#### On estimating the trace of quantum state powers

Yupan Liu<sup>1</sup> Qisheng Wang<sup>2,1</sup>

<sup>1</sup>Graduate School of Mathematics, Nagoya University

<sup>2</sup>School of Informatics, University of Edinburgh

To appear in SODA 2025. Available on arXiv soon.

SEAS, Harvard University, October 2024

- 2 Main results: Upper and lower bounds
- **③** Proof techniques: Uniform polynomial approximation and QJT<sub>q</sub>-based reductions
- Open problems

# What is quantum state testing

#### Task: Quantum state testing

Given two quantum devices  $Q_0$  and  $Q_1$  that prepare *n*-qubit quantum states  $\rho_0 \in \mathbb{C}^{N \times N}$ and  $\rho_1 \in \mathbb{C}^{N \times N}$ , respectively. Decide whether  $\operatorname{dist}(\rho_0, \rho_1) \leq \varepsilon_1$  or  $\operatorname{dist}(\rho_0, \rho_1) \geq \varepsilon_2$ .

Three types of access to quantum devices  $Q_b$  for  $b \in \{0,1\}$  are considered:

- **Sample access**: Receive copies of the state  $\rho_b$  from the device  $Q_b$ .
- Query access:  $Q_b$  denotes the state-preparation circuit of the state  $\rho_b$ :
  - $\diamond$  **Black-box model**.  $Q_b$  is given as a black box (oracle).
  - $\diamond$  White-box model. The (gate-based) description of  $Q_b$  is provided.

Type of access	Complexity measure	
Sample access	ss Sample complexity (the number of copies	
Query access (black-box)	Query complexity (the number of queries)	
Query access (white-box)	Complexity class	

Typical goal. Minimize the	"complexity" of $\rho_b$	(or its corresponding	$Q_b$ ) for $b \in \{$	$\{0,1\}$ :
----------------------------	--------------------------	-----------------------	------------------------	-------------

In this talk: We focus on query access, primarily the white-box model (i.e., a promise problem), while addressing all three types of access in our work.

### Quantum state testing: Hard and easy examples

Quantum state testing is *hard* in general, with complexity (linearly) depending on the dimension N (or rank r), through some distance-like measures make these task *easy*.

Hard examples. Quantum state testing with respect to von Neumann entropy:

- ▶ QUANTUM ENTROPY DIFFERENCE (QED):  $S(\rho_0) S(\rho_1)$  is  $\geq 1/2$  or  $\leq -1/2$ .
  - ◊ [Ben Aroya-Schwartz-Ta-Shma'08] QED is QSZK-complete.
- ▶ QUANTUM ENTROPY APPROXIMATION (QEA).  $S(\rho)$  is  $\geq t(n) + 1/2$  or  $\leq t(n) 1/2$ .
  - ◊ [BASTS08, Chailloux-Ciocan-Kerenidis-Vadhan'08] QEA is NIQSZK-complete.
  - ♦ [Bun-Kothari-Thaler'18] Query complexity lower bound for QED and QEA is  $\Omega(\sqrt{N})$ .

**Easy example.** PURITY ESTIMATION: Decide whether  $Tr(\rho^2)$  is  $\geq 2/3$  or  $\leq 1/3$ .

- ► [Buhurman-Cleve-Watrous-de Wolf'01] Query complexity for approximating  $Tr(\rho^2)$  to within additive error  $\varepsilon$  is  $O(1/\varepsilon)$ , with BQP containment in the white-box setting.
- ► [Ekert-Alves-Oi-Horodecki-Horodecki-Lwek'02] The same bound and the BQP containment apply for estimating Tr(ρ<sup>q</sup>) for integer q > 1.
- These examples raise questions on estimating the trace of quantum state powers:
  - **()** Is there an efficient quantum algorithm for estimating  $Tr(\rho^q)$  for *non-integer* q > 1?
  - **2** Is estimating the trace of quantum state powers, e.g.,  $Tr(\rho^2)$ , BQP-*complete*?

# Quantum state testing with respect to quantum q-Tsallis entropy

Quantum q-Tsallis entropy: power quantum entropy of order q

$$S_q(\rho) = \frac{1 - \text{Tr}(\rho^q)}{q - 1} = -\text{Tr}(\rho^q \ln_q(\rho)), \text{ where } \ln_q(x) \coloneqq \frac{1 - x^{1 - q}}{q - 1}.$$

As  $q \to 1$ , the von Neumman entropy is recovered:  $S_q(\rho) = S(\rho)$  and  $\ln_q(x) = \ln(x)$ .

