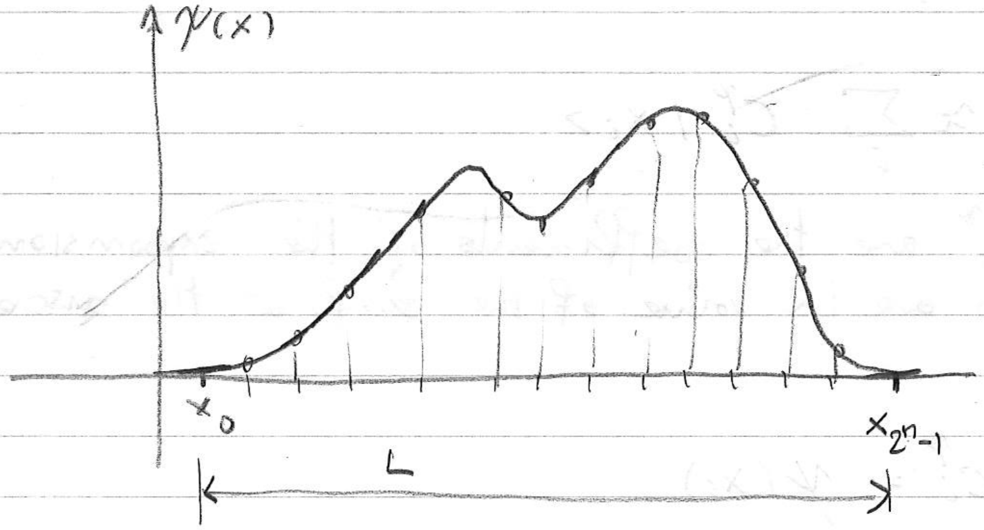
Notes on writing a variational wave function on a discretized lattice.

We are looking the Schrödinger eq. in 1D

$$-\nabla^2 \psi(x) + V(x)\,\psi(x) = E\,\psi(x) \tag{1}$$

Assume the w.f. is defined on a integration interval of lengh L ($V(x) \rightarrow \infty$ and $\psi(x) \approx 0$ outside L):

(2)



The eigenstate for a particle at a position $\bar{x}$ is given by:

$$|\bar{x}\rangle = \delta(x - \bar{x}) \tag{3}$$

The w.f. can be expanded on this basis:

$$|\psi(x)\rangle = \int d\bar{x}\; c^{\psi}_{\bar{x}}\, |\bar{x}\rangle \tag{4}$$

Note that the coefficients $C_{\bar{x}}^{\psi}$ are in fact the w.f.

(5) $$|\psi(x)\rangle = \int d\bar{x}\ C_{\bar{x}}^{\psi}\ \delta(x-\bar{x}) = C_x^{\psi}$$

In practice, we discretize the integration range L into 2^n points equally distant.

(6)
$$|\psi\rangle = \int d\bar{x}\ \overbrace{\psi(\bar{x})}^{C_{\bar{x}}^{\psi}}\ |\bar{x}\rangle$$

$$\approx \sum_i C_i^{\psi}\ |x_i\rangle$$

where c_i^{ψ} are the coefficients of the expansion. Obviously, they also are the value of the w.f. at the discretization points:

(7) $$C_i^{\psi} = \psi(x_i)$$

$|x_i\rangle$ are our basis to expand the w.f. ψ, and C_i^{ψ} are the coefficients of the expansion.

Note that any wave function of the basis can also be expanded in the $|\bar{x}_i\rangle$ too. So:

(8) $$|x_j\rangle = \sum_i C_i^j\ |x_i\rangle$$

Since,

(9) $$\langle x_k | x_j \rangle = \delta_{kj}$$

wee have:

$$(10)\quad \langle x_i | x_j \rangle = \delta_{ij} = \langle x_i | \sum_k C_k^j | x_k \rangle = \sum_k C_k^j \underbrace{\langle x_i | x_k \rangle}_{\delta_{kj}} = C_i^j$$

Thus: $C_i^j = \delta_{i,j}$ (11)

For the Heisenberg and Ising models, Carleo expands the QS into a basis for his Hilbert space. In this case the states of the basis are each possible configuration of the spins $\{\sigma\}$. The equivalents of eqs (8) is:

$$(12)\quad |\Psi\rangle = \sum_{\{\sigma\}} \Psi(\{\sigma\}) \underbrace{|\{\sigma\}\rangle}$$

↳ basis states: $|\{\sigma\}\rangle = |+,+,-,-,+\dots\rangle$, $|+,-,+,+,\dots\rangle$, etc...

Once again, the coefficient of the expansion are obtained projecting the entire QS on each state of the basis:

$$(13)\quad \langle\{\sigma\}|\Psi\rangle = \Psi(\{\sigma\})$$

This is thee wave function that is approximated by a RBM neural network function.

