2\left(\frac{\partial A}{\partial x_p}+\frac{\partial B}{\partial x_p}\right) = \frac{1}{\sigma^2}(a_p-x_p)+\frac{1}{\sigma^2}\sum_{i=1}^{M}W_{ip}\left(\exp\left(-b_i-\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)+1\right)^{-1}
\end{aligned}$$

Derivatives for the gradient of average local energy:

$$\begin{aligned}
\frac{\partial \ln\Psi_T}{\partial W_{ip}} &= \exp(-A-B)\frac{\partial}{\partial W_{ip}}\exp(A+B) = \frac{\partial B}{\partial W_{ip}} \\
&= \frac{\partial}{\partial W_{ip}}\left[\frac{1}{2}\sum_{j=1}^{M}\ln\left(1+\exp\left(b_j+\frac{1}{\sigma^2}\vec{W}_j^T\vec{x}\right)\right)\right] \\
&= \frac{1}{2\sigma^2}\left(1+\exp\left(b_i+\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\right)^{-1}\exp\left(b_i+\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)\frac{\partial}{\partial W_{ip}}\left[\sum_{q=1}^{N}W_{iq}x_q\right] \\
&= \frac{1}{2\sigma^2}\left(\exp\left(-b_i-\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)+1\right)^{-1}x_p
\end{aligned}$$

$$
\begin{aligned}
\frac{\partial \ln \Psi_T}{\partial b_i} &= \frac{\partial B}{\partial b_i} = \frac{\partial}{\partial b_i}\left[\frac{1}{2}\sum_{j=1}^{M}\ln\left(1+\exp\left(b_j+\frac{1}{\sigma^2}\vec{W}_j^T\vec{x}\right)\right)\right] \\
&= \frac{1}{2}\left(\exp\left(-b_i-\frac{1}{\sigma^2}\vec{W}_i^T\vec{x}\right)+1\right)^{-1} \\
\frac{\partial \ln \Psi_T}{\partial a_p} &= \frac{\partial A}{\partial a_p} = \frac{\partial}{\partial a_p}\left[-\frac{1}{4\sigma^2}\sum_{q=1}^{N}(x_q-a_q)^2\right] = \frac{1}{2\sigma^2}(x_p-a_p)
\end{aligned}
$$

Define the vectors $\vec{z}, \vec{\sigma} \in \mathbb{R}^M$ with elements

$$
z_i \equiv b_i + \frac{1}{\sigma^2}\vec{W}_i^T\vec{x}, \quad \sigma_i \equiv \frac{1}{\exp(-z_i)+1},
$$

so that we have

$$
\begin{aligned}
E_L &= -\frac{1}{2}\sum_{p=1}^{N}\left[-\frac{1}{2\sigma^2}+\frac{1}{2\sigma^4}\sum_{i=1}^{M}W_{ip}^2\sigma_i^2\exp(-z_i)+\left(\frac{1}{2\sigma^2}(a_p-x_p)+\frac{1}{2\sigma^2}\sum_{i=1}^{M}W_{ip}\sigma_i\right)^2\right] \\
&\quad+\frac{1}{2}\sum_{p=1}^{N}x_p^2+\sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2} \\
&= \frac{N}{4\sigma^2}-\frac{1}{4\sigma^4}\sum_{p=1}^{N}\sum_{i=1}^{M}W_{ip}^2\sigma_i^2\exp(-z_i)-\frac{1}{8}\|\vec{F}(\vec{x})\|^2+\frac{1}{2}\|\vec{x}\|^2+\sum_{p<q}\frac{\nu(\nu-1)}{(x_p-x_q)^2} \\
F_p(\vec{x}) &= \frac{1}{\sigma^2}(a_p-x_p)+\frac{1}{\sigma^2}\vec{\sigma}^T\vec{W}_p \\
\frac{\partial \ln \Psi_T}{\partial W} &= \frac{1}{2\sigma^2}\vec{\sigma}\vec{x}^T \\
\frac{\partial \ln \Psi_T}{\partial \vec{b}} &= \frac{1}{2}\vec{\sigma} \\
\frac{\partial \ln \Psi_T}{\partial \vec{a}} &= \frac{1}{2\sigma^2}(\vec{x}-\vec{a})
\end{aligned}
$$