Tsallis entropy has been independently rediscovered several times: [Havrda-Charváť67, Daróczy'70, Tsallis'88], with the quantum version introduced in [Raggio'95].

#### Quantum state testing with respect to quantum Tsallis entropy:

- ▶ QUANTUM *q*-TSALLIS ENTROPY DIFFERENCE (TSALLISQED*q*): Decide whether  $S_q(\rho_0) - S_q(\rho_1) \ge 0.001$  or  $S_q(\rho_0) - S_q(\rho_1) \le -0.001$ .
- ► QUANTUM *q*-TSALLIS ENTROPY APPROXIMATION (TSALLISQEA<sub>*q*</sub>): Decide whether  $S_q(\rho) \ge t(n) + 0.001$  or  $S_q(\rho) \le t(n) - 0.001$ .

#### Why investigate $S_q(\rho)$ for non-integer q?

• Since  $S_q(\rho) \le S(\rho)$ ,  $S_{q=1+\varepsilon}(\rho)$  serves as a reasonable lower bound for  $S(\rho)$ . "Hardness of approximating von Neumann entropy"?

Ø H<sub>q=3/2</sub>(p) captures systems where both frequent and rare events matter. Meanwhile, estimating S<sub>q</sub>(ρ) for non-integer 1 < q < 2 seems to be challenging:</p>

- $\diamond H_{q=2}(p)$ , also known as *Gini impurity*, is very sensitive to rare events.
- Examples in fluid dynamics: modeling velocity changes in turbulent flows [Beck'02].

- 2 Main results: Upper and lower bounds
- 3 Proof techniques: Uniform polynomial approximation and QJT<sub>q</sub>-based reductions
- Open problems

# Main result (upper bounds): Quantum estimator for q-Tsallis entropy

**Theorem 1** (Quantum estimator for *q*-Tsallis entropy).

Given quantum query access to the state-preparation circuit Q of an *n*-qubit state  $\rho$ , for any  $q \ge 1 + \Omega(1)$ , there exists a quantum algorithm that estimates  $S_q(\rho)$  to within additive error  $\varepsilon$  with query complexity  $O(1/\varepsilon^{1+\frac{1}{q-1}}) = \text{poly}(1/\varepsilon)$ .

► If the description of the state-preparation circuit is of size L(n), the time complexity is  $O(L/\varepsilon^{1+\frac{1}{q-1}}) = poly(n, 1/\varepsilon)$ .

 $\diamond$  As a corollary, for any  $q \ge 1 + \Omega(1)$ , TSALLISQED<sub>q</sub> and TSALLISQEA<sub>q</sub> are in BQP.

Using the samplizer [Wang-Zhang'24], allowing a quantum query-to-sample simulation, the sample complexity required to estimate S<sub>q</sub>(ρ) is Õ(1/ε<sup>3+ <sup>2</sup>/<sub>q-1</sub></sup>).

Prior works have complexity depending on the dimension  $N = 2^n$  or the rank *r* of  $\rho$ :

- 1 Dimension dependence: [Acharya-Issa-Shende-Wagner'19].
- 2 Rank dependence: [Wang-Guan-Liu-Zhang-Ying'22, Wang-Zhang-Li'22, Wang-Zhang'24].

#### Main results (lower bounds): Hardness for TSALLISQED<sub>q</sub> and TSALLISQEA<sub>q</sub>

Let CONSTRANKTSALLISQED<sub>q</sub> and CONSTRANKTSALLISQEA<sub>q</sub> be restricted variants of TSALLISQED<sub>q</sub> and TSALLISQEA<sub>q</sub>, respectively, where the rank of the state(s) is  $\leq O(1)$ .

**Theorem 2** (Computational hardness for TSALLISQED<sub>q</sub> and TSALLISQEA<sub>q</sub>).

The promise problems TSALLISQED<sub>q</sub> and TSALLISQEA<sub>q</sub> capture the computational power of respective complexity classes, depending on the regime of q:

**• Easy regimes**. For  $q \in [1,2]$ , CONSTRANKTSALLISQED<sub>q</sub> and CONSTRANKTSALLISQEA<sub>q</sub> are BQP-hard. The following corollaries holds:

- ◊ For 1 + Ω(1) ≤ q ≤ 2, TSALLISQED<sub>q</sub> and TSALLISQEA<sub>q</sub> are BQP-complete.
- ♦ PURITY ESTIMATION is BQP-complete.
- **@ Hard regimes.** For  $q \in (1, 1 + \frac{1}{n-1}]$ , TSALLISQED<sub>q</sub> is QSZK-hard under Karp reduction, and consequently, TSALLISQEA<sub>q</sub> is QSZK-hard under Turing reduction. For  $q = 1 + \frac{1}{n-1}$ , TSALLISQEA<sub>q</sub> is NIQSZK-hard under Karp reduction.

