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Performance Guarantees for Quantum Neural Estimation of Entropies

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Estimating quantum entropies and divergences is an important problem in quantum physics, information theory, and machine learning. Quantum neural estimators (QNEs), which utilize a hybrid classical-quantum architecture, have recently emerged as an appealing computational framework for estimating these measures. Such estimators combine classical neural networks with parametrized quantum circuits, and their deployment typically entails tedious tuning of hyperparameters controlling the sample size, network architecture, and circuit topology. This work initiates the study of formal guarantees for QNEs of measured (Rényi) relative entropies in the form of non-asymptotic error risk bounds. We further establish exponential tail bounds showing that the error is sub-Gaussian and thus sharply concentrates about the ground truth value. For an appropriate sub-class of density operator pairs on a space of dimension d with bounded Thompson metric, our theory establishes a copy complexity of $O(|\Theta(\mathcal{U})|d/\epsilon^2)$ for QNE with a quantum circuit parameter set $\Theta(\mathcal{U})$, which has minimax optimal dependence on the accuracy ϵ. Additionally, if the density operator pairs are permutation invariant, we improve the dimension dependence above to $O(|\Theta(\mathcal{U})|\text{polylog}(d)/\epsilon^2)$. Our theory aims to facilitate principled implementation of QNEs for measured relative entropies and guide hyperparameter tuning in practice.

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1 Introduction

Entropy, a concept rooted in thermodynamics and statistical mechanics, plays a fundamental role in quantifying the amount of uncertainty or disorder in physical systems. Von Neumann and Shannon introduced these concepts to quantum mechanics and classical information theory, now referred to as the von Neumann entropy [1] and Shannon entropy [2], respectively. Rényi generalized this concept axiomatically, showing that any uncertainty measure satisfying a set of natural axioms can be characterized in terms of a single parameter family of entropy measures now known as Rényi entropies [3]. Since their seminal works, related measures of information and discrepancy, such as mutual information, relative entropy [4, 5], and their Rényi counterparts [6–9], have found operational interpretations in classical and quantum hypothesis testing [6, 10–14], channel coding, data compression, and other related tasks.

Given the significance of entropic measures in characterizing the fundamental limits of quantum information systems, computing them is an important problem. However, often the underlying state is unknown, which necessitates estimating these quantities based on measurements of the quantum system. To this end, several estimators have been proposed in both the classical and quantum settings [15–28]. Recently, quantum neural estimation (QNE), employing a hybrid classical-quantum architecture composed of neural nets and

Rényi order and state class	Minimax risk upper bound	Minimax risk lower bound
$\alpha = 1$ and $\mathcal{S} \subseteq \mathcal{S}_d(b)$	$O_b\left(\delta + \sqrt{\frac{d\,\Theta(\delta,\mathcal{S})}{n}}\right)$	$\Omega_b\left(\frac{1}{\sqrt{n}} + \frac{d}{n \log d}\right)$
$0 < \alpha \neq 1$ and $\mathcal{S} \subseteq \mathcal{S}_d(b)$	$O_{\alpha,b}\left(\delta + \sqrt{\frac{d\,\Theta(\delta,\mathcal{S})}{n}}\right)$	$\Omega_{\alpha,b}\left(\frac{1}{\sqrt{n}} + \frac{d}{n \log d}\right)$

Table 1: Minimax risk bounds for estimation of measured relative entropies over the class $\mathcal{S} \subseteq \mathcal{S}_d(b)$. Here, b is a uniform upper bound on the Thompson metric between density operator pairs in $\mathcal{S}_d(b)$, δ is an approximation error parameter for PQC parametrized by $\Theta(\delta, \mathcal{S})$, and n is the number of copies of quantum states on a Hilbert space of dimension d used by the QNE. The upper bound holds for any $\mathcal{S} \subseteq \mathcal{S}_d(b)$ while the lower bound holds for any $\mathcal{S} \subseteq \mathcal{S}_d(b)$ containing all state pairs in any fixed eigen-basis, when $db \lesssim n \log d$ and $b \geq (\log d)^2 \vee 2$.

quantum circuits, has been proposed for estimating quantum entropies and measured relative entropies [29] (see also [30, 31]). QNE utilizes the variational form of the entropic measure given as the supremum over Hermitian operators of a trace functional with respect to the underlying states [32–34]. By parametrizing the eigenvalues and eigenvectors of the Hermitian operator by the neural net and quantum circuit, respectively, the QNE leverages their expressivity to construct scalable estimators. In [29], it was shown via numerical simulations that the QNE is consistent.

1.1 Summary of Contributions

In this paper, we provide the first theoretical guarantees for QNE in the form of sharp bounds on the expected absolute error. The bounds depend on the number of quantum state copies the algorithm uses, parameters defining the class of underlying density operators, and the classical-quantum circuit parameters. Furthermore, we also derive concentration inequalities for the absolute error about the ground truth, which leads to an upper bound on the copy complexity of QNE, i.e., the minimum number of copies of the quantum states required for estimating measured relative entropies.

To summarize our main contributions, let $\mathcal{S}_d(b)$ be the set of density operator pairs (ρ, σ) for a Hilbert space of dimension d, such that their Thompson metric [35] is bounded from above by $\log b$. Assuming that the neural net and quantum circuit are sufficiently expressive and have bounded statistical complexity (see Assumption 1 and Section 2.5.2), we show the following:

(i) We derive an upper bound on the expected absolute error achieved by QNE for estimating the measured relative entropy (Theorem 1) and the measured Rényi relative entropy (Theorem 5) over the class $\mathcal{S}_d(b)$. Further, we establish an exponential deviation inequality that shows that the absolute error has sub-Gaussian tails.

