Rank–dependent complexity in estimating traces of quantum state powers

[2408.00314] Rank Is All You Need: Estimating the Trace of Powers of Density Matrices

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Overview

- Trace of powers & Literature review
- Mathematical intuitions
- Main results: algorithm, lemmas, theorems, corollaries
- Numerical simulations
- Computational hardness of $\mathrm{TsallisQED}_q$ and $\mathrm{TsallisQEA}_q$
- Applications
- Concluding remarks

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Property testing

- **(Property testing)** Let $\mathcal{X}$ be a set of objects and $d : \mathcal{X} \times \mathcal{X} \to [0,1]$ be a distance measure on $\mathcal{X}$.
  - A subset $\mathcal{P} \subseteq \mathcal{X}$ is called a *property*.
  - An object $x \in \mathcal{X}$ is ε-*far* from $\mathcal{P}$ if $d(x, y) \geq \varepsilon$ for all $y \in \mathcal{P}$; x is ε-*close* to $\mathcal{P}$ if there is a $y \in \mathcal{P}$ such that $d(x, y) \leq \varepsilon$.
  - An ε-property tester (sometimes abbreviated to ε-tester) for $\mathcal{P}$ is an algorithm that receives as input either an $x \in \mathcal{P}$ or an x that is ε-far from $\mathcal{P}$.
  - In the former case, the algorithm accepts with probability at least 2/3; in the latter case, the algorithm rejects with probability at least 2/3.

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- One can view classical property testing algorithms in two ways:
  - either as testing **properties of data** (such as graph isomorphism),
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  - either as testing **properties of data** (such as graph isomorphism),
  - or **properties of functions** (such as linearity).

- If one wishes to generalize property testing to the quantum realm, one is thus naturally led to two different generalizations:
  - testing **properties of quantum states**,
  - and **properties of quantum operations**.

Property testing

- **(Quantum testing of quantum properties)** Consider cases where $\mathscr{X}$ is a set of quantum objects and our tester is also quantum.

[1310.2035] A Survey of Quantum Property Testing

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	Coherent	**Incoherent**
Static	Pure state (§4.1)	Mixed state (§4.2)
Dynamic	Unitary operator (§5.1)	Quantum channel (§5.2)

Table 1: The taxonomy of quantum properties

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Table 1: The taxonomy of quantum properties

Equality, Separability

Unitarily invariant properties

(Purity, Mixedness, …)

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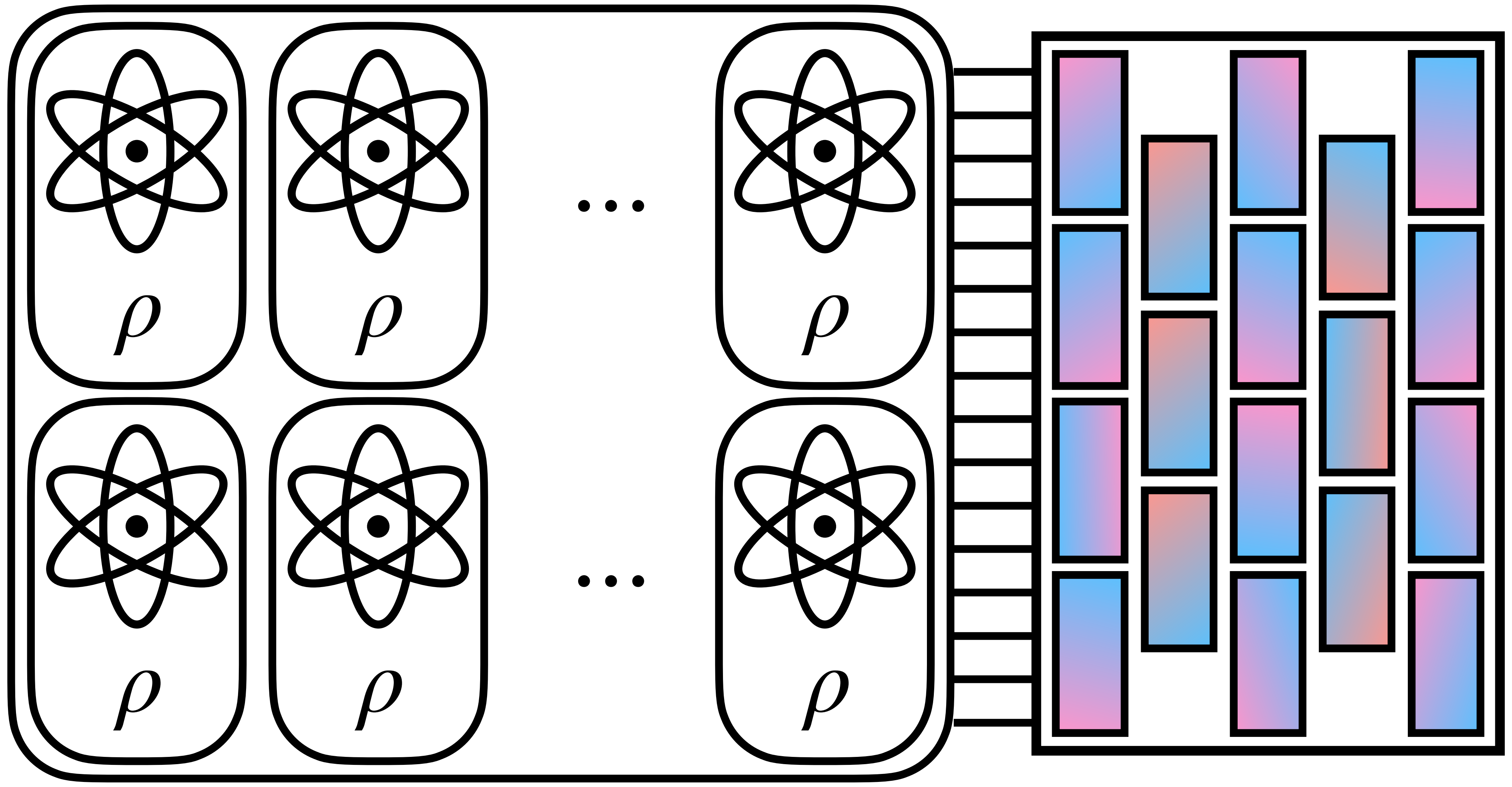


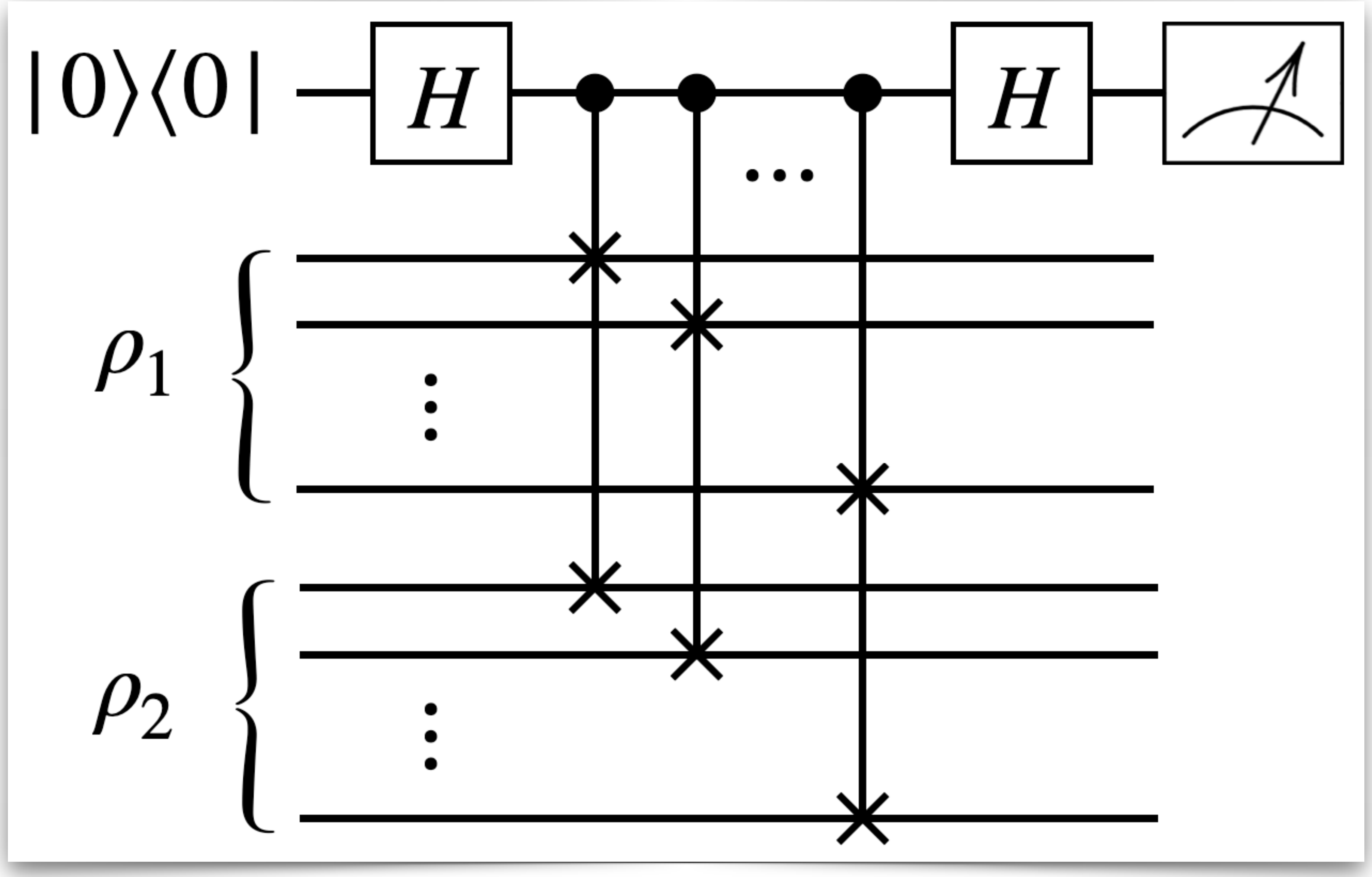
Given $\rho^{\otimes k}$

(efficient) quantum protocol
& some post processing

$\Rightarrow$ ε-approximate $\mathrm{Tr}\left(\rho^k\right)$

- Nonlinear function calculations
- Entanglement spectroscopy
- Quantum error mitigation
- Quantum Gibbs state preparation

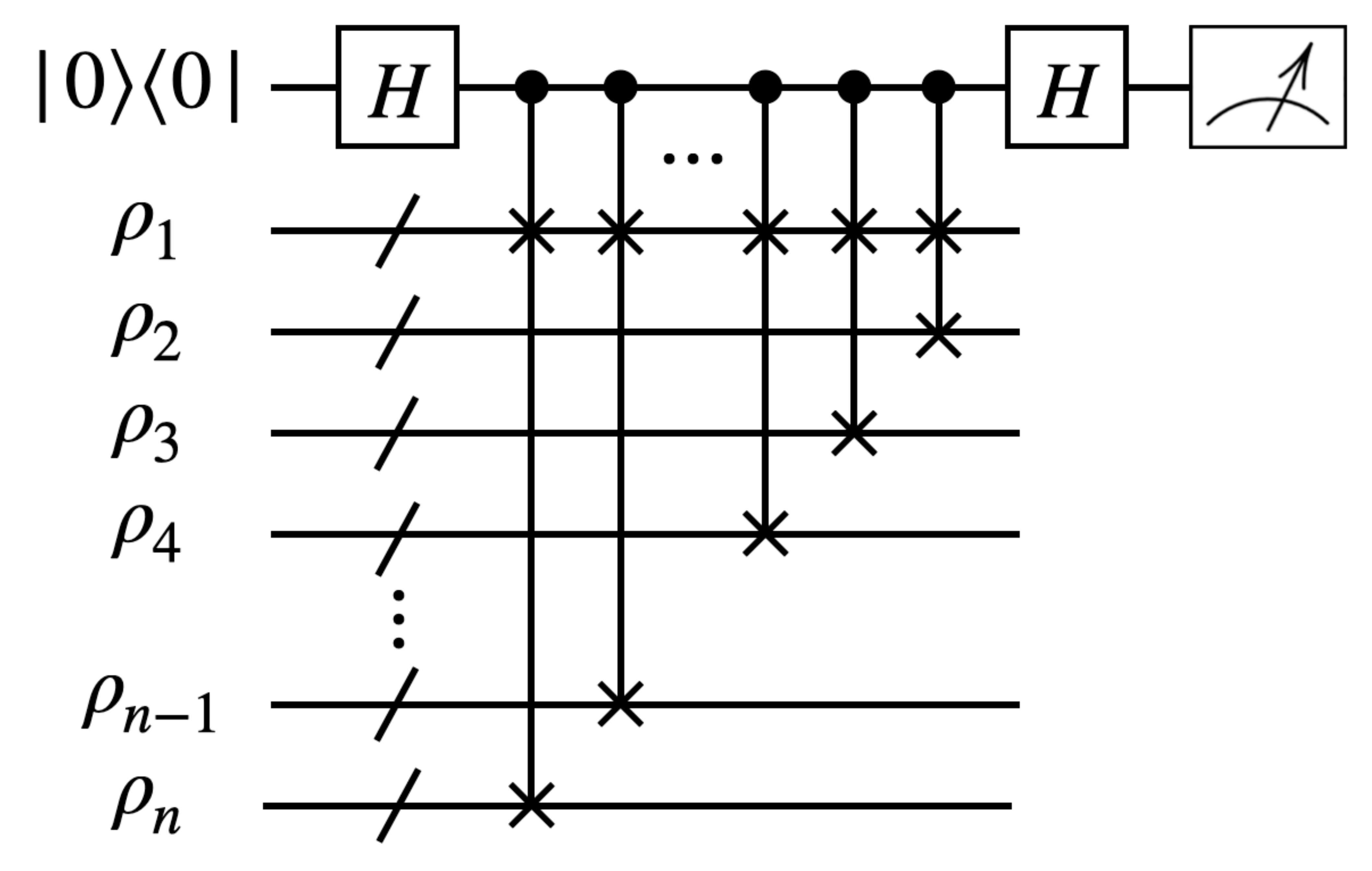
Swap test



$$\mathrm{Tr}\left(S\left(\rho_1 \otimes \rho_2\right)\right) = \mathrm{Tr}\left(\rho_1 \rho_2\right)$$

