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Estimating quantum relative entropies on quantum computers

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Quantum relative entropy serves as a fundamental measure of the distinguishability between quantum states and plays a pivotal role in quantum information science. Despite its importance, efficiently estimating quantum relative entropy between two quantum states on quantum computers remains a significant challenge. In this work, we propose a quantum algorithm for directly estimating quantum relative entropy and Petz Rényi divergence from two unknown quantum states on quantum computers. The circuit size of our algorithm is at most $2n + 1$ with n being the number of qubits in the quantum states and it is directly applicable to distributed scenarios, where quantum states to be compared are hosted on cross-platform devices. We validate the effectiveness of our method through numerical experiments and observe the absence of the barren plateau phenomenon. As an application, we employ our algorithm to investigate the superadditivity of quantum channel capacity. Numerical simulations reveal new examples of qubit channels exhibiting strict superadditivity of coherent information, highlighting the potential of quantum machine learning to address quantum-native problems.

Relative entropy, also known as the Kullback-Leibler (KL) divergence¹, quantifies the difference between a model probability distribution and the true distribution. It is a fundamental concept in classical information theory and has widespread applications across various fields. For example, KL divergence serves as a standard loss function in machine learning², including in Boltzmann Machines³, which were recognized with the 2024 Nobel Prize in Physics for their foundational impact. Additionally, it is used to assess the efficiency of data compression schemes^{4,5} and to measure deviations from thermodynamic equilibrium in statistical mechanics^{6,7}. Building on advances in quantum information science, several quantum generalizations of KL divergence have been developed to quantify the distinguishability between quantum states^{8–11}. Moreover, the formulations introduced by Umegaki⁸ and Petz¹² are particularly important due to their operational relevance in a wide range of quantum information processing tasks^{11,13–17}. These measures are widely used in quantum machine learning¹⁸, quantum channel coding^{19–21}, quantum error correction²², quantum resource theories²³, and quantum cryptography²⁴.

Despite its broad utility, efficiently estimating quantum relative entropy remains challenging: classical approaches require density-matrix reconstruction via quantum state tomography with exponentially many measurements^{25,26}, followed by manipulation of exponentially large matrices. Direct estimation on quantum computers offers a promising and potentially more efficient alternative, but the nonlinear nature of quantum relative entropy makes this approach difficult. Estimating quantum

entropies and divergences is a central problem in quantum information science and has attracted significant recent attention^{27–30}. Existing approaches can be broadly categorized into two classes, as summarized in Supplementary Table S1 of the Supplementary Note 1. The first class relies on the “purified quantum query access” model within the framework of quantum singular value transformation (QSVT)^{27,31–33}. The second class employs variational quantum algorithms (VQAs), which are well suited for problems that are difficult to solve exactly^{28,30,34–36}. Related works and other approaches are summarized in “Related works” section of the Supplementary Note 1. However, all current methods fail to estimate quantum relative entropy and Petz–Rényi divergences from unknown quantum states due to various inherent limitations.

In this work, we develop a variational quantum algorithm for directly estimating quantum relative entropy and Petz–Rényi divergence between two unknown quantum states on quantum computers, addressing open problems highlighted in refs. 27,30. An overview of our method is provided in Fig. 1. Our approach combines quadrature approximations, the variational representation of quantum f -divergences, and a parameterization of Hermitian polynomial operators, leading to a scalable framework with circuit size at most $2n + 1$ for n -qubit states. The algorithm is naturally suited to distributed settings, which is particularly relevant for cross-platform quantum verification^{37–41}. We prove that the associated loss function is operator-convex, ensuring a well-behaved optimization landscape. Numerical simulations demonstrate reliable trainability with simple

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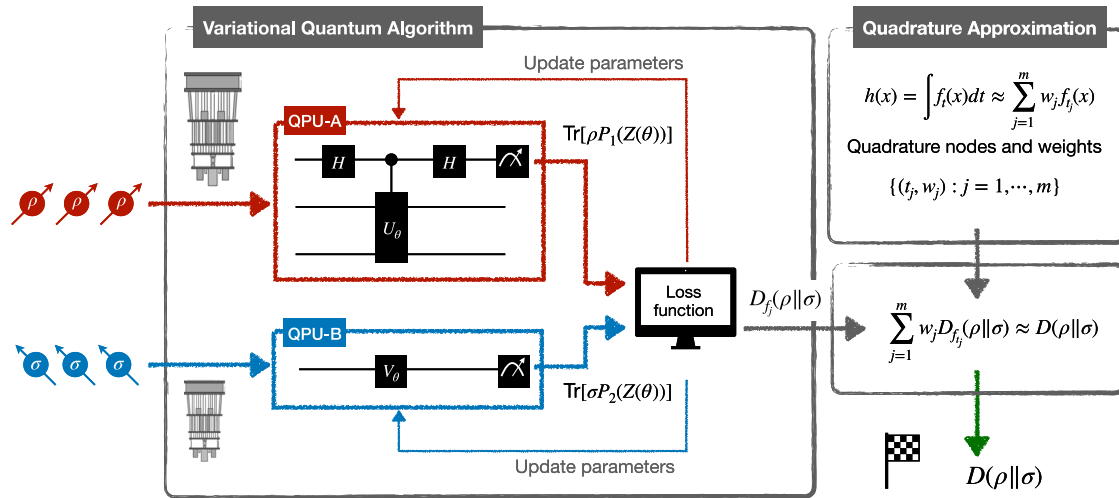


Fig. 1 | Estimating quantum relative entropy using a variational quantum algorithm. Identical copies of quantum states ρ and σ , possibly hosted on different quantum computers (QPU-A in red and QPU-B in blue), are processed through parameterized quantum circuits to extract relevant information. The variational

algorithm estimates quantum f -divergences $D_{f_j}(\rho||\sigma)$, and the quantum relative entropy $D(\rho||\sigma)$ is computed as a weighted average of these f -divergences, determined by the quadrature nodes t_j and weights w_j . The estimation of Petz–Rényi divergence follows a similar procedure.

optimizers, accurate estimates, and the absence of barren plateaus^{42,43}. As an application, we employ our algorithm to investigate the superadditivity of quantum channel capacity and discover new qubit channels exhibiting strict superadditivity of coherent information. Compared with approaches based on classical neural networks and optimization^{44–46}, our method leverages quantum systems directly, highlighting the potential of quantum machine learning for quantum-native problems.

Results

A quantum state is a positive semidefinite operator with unit trace, denoted by ρ and σ . We write $\text{supp}(\rho)$ and $\text{supp}(\sigma)$ for their supports. Logarithms with base 2 are denoted by $\log$, while natural logarithms (base e) are denoted by $\ln$. The set of integers $\{1, 2, \dots, p\}$ is abbreviated as $[p]$. Estimated values are distinguished by a hat, such as $\hat{x}$. Throughout this work, these notations are adopted consistently.

Variational expression of quantum relative entropies

In this section, we introduce the standard quantum f -divergence and present its variational expression for a specific class of f_j -divergences. We then derive variational forms for the quantum relative entropy and Petz–Rényi divergence, utilizing the Gauss–Radau–Jacobi (GRJ) quadrature approximation. The GRJ quadrature method efficiently approximates integrals with weight functions of the form $(1-t)^a(1+t)^b$ by discretizing the integral into a weighted sum over carefully selected quadrature nodes. By exploiting the linearity of the standard quantum f -divergence in f , we reformulate the integral representations of quantum relative entropy and Petz–Rényi divergence as sums of f_j -divergences. This approach enables these quantities to be efficiently estimated within the variational framework later.

Standard quantum f -divergence. The definition of standard quantum f -divergence is as follows^{12,47}.

Definition 1. (Standard quantum f -divergence) Let ρ, σ be positive semidefinite operators on a finite-dimensional Hilbert space $\mathcal{H}$ with spectral decompositions $\rho = \sum_j \eta_j P_j$ and $\sigma = \sum_k \mu_k Q_k$. The standard quantum f -divergence is defined by

$$D_f(\rho||\sigma) := \sum_{j:\eta_j>0} \sum_{k:\mu_k>0} \eta_j f(\mu_k^{-1} \eta_j) \text{Tr}[P_j Q_k] + f(0^+) \text{Tr}[\rho(I - \sigma^0)], \quad (1)$$

where σ^0 denotes the projector onto the support of σ and $f(0^+)$ denotes the right-hand limit of $f(x)$ as $x \rightarrow 0$.

For quantum states ρ and σ with $\text{supp}(\rho) \subseteq \text{supp}(\sigma)$, the second term in Eq. (1) vanishes since $\text{Tr}[\rho(I - \sigma^0)] = 0$. When we set the function f in the definition above as

$$f_t(x) := \frac{x-1}{t(x-1)+1} \text{ for } t \in [0, 1], \quad (2)$$

its corresponding standard divergence $D_{f_t}(\rho||\sigma)$ has the following variational expression.

Lemma 2. (⁴⁸) Let ρ and σ be positive semidefinite operators on a finite-dimensional Hilbert space $\mathcal{H}$ and $t \in (0, 1]$. Then we have

$$D_{f_t}(\rho||\sigma) = \inf_Z \frac{1}{t} \{ \text{Tr}[\rho] + \text{Tr}[\rho(Z + Z^\dagger)] + (1-t) \text{Tr}[\rho Z^\dagger Z] + t \text{Tr}[\sigma Z Z^\dagger] \}, \quad (3)$$

where the infimum on the right-hand side is taken over all bounded linear operators Z on $\mathcal{H}$.

