Title: Matchgate Shadows for Fermionic Quantum Simulation

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Abstract: In this talk, I'll describe new tomographic protocols for efficiently estimating various fermionic quantities, including both local observables (i.e., expectation values of local fermionic operators) and certain global properties (e.g., inner products between an unknown quantum state and arbitrary fermionic Gaussian states). Our protocols are based on classical shadows arising from random matchgate circuits. As a concrete application, they enable us to implement the recently introduced quantum-classical hybrid quantum Monte Carlo algorithm, without the exponential post-processing cost incurred by the original approach.

Matchgate shadows for fermionic quantum simulation

Kianna Wan, William J. Huggins, Joonho Lee, Ryan Babbush

overview

original motivation: remove the exponentially scaling classical post-processing cost of the *quantum-classical quantum Monte Carlo* (QC-QMC) algorithm [HOR+21]

- QC-QMC is a hybrid algorithm for simulating fermionic systems;
  enabled high-accuracy chemistry experiment on 16 qubits (largest to date!)
- idea: use quantum computer to prepare a better "trial wavefunction" $|\Psi_{\text{trial}}\rangle$, which guides (classical) QMC calculation
- crucial step: estimate overlaps $\langle\Psi_{\text{trial}}|\varphi_i\rangle$ with **many** "walker states" $|\varphi_i\rangle$ — do this using (Clifford-based) *classical shadows* protocol of [HKP20], to reduce quantum resources

but classical cost is exponential in $n = \#$ qubits ($= \#$ fermionic modes)

[HOR+21] *Unbiasing fermionic quantum Monte Carlo with a quantum computer.* arXiv:2106.16235

[HKP20] *Predicting many properties of a quantum system from very few measurements.* arXiv:2002.08953

overview

original motivation: remove the exponentially scaling classical post-processing cost of the *quantum-classical quantum Monte Carlo* (QC-QMC) algorithm [HOR+21]

our results: tomographic protocols for **efficiently** estimating various properties of fermionic systems, including

- expectation values of local fermionic operators
- fidelities w.r.t. fermionic Gaussian states
- overlaps required for QC-QMC

our protocols are based on the classical shadows framework of [HKP20], but we use different ensembles of random measurements

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classical shadows [review]

goal: estimate $\mathrm{tr}(O_1\rho),\ldots,\mathrm{tr}(O_M\rho)$ for observables $O_1,\ldots,O_M$, given any unknown state ρ

how? decide on a distribution over unitaries, D

procedure: randomly draw a unitary $U \sim D$
measure ρ in the basis $\{U^\dagger|b\rangle\}_{b\in\{0,1\}^n}$

repeat N_{sample} times

corresponding channel:

$$\mathcal{M}(\rho) = \mathop{\mathbb{E}}_{U\sim D} \sum_{b\in\{0,1\}^n} \langle b|U\rho U^\dagger|b\rangle U^\dagger|b\rangle\langle b|U$$

if $\mathcal{M}$ is invertible,

"classical shadow"

$$\mathop{\mathbb{E}}_{\substack{U\sim D\\ b\sim U\rho U^\dagger}} \left[\mathcal{M}^{-1}(U^\dagger|b\rangle\langle b|U)\right] = \rho$$

$$\hookrightarrow \mathop{\mathbb{E}}_{\substack{U\sim D\\ b\sim U\rho U^\dagger}} \left[\mathrm{tr}\left(O_i\mathcal{M}^{-1}(U^\dagger|b\rangle\langle b|U)\right)\right] = \mathrm{tr}(O_i\rho)$$

classical shadows [review]

$$\mathop{\mathbb{E}}_{\substack{U\sim D\\ b\sim U\rho U^\dagger}}\left[\mathrm{tr}\left(O_i \underbrace{\mathcal{M}^{-1}(U^\dagger|b\rangle\langle b|U)}_{\text{“classical shadow”}}\right)\right] = \mathrm{tr}(O_i\rho)$$

not all classical shadows protocols are efficient!
efficiency depends on $O_1, \ldots, O_M$ and choice of D