S = swap operator

Generalized swap test



To estimate $\mathrm{Tr}\left(\rho^k\right)$

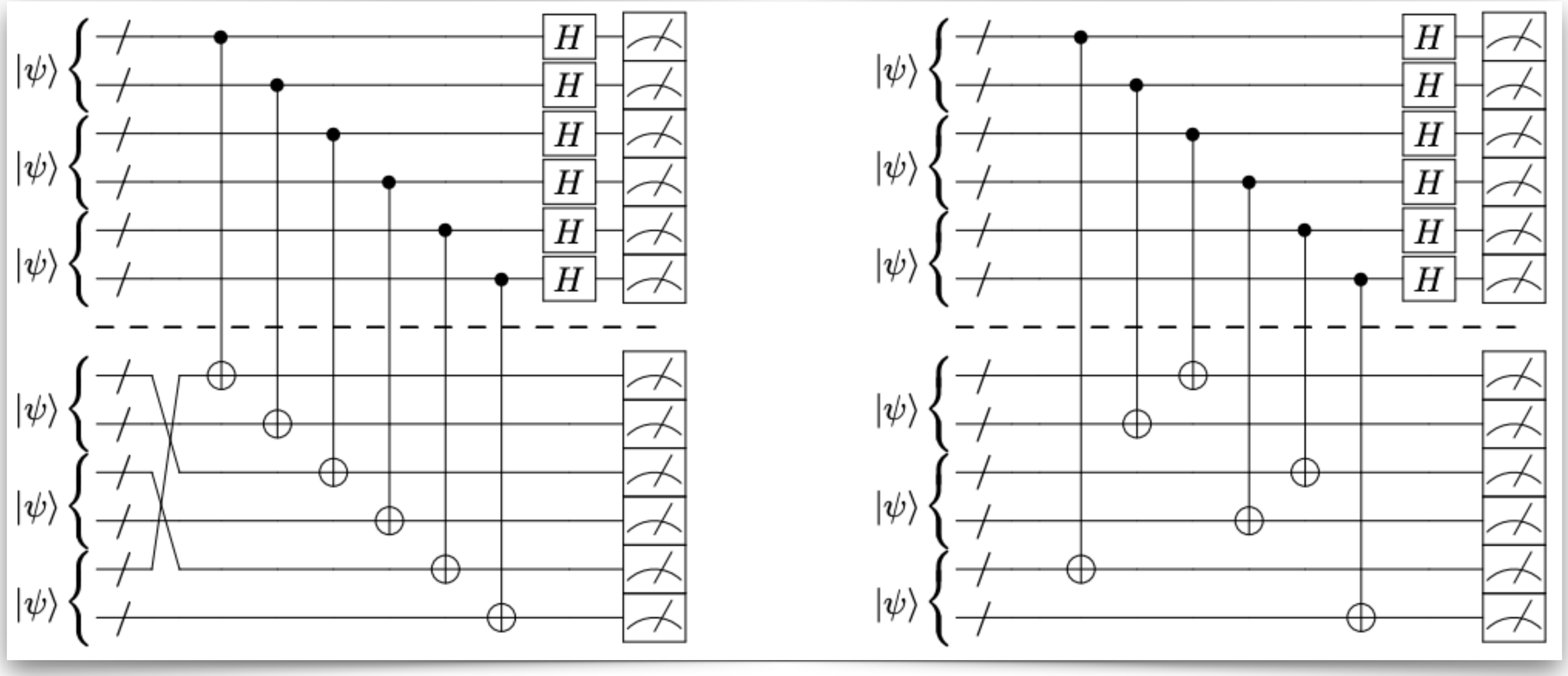
* Depth: $\mathcal{O}(k)$
* Width: $\mathcal{O}(k)$
* Copies: $\mathcal{O}(k)$
* Multi-qubit gates: $\mathcal{O}(k)$

$$\mathrm{Tr}\left(W^\pi\left(\rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_{n-1} \otimes \rho_n\right)\right) = \mathrm{Tr}\left(\rho_1\rho_2\cdots\rho_{n-1}\rho_n\right)$$

W^π = cyclic shift permutation operator

"Direct estimations of linear and nonlinear functionals of a quantum state". Physical Review Letters 88, 217901 (2002).

Two copy test



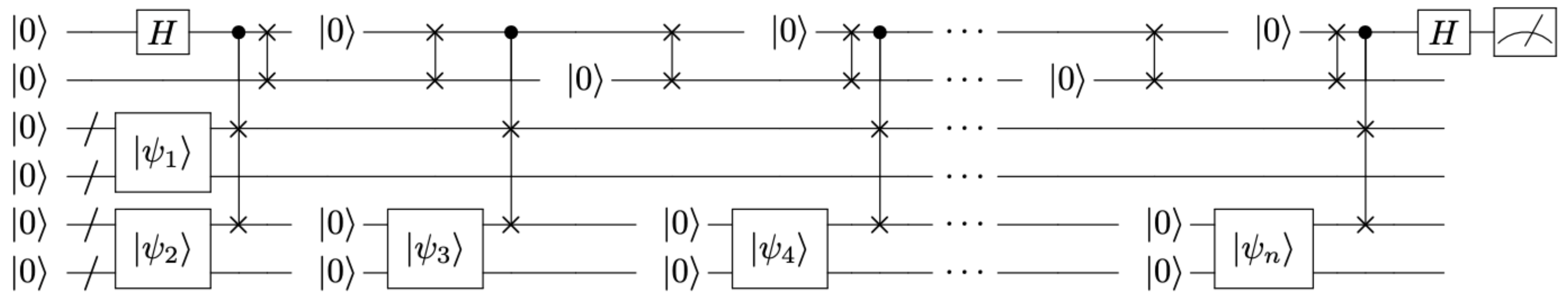
To estimate Tr $\left(\rho^k\right)$

* **Depth: $\mathcal{O}(1)$**
* Width: $\mathcal{O}(k)$
* Copies: $\mathcal{O}(k)$
* Multi-qubit gates: $\mathcal{O}(k)$

* Note that original entangled pure state $|\psi_{AB}\rangle$ needed, where $\rho_A = \mathrm{Tr}_B\left(|\psi\rangle\langle\psi|_{AB}\right)$

"Entanglement spectroscopy with a depth-two quantum circuit". Journal of Physics A: Mathematical and Theoretical 52, 044001 (2019).

Qubit-efficient two copy test



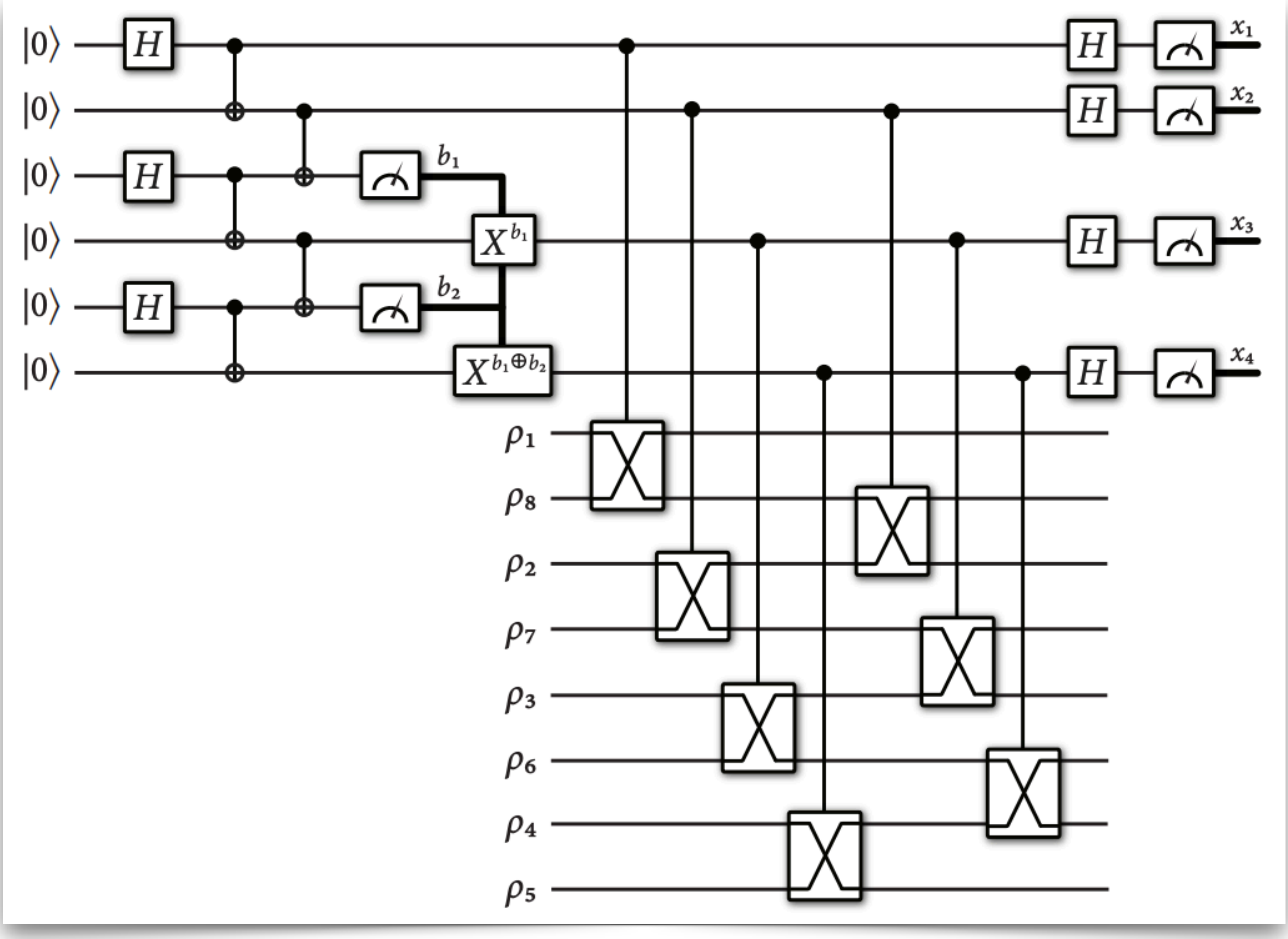
To estimate $\mathrm{Tr}\left(\rho^k\right)$

* Depth: $\mathcal{O}(k)$
* **Width: $\mathcal{O}(1)$**
* Copies: $\mathcal{O}(k)$
* Multi-qubit gates: $\mathcal{O}(k)$

* Using qubit-reset strategies
* Original entangled pure state $|\psi_{AB}\rangle$ needed

"Qubit- efficient entanglement spectroscopy using qubit resets". Quantum 5, 535 (2021).

Multivariate trace estimation algorithm



To estimate $\mathrm{Tr}\left(\rho^k\right)$

- **Depth: $\mathcal{O}(1)$**
- Width: $\mathcal{O}(k)$
- Copies: $\mathcal{O}(k)$
- Multi-qubit gates: $\mathcal{O}(k)$

* Inspired by Shor's error correction code

"Multivariate trace estimation in constant quantum depth". Quantum 8, 1220 (2024)

Comparison

Summary of resources required by different algorithms to estimate the values of $\{\mathrm{Tr}(\rho^i)\}_{i=1}^k$ within an error margin of ϵ

Algorithm	# Depth	# Qubits	# CSWAP	# Copies	Original $\lvert\psi\rangle$
Generalized swap test	$\mathcal{O}(k)$	$\mathcal{O}(k)$	$\mathcal{O}(k)$	$\mathcal{O}\left(\frac{k^2}{\epsilon^2}\right)$	***NOT*** required
Hadamard test	$\mathcal{O}(k)$	$\mathcal{O}(k)$	$\mathcal{O}(k)$	$\mathcal{O}\left(\frac{k^2}{\epsilon^2}\right)$	Required
Two copy test	$\mathcal{O}(1)$	$\mathcal{O}(k)$	$\mathcal{O}(k)$	$\mathcal{O}\left(\frac{k^2}{\epsilon^2}\right)$	Required
Qubit-efficient two copy test	$\mathcal{O}(k)$	$\mathcal{O}(1)$	$\mathcal{O}(k)$	$\mathcal{O}\left(\frac{k^2}{\epsilon^2}\right)$	Required
Multivariate trace estimation	$\mathcal{O}(1)$	$\mathcal{O}(k)$	$\mathcal{O}(k)$	$\mathcal{O}\left(\frac{k^2}{\epsilon^2}\right)$	***NOT*** required
Ours (this work)	$\mathcal{O}(1)$	$\mathcal{O}(r)$	$\mathcal{O}(r)$	$\mathcal{O}\left(\frac{k^2 r^4 \ln^2 r}{\epsilon^2}\right)$, $p_1 \approx 1$ $\mathcal{O}\left(\frac{r^2 \ln^2 r}{\epsilon^2}\right)$, otherwise	***NOT*** required

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Intuition

Consider two quantum states: $\rho = \sum_{i=1}^{r} p_i |\psi_i\rangle\langle\psi_i|$, $\sigma = \sum_{i=1}^{r} q_i |\phi_i\rangle\langle\phi_i|$

(assume descending order $p_1 \geq p_2 \geq \ldots \geq p_{r-1} \geq p_r \geq 0$ and also for q_i)

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If $\begin{cases} \mathrm{Tr}(\rho^1) = \mathrm{Tr}(\sigma^1) \\ \mathrm{Tr}(\rho^2) = \mathrm{Tr}(\sigma^2) \\ \vdots \\ \mathrm{Tr}(\rho^{r-1}) = \mathrm{Tr}(\sigma^{r-1}) \\ \mathrm{Tr}(\rho^r) = \mathrm{Tr}(\sigma^r) \end{cases}$ then, $\begin{cases} p_1 = q_1 \\ p_2 = q_2 \\ \vdots \\ p_{r-1} = q_{r-1} \\ p_r = q_r \end{cases}$?

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Answer: YES

Newton-Girard method

Key observation: exactly knowing $\{\mathrm{Tr}(\rho^i)\}_{i=1}^r$ is equivalent to knowing $\{p_i\}_{i=1}^r$.

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Consider the equation having these eigenvalues as root in the form of

$$\prod_{m=1}^{r}(x - p_m) = 0.$$

The values of $\mathrm{Tr}(\rho^i)$ are now the i-th power sum of the roots. Denote the power sum as

$$P_i := \sum_{m=1}^{r} p_m^i = \mathrm{Tr}(\rho^i)\,.$$

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Simply expanding the terms to get: $\prod_{m=1}^{r}(x - p_m) = \sum_{k=0}^{r}(-1)^k a_k x^{r-k},$

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where

$$
\begin{aligned}
a_0 &= 1, \\
a_1 &= p_1 + p_2 + \cdots + p_r = \sum_{1 \le \alpha \le r} p_\alpha, \\
a_2 &= p_1 p_2 + p_1 p_3 + \cdots + p_{r-1} p_r = \sum_{1 \le \alpha < \beta \le r} p_\alpha p_\beta, \\
a_3 &= \sum_{1 \le \alpha < \beta < \gamma \le r} p_\alpha p_\beta p_\gamma, \\
&\vdots \\
a_r &= \prod_{i=1}^{r} p_i \,.
\end{aligned}
$$

Newton-Girard method

The Newton-Girard method states the relationship between

the elementary symmetric polynomials and the power sums recursively.

For all $r \geq k \geq 1, \;\; a_k = \dfrac{1}{k}\sum_{i=1}^{k}(-1)^{i-1}a_{k-i}P_i.$

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Therefore, the set of eigenvalues is **uniquely determined**

as the roots of the equation $\prod_{m=1}^{r} (x - p_m)$.

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Answer: NO

Counterexample – *Wilkinson's polynomial*

* The location of the roots can be very sensitive to perturbations
in the coefficients of the polynomial

Wilkinson's polynomial

$$w(x) = \prod_{i=1}^{20} (x - i) = (x - 1)(x - 2)\cdots(x - 20)$$

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The 20 roots become:

1.00000	2.00000	3.00000	4.00000	5.00000
6.00001	6.99970	8.00727	8.91725	20.84691
$10.09527 \pm 0.64350i$	$11.79363 \pm 1.65233i$	$13.99236 \pm 2.51883i$	$16.73074 \pm 2.81262i$	$19.50244 \pm 1.94033i$

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* Some of the roots are greatly displaced, even though the change to the coefficient is tiny and the original roots seem widely spaced.

