QI 113

Adaptive and provably accurate estimation of quantum expectation values using the empirical Bernstein stopping rule

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Motivation

Goal

- Reduce measurement effort of quantum measurements while retaining a target accuracy

Applications

- Variational quantum algorithms (VQAs), e.g. for quantum chemistry, combinatorics
- any quantum experiment of increasing system size

Challenges

- Many non-commuting observables
- Unclear hyperparameter optimization
- High precision required:

Use-case: Quantum Chemistry

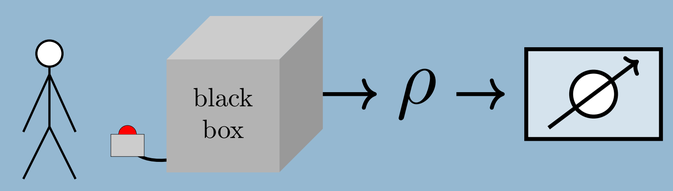
Chemical accuracy (1.6 mHa) required

Fermionic operators:
$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$

Spin Operators:
$H = \sum_i c_i P_i$

Problem Setting

Experiment (as a theoretician)



estimate energy of ρ: $E = \mathrm{Tr}[H\rho]$
s.t. estimate $\hat{E}$ fulfills $|\hat{E} - E| \leq \epsilon$

Measurement strategy

- two commuting operators can be measured simultaneously

→ put them into one group σ

- grouped Hamiltonian decomposition:

$$H = \sum_{i=1}^{N} c_i P_i = \sum_{j=1}^{N_g} \sum_{k=1}^{N_j} c_{\sigma_j(k)} P_{\sigma_j(k)}$$

$c_i \in \mathbb{R}$, $P_i \in \{X, Y, Z, \mathbb{1}\}^{\otimes n}$
s.t. every P_i belongs to at least one σ_j

- numerically cheap to group [2], i.e., to find the groups σ_j

→ $N_g \ll N$ distinct measurement settings needed to estimate E

References

[1] Mnih, Volodymyr and Szepesvári, Csaba and Audibert, Jean-Yves: *Empirical Bernstein stopping*, Proc. 25th Int. Conf. Mach. Learning (2008).

[2] Alexander Gresch and Martin Kliesch: *Guaranteed efficient energy estimation of quantum many-body Hamiltonians using ShadowGrouping*, arXiv (2023).

[3] O'Malley, Peter JJ and Babbush, et. al.: *Scalable quantum simulation of molecular energies*, APS (2016).

[4] Arrasmith, Cincio, Somma and Coles: *Operator Sampling for shot-frugal Optimization in Variational Algorithms*, arXiv (2020).

Empirical Bernstein stopping algorithm (EBS)

- **Goal:** Estimate E with accuracy ϵ and confidence $1 - \delta$
- **Idea:** Use empirical Bernstein bound to adaptively terminate the estimation process

Algorithm EBGStop [1]

Require: Accuracy ϵ & inconfidence δ
Require: Range $R = 2\sum_{i=1}^{N} |c_i|$
Require: iid samples E_t with mean E
  $c_0 \leftarrow \infty$
  $t \leftarrow 1$
  while $\epsilon_t > \epsilon$ **do**
    Sample Energy E_t
    Update MEAN(E_t) & VAR(E_t)
    Update $\epsilon_t(d_t)$ using Eq. (2)
    $t \leftarrow t + 1$
  end while
  $\hat{E} \leftarrow$ MEAN(E_t)
  return $\hat{E}$
Ensure: $|\hat{E} - E| \leq \epsilon$ with prob. $1 - \delta$

Hoeffding

$$|\hat{E} - E| \leq R\sqrt{\frac{\ln(2/\delta)}{2t}} \quad (1)$$

Empirical Bernstein

$$|\hat{E} - E| \leq \hat{\sigma}_t \sqrt{\frac{2\ln(3/\delta)}{t}} + \frac{3R\ln(3/\delta)}{t} \quad (2)$$

