Matrix-Product states: Properties and Extensions

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Outline

- Variational optimization of periodic MPS
- Mechanism of symmetry breaking with MPS
  - 1-d periodic transverse-field Ising model
  - critical form of the magnetization curve (finite N, N=∞)
  - limitations of finite computer precision(?)
- Criticality in 2D iPEPS (transverse-field Ising)
- MPS with variational Monte Carlo (time permitting)
Matrix product states (MPS)

Consider a periodic chain of S=1/2 spins

\[ |\Psi\rangle = \sum_{\{s_i\}} W(s_1, s_2, \ldots, s_N) |s_1, s_2, \ldots, s_N\rangle, \quad s_i = \uparrow, \downarrow \]

\[ W(s_1, s_2, \ldots, s_N) = \text{Tr}[A(s_1)A(s_2) \cdots A(s_N)] \]

• MPSs can be implicitly generated by DMRG (Ostlund & Romer, 1995)
• Can be used independently of DMRG as a class of variational 1-d states

**Graphical representation** of \(a^{l,s}_r\) and MPSs

Normalization \(\langle \Psi | \Psi \rangle\)

Expectation value \(\langle \Psi | S^a_i S^b_{i+1} \Psi \rangle\)

Can be easily evaluated; scaling for periodic chain: standard way costs \(ND^5\)
• Pippan, White, Evertz (PRB 2010); good approximation (SVD) with \(ND^3\)
• Monte Carlo sampling (Sandvik & Vidal, PRL 2007); \(ND^3\)
How to optimize the matrices in MPS calculations
• Local energy minimization, “sweep” through the lattice (Verstraete et al., ...)
• Imaginary-time evolution (projecting out the ground state) (Vidal, ...)

Minimize the energy with maintained translational invariance?
Stochastic Optimization (using first derivatives)

The stochastic method is guaranteed to reach the global minimum if:
• “cooled” sufficiently slowly
• if all local minima on “funnel walls”: b<a

Seems to work well for MPS optimization
• Starting from random matrices or ones optimized for smaller D
• Steepest decent can be faster at final stages
• But much slower than conventional methods
Test: Antiferromagnetic Heisenberg chain

\[ H = \sum_{i=1}^{N} S_i \cdot S_{i+1} = \sum_{i=1}^{N} [S_{i}^z S_{i+1}^z + \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)] \]

Comparison with N=100 results by: Pippan, White, Evertz (PRB 2010)

Good results, but the method is very slow
Infinite chain MPS

Exactly as in classical transfer-matrix method;
- keep only largest eigenvalue of $P$ when $N \to \infty$
- Imaginary-time evolution (ground state projection) or DMRG-type optimization can be applied (Vidal, Cirac, McCulloch,...)

$<\Psi | \Psi> = \text{Tr} \{ P_N \}$

(b) $c \quad d \quad a+(c-1)D \quad b+(d-1)D \quad = \quad A_{ab}(\uparrow)A^*_{cd}(\uparrow) + A_{ab}(\downarrow)A^*_{cd}(\downarrow) \quad = \quad P$

For some operator $M$ (single-site, e.g., magnetization)

$$\langle M \rangle = \frac{\text{Tr}\{ MP^{N-1} \}}{\text{Tr}\{ P^N \}} \quad \to \quad \frac{1}{\lambda_1} \sum_{i,j} v^*_{1i} v_{1j} M_{ij}$$
Question: **How is symmetry breaking manifested in MPS?**
- for finite N and N→∞

**Test: transverse-field Ising model**
- true critical magnetization exponent β=1/8
- how does this exponent emerge?
- what is the h→h_c behavior for finite D?

\[
H = - \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - \frac{h}{2} \sum_{i=1}^{N} (\sigma_i^+ + \sigma_i^-)
\]

**Stochastic optimization**
- Energy derivatives involve summing N different contributions
  ‣ time-consuming for N→∞

**Optimize in a trivial (slow) way for N=∞**
- Propose random changes in the matrix elements
  ‣ accept if and only if the energy improves
- easy to do in **quadruple precision** (but very slow)
Symmetry breaking for finite N

First-order transition (D fixed)
- discontinuity decreases with increasing N
- continuous for $N \to \infty$
- two $E$ minimums
  - symmetric and symmetry-broken states
- “level” crossing