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Main result: iterative $\mathrm{Tr}(\rho^i)$ estimation algorithm

[1] Estimate $P_i = \mathrm{Tr}(\rho^i)$ for $i = 1,2,\ldots,r$, using a constant-depth quantum circuit consisting of $\mathcal{O}(i)$ qubits and $\mathcal{O}(i)$ CSWAP operations using multivariate trace estimation, where r is the rank of ρ, and denote the estimated value as Q_i. $\rightarrow \quad Q_1, \ldots, Q_r$

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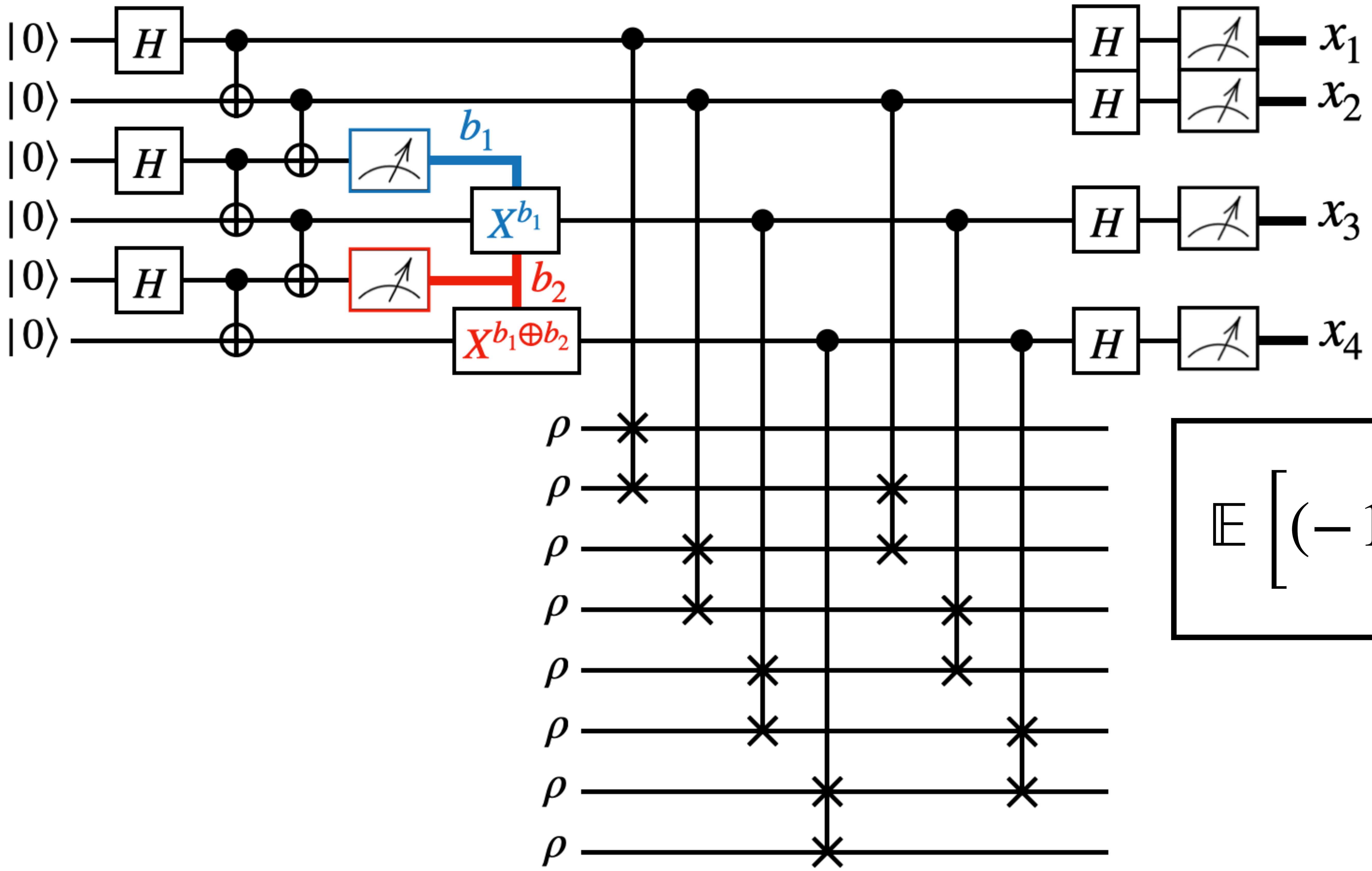
Example ($i = 8$)



$$\mathbb{E}\left[(-1)^{\sum_{i=1}^{4} x_i}\right] = \mathrm{Re}\left(\mathrm{Tr}(\rho^8)\right)$$

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$\rightarrow \; Q_1, \ldots, Q_r$

[2] Calculate the elementary symmetric polynomial $b_i = \frac{1}{i}\sum_{\ell=1}^{i}(-1)^{\ell-1} b_{i-\ell} Q_\ell, \; b_1 = 1, \; 1 \le i \le r$.

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[3] Calculate the estimated value Q_i $(i > r)$ by $Q_i = \sum_{\ell=1}^{r}(-1)^{\ell-1} b_\ell Q_{i-\ell} \sim \mathrm{Tr}(\rho^i)$.

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The output of our algorithm Q_i guarantees an *ϵ-approximate trace of powers* $\mathrm{Tr}(\rho^i)$

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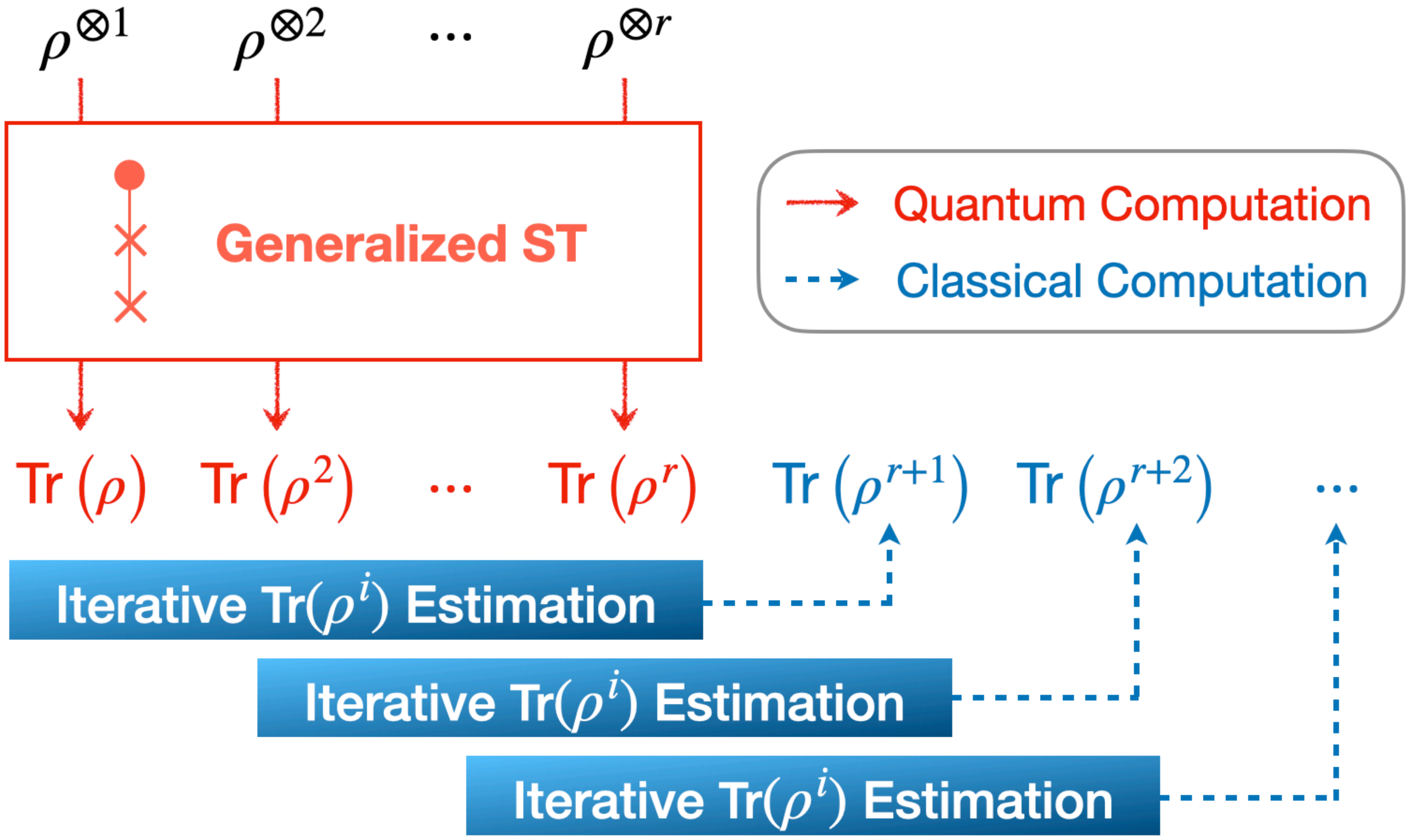

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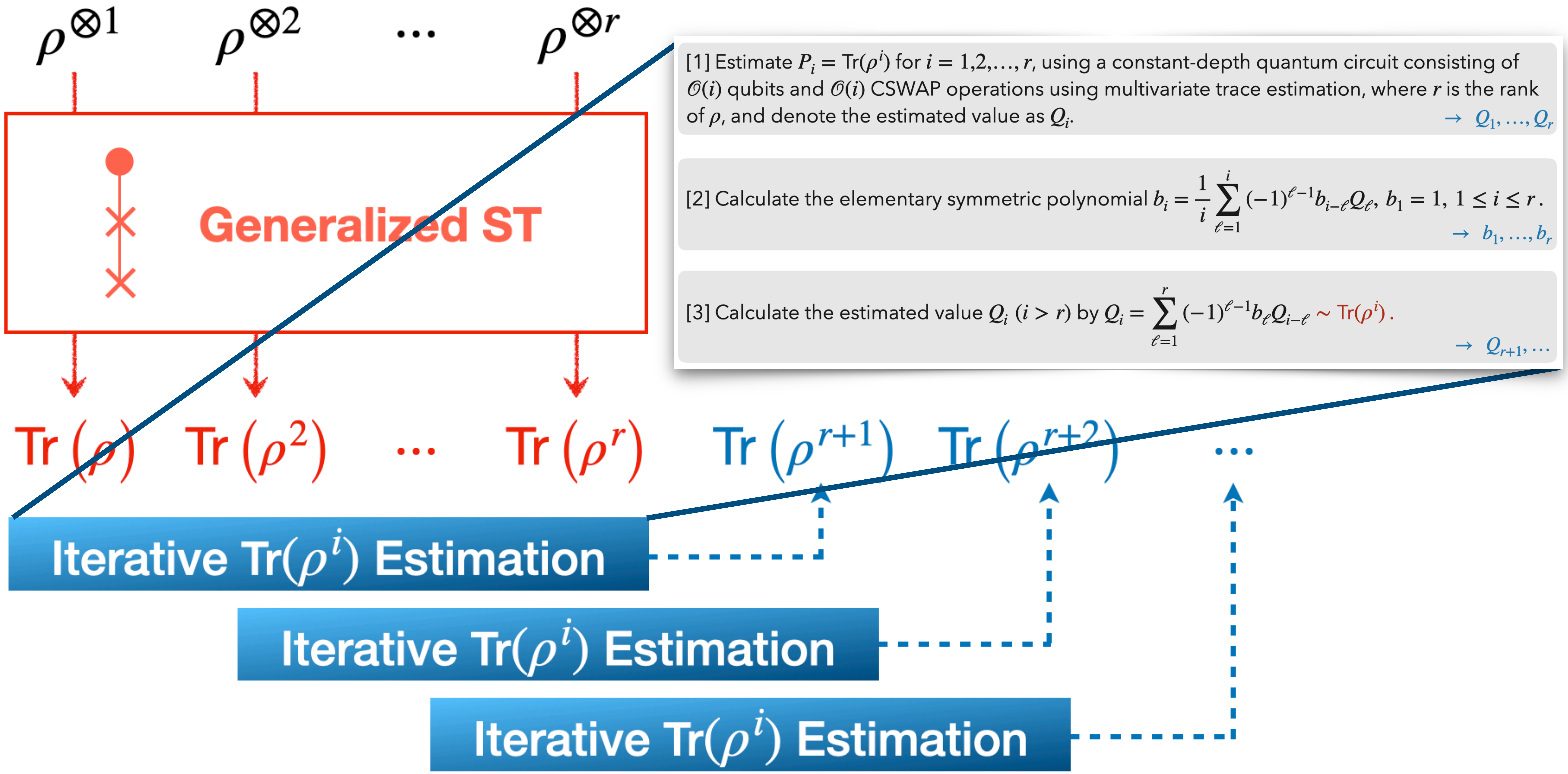

Rank is all you need — Lemma 1

- $a_k, b_k =$ the elementary symmetric polynomials corresponding to each P_i and Q_i.
- Q_i is defined as the estimated value of $P_i = \mathrm{Tr}(\rho^i)$ on a quantum device for $i \leq r$ otherwise $Q_i = \sum_{\ell=1}^{r} (-1)^{\ell-1} b_\ell Q_{i-\ell}$.

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Lemma 1

Let $t_k := b_k - a_k$, then the following holds: $|t_k| \leq \sum_{j=1}^{k} \frac{|\epsilon_j|}{j}$

where $\epsilon_j = Q_j - P_j$ is the error that occurred by the estimation of $P_j = \mathrm{Tr}(\rho^j)$.

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Proof. By strong mathematical induction logic.

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Suppose that

$$\varepsilon_i := |\epsilon_i| = |P_i - Q_i| < \frac{\epsilon}{2T \ln r}$$

holds for $i = 1,2,\ldots,r$, where T is defined as:

$$T = \sum_{i=1}^{r} \frac{p_i(1 - p_i^k)(1 - p_i^r)}{(1 - p_i)^2} \leq kr\,.$$

Then the following relation always holds:

$$|\epsilon_i| = |P_i - Q_i| \leq \epsilon$$

for $i = 1,2,\ldots,k$.

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Proof. By applying **Lemma 1** + long calculation with some mathematical trick.

Rank is all you need – Corollary 1

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To estimate $\mathrm{Tr}(\rho^i)$ for all $i \leq k$ within an additive error of ϵ and with a success probability of at least $1-\delta$, where $\delta \in (0,1)$, it is necessary to estimate each $\mathrm{Tr}(\rho^j)$ for $j \leq r$ within an additive error of ε_j, as defined in **Theorem 1.** This can be achieved by using

$$\mathcal{O}\left(\frac{T^2}{\epsilon^2}\ln^2 r \ln\left(\frac{1}{\delta}\right)\right)$$

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runs on a constant-depth quantum circuit consisting of $\mathcal{O}(j)$ qubits and $\mathcal{O}(j)$ CSWAP operations. Here, T is defined in **Theorem 1.**

* Note that T scales from a constant to kr, mainly depending on the largest eigenvalue p_1 of ρ.
* If p_1 is not close to 1, then $T = \mathcal{O}(1)$. (This implies that if ρ is far from a pure state.)

Rank is all you need – Theorem 2

Extension: Estimating $\mathrm{Tr}(M\rho^k)$, the trace of powers with arbitrary observables M.

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Theorem 2

Suppose that $\varepsilon_{i,M} := |\epsilon_{i,M}| = |P_{i,M} - Q_{i,M}| < \frac{\epsilon}{2}$, and $\varepsilon_i = |\epsilon_i| = |P_i - Q_i| < \frac{\epsilon}{2T\|M\|_\infty \ln r}$, holds for $i = 1,2,\ldots,r$, where the operator norm $\|M\|_\infty$ is defined corresponding to the ∞-norm for vectors $\|x\|_\infty$, as $\|M\|_\infty = \sup_{x\neq 0} \frac{\|Mx\|_\infty}{\|x\|_\infty}$, $T = \sum_{i=1}^{r} \frac{p_i(1-p_i^k)(1-p_i^r)}{(1-p_i)^2} \leq kr$.

Then the following holds:

$$|\epsilon_{i,M}| = |P_{i,M} - Q_{i,M}| \leq \epsilon$$

for $i = 1,2,\ldots,k$.