- in general, $N_{\text{samples}} = \mathcal{O}\left(\frac{\log M}{\varepsilon^2}\max_i \mathrm{Var}(O_i)\right)$ copies of ρ suffice

  [HKP20]: $D = \textsc{Uniform}(\mathrm{Cl}_n) \rightarrow \mathrm{Var}(O_i)$ small if $\|O_i\|_{\text{H-S}}$ small
  $D = \textsc{Uniform}(\mathrm{Cl}_1^{\otimes n}) \rightarrow \mathrm{Var}(O_i)$ small for local O_i

- but even when $\mathrm{Var}(O_i)$ small, classical post-processing [computing $\mathrm{tr}\left(O_i\mathcal{M}^{-1}(U^\dagger|b\rangle\langle b|U)\right)$] can still be exponentially costly!

[HKP20] Huang, Kueng, Preskill. *Predicting many properties of a quantum system from very few measuremer*

classical shadows [review]

$$\mathop{\mathbb{E}}_{\substack{U\sim D\\ b\sim U\rho U^\dagger}}\left[\mathrm{tr}\left(O_i\underbrace{\mathcal{M}^{-1}(U^\dagger|b\rangle\langle b|U)}_{\text{“classical shadow”}}\right)\right]=\mathrm{tr}(O_i\rho)$$

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[HKP20]: $D=\textsc{Uniform}(\mathrm{Cl}_n)$ $\rightarrow$ $\mathrm{Var}(O_i)$ small if $\|O_i\|_{\text{H-S}}$ small

e.g., relevant observables O_i for QC-QMC all have $\|O_i\|_{\text{H-S}}=\text{const.}$
but can't efficiently compute $\mathrm{tr}\left(O_i\mathcal{M}^{-1}(U^\dagger|b\rangle\langle b|U)\right)$ for Clifford circuits U

[HKP20] Huang, Kueng, Preskill. *Predicting many properties of a quantum system from very few measuremen*

classical shadows **checklist**

for observables of interest $\{O_i\}_{i\in[M]}$ and a candidate distribution D, need to

0. efficiently sample unitaries from D, and compile them into small quantum circuits

1. determine the measurement channel $\mathcal{M}$ (then $\mathcal{M}^{-1}$) to find the form of the classical shadow samples associated with D

D

2. figure out how to efficiently compute the expectation values of the O_i's with respect to the classical shadow samples

   i.e., $\mathrm{tr}\left(O_i \mathcal{M}^{-1}(U^\dagger|b\rangle\langle b|U)\right)$ for all $i \in [M]$, $U \in D$, $b \in \{0,1\}^n$

3. evaluate and bound the variance

$D, \{O_i\}$

we'll do all this for $D =$ Uniform(matchgate circuits) and various fermionic observables O_i

wait, what are matchgate circuits?

matchgate circuits $\overset{\text{J-W}}{=}$ fermionic Gaussian unitaries

for n qubits/n fermionic modes, consider the $2n$ Majorana operators $\gamma_1, \ldots, \gamma_{2n}$:

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2\delta_{\mu\nu} I$$

$\{\gamma_S : S \subseteq [2n]\}$ forms a (H-S orthogonal) basis for the space of n-qubit operators

$\gamma_S := \gamma_{\mu_1} \ldots \gamma_{\mu_k}$ for $S = \{\mu_1, \ldots, \mu_k\}$ (with $\mu_1 < \cdots < \mu_k$)

(under the Jordan-Wigner transformation,

$$\gamma_1 = X \otimes I \otimes \cdots \otimes I \qquad \gamma_3 = Z \otimes X \otimes I \otimes \cdots \otimes I$$
$$\gamma_2 = Y \otimes I \otimes \cdots \otimes I \qquad \gamma_4 = Z \otimes Y \otimes I \otimes \cdots \otimes I \qquad \text{etc.})$$

