Simulating Quantum Systems through Matrix Product States

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Journal Club 15-04-2010
Motivations

- Theoretical interest in Matrix Product States
- Wide spectrum of their numerical applications
- Eventual relations with methods which work on the same geometries
Motivations
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- Quantum information perspective
- Quantum Many-Body simulations
- Simplified models (spin chains, Bose-Hubbard..) capture the relevant physics, but still they are not simple!

Equilibrium
- Quenches
- Time-dependent Hamiltonian

Out of Equilibrium
Why are quantum many-body systems so hard to simulate?

Hilbert space grows exponentially with the system size.

Ex: Bose-Hubbard model

\[ \hat{H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \]

# states:

\[ W(N, M) = \frac{(M + N - 1)!}{(M - 1)! N!} \]

<table>
<thead>
<tr>
<th>N</th>
<th>M</th>
<th>W</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>5</td>
<td>126</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>~10000</td>
</tr>
<tr>
<td>15</td>
<td>15</td>
<td>~10^8</td>
</tr>
</tbody>
</table>
SCHMiDT Decomposition

\[ |\psi\rangle = \sum_{\alpha=1}^{\chi_A} \lambda_\alpha |\phi^A_\alpha\rangle |\phi^B_\alpha\rangle \]

\[ \hat{\rho}_A |\phi^A_\alpha\rangle = |\lambda_\alpha|^2 |\phi^A_\alpha\rangle \quad \hat{\rho}_B |\phi^B_\alpha\rangle = |\lambda_\alpha|^2 |\phi^B_\alpha\rangle \]

\[ \sum_\alpha |\lambda_\alpha|^2 = 1 \]

Schmidt number
\[ \chi = \max_A \chi_A \]

For a general state \(1 \leq \chi \leq 2^{n/2}\)
Schmidt decomposition from SVD

\[ |\psi\rangle = \sum_{ij} c_{ij} |i\rangle_A |j\rangle_B \]

Singular Value Decomposition

\[ C = UDV \]

- \( C \) mxn matrix
- \( U, V \) unitary. \( D = \delta_{ii} \delta_{jj} \)

\[ \sum_k d_{kk} \sum_i u_{ik} |i\rangle_A \sum_j v_{kj} |j\rangle_B = \sum_k \lambda_k |\phi_k^A\rangle |\phi_k^B\rangle \]
\[ |\psi\rangle = \sum_{i_1, \ldots, i_n} c_{i_1 \ldots i_n} |i_1\rangle \otimes \cdots \otimes |i_n\rangle \]

Matrix Product State

\[ c_{i_1 \ldots i_n} = \sum_{\alpha_1 \ldots \alpha_n = 1} \chi \Gamma_{\alpha_1}^{[1]} \lambda_{\alpha_1}^{[1]} \Gamma_{\alpha_1 \alpha_2}^{[2]} \lambda_{\alpha_2}^{[2]} \Gamma_{\alpha_2 \alpha_3}^{[3]} \cdots \Gamma_{\alpha_{n-1}}^{[n]} \]

Site numbers

State index

\[ |\psi\rangle = \sum_{\alpha} \lambda_{\alpha} |\phi_{A=\{1,2\}}\rangle |\phi_{B=\{3,\ldots,n\}}\rangle \]
We have expressed $2^n$ coefficients with $(2\chi^2 + \chi)n$

We want to retain a fixed $\chi'$ number of states. In order to have a small error the choice of $\chi'$ depends on the entanglement entropy

$$S_L = -\sum_{\alpha} |\lambda_\alpha|^2 \log |\lambda_\alpha|^2$$

$\chi' \approx 2^{S_L}$

if $S_L \sim O(n^\delta)$ nothing gained

if $S_L \sim \text{const}$ we can exploit small entanglement

for general systems in $D>1$

true for gapped systems in $D=1$
Single site operations

only the corresponding $\Gamma$ tensor has to be updated ($\chi^2$ operations)

$$c_{i_1..i_n} = \sum_{\alpha_1..\alpha_{n-1}} \Gamma^{1,i_1}_{\alpha_1} \lambda^{1}_{\alpha_1} \Gamma^{2,i_2}_{\alpha_1,\alpha_2} \lambda^{2}_{\alpha_2} \Gamma^{3,i_3}_{\alpha_2,\alpha_3} .. \Gamma^{n,i_n}_{\alpha_{n-1}}$$

Two-site operations

only the corresponding $\Gamma$ tensors and $\lambda$ vector has to be updated ($\chi^3$ operations)
Time Evolution

\[ \hat{H} = \sum_k \hat{H}_{2k,2k+1} + \sum_k \hat{H}_{2k+1,2k+2} \]

Suzuki-Trotter decomposition

\[ e^{-i\delta t \hat{H}} \approx e^{-i\delta t \hat{H}_{\text{odd}}} e^{-i\delta t \hat{H}_{\text{even}}} + O(\delta t^2) \]
\[ \approx e^{-i\frac{\delta t}{2} \hat{H}_{\text{even}}} e^{-i\delta t \hat{H}_{\text{odd}}} e^{-i\frac{\delta t}{2} \hat{H}_{\text{even}}} + O(\delta t^3) \]