It is important to note that the variational expression in Lemma 2 does not apply at $t = 0$. However, in this boundary case, the value can be directly computed from the definition of the standard quantum f -divergence (Eq. (1)), which gives $D_{f_0}(\rho||\sigma) = \text{Tr}[\rho^0 \sigma] - 1$. For the remainder of this paper, we assume $\text{supp}(\rho) = \text{supp}(\sigma)$ for simplicity, which is the typical scenario of practical interest since noise is ubiquitous in realistic settings. In this case, we have $D_{f_0}(\rho||\sigma) = 0$.

Quantum relative entropy. Let ρ and σ be two quantum states. Their quantum relative entropy is defined as⁸

$$D(\rho||\sigma) := \text{Tr}[\rho(\log \rho - \log \sigma)], \quad (4)$$

if $\text{supp}(\rho) \subseteq \text{supp}(\sigma)$ and $+\infty$ otherwise. In particular, let $f(x) = -\log(x)$. The corresponding standard quantum f -divergence simplifies to the quantum relative entropy,

$$D_{-\log}(\rho||\sigma) = D(\rho||\sigma). \quad (5)$$

With the integral representation of logarithm, $\ln(x) = \int_0^1 f_t(x) dt$, we can approximate the logarithm using GRJ quadrature as follows⁴⁸, Theorem 3.8,

$$\log(x) \approx r_m(x) := \frac{1}{\ln 2} \sum_{j=1}^m w_j f_{t_j}(x), \quad (6)$$

where $\{t_j\}_{j=1}^m$ is the set of GRJ quadrature nodes with a fixed node $t_1 = 0$ or $t_m = 1$, and $\{w_j\}_{j=1}^m$ are corresponding weights. The quadrature approximation for $\log x$ is shown in the Supplementary Fig. S1a, which converges to the exact value as the number of quadrature nodes m increases. Combining Eqs. (5) and (6), we obtain the approximation of quantum relative entropy as follows:

$$D(\rho \parallel \sigma) \approx D_{-r_m}(\rho \parallel \sigma) = - \sum_{j=1}^m \frac{w_j}{\ln 2} D_{f_{t_j}}(\rho \parallel \sigma), \quad (7)$$

where each $D_{f_{t_j}}(\rho \parallel \sigma)$ on the right-hand side can be evaluated using the variational expression provided in Lemma 2.

Petz-Rényi divergence. Let ρ and σ be two quantum states. The Petz-Rényi divergence is defined as¹²

$$D_\alpha(\rho \parallel \sigma) := \frac{1}{\alpha - 1} \log Q_\alpha(\rho \parallel \sigma), \quad (8)$$

if $\alpha < 1$ and $\rho \not\perp \sigma$ or $\text{supp}(\rho) \subseteq \text{supp}(\sigma)$. It is defined as $+\infty$ otherwise. Here $Q_\alpha(\rho \parallel \sigma) := \text{Tr}[\rho^\alpha \sigma^{1-\alpha}]$ is the quasi-relative entropy, and we focus on $\alpha \in (0, 1) \cup (1, 2]$ which is the range of particular interest. Let $f(x) = x^{1-\alpha}$. The corresponding standard quantum f -divergence reduces to

$$D_{x^{1-\alpha}}(\rho \parallel \sigma) = Q_\alpha(\rho \parallel \sigma). \quad (9)$$

To implement the quadrature approximation, an integral representation for the power function is required, which is provided by the Löwner's Theorem⁴⁹, for $\alpha \in (0, 1) \cup (1, 2)$,

$$x^{1-\alpha} - 1 = \frac{\sin(\alpha\pi)}{\pi} \int_0^1 f_t(x) t^{\alpha-1} (1-t)^{1-\alpha} dt. \quad (10)$$

The integral on the right-hand side can be approximated via GRJ quadratures by⁵⁰, Theorem 1 or⁵¹, Proposition 3.12,

$$\sum_{j=1}^m w_j^1 f_{t_j^1}(x) \leq \int_0^1 f_t(x) t^{\alpha-1} (1-t)^{1-\alpha} dt \leq \sum_{j=1}^m w_j^0 f_{t_j^0}(x). \quad (11)$$

Here, $\{t_j^0\}_{j=1}^m$ and $\{w_j^0\}_{j=1}^m$ denote the nodes and weights of the GRJ quadrature with a fixed node at $t_1^0 = 0$, while $\{t_j^1\}_{j=1}^m$ and $\{w_j^1\}_{j=1}^m$ correspond to the nodes and weights with a fixed node at $t_m^1 = 1$. As $m \rightarrow \infty$, both the lower and upper bounds converge to the exact value of the integral. Thus, the integral in Eq. (11) can be approximated using either bound. For simplicity, we omit the superscripts in the following discussion.

Combining Eqs. (10) and (11), we have

$$x^{1-\alpha} \approx h_m(x) := 1 + \frac{\sin(\alpha\pi)}{\pi} \sum_{j=1}^m w_j f_{t_j}(x). \quad (12)$$

The performance of this quadrature approximation is shown in the Supplementary Fig. S1b, where we take $\alpha = 1.5$ as an example. As given in Eq. (9), we have the approximation to $Q_\alpha(\rho \parallel \sigma)$ by

$$Q_\alpha(\rho \parallel \sigma) \approx D_{h_m}(\rho \parallel \sigma) = 1 + \frac{\sin(\alpha\pi)}{\pi} \sum_{j=1}^m w_j D_{f_{t_j}}(\rho \parallel \sigma), \quad (13)$$

where each $D_{f_{t_j}}(\rho \parallel \sigma)$ on the right-hand side can be evaluated using the variational expression provided in Lemma 2.

In the case of $\alpha = 2$, we can consider $t = 1$ and the standard quantum f -divergence gives $Q_2(\rho \parallel \sigma) = 1 - D_{f_1}(\rho \parallel \sigma)$ and $D_2(\rho \parallel \sigma) = \log Q_2(\rho \parallel \sigma)$, Remark 3.6.

Estimating standard f_t -divergence with quantum computers

The variational expression introduced in the previous section is a special case of the following general optimization problem:

$$\inf_{\{Z_1, \dots, Z_N\}} \{ \text{Tr}[\rho P(Z_1, \dots, Z_N)] + \text{Tr}[\sigma Q(Z_1, \dots, Z_N)] \}, \quad (14)$$

where $\{Z_1, Z_2, \dots, Z_N\}$ is a set of linear operators, and P and Q are Hermitian polynomials satisfying $P^\dagger = P$ and $Q^\dagger = Q$. In this work, we present a method for parameterizing the polynomial observables P and Q by singular value decomposition, along with a sampling procedure for estimating $\text{Tr}[\rho P]$ and $\text{Tr}[\sigma Q]$ that is well-suited for implementation on quantum computers. See “Parameterization of Hermitian polynomial operators” subsection in the Methods for details. We apply this method to estimate the standard f_t -divergence via Eq. (3). The evaluation procedure involves parameterizing the linear operator Z , estimating the individual terms $\text{Tr}[\rho(Z + Z^\dagger)]$, $\text{Tr}[\rho Z^\dagger Z]$, and $\text{Tr}[\sigma Z Z^\dagger]$, and finally optimizing the loss function. The detailed steps are as follows.

The first step is to parameterize the linear operator Z with singular value decomposition, i.e., $Z = U\Lambda V$, where U and V are two unitary operators, Λ is non-negative real diagonal matrix. We choose a set of basis $\{|i\rangle\}_{i=1}^d$ and parameterize Λ as $\sum_{i=1}^d \lambda_i |i\rangle\langle i|$, where $\lambda_i \geq 0$ and $\lambda_i \in \mathbb{R}$ for all i . All parameters λ_i are collectively represented as λ . Then the unitaries U and V are represented by two parameterized quantum circuit $U(\theta)$ and $V(\beta)$ with parameters $\theta \in \mathbb{R}^q$ and $\beta \in \mathbb{R}^r$. For the sake of simplicity, we denote $U(\theta)$ as U_θ and $V(\beta)$ as V_β . Then the linear operator Z is then parameterized as

$$Z = \sum_{i=1}^d \lambda_i U_\theta |i\rangle\langle i| V_\beta. \quad (15)$$

Note that the contribution of each term in Eq. (3) depends on how the linear operator Z acts within the support of ρ and σ . In practice, when the quantum states are not full-rank, i.e., $\text{rank}(\rho) = \text{rank}(\sigma) = s$, we can restrict Z to an at most s -dimensional subspace without affecting the value of the optimization problem. Any contribution from Z outside the support of ρ and σ does not affect the traces involving ρ and σ . Thus, to ensure the efficiency, we can parameterize Λ with a sparse diagonal matrix that only contains at most s nonzero elements, i.e., $\Lambda = \sum_{k=1}^s \lambda_{i_k} |i_k\rangle\langle i_k|$, where $i_k \in [d]$.