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"matchgate group"

for any matchgate circuit $U_Q \in \mathrm{M}_n$,

$$U_Q{}^\dagger \gamma_\mu U_Q = \sum_{\nu=1}^{2n} Q_{\mu\nu} \gamma_\nu \qquad \text{for some } Q \in \mathrm{O}(2n)$$

so each matchgate circuit is specified (up to global phase) by some $Q \in \mathrm{O}(2n)$

define the channel $\mathcal{U}_Q(\,\cdot\,) := U_Q^\dagger(\,\cdot\,)U_Q$

matchgate shadows **checklist**

$:=$ samples of the classical shadow estimator associated with $D = \textsc{Uniform}(\mathrm{M}_n)$

0. efficiently sample from $\textsc{Uniform}(\mathrm{M}_n)$, and compile all $U_Q \in \mathrm{M}_n$ into small quantum circuits

1. determine the measurement channel $\mathcal{M}$ (then $\mathcal{M}^{-1}$) to find the form of the matchgate shadows

2. figure out how to efficiently compute the expectation values of the observables of interest with respect to the matchgate shadows

   i.e., $\mathrm{tr}\left(O_i \mathcal{M}^{-1}(U_Q^\dagger |b\rangle\langle b| U_Q)\right)$

3. evaluate and bound the variance

0. compile random matchgate circuits

"matchgate group"

for any matchgate circuit $U_Q \in \mathrm{M}_n$,

$$U_Q{}^\dagger \gamma_\mu U_Q = \sum_{\nu=1}^{2n} Q_{\mu\nu}\gamma_\nu \qquad \text{for some } Q \in \mathrm{O}(2n)$$

- sample $Q \in \mathrm{O}(2n)$ according to the Haar measure $d\mu$ on $\mathrm{O}(2n)$
- decompose Q into Givens rotations, followed by a reflection if $\det(Q) = -1$

1- and (nearest-neighbour) 2-qubit Pauli rotations

e.g., Pauli X on nth qubit

any U_Q can be implemented using $\mathcal{O}(n^2)$ 1- and (nearest-neighbour) 2-qubit gates in $\mathcal{O}(n)$ depth

matchgate shadows checklist

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1. determine the channel $\mathcal{M}$

$$\mathcal{M}(\rho) = \mathop{\mathbb{E}}_{U\sim D} \sum_{b\in\{0,1\}^n} \langle b|U\rho U^\dagger|b\rangle U|b\rangle\langle b|U$$

$$= \mathop{\mathbb{E}}_{U\sim D} \sum_{b\in\{0,1\}^n} \mathrm{tr}_1\left[U^\dagger|b\rangle\langle b|U\rho \otimes U^\dagger|b\rangle\langle b|U\right] \qquad \mathcal{U}(\cdot) := U^\dagger(\cdot)U$$

$$= \mathop{\mathbb{E}}_{U\sim D} \sum_{b\in\{0,1\}^n} \mathrm{tr}_1\left[\mathcal{U}(|b\rangle\langle b|)\rho \otimes \mathcal{U}(|b\rangle\langle b|)\right]$$

$$= \sum_{b\in\{0,1\}^n} \mathrm{tr}_1\left[\underbrace{\mathop{\mathbb{E}}_{U\sim D}\mathcal{U}^{\otimes 2}}_{=:\ \mathcal{E}_2}(|b\rangle\langle b|^{\otimes 2})(\rho\otimes I)\right]$$

$=: \mathcal{E}_2$ ["2-fold twirl channel"]

$$D = \mathrm{UNIFORM}(\mathrm{M}_n) \ \rightarrow\ \mathcal{E}_2 = \int_{\mathrm{O}(2n)} d\mu(Q)\,\mathcal{U}_Q^{\otimes 2}$$

1. determine the channel $\mathcal{M}$

how to evaluate $\mathcal{E}_2 := \int_{O(2n)} d\mu(Q)\, \mathcal{U}_Q^{\otimes 2}$?

