Neural Network Solutions of Bosonic and Fermionic Systems in One Dimension

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Finding Ground States

- Finding the ground state energy is difficult for many-body quantum systems
  - High dimensionality makes exact solutions hard to solve for
- Models with analytic solutions are uncommon
- Instead, apply numerical methods to obtain estimates of ground state properties

Variational Method

Given an arbitrary Hamiltonian $\hat{H}$, and state $|\psi\rangle$, the variational principle provides a bound on the value of the ground state energy of the Hamiltonian

The Variational Principle

For Hamiltonian $\hat{H}$, and arbitrary state $|\psi\rangle$:

$$E_0 \langle\psi|\psi\rangle \leq \langle\psi|\hat{H}|\psi\rangle$$

- Choose $\psi(\boldsymbol{\theta})$, then vary $\boldsymbol{\theta}$ to minimize $\langle\psi|\hat{H}|\psi\rangle \rightarrow$ estimate for E_0.
- In practice, we have many variational parameters, minimization of $\langle\hat{H}\rangle$ requires Monte Carlo sampling and gradient descent.

Monte Carlo Methods

We need to compute the expectation value:

$$\langle \hat{H} \rangle = \frac{\int d\boldsymbol{x}\, \psi\left(\boldsymbol{x}\right)^{\dagger} \hat{H} \psi\left(\boldsymbol{x}\right)}{\int d\boldsymbol{x}\, \psi\left(\boldsymbol{x}\right)^{\dagger} \psi\left(\boldsymbol{x}\right)}$$

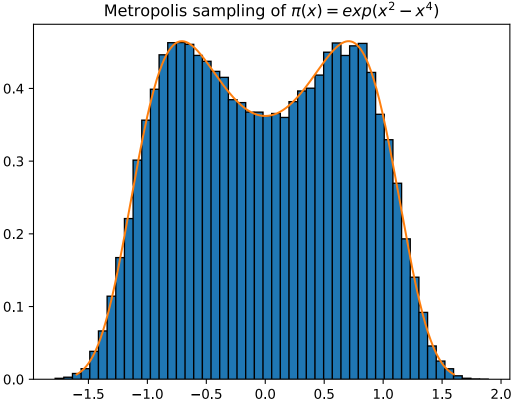
This is difficult for systems with many particles, so instead, we write it as a statistical average

$$\langle \hat{H} \rangle = \left\langle \psi^{-1}\left(\boldsymbol{x}\right) \hat{H} \psi\left(\boldsymbol{x}\right) \right\rangle_{\psi^2}$$

Where the average is taken over samples from ψ^2.

Metropolis Algorithm

- Metropolis-Hastings allows for sampling from probability distributions
- Easily generalizes to multiple dimensions $\rightarrow$ many-body quantum systems



Metropolis Algorithm

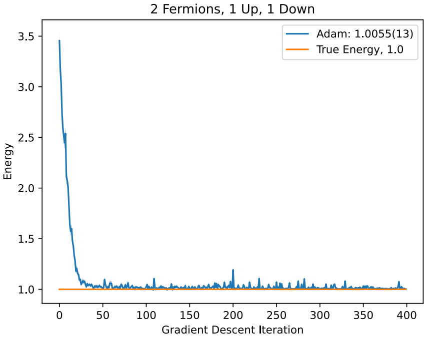
Given a probability distribution function $P(\boldsymbol{x})$:

1. Generate a starting sample, $\boldsymbol{x}_t$.
2. Generate a random shift, $\boldsymbol{r}$ (sampled uniformly within a range).
3. Let $\boldsymbol{x}' = \boldsymbol{x}_t + \boldsymbol{r}$. This is the proposed next sample.
4. Generate random $p \in [0, 1]$. If $p < \frac{P(\boldsymbol{x}')}{P(\boldsymbol{x})}$, accept the sample, and use it as the next starting sample. Otherwise, reject the sample, and keep the starting sample the same.

The algorithm draws samples from high-density regions, and rejects proposals from low-density regions $\rightarrow$ samples mimic the given probability distribution.

Variational Monte Carlo

- Applying Variational Method to obtain estimate for $E_0 \rightarrow$ using Monte Carlo to compute expectation values
- Use gradient descent algorithm to minimize $\mathcal{E}$ by varying $\boldsymbol{\theta}$.
  - Compute $\frac{d\mathcal{E}}{d\boldsymbol{\theta}}$, shift values of $\boldsymbol{\theta}$, repeat until $\mathcal{E}$ converges
- Determine convergence by comparison to theory or by increasing the number of samples



Why Neural Networks?

The Variational Principle gives no information about how close the estimate is to E_0.