(ii) To obtain concrete bounds, we specialize the aforementioned results to shallow neural nets with sufficiently large width (Corollary 2 and Corollary 6) and deep neural nets with a sufficient number of layers (Proposition 4 and Proposition 7). An upper bound on the absolute error achieved by a QNE with a shallow net over the class $\mathcal{S}_d(b)$ is illustrated in Table 1, along with a lower bound on the minimax risk (valid for any estimator) over the same class.

(iii) Let $d = m^N$, with N denoting the number of qudits, and let ρ, σ be density operators defined on N qudits. While the QNE has a worst-case copy complexity that scales exponentially in N, we show that for a subclass (which depends on the quantum circuit) of permutation invariant states across N qudits within $\mathcal{S}_d(b)$, the algorithm

has a much better polynomial dependence (see Proposition 9). This is possible due to Schur–Weyl duality from representation theory, which implies that the number of degrees of freedom for such states scales polynomially in N.

1.2 Literature Review and Related Work

Measured relative entropy was introduced in [36, 37] and since then has found operational significance in terms of characterizing the Stein's and strong converse exponents in centralized, adversarial, and distributed hypothesis testing (see e.g., [38–43]). There is an extensive literature on estimation of entropic, information and divergence measures in the classical setting. Given this, we focus primarily on the finite-dimensional quantum setting. The reader is referred to, e.g., [44, 45] and references therein, for a detailed account of relevant works in the classical setting. In the quantum setting, a pertinent approach for estimating such measures is to use quantum tomography to learn the entire density matrix, from which the desired entropic quantity of interest can be computed. The copy complexity of this approach is linear in the dimension of the state (or, equivalently, exponential in the number of qudits) [46–49].

A possibly more efficient approach is to estimate the entropies directly, without estimating the underlying states. In this regard, several estimators have been proposed and their computational complexities investigated under different input models [15–27]. In particular, [17] provided algorithms for estimating the von Neumann entropy and Rényi entropies, given access to independent copies of the input quantum state, which achieves the copy complexity (sub-linear in dimension) for integer orders greater than one. Entropy estimation under the quantum query model, i.e., where one has access to an oracle that prepares the input quantum state, was explored in [18, 20]. These works also established sub-linear (in dimension) query complexity bounds for estimating the von Neumann and Rényi entropies.

In contrast to the estimators mentioned above, QNE proposed in [29] is based on variational methods, which have become a prominent research area in quantum computing and machine learning [50–53]. Specifically, QNEs utilize a hybrid quantum-classical algorithm that extends the approach from [54–60] to the quantum framework. The appeal of such estimators stems from their scalability to high-dimensional problems and large datasets, as well as their compatibility with modern gradient-based optimization techniques. This makes them particularly relevant in the quantum context, where the dimension of the underlying Hilbert space scales exponentially in the number of qudits. Although QNE was shown to perform empirically well in [29], theoretical performance guarantees are still lacking, which this work aims to advance upon. We note that variational methods have also been used in [61] for estimating fidelity, entropies and Fisher information, in [30] for estimating quantum mutual information and in [31] for estimating entanglement entropy, which indicates their versatility.

In the framework of [29] for estimating measured relative entropies, the optimization is performed over Hermitian operators of the form $H(\theta, \phi) = U(\boldsymbol{\theta})\,\mathrm{diag}(\Lambda_\phi)\,U(\boldsymbol{\theta})^\dagger$, where a parameterized quantum circuit (PQC) $U(\boldsymbol{\theta})$ specifies the eigenvectors and a neural network defines the eigenvalues Λ_ϕ. Although this hybrid parameterization effectively captures the optimization of the variational formula $\mathrm{Tr}[H\rho] + 1 - \mathrm{Tr}[e^H\sigma]$ for measured relative entropy (and a related formula for measured Rényi relative entropy), it remains susceptible to barren plateaus [62–64]. In particular, if the PQC is sufficiently deep and unstructured, $U(\boldsymbol{\theta})$ approximates a unitary two-design, causing $\mathrm{Tr}[H\rho]$ and $\mathrm{Tr}[e^H\sigma]$ to concentrate around their means and the gradient variances to vanish exponentially in the number of qubits. This leads to vanishing gradients in the quantum parameters $\boldsymbol{\theta}$ and, indirectly, to weak-

ened gradient signals for the classical parameters ϕ. Barren plateaus can be mitigated by employing shallow or symmetry-informed ansätze [65, 66], initializing $U(\boldsymbol{\theta})$ near the identity [67], or adopting layer-wise or hybrid training strategies that preserve gradient signal throughout optimization [68]. Importantly, despite its variational structure, the QNE framework is not susceptible to the classical-simulability arguments discussed in [69], since it assumes direct access to quantum samples of the states ρ and σ rather than classical descriptions or measurement data. The learning task thereby exploits intrinsically quantum input data, placing it outside the regime of efficiently classically simulable models identified in [69].

Paper Organization

The rest of the paper is organized as follows. Section 2 introduces the notation and preliminary concepts along with QNE. Section 3 obtains performance guarantees in terms of expected absolute error bounds and deviation inequalities for estimating measured relative entropies using QNE. Section 4 discusses the copy complexity achieved by QNE. Section 5 presents proofs of the main results, with proofs of the auxiliary results deferred to the Appendix. Finally, Section 6 concludes the paper with suggestions of avenues for future research.