Our reductions for the hard regimes also leads to query and sample complexity lower bounds for estimating  $S_q(\rho)$  to within additive error  $\varepsilon$ :

The regime of $q$	Query complexity	Sample complexity
$q \geq 1 + \Omega(1)$	$\Omega(1/\sqrt{\epsilon})$	$\Omega(1/arepsilon)$
$1 < q \le 1 + \tfrac{1}{n-1}$	$\Omega(r^{1/3})$	$\Omega(r^{2/3})$

# Summary: "Hardness of approximating von Neumann entropy"

Quick summary for estimating  $S_q(\rho)$  for q = 1 (von Neumann entropy) and q > 1:

	q = 1	$1 < q \leq 1 + \tfrac{1}{n-1}$	$1 + \Omega(1) \leq q \leq 2$	q > 2
TsallisQED <sub>q</sub>	QSZK-complete	QSZK-hard	BQP-complete	in BQP
	[BASTS08]	Theorem 2(2)	Theorem 1 & Theorem 2(1)	Theorem 1
TSALLISQEAq	NIQSZK-complete	NIQSZK-hard*	BQP-complete	in BQP
	[BASTS08,CCKV08]	Theorem 2(2)	Theorem 1 & Theorem 2(1)	Theorem 1

A sharp phase transition occurs between the case of q = 1 and constant q > 1.

#### Why is the regime $q \ge 1 + \Omega(1)$ computationally easy?

Let's focus on PURITY ESTIMATION (q = 2). Let  $\{\lambda_k\}_{k \in [2^n]}$  be eigenvalues of an *n*-qubit state  $\rho$ . For any state  $\hat{\rho}$  having eigenvalues at most 1/n, we have  $\operatorname{Tr}(\hat{\rho}^2) = \sum_k \lambda_k^2 \leq 1/n$ . Hence, *zero* serves as a good estimate of  $\operatorname{Tr}(\hat{\rho}^2)$  to within additive error 1/3.

**4** Only (sufficiently) large eigenvalues contribute to the estimate of  $Tr(\rho^2)$ !

**Q**: How to estimate  $\sum_{k \in \mathcal{I}_{large}} \lambda^2$ , where  $\mathcal{I}_{large}$  is the index set of large eigenvalues  $\lambda_k$ ?

For integer  $q \ge 2$ , SWAP test-like techniques [BCWdW01,EAO+02] provide a solution.

For non-integer  $q \ge 1 + \Omega(1)$ , our result (Theorem 1) solves the problem.

2 Main results: Upper and lower bounds

**8** Proof techniques: Uniform polynomial approximation and QJT<sub>q</sub>-based reductions

Open problems

# BQP containment for the regime $q \ge 1 + \Omega(1)$

We begin with a procedure that accepts with probability  $\frac{1}{2}(1 + \text{Tr}(\rho U_{f(\rho)}))$ , utilizing the Hadamard test [Kitaev'95, Aharonov-Jones-Landau'06]:



- ►  $U_{f(\rho)}$  is an *approximate* unitary block-encoding of  $f(\rho) = \rho^{q-1}$ , constructed from the state-preparation circuit *Q* and implemented using quantum singular value transformation [Gilyén-Su-Low-Wiebe'19], with an appropriate polynomial approximation  $P_d(x)$  of  $f(x) = x^{q-1}$ .
- This approach has been applied to estimate fidelity [Gilyén-Poremba'22], trace distance [Wang-Zhang'23, Le Gall-L.-Wang'23], and von Neumann entropy [Le Gall-L.-Wang'23, Wang-Zhang'24].
- The acceptance probability of this procedure can be further *boosted*, to say at least 2/3 for *yes* instances, through quantum amplitude estimation.

## BQP containment (Cont.): Removing the rank dependence

**Rank dependence in prior works.** Prior works based on this approach require time (or query) complexity that depends at least *linearly* on the rank. Specifically,

$$\begin{split} |\mathrm{Tr}(
ho f(oldsymbol{
ho}) - \mathrm{Tr}(
ho P_d(
ho))| &\leq \sum_{0\leq\lambda_j<\delta} \left|\lambda_j f(\lambda_j) - \lambda_j P_d(\lambda_j)\right| + \sum_{\lambda_j\geq\delta} \left|\lambda_j f(\lambda_j) - \lambda_j P_d(\lambda_j)\right| \ &\leq r\cdot\mathrm{poly}(\delta) + O(arepsilon). \end{split}$$

