Semistochastic importance sampling of second-quantized operators in determinant space

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Overview

1. Motivation
2. Algorithm
3. Applications

Motivation

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    4. Full CI Quantum Monte Carlo (FCIQMC)

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4. FCIQMC: Stochastically simulate the power method,

$$\psi_0 \propto \lim_{n \to \infty} (1 - \tau H)^n \psi_T \tag{3}$$

Approaches for computing $H\left|D_i\right\rangle$

Broadly, there are three main approaches:

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3. **Semistochastic:** Evaluating the largest-magnitude components, and sampling the remaining, smaller components. Reduces complexity relative to the deterministic approach, but with a **greatly reduced stochastic uncertainty** relative to fully stochastic methods. In projector methods, it also mitigates the bias incurred in taming the fermion sign problem, such as the initiator bias in FCIQMC.

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$$H\left|D_i\right\rangle = \sum_j H_{ji} \tag{4}$$

$$= \underbrace{\sum_j H_{ji}\Big|_{|H_{ji}|\geq\epsilon}}_{\substack{\text{few large terms:}\\ \text{sum deterministically}}} + \underbrace{\sum_j H_{ji}\Big|_{|H_{ji}|<\epsilon}}_{\substack{\text{many small terms:}\\ \text{importance sample}}} \tag{5}$$

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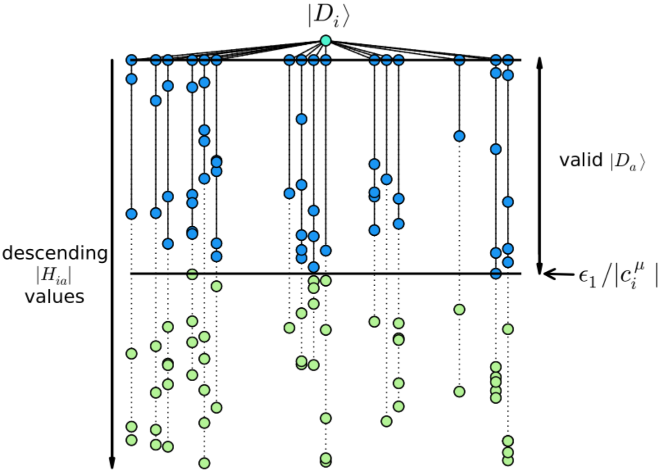
- **Finding important connected determinants** D_j (for which $|H_{ji}| \geq \epsilon$):
  - For each pair of occupied orbitals $\{p, q\}$, look up the stored list of $\{r, s, |H(rs \leftarrow pq)|\}$ and iterate until $|H(rs \leftarrow pq)| < \epsilon$

Deterministic component



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- Usually, Alias sampling is preferred because it has lower sampling complexity, but CDF searching has a unique use case that we will need...

CDF searching's unique use case

Suppose we have a stored CDF, and we want to be able to efficiently sample one of the first n elements, where n is not known ahead of time. CDF searching can do this efficiently with a small modification:

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- Examples of importance-sampling distributions include:

$$f(|H_{ji}|) = |H_{ji}|, \qquad f(|H_{ji}|) = |H_{ji}|^2 \tag{8}$$

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- This enables **importance-sampling an exciting electron pair in $\mathcal{O}(1)$ time**

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- So, we just use CDF searching to **sample a target orbital pair in $\mathcal{O}(\log M)$ time**

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  where $|H(p \to r)|_{\max}$ is the largest magnitude the $p \to r$ excitation can have from *any* initial determinant
- The simplest way to incorporate singles is to sample them with probability $P(|H(p \to r)|) \propto f(|H(p \to r)|_{\max})$ and skip them in the deterministic step

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  2. Scale the sample probabilities by a constant factor so they remain normalized (can be performed in $\mathcal{O}(N^4 + N_{\det} N^3)$ time during deterministic step)

Applications

Epstein-Nesbet perturbation theory

Given a variational wavefunction $\psi_0 = \sum_i c_i \left|D_i\right\rangle$ with energy E_0, the Epstein-Nesbet perturbative correction to the energy is give by

$$\Delta E\left[V\left|\psi_0\right\rangle\right] = \left\langle \psi_0 \left| V \frac{1}{E_0 - H_0} V \right| \psi_0 \right\rangle \tag{10}$$

$$= \sum_{\substack{a \in \mathcal{C}(\mathcal{V}) \\ \notin \mathcal{V}}} \frac{1}{E_0 - E_a} \left(\sum_{ij \in \mathcal{V}} c_j H_{ja} H_{ai} c_i \right), \tag{11}$$

so we can now evaluate the H_{ai} components semistochastically using importance sampling.

Semistochastic Epstein-Nesbet Perturbation Theory

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3. Stochastically evaluate the difference between the exact and approximate ΔE

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    - Wastes time on small-magnitude H_{ai} elements

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    - No time or memory is wasted on deterministically evaluating contributions from small-magnitude H_{ai} elements!

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- The energy can be estimated using a mixed estimator:

$$E_0 = \frac{\langle \psi_T \left| H \right| \psi_0 \rangle}{\langle \psi_T | \psi_0 \rangle}, \tag{18}$$

using a precomputed ψ_T (e.g. from Selected CI)

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    3. Importance-sample off-diagonal elements, discard the ones that were already treated deterministically

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  - Deterministic/stochastic division is dynamic: it depends on the current $\psi^{(t)}$, which should greatly reduce the stochastic fluctuations and mitigate the fermion sign problem

Semistochastic algorithm in FCIQMC

- New approach (Dynamic, importance-sampled semistochastic FCIQMC):

  1. Apply the Hamiltonian using semistochastic importance sampling to each determinant in $\psi^{(t)}$

- Advantages:

  - Deterministic/stochastic division is dynamic: it depends on the current $\psi^{(t)}$, which should greatly reduce the stochastic fluctuations and mitigate the fermion sign problem

  - Directly samples the off-diagonal H elements that were not treated deterministically, which should greatly reduce the computational time