Scalable variational embedding for quantum many-body problems

SIAM MS21
Electronic structure methods: quantum magnetism and numerical approaches beyond density functional Theory

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The ground-state eigenvalue problem

- The basic quantum many-body problem is the *ground state eigenvalue problem*
  - Find lowest eigenvalue E_0 of an operator $\hat{H}$ on a Hilbert space $\mathcal{Q}$ of exponentially high dimension
  - Variational formulation

$$E_0 = \min_{\phi \in \mathcal{Q} \,:\, \phi^* \phi = 1} \phi^* \hat{H} \phi$$

- Wide-reaching applications in chemistry, physics, and materials science
  - Include equilibrium geometry of molecules, *ab initio* molecular dynamics
  - Moreover, expectations of the form $\phi^* \hat{O} \phi$ predict physically observable quantities within the ground state

Quantum spin systems

- Consider a model consisting of M sites, indexed by $i \in [M] := \{1, \ldots, M\}$
- Classically, each site can assume a binary state $s_i \in \{0, 1\}$
- The classical states are then binary strings

$$\mathbf{s} = (s_1, \ldots, s_M) \in \{0, 1\}^M$$

- We will consider the 'quantum analog' of classical combinatorial (0-1) optimization problems

$$\min_{\mathbf{s} \in \{0,1\}^M} f(\mathbf{s})$$

  - e.g., MaxCut: $f(\mathbf{s}) = \mathbf{s}^\top A \mathbf{s}$, where A is an adjacency matrix for a graph on $[M]$
- .Quantum wavefunctions are complex functions $\phi : \{0, 1\}^M \to \mathbb{C}$
  - Can be viewed as tensors in $\mathcal{Q} := \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$ (M times) via

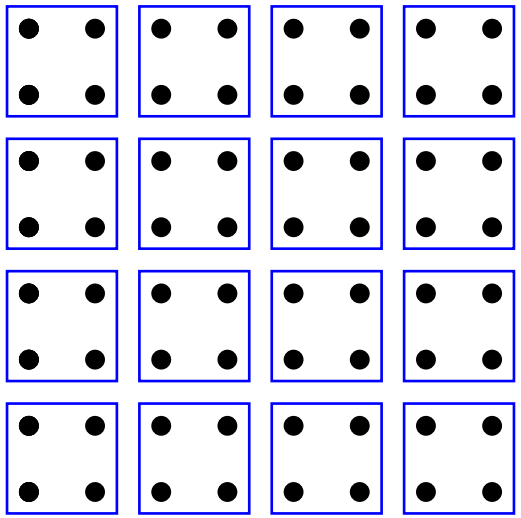
$$\phi_{s_1 s_2 \cdots s_M} = \phi(\mathbf{s})$$

- This is the Hilbert space for quantum spin-$\frac{1}{2}$ systems
  - Also the Hilbert space for electronic structure problems after passing to the second-quantized fermionic formalism

Algebras of operators

- Let $\mathcal{A}$ be the algebra of operators on $\mathcal{Q}$
  - Classical analog is functions on $\{0,1\}^M$
- For any subset $S \subset [M]$, we have a subalgebra $\mathcal{A}_S$ of *local* operators
  - Classical analog is functions that depend only on a subset of variables
  - For quantum spin systems, $\mathcal{A}_S$ consists of operators obtained by tensoring with the identity operator on sites in $[M] \backslash S$
  - For fermions, $\mathcal{A}_S$ is generated by the creation/annihilation operators $a_i^\dagger, a_i$ for $i \in S$

Algebras of operators



- Then given a partition of $[M]$ into disjoint clusters C_γ, assume our Hamiltonian operator can be written

$$\hat{H} = \sum_\gamma \hat{H}_\gamma + \sum_{\gamma\delta} \hat{H}_{\gamma\delta},$$

where $\hat{H}_\gamma \in \mathcal{A}_\gamma := \mathcal{A}_{C_\gamma}$ and $\hat{H}_{\gamma\delta} \in \mathcal{A}_{\gamma\delta} := \mathcal{A}_{C_\gamma \cup C_\delta}$ are Hermitian

  - True of many physical problems, including suitable discretizations of electronic structure problems