Ansatze are human-generated, based on knowledge of the Hamiltonian or ground state behavior:

- Harmonic oscillator potential $\rightarrow$ inverted quadratic, $\left(x+\frac{a}{2}\right)\left(x-\frac{a}{2}\right)$
- Helium atom $\rightarrow$ Hydrogen atom ground state with added variational parameters

Ideal ansatz is something that can take on a large range of functional forms.

Neural Networks

Define a network of L layers, weights $\{\boldsymbol{W}_i\}$, biases $\{\boldsymbol{b}_i\}$, and activation function f:

$$\begin{aligned} I_{i+1} &= O_i = f(\mathbf{W}_i \boldsymbol{I_i} + \boldsymbol{b}_i), \qquad 1 \leq i \leq L-1 \\ O_L &= \mathbf{W}_L \boldsymbol{I}_L + \boldsymbol{b}_L \end{aligned}$$

- O_L has no activation function, so that the network can produce any value as output
- We use $f = \text{CELU}$:

$$\text{CELU}\,(x, \alpha) = \begin{cases} x & x > 0 \\ \alpha \left(\exp\left(\frac{x}{\alpha}\right) - 1 \right) & x \leq 0 \end{cases}$$

Neural Networks

- Neural networks have been shown to be universal function approximators[1]
- **Why not use neural networks as the VMC ansatz?**
- Weights and biases of the network serve as variational parameters
- Neural network should converge to ground state wavefunction given enough weights and biases
- Caveat: Systems of bosons and fermions have exchange (anti)symmetries that need to be encoded

[1] K. Hornik, M. Stinchcombe, and H. White, Multilayer feedforward networks are universal approximators, Neural networks **2**, 359 (1989)

Bosonic Exchange Symmetry

- Neural network output should be invariant under coordinate exchange
- Use a bijection from $\{x_i\}$ to some exchange symmetric $\{\xi_i\}$

$$\xi_i = \sum_{k=1}^{N} \left(\frac{x_k}{w}\right)^i$$

- Exchanging x_i and x_j produces the same $\{\xi_i\}$

$$\begin{aligned} \xi_1 &= x_1^1 + x_2^1 + \cdots + x_N^1 \\ \xi_2 &= x_1^2 + x_2^2 + \cdots + x_N^2 \\ &\vdots \\ \xi_N &= x_1^N + x_2^N + \cdots + x_N^N \end{aligned}$$

Bosonic Ansatz

- We define our bosonic ansatz:

$$\psi\left(x_1, x_2, \ldots, x_N\right) = e^{-\mathcal{A}(\xi_1, \xi_2, \ldots, \xi_N))} \cdot e^{-\Omega \sum_{i=1}^{N} x_i^2}$$

- Gaussian ensures that ψ vanishes at infinity
- ψ is real-valued $\rightarrow$ real-valued weights and biases
- Exchange symmetry is maintained using $\{\xi_i\}$ as neural network inputs

Fermionic Ansatz

- For a system of $N_\uparrow$ spin-up and $N_\downarrow$ spin-down fermions (N total), we expect exchange antisymmetry between same spin fermions

$$\underbrace{x_1, x_2, \ldots, x_{N_\uparrow}}_{\text{up-spin}}, \underbrace{x_{N_\uparrow+1}, x_{N_\uparrow+2}, \ldots x_N}_{\text{down-spin}}$$

- Ansatz constructed using two Slater determinants, one for each set of spins
  - Each determinant is antisymmetric for its species of fermion

Fermionic Ansatz

$$\Phi^{\uparrow}(\boldsymbol{x}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{1,1} & \phi_{1,2} & \cdots \\ \phi_{2,1} & \phi_{2,2} & \\ \vdots & & \ddots \end{vmatrix}$$

$$\Phi^{\uparrow}(\boldsymbol{x}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{N_\uparrow+1,N_\uparrow+1} & \phi_{N_\uparrow+1,N_\uparrow+2} & \cdots \\ \phi_{N_\uparrow+2,N_\uparrow+1} & \phi_{N_\uparrow+2,N_\uparrow+2} & \\ \vdots & & \ddots \end{vmatrix}$$

Where $\phi_{i,j}$ is a neural network function $\phi_i(x_j, x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N)$ which is symmetric with respect to all but x_j.

$$\psi(\boldsymbol{x}) = \Phi^{\uparrow}(\boldsymbol{x})\,\Phi^{\downarrow}(\boldsymbol{x})\,e^{-\sum_i^N x_i^2}$$

Bosonic Models

We consider 2 models of interacting bosons, both with harmonic potentials.