With the above parameterization, we obtain

$$\text{Tr}[\rho Z^\dagger Z] = \sum_{i=1}^d \lambda_i^2 \text{Tr}[\rho V_\beta^\dagger |i\rangle\langle i| V_\beta], \quad (16)$$

$$\text{Tr}[\sigma Z Z^\dagger] = \sum_{i=1}^d \lambda_i^2 \text{Tr}[\sigma U_\theta |i\rangle\langle i| U_\theta^\dagger], \quad (17)$$

$$\begin{aligned} \text{Tr}[\rho(Z + Z^\dagger)] &= 4 \sum_{i=1}^d \lambda_i \text{Tr}[(|0\rangle\langle 0| \otimes I) \\ &\quad \cdot \chi(|0\rangle\langle 0| \otimes \rho \otimes |i\rangle\langle i|) \chi^\dagger] - 2, \end{aligned} \quad (18)$$

where χ is a unitary operation constructed according to the quantum circuit shown in Fig. 2. Then each individual term above can be estimated on quantum computers.

More specifically, denote the probability distributions as

$$p_\beta^{(i)} := \text{Tr}[V_\beta \rho V_\beta^\dagger |i\rangle\langle i|], \quad (19a)$$

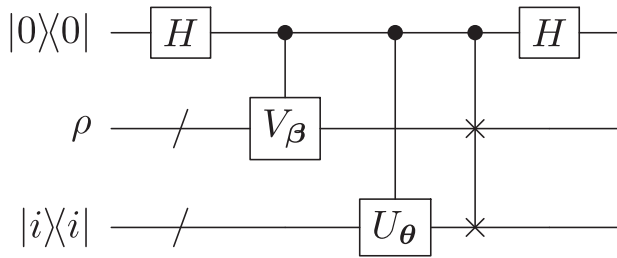


Fig. 2 | Visualization of unitary operation χ . It consists of two Hadamard gates H , controlled U_θ , V_β gates, and a controlled swap gate.

$$p_\theta^{(i)} := \text{Tr}[U_\theta^\dagger \sigma U_\theta |i\rangle\langle i|], \quad (19b)$$

$$p_\chi^{(i)} := \text{Tr}[|0\rangle\langle 0| \otimes I \chi |0\rangle\langle 0| \otimes \rho \otimes |i\rangle\langle i| \chi^\dagger]. \quad (19c)$$

Then, $p_\beta^{(i)}$ can be estimated by evolving the quantum state ρ using V_β and performing measurements in the computational basis. The same procedure applies to $p_\theta^{(i)}$. Finally, $p_\chi^{(i)}$ can be estimated by evolving the initial state $|0\rangle\langle 0| \otimes \rho \otimes |i\rangle\langle i|$ with the unitary χ and measuring the first qubit in the computational basis. With these sampling results, we can obtain from classical computations that

$$\text{Tr}[\rho Z^\dagger Z] = \sum_{i=1}^d \lambda_i^2 p_\beta^{(i)}, \quad (20)$$

$$\text{Tr}[\sigma Z Z^\dagger] = \sum_{i=1}^d \lambda_i^2 p_\theta^{(i)}, \quad (21)$$

$$\text{Tr}[\rho(Z + Z^\dagger)] = 4 \sum_{i=1}^d \lambda_i p_\chi^{(i)} - 2. \quad (22)$$

We are now well-prepared to introduce our variational quantum algorithms.

Variational quantum algorithms

Based on the method provided in previous section, we can estimate $D_{f_i}(\rho \parallel \sigma)$ by solving the optimization problem defined in Eq. (3), where we define the loss function as follows:

$$\mathcal{L}(\lambda, \theta, \beta) := \sum_{i=1}^d \left\{ t \lambda_i^2 p_\theta^{(i)} + (1-t) \lambda_i^2 p_\beta^{(i)} + \lambda_i (4 p_\chi^{(i)} - 2) \right\}, \quad (23)$$

The optimization problem is thus $\hat{\mathcal{L}} = \min_{\lambda, \theta, \beta} \mathcal{L}(\lambda, \theta, \beta)$, and the approximation value of $D_{f_i}(\rho \parallel \sigma)$ is $\hat{D}_{f_i}(\rho \parallel \sigma) = \frac{1}{t} (1 + \hat{\mathcal{L}})$. Since the loss function is quadratic with respect to each λ_i we can write the solution of λ_i as follows:

$$\lambda_i^{\text{opt}} = \max \left\{ 0, \frac{1 - 2 p_\chi^{(i)}}{t p_\theta^{(i)} + (1-t) p_\beta^{(i)}} \right\}, \quad (24)$$

and the optimization problem is simplified as

$$\hat{\mathcal{L}} = \min_{\theta, \beta} \mathcal{L}(\lambda^{\text{opt}}, \theta, \beta). \quad (25)$$

We utilize the gradient descent algorithm to optimize the loss function defined by Eq. (23), which requires the gradients of the loss function with respect to each parameter. The values of $p_\theta^{(i)}$, $p_\beta^{(i)}$, and $p_\chi^{(i)}$ are estimated by

sampling on quantum computers. The quantum circuit parameters θ and β are updated with respect to the parameter-shift rule⁵². The algorithm for estimating D_{f_i} is shown in Algorithm 1.

Algorithm 1. Variational quantum algorithm for estimating standard f_i -divergence

Input:

K	number of iterations
ℓ_r	learning rate
N	number of samples
t	function parameter
ρ, σ	quantum states with the same support

Output:

$\hat{D}_{f_i}(\rho \parallel \sigma)$ estimate of $D_{f_i}(\rho \parallel \sigma)$

$\theta^1 \leftarrow$ Random initialization in $[0, 2\pi]^q$.

$\beta^1 \leftarrow$ Random initialization in $[0, 2\pi]^r$.

if $t = 0$ **then**

return $\hat{D}_{f_0}(\rho \parallel \sigma) \leftarrow 0$.

end

foreach $k \in \{1, 2, \dots, K\}$ **do**

 Sample N times to evaluate $p_\theta^{(i)}$, $p_\beta^{(i)}$ and $p_\chi^{(i)}$
 for $i = 1, \dots, d$, with θ^k and β^k on quantum computers.

 Compute λ^{opt} with Eq. (24).

 Sample N times to evaluate $\nabla_\theta \mathcal{L}$ and $\nabla_\beta \mathcal{L}$
 using the parameter shift rule.

$\theta^{k+1} \leftarrow \theta^k + \ell_r \nabla_\theta \mathcal{L}$

$\beta^{k+1} \leftarrow \beta^k + \ell_r \nabla_\beta \mathcal{L}$

end

$\hat{\mathcal{L}} \leftarrow \mathcal{L}(\theta^{K+1}, \beta^{K+1})$.

return $\hat{D}_{f_i}(\rho \parallel \sigma) \leftarrow (1 + \hat{\mathcal{L}})/t$

Based on the algorithm for estimating $D_{f_i}(\rho \parallel \sigma)$ presented in Algorithm 1, we can approximate the quantum relative entropy and Petz-Rényi divergence by iterating over the quadrature nodes. The idea is to solve the optimization problem Eq. (25) for m times to get the estimates of $D_{f_{i_j}}(\rho \parallel \sigma)$ for $j \in \{1, \dots, m\}$, and then obtain the estimation value of $D_{-r_m}(\rho \parallel \sigma)$ with Eq. (7) and $D_{h_m}(\rho \parallel \sigma)$ with Eq. (13). The approximations are thus given by $\hat{D}(\rho \parallel \sigma) \approx \hat{D}_{-r_m}(\rho \parallel \sigma)$ and $\hat{D}_\alpha(\rho \parallel \sigma) \approx \frac{1}{\alpha-1} \log D_{h_m}(\rho \parallel \sigma)$. In the case of $\alpha = 2$, the approximation is directly obtained by the estimation of $D_{f_1}(\rho \parallel \sigma)$, i.e., $\hat{D}_2(\rho \parallel \sigma) \approx \log(1 - D_{f_1}(\rho \parallel \sigma))$. Further details are provided in Supplementary Note 3.

It is worth noting that the only step requiring quantum computers is obtaining the sampling results $p_\theta^{(i)}$, $p_\beta^{(i)}$ and $p_\chi^{(i)}$. All other computations can be performed on classical computers. Furthermore, the quantum sampling procedure is naturally suited to distributed scenarios. Specifically, according to Eq. (19), the probability distributions $p_\theta^{(i)}$ and $p_\beta^{(i)}$ can be sampled on a quantum computer preparing the state ρ , while $p_\chi^{(i)}$ can be obtained on a quantum computer preparing σ . This enables the comparison of quantum data generated by distributed quantum devices, making the approach directly applicable to cross-platform verification and related distributed quantum information tasks^{37–40}.

Numerical simulations

In this section, we present numerical simulations to validate the effectiveness of our variational algorithms via the PennyLane package⁵³. We begin by outlining our methodology and parameter settings, followed by a discussion of the simulation results.

Numerical setup. We consider scenarios where the input states are one-qubit and two-qubit mixed states. For this, we use the interface `qml.QubitStateVector` from PennyLane to generate two pure quantum

states $|\rho\rangle_{RS}$ and $|\sigma\rangle_{RS}$. These states effectively produce two mixed states on the marginal system S , that is, $\rho_S = \text{Tr}_R[|\rho\rangle\langle\rho|]$ and $\sigma_S = \text{Tr}_R[|\sigma\rangle\langle\sigma|]$.