- observe that $\mathcal{E}_2$ is an orthogonal (super)projector: ${\mathcal{E}_2}^2 = \mathcal{E}_2, \quad \mathcal{E}_2^\dagger = \mathcal{E}_2$
- then determine its image, using symmetries of the matchgate group

e.g., **lemma**: $\mathcal{E}_2(\gamma_{S_1} \otimes \gamma_{S_2}) = 0$ unless $S_1 = S_2$

proof: for $S_1 \neq S_2$, $\exists\, \mu \in S_1$ such that $\mu \notin S_2$ (wlog)

consider the reflection $\mathcal{U}_{Q'} : \gamma_\mu \mapsto -\gamma_\mu, \quad \gamma_\nu \mapsto \gamma_\nu$ for all $\nu \neq \mu$

- $\mathcal{U}_{Q'}^{\otimes 2}(\gamma_{S_1} \otimes \gamma_{S_2}) = -\gamma_{S_1} \otimes \gamma_{S_2}$
- but $\mathcal{E}_2 \circ \mathcal{U}_{Q'}^{\otimes 2} = \mathcal{E}_2$ by Haar invariance

$\hookrightarrow \mathcal{E}_2(\gamma_{S_1} \otimes \gamma_{S_2}) = -\mathcal{E}_2(\gamma_{S_1} \otimes \gamma_{S_2})$

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$\hookrightarrow \mathcal{E}_2(\gamma_{S_1} \otimes \gamma_{S_2}) = -\mathcal{E}_2(\gamma_{S_1} \otimes \gamma_{S_2})$

and so on... (also use the fact that permutation matrices are in $O(2n)$, to fully determine $\mathcal{E}_2$)

1. determine the channel $\mathcal{M}$

$$\mathcal{M}(A) = \sum_{\ell=0}^{n} \binom{n}{\ell} \binom{2n}{2\ell}^{-1} \mathcal{P}_{2\ell}(A)$$

where $\mathcal{P}_k :=$ (super)projector onto $\Gamma_k := \text{span}\{\gamma_S : S \subseteq [2n], |S| = k\}$

so $\mathcal{M}$ is *not* invertible on the full space of operators!
but invertible on $\Gamma_{\text{even}} := \bigoplus_{k \text{ even}} \Gamma_k$

$\hookrightarrow$ define the (pseudo)inverse

$$\mathcal{M}^{-1}(A) = \sum_{\ell=0}^{n} \binom{2n}{2\ell} \binom{n}{\ell}^{-1} \mathcal{P}_{2\ell}(A)$$

$\Rightarrow$ matchgate shadows give unbiased estimates for $\text{tr}(O\rho)$ whenever $O \in \Gamma_{\text{even}}$, or $\rho \in \Gamma_{\text{even}}$

matchgate shadows checklist

:= samples of the classical shadow estimator associated with $D = \textsc{Uniform}(\mathrm{M}_n)$

- [x] 0. efficiently sample from $\textsc{Uniform}(\mathrm{M}_n)$, and compile all $U_Q \in \mathrm{M}_n$ into small quantum circuits

- [x] 1. determine the measurement channel $\mathcal{M}$ (then $\mathcal{M}^{-1}$) to find the form of the matchgate shadows

2. figure out how to efficiently compute the expectation values of the observables of interest with respect to the matchgate shadows

   i.e., $\mathrm{tr}\left(O_i \mathcal{M}^{-1}(U_Q^\dagger |b\rangle\langle b| U_Q)\right)$

3. evaluate and bound the variance

2. compute expectation values

recall $\underset{\substack{U\sim D \\ b\sim U\rho U^\dagger}}{\mathbb{E}}\left[\mathrm{tr}\left(O\,\underbrace{\mathcal{M}^{-1}(U^\dagger|b\rangle\langle b|U)}_{\text{“classical shadow”}}\right)\right] = \mathrm{tr}(O\rho)$

and $\mathcal{M}^{-1}(A) = \sum_{\ell=0}^{n} \binom{2n}{2\ell}\binom{n}{\ell}^{-1} \mathcal{P}_{2\ell}(A)$ for $D = \textsc{Uniform}(\mathrm{M}_n)$