Behavior versus D
- for given $N$, $h_c(D) \to 0$
- no symmetry-breaking for $N<\infty$, $D=\infty$
Infinite chain MPS - optimization using derivatives

The derivative of the energy with respect to a matrix element is of the form

\[
\frac{\partial E}{\partial a_{\sigma ij}} = C_{ij}^\sigma + \sum_{l=1}^{N-2} D_{ij}^\sigma (l) \quad D(l) \sim \text{Tr}\{X B^l X B^{N-2-l}\}
\]

D(l) is a correlation function; D(l)→0 when l→∞

- impose cut-off \( l_{\text{cut}} \) in optimization for \( N=\infty \); dependence on \( l_{\text{cut}} \)

\[
D = 2
\]
**N=∞: Optimization using trivial random updates**

Does not require derivatives
- propose random changes in all parameters; maximum change=\(\delta\)
- accept only if the energy decreases
- for \(\delta \to 0\) the acceptance rate should be 50%
- adjust \(\delta\) to give (e.g.) 10% acceptance rate

- find largest eigenvalue of \(P\) using

\[
P^m v = \lambda_1^m v, \quad m \to \infty
\]

- efficient with \(m=1,2,4,8,\ldots\) → \(P, P^2, P^4, P^8, \ldots\)
- numerically stable
- easy to go to high precision (quadruple, 128 bit)
Example: D=4, h=1.01432

- $10^4$ update attempts per “step”
- $\delta \rightarrow \delta/1.1$ after each step if <10% accepted updates
- **stage 1:** double precision, **stage 2:** quadruple precision
- $E = -1.282445246576107642...$, $M_z = 0.0318141670...$ (quad precision)

Errors relative to converged results (for given D)

$$\Delta_E = \frac{(E - E_{\text{conv}})}{E_{\text{conv}}}$$

$$\Delta_m = \frac{(m - m_{\text{conv}})}{m_{\text{conv}}}$$

![Graph showing evolution of $\delta$ and acceptance rate](image-url)
Close to the critical point:
Small change in E → large (relative) change in m^Z
• can be a serious issue when analyzing the critical behavior

\[ \frac{E}{N} \quad m^Z = \frac{1}{N} \sum_{i=1}^{N} S_i^Z \quad \delta = \text{max change in matrix elements} \]

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<th>( \delta )</th>
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Relative change \( = 3 \times 10^{-14} = 3 \times 10^{-3} \)

Comparison with imaginary-time projection (TEBD); D=4, h=1.014334
E=-1.282454538906097   \( m=0.004589923026775 \) (I. McCulloch, standard)
E=-1.28245453890609554713490 \( m=0.004589765790234 \) (Random optimization)
Analysis of the critical behavior

Power-law fit for small $m^z$ always gives $\beta \approx 0.50$
- indicates asymptotic mean-field behavior

For finite $D$, asymptotic critical behavior is of mean-field type
- cross-over to the true critical exponent
- numerical precision may limit access to critical behavior
The asymptotic mean-field behavior for MPS is not surprising
• finite D $\rightarrow$ maps to classical 1D transfer matrix
• criticality in 1D classical system requires long-range interactions

**How about 2D PEPS?**

Finite D $\rightarrow$ classical 2D partition function; critical points exist
• non-trivial exponents have been seen (?) for D=2,3 iPEPS

**Infinite-size PEPS (iPEPS)** [Orus & Vidal (2009)]
• Generalization of the N=\(\infty\) MPS (but more complicated, approximations)
• We use new stable optimization/contraction [Wang & Verstraete]

$\leftarrow$ 2D transverse-field Ising
• mean-field cross-over
• to extract the true exponent requires careful check of convergence with D
• the true exponent emerges in a window away from \(h_c\)
• similar cross-overs in classical systems (Baxter, Nishino et al.,...)
Conclusions

Symmetry-breaking in MPS
• first-order for finite $N$, finite $D$
• continuous mean-field transition for $N=\infty$, finite $D$
  - mean-field window shrinks as $D \to \infty$
  - true exponents emerge through cross-over behavior

Numerical precision issues (variational optimization)
• $N=\infty$ optimization difficult close to phase transition
  - relative error of order parameter large even if $E$ converged
  - difficult to extract the critical point precisely

$N=\infty$ PEPS (IPEPS)
• mean-field criticality for finite $D$
  - existence of non-trivial critical points for finite $D$ does not mean that one automatically obtains correct critical behavior for a given $H$