Rank is all you need – Corollary 2

Corollary 2

Suppose there is an efficient decomposition $M = \sum_{\ell=1}^{N_M} a_\ell P_\ell$, where $a_\ell \in \mathbb{R}$ and $P_\ell = \sigma_{\ell_1} \otimes \cdots \otimes \sigma_{\ell_n}$ are tensor products of Pauli operators $\sigma_{\ell_1}, \ldots, \sigma_{\ell_n} \in \{\sigma_x, \sigma_y, \sigma_z, I\}$. The quantity $\sum_{\ell=1}^{N_M} |a_\ell| = \mathcal{O}(c)$ is bounded by a constant c.

To estimate $\mathrm{Tr}(M\rho^i)$ for all $i \leq k$ within an additive error of ϵ and with a success probability of at least $1-\delta$, where $\delta \in (0,1)$, it is necessary to estimate each $\mathrm{Tr}(M\rho^j)$ for $j \leq r$ within an additive error of $\varepsilon_{j,M}$.

This can be achieved by using $\mathcal{O}\left(\frac{c^2 N_M}{\epsilon^2} \ln\left(\frac{1}{\delta}\right)\right)$ runs on a constant-depth quantum circuit consisting of $\mathcal{O}(j)$ qubits and $\mathcal{O}(j)$ CSWAP operations, and estimating each $\mathrm{Tr}(\rho^{j'})$ for $j' \leq r$ within an additive error of $\varepsilon_{j'}$, by using $\mathcal{O}\left(\frac{T^2}{\epsilon^2} \ln^2 r \ln\left(\frac{1}{\delta}\right)\right)$ runs on a constant-depth quantum circuit consisting of $\mathcal{O}(j')$ qubits and $\mathcal{O}(j')$ CSWAP operations. Here, $\varepsilon_{j,M}$, $\varepsilon_{j'}$ and T are defined in **Theorem 2.**

(Effective) Rank is all you need – Lemma 2

$$\mathcal{O}\left(\frac{T^2}{\epsilon^2}\ln^2 r \ln\left(\frac{1}{\delta}\right)\right)$$

* If p_1 is not close to 1, then $T = \mathcal{O}(1)$.
* ***Our algorithm may perform suboptimally on pure states.***

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As the maximum eigenvalue of ρ approaches 1, the r_ϵ decreases!

(Possible to resolve issues with pure states)

Finding the $r = \text{rank}(\rho)$

- To proceed with our algorithm, we need to know the rank of quantum state.
- Due to the concept of effective rank, **the estimated rank doesn't have to be precise.**
- Several approaches:
  - Variational algorithms via purity minimization
  - Binary search-based heuristic

Variational algorithms via purity minimization

$$C(\theta) = \mathrm{Tr}\left[\left[\frac{\eta(\theta)^k \rho \eta(\theta)^k}{\mathrm{Tr}\left(\eta(\theta)^k \rho \eta(\rho)^k\right)}\right]^2\right]$$

[Phys. Rev. Research **3**, 033251]

- where k is any positive integer, ρ is the density matrix of a possibly unnormalized mixed state, and $\eta(\theta)$ is some normalized ansatz state. The goal is to minimize the cost function $C(\theta)$ by varying θ in order to find the optimal ansatz $\eta(\theta^*)$.
- Purity optimization allows one to find a lower bound estimate of the rank.
- This comes directly from the fact that $r = \mathrm{rank}(\rho) \approx \dfrac{1}{C(\theta^*)}$ and that in general for any θ, we have $d \geq \dfrac{1}{C(\theta)}$.

Binary search-based heuristic

1. Choose r to be reasonably large.

2. Apply our algorithm to obtain estimated values for $\mathrm{Tr}(\rho^i)$, for $r+1 \leq i \leq 2r$.

3. Analyze the difference between the estimated values and the measurements for $r+1 \leq i \leq 2r$.

4. Do the following:

   A. If the difference is significant, double the value of r.

   B. Otherwise, keep the current value of r.

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Reduction of required runs

Analyze the behavior of $T = \sum_{i=1}^{r} \frac{p_i(1-p_i^k)(1-p_i^r)}{(1-p_i)^2}$ as the eigenvalues of ρ change.

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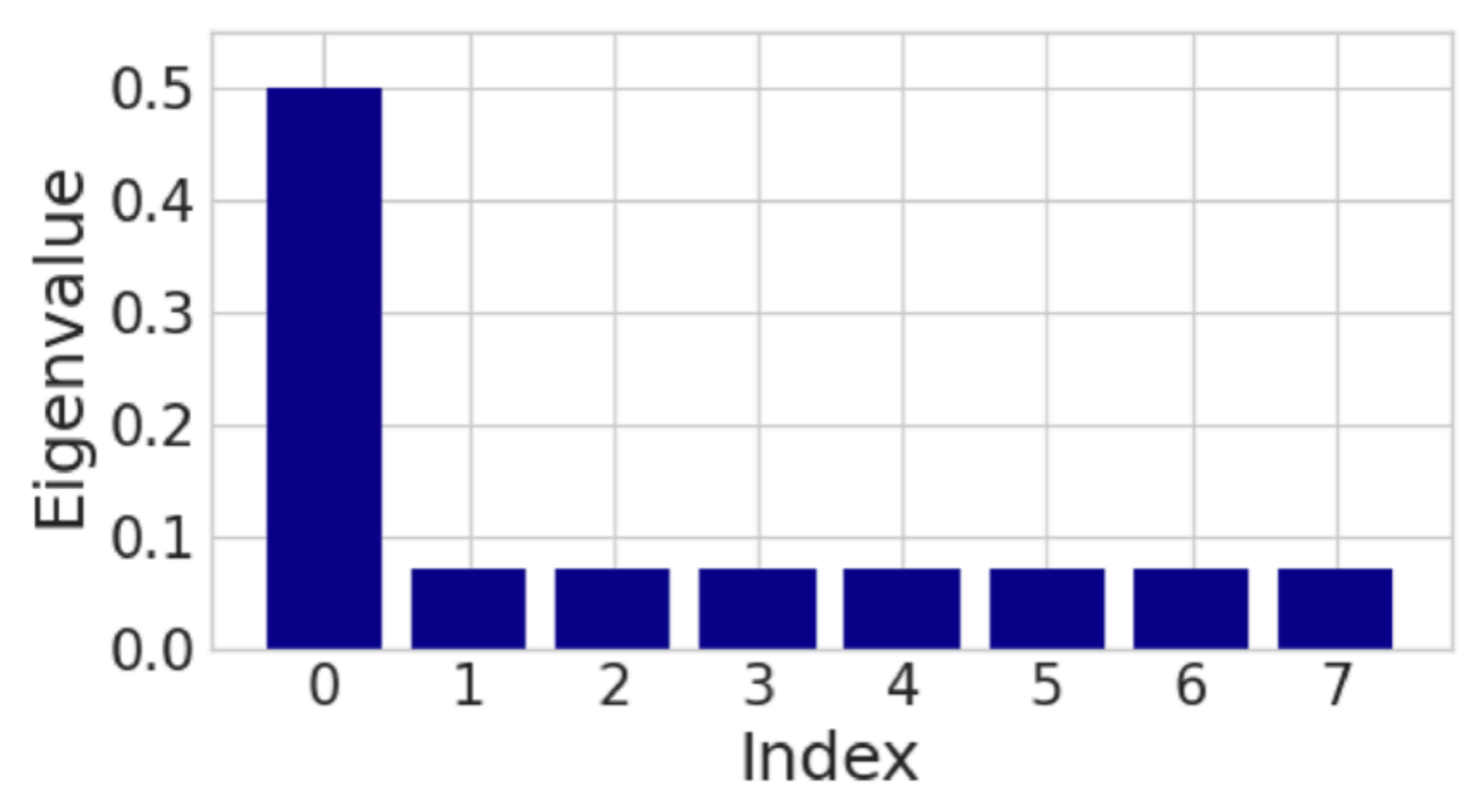
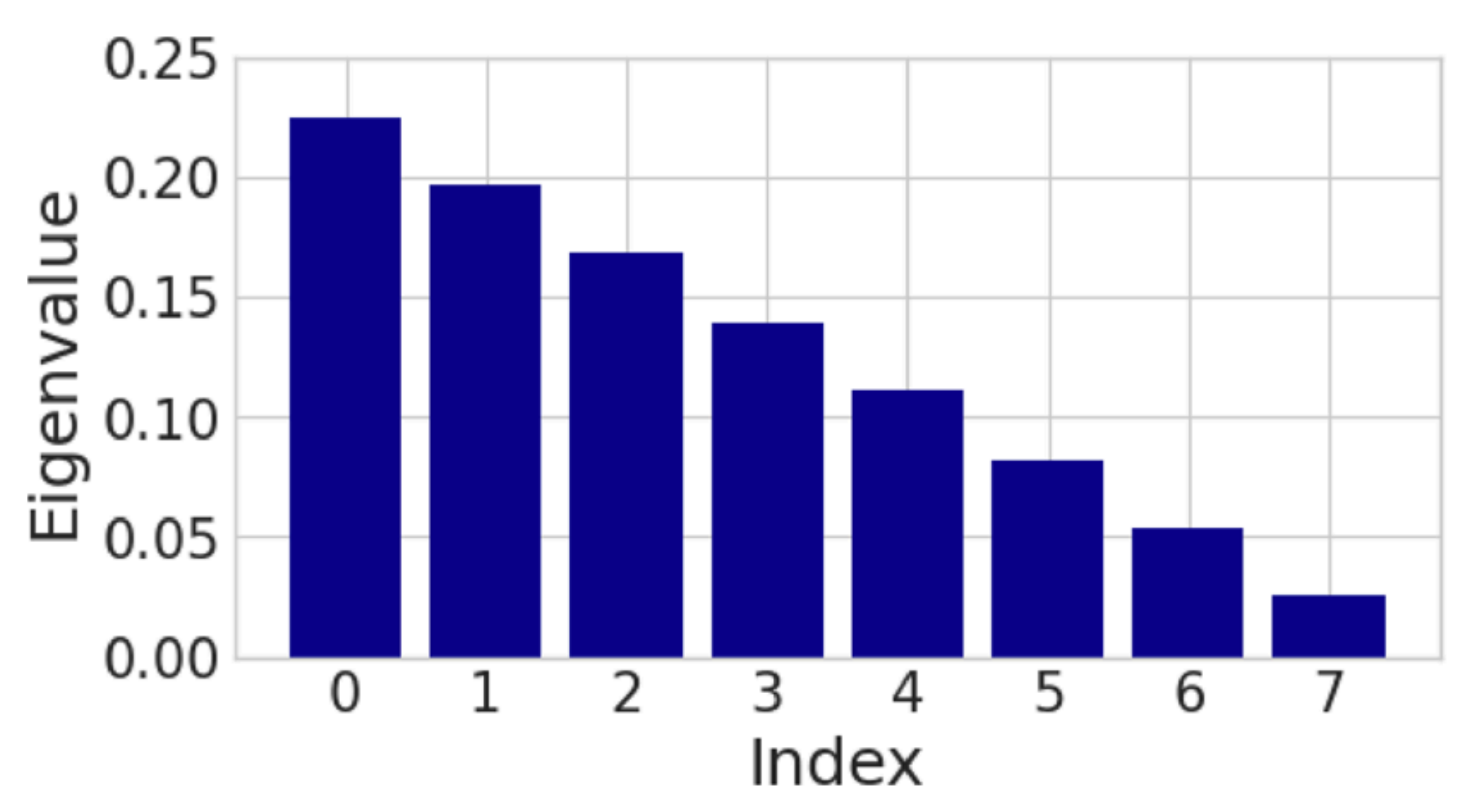
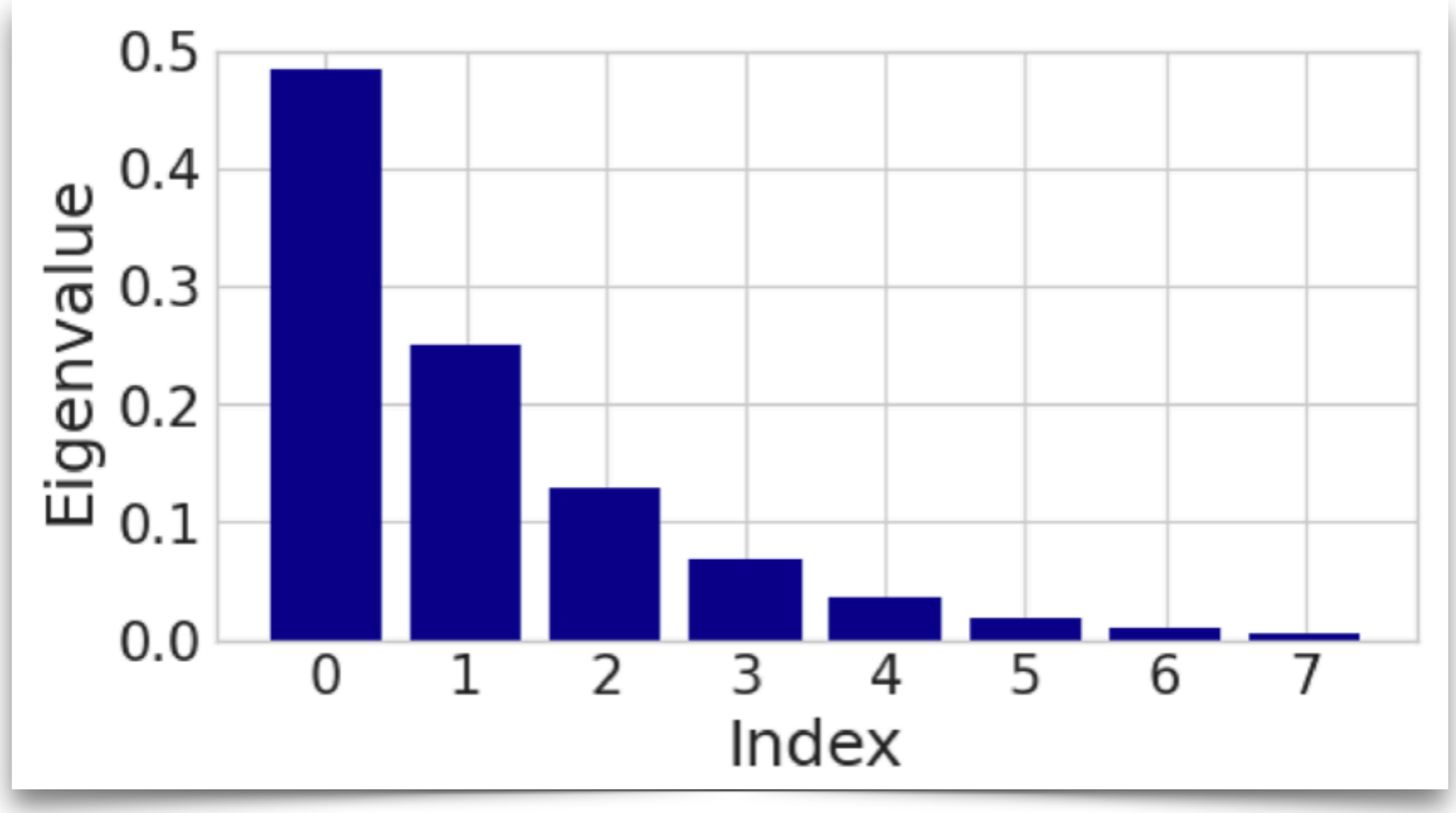
Since we don't know the exact distribution of the eigenvalues of an arbitrary density matrix ρ, we consider several typical cases.