Our ansatz is shown in Fig. 3. For one-qubit cases, we set U_θ and V_β as the general single-qubit rotation gate U_3 in Fig. 3a. For two-qubit cases, we set U_θ and V_β as the ansatz in Fig. 3b with different parameters. We use 4 layers of the two-qubit ansatz. To evaluate the gradient of the parameters in the parameterized quantum circuit, we utilize the function `qml.gradient-s.param_shift` in PennyLane.

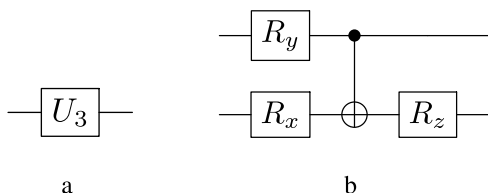


Fig. 3 | Visualization of a single layer of our ansatz. **a** Single-qubit cases: the ansatz is a general single-qubit rotation gate U_3 ; **b** Two-qubit cases: the ansatz is constructed with three single-qubit rotation gates R_x , R_y , and R_z around each axis and a CNOT gate that generates entanglement.

Table 1 | Numerical results that compares exact values with their estimated values

Relative entropies		Exact value	Quadrature approx.	Estimated value	Relative error
1-qubit cases	$D(\rho\ \sigma)$	0.2470	0.2470	0.2455	0.59%
	$D_{1.5}(\rho\ \sigma)$	0.3381	0.3381	0.3314	2.01%
	$D_2(\rho\ \sigma)$	0.4073	\	0.4096	0.56%
2-qubit cases	$D(\rho\ \sigma)$	0.6585	0.6585	0.6514	1.07%
	$D_{1.5}(\rho\ \sigma)$	0.9308	0.9308	0.9244	0.70%
	$D_2(\rho\ \sigma)$	1.1430	\	1.1377	0.46%

We estimate the values in Eq. (19) with sample means. The number of samples is set to be 10,000. The number of quadrature nodes m is taken at 6. The learning rate ℓ_r and the number of iterations K depend on specific situations. The choices of these parameters are empirical. In particular, if m is required to be large, a smaller learning rate ℓ_r and a larger number of iterations K are required to ensure the precision of estimation. An adaptive learning rate strategy for large m is shown in the “Training with adaptive learning rate” section of the Supplementary Note 7. The final loss is determined as the average of the loss values from the last 10 iterations.

Numerical results. The numerical results of our simulations are shown in Table 1. For one-qubit simulations, we set the iteration number K as 300; while for two-qubit simulations, we set K as 200. The loss over the first 100 iterations for a representative case is shown in Fig. 4. Additional results are provided in the Supplementary Note 6 “Additional numerical results”. For all the cases, we set the learning rate ℓ_r as 0.1. We choose $\alpha = 1.5$ as an example for Petz–Rényi divergence. We also note that the Petz-2 Rényi divergence $D_2(\rho\|\sigma)$ does not require a quadrature approximation, as it can be directly obtained from $D_{f_1}(\rho\|\sigma)$.

All exact and estimated values in the table are retained to four decimal places. It is easy to see that the quadrature approximations match the corresponding exact values to four decimal places and the relative errors of our estimated values are sufficiently small, most of which are within 1%.

Application in quantum channel capacity

As an application, we utilize our algorithm to explore the superadditivity of quantum channel capacity. It’s a famous phenomenon where the combined use of quantum channels exceeds the sum of their individual capacities. Specifically, we propose a variational approach to compute the quantum channel coherent information, employing our algorithm for quantum relative entropy as a subroutine. Numerical simulations uncover new examples of qubit channels exhibiting strict superadditivity of coherent information.

Theoretical framework. Quantum channels exhibit several fascinating properties that distinguish them from their classical counterparts. One such property is the ability to transmit information superadditively,

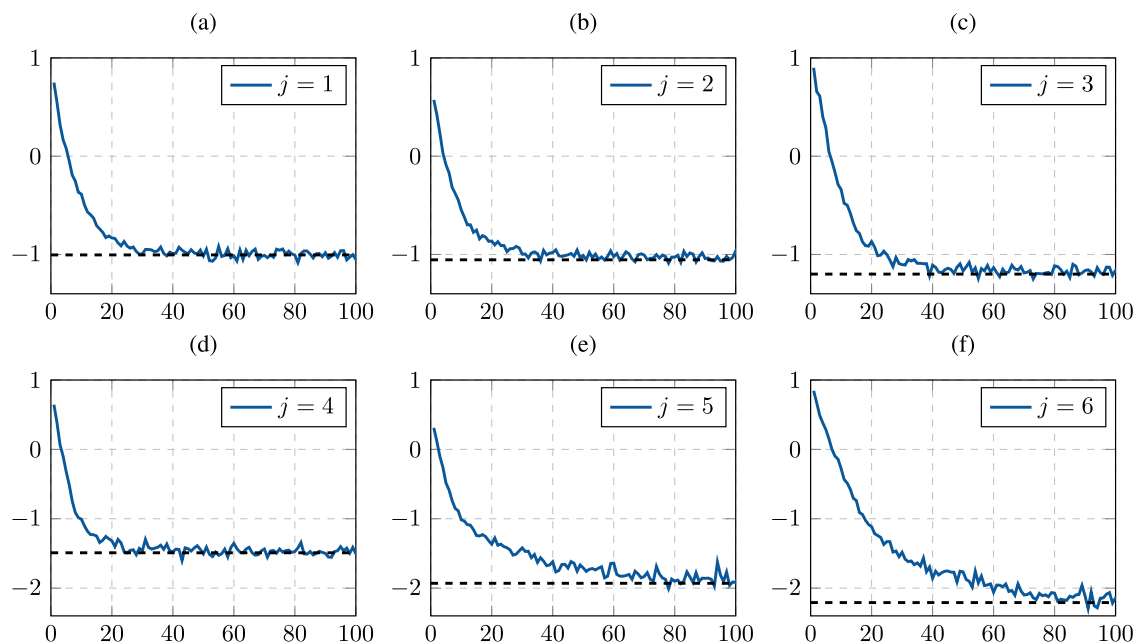
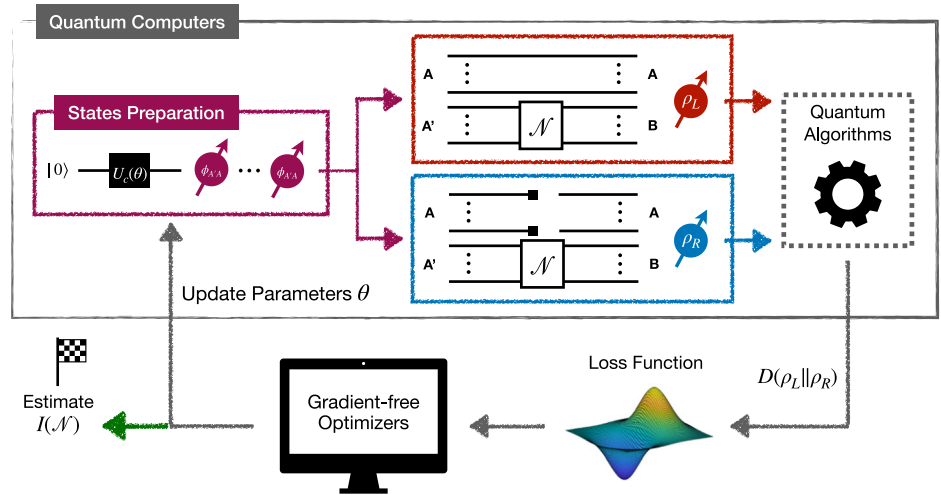


Fig. 4 | Two-qubit case of estimating $D(\rho\|\sigma)$. Each subplot from (a) to (f) corresponds to a different quadrature node, where j represents the index of the quadrature nodes $\{t_j\}_{j=1}^6$. The horizontal axis represents the number of iterations, and the

vertical axis gives the loss value. The dashed line indicates the exact loss value, while the blue line is the loss value during training.

Fig. 5 | Estimating channel coherent information within the variational framework. Using a parameterized quantum circuit $U_c(\theta)$ and the target quantum channel $\mathcal{N}$, we prepare the states ρ_L (in red) and ρ_R (in blue) and estimate their quantum relative entropy using our algorithm. The circuit parameters are then updated using a gradient-free optimizer. Once the optimization process is complete, $D(\rho_L\|\rho_R)$ is returned as an estimate of the channel coherent information $I(\mathcal{N})$.



where multiple uses of the same channel can increase the total amount of information that can be reliably transmitted. Let $I(AB)_\sigma := D(\sigma_{AB} \| I_A \otimes \text{Tr}_A(\sigma_{AB}))$ denote the coherent information of a quantum state σ_{AB} , where I_A is the identity operator. The well-known quantum capacity theorem^{54–56} states that the quantum capacity $Q(\mathcal{N})$ of a quantum channel is given by the regularized channel coherent information:

$$Q(\mathcal{N}) = \lim_{k \rightarrow \infty} \frac{1}{k} I(\mathcal{N}^{\otimes k}), \quad (26)$$

where

$$I(\mathcal{N}) \equiv \sup_{\phi_{AA'}} I(A)B_{\mathcal{N}_{A' \rightarrow B}(\phi_{AA'})} \quad (27)$$

is the channel coherent information, and the optimization is performed over all pure, bipartite quantum states $\phi_{AA'}$. Due to the superadditivity of channel coherent information, the limit in Eq. (26) is generally necessary.