$\mathcal{P}_{2\ell} :=$ projector onto $\mathrm{span}\{\gamma_S : |S| = 2\ell\}$

↪ need to compute

$$\mathrm{tr}\left(O\,\underbrace{\mathcal{M}^{-1}(U_Q^\dagger|b\rangle\langle b|U_Q)}_{\text{“matchgate shadow”}}\right) = \sum_{\ell=0}^{n}\binom{2n}{2\ell}\binom{n}{\ell}^{-1} \underbrace{\mathrm{tr}\left(O\,\mathcal{P}_{2\ell}(U_Q^\dagger|b\rangle\langle b|U_Q)\right)}_{\text{can we efficiently evaluate this?}}$$

naive approach: expand in $\{\gamma_S\}$ basis

...but exponentially many (i.e., $\binom{2n}{2\ell}$) terms to consider!

2. compute expectation values

$$\mathrm{tr}\left(O\,\mathcal{M}^{-1}(U_Q^\dagger|b\rangle\langle b|U_Q)\right) = \sum_{\ell=0}^{n}\binom{2n}{2\ell}\binom{n}{\ell}^{-1}\underbrace{\mathrm{tr}\left(O\,\mathcal{P}_{2\ell}(U_Q^\dagger|b\rangle\langle b|U_Q)\right)}$$

<u>warm-up:</u> consider $\mathrm{tr}\left(O\,\mathcal{P}_{2\ell}(|\vec{0}\rangle\langle\vec{0}|)\right)$

recall $|\vec{0}\rangle\langle\vec{0}| = \prod_{j=1}^{n}\frac{1}{2}(I - i\gamma_{2j-1}\gamma_{2j})$

trick: introduce a formal variable z and define

$$p(z) = \mathrm{tr}\left(O\,\underbrace{\prod_{j=1}^{n}\frac{1}{2}(I - iz\gamma_{2j-1}\gamma_{2j})}\right)$$

$$= \sum_{\ell} z^{\ell}\mathcal{P}_{2\ell}(|\vec{0}\rangle\langle\vec{0}|)$$

the coefficient of z^{ℓ} in $p(z)$ is $\mathrm{tr}\left(O\,\mathcal{P}_{2\ell}(|\vec{0}\rangle\langle\vec{0}|)\right)$!!

2. compute expectation values

$$\mathrm{tr}\left(O\,\mathcal{M}^{-1}(U_Q^\dagger|b\rangle\langle b|U_Q)\right) = \sum_{\ell=0}^{n}\binom{2n}{2\ell}\binom{n}{\ell}^{-1}\underbrace{\mathrm{tr}\left(O\,\mathcal{P}_{2\ell}(U_Q^\dagger|b\rangle\langle b|U_Q)\right)}$$

general case: consider $\mathrm{tr}\left(O\,\mathcal{P}_{2\ell}(U_Q^\dagger|b\rangle\langle b|U_Q)\right)$

recall $U_Q^\dagger|b\rangle\langle b|U_Q = \prod_{j=1}^{n}\frac{1}{2}(I - i(-1)^{b_j}\widetilde{\gamma}_{2j-1}\widetilde{\gamma}_{2j})$, $\quad \widetilde{\gamma}_\mu := U_Q^\dagger\gamma_\mu U_Q = \sum_{\nu=1}^{2n} Q_{\mu\nu}\gamma_\nu$

trick: introduce a formal variable z and define

$$p(z) = \mathrm{tr}\left(O\,\underbrace{\prod_{j=1}^{n}\frac{1}{2}\left(I - i(-1)^{b_j}\,z\widetilde{\gamma}_{2j-1}\widetilde{\gamma}_{2j}\right)}\right)$$

$$= \sum_{\ell} z^\ell\mathcal{P}_{2\ell}(U_Q^\dagger|b\rangle\langle b|U_Q)$$

the coefficient of z^ℓ in $p(z)$ is $\mathrm{tr}\left(O\,\mathcal{P}_{2\ell}(U_Q^\dagger|b\rangle\langle b|U_Q)\right)$!!