State formulation

- Call a linear functional $\omega : \mathcal{A} \to \mathbb{C}$ a *state* on $\mathcal{A}$ if $\omega(\hat{A}^*) = \omega(\hat{A})^*$, $\omega(\hat{A}^*\hat{A}) \geq 0$ for all $\hat{A} \in \mathcal{A}$, and $\omega(\mathrm{Id}) = 1$
  - $\omega(\hat{A}) = \mathrm{Tr}\left[\hat{A}\rho\right]$ for some density operator ρ on $\mathcal{Q}$ ($\rho \succeq 0$, $\mathrm{Tr}[\rho] = 1$)
  - Let Ω, Ω_γ, $\Omega_{\gamma\delta}$ be the (convex) sets of states on $\mathcal{A}$, $\mathcal{A}_\gamma$, and $\mathcal{A}_{\gamma\delta}$
- Ground state eigenvalue problem can be rephrased as

$$E_0 = \min_{\omega \in \Omega} \omega(\hat{H})$$

  - The optimizer ω is given by $\omega(\hat{A}) = \mathrm{Tr}\left[\hat{A}\phi\phi^*\right] = \phi^*\hat{A}\phi$, where ϕ is the ground-state eigenvector
- Note that we can rewrite

$$E_0 = \inf\left\{\sum_\gamma \omega_\gamma(\hat{H}_\gamma) + \sum_{\gamma\delta} \omega_{\gamma\delta}(\hat{H}_{\gamma\delta}) \;:\; \omega_\gamma \in \Omega_\gamma,\ \omega_{\gamma\delta} \in \Omega_{\gamma\delta} \text{ are jointly representable}\right\}$$

  - Joint representability means that the $\omega_\gamma \in \Omega_\gamma$, $\omega_{\gamma\delta} \in \Omega_{\gamma\delta}$ *all* could have come from the *same* $\omega \in \Omega$ by restriction
  - We have changed exponential size of optimization space for exponential complexity of constraints

Semidefinite relaxation

- We aim to relax the joint representability constraint to get a lower bound
- That is, enforce some necessary (but not sufficient) constraints for joint representability:
  1. **State:** $\omega_{\gamma\delta} \in \Omega_{\gamma\delta}$
     - Yields independent semidefinite constraints for each pair (γ, δ)
  2. **Local consistency:** $\omega_{\gamma\delta}(\hat{A}) = \omega_\gamma(\hat{A})$ for $\hat{A} \in \mathcal{A}_\gamma$, $\omega_{\gamma\delta}(\hat{A}) = \omega_\delta(\hat{A})$ for $\hat{A} \in \mathcal{A}_\delta$
     - Yields linear equality constraints coupling overlapping pairs of clusters
  3. ***Global consistency***: $\omega\left[\left(\sum_\gamma \hat{A}_\gamma\right)^\dagger \left(\sum_\gamma \hat{A}_\gamma\right)\right] \geq 0$ for any $\hat{A}_\gamma \in \mathcal{A}_\gamma$
     - Yields global semidefinite constraint coupling all pairs (γ, δ)

Semidefinite relaxation

- Concretely one obtains

$$
\begin{aligned}
\underset{\{\rho_i\},\,\{\rho_{ij}\}_{i<j}}{\text{minimize}} \quad & \sum_i \mathrm{Tr}\left[H_i \rho_i\right] + \sum_{i<j} \mathrm{Tr}\left[H_{ij} \rho_{ij}\right] \\
\text{subject to} \quad & \rho_{ij} \succeq 0, \quad 1 \le i < j \le M, \\
& \rho_i = A_1[\rho_{ij}], \;\; \rho_j = A_2[\rho_{ij}], \quad 1 \le i < j \le M, \\
& \mathrm{Tr}[\rho_i] = 1, \quad i = 1, \ldots, M, \\
& G[\{\rho_i\}, \{\rho_{ij}\}_{i \le j}] \succeq 0.
\end{aligned}
$$

  for suitable matrices H_i, H_{ij}

  - For simplicity now use i, j to index clusters, not sites

- Call it the *2-marginal relaxation*, optimal value $E_0^{(2)}$
  - Analogy of local states to marginals in classical probability