Note that $\Psi(\{\sigma\})$ is a complex valued funcion of discretized variables, just like $\psi(x_i) = C_i^{\psi}$ in eq. (7)

<u>Thus, we just need to map the spin confs. $\{\sigma\}$ into the $\{x_i\}$ basis.</u>

The mapping must be a 1-to-1 correspondence between each spin configuration and the discrete positions x_i:

$$(14)\quad \begin{cases} X(\{\sigma\}) \longmapsto x_i \\ S'(x_i) \longmapsto \{\sigma\} \end{cases}$$

Given that spins have 2 possible values, we can take these as binary numbers that label each coordinate x_i:

$$(15)\quad i = \sum_{\ell=0}^{n-1} b(\sigma_\ell)\, 2^\ell$$

where the bit value is either 0, or 1:

$$(16)\quad b(\sigma_\ell) = \begin{cases} 0 & \text{if } \sigma_\ell = -1 \\ 1 & \text{if } \sigma_\ell = +1 \end{cases}$$

The coordinate points x_i are then

$$(17)\quad x_i = x_0 + i \times \Delta x \quad , \text{ with } \Delta x = \frac{L}{2^n - 1}$$

The VMC approach by Carleo samples spin configs. and calculates the local energy each time.

For a conf. $|\{\sigma\}\rangle$, we have:

(18) $$E_{loc} = \frac{\langle\sigma|H|\Psi\rangle}{\langle\sigma|\Psi\rangle}$$

By inserting an identity and using eq. (13), we have:

(19) $$E_{loc} = \frac{\sum_{\{\sigma'\}} \langle\sigma|H|\sigma'\rangle\langle\sigma'|\Psi\rangle}{\langle\sigma|\Psi\rangle} = \frac{\sum_{\sigma'} \langle\sigma|H|\sigma'\rangle \cdot \Psi(\sigma')}{\Psi(\sigma')}$$

Thus, Carleo needs the matrix elements of the Hamiltonian in the basis states $|\{\sigma\}\rangle$.

Things are exacly the same for our particle in a box:

(20) $$E_{loc} = \frac{\langle x_i|H|\Psi\rangle}{\langle x_i|\Psi\rangle} = \frac{\sum_j \langle x_i|H|x_j\rangle \psi(x_j)}{\psi(X_i)}$$

Using our mapping, we can solve our eq. using the spin and RBM setup of Carleo:

(21) $$\langle\sigma_i|H|\sigma_j\rangle \longrightarrow \langle X(\sigma_i)|H|X(\sigma_j)\rangle$$

(22) $$\Psi(\sigma_i) \longrightarrow \psi(X(\sigma_i))$$

Note that the routines of Carleo's code pre-stores the mtx els of

$$\langle \sigma | H | \sigma' \rangle \tag{23}$$

by giving sate $|\sigma'\rangle$ and then $|\sigma\rangle$ is expressed as a set of spin flips w.r.t. $|\sigma'\rangle$. Then the mtx els of eq.(23) are used to calculate E_{loc} from Eq.(19).

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We now need to evaluate the mtx. elements of the hamiltonian in the discretized coord. space basis:

$$\langle x_i | \hat{H} | x_j \rangle = \langle x_i | -\nabla^2 + \hat{V} | x_j \rangle \tag{24}$$

The double derivative of the wave function can be expanded on the basis $|x_i\rangle$, exactly as for $|\psi\rangle$ in eq. (6). This gives:

$$|\nabla^2 \psi\rangle = \int d\bar{x} \quad \psi''(\bar{x}) \, |\bar{x}\rangle = \sum_i \psi''(x_i) \, |x_i\rangle \tag{25}$$

where $\psi''(x_i)$ needs to be calculated from the values of $\psi(x_i)$ at neighbouring points:

$$\psi''(x_i) = \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{(\Delta x)^2} \tag{26}$$

Note that other approximation of the kinetic energy term exist, besides eq. (26).

We can apply eqs. (25) and (26) together to get the effect of ∇^2 operator on the basis states:

(27) $$\nabla^2 | x_j \rangle = \sum_k \left(C^j_{k+1} - 2C^j_k + C^j_{k-1} \right) \frac{1}{(\Delta x)^2} | x_k \rangle$$

Then, using eqs. (9) and (11), we get:

(28) $$\langle x_i | \nabla^2 | x_j \rangle = \frac{\delta_{j,i+1} - 2\delta_{i,j} + \delta_{j,i-1}}{(\Delta x)^2} = \begin{cases} \frac{1}{(\Delta x)^2} & \text{if } i = j \pm 1 \\ \frac{-2}{(\Delta x)^2} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

Let's check eq. (28) by applying it to a generic function $\psi(x)$

$$\langle x_i | \nabla^2 | \psi \rangle = \sum_j \langle x_i | \nabla^2 | x_j \rangle \cdot \langle x_j | \psi \rangle$$

(29) $$= \sum_j \frac{(\delta_{j,i+1} + \delta_{j,i-1} - 2\delta_{ij})}{(\Delta x)^2} \cdot \psi(x_j)$$

$$= \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{(\Delta x)^2} = \psi''(x_i) \quad ,$$

which confirms eqs. (25) and (26).

Obviously:

(30) $$\langle x_i | V(x) | x_j \rangle = V(x_i)\, \delta_{ij} \; .$$