- Harmonically trapped bosons with a delta function potential
  - $\hat{H} = \sum_{i=1}^{N} \left(-\frac{1}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m\omega^2 x_i^2 \right) + \sum_{i<j}^{N} g\delta\left(x_i - x_j\right)$
  - Exactly solvable in the 2 particle case

- Harmonically trapped bosons with short and long range interactions
  - $\hat{H} = \sum_{i=1}^{N} \left(-\frac{1}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m\omega^2 x_i^2 \right) + \sum_{i<j}^{N} g\delta\left(x_i - x_j\right) + \sigma|x_i - x_j|$
  - Exactly solvable in the case where $\sigma = -m\omega g/2$

Fermionic Models

We consider 2 models of fermions, with harmonic potentials.

- $N = N_\uparrow + N_\downarrow$ non-interacting fermions
  - $\hat{H} = \sum_i^N \left(-\frac{1}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m\omega^2 x_i^2 \right)$
  - Exactly solvable
- $N = N_\uparrow = N_\downarrow$ fermions with a contact potential
  - $\hat{H} = \sum_i^N \left(-\frac{1}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m\omega^2 x_i^2 \right) + \sum_{i<j} g\delta\left(x_i - x_j\right)$
  - $N_\downarrow = 1$, $N_\uparrow = 1, 2, \ldots, 10$ cases are solved exactly

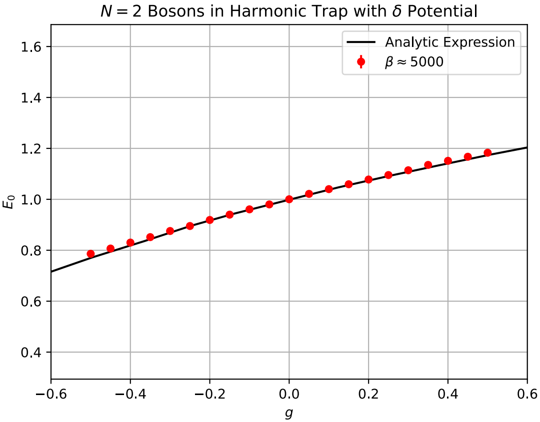
Implementation

- Python: numpy + Jax
- Optimize Monte Carlo computations using vectorization
- Jax just-in-time (jit) compilation optimizes code reuse
- Gradient descent using ADAM optimizer

Bosons with Contact Potential

$N = 2$ case has exact solution:

$$\sqrt{2}\left(\frac{\Gamma\left(1-\frac{E_0}{2}\right)}{\Gamma\left(\frac{1}{2}-\frac{E_0}{2}\right)}\right) = -\frac{2}{g}$$



Bosons with Short and Long Range Potentials

Look at two regimes:

- Exactly solvable regime: $\sigma = -g/2$
- A non-analytically solvable regime: $\sigma = -g$

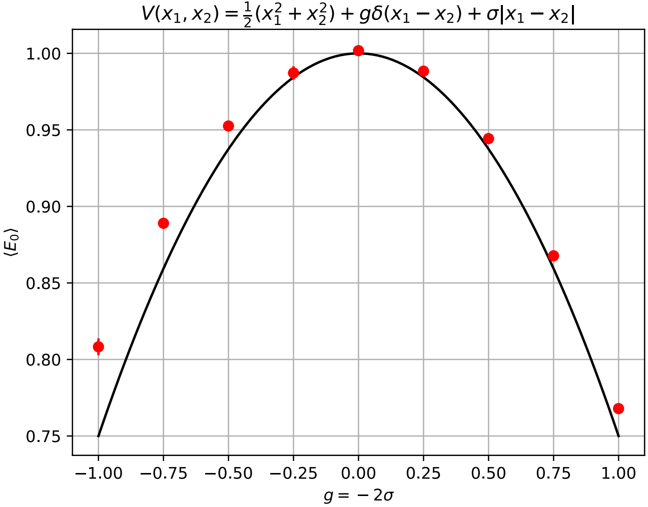
In the exactly solvable regime:

$$E_0 = \frac{N\omega}{2} - mg^2 \frac{N\left(N^2 - 1\right)}{24}$$

$$\psi\left(\boldsymbol{x}\right) = \prod_{i<j} e^{-|x_i - x_j|/a_s} \prod_{i} e^{-x_i^2/\left(2a_{ho}^2\right)}$$

Where $a_s = -\frac{2}{mg}$ and $a_{ho} = \sqrt{\frac{1}{m\omega}}$.

