Error estimates for extrapolations of observables with matrix-product states

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MPQ

2 March 2018; Benasque

with Jutho Haegeman & Uli Schollwöck

DMRG as ground-state solver

2DMRG

- "original" system/environment
- well-established, widely used
- typically converges, esp. with additional noise terms
- $O(m^3d^2w + m^3d^3 + m^2d^2w^2)$
- truncation error allows linear extrapolation $m \to \infty$

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1DMRG

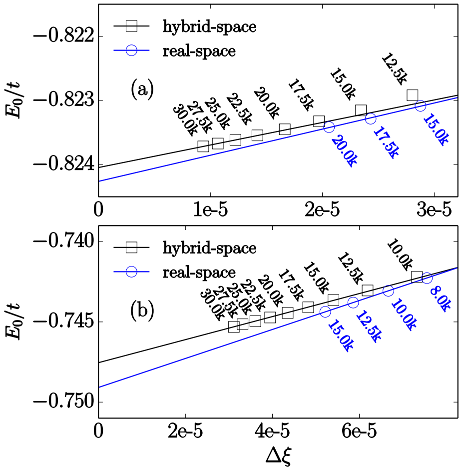
- easy to implement
- "natural" variant for MPS
- converges with subspace expansion
- $O(m^3dw + m^2d^2w^2)$
- speedup: 3-4 (spins/electrons), large (bosons)
- same factor in memory savings
- no error measure

Usefulness of extrapolations

- $m \approx 5'000$ to $m \approx 100'000$ upper limit (large-scale)
- $m \approx 1'000$ much nicer
- not always sufficient to evaluate observables to desired precision
- extrapolation in 2DMRG truncation error lowers error in observable by approx. order of magnitude
- extrapolation in m directly not possible
- applications: DMRG on 2D cylinders, critical 1D systems, DMET(?)

2DMRG Example

G. Ehlers, S. R. White, R. M. Noack, PRB 95, 125125



Alternative to 2DMRG truncation error: variance v

- $v = \langle\psi| \left(\hat{H} - E\right)^2 |\psi\rangle = \left|\left|\hat{H}|\psi\rangle - E|\psi\rangle\right|\right|^2$: squared norm of residual
- if $|\psi\rangle$ is "mostly ground state", v measures error
- extrapolation of energy in v possible
- $v(\hat{H}, |\psi\rangle)$, not $v(\hat{H}, \mathrm{DMRG\ method,\ sweeping\ procedure,\ \#sweeps})$

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- $v(\hat{H}, |\psi\rangle)$, not $v(\hat{H}, \mathrm{DMRG\ method, sweeping\ procedure, \#sweeps})$
- $O(m^3 d w^2 + \ldots)$ or $O(m^3 d (2w))$

n-site variation spaces on a MPS $|\psi\rangle$

- $\mathcal{W}_0 = \mathrm{span}\left(|\psi\rangle\right)$
- $\mathcal{W}_1$: single-site variations of $|\psi\rangle$ orthogonal to $|\psi\rangle$
- $\mathcal{W}_2$: consecutive two-site variations of $|\psi\rangle$ orthogonal to $|\psi\rangle$ and $\mathcal{W}_1$
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- $\mathcal{H} = \bigoplus_{k=0}^{L} \mathcal{W}_k$

Left- and right-complement MPS tensors

- $A_i : \mathcal{H}_L \otimes \mathcal{H}_p \mapsto \mathcal{H}_R \qquad B_i : \mathcal{H}_R \otimes \mathcal{H}_p \mapsto \mathcal{H}_L$

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- $\sum_{m_i,\sigma_i} F_{i;m'_{i+1}}^{\sigma_i m_i} F_{i;\sigma_i m_i}^{\dagger \tilde{m}'_{i+1}} = \mathbf{1}_{m'_{i+1}}^{\tilde{m}'_{i+1}}$
- $\sum_{m_i,\sigma_i} F_{i;m'_{i+1}}^{\sigma_i m_i} A_{i;\sigma_i m_i}^{\dagger \tilde{m}_{i+1}} = 0$