Partial duality

- Dualize only the global semidefinite constraint to obtain

$$E_0^{(2)} = \sup_{X \succeq 0} \ \mathcal{F}[X],$$

where $\mathcal{F}[X]$ is optimal value of 'effective problem'

$$\begin{aligned} \underset{\{\rho_i\},\, \{\rho_{ij}\}_{i<j}}{\text{minimize}} \quad & \sum_i \mathrm{Tr}\left[H_i(X)\rho_i\right] + \sum_{i<j} \mathrm{Tr}\left[H_{ij}(X)\rho_{ij}\right] \\ \text{subject to} \quad & \rho_{ij} \succeq 0, \quad 1 \leq i < j \leq M, \\ & \rho_i = A_1[\rho_{ij}], \ \rho_j = A_2[\rho_{ij}], \quad 1 \leq i < j \leq M, \\ & \mathrm{Tr}[\rho_i] = 1, \quad i = 1, \ldots, M \end{aligned}$$

- Effective problem has similar structure to original SDP
  - But global semidefinite constraints omitted, exchanged for effective contribution dependent on X
- Gives the interpretation of a *quantum embedding theory*

Partial dual gradient ascent approach

- Want to perform projected gradient ascent on $\mathcal{F}[X]$ over $X \succeq 0$
- Alternate between:
  1. Obtain $\{\rho_i\}$, $\{\rho_{ij}\}_{i<j}$ by solving the effective problem (holding X fixed)
  2. Update $X \leftarrow \Pi_{\succeq 0}\left(X - \varepsilon G\left[\{\rho_i\}, \{\rho_{ij}\}_{i<j}\right]\right)$
- In practice, we replace step (1) with a single iteration of an augmented Lagrangian-type solver
- Translation-invariance can be exploited for a per-iteration cost scaling *linearly* in number K of clusters
  - *Bottleneck*: K full matrix diagonalizations
    - These are decoupled and can be perfectly parallelized
- Otherwise the global semidefinite constraint is generally cubic in K
- Scaling is exponential in cluster size $L = |C_\gamma|$
  - In our experiments, $L \leq 4$
  - *Ongoing*: further (local) relaxation may enable larger clusters for *ab initio* quantum chemistry