but $p(z)$ doesn't involve the projector $\mathcal{P}_{2\ell}$ ☺

2. compute expectation values

but now, how to **efficiently** compute

$$p(z) = \mathrm{tr}\left(O \prod_{j=1}^{n} \frac{1}{2} \left(I - i(-1)^{b_j} z \widetilde{\gamma}_{2j-1} \widetilde{\gamma}_{2j} \right) \right) \ ?$$

two approaches:

(a) exploit structure of the Clifford algebra generated by the γ_μ's, to obtain **explicit**, efficiently evaluable expressions for $p(z)$ for various O

- $O = \gamma'_S = U_{Q'} \gamma_S U_{Q'}$, for any $Q' \in \mathrm{O}(2n)$ → e.g., k-RDMs, local observables
- $O =$ density operator of any fermionic Gaussian state → e.g., fidelities
- $O = |\varphi\rangle\langle\vec{0}|$, for any Slater determinant $|\varphi\rangle$ → e.g., overlaps for QC-QMC

$$p(z) = \frac{i^{\zeta/2}}{2^{n-\zeta/2}} \mathrm{Pf}(M_1 + z M_2) \qquad (\zeta := \# \text{ of particles in } |\varphi\rangle)$$

efficiently computable $(2n-\zeta) \times (2n-\zeta)$ matrices

2. compute expectation values

but now, how to **efficiently** compute

$$p(z) = \mathrm{tr}\left(O \prod_{j=1}^{n} \frac{1}{2} \left(I - i(-1)^{b_j} z \widetilde{\gamma}_{2j-1} \widetilde{\gamma}_{2j} \right) \right) \ ?$$

two approaches:

(a) exploit structure of the Clifford algebra generated by the γ_μ's, to obtain **explicit**, efficiently evaluable expressions for $p(z)$ for various O

(b) develop a **general method** for efficiently computing any $\mathrm{tr}(A_1 \dots A_m)$, where each A_i is (i) a linear combination of γ_μ's, (ii) a Gaussian density operator ϱ, or (iii) a Gaussian unitary U_Q [this encompasses all cases treated using (a)]

e.g., $\mathrm{tr}(U_{Q_1} U_{Q_2} \gamma'_S \varrho_1 U_{Q_3} a^\dagger_{j_1} \dots a^\dagger_{j_k} \varrho_2 \gamma''_S)$,

$\mathrm{tr}(U_Q \varrho_1 \varrho_2)$ $\rightarrow$ overlaps with arbitrary Gaussian states

high-level procedure: convert to an expression in a related, higher-dimensional Grassmann algebra, then use Grassmann integral identities

matchgate shadows checklist

$:=$ samples of the classical shadow estimator associated with $D = \textsc{Uniform}(\mathrm{M}_n)$

- [x] 0. efficiently sample from $\textsc{Uniform}(\mathrm{M}_n)$, and compile all $U_Q \in \mathrm{M}_n$ into small quantum circuits
- [x] 1. determine the measurement channel $\mathcal{M}$ (then $\mathcal{M}^{-1}$) to find the form of the matchgate shadows
- [x] 2. figure out how to efficiently compute the expectation values of the observables of interest with respect to the matchgate shadows

  i.e., $\mathrm{tr}\left(O_i \mathcal{M}^{-1}(U_Q^\dagger |b\rangle\langle b| U_Q)\right)$

3. evaluate and bound the variance

3. bound the variance

recall $\mathcal{M}(\rho) = \mathrm{tr}_1 \left[\sum_{b \in \{0,1\}^n} \underbrace{\mathop{\mathbb{E}}_{U\sim D} \mathcal{U}^{\otimes 2}}_{=:\, \mathcal{E}_2} (|b\rangle\langle b|^{\otimes 2})(\rho \otimes I) \right]$

