Ordered sampling of a Slater determinant

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1 Sampling ordered particle positions from a Slater determinant

In order to combine the autoregressive neural network (MADE) ansatz representing the Jastrow factor with a Slater determinant one needs to be able to sample particle positions from the Slater determinant in an ordered fashion. Let D be the number of sites and N the number of fermions.

First of all, ordered sampling implies that the support of the conditional probabilities changes depending on the position i_{k-1} of the previously sampled particle and depending on the number of particles, $N-k$, that still need to be placed somewhere: Thus, for the k-th particle the possible positions (in the fermion ordering) are

$$x_k \in [i_{k-1}+1, \ldots, D-(N-k)], \tag{1}$$

where D is the number of sites and N the number of particles.

In the grand-canonical ensemble the joint probability for a set of occupation numbers $n_i \in \{0,1\}$ is:

$$\begin{aligned} p(n_1, n_2, \cdots n_k) &= (-)^{n_1+n_2+\cdots n_k} \det \begin{pmatrix} G_{11}-n_1 & G_{12} & \cdots & G_{1k} \\ G_{21} & G_{22}-n_2 & \cdots & G_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ G_{k1} & G_{k2} & \cdots & G_{kk}-n_k \end{pmatrix} \\ &= (-)^{n_1+n_2+\cdots n_k} \det\left(G_{K,K}-N_K\right) \end{aligned} \tag{2}$$

with the submatrix $G_{K,K} = (G)_{K=\{1,\ldots,k\},K=\{1,\ldots,k\}}$ of the single-particle Green's function in position space and the diagonal matrix $N_K = \mathrm{diag}(n_1, \ldots, n_k)$. Everything that follows is based on this formula, even though we wish to sample in the ensemble of fixed particle number N.

We wish to sample particle positions $i_1 < i_2 < \ldots < i_N$ in such a way that position i_1 is sampled first, i_2 is sampled second, and so on. The probability of having a particle at position i_1 and this being the first one, i.e. left-most in the fermion ordering, in terms of the above joint probabilities for occupation numbers is

$$\begin{aligned} p_1(x_1 = 1) &= p(n_1 = 1) \\ p_1(x_1 = 2) &= p(n_1 = 0, n_2 = 1) \\ &\cdots \\ p_1(x_1 = k) &= p(n_1 = 0, n_2 = 0, \ldots, n_{k-1} = 0, n_k = 1), \end{aligned}$$

that is, it needs to be assured all sites to the left (in the fermion ordering) of x_1 are empty. The conditional

probabilities for the position of the second particle, given the first particle's position is $x_1 = i_1$, are

$$
\begin{aligned}
p_2(x_2 = i_1{+}1 | x_1 = i_1) &= \frac{p(x_2 = i_1 + 1, x_1 = i_1 \wedge x_1 \text{is left-most particle})}{p(x_1 = i_1 \wedge x_1 \text{is left-most particle})} \\
&= \frac{p(n_1 = 0, \ldots, n_{i_1-1} = 0, n_{i_1} = 1, n_{i_1+1} = 1)}{p(n_1 = 0, \ldots, n_{i_1-1} = 0, n_{i_1} = 1)} \\
&\vdots \\
p_2(x_2 = i_1{+}m | x_1 = i_1) &= \frac{p(n_1 = 0, \ldots, n_{i_1-1} = 0, n_{i_1} = 1, n_{i_1+1} = 0, \ldots, n_{i_1+m-1} = 0, n_{i_1+m} = 1)}{p(n_1 = 0, \ldots, n_{i_1-1} = 0, n_{i_1} = 1)} \\
&\vdots
\end{aligned}
\tag{3}
$$

Here, the range of m is restricted according to Eq. (1). The ratios of determinants are computed using the formula for block determinants and by iteratively updating the required submatrices.