2 Preliminaries

Notation

Throughout, we consider a d-dimensional complex Hilbert space $\mathbb{H}_d$. The set of (linear) operators from $\mathbb{H}_d$ to itself is denoted by $\mathcal{L}(\mathbb{H}_d)$. The set of density operators (or quantum states) on $\mathbb{H}_d$, i.e., positive semi-definite operators with unit trace is denoted by $\mathbb{S}_d$. $\mathrm{Tr}[\cdot]$ and $\|\cdot\|_p$ for $p \geq 1$ signify the trace operation and Schatten p-norm, respectively. For normal operators A (which includes Hermitian and unitary operators), $\|A\|_\infty = \|A\|$, where $\|A\|$ represents the operator norm of A. The usual norm associated with the Lebesgue space of p-integrable functions ($p \geq 1$) on $\mathcal{X} \subseteq \mathbb{R}^d$ with respect to a measure μ is denoted by $\|\cdot\|_{p,\mu}$, while $\|\cdot\|_{\infty,\mathcal{X}}$ designates the standard sup-norm, i.e., $\|f\|_{\infty,\mathcal{X}} = \sup_{x\in\mathcal{X}} |f(x)|$. $\mathbb{1}_{\mathcal{X}}$ denotes the indicator of a set $\mathcal{X}$. For reals a, b, we define $a \wedge b := \min\{a, b\}$ and $a \vee b := \max\{a, b\}$. Further, $a \lesssim_x b$ indicates that $a \leq c_x b$ for a constant $c_x > 0$ that depends only on x, and $a \gtrsim_x b$ means that $b \lesssim_x a$.

2.1 Measured Relative Entropy and Measured Rényi Relative Entropy

The *measured relative entropy* between $\rho, \sigma \in \mathbb{S}_d$ is defined as [36, 37]

$$\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) := \sup_{\mathcal{Z},\{M_z\}_{z\in\mathcal{Z}}} \sum_{z\in\mathcal{Z}} \mathrm{Tr}[M_z\rho] \log\left(\frac{\mathrm{Tr}[M_z\rho]}{\mathrm{Tr}[M_z\sigma]}\right), \tag{1}$$

where the supremum is over all finite sets $\mathcal{Z}$ and positive operator-valued measures[1] (POVMs) $\{M_z\}_{z\in\mathcal{Z}}$ indexed by $\mathcal{Z}$. The measured relative entropy can be expressed in terms of the following variational expression [34, Lemma 1]:

$$\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) = \sup_H \mathrm{Tr}[H\rho] - \mathrm{Tr}[e^H\sigma] + 1, \tag{2}$$

[1] A POVM $\{M_z\}_{z\in\mathcal{Z}}$ on $\mathbb{H}_d$ indexed by a discrete $\mathcal{Z}$ is a set of positive semi-definite operators satisfying $\sum_{z\in\mathcal{Z}} M_z = I$.

where the supremum is over the class of Hermitian operators H on $\mathbb{H}_d$.

The *measured Rényi relative entropy* of order $\alpha \in (0,1) \cup (1,\infty)$ between $\rho, \sigma \in \mathbb{S}_d$ is defined as follows [70, Eqs. (3.116)–(3.117)]:

$$\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) \coloneqq \sup_{\mathcal{Z},\{M_z\}_{z\in\mathcal{Z}}} \frac{1}{\alpha-1} \log \sum_{z\in\mathcal{Z}} \operatorname{Tr}[M_z\rho]^\alpha \operatorname{Tr}[M_z\sigma]^{1-\alpha}, \tag{3}$$

where the supremum is over all finite sets $\mathcal{Z}$ and POVMs $\{M_z\}_{z\in\mathcal{Z}}$. Recall that it satisfies the variational expression [34, Lemma 3]:

$$\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) = \sup_H \frac{\alpha}{\alpha-1} \log \operatorname{Tr}[e^{(\alpha-1)H}\rho] - \log \operatorname{Tr}[e^{\alpha H}\sigma]. \tag{4}$$

When $\rho, \sigma > 0$, the suprema in (2) and (4) are achieved for some $H^\star_\alpha(\rho,\sigma)$ [34, Lemma 1 and Lemma 3] ($H^\star_1(\rho,\sigma)$ corresponds to the optimizer of (2)). Specifically, the proof of [34, Lemma 1 and Theorem 2] shows that

$$H^\star_\alpha(\rho,\sigma) = \sum_{i=1}^d \lambda^\star_{i,\alpha} P^\star_{i,\alpha}, \qquad \text{with } \lambda^\star_{i,\alpha} \coloneqq \log\left(\frac{\operatorname{Tr}[P^\star_{i,\alpha}\rho]}{\operatorname{Tr}[P^\star_{i,\alpha}\sigma]}\right), \tag{5}$$

where $\{P^\star_{i,\alpha}\}_{i=1}^d$ denotes a set of orthonormal rank-one projectors from the spectral decomposition of $H^\star_\alpha(\rho,\sigma)$. When $\alpha = 1$, we henceforth simply write $\{\lambda^\star_i\}_{i=1}^d$, $\{P^\star_i\}_{i=1}^d$, and $H^\star(\rho,\sigma)$. Note that while $\{P^\star_{i,\alpha}\}_{i=1}^d$ need not be unique in general, $H^\star_\alpha(\rho,\sigma)$ is unique (see Appendix A). Also, although a closed form expression for $H^\star_\alpha(\rho,\sigma)$ is not known, it can be shown by setting matrix (Fréchet) derivatives with respect to H in (2) and (4) to zero that $H^\star_\alpha(\rho,\sigma)$ satisfies

$$\int_0^1 e^{t(\alpha-1)H^\star_\alpha(\rho,\sigma)} \rho e^{(1-t)(\alpha-1)H^\star_\alpha(\rho,\sigma)} dt = \int_0^1 e^{t\alpha H^\star_\alpha(\rho,\sigma)} \sigma e^{(1-t)\alpha H^\star_\alpha(\rho,\sigma)} dt. \tag{6}$$

Furthermore, we note from the proof of [34, Lemma 1 and Theorem 2] that the projective POVMs formed by the optimizers $\{P^\star_i\}_{i=1}^d$ and $\{P^\star_{i,\alpha}\}_{i=1}^d$ turn out to be optimal measurements achieving the suprema in (1) and (3), respectively.