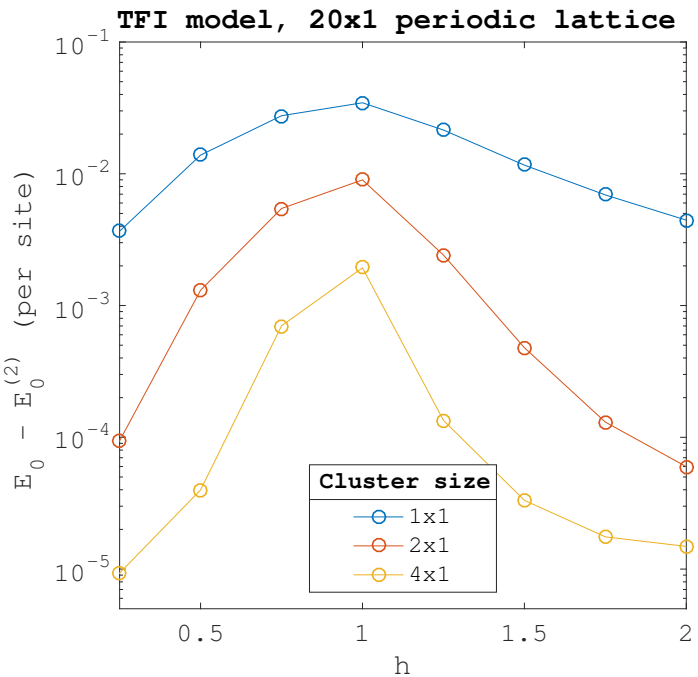
Selected results

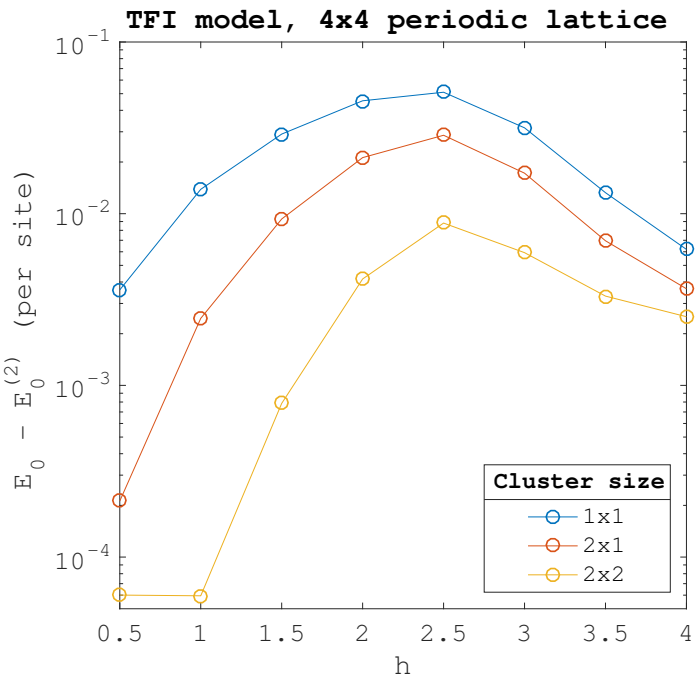
- I'll present results for the transverse-field Ising (TFI) and anti-ferromagnetic Heisenberg (AFH) model

$$\mathcal{H}_{\mathrm{TFI}} = -h \sum_i \sigma_i^x - \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z$$

$$\mathcal{H}_{\mathrm{AFH}} = \sum_{\langle i,j \rangle} \left[\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z \right]$$

TFI exact benchmark





AFH exact benchmark

1×1 clusters	2×1 clusters	4×1 clusters
0.5383	0.0521	0.0034

Table: Relaxation error per site for the AFH model on a 20×1 periodic lattice for various cluster sizes.

1×1 clusters	2×1 clusters	2×2 clusters
0.6634	0.1851	0.0034

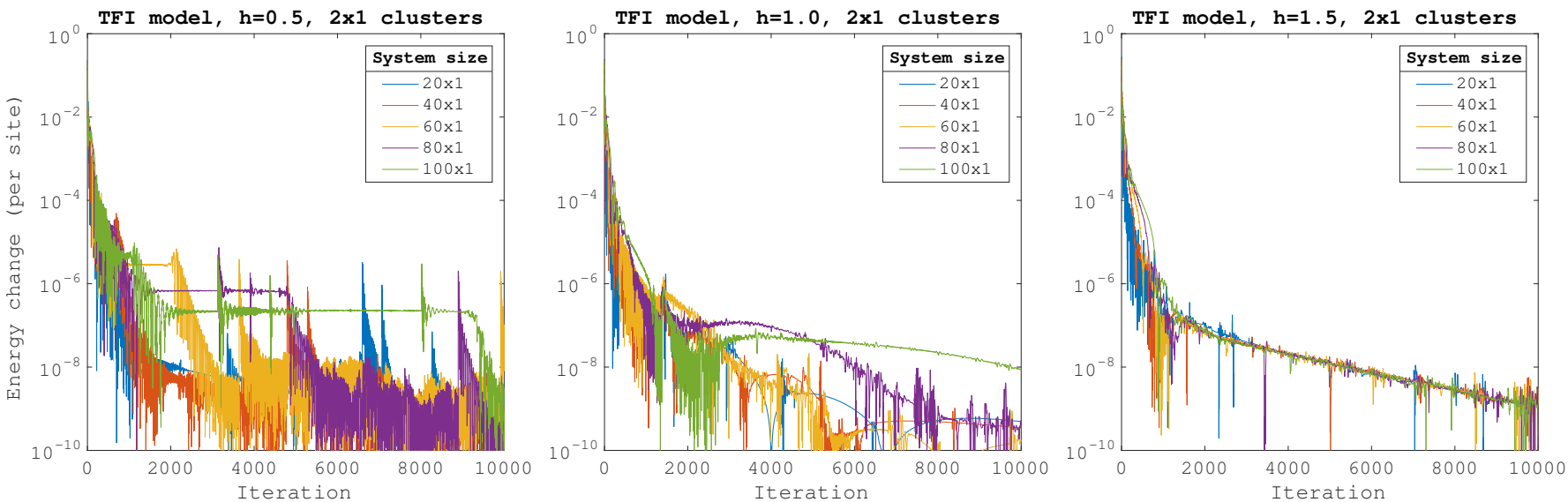
Table: Relaxation error per site for the AFH model on a 4×4 periodic lattice for various cluster sizes.