$=: \mathcal{E}_2$ ["2-fold twirl channel"]

variance of classical shadows estimator for $\mathrm{tr}(O\rho)$:

$$\mathrm{Var}(O) = \mathrm{tr} \left[\sum_{b \in \{0,1\}^n} \underbrace{\mathop{\mathbb{E}}_{U\sim D} \mathcal{U}^{\otimes 3}}_{=:\, \mathcal{E}_3} (|b\rangle\langle b|^{\otimes 3}) \left(\rho \otimes \mathcal{M}^{-1} \otimes \mathcal{M}^{-1}(O^\dagger)\right) \right]$$

$=: \mathcal{E}_3$ ["3-fold twirl channel"]

$$D = \textsc{Uniform}(\mathrm{M}_n) \;\rightarrow\; \mathcal{E}_3 = \int_{\mathrm{O}(2n)} d\mu(Q)\, \mathcal{U}_Q^{\otimes 3}$$

3. bound the variance

how to evaluate $\mathcal{E}_3 := \mathbb{E}_{U \in \mathrm{M}_n} \mathcal{U}^{\otimes 3} = \int_{\mathrm{O}(2n)} d\mu(Q) \mathcal{U}_Q^{\otimes 3}$?

just like for $\mathcal{E}_2$, use symmetry:

by considering the action of certain reflections and permutations, and using Haar invariance ($\mathcal{E}_3 \circ \mathcal{U}_{Q'}^{\otimes 3} = \mathcal{E}_3$), can fully determine $\mathcal{E}_3$

but this would lead to the **same expression** if we randomised only over the ***discrete*** **group generated by reflections and permutations**!

$\cong$ matchgate circuits that are also Clifford

3. bound the variance

how to evaluate $\mathcal{E}_3 := \mathop{\mathbb{E}}_{U \in \mathrm{M}_n} \mathcal{U}^{\otimes 3} = \int_{\mathrm{O}(2n)} d\mu(Q)\, \mathcal{U}_Q^{\otimes 3}$?

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$\cong$ matchgate circuits that are also Clifford

i.e.,

$$\mathop{\mathbb{E}}_{U \in \mathrm{M}_n} \mathcal{U}^{\otimes 3} = \mathop{\mathbb{E}}_{U \in \mathrm{M}_n \cap \mathrm{Cl}_n} \mathcal{U}^{\otimes 3}$$

$\Leftrightarrow$ $\mathrm{M}_n \cap \mathrm{Cl}_n$ = "matchgate 3-design" !!!

3. bound the variance

$\mathrm{M}_n \cap \mathrm{Cl}_n =$ "matchgate 3-design"

$\Rightarrow$ in the context of classical shadows, doesn't matter whether we use $D = \textsc{Uniform}(\textbf{all}$ matchgate circuits) or $\textsc{Uniform}(\textbf{Clifford}$ matchgate circuits)

- practical implications...?
- one mathematical payoff: can use the more explicit symmetry of the *continuous* matchgate group to analyse its *discrete* subgroup $\mathrm{M}_n \cap \mathrm{Cl}_n$

  $\rightarrow$ basis-independent variance bound for *both* distributions

$$\mathrm{Var}(O) \leq \frac{1}{2^{2n}} \sum_{\substack{\ell_1,\ell_2,\ell_3 \geq 0 \\ \ell_1+\ell_2+\ell_3 \leq n}} \alpha_{\ell_1,\ell_2,\ell_3} \sum_{\substack{S_1,S_2,S_3 \subseteq [2n] \text{ disjoint} \\ |S_i| = 2\ell_i}} \left|\mathrm{tr}(O\widetilde{\gamma}_{S_2 \cup S_3})\mathrm{tr}(O\widetilde{\gamma}_{S_3 \cup S_1})\right|$$

$\widetilde{\gamma}_S = U_Q^\dagger \gamma_S U_Q$ for any $Q \in \mathrm{O}(2n)$

this lets us analyse the variance for continuous families of fermionic observables

3. bound the variance

- $\mathrm{Var}(\gamma'_S) \leq \binom{2n}{|S|}\binom{n}{|S|/2}^{-1}$ where $\gamma'_S = U_{Q'}\gamma_S U_{Q'}$, for any $Q' \in \mathrm{O}(2n)$