There exists an alternative variational form for measured relative entropies, as given in [34, Lemma 1 and Lemma 2]:

$$\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) = \sup_{\omega>0} \operatorname{Tr}[\rho \log \omega] + 1 - \operatorname{Tr}[\sigma\omega], \tag{7}$$

$$\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) = \frac{1}{\alpha-1} \log Q_\alpha(\rho\|\sigma), \quad \alpha \in (0,1)\cup(1,\infty), \tag{8}$$

where

$$Q_\alpha(\rho\|\sigma) = \begin{cases} \inf_{\omega>0} \{\alpha \operatorname{Tr}[\rho\omega] + (1-\alpha)\operatorname{Tr}[\sigma\omega^{\frac{\alpha}{\alpha-1}}]\}, & \text{for } \alpha \in \left(0, \frac{1}{2}\right), \\ \inf_{\omega>0} \{\alpha \operatorname{Tr}[\rho\omega^{1-\frac{1}{\alpha}}] + (1-\alpha)\operatorname{Tr}[\sigma\omega]\}, & \text{for } \alpha \in \left[\frac{1}{2}, 1\right), \\ \sup_{\omega>0} \{\alpha \operatorname{Tr}[\rho\omega^{1-\frac{1}{\alpha}}] + (1-\alpha)\operatorname{Tr}[\sigma\omega]\}, & \text{for } \alpha \in (1,\infty). \end{cases} \tag{9}$$

The advantage of these forms is that (7) and (8) are (strictly) convex optimization problems over the cone of positive definite matrices when $\rho, \sigma > 0$, which can be utilized to obtain a necessary and sufficient condition that is satisfied by $H^\star_\alpha(\rho,\sigma)$. For instance, setting the matrix derivatives of the expressions on the right-hand side (RHS) of (9) to zero yields that, for $\alpha \in [1/2, 1) \cup (1,\infty)$, the unique optimizer $\omega^\star_\alpha(\rho,\sigma)$ $(= e^{\alpha H^\star_\alpha(\rho,\sigma)})$ satisfies

$$\sigma = \left(\frac{\alpha}{1-\alpha}\right) \frac{\sin\left(\left(\frac{1-\alpha}{\alpha}\right)\pi\right)}{\pi} \int_0^\infty t^{\frac{\alpha-1}{\alpha}} \left(\omega^\star_\alpha(\rho,\sigma) + tI\right)^{-1} \rho \left(\omega^\star_\alpha(\rho,\sigma) + tI\right)^{-1} dt. \tag{10}$$

Note that ρ and σ above are related by a completely positive map involving $H_\alpha^\star(\rho,\sigma) = \log \omega_\alpha^\star(\rho,\sigma)$. Details of the above are provided in Appendix A. See also [71] for how to compute the measured (Rényi) relative entropies by means of semi-definite optimization.

2.2 Minimax Estimation of Measured Relative Entropies

Consider the problem of estimating measured relative entropies $\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma)$ and $\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)$ based on n copies of both ρ and σ. We are interested in the decay rate of the QNE absolute error with n, and how it compares to the performance of an optimal algorithm for estimating entropies. It is well known from classical results that estimating entropies, in general, suffers from the so-called curse of dimensionality [72], in that, the estimation error is $\Omega(n^{-\frac{1}{d}})$. In other words, estimating entropies is hard in high dimensions without additional assumptions that restrict the class of density operators.

The performance of an estimator is quantified by the minimax risk, namely, the error of the best estimator uniformly over a class of density operators. Formally, the minimax risk for measured relative entropy over a class $\mathcal{S}$ is defined as follows:

$$R_n^\star(\mathcal{S}) \coloneqq \inf_{\hat{\mathsf{D}}_n} \sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{E}\Big[\Big|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}_n(\rho^{\otimes n},\sigma^{\otimes n})\Big|\Big], \tag{11}$$

where the infimum is over all estimators $\hat{\mathsf{D}}_n$, i.e., a map $(\rho^{\otimes n},\sigma^{\otimes n}) \mapsto \hat{\mathsf{D}}_n(\rho^{\otimes n},\sigma^{\otimes n})$, which is allowed to perform quantum operations (apply quantum channels, measurements, etc.) and the expectation is over any randomness resulting from such quantum operations. Note that the minimax risk is a property of the estimation setting—the best possible performance uniformly over the class—as opposed to the specific estimator. The minimax risk for measured Rényi relative entropy, $R_{n,\alpha}^\star(\mathcal{S})$, is defined analogously by replacing $\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)$ with $\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma)$ in (11).