Uniform non-maximum



Arithmetically decaying



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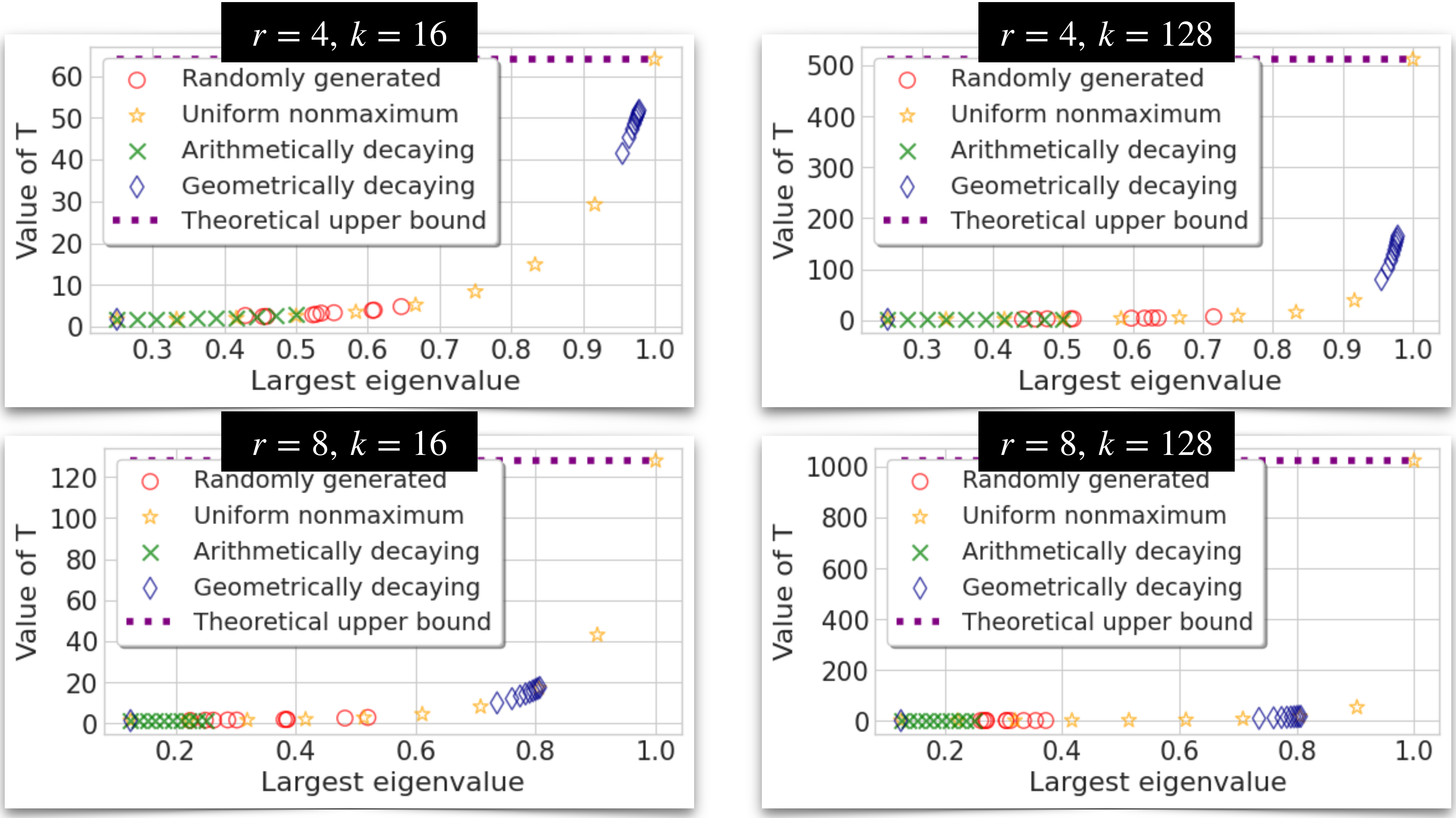

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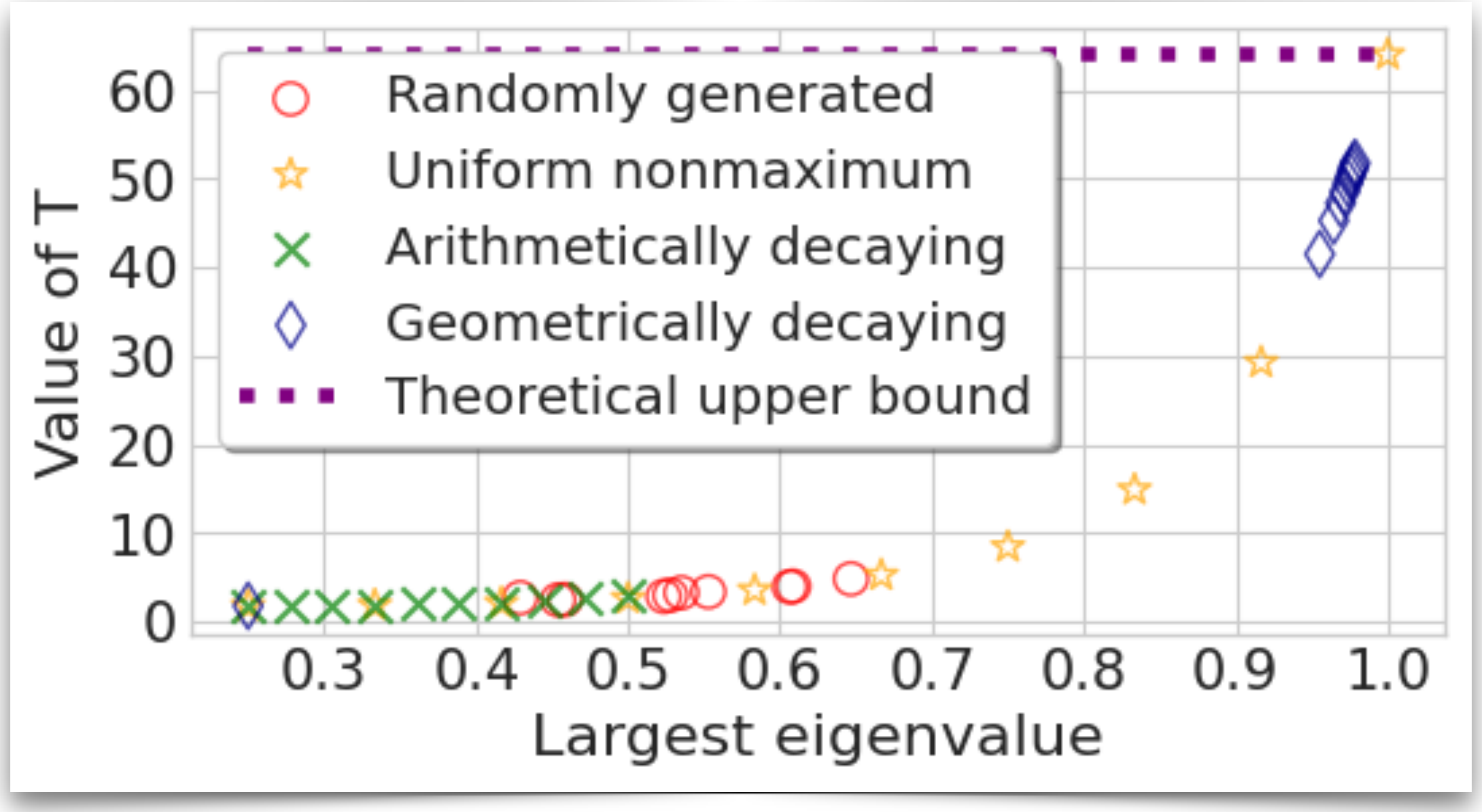

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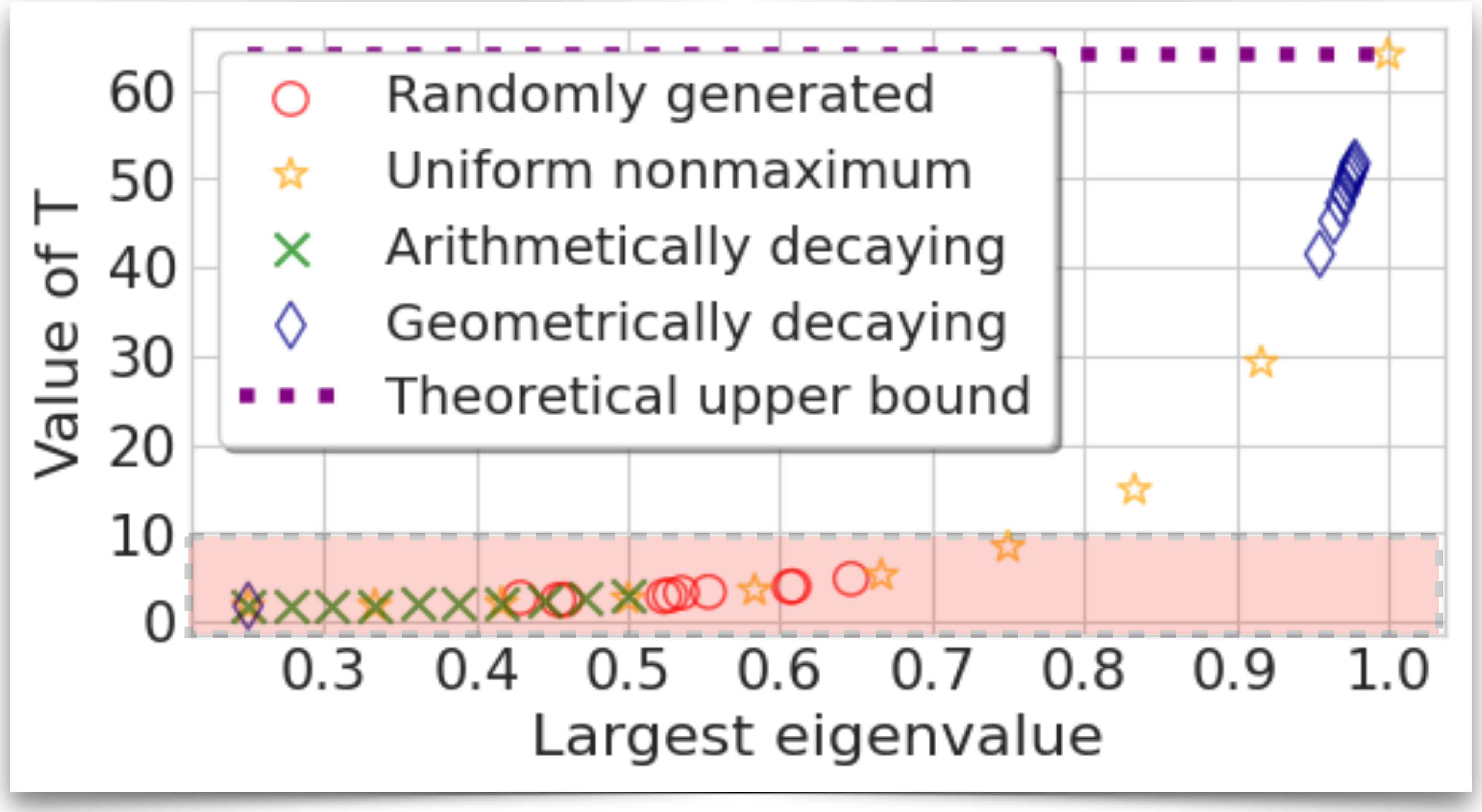

~ constant

$$\mathcal{O}(1) \leq T = \sum_{i=1}^{r} \frac{p_i(1-p_i^k)(1-p_i^r)}{(1-p_i)^2}$$

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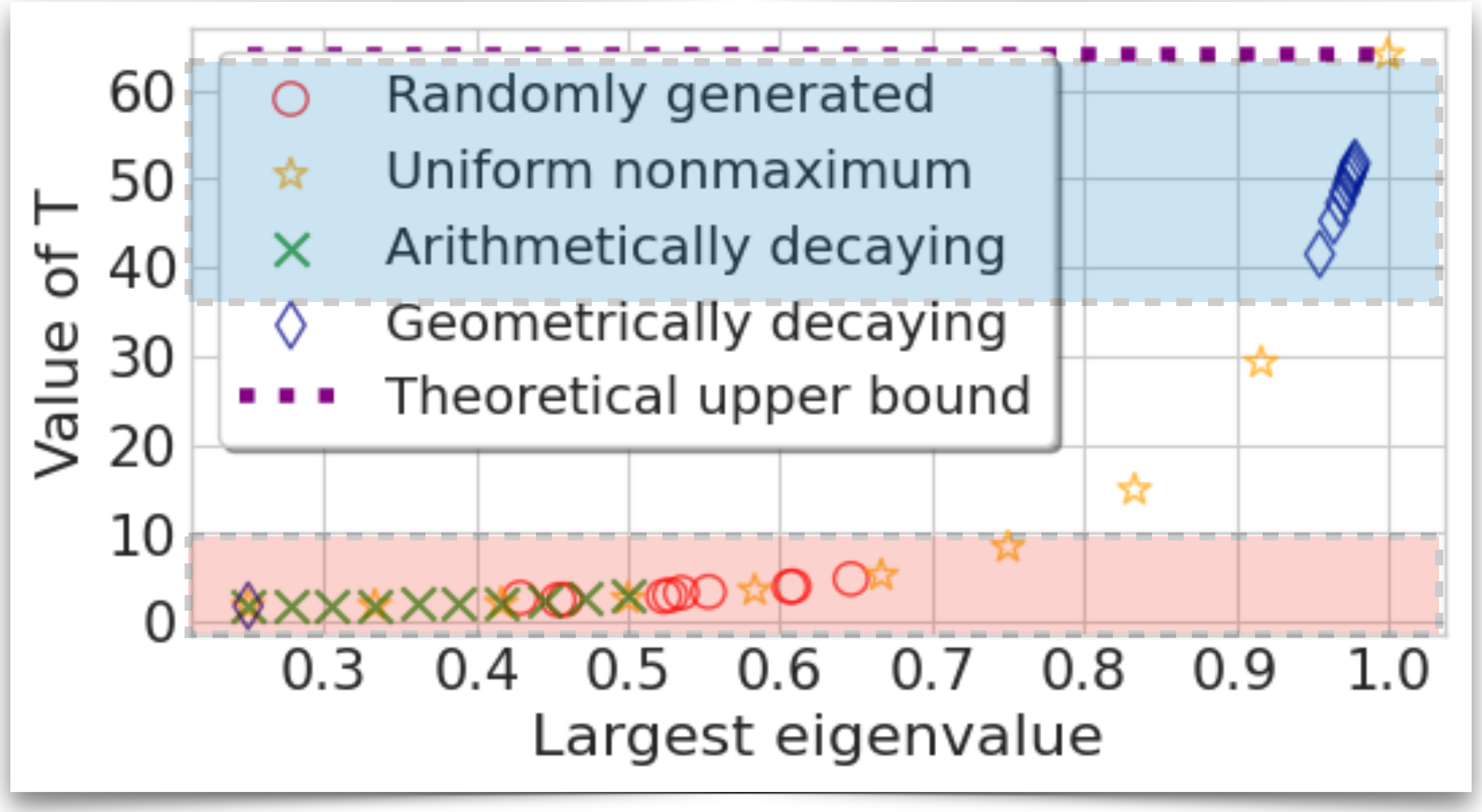