An important question in quantum Shannon theory is to identify channels that exhibit strict superadditivity of coherent information, i.e., $I(\mathcal{N}^{\otimes n}) > nI(\mathcal{N})$. This phenomenon indicates that entangled channel coding or error correction strategies can outperform non-entangled ones, which has profound implications for quantum communication and quantum error correction. Existing studies have addressed this problem by classical neural networks and optimizations^{44–46}. In this work, we take a different approach and propose a variational quantum algorithm to estimate the quantum channel coherent information directly on quantum computers.

First of all, the quantum channel coherent information can be expressed as:

$$I(\mathcal{N}) = \sup_{\phi_{AA'}} I(A)B_\sigma = \sup_{\phi_{AA'}} D(\sigma_{AB} \| I_A \otimes \text{Tr}_A[\sigma_{AB}]), \quad (28)$$

where $\sigma_{AB} = \mathcal{N}_{A' \rightarrow B}(\phi_{AA'})$. Let $\mathcal{R}_A^I = \text{Tr}_A[\cdot] I_A$ represent the replacement channel on system A . Then, the channel coherent information can be rewritten as:

$$I(\mathcal{N}) = \sup_{\phi_{AA'}} D(\mathcal{N}_{A' \rightarrow B}(\phi_{AA'}) \| \mathcal{R}_A^I \otimes \mathcal{N}_{A' \rightarrow B}(\phi_{AA'})). \quad (29)$$

Using the quantum algorithm for estimating quantum relative entropy, we can solve the supremum optimization problem in Eq. (29) within a variational framework. As illustrated in Fig. 5, the process begins with the input state $|0\rangle$. A parameterized quantum circuit $U_c(\theta)$ is applied to prepare the state $|\phi(\theta)\rangle = U_c(\theta)|0\rangle$. The quantum channel $\mathcal{N}$ is then applied to

generate the states ρ_L and ρ_R defined as:

$$\begin{aligned} \rho_L &= \mathcal{N}_{A' \rightarrow B}(\phi(\theta)), \\ \rho_R &= \mathcal{R}_A^I \otimes \mathcal{N}_{A' \rightarrow B}(\phi(\theta)). \end{aligned} \quad (30)$$

The states ρ_L and ρ_R are used as inputs to the quantum algorithm for estimating quantum relative entropy. The parameters θ are updated iteratively using a gradient-free optimizer, such as a genetic algorithm. This is because the coherent information landscape is dominated by local maxima, making traditional optimization methods like gradient descent less effective⁴⁵. The genetic algorithm used here follows the approach in ref. 46. Once the optimization process converges, the algorithm outputs $D(\rho_L\|\rho_R)$ as an estimate of the channel coherent information $I(\mathcal{N})$.

Numerical experiments. We conduct numerical experiments to explore superadditive quantum channels. For this, we identify a quantum channel with a readily computable one-shot coherent information $I(\mathcal{N})$ and estimate its n -shot coherent information $I(\mathcal{N}^{\otimes n})$ using the method outlined previously. According to Eq. (44) in Methods, our estimate $\hat{I}(\mathcal{N}^{\otimes n})$ always serves as a lower bound for $I(\mathcal{N}^{\otimes n})$, i.e., $I(\mathcal{N}^{\otimes n}) \geq \hat{I}(\mathcal{N}^{\otimes n})$. This implies that if our estimated value $\hat{I}(\mathcal{N}^{\otimes n})$ is strictly greater than $nI(\mathcal{N})$, then superadditivity must exist, as $I(\mathcal{N}^{\otimes n}) \geq \hat{I}(\mathcal{N}^{\otimes n}) > nI(\mathcal{N})$.

In particular, we choose the set of three-parameter family of Pauli channels, defined as

$$\mathcal{P}(\rho) = p_0 \sigma_0 \rho \sigma_0 + p_1 \sigma_1 \rho \sigma_1 + p_2 \sigma_2 \rho \sigma_2 + p_3 \sigma_3 \rho \sigma_3, \quad (31)$$

where $p_i \geq 0$, $\sum_{i=0}^3 p_i = 1$, and $\{\sigma_i\}_{i=0}^3$ is the set of Pauli matrices. It is well known that the coherent information of a Pauli channel is^{57,58}

$$I(\mathcal{P}) = 1 + \sum_{i=0}^3 p_i \log p_i. \quad (32)$$

Set $n = 2$ and the loss function as

$$L(\mathbf{p}) = \frac{1}{2} D(\rho_L\|\rho_R) - I(\mathcal{P}), \quad (33)$$

where ρ_L and ρ_R are defined in Eq. (30), and $\mathbf{p} = (p_0, p_1, p_2, p_3)$. The superadditivity is evident when we observe $L(\mathbf{p}) > 0$.

We discretize the channel parameters $(p_1, p_2, p_3) \in [0, 0.2]^3$ with a step size of 0.01, resulting in a total of 8000 Pauli channels. To construct the parameterized quantum circuit $U_c(\theta)$, we use a 2-layer complex entangled ansatz, as shown in Fig. 6, with 4 input qubits. The initial parameters θ are randomly selected from the interval $[0, 2\pi]$. For optimization, we employ a

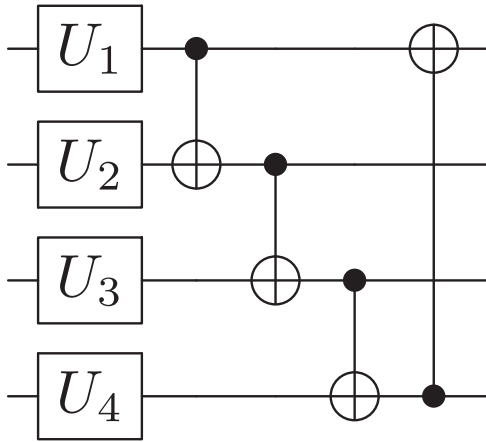


Fig. 6 | Complex entangled ansatz for $U_i(\theta)$. Each U_i ($i \in \{1, 2, 3, 4\}$) represents an arbitrary single-qubit rotation gate.

simple genetic algorithm, available in the *Global Optimization Toolbox* of MATLAB, as our gradient-free optimizer.

Out of the 8000 Pauli channels analyzed, our method identifies 69 channels exhibiting strict superadditivity. The largest superadditivity gap is approximately $\frac{1}{2}D(\rho_L \parallel \rho_R) - I(P) \approx 0.0078$, which matches the state-of-the-art gap found for Pauli channels⁴⁶. Supplementary Fig. S5 in the Supplementary Note 6 provides a visualization of these channels and their corresponding superadditivity values. This confirms the effectiveness of our method in identifying superadditive channels and showcases the potentials of quantum computers to address quantum-native problems.

Conclusions

We have proposed a variational quantum algorithm for directly estimating quantum relative entropy and Petz–Rényi divergence between two unknown quantum states on quantum computers, addressing open problems highlighted by Goldfeld et al.³⁰ and Wang et al.²⁷. The feasibility and effectiveness of this approach have been validated through theoretical analysis and numerical simulations.

Efficiently computing information-theoretic quantities such as quantum relative entropy and Petz–Rényi divergence on quantum hardware represents a significant step toward realizing the full potential of quantum technologies for scientific discovery. Our demonstration of the application of this method to a well-known problem in quantum Shannon theory highlights the potential of quantum machine learning to tackle quantum-native problems and paving the way for advancing quantum science through quantum computation.

In terms of hardware implementation, a notable feature of our algorithm is its applicability to distributed quantum computing scenarios, where the quantum states to be compared are hosted on cross-platform quantum devices. This capability opens up a wide range of potential applications. Furthermore, the circuit size of our algorithm closely matches the size of the quantum states being compared, making it feasible for immediate implementation on existing quantum hardware. We leave the exploration of quantum hardware experiments as a direction for future work.

Another direction for future research is to extend the class of quantum divergences that can be efficiently estimated. In this work, the function f_i in Eq. (2) is particularly useful because its connection to a resolvent representation enables a quadratic variational formulation. Within our current framework, different divergences can be estimated by modifying the measurement schemes and weighting in the quadrature approximation, without altering the underlying variational structure. More broadly, other quantum divergences may admit alternative variational characterizations with similar structural properties. However, such formulations are not yet known in general and might involve non-polynomial operator functions, which could lead to non-quadratic objectives. Discovering broader families of

divergences with similarly tractable variational characterizations remains an open problem for future work.

Complementary to the methodological extensions discussed above, we identify several numerical aspects that warrant further investigation. In particular, we observe that the proposed algorithm can become more sensitive when the number of quadrature nodes m is large, potentially leading to instability during optimization. To mitigate this issue, we employ an adaptive learning rate strategy that significantly improves convergence behavior in this regime, as detailed in “Training with adaptive learning rate” section of the Supplementary Note 7. Beyond this approach, it is natural to combine our variational framework with more advanced optimization techniques, such as natural-gradient methods or stochastic variance-reduced schemes, to further enhance robustness and scalability.

Methods

Parameterization of Hermitian polynomial operators

In this section, we present our general method for parameterizing the polynomial observables P and Q , along with a sampling procedure for estimating $\text{Tr}[\rho P]$ and $\text{Tr}[\sigma Q]$ that is well-suited for implementation on quantum computers.