Recalling the Thompson metric $T(\rho,\sigma) \coloneqq \log(\|\sigma^{-1/2}\rho\sigma^{-1/2}\| \vee \|\rho^{-1/2}\sigma\rho^{-1/2}\|)$ [35] ($\|\sigma^{-1/2}\rho\sigma^{-1/2}\| \wedge \|\rho^{-1/2}\sigma\rho^{-1/2}\| \geq 1$ with equality iff $\rho = \sigma$), in what follows, we are interested in the minimax risk over a subclass $\mathcal{S} \subseteq \mathcal{S}_d(b)$, where for $b \geq 1$,

$$\mathcal{S}_d(b) \coloneqq \{(\rho,\sigma) : 0 < \rho,\sigma \in \mathbb{S}_d, T(\rho,\sigma) \leq \log b\}. \tag{12}$$

Note that $T(\rho,\sigma)$ being bounded constrains the minimal eigenvalue of both ρ and σ to be bounded away from zero. In fact, it is equivalent to $D_{\max}(\rho\|\sigma) \vee D_{\max}(\sigma\|\rho) \leq \log b$, where $D_{\max}(\rho\|\sigma)$ denotes the max-relative entropy between ρ and σ [73] (see Appendix D). We will use the fact that the Thompson metric contracts under the application of a quantum channel [73, Lemma 7], i.e., $T(\rho,\sigma) \geq T(\mathcal{N}(\rho),\mathcal{N}(\sigma))$ for every quantum channel $\mathcal{N}$.

2.3 Quantum Neural Estimator for Estimating Measured Relative Entropies

The QNE proposed in [29] has a classical neural class $\mathcal{F}$ and parametrized quantum circuit (PQC) $\mathcal{U}(\Theta)$, indexed by a set Θ. It estimates $\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)$ as follows:

$$\hat{\mathsf{D}}^n_{\mathsf{M},\Theta,\mathcal{F}} \coloneqq \sup_{\boldsymbol{\theta}\in\Theta} \hat{\mathsf{D}}^n_{\mathsf{M},\boldsymbol{\theta},\mathcal{F}}, \tag{13a}$$

where

$$\hat{\mathsf{D}}^n_{\mathsf{M},\boldsymbol{\theta},\mathcal{F}} \coloneqq \sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{\ell=1}^n f(i_\ell(\boldsymbol{\theta})) - \frac{1}{n}\sum_{\ell=1}^n e^{f(j_\ell(\boldsymbol{\theta}))} + 1, \tag{13b}$$

and $i_\ell(\boldsymbol{\theta}) \sim p^\rho_{\boldsymbol{\theta}}$, $j_\ell(\boldsymbol{\theta}) \sim q^\sigma_{\boldsymbol{\theta}}$, with

$$p^\rho_{\boldsymbol{\theta}}(i) \coloneqq \mathrm{Tr}\left[U(\boldsymbol{\theta})|i\rangle\langle i|U^\dagger(\boldsymbol{\theta})\rho\right], \tag{14a}$$

$$q^\sigma_{\boldsymbol{\theta}}(i) \coloneqq \mathrm{Tr}\left[U(\boldsymbol{\theta})|i\rangle\langle i|U^\dagger(\boldsymbol{\theta})\sigma\right]. \tag{14b}$$

The analogous QNE estimate for measured Rényi relative entropy is given by

$$\hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta,\mathcal{F}} \coloneqq \sup_{\boldsymbol{\theta}\in\Theta} \hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\boldsymbol{\theta},\mathcal{F}},$$

where

$$\hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\boldsymbol{\theta},\mathcal{F}} \coloneqq \frac{\alpha}{\alpha-1}\log\frac{1}{n}\sum_{k=1}^n e^{(\alpha-1)f(i_k(\boldsymbol{\theta}))} - \log\frac{1}{n}\sum_{k=1}^n e^{\alpha f(j_k(\boldsymbol{\theta}))},$$

and $i_\ell(\boldsymbol{\theta}) \sim p^\rho_{\boldsymbol{\theta}}$, $j_\ell(\boldsymbol{\theta}) \sim q^\sigma_{\boldsymbol{\theta}}$ with $p^\rho_{\boldsymbol{\theta}}$ and $q^\sigma_{\boldsymbol{\theta}}$ as given in (14). In practice, $\hat{\mathsf{D}}^n_{\mathsf{M},\Theta,\mathcal{F}}$ and $\hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta,\mathcal{F}}$ are computed via alternating optimization, by performing gradient ascent iteratively over the neural net class $f \in \mathcal{F}$ (for a fixed $\boldsymbol{\theta}$) followed by that over Θ.

For flexibility of the framework, we will also allow applying a fixed quantum channel to each copy of ρ and σ before performing measurements using the PQC; i.e., ρ and σ in (14) are replaced by $\mathcal{N}(\rho)$ and $\mathcal{N}(\sigma)$, respectively, for a channel $\mathcal{N}$, with $\mathcal{U}(\Theta)$ adjusted to be a set of unitary operators on the channel's output space. The rationale behind this is to leverage any additional known structure on the quantum states to reduce the copy complexity of QNE. For instance, when ρ and σ are permutationally invariant, it is known from Schur–Weyl duality that the number of degrees of freedom in such states scales polynomially in the number of qubits (as opposed to exponential in the general case). In this case, the complexity of QNE can be reduced by applying a pre-processing channel $\mathcal{N}$ chosen based on the Schur transform and running QNE on its output space. We note that there are various efficient quantum circuit implementations [74–77] for the Schur transform. In the general case (without any additional known structure), we take the pre-processing channel to be the identity channel.