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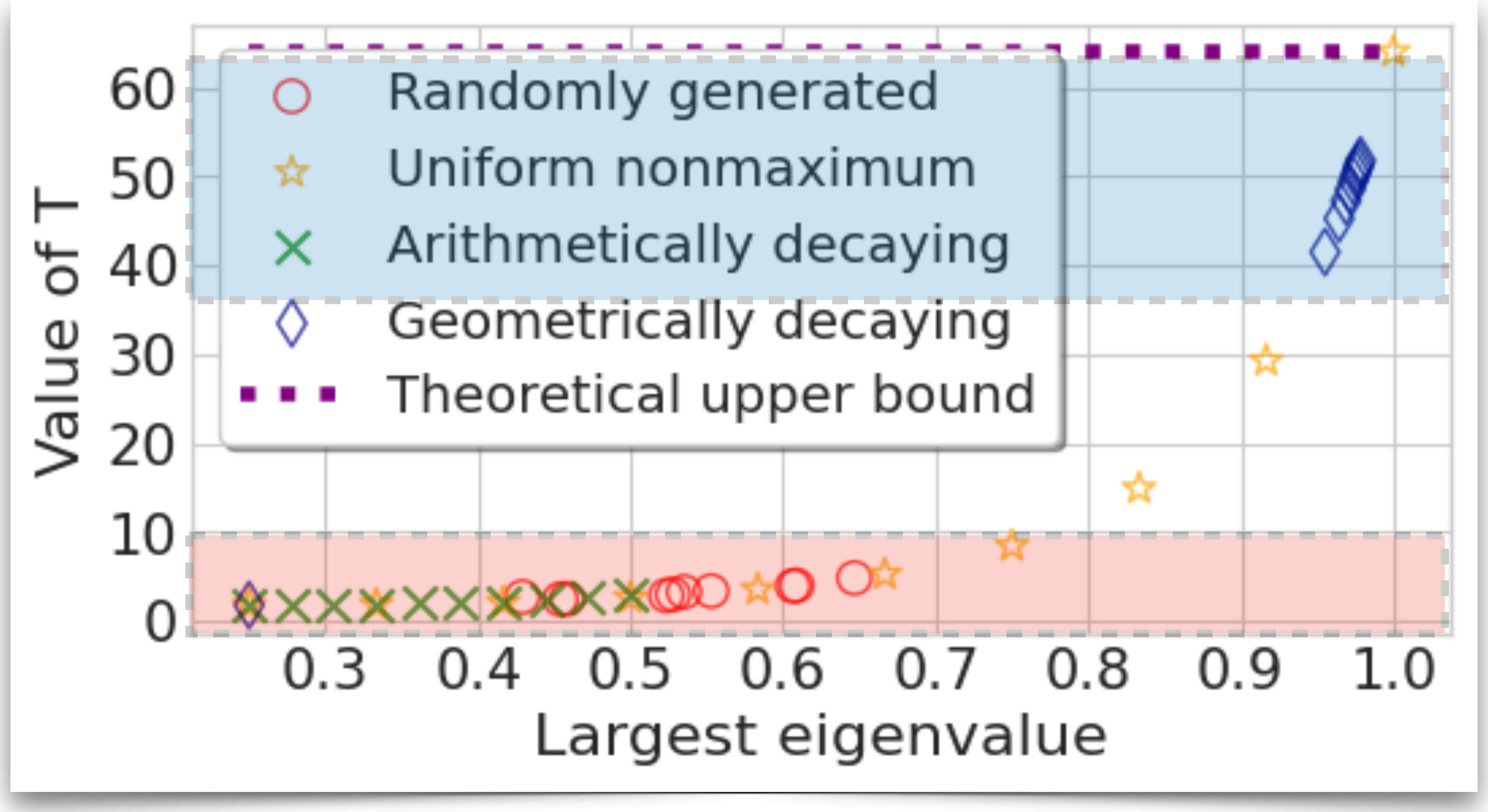

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To estimate $\mathrm{Tr}(\rho^i)$ for all $i \leq k$ within an additive error of ϵ and with a success probability of at least $1-\delta$, where $\delta \in (0,1)$, it is necessary to estimate each $\mathrm{Tr}(\rho^j)$ for $j \leq r$ within an additive error of ε_j, as defined in **Theorem 1.** This can be achieved by using

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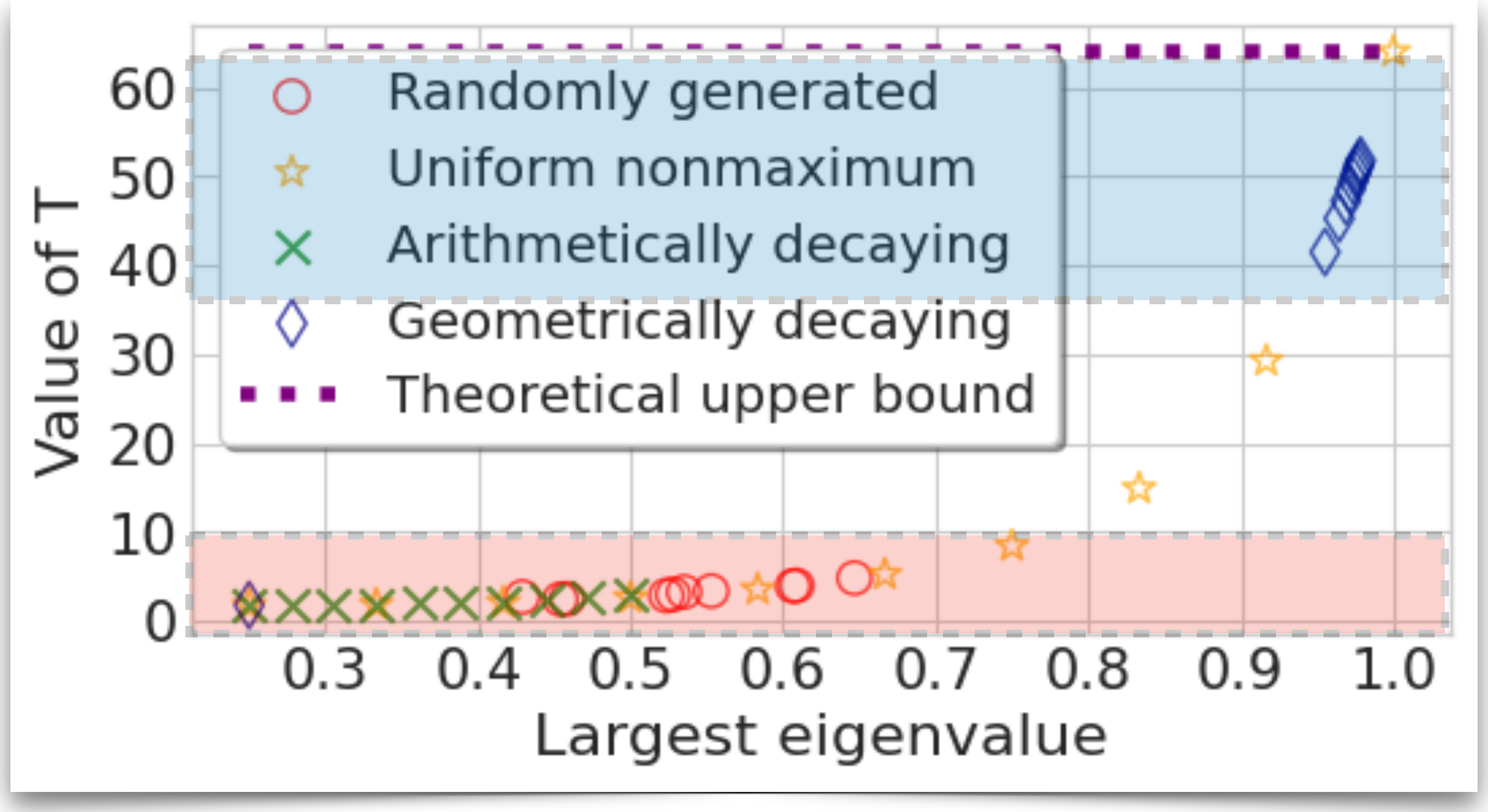

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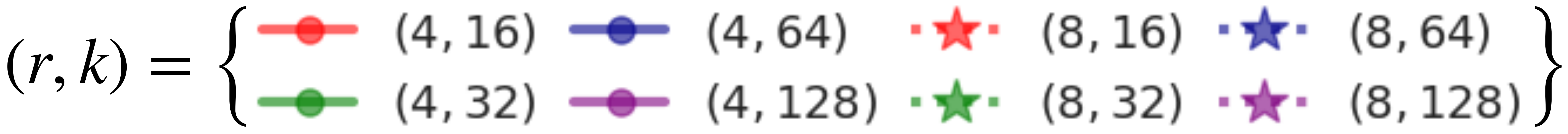
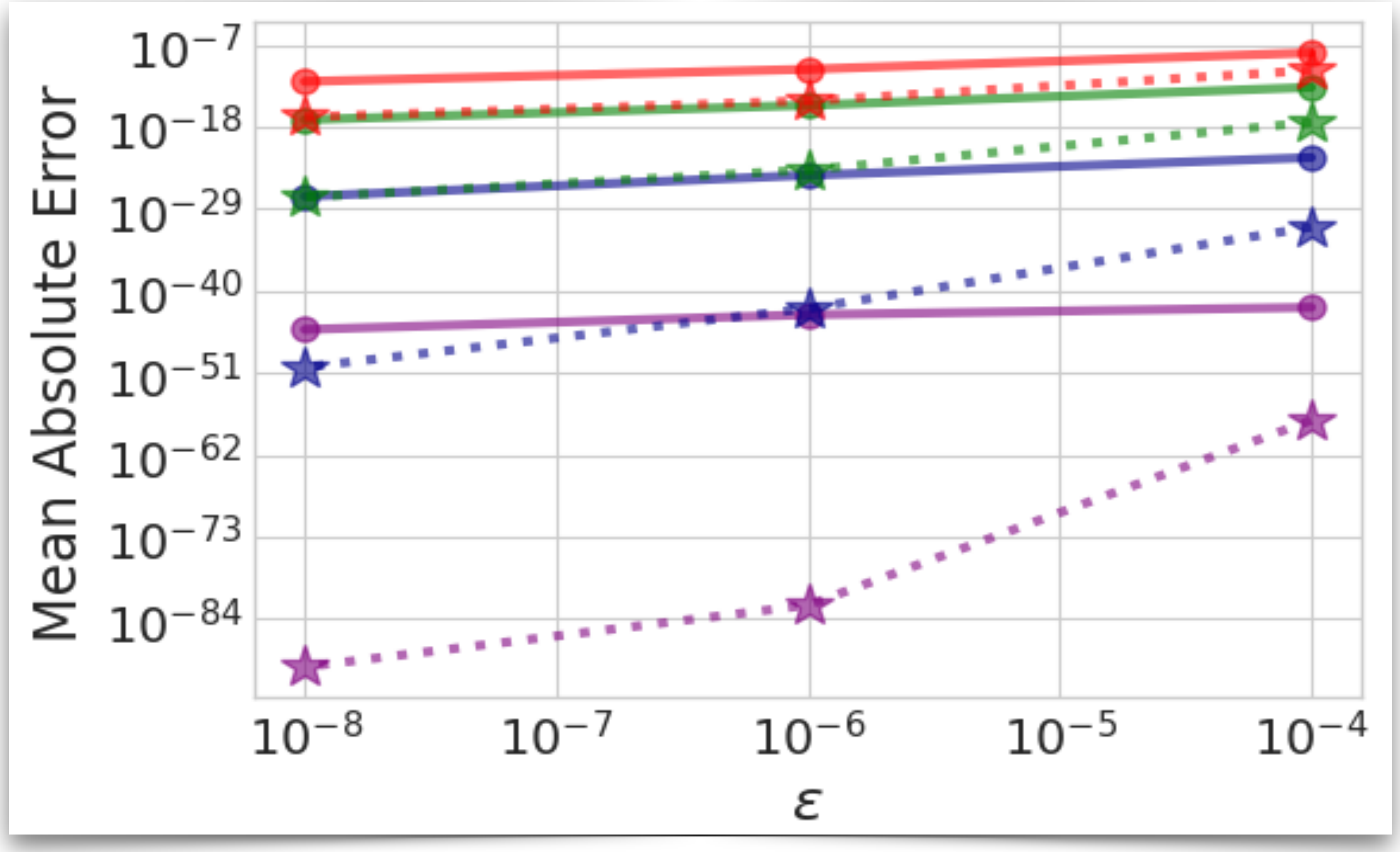
runs on a constant-depth quantum circuit consisting of $\mathcal{O}(j)$ qubits and $\mathcal{O}(j)$ CSWAP operations. Here, T is defined in **Theorem 1.**

The value of T is significantly less than the kr in most cases.

Especially when the state is *mixed* (e.g., the largest eigenvalue is small), the system is large (e.g., r is large), or k grows large, the expected advantage becomes more dramatic compared to the upper bound.

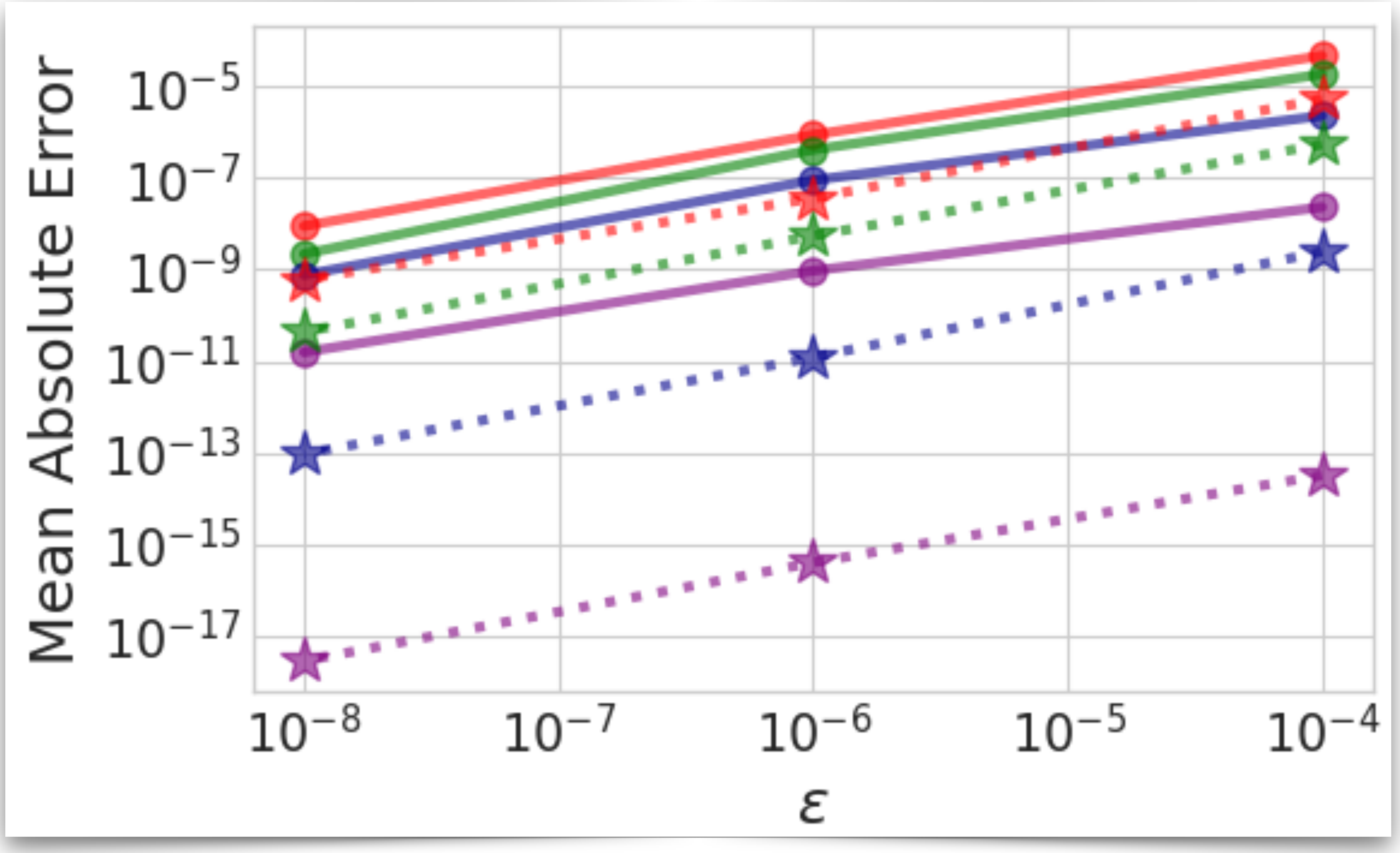
Numerical simulation





Arithmetically decaying

$T \sim \mathcal{O}(1)$



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Computational hardness of TsallisQED$_q$ and TsallisQEA$_q$

$$S_q(\rho) = \frac{1 - \mathrm{Tr}(\rho^q)}{q-1}$$

- **Quantum q-Tsallis Entropy Difference Problem (TsallisQED$_q$):**
  - Two polynomial-size quantum circuits, denoted as Q_0 and Q_1, prepare n-qubit quantum states ρ_0 and ρ_0.
  - The goal is to decide whether the difference between their q-Tsallis entropy values, $S_q(\rho_0) - S_q(\rho_1)$, is:
    - At least 0.001, or
    - At most −0.001.
  - The problem involves access to the descriptions of the quantum circuits Q_0 and Q_1.