Our method is based on the singular value decomposition and the extended SWAP test⁵⁹. Without loss of generality, we consider the p -th order term in the polynomial, which takes the form

$$\sum_{i \in [N]^p} a_i (Z_i + Z_i^\dagger) Z_i = \prod_{k=1}^p Z_{i_k}, \quad (34)$$

where $a_i \in \mathbb{R}$, $i := (i_1, i_2, \dots, i_p) \in [N]^p$ is an index-sequence of length p . For possible terms such as $Z_1 Z_1^\dagger$, it can be included by considering a polynomial $P(Z_1, Z_1^\dagger, \dots)$. To parameterize the polynomial $P(Z_1, \dots, Z_N)$ and estimate the value $\text{Tr}[\rho P]$, it suffices to parameterize the linear operator $\mathcal{Z}_i$ and then estimate the value $\text{Tr}[\rho(\mathcal{Z}_i + \mathcal{Z}_i^\dagger)]$. Detailed procedures are given as follows.

With singular value decomposition, a linear operator can be parameterized by

$$\mathcal{Z}_{i_k} = \sum_{j_k=1}^d \lambda_{k,j_k} U_{i_k} |j_k\rangle \langle j_k| V_{i_k}, \quad (35)$$

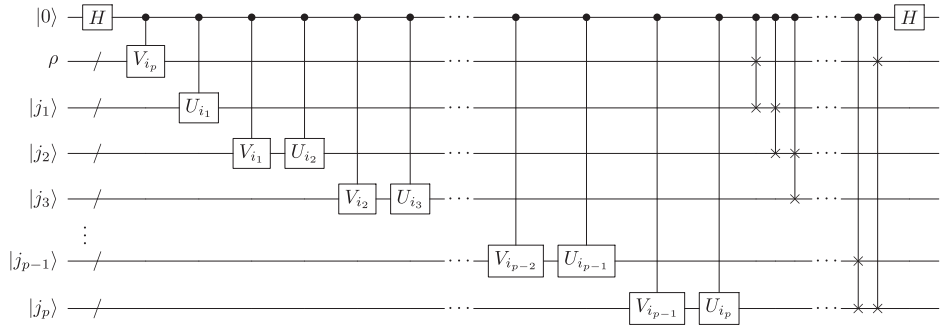
where $\lambda_{k,j_k} \geq 0$ and $\{|1\rangle, |2\rangle, \dots, |d\rangle\}$ denotes a set of computational basis. Then we have

$$\mathcal{Z}_i = \sum_{(j_1, \dots, j_p) \in [d]^p} \prod_{k=1}^p \lambda_{k,j_k} U_{i_k} |j_k\rangle \langle j_k| V_{i_k}. \quad (36)$$

We parameterize the unitaries U_{i_k} and V_{i_k} with a set of parameterized quantum circuits $U_{i_k}(\theta_{i_k})$ and $V_{i_k}(\beta_{i_k})$, where the circuit structures are tailored to the specific problems being addressed and the available quantum hardware. The dimensions of vectors θ_{i_k} and β_{i_k} depend on the structure of the parameterized quantum circuits.

When the linear operators $\mathcal{Z}_i$ are bounded, Eq. (14) transforms into a constrained optimization problem, expressed as $0 \leq \|Z_i\| \leq M_i$ for all i , where $\|\cdot\|$ denotes a suitable operator norm and M_i are given constants. This optimization can be efficiently handled by imposing constraints on the parameters λ_{k,j_k} during data processing on classical computers. Moreover, an alternative approach for parameterizing a linear operator, which involves incorporating classical neural networks (CNNs) as used in ref. 30, is detailed in Supplementary Note 2 “Alternative approach to parameterizing linear operator”.

Fig. 7 | Visualization of unitary operation χ_i . We evolve the input state $|0\rangle\langle 0| \otimes \rho \otimes |j\rangle\langle j|$ with a unitary operation χ_i , and then measure the first qubit in the computational basis. The probability of outcome 0 of the measurement gives the value of $(\Theta_{j,i} + 1)/2$.



Denote $\mathbf{j} := (j_1, j_2, \dots, j_p) \in [d]^p$, $a_j := \prod_{k=1}^p \lambda_{k,j_k}$, and

$$\Theta_{j,i} := \text{Re} \left[\text{Tr} \left(\rho \prod_{k=1}^p U_{i_k} |j_k\rangle\langle j_k| V_{i_k} \right) \right]. \quad (37)$$

Due to Eq. (36), after parameterization, the quantity we need to estimate becomes

$$\text{Tr}[\rho(Z_i + Z_i^\dagger)] = 2 \sum_{j \in [d]^p} a_j \Theta_{j,i}. \quad (38)$$

We can estimate the quantity above based on the extended SWAP test provided in ref. 59, Theorem 2.3, as adapted in the following lemma.

Lemma 3. Let ρ be a quantum state of dimension d , and Z_i be the linear operator defined in Eq. (34), the corresponding parameterization of which is Eq. (36). Denote $\mathbf{j} = (j_1, j_2, \dots, j_p) \in [d]^p$ and $|j\rangle = |j_1\rangle|j_2\rangle \cdots |j_p\rangle$. Then the unitary circuit χ_i shown in Fig. 7 gives

$$\Theta_{j,i} = 2\text{Tr} \left[(|0\rangle\langle 0| \otimes I) \chi_i (|0\rangle\langle 0| \otimes \rho \otimes |j\rangle\langle j|) \cdot \chi_i^\dagger \right] - 1. \quad (39)$$

More specifically, the unitary operation χ_i consists of two Hadamard gates, a series of controlled unitaries, and a controlled cyclic permutation. We implement the unitary χ_i on the input state $|0\rangle\langle 0| \otimes \rho \otimes |j\rangle\langle j|$, and then measure the first qubit. The probability of outcome 0 of the measurement is given by $(\Theta_{j,i} + 1)/2$.

With the parameterization and sampling procedure mentioned above, we can estimate the loss function in the optimization problem Eq. (14) by sampling on quantum computers, which paves the way for estimating quantum relative entropies (where $p = 1$).

Convergence analysis

In this section, we prove that our loss function is operator-convex, ensuring a well-behaved optimization landscape. We further discuss the convergence and trainability of our approach, and present numerical evidence indicating that our loss function is absent of the barren plateau phenomenon.

Convexity and global optimality. Let $\mathcal{L}(\mathcal{H})$ denote the set of all bounded linear operators on the Hilbert space $\mathcal{H}$. Consider a function $g : \mathcal{L}(\mathcal{H}) \rightarrow \mathbb{R}$. We say that g is operator-convex⁶⁰ if, for all $X, Y \in \mathcal{L}(\mathcal{H})$ and $\omega \in [0, 1]$, the following holds: $g((1 - \omega)X + \omega Y) \leq (1 - \omega)g(X) + \omega g(Y)$. We show that the loss function in Eq. (3) is operator-convex with respect to Z and we also characterize its optimal solution.

Lemma

4.

Let

$g(Z, Z^\dagger) = \text{Tr}[\rho] + \text{Tr}[\rho(Z + Z^\dagger)] + (1 - t)\text{Tr}[\rho Z^\dagger Z] + t\text{Tr}[\sigma Z Z^\dagger]$, where $\text{supp}(\rho) \subseteq \text{supp}(\sigma)$. Then $g(Z, Z^\dagger)$ is operator-convex with respect to Z .

Moreover, any solution $\tilde{Z}$ of the following Sylvester's equation,

$$\begin{aligned} (1 - t)\rho \tilde{Z}^\dagger + t\tilde{Z}^\dagger \sigma &= -\rho \\ \text{or } (1 - t)\tilde{Z}\rho + t\sigma \tilde{Z} &= -\rho, \end{aligned} \quad (40)$$

is an optimizer of the infimum problem $\inf_{Z \in \mathcal{L}(\mathcal{H})} g(Z, Z^\dagger)$. The above equation always admits at least one solution, which is unique if and only if at least one of ρ and σ is full-rank.

Lemma 4 shows that our loss function is operator-convex in Z , implying that any local minimum is also a global minimum. Consequently, our optimization landscape is free of spurious local minima, ensuring a simple and well-behaved structure. The proof is given in Supplementary Note 4.