Effect of global consistency constraints

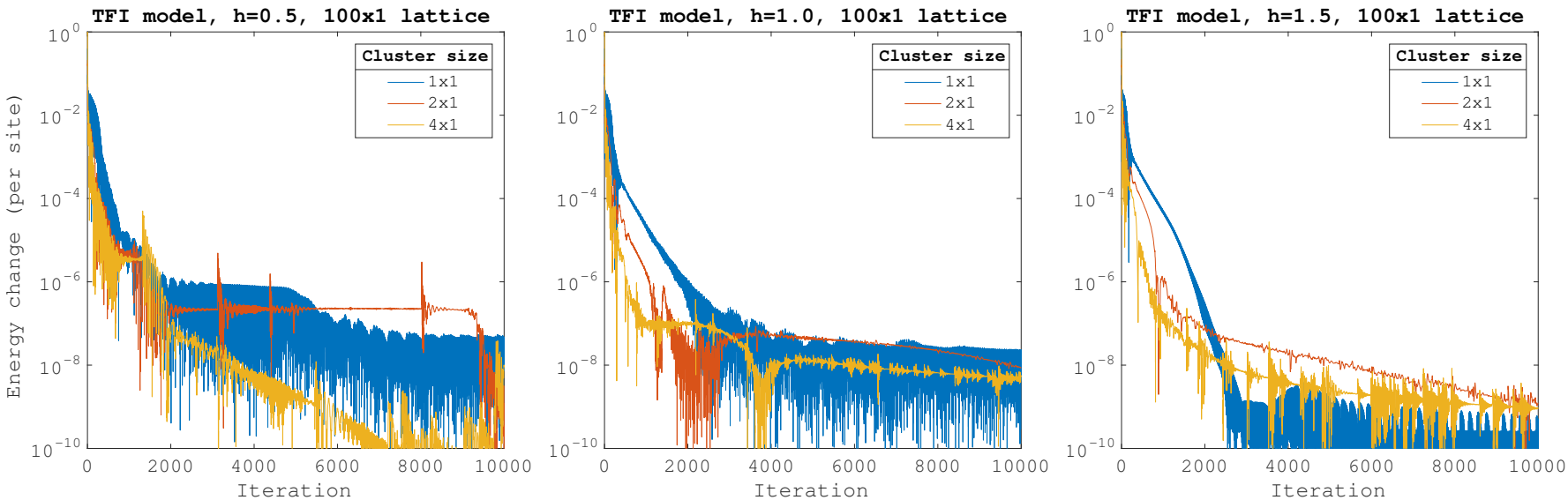
	1×1 clusters	2×1 clusters	1×3 clusters
With global constraints	1.0439	0.3937	0.0410
W/o global constraints	3.5439	2.1897	0.8773

Table: Relaxation error per site for the AFH model on a 4×3 periodic lattice for various cluster sizes

Dependence of convergence on system size



Dependence of convergence on cluster size



References and related work

- References for the talk
  - L. Lin and **M.L.**, Variational embedding for quantum many-body problems, *CPAM* (2021)
  - Y. Khoo and **M.L**., Scalable semidefinite programming approach to variational embedding for quantum many-body problems (*in preparation*)
- Classical 0-1 optimization, graphical models
  - [Goemans and Williamson (1995)] (MaxCut)
  - [Jordan and Wainwright (2008)] (Variational inference, marginal polytope relaxations)
- 2-RDM theory (electronic structure)
  - e.g., many papers of D. Mazziotti et al and M. Nakata et al
- Other quantum marginal-type relaxations
  - [Ferris and Poulin (2013)] (quantum belief propagation)
  - [Barthel and Hübener (2012)]
- Classical analogs of the relaxation in this talk
  - [Khoo, Lin, **M.L.**, Ying (2020)] (multi-marginal optimal transport)
  - [Chen, Khoo, **M.L.** (2020)] (marginal relaxation for global optimization)