[arXiv:2410.13559]

Computational hardness of TsallisQED$_q$ and TsallisQEA$_q$

$$S_q(\rho) = \frac{1 - \mathrm{Tr}(\rho^q)}{q - 1}$$

- **Quantum q-Tsallis Entropy Approximation Problem (TsallisQEA$_q$)**
  - Similar to TsallisQED$_q$, but involves only a single n-qubit quantum state ρ.
  - The task is to decide whether the difference between the q-Tsallis entropy of ρ and a known threshold $t(n)$, $S_q(\rho) - t(n)$is:
    - At least 0.001, or
    - At most -0.001.

[arXiv:2410.13559]

Computational hardness of TsallisQED$_q$ and TsallisQEA$_q$

- Given quantum query access to the state-preparation circuit of an n-qubit quantum state ρ, for any $q \geq 1 + \Omega(1)$, there is a quantum algorithm for estimating $S_q(\rho)$ to additive error 0.001 with query complexity $O(1)$.
- Moreover, if the description of the state-preparation circuit is of size poly(n), then the time complexity of the quantum algorithm is poly(n).

∴ For any $q \geq 1 + \Omega(1)$, TsallisQEC$_q$ and TsallisQEA$_q$ are in BQP.

Computational hardness of TsallisQED$_q$ and TsallisQEA$_q$

	$q = 1$	$1 < q \leq 1 + \frac{1}{n-1}$	$1+\Omega(1) \leq q \leq 2$	$q > 2$
TsallisQED$_q$	QSZK-complete [BASTS10]	QSZK-hard Theorem 1.2(2)	BQP-complete Theorem 1.1 and Theorem 1.2(1)	in BQP Theorem 1.1
TsallisQEA$_q$	NIQSZK-complete [BASTS10, CCKV08]	NIQSZK-hard* Theorem 1.2(2)	BQP-complete Theorem 1.1 and Theorem 1.2(1)	in BQP Theorem 1.1

Leading to hardness of approximating von Neumann entropy

because $S_q(\rho) \leq S(\rho)$, as long as **BQP** $\subsetneq$ **QSZK**

Purity Estimation = BQP-complete

QSZK $\subseteq$ QIP(2) $\subseteq$ PSPACE = IP

NIQSZK $\subseteq$ qq-QAM $\subseteq$ QIP(2) $\subseteq$ PSPACE = IP

Computational hardness of TsallisQED_q and TsallisQEA_q

- In terms of *quantitative bounds* on quantum query and sample complexities, **QSZK-hard or NIQSZK-hard correspond to rank-dependent complexities.**

Regime of q	Query Complexity		Sample Complexity	
	Upper Bound	Lower Bound	Upper Bound	Lower Bound
$q \geq 1 + \Omega(1)$	$O(1/\epsilon^{1+\frac{1}{q-1}})$ Theorem 3.2	$\Omega(1/\sqrt{\epsilon})$ Theorem 5.12	$\widetilde{O}(1/\epsilon^{3+\frac{2}{q-1}})$ Theorem 3.3	$\Omega(1/\epsilon)$ Theorem 5.14
$1 < q \leq 1 + \frac{1}{n-1}$	$\widetilde{O}(r/\epsilon^2)$ [WZL24]	$\Omega(r^{1/3})$ Theorem 5.13	$\widetilde{O}(r^2/\epsilon^5)$[7] [WZ24b]	$\Omega(r^{0.51-c})$[8] Theorem 5.15
$q = 1$	$\widetilde{O}(r/\epsilon^2)$[9] [WGL+24]	$\widetilde{\Omega}(\sqrt{r})$ [BKT20]	$\widetilde{O}(r^2/\epsilon^5)$[7] [WZ24b]	$\Omega(r/\epsilon)$ [WZ24b]

Computational hardness of $\mathrm{TsallisQED}_q$ and $\mathrm{TsallisQEA}_q$

The quantum query complexities are also extensively studied. For von Neumann entropy estimation, the dimension-dependence was studied in [GL20], the dependence on the reciprocal of the minimum non-zero eigenvalue of the quantum state was studied in [CLW20], the multiplicative error-dependence was studied in [GHS21], and the rank-dependence was studied in [WGL+24]. In [SLLJ24], they presented a rank-dependent estimator for the q-Tsallis entropy with integer q larger than the rank of quantum states. For Rényi entropy estimation, the query complexity was first studied in [SH21], the rank-dependence was studied in [WGL+24], and was later improved in [WZL24]. Other problems include tomography [vACGN23], and the estimations of fidelity and trace distance [WZC+23, WGL+24, GP22, WZ24a, Wan24].

In [GH20], the Quantum Entropy Difference Problem (with respect to von Neumann entropy) with shallow circuits was shown to have (conditional) hardness. The computational complexity of the space-bounded versions of the Quantum Entropy Difference Problem and Quantum State Distinguishability Problem were studied in [LGLW23].

[3] Calculate the estimated value Q_i $(i > r)$ by $Q_i = \sum_{\ell=1}^{r} (-1)^{\ell-1} b_\ell Q_{i-\ell} \sim \mathrm{Tr}(\rho^i)$.

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Applications

Nonlinear functions

Computation of the **partition function** and other **thermodynamical** variables for the systems with finite energy levels and finite # of non interacting particles

e.g.

$$g(x) = e^{\beta x},\ \beta \in \mathbb{R}$$

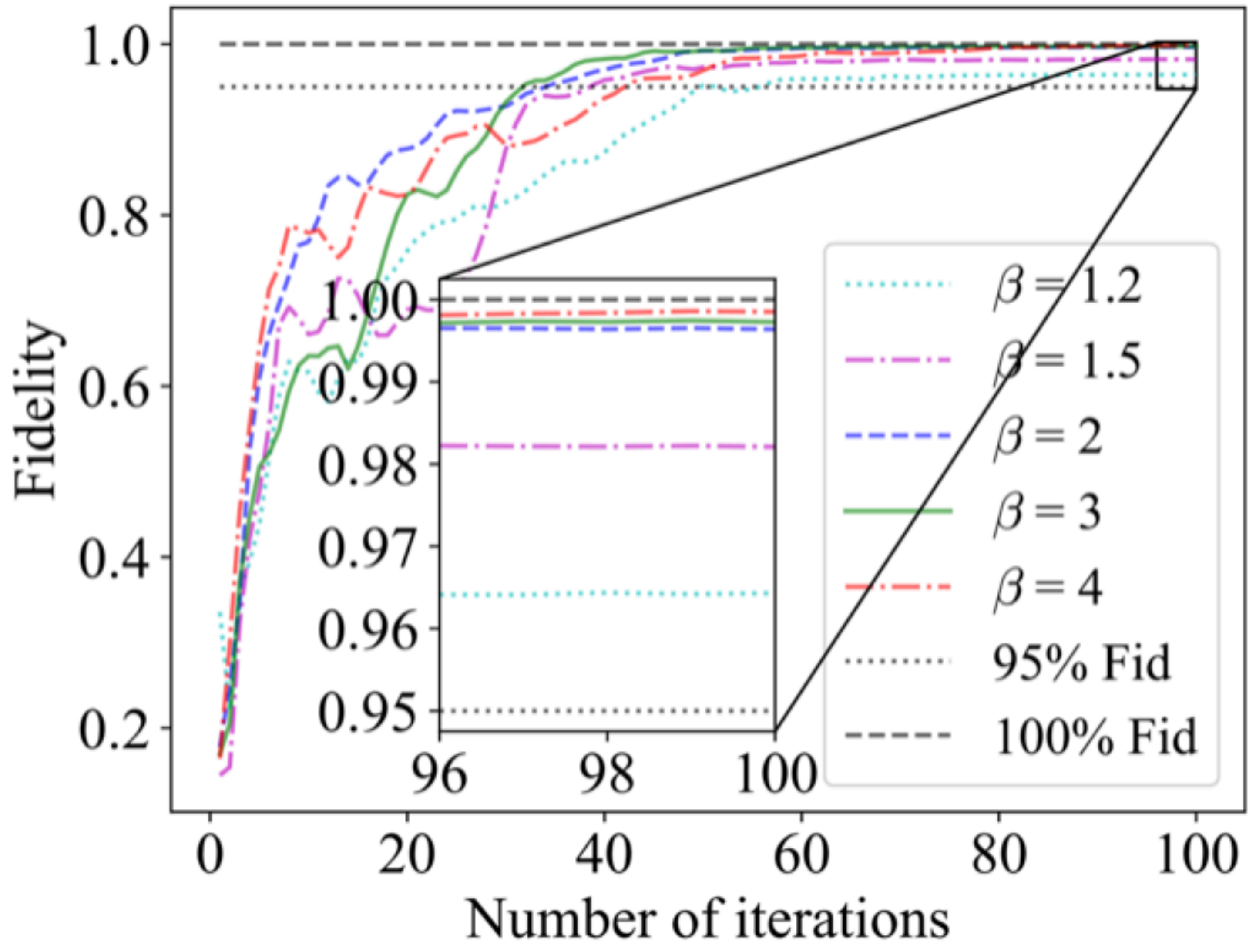
$$g(x) = (1+x)^{\alpha},\ \alpha \in \mathbb{R}^{+}$$

and more

Quantum Gibbs states

Variational quantum Gibbs state preparation with a **truncated Taylor series**

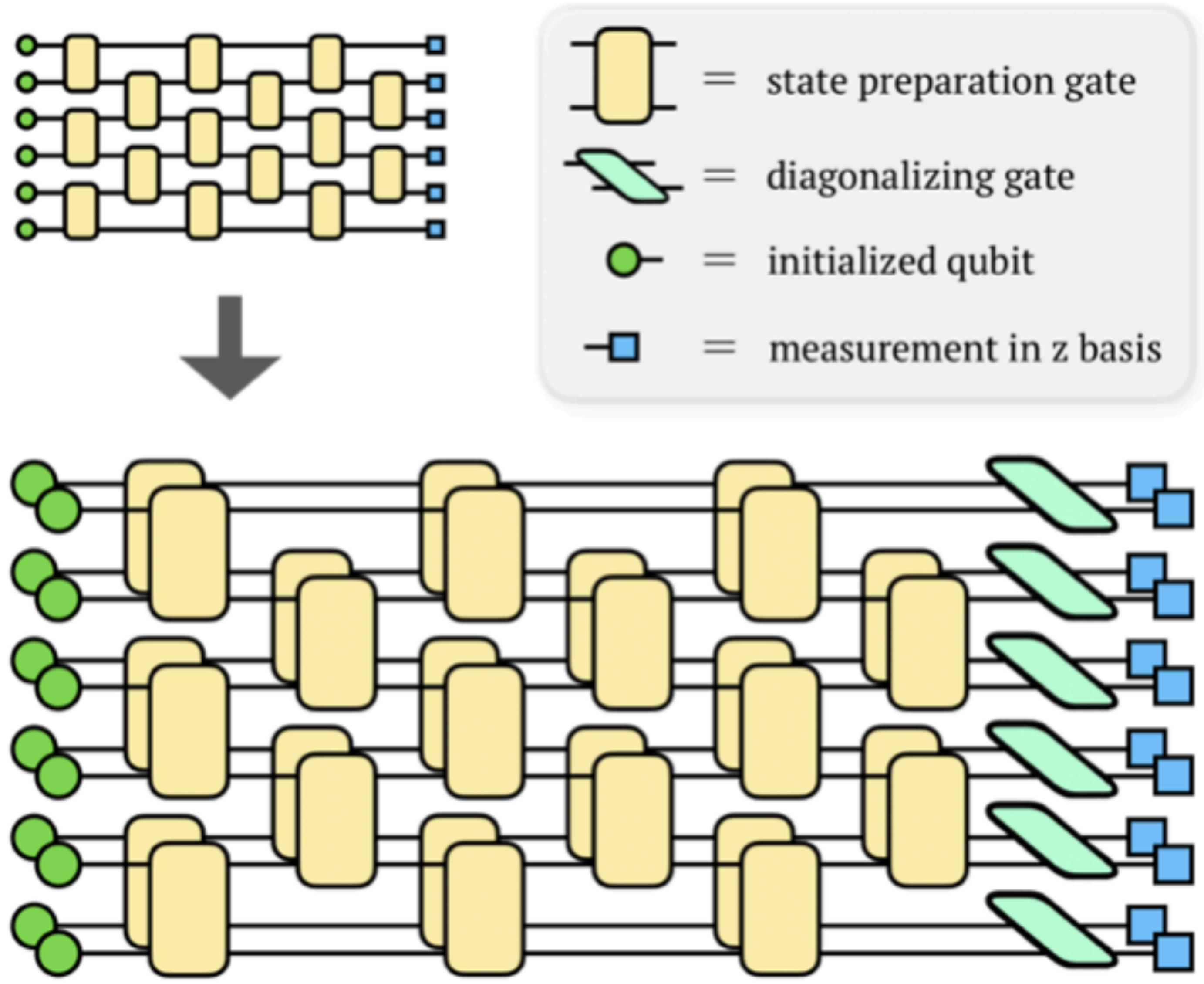
[Phys. Rev. Applied 16, 054035 (2021)]



Quantum error mitigation

Virtual distillation for quantum error mitigation

[Phys. Rev. X 11, 041036 (2021)]



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Calculating the nonlinear functions of quantum state

Let ρ be a quantum state with rank r.

Suppose there exist $\epsilon > 0$ and a slowly-growing function C (as a function of m) such that $g : \mathbb{R} \to \mathbb{R}$ is approximated by a degree m polynomial $f(x) = \sum_{k=0}^{m} c_k x^k$ on the interval $[0,1]$, in the sense that $\sup_{x \in [0,1]} |g(x) - f(x)| < \frac{\epsilon}{2r}$, and $\sum_{k=0}^{m} |c_k| < C$.

Calculating the nonlinear functions of quantum state

Then estimating Tr$(g(\rho))$ within an ϵ additive error and with a success probability of at least $1-\delta$, where $\delta \in (0,1)$ requires

Calculating the nonlinear functions of quantum state

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$\mathcal{O}\left(\frac{T^2C^2r^2}{\epsilon^2}\ln^2 r \ln\left(\frac{1}{\delta}\right)\right)$ copies of ρ and

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Ours: $\mathcal{O}\left(\frac{T^2C^2r^2}{\epsilon^2}\ln^2 r\ln\left(\frac{1}{\delta}\right)\right)$ copies of ρ and $\mathcal{O}\left(\frac{T^2C^2r}{\epsilon^2}\ln^2 r\ln\left(\frac{1}{\delta}\right)\right)$ runs on a circuit consisted of $\mathcal{O}(1)$ depth, $\mathcal{O}(r)$ qubits and $\mathcal{O}(r)$ CSWAP operations.