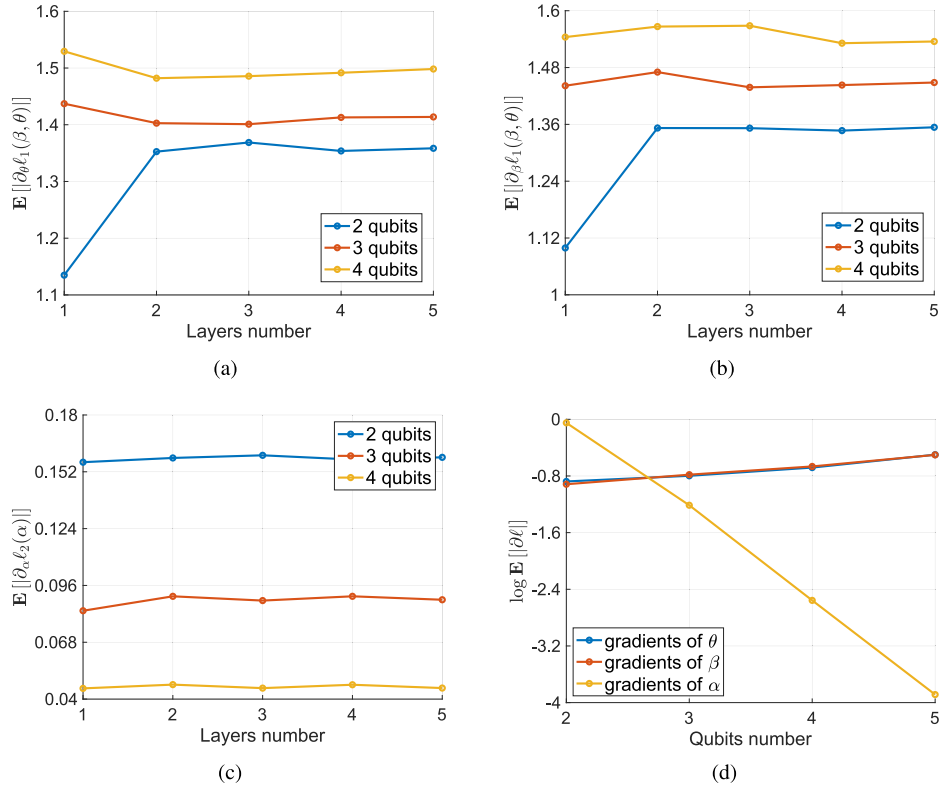
Convergence, trainability and barren plateau. The convergence of a variational quantum algorithm is fundamentally determined by the structure of its loss function and the resulting optimization landscape. As our loss function is operator-convex, this guarantees the existence of a global optimum at the operator level. Provided that the parameterized circuit is sufficiently expressive to represent all linear operators, the optimal solution can be reached. Achieving adequate expressibility typically requires deeper or more complex circuit architectures, which may increase computational overhead and resource requirements. In practice, this can be addressed by employing a well-designed ansatz and repeating it over a moderate number of layers. As the circuit depth increases, the expressibility of the ansatz improves, enhancing the chances of finding a better solution.

However, prior studies have shown that highly expressive parameterized quantum circuits can suffer from barren plateaus—regions in the optimization landscape where gradients vanish exponentially, making training infeasible^{34,42}. In particular, Holmes et al.⁴³ demonstrated that for a broad class of loss functions, such as energy expectation values $C(\theta) = \text{Tr}[HU(\theta)\rho U^\dagger(\theta)]$, there is a fundamental trade-off: highly expressive ansatzes tend to produce vanishing gradients, resulting in barren plateaus. Nevertheless, for certain specialized cost functions—particularly those with specific symmetries or locality properties—this trade-off does not always apply, even for highly expressive circuits. This raises a key question: can our loss function avoid the barren plateau phenomenon?

Intuitively, our loss function defined in Eq. (23) may partially circumvent the barren plateau problem. Unlike most cost functions, our loss function combines contributions from terms such as $\text{Tr}[\rho Z^\dagger Z]$, $\text{Tr}[\sigma Z Z^\dagger]$, and $\text{Tr}[\rho(Z + Z^\dagger)]$, which is non-global as $Z^\dagger Z$, $Z Z^\dagger$ and $Z + Z^\dagger$ are decomposed into projectors $|i\rangle\langle i|$ rather than a single global expectation value. Additionally, the mixture of quadratic and linear dependence on the eigenvalue weights λ_i ensures that gradients are sourced from multiple, non-identical directions in parameter space, reducing the extent to which gradients are averaged out under random circuit exploration.

To verify this intuition, we conduct numerical experiments comparing two different loss functions. The first is our proposed loss function from Eq.

Fig. 8 | Gradient scaling with respect to the number of layers and qubits. Error bars that represent the standard error of the mean are not shown since they are smaller than the marker size. **a** Mean gradient norm $\mathbb{E}[|\partial_{\theta} \ell_1(\beta, \theta)|]$ as a function of the number of layers for 2, 3, and 4 qubits. **b** Mean gradient norm $\mathbb{E}[|\partial_{\beta} \ell_1(\beta, \theta)|]$ as a function of the number of layers for 2, 3, and 4 qubits. **c** Mean gradient norm $\mathbb{E}[|\partial_{\alpha} \ell_2(\alpha)|]$ as a function of the number of layers for 2, 3, and 4 qubits. **d** Dependence of the mean gradient norm on the number of qubits for a 5-layer circuit, shown separately for the gradients with respect to θ , β , and α . For visual clarity, the data vectors are normalized before plotting.



(23):

$$\ell_1(\theta, \beta) = \mathcal{L}(\lambda, \theta, \beta). \quad (41)$$

The second loss function is a standard global cost:

$$\ell_2(\alpha) = \text{Tr}[W_{\alpha} \rho W_{\alpha}^{\dagger} \sigma]. \quad (42)$$

For all parameterized quantum circuits U_{θ} , V_{β} , and W_{α} , we employ a fixed ansatz. Specifically, we adopt Circuit-9 from ref. 61 (Fig. 2), since it has been shown that its expressibility increases monotonically with the number of layers from 1 to 5. To assess the scale of the gradients, we compute $\partial_{\theta} \ell_1(\theta, \beta)$, $\partial_{\beta} \ell_1(\theta, \beta)$, and $\partial_{\alpha} \ell_2(\alpha)$ at $N = 10,000$ uniformly random samples $\{\theta_i, \beta_i, \alpha_i\}_{i=1}^N$, and evaluate the following mean absolute values, $\mathbb{E}[|\partial_{\theta} \ell_1(\theta, \beta)|] = \frac{1}{N} \sum_{i=1}^N |\partial_{\theta} \ell_1(\theta_i, \beta_i)|$, $\mathbb{E}[|\partial_{\beta} \ell_1(\theta, \beta)|] = \frac{1}{N} \sum_{i=1}^N |\partial_{\beta} \ell_1(\theta_i, \beta_i)|$, and $\mathbb{E}[|\partial_{\alpha} \ell_2(\alpha)|] = \frac{1}{N} \sum_{i=1}^N |\partial_{\alpha} \ell_2(\alpha_i)|$. For computational reasons, results for 5-qubit cases are obtained using $N = 1,000$ random samples.

The results are shown in Fig. 8, where the subfigures (a)–(c) show the gradient scaling with respect to the number of layers⁶². Moreover, the gradient scaling of both $\ell_1(\theta, \beta)$ and $\ell_2(\alpha)$ does not decrease with the number of layers, despite the increasing expressibility of the parameterized circuits. However, as shown in Fig. 8d, the gradient scaling of $\ell_2(\alpha)$ decreases exponentially with respect to the number of qubits, while the gradient scaling of our loss function $\ell_1(\theta, \beta)$ remains essentially unchanged. These observations provide preliminary evidence that our proposed loss function circumvents the barren plateau phenomenon, maintaining trainability even as circuit expressibility increases.

A standard approach to analyzing barren plateaus involves examining the statistical properties of the cost function's gradient. When the cost landscape is unbiased, that is, $\mathbb{E}_{\theta}[\partial_{\theta_k} \ell_1] = 0$, Chebyshev's inequality shows that the probability of observing a gradient with magnitude exceeding δ is

bounded by $\text{Var}[\partial_{\theta_k} \ell_1] / \delta^2$ ⁴³. Thus, exponentially small gradient variance directly induces barren plateau behavior. However, our loss function differs fundamentally from standard cost functions. Rather than consisting of a single expectation value of a fixed observable, its gradient is given by a structured sum of multiple measurement contributions with variationally optimized coefficients. Consequently, the gradient variance cannot be determined by analyzing isolated terms under standard Haar-random assumptions. Instead, one must compute the variance of each contribution and account for covariance terms between different measurement components. This presents a significant technical challenge: the distinct measurement terms are neither independent nor generated by global observables drawn from a unitary 2-design. Rather, they arise from correlated measurements and optimization-dependent coefficients λ_i , introducing nontrivial statistical dependencies across terms. These structural correlations render standard barren plateau analyses inapplicable and make a rigorous variance analysis considerably more involved. Despite the lack of a complete theoretical explanation, our empirical observations provide evidence that the proposed loss function avoids barren plateaus and maintains trainability. We believe this warrants further investigation in future work.

Error analysis

In this section, we first show that our estimates for quantum relative entropy and Petz–Rényi divergence serve as rigorous lower bounds for their true values, despite the heuristic nature of the algorithms. We also provide an error analysis for these estimates, given the relative error of Algorithm 1.