Our objective is to quantify the performance of QNE in terms of d, n, and the parameters defining $\mathcal{F}$, $\mathcal{U}$, and $\mathcal{S}$. To that end, we split the error of QNE into two components[2]: *approximation* and *statistical*. The approximation error depends on the ability of the classical neural net and PQC to approximate, respectively, the eigenvalues and eigenvectors of the optimizer $H^\star(\rho,\sigma)$ given in (5). The statistical error, on the other hand, is the random component of the overall error that depends on the complexity of the classical-quantum model used by the QNE. We briefly note that a QNE for measured relative entropies may also be constructed by using the variational forms given in (7) and (8) (by estimating $Q_\alpha(\rho\|\sigma)$ when $\alpha \neq 1$ and substituting in (8)). An analysis of this estimator could be performed similarly to that of (13), with the resulting performance guarantees differing only in terms of constants that depend on b and α. Hence, we omit it.

2.4 Relevant Concepts from Probability Theory

Here, we introduce some notions from probability theory (see e.g. [78]) which will be useful in our analysis of QNE performance. We will require that the neural class used in QNE has

[2]In practice, there is also an optimization error component, which arises when the suprema in (13) are only approximately computed, e.g., by gradient-based methods. This can be incorporated as an additive factor in the overall error. A detailed analysis however has to take into account the specific parameterizations of the classical neural net and quantum circuit. Hence, we ignore this aspect in our analysis and leave its quantification as part of future work.

bounded complexity (see Assumption 1 below), as quantified using the notion of covering entropy [79] of a function class in a suitable metric.

Definition 1 (Covering entropy)**.** *Let* (Θ, d) *be a metric space. A set* $\Theta' \subseteq \Theta$ *is an* ϵ*-covering of* (Θ, d) *if, for every* $\theta \in \Theta$*, there exists* $\theta' \in \Theta'$ *such that* $\mathsf{d}(\theta, \theta') \leq \epsilon$*. The* ϵ*-covering number is defined as*

$$N(\epsilon, \Theta, \mathsf{d}) \coloneqq \inf \left\{ |\Theta'| : \Theta' \text{ is an } \epsilon\text{-covering of } \Theta \right\},$$

and the ϵ*-covering entropy is* $\log N(\epsilon, \Theta, \mathsf{d})$*.*

To obtain a handle on the statistical component of the overall error, we will upper bound it in terms of suprema of separable sub-Gaussian processes indexed by neural class and quantum circuit parameters.

Definition 2 (Separable sub-Gaussian process)**.** *A real-valued stochastic process* $(X_\theta)_{\theta \in \Theta}$ *on a metric space* (Θ, d) *is sub-Gaussian if it is centered, i.e.,* $\mathbb{E}[X_\theta] = 0$ *for all* $\theta \in \Theta$*, and* $\mathbb{E}[e^{t(X_\theta - X_{\tilde{\theta}})}] \leq e^{\frac{1}{2}t^2 \mathsf{d}(\theta, \tilde{\theta})^2}, \quad \forall\ \theta, \tilde{\theta} \in \Theta,\ t \geq 0$*. A stochastic process* $(X_\theta)_{\theta \in \Theta}$ *is separable if there exists a countable subset* $\Theta_0 \subseteq \Theta$ *and a probability null set* $\mathcal{N}$ *such that for every* $\omega \notin \mathcal{N}$ *and* $\theta \in \Theta$*, there exists a sequence* $(\theta_n)_{n \in \mathbb{N}}$ *in* Θ_0 *such that* $\mathsf{d}(\theta_n, \theta) \to 0$ *and* $X_{\theta_n}(\omega) \to X_\theta(\omega)$*.*

2.5 Approximating Functions and Operators in Quantum Neural Estimation

At the core of our framework is the question of approximating the eigenvalues and eigenvectors of Hermitian operators. In order for this approximation to hold uniformly over a class of density operators of interest, we require the neural class and quantum circuit to be sufficiently expressive. On the other hand, the complexity of these approximating classes should be balanced so that the statistical component of the estimation error is minimized. To this end, we assume that the neural class satisfies the (mild) high-level assumptions stated below, which, in particular, are satisfied by feedforward neural nets with finite width and depth, bounded parameters and common continuous activations such as rectified linear (ReLU) and sigmoid. After stating these for the neural class, we provide some basic definitions for quantum circuits.

2.5.1 Classical Neural Networks

To handle the approximation error, we will employ bounds from approximation theory for neural networks. For this purpose, we embed the set $\{1, \ldots, d\}$ indexing the eigenvalues as points into the Euclidean space $\mathbb{R}^m$, and we consider the neural net approximation of a function whose values at these points are equal to the eigenvalues of $H^\star(\rho, \sigma)$ or $H^\star_\alpha(\rho, \sigma)$. To account for a broad class of embeddings (an injective map) and classical neural nets, we formulate a general framework and state the assumptions under which our bounds hold. Later, we consider natural instances of embeddings and neural nets that satisfy these assumptions. To obtain a handle on the statistical error, we require that the neural class has bounded complexity, quantified in terms of the covering entropy as stated below.

For a positive integer $\ell \leq d$, let $e_m \colon \{1, \ldots, d\} \mapsto \mathbb{R}^m$ denote an embedding, and let $\mathcal{X} \coloneqq \{e_m(i)\}_{i=1}^d$ be the set of embedded points. Let $\mathcal{F}_{b,\mathcal{X}}$ denote the class of continuous functions $f \colon \mathbb{R}^m \mapsto \mathbb{R}$ such that $\|f\|_{\infty,\mathcal{X}} \leq \log b$, which we will simply denote by $\mathcal{F}_b$.