To ensure that the last line is bounded by  $O(\varepsilon)$ ,  $\delta$  must be *sufficiently small*, e.g., 1/poly(r), introducing rank dependence. The target function f(x) is approximated by a polynomial  $P_d(x)$  of degree  $d = O(\frac{1}{\delta} \log \frac{1}{\varepsilon})$  such that

$$\max_{x \in [\delta,1]} |P_d(x) - f(x)| \le \varepsilon \quad \text{and} \quad \max_{x \in [-1,1]} |P(x)| \le 1.$$

**Removing the rank dependence.** Instead, we need a polynomial that *uniformly* approximates f(x). The best uniform (polynomial) approximation of  $x^q$  was investigated in [Bernstein'38], with a non-constructive proof in [Timan'63], satisfies:

$$\max_{x\in[0,1]} \left| P^*_{d'}(x) - x^q \right| \to 1/d'^q, \quad \text{ as } d' \to \infty.$$

The remaining challenge is to make the coefficients of  $P_{d'}^*(x)$  efficiently computable. This can be achieved using the asymptotically best uniform (polynomial) approximation  $\widehat{P}_{d}(x)$ , particularly via Chebyshev truncation and the de La Vallée Poussin partial sum:

$$\max_{x\in[0,1]} \left|\widehat{P}_{\hat{d}}(x) - x^q/2\right| \leq \varepsilon \quad \text{and} \quad \max_{x\in[-1,1]} |P(x)| \leq 1, \quad \text{where } \hat{d} = O(1/\varepsilon^{1/q}).$$

# Hardness results via QJT<sub>q</sub>-based reductions

The key quantity underlying our proof is the quantum q-Jensen-(Shannon-)Tsallis divergence, as defined in [Briët-Harremoës'09]:

$$\mathsf{QJT}_{\boldsymbol{q}}(\boldsymbol{\rho}_0,\boldsymbol{\rho}_1) \coloneqq \frac{1}{2} \big( \mathsf{S}_{\boldsymbol{q}}(\boldsymbol{\rho}_0) + \mathsf{S}_{\boldsymbol{q}}(\boldsymbol{\rho}_1) \big) - \mathsf{S}_{\boldsymbol{q}} \Big( \frac{\boldsymbol{\rho}_0 + \boldsymbol{\rho}_1}{2} \Big).$$

Specifically, we focus on reductions from restricted versions of quantum state testing with respect to the trace distance (QSD), particularly decide whether  $T(\rho_0, \rho_1)$  is at least  $1 - \varepsilon(n)$  or at most  $\varepsilon(n)$ , to TSALLISQED<sub>q</sub> or TSALLISQEA<sub>q</sub>:

Problem	Regime of $q$	Reduction from	New inequalities
ConstRank- TsallisQED <sub>q</sub>	$1 \le q \le 2$	PUREQSD is BQP-hard [RASW23]	$H_{q}\left(\tfrac{1}{2}\right)\!-\!H_{q}\!\left(\tfrac{1-T}{2}\right) \leq QJT_{q} \leq H_{q}\!\left(\tfrac{1}{2}\right)\!T^{q}$
TSALLISQEDq	$1\!\leq\!q\!\leq\!1\!+\!\tfrac{1}{n\!-\!1}$	QSD is QSZK-hard [Wat02, Wat09]	$\mathbf{H}_{q}\left(\frac{1}{2}\right) - \mathbf{H}_{q}\left(\frac{1-\mathrm{T}}{2}\right) \leq QJT_{q}$
TSALLISQEA <sub>q</sub>	$q = 1 + \frac{1}{n-1}$	QSCMM is NIQSZK-hard [Kob03, BASTS10, CCKV08]	$\left(1\!-\!\mathbf{T}\!-\!\frac{1}{2^n}\right)\ln_q(2^n)\leq\mathbf{S}_q\leq\ln_q(2^n(1\!-\!\mathbf{T}))$

Our upper bound for Tsallis binary entropy is also crucial:  $H_q(x) \le H_q(\frac{1}{2})\sqrt{x(1-x)}$ .