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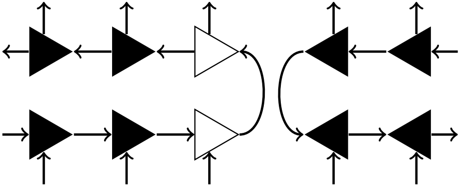
- $\hat{P}_1$: $\sum_{i=1}^{L}$ 

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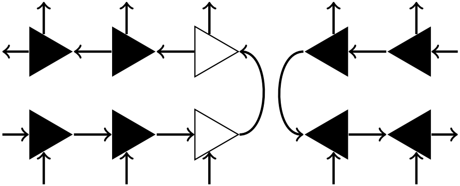
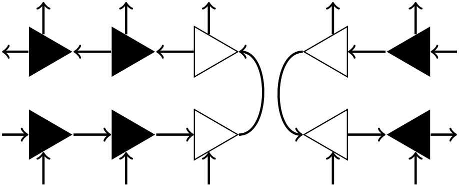


- $\hat{P}_2$: $\sum_{i=1}^{L-1}$



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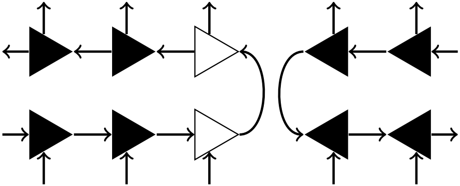
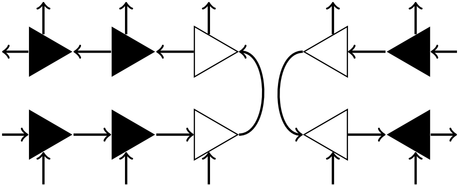
- $\hat{P}_1$: $\sum_{i=1}^{L}$ 
- $\hat{P}_2$: $\sum_{i=1}^{L-1}$ 
- $\hat{\mathbf{1}} = \sum_{k=0}^{L} \hat{P}_k$

Two-site variance

$$v = \langle\psi| \left(\hat{H} - E\right) \left(\hat{H} - E\right) |\psi\rangle$$

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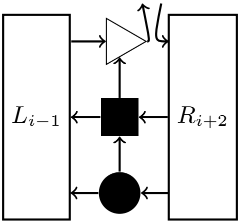
$$= \langle\psi|\hat{H} \left(\hat{P}_1 + \hat{P}_2\right) \hat{H}|\psi\rangle$$

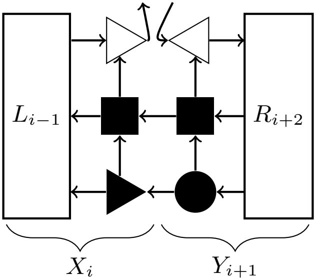
Two-site variance

$$v \approx \langle\psi|\hat{H}\left(\hat{P}_1 + \hat{P}_2\right)\hat{H}|\psi\rangle$$

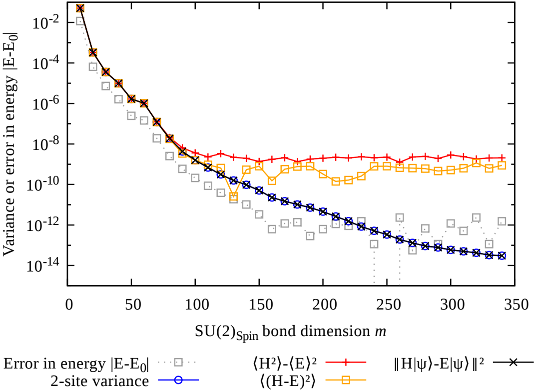
- exact if $\hat{H} = \sum_{i=1}^{L-1} \hat{h}_{i,i+1}$
- only small, positive terms to sum
- relatively fast: $O\left(m^3 dw + m^3 d^2 w\right)$
- easy to parallelise costly part by $2L - 1$ workers