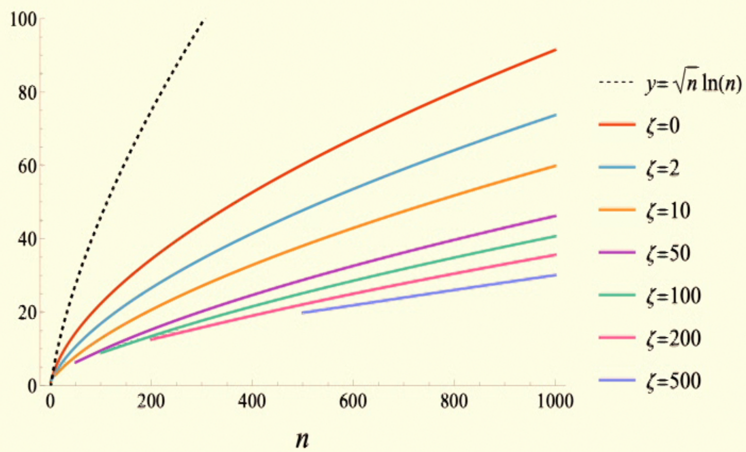
  $= \mathcal{O}\left(n^{|S|/2}\right)$ for constant $|S|$

- $\mathrm{Var}(\varrho) = \mathcal{O}(\sqrt{n}\log n)$

  where $\varrho =$ density operator of any fermionic Gaussian state

- $\mathrm{Var}(|\varphi\rangle\langle\vec{0}|)$ for any Slater determinant $|\varphi\rangle$:

  $\hookrightarrow$ overlaps with Slater determinants (as required for QC-QMC)



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$:=$ samples of the classical shadow estimator associated with $D = \textsc{Uniform}(\mathrm{M}_n)$

- ✓ 0. efficiently sample from $\textsc{Uniform}(\mathrm{M}_n)$, and compile all $U_Q \in \mathrm{M}_n$ into small quantum circuits
- ✓ 1. determine the measurement channel $\mathcal{M}$ (then $\mathcal{M}^{-1}$) to find the form of the matchgate shadows
- ✓ 2. figure out how to efficiently compute the expectation values of the observables of interest with respect to the matchgate shadows

  i.e., $\mathrm{tr}\left(O_i \mathcal{M}^{-1}(U_Q^\dagger |b\rangle\langle b| U_Q)\right)$
- ✓ 3. evaluate and bound the variance

summary

observable	classical post-processing cost	variance
$\gamma'_S = U_{Q'} \gamma_S U_{Q'}$ $\rightarrow$ k-RDMs, local fermionic observables	$\mathcal{O}(n^3)$	$\binom{2n}{\lvert S\rvert}\binom{n}{\lvert S\rvert/2}^{-1}$
fermionic Gaussian state ϱ $\rightarrow$ fidelities with Gaussian states	$\mathcal{O}(n^3)$	$\mathcal{O}\left(\sqrt{n}\log n\right)$
$\lvert\varphi\rangle\langle\vec{0}\rvert$ for Slater determinant $\lvert\varphi\rangle$ $\rightarrow$ overlaps with Slater determinants	$\mathcal{O}\left((n-\zeta/2)^4\right)$	$< \mathrm{Var}(\varrho)$ (?)
$A_1 \ldots A_m$ $\rightarrow$ e.g., overlaps with Gaussian states	$\mathrm{poly}(n, m)$	?

auxiliary results:

- Clifford matchgate circuits form a "matchgate 3-design"

  $\Rightarrow$ classical shadows from M_n are functionally equivalent to those from $\mathrm{M}_n \cap \mathrm{Cl}_n$

- general method for efficiently computing any quantity of the form $\mathrm{tr}(A_1 \ldots A_m)$, where each A_i is a linear combination of γ_μ's, a Gaussian density operator, or a Gaussian unitary