# Hardness results via QJT<sub>q</sub>-based reductions (Cont.)

**Proof Sketch** (New Inequalities between  $QJT_q$  and T). We follow the approach for proving the inequalities for QJS from [Briët-Harremoës'09]. The key step is to establish the data-processing inequality  $QJT_q(\Phi(\rho_0), \Phi(\rho_1)) \leq QJT_q(\rho_0, \rho_1)$  for  $1 \leq q \leq 2$ :

- ► For q = 1 (QJS), this follows from  $QJS(\rho_0, \rho_1) = \frac{1}{2} \left( D(\rho_0 \| \frac{\rho_0 + \rho_1}{2}) + D(\rho_1 \| \frac{\rho_0 + \rho_1}{2}) \right)$ .
- For  $1 < q \le 2$ , we need the joint convexity for  $QJT_q$  [Chen-Tropp'14, Virosztek'17]:

$$\mathsf{QJT}_q\big((1-\lambda)\rho_0 + \lambda\rho_0', (1-\lambda)\rho_1 + \lambda\rho_1'\big) \leq (1-\lambda)\mathsf{QJT}_q\big(\rho_0,\rho_1\big) + \lambda\mathsf{QJT}_q\big(\rho_0',\rho_1'\big).$$

**Proof Sketch** (Reductions from variants of QSD to (CONSTRANK)TSALLISQED<sub>q</sub>). **Pure-state reductions** are inspired by [L.'23], namely QJT<sub>q</sub> can be viewed as a distance version of  $S_q(\rho_0) - S_q(\rho_1)$  for  $1 \le q \le 2$ . Consider the following states

$$\begin{split} \rho_0' &:= (p_0 | 0 \rangle \langle 0 | + p_1 | 1 \rangle \langle 1 |) \otimes \frac{1}{2} (| \psi_0 \rangle \langle \psi_0 | + | \psi_1 \rangle \langle \psi_1 |), \\ \rho_1' &:= \frac{1}{2} | 0 \rangle \langle 0 | \otimes | \psi_0 \rangle \langle \psi_0 | + \frac{1}{2} | 1 \rangle \langle 1 | \otimes | \psi_1 \rangle \langle \psi_1 |. \end{split}$$

Using the pseudo-additivity and the joint entropy theorem for  $S_q$ , we obtain

$$\mathbf{S}_q(\boldsymbol{\rho}_0') - \mathbf{S}_q(\boldsymbol{\rho}_1') = (1 - (q - 1)\mathbf{H}_q(p_0)) \cdot \mathsf{QJT}_q(|\boldsymbol{\psi}_0\rangle \langle \boldsymbol{\psi}_0|, |\boldsymbol{\psi}_1\rangle \langle \boldsymbol{\psi}_1|) + \mathbf{H}_q(p_0) - \mathbf{H}_q(\frac{1}{2}).$$

By choosing a suitable  $p_0 \in (0, 1/2)$ , the bounds for  $S_q(\rho'_0) - S_q(\rho'_1)$  follow from the inequalities between  $QJT_q$  and the trace distance.

**② Mixed-state reductions**, inspired by [BASTS'08], are a bit more complicated. The upper bound for  $S_q(\rho'_0) - S_q(\rho'_1)$  now needs the Fannes' inequality for  $QJT_q$  [Zhang'07]:

$$\forall q > 1, \quad \left| S_q(\rho_0) - S_q(\rho_1) \right| \le T(\rho_0, \rho_1)^q \cdot \ln_q(2^n - 1) + H_q(T(\rho_0, \rho_1)).$$

- 2 Main results: Upper and lower bounds
- **③** Proof techniques: Uniform polynomial approximation and QJT<sub>q</sub>-based reductions
- Open problems

# Conclusions and open problems

#### Take-home messages on our work

● For the regime q ≥ 1 + Ω(1), estimating the quantum Tsallis entropy S<sub>q</sub>(ρ), equivalently the trace of quantum state powers, is computationally *easy* and has query or sample complexity that is *independent* of the rank of the state. This provides an efficiently computable lower bound for the von Neumann entropy!

Ø For the regime 1 < q ≤ 1 +  $\frac{1}{n-1}$ , estimating the quantum Tsallis entropy S<sub>q</sub>(ρ) is computationally *hard*:

- $\diamond~$  The white-box problems cannot be solved efficiently unless BQP = QSZK;
- $\diamond~$  The rank dependence in query or sample complexity is unavoidable in black-box settings.

This can be interpreted as "hardness of approximating the von Neumann entropy".

#### Open problems

- Are there more applications for estimating quantum *q*-Tsallis entropy S<sub>q</sub>(ρ) in the regime 1 < q < 2, which has previously been challenging to compute?</p>
- **②** Can we improve query and sample complexity bounds for the regime  $q \ge 1 + \Omega(1)$ ?
- **(a)** What are the computational complexity and hardness for estimating  $S_q(\rho)$  for the regime 0 < q < 1? Can we show that TSALLISQED<sub>q</sub> (or TSALLISQEA<sub>q</sub>) for the regime  $1 < q < 1 + \frac{1}{n-1}$  is contained in QSZK (or NIQSZK)?

# Thanks!