Individual terms

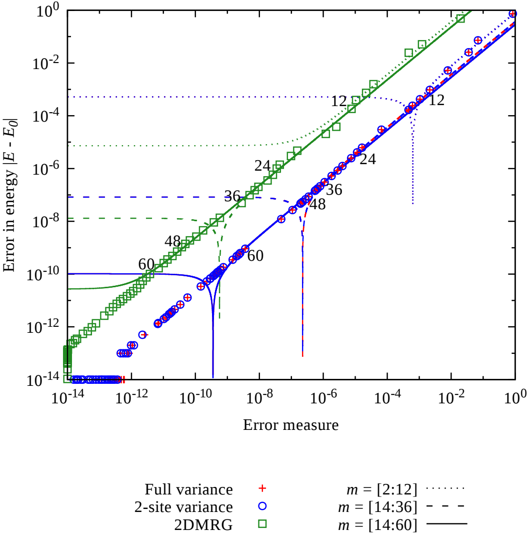




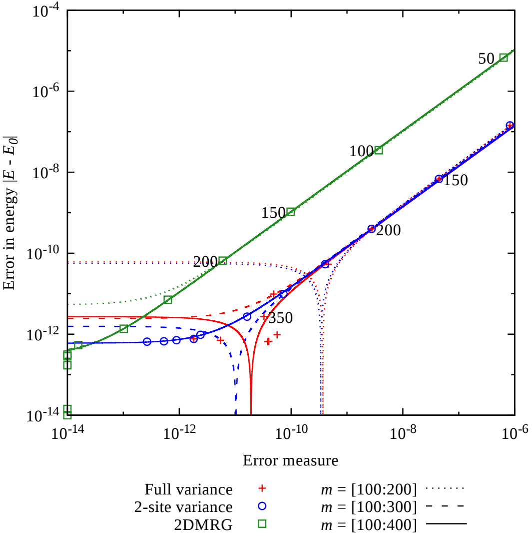
Accuracy: $L = 200, S = 1$ Heisenberg model



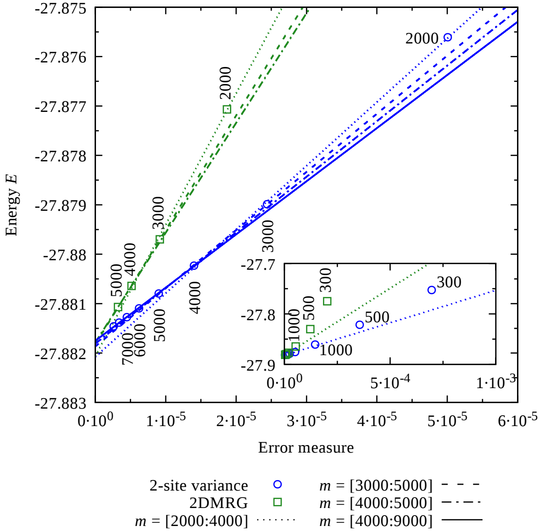
Extrapolation: $L = 30, S = 1/2$ Heisenberg model



Extrapolation: $L = 20$ Hubbard, Coulomb-like interactions



Extrapolation: 10×4 Hubbard, $U = 8$, $n = 0.9$



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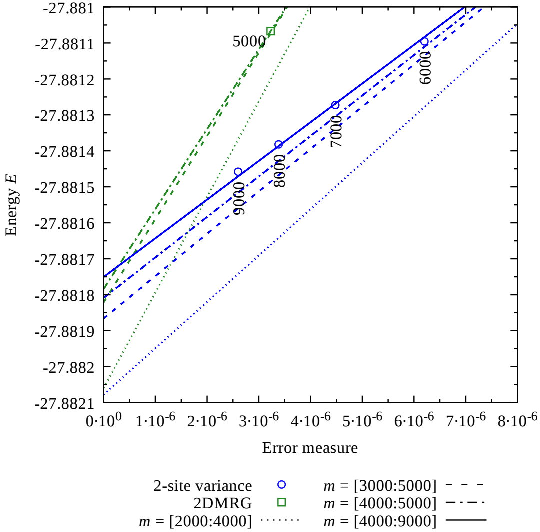

Summary

- extrapolations lower error in energy by approx. one order of magnitude
- 2-site variance/full variance work as well as 2DMRG truncation error
- 2-site variance much faster than full variance
- 2-site variance also reliable for long-range $\hat{H}$, extensible to n-site
- 1DMRG + 2-site variance faster than 2DMRG for same energies, much larger bond dimensions possible
- *variational property of DMRG lost when extrapolating*