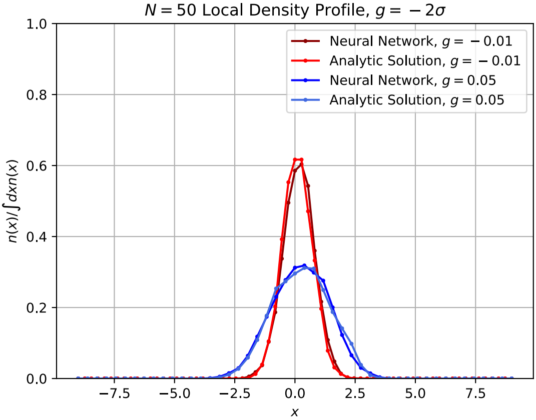
Analytic Regime ($\sigma = -g/2$)



Large N Systems

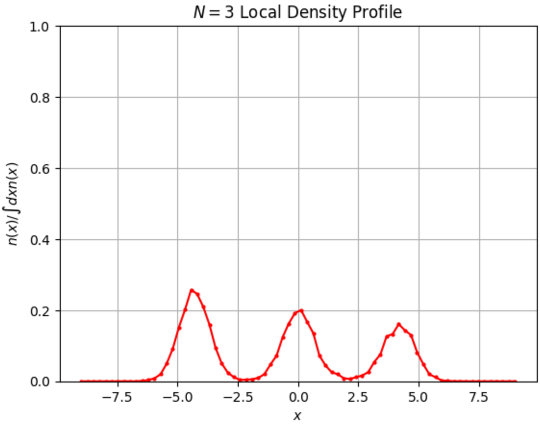
Compute the local density profile:

$$n(x) = \int dx_2, \ldots, dx_N \left|\psi(x_1, x_2, \ldots, x_N)\right|^2$$



Nonanalytic Regime ($\sigma = -g$)

Neural network ansatz encodes correct qualitative behavior of the ground state for repulsive g:

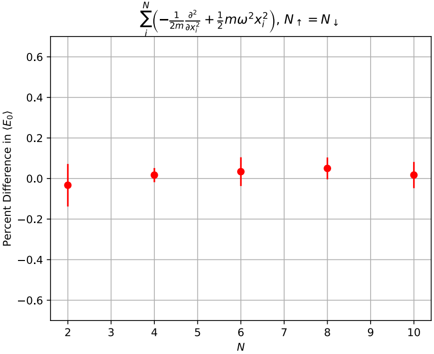


Fermions in Harmonic Well

System of fermions with no interactions has known ground state solution:

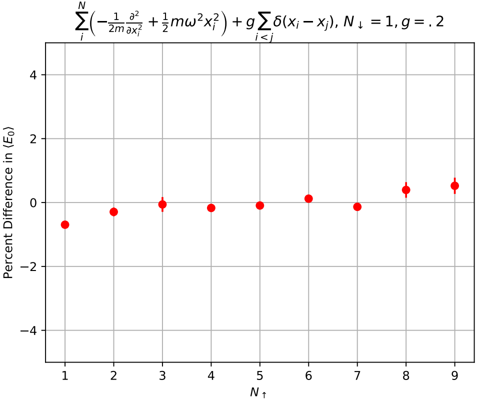
$$E_0 = \frac{N_\uparrow^2 + N_\downarrow^2}{2}$$

Percent difference from exact ground state energy:



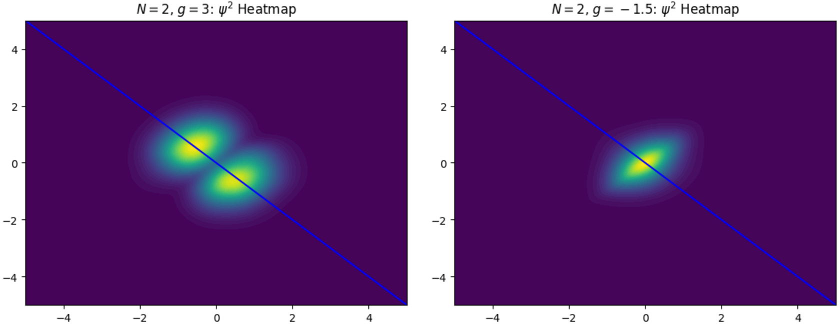
Fermions with Contact Potential

Percent difference between neural network and exact results:



Fermion Probability Density

Position-space probability density of repulsive and attractive ground states of fermions with delta function interaction:



Conclusion

- Neural networks can provide general wavefunctions for bosonic and fermionic models
- Allow for straightforward increases in the number of variational parameters, and number of particles
- Ability to probe systems with no analytic solutions

Further Work

- Expand to higher dimensional systems
  - 3D $\rightarrow$ requires 3 dimensional symmetrization method
- Explore GPU parallelization for MC computations
- Study scaling of parameter counts
- Explore transfer learning for different interaction strengths
- Explore methods for systematically choosing optimization hyperparameters

Questions?