Imaginary Time Evolution

Ground State Properties

\[ |\psi_\tau\rangle = \frac{e^{-\tau \hat{H}} |\psi_0\rangle}{||e^{-\tau \hat{H}} |\psi_0\rangle||} \]
Algorithm
1. Apply $e^{-i\delta t H_{2k,2k+1}}$ on all even bonds
2. Carry out a Schmidt decomposition and retain a fixed number of states
3. Repeat point (1) and (2) for the odd bounds
4. This completes one Trotter time step which has to be iterated

Translationally Invariant Infinite Chain

Two kinds of tensors are enough to represent the infinite chain

Computational cost reduction of a factor $n$ due to parallelized, local updates
Matrix Product States on trees

Bethe lattice

\[ \text{MPS: write } |\psi\rangle \text{ in terms of } \Gamma_{\alpha_1 \alpha_2 \alpha_3} \text{ for each site and } \lambda_{\alpha_k} \text{ for each bound} \]
Matrix Product States on trees

MPS: write $|\psi\rangle$ in terms of $\Gamma_{\alpha_1\alpha_2\alpha_3}$ for each site and $\lambda_{\alpha k}$ for each bound
Matrix Product States on trees

Bethe lattice

\[ |\psi\rangle = \sum_{\alpha} \lambda_{\alpha} |\phi^{A}_{\alpha}\rangle |\phi^{B}_{\alpha}\rangle \]

MPS: write \( |\psi\rangle \) in terms of \( \Gamma_{\alpha_{1}\alpha_{2}\alpha_{3}} \) for each site and \( \lambda_{\alpha_{k}} \) for each bound
Consider a translationally invariant system
Define two kind of tensor on the bipartite graph, $\Gamma^A \Gamma^B$ and an “incoming” direction

Update in two steps
(Analogous to the “even-odd” update of the chain)
Correlation Functions

In general Correlations over MPS are computed as contractions of tensors one can look at the second eigenvalues of a given matrix $B$ function of the tensors $\Gamma$

$$\langle \hat{O}_i \hat{O}_j \rangle - \langle \hat{O}_i \rangle \langle \hat{O}_j \rangle \propto \mu_2^{|i-j|}$$

$$\xi = -1/\log \mu_2$$

$\mu_2$ second eigenvalue of $B$

$\xi$ correlation length

$\mu_2 \leq 1$. As far as $\mu_2 < 1$ correlations falls exponentially
Some results for the quantum transverse field Ising model

$$\frac{s}{2} \sum_{\langle ij \rangle} (1 - \hat{\sigma}_z^i \hat{\sigma}_z^j) + \frac{c(1 - s)}{2} \sum_i (1 - \hat{\sigma}_x^i)$$

Infinite Chain

### Figures

1. **FIG. 11.**
   - Caption: Magnetization obtained using MPS vs $s$ on the line.
   - Description: Some results for the quantum transverse field Ising model.

2. **FIG. 12.**
   - Caption: Transverse Ising model on an infinite tree.
   - Description: The computational cost of the tree simulation is more ex-

### Equations

- $s$ is the ratio of the interaction term with the value $s = 8$.
- The energy scale is logarithmic.
- Away from criticality, it behaves like $\log L$. Already at low $s$, $\xi$ becomes a projector, expressed in the $L = \frac{c(1 - s)}{2}$.

### Graphs

- **Left Graph**: Shows $M$ vs $s$ for different $\chi$.
- **Middle Graph**: Shows $\xi$ vs $s$ for different $\chi$.
- **Right Graph**: Shows $E_x - E_{\text{max}}$ vs $s$ for different $\chi$.

- **Legend**:
  - $\chi=4$
  - $\chi=8$
  - $\chi=16$
  - $\chi=30$

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Tuesday, May 18, 2010
Some results for the quantum transverse field Ising model

\[ \frac{s}{2} \sum_{\langle ij \rangle} (1 - \hat{\sigma}^i_z \hat{\sigma}^j_z) + \frac{c(1 - s)}{2} \sum_i (1 - \hat{\sigma}^i_x) \]
Some results for the quantum transverse field Ising model

\[
\frac{s}{2} \sum_{\langle ij \rangle} (1 - \hat{\sigma}_z^i \hat{\sigma}_z^j) + \frac{c(1 - s)}{2} \sum_i (1 - \hat{\sigma}_x^i)
\]

Bethe Lattice
Some results for time evolving quantities

$$\hat{H} = \sum_r \hat{\sigma}_x^r \hat{\sigma}_x^{r+1} + h_z \hat{\sigma}_z$$

The infinite chain. At $t=0$ $h_z=10 \rightarrow h_z=3$

Main sources of errors

- Suzuki-Trotter decomposition
- Truncation error ($\chi$)

The error grows with time
Comments & Conclusions

- General requirement: the entanglement must not grow too fast with time evolution in order to have a reliable simulation
- The algorithm establishes that any quantum evolution involving restricted amount of entanglement can be performed with classical computers
- It can be integrated into DMRG codes
- Lots of applications
    (and many others...)
- Many generalizations (D>1, critical systems, finite temperature,...)

[cond-mat/0605597v2]

[cond-mat/0712.1806v1]