Assumption 1 (Assumptions on neural class)**.** *The neural class* $\mathcal{F}$ *is a closed subset of* $\mathcal{F}_b$ *and satisfies*

$$\log N(2\epsilon \log b, \mathcal{F}, \|\cdot\|_{\infty,\mathcal{X}}) \leq \bar{\kappa}(\mathcal{F}, \epsilon), \qquad \forall \epsilon \in (0, 1], \tag{15a}$$

where $\bar{\kappa}(\mathcal{F},\epsilon) \geq 0$ *is such that*

$$\kappa(\mathcal{F}) \coloneqq \int_0^1 \sqrt{\bar{\kappa}(\mathcal{F},\epsilon)}\, d\epsilon < \infty. \tag{15b}$$

2.5.2 Parametrized Quantum Circuits

For a fixed enumeration $\mathbf{P} \coloneqq \{P_i^\star\}_{i=1}^d$ of the set of orthogonal rank-one projectors in the spectral decomposition of $H_\alpha^\star(\rho,\sigma)$ satisfying (5) and (6), let $U^\star(\mathbf{P})$ be the unitary such that $U^\star(\mathbf{P})|i\rangle\langle i|\left(U^\star(\mathbf{P})\right)^\dagger = P_i^\star$ for all i. For $\mathcal{S} \subseteq \mathbb{S}_d \times \mathbb{S}_d$, let

$$\mathcal{U}_\alpha^\star(\mathcal{S}) \coloneqq \{U^\star(\mathbf{P}) : \mathbf{P} \text{ is a given enumeration of eigenprojectors of } H_\alpha^\star(\rho,\sigma) \text{ for } (\rho,\sigma) \in \mathcal{S}\}. \tag{16}$$

Note that although the RHS of (16) implicitly depends on the specific enumeration $\mathbf{P}$ of the eigen-projectors (which is not necessarily unique) of $H_\alpha^\star(\rho,\sigma)$ for $(\rho,\sigma) \in \mathcal{S}$, we suppress this dependence for simplicity. Let $\mathcal{U}_\alpha(\delta,\mathcal{S})$ denote a δ-covering of $\mathcal{U}_\alpha^\star(\mathcal{S})$ in the operator norm. In other words, $\mathcal{U}_\alpha(\delta,\mathcal{S})$ denotes a PQC composed of a (finite) set of unitary operators, parametrized by $\boldsymbol{\theta} \in \Theta_\alpha(\delta,\mathcal{S})$ such that for every $U^\star \in \mathcal{U}_\alpha^\star(\mathcal{S})$, there exists $U(\boldsymbol{\theta})$ satisfying

$$\|U^\star - U(\boldsymbol{\theta})\| \leq \delta. \tag{17}$$

For all $\mathcal{S}$, an application of the Solovay–Kitaev theorem (see Appendix E) guarantees that such a $\mathcal{U}_\alpha(\delta,\mathcal{S})$ exists. Set $\mathcal{U}^\star(\mathcal{S}) \coloneqq \mathcal{U}_1^\star(\mathcal{S})$, $\mathcal{U}(\delta,\mathcal{S}) \coloneqq \mathcal{U}_1(\delta,\mathcal{S})$ and $\Theta(\delta,\mathcal{S}) \coloneqq \Theta_1(\delta,\mathcal{S})$. In practice, PQCs generated by commonly employed ansätze such as the hardware efficient ansatz [80], alternating layered ansatz [63], or alternating operator ansatz for quantum approximate optimization algorithm (QAOA) could be used for QNE, among which the latter is known to be universal for emulating a general quantum circuit given sufficient circuit length [81, 82]. Since the construction of the PQC is not our focus, we henceforth assume that an efficient parametrized quantum circuit architecture implementing $\mathcal{U}_\alpha(\delta,\mathcal{S})$ is given.

3 Performance Guarantees for Quantum Neural Estimation

In this section, we obtain upper bounds on the expected absolute error achieved by the QNE for estimating measured relative entropy, along with a sub-Gaussian concentration inequality for this error. Before doing so, let us establish a few definitions. Let $\Lambda_\alpha^\star(\rho,\sigma)$ be the set of eigenvalues of $H_\alpha^\star(\rho,\sigma)$, where $H_\alpha^\star(\rho,\sigma)$ is a Hermitian operator satisfying (5) and (6). For a given set $\mathcal{S}$ of density operators and a set $\mathcal{F}$ of real-valued functions supported on $\mathcal{X}$, set

$$\varepsilon_\alpha(\mathcal{F},\mathcal{S}) \coloneqq \min_{f\in\mathcal{F}} \sup_{(\rho,\sigma)\in\mathcal{S}} \max_{\{\lambda_{i,\alpha}^\star\}_{i=1}^d} \max_{i\in[1:d]} \left| f(e_m(i)) - \lambda_{i,\alpha}^\star \right|, \tag{18}$$

where the inner maximization is over all possible enumerations $\{\lambda_{i,\alpha}^\star\}_{i=1}^d$ of $\Lambda_\alpha^\star(\rho,\sigma)$. Set $\varepsilon(\mathcal{F},\mathcal{S}) \coloneqq \varepsilon_1(\mathcal{F},\mathcal{S})$. These quantities provide a uniform upper bound (over the class $\mathcal{S}$) on the component of error arising due to neural network approximation of any enumeration of the eigenvalues of $H_\alpha^\star(\rho,\sigma)$, and will play a role in the performance guarantees for QNE given below.

3.1 Measured Relative Entropy

We start with our main result for measured relative entropy QNE.