2 Benchmark

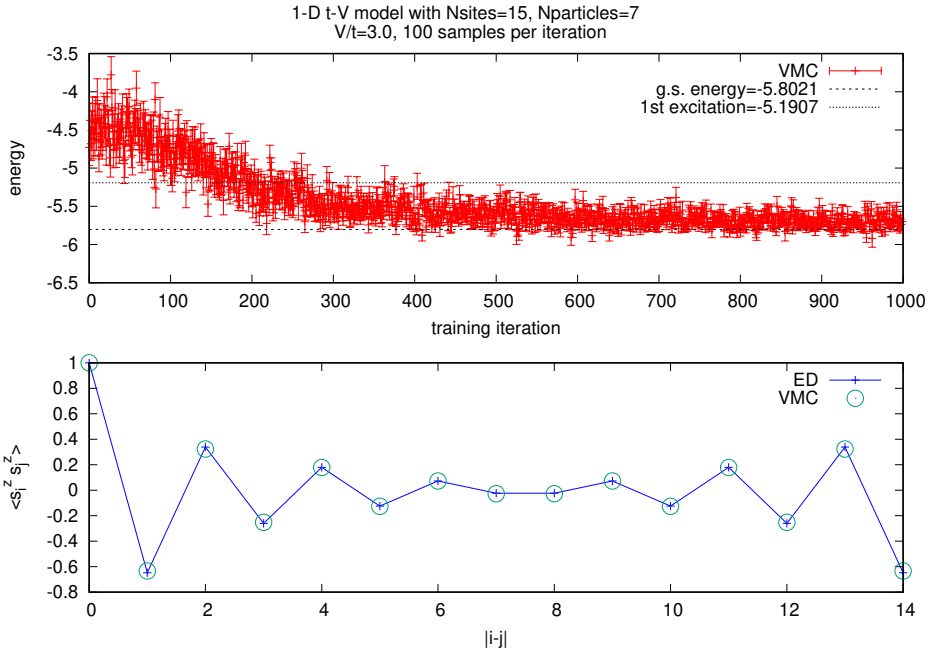

Figure 1: Autoregressive Slater-Jastrow ansatz with a single Slater determinant, for which the Hartree-Fock ground state is used. Lower panel: Comparison of $\langle s_i^z s_j^z \rangle$ correlation function (with $s_i^z = 2n_i - 1$) between ED and VMC.

Consider the one-dimensional t-V model of spin-polarized fermions with periodic boundary conditions:

$$
H = -t \sum_i (\hat{c}_i^\dagger \hat{c}_{i+1} + h.c.) + V \sum_i \hat{n}_i \hat{n}_{i+1}. \tag{4}
$$

The Hartree-Fock Hamiltonian

$$
H_{HF}(|\psi\rangle) = -t \sum_i (\hat{c}_i^\dagger \hat{c}_{i+1} + h.c.) + V \sum_i \left(\hat{n}_i \langle \psi | \hat{n}_{i+1} | \psi \rangle - [\hat{c}_i^\dagger \hat{c}_{i+1} \langle \psi | \hat{c}_{i+1}^\dagger c_i | \psi \rangle + h.c.] \right) \tag{5}
$$

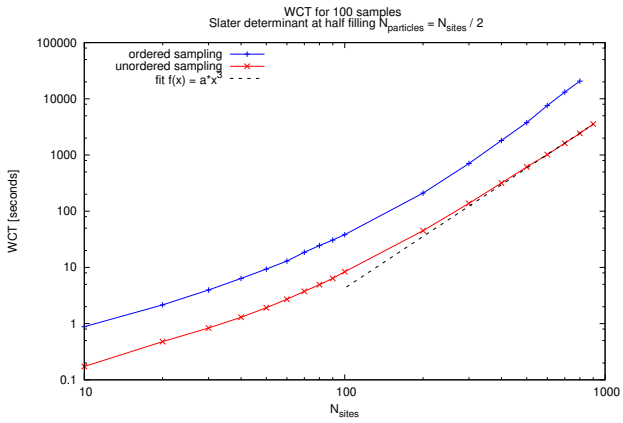

Figure 2: Wall clock time for producing 100 samples from a Slater determinant for ordered and unordered sampling (no Jastrow factor).

is solved iteratively and its ground state $|\psi_{HF}\rangle$ is taken as the reference Slater determinant for autoregressive VMC. The result of stochastic gradient descent training is shown in Fig. 1.

Unordered sampling is significantly slower than ordered sampling because unoccupied positions also appear in the determinants (see Fig. 2).

3 Continuation

1. Backflow transformation using an autoregressive neural network.
2. Multi-determinant ansatz.
3. Use other reference wavefunctions such as antisymmetrized geminal powers (AGP), Pfaffian wavefunctions, etc. and sample directly from them.
4. Other autoregressive neural network architectures, e.g. recurrent NN.