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 basic quantum many-body problem is the \textit{ground state eigenvalue problem}

- Find lowest eigenvalue $E_0$ of an operator $\hat{H}$ on a Hilbert space $Q$ of exponentially high dimension
- Variational formulation

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

Wide-reaching applications in chemistry, physics, and materials science

- Include equilibrium geometry of molecules, \textit{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 $s = (s_1, \ldots, s_M) \in \{0, 1\}^M$
- We will consider the ‘quantum analog’ of classical combinatorial (0-1) optimization problems
  $$\min_{s \in \{0,1\}^M} f(s)$$
  - e.g., MaxCut: $f(s) = s^\top As$, where $A$ is an adjacency matrix for a graph on $[M]$
- Quantum wavefunctions are complex functions $\phi : \{0, 1\}^M \rightarrow \mathbb{C}$
  - Can be viewed as tensors in $Q := \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$ ($M$ times) via
    $$\phi_{s_1 s_2 \cdots s_M} = \phi(s)$$
- 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 $Q$.
  - 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 $[M] \setminus S$.
  - For fermions, $\mathcal{A}_S$ is generated by the creation/annihilation operators $a_i^\dagger, a_i$ for $i \in S$. 
Then given a partition of \([M]\) into disjoint clusters \(C_\gamma\), 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 $\omega(\text{Id}) = 1$
  - $\omega(\hat{A}) = \text{Tr} \left[ \hat{A} \rho \right]$ for some density operator $\rho$ on $\mathcal{Q}$ ($\rho \succeq 0$, $\text{Tr}[\rho] = 1$)
  - Let $\Omega$, $\Omega_\gamma$, $\Omega_{\gamma\delta}$ 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 $\omega$ is given by $\omega(\hat{A}) = \text{Tr} \left[ \hat{A} \phi \phi^* \right] = \phi^* \hat{A} \phi$, where $\phi$ 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 \((\gamma, \delta)\)
  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 \((\gamma, \delta)\)
Semidefinite relaxation

Concretely one obtains

\[
\begin{align*}
\text{minimize} & \quad \sum_i \text{Tr} [H_i \rho_i] + \sum_{i<j} \text{Tr} [H_{ij} \rho_{ij}] \\
\text{subject to} & \quad \rho_{ij} \succeq 0, \quad 1 \leq i < j \leq M, \\
& \quad \rho_i = A_1[\rho_{ij}], \quad \rho_j = A_2[\rho_{ij}], \quad 1 \leq i < j \leq M, \\
& \quad \text{Tr}[\rho_i] = 1, \quad i = 1, \ldots, M, \\
& \quad G[\{\rho_i\}, \{\rho_{ij}\}_{i\leq j}] \succeq 0.
\end{align*}
\]

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’

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

- 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 $X \leftarrow \Pi_{\succeq 0} (X - \varepsilon G [\{\rho_i\}, \{\rho_{ij}\}_{i<j}])$

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

\[ H_{\text{TFI}} = -h \sum_i \sigma_i^x - \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z \]

\[ H_{\text{AFH}} = \sum_{\langle i,j \rangle} \left[ \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z \right] \]
TFI exact benchmark

TFI model, 20x1 periodic lattice

TFI model, 4x4 periodic lattice

Cluster size

$E_0 - E^{(2)}$ (per site)
AFH exact benchmark

<table>
<thead>
<tr>
<th>Cluster Size</th>
<th>Relaxation Error (20 × 1)</th>
<th>Relaxation Error (4 × 4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 × 1 clusters</td>
<td>0.5383</td>
<td>0.6634</td>
</tr>
<tr>
<td>2 × 1 clusters</td>
<td>0.0521</td>
<td>0.1851</td>
</tr>
<tr>
<td>4 × 1 clusters</td>
<td>0.0034</td>
<td>0.0034</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Cluster Size</th>
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</tr>
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<tr>
<td>1 × 1 clusters</td>
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<td>0.1851</td>
</tr>
<tr>
<td>2 × 2 clusters</td>
<td>0.0034</td>
</tr>
</tbody>
</table>

**Table:** Relaxation error per site for the AFH model on a 4 × 4 periodic lattice for various cluster sizes.
Effect of global consistency constraints

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

<table>
<thead>
<tr>
<th></th>
<th>$1 \times 1$ clusters</th>
<th>$2 \times 1$ clusters</th>
<th>$1 \times 3$ clusters</th>
</tr>
</thead>
<tbody>
<tr>
<td>With global constraints</td>
<td>1.0439</td>
<td>0.3937</td>
<td>0.0410</td>
</tr>
<tr>
<td>W/o global constraints</td>
<td>3.5439</td>
<td>2.1897</td>
<td>0.8773</td>
</tr>
</tbody>
</table>
Dependence of convergence on system size

TFI model, $h=0.5$, 2x1 clusters

TFI model, $h=1.0$, 2x1 clusters

TFI model, $h=1.5$, 2x1 clusters

Energy change (per site) vs. iteration for different system sizes.
Dependence of convergence on cluster size

TFI model, $h=0.5$, 100x1 lattice

TFI model, $h=1.0$, 100x1 lattice

TFI model, $h=1.5$, 100x1 lattice
References and related work

- References for the talk
  - 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)