Rigorous lower bounds. We consider the estimate of quantum relative entropy. The rigorous lower bound is obtained using quadrature approximations with the fixed node at $t_1 = 0$. Denote $r_m^1(x)$ and $r_m^0(x)$ as the quadrature approximations of $\log x$ with fixed nodes at $t_m = 1$ and $t_1 = 0$, respectively. According to ref. 50, Theorem 1, we have $r_m^0(x) \geq \log x \geq r_m^1(x)$. The infimum optimization in Lemma 2 ensures

that our approximation is always larger than the exact value, i.e., $\widehat{D}_{f_i}(\rho \parallel \sigma) \geq D_{f_i}(\rho \parallel \sigma)$. Therefore, we have

$$\begin{aligned} D_{-r_m^0}(\rho \parallel \sigma) &= - \sum_{j=1}^m \frac{w_j}{\ln 2} D_{f_{t_j}}(\rho \parallel \sigma) \\ &\geq - \sum_{j=1}^m \frac{w_j}{\ln 2} \widehat{D}_{f_{t_j}}(\rho \parallel \sigma) = \widehat{D}(\rho \parallel \sigma). \end{aligned} \quad (43)$$

This shows that our approximation serves as a lower bound,

$$D(\rho \parallel \sigma) \geq D_{-r_m^0}(\rho \parallel \sigma) \geq \widehat{D}(\rho \parallel \sigma). \quad (44)$$

The reasoning is analogous for Petz–Rényi divergence. Denote $h_m^1(x)$ and $h_m^0(x)$ as the quadrature approximations of $h(x) = x^{1-\alpha}$ with fixed nodes at $t_m = 1$ and $t_1 = 0$, respectively. For $\alpha \in (0, 1)$, we have $h_m^1(x) \leq h(x) \leq h_m^0(x)$, while for $\alpha \in (1, 2)$, we have $h_m^0(x) \leq h(x) \leq h_m^1(x)$. For $\alpha \in (0, 1)$, it follows that $Q_\alpha(\rho \parallel \sigma) = D_h(\rho \parallel \sigma) \leq D_{h_m^0}(\rho \parallel \sigma) \leq \widehat{D}_{h_m^0}(\rho \parallel \sigma)$. Similarly, for $\alpha \in (1, 2)$, we have $Q_\alpha(\rho \parallel \sigma) = D_h(\rho \parallel \sigma) \geq D_{h_m^0}(\rho \parallel \sigma) \geq \widehat{D}_{h_m^0}(\rho \parallel \sigma)$. Therefore, in both cases, the lower bound for Petz–Rényi divergences holds:

$$\begin{aligned} D_\alpha(\rho \parallel \sigma) &= \frac{1}{\alpha-1} \log Q_\alpha(\rho \parallel \sigma) \\ &\geq \frac{1}{\alpha-1} \log \widehat{D}_{h_m^0}(\rho \parallel \sigma) = \widehat{D}_\alpha(\rho \parallel \sigma). \end{aligned} \quad (45)$$

Error bound for estimating quantum relative entropy. The total error of our estimate comprises two components: ε_Q , which arises from the quadrature approximation and can be reduced by increasing the number of quadrature nodes m ; and ε_V , which stems from the heuristic nature of the variational algorithms. For the two different choices of GRJ quadrature nodes, i.e., with fixed node at $t_m = 1$ and at $t_1 = 0$, the analysis is different but essentially the same. All the proofs are shown in “Proofs of the error bounds” section of the Supplementary Note 5.

Proposition 5. (Error bound for estimating $D(\rho \parallel \sigma)$) For any quantum states ρ and σ with their supports $\text{supp}(\rho) \subseteq \text{supp}(\sigma)$, if the relative error of Algorithm 1 is within ε_V , i.e.,

$$\left| \frac{\widehat{D}_{f_j}(\rho \parallel \sigma) - D_{f_j}(\rho \parallel \sigma)}{D_{f_j}(\rho \parallel \sigma)} \right| \leq \varepsilon_V, \quad (46)$$

where $j = 1, 2, \dots, m$. Then the relative error of estimating $D(\rho \parallel \sigma)$ can be bounded by

$$\left| \frac{\widehat{D}(\rho \parallel \sigma) - D(\rho \parallel \sigma)}{D(\rho \parallel \sigma)} \right| \leq C \frac{1 + \varepsilon_V}{m^2} + \varepsilon_V, \quad (47)$$

where $C = (Q_0(\rho \parallel \sigma) + Q_2(\rho \parallel \sigma))/(D(\rho \parallel \sigma) \ln 2)$ and m is the number of quadrature nodes.

Error bound for estimating Petz–Rényi divergence. Similarly, for estimating the Petz–Rényi divergence, the error ε_Q arises from the difference between the quadrature approximation $h_m(x)$ and the exact function $h(x) = x^{1-\alpha}$. This difference can be bounded by using Theorem 1 and Theorem 9 from ref. 50.

Lemma 6. ⁽⁵⁰⁾ Consider the function $h(x) = x^{1-\alpha}$, whose integral representation is $h(x) = 1 + \int_0^1 f_t(x) dv_\alpha(t)$, where $\alpha \in (0, 1) \cup (1, 2)$, $f_t(x)$ is defined in Eq. (2), and $dv_\alpha(t) = \frac{\sin(\alpha\pi)}{\pi} t^{\alpha-1} (1-t)^{1-\alpha} dt$. Let $h_m(x)$ be the GRJ quadrature approximations to $h(x)$ with the fixed node at 1. Then for

$m \geq 1$ and $x > 0$, we have

$$0 \leq \frac{h(x) - h_m(x)}{1 - \alpha} \leq \alpha v_{\alpha,m} \frac{(x-1)^2}{x}, \quad (48)$$

where $v_{\alpha,m} = \max\{v_{\alpha,m}^0, v_{\alpha,m}^1\}$ and

$$\begin{aligned} v_{\alpha,m}^0 &= O\left(\frac{\Gamma(\alpha)}{m^{2\alpha}\Gamma(2-\alpha)}\right), \\ v_{\alpha,m}^1 &= O\left(\frac{\Gamma(2-\alpha)}{m^{2(2-\alpha)}\Gamma(\alpha)}\right). \end{aligned} \quad (49)$$

We note here that for $\alpha \in (0, 1)$, $h(x) - h_m(x) \geq 0$; while for $\alpha \in (1, 2)$, $h(x) - h_m(x) \leq 0$. When $m \rightarrow \infty$, $h_m(x)$ converges to $h(x)$.

Based on this lemma, we have the following error bound for estimating $Q_\alpha(\rho \parallel \sigma)$ and $D_\alpha(\rho \parallel \sigma)$.

Lemma 7. (Error bound for estimating $Q_\alpha(\rho \parallel \sigma)$) Let $\alpha \in (0, 1) \cup (1, 2)$. For any quantum states ρ and σ with $\text{supp}(\rho) \subseteq \text{supp}(\sigma)$, if the relative error of Algorithm 1 is within ε_V (as defined in Eq. (46)), then the error of estimating $Q_\alpha(\rho \parallel \sigma)$ is bounded as follows:

$$|Q_\alpha(\rho \parallel \sigma) - \widehat{Q}_\alpha(\rho \parallel \sigma)| \leq C_1 v_{\alpha,m} (1 + \varepsilon_V) + C_2 \varepsilon_V, \quad (50)$$

where $C_1 = 2|\alpha(1-\alpha)| \cdot (Q_2(\rho \parallel \sigma) - 1)$, $C_2 = |Q_\alpha(\rho \parallel \sigma) - 1|$ and $v_{\alpha,m}$ defined in Lemma 6.

This lemma implies that when $m \rightarrow \infty$, the error stems from quadrature approximation vanishes as $v_{\alpha,m} \rightarrow 0$. It also leads to the error bound for $D_\alpha(\rho \parallel \sigma)$ as follows.

Proposition 8. (Error bound for estimating $D_\alpha(\rho \parallel \sigma)$) Let $\alpha \in (0, 1) \cup (1, 2)$. For any quantum states ρ and σ with $\text{supp}(\rho) \subseteq \text{supp}(\sigma)$, if the relative error of Algorithm 1 is within ε_V (as defined in Eq. (46)), then the total relative error of estimating $D_\alpha(\rho \parallel \sigma)$ can be bounded by

$$\left| \frac{D_\alpha(\rho \parallel \sigma) - \widehat{D}_\alpha(\rho \parallel \sigma)}{D_\alpha(\rho \parallel \sigma)} \right| \leq O(v_{\alpha,m}) + O(\varepsilon_V), \quad (51)$$

where $v_{\alpha,m}$ is defined in Lemma 6 and m is the number of quadrature nodes.

In the case of $\alpha = 2$, the error arises solely from the heuristic nature of the variational process, because the value of $Q_2(\rho \parallel \sigma)$ can be exactly determined from the value of $D_{f_1}(\rho \parallel \sigma)$. Therefore, if the relative error of Algorithm 1 can be controlled within ε_V , the error bound for estimating $D_2(\rho \parallel \sigma)$ is given by:

$$\begin{aligned} &\left| \frac{D_2(\rho \parallel \sigma) - \widehat{D}_2(\rho \parallel \sigma)}{D_2(\rho \parallel \sigma)} \right| \\ &\leq O\left(\varepsilon_V \cdot \frac{Q_2(\rho \parallel \sigma) - 1}{Q_2(\rho \parallel \sigma) D_2(\rho \parallel \sigma)}\right) = O(\varepsilon_V). \end{aligned} \quad (52)$$

Data availability

The data that support the findings of this study are available from the corresponding author upon request.

Code availability

The code for our numerical simulations is available on Zenodo <https://doi.org/10.5281/zenodo.19322126>.

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Author contributions

K.F. developed the main idea of this work and supervised the project. Y.L. derived the theoretical results and conducted the numerical simulations. Both authors contributed to the writing, discussions and interpretations of the results. Corresponding author: Kun Fang.

Competing interests

The authors declare no competing interests.

Additional information

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