Algorithm key ideas

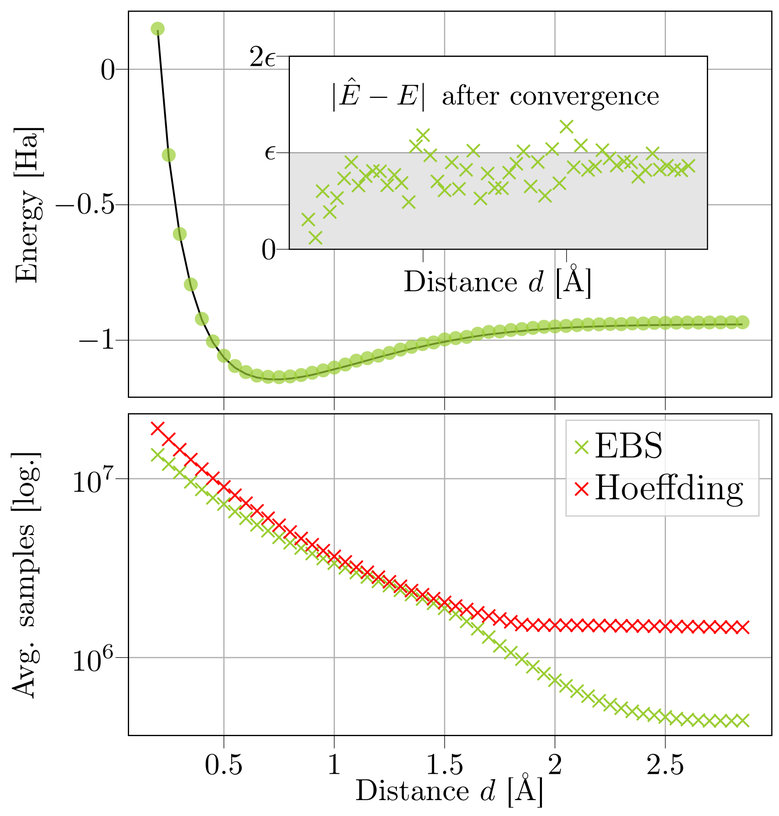
(1) $\mathbb{P}[\text{premature stopping}] \overset{!}{\leq} \delta$
(2) partition into steps, s.t. $\sum_{t=1}^{\infty} d_t \leq \delta$
(3) use tail bound at step t with prob. of premature stopping at most d_t
(4) Batch-sampling: updating after $\lceil \beta^k \rceil > 1$ samples reduces variance of the estimator
(5) Mid-interval sampling to reduce over-shooting

Results

Variational quantum eigensolver (VQE)

- VQE for H_2 molecule (2 qubits) at various bond lengths d
- Ham. $H(d)$ and VQE ansatz based on [3]
- 3 distinct measurements needed to gain one energy sample
- Each $E(d)$ estimated using EBS
- benchmark EBS on this estimator against the Hoeffding guarantee [4]

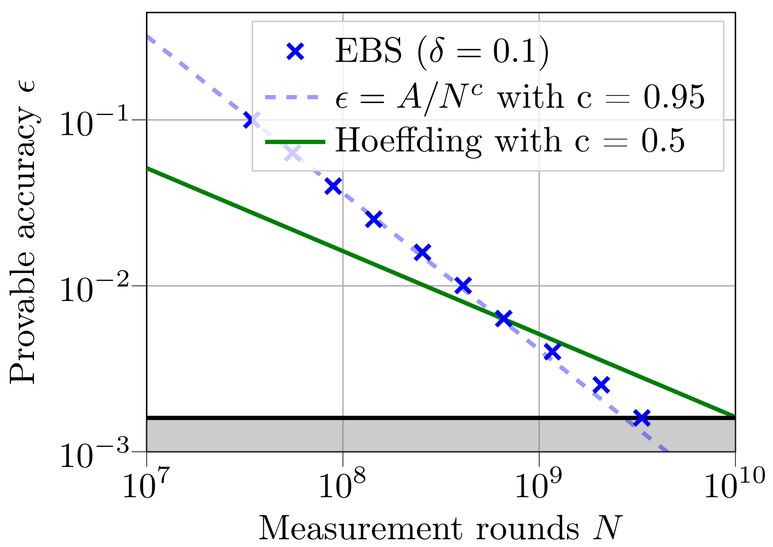
→ performance improvement over most d

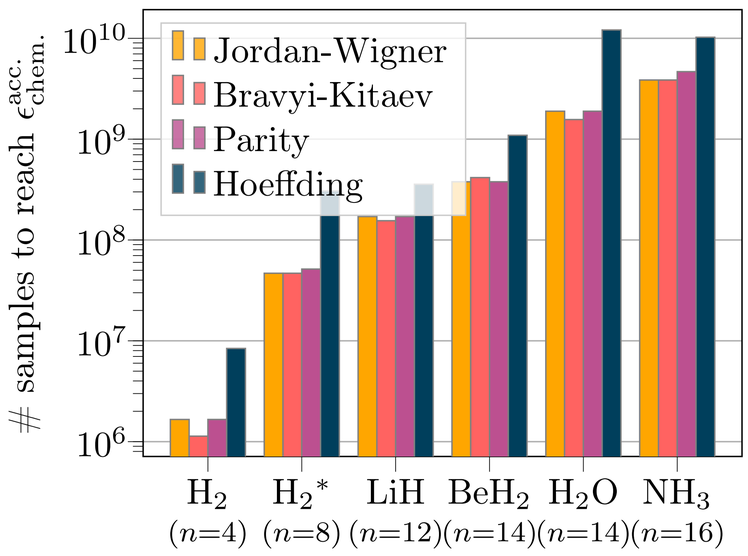


Sampling from molecular ground-states

- group H using ShadowGrouping [2]
- measure each group once to obtain a single sample E_t (using $N = \mathcal{O}(n^4)$ shots in total)
- repeat for various molecules and fermion-to-qubit mappings

→ consistently outperforms the basic Hoeffding guarantee for various system sizes n





Outlook

- extension of the empirical Bernstein bound to random vectors

→ much more efficient estimators available [2]

- hyperparameter optimization of EBS still possible: overshooting?
- application of EBS to other contexts, such as estimating the fidelity, purity, entanglement ...

github.com/UgurTepe/EmpiricalBernsteinAlgorithm