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When $g(x) = e^{\beta x}$, C becomes $e^{|\beta|}$. We can efficiently estimate $\mathrm{Tr}(e^{\beta\rho})$ which has applications in thermodynamics and the density exponentiation algorithm.

Applications

Nonlinear functions

Computation of the **partition function** and other **thermodynamical** variables for the systems with finite energy levels and finite # of non interacting particles

e.g.

$$g(x) = e^{\beta x},\ \beta \in \mathbb{R}$$

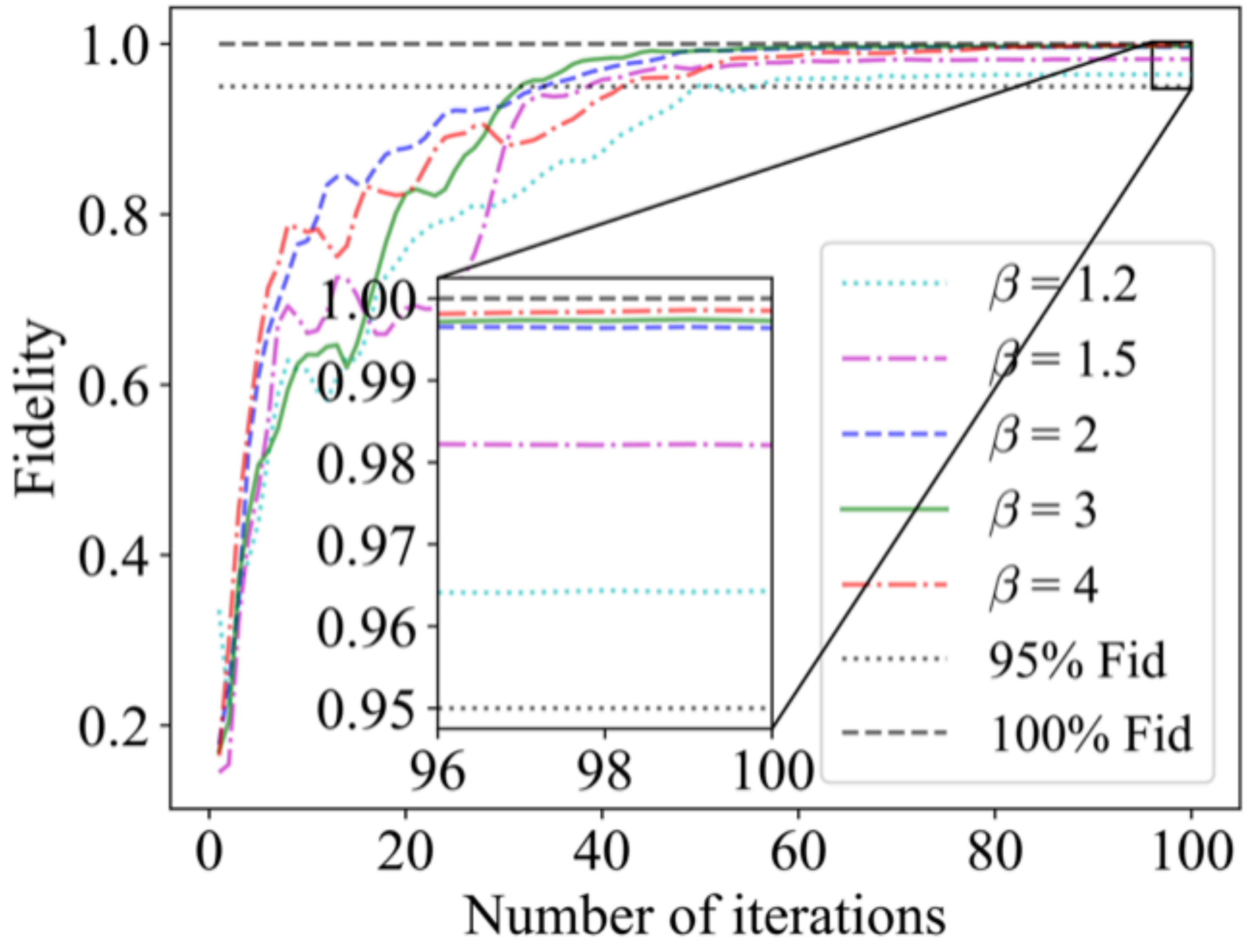
$$g(x) = (1+x)^{\alpha},\ \alpha \in \mathbb{R}^{+}$$

and more

Quantum Gibbs states

Variational quantum Gibbs state preparation with a **truncated Taylor series**

[Phys. Rev. Applied 16, 054035 (2021)]



Quantum error mitigation

Virtual distillation for quantum error mitigation

[Phys. Rev. X 11, 041036 (2021)]

Quantum Gibbs state preparation

The truncated Taylor series $S_k(\rho) = \sum_{i=1}^{k} \mathrm{Tr}\left(\left(\rho - I\right)^k \rho\right)$

is used as the **cost function for variational quantum Gibbs state preparation.**

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The truncated Taylor series $S_k(\rho) = \sum_{i=1}^{k} \mathrm{Tr}\left(\left(\rho - I\right)^k \rho\right)$

is used as the **cost function for variational quantum Gibbs state preparation.**

It is shown that the fidelity $F\left(\rho(\theta_0), \rho_G\right)$ between the optimized state $\rho(\theta_0)$ and the Gibbs state ρ_G is bounded by $F(\rho(\theta_0), \rho_G) \geq 1 - \sqrt{2\left(\beta\epsilon + \frac{2r}{k+1}(1-\Delta)^{k+1}\right)}$

where β is the inverse temperature of the system,

and Δ is a constant that satisfies $-\Delta \ln(\Delta) < \frac{1}{k+1}(1-\Delta)^{k+1}$.

Quantum Gibbs state preparation

By using the inequality $D(\rho(\theta_0), \rho_G) < \sqrt{1 - F\left(\rho\left(\theta_0\right), \rho_G\right)}$, to achieve

$T\left(\rho(\theta_0), \rho_G\right) < \epsilon$, we need to set $k = \mathcal{O}\left(\,\cdot\,\right)$, where T is the trace distance.

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Ours: $k = \mathcal{O}\left(r\right)$ qubits and CSWAP operations are needed.

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Previous: $k = \mathcal{O}\left(\frac{r}{\epsilon^4}\right)$ qubits and CSWAP operations are needed.

Significantly reduces the number of qubits and CSWAP operations.

* Independent of the desired error bound ϵ.

Ours: $k = \mathcal{O}(r)$ qubits and CSWAP operations are needed.

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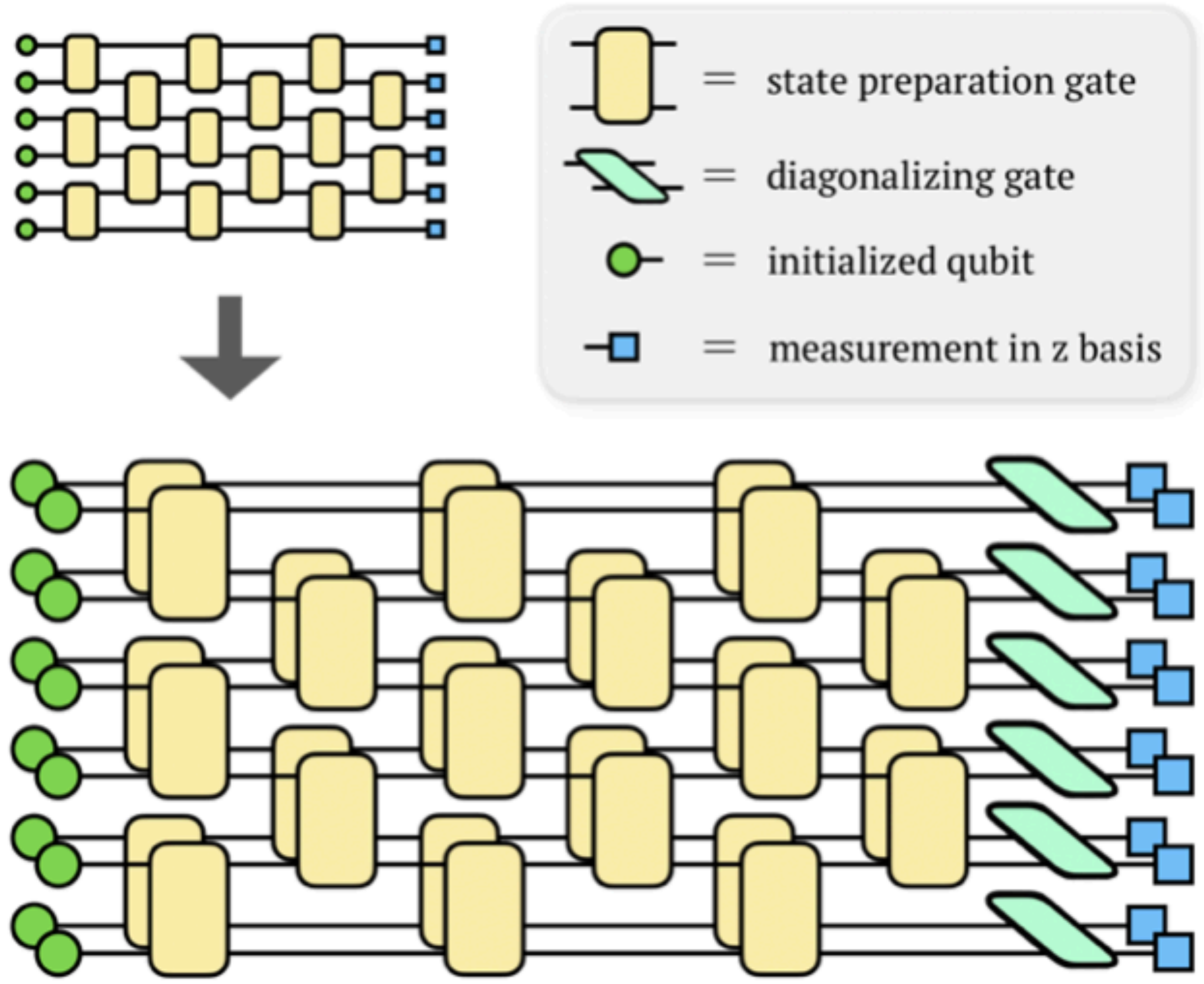

Quantum error mitigation

The expected value of a Hermitian operator M is given by $\langle M \rangle = \mathrm{Tr}(M |\psi\rangle\langle\psi|)$.

Due to noise, this value becomes $\langle M \rangle_{\text{noise}} = \mathrm{Tr}(M\rho) \neq \langle M \rangle$.

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Virtual distillation protocol offers a method to address this issue.

The protocol involves using collective measurements of k copies of the mixed state ρ to suppress incoherent errors.

This approach approximates the error-free expectation value $\langle M \rangle_{\text{vd}}^{(k)} = \dfrac{\mathrm{Tr}(M\rho^k)}{\mathrm{Tr}(\rho^k)}$,

where k denotes the number of copies used.

Quantum error mitigation

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$$\langle M \rangle_{\mathrm{vd}}^{(k)} = \frac{\mathrm{Tr}(M\rho^k)}{\mathrm{Tr}(\rho^k)}$$

Corollary 1

To estimate $\mathrm{Tr}(\rho^i)$ for all $i \leq k$ within an additive error of ϵ and with a success probability of at least $1 - \delta$, where $\delta \in (0,1)$, it is necessary to estimate each $\mathrm{Tr}(\rho^j)$ for $j \leq r$ within an additive error of ε_j, as defined in **Theorem 1.** This can be achieved by using

$$\mathcal{O}\left(\frac{T^2}{\epsilon^2} \ln^2 r \ln\left(\frac{1}{\delta}\right)\right)$$

runs on a constant-depth quantum circuit consisting of $\mathcal{O}(j)$ qubits and $\mathcal{O}(j)$ CSWAP operations. Here, T is defined in **Theorem 1.**

Quantum error mitigation

$$\langle M \rangle^{(k)}_{\text{vd}} = \frac{\mathrm{Tr}(M\rho^k)}{\mathrm{Tr}(\rho^k)}$$

Corollary 2

Suppose there is an efficient decomposition $M = \sum_{\ell=1}^{N_M} a_\ell P_\ell$, where $a_\ell \in \mathbb{R}$ and $P_\ell = \sigma_{\ell_1} \otimes \cdots \otimes \sigma_{\ell_n}$ are tensor products of Pauli operators $\sigma_{\ell_1}, \ldots, \sigma_{\ell_n} \in \{\sigma_x, \sigma_y, \sigma_z, I\}$. The quantity $\sum_{\ell=1}^{N_M} |a_\ell| = \mathcal{O}(c)$ is bounded by a constant c.

To estimate $\mathrm{Tr}(M\rho^i)$ for all $i \leq k$ within an additive error of ϵ and with a success probability of at least $1-\delta$, where $\delta \in (0,1)$, it is necessary to estimate each $\mathrm{Tr}(M\rho^j)$ for $j \leq r$ within an additive error of $\varepsilon_{j,M}$.

This can be achieved by using $\mathcal{O}\left(\frac{c^2 N_M}{\epsilon^2} \ln\left(\frac{1}{\delta}\right)\right)$ runs on a constant-depth quantum circuit consisting of $\mathcal{O}(j)$ qubits and $\mathcal{O}(j)$ CSWAP operations, and estimating each $\mathrm{Tr}(\rho^{j'})$ for $j' \leq r$ within an additive error of $\varepsilon_{j'}$, by using $\mathcal{O}\left(\frac{T^2}{\epsilon^2} \ln^2 r \ln\left(\frac{1}{\delta}\right)\right)$ runs on a constant-depth quantum circuit consisting of $\mathcal{O}(j')$ qubits and $\mathcal{O}(j')$ CSWAP operations. Here, $\varepsilon_{j,M}$, $\varepsilon_{j'}$ and T are defined in **Theorem 2.**

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runs on a constant-depth quantum circuit consisting of $\mathcal{O}(j)$ qubits and $\mathcal{O}(j)$ CSWAP operations. Here, T is defined in **Theorem 1.**

Overview

- Trace of powers & Literature review
- Mathematical intuitions
- Main results: algorithm, lemmas, theorems, corollaries
- Numerical simulations
- Computational hardness of $\mathrm{TsallisQED}_q$ and $\mathrm{TsallisQEA}_q$
- Applications
- **Concluding remarks**

Concluding remarks

- Our main contribution lies in proving that the **error increases linearly at most** when applying the Newton-Girard method with a recursive strategy.
- We also generalize the result to traces of powers with observables M, which are represented as $\mathrm{Tr}(M\rho^k)$.
- Our work can enhance any previous algorithms, including $\mathrm{Tr}(\rho^k)$ and/or $\mathrm{Tr}(M\rho^k)$.
- We can estimate the trace of powers with $\mathcal{O}(1)$-depth, $\mathcal{O}(r)$-width, and only $\mathcal{O}(r)$ -CSWAP operations.
- Our method also provides advantages in copy complexity when estimating the trace of large powers **with low-rank states or sufficiently mixed states.**

Future work

- It remains open for future work to find more applications that can take advantage of our work.
- Generalizing this result to multivariate trace estimation, or even Tr$(\rho^k \sigma^l)$, can open up more possibilities, such as calculating functions that satisfy the data-processing inequality under unital quantum channels, which can be an alternative tool for distance measures.
- Tightening the bounds on Theorems 1 and 2 is an interesting future research topic.
- **More algorithms for low-rank quantum states.**

Thank you for listening!

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