Theorem 1 (Performance guarantees for measured relative entropy)**.** *Consider a QNE for estimating* $\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)$ *with classical neural net* $\mathcal{F} \subseteq \mathcal{F}_b$ *satisfying Assumption 1 and a PQC* $\mathcal{U}(\delta, \mathcal{S})$ *parametrized by* $\Theta(\delta, \mathcal{S})$ *for* $\mathcal{S} \subseteq \mathcal{S}_d(b)$*. Setting* $\xi_{\mathcal{F},\mathcal{S},\delta,b} \coloneqq \varepsilon(\mathcal{F}, \mathcal{S})(b+1) + 2\delta(b + \log b)$*, we have*

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{E}\Big[\Big|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}^{n}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}\Big|\Big] \leq \xi_{\mathcal{F},\mathcal{S},\delta,b} + 48(b+1)(\log b)\,\kappa(\mathcal{F})\,n^{-\frac{1}{2}}, \tag{19}$$

where $\kappa(\mathcal{F})$ *and* $\varepsilon(\mathcal{F}, \mathcal{S})$ *are as given in* (15b) *and* (18)*, respectively. Moreover, for all* $z \geq 0$*, we have*

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{P}\left(\Big|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}^{n}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}\Big| \geq \xi_{\mathcal{F},\mathcal{S},\delta,b} + 128(b+1)(\log b)\big(n^{-\frac{1}{2}}\kappa(\mathcal{F}) + z\big)\right) \leq 2e^{-nz^2}. \tag{20}$$

The proof of Theorem 1 is given in Section 5.1, and relies on upper bounding the (absolute) error as the sum of approximation and statistical components, i.e., $\mathbb{E}[\text{error}] \leq$ approx. err $+ \mathbb{E}[$stat. err$]$. This is enabled by the compatible structure of the variational form of measured relative entropy (see (4)) and its QNE (see (13b)). The approximation error arises as a consequence of parameterizing the Hermitian operator in the variational form using a hybrid model composed of PQCs and neural nets, while the statistical error is due to replacing expectations therein by the corresponding empirical averages with respect to measurement outcomes. The approximation error can be made arbitrary small by choosing a sufficiently large hybrid model, thanks to the universal approximation property of suitable neural nets and PQCs for approximating continuous functions and unitaries, respectively.

Choosing an expressive model to reduce the approximation error, however, comes at the cost of increased statistical complexity of the model. The associated statistical error can be bounded in terms of the suprema of separable sub-Gaussian processes indexed by the neural class and quantum circuit parameters, which is a key object of interest in empirical process theory and can be analyzed using the tools therein. In particular, the expected statistical error can be upper bounded in terms of a covering entropy integral [78, Corollary 5.25] with the random fluctuations around the latter exhibiting sub-Gaussian concentration [78, Theorem 5.29] (see Theorem 12 below). Leveraging the aforementioned results, Theorem 1 quantifies the approximation and statistical errors for a given neural net $\mathcal{F}$ satisfying Assumption 1 and PQC $\mathcal{U}(\delta, \mathcal{S})$. In (19), the term $\xi_{\mathcal{F},\mathcal{S},\delta,b}$ corresponds to the approximation error component, with $\varepsilon(\mathcal{F}, \mathcal{S})$ and δ denoting the neural net and PQC approximation parameter, respectively. The second term in (19), which decays at rate $n^{-\frac{1}{2}}$, corresponds to the statistical component. Below, we will instantiate Theorem 1 to shallow (Corollary 2) and deep (Proposition 4) nets, where we explicitly quantify $\xi_{\mathcal{F},\mathcal{S},\delta,b}$ and $\kappa(\mathcal{F})$ in terms of neural net parameters.

Remark 1 (Effective copy complexity)**.** *Since each inner loop of the QNE consumes* n *copies of both* ρ *and* σ*, the effective copy complexity of the algorithm that achieves the expected absolute error bound given in Theorem 1 is* $O\big(n|\Theta(\delta, \mathcal{S})|\big)$*. Given this, it is of interest to determine or characterize the classes* $\mathcal{S}$ *for which* $|\Theta(\delta, \mathcal{S})|$ *scales benignly as a function of* δ*. However, this turns out to be a non-trivial problem, closely related to that of characterizing the class of unitaries which can be efficiently approximated. Nevertheless, in Section 4 below, we will consider certain classes of states exhibiting symmetries for which the copy complexity scales efficiently.*

Next, we specialize Theorem 1 by considering specific embeddings and neural classes. We first define the neural class of interest.

Definition 3 (Neural network class)**.** *Let $2 \leq L \in \mathbb{N}$, $k_0 = m$, $k_1, \ldots, k_{L-1} \in \mathbb{N}$, and $k_L = 1$. A neural network with L layers and activation $\varphi\colon \mathbb{R} \mapsto \mathbb{R}$ is a map $f\colon \mathbb{R}^{k_0} \mapsto \mathbb{R}$ given by*

$$f \coloneqq \begin{cases} W_2 \circ \varphi \circ W_1, & L = 2, \\ W_L \circ \varphi \circ W_{L-1} \circ \varphi \circ \cdots \circ \varphi \circ W_1, & L \geq 3, \end{cases} \tag{21}$$

where for $\ell \in \{1, \ldots, L\}$, $W_\ell\colon \mathbb{R}^{k_\ell} \mapsto \mathbb{R}^{k_{\ell-1}}$, $W_\ell x \coloneqq A_\ell x + b_\ell$ are affine maps with matrices $A_\ell \in \mathbb{R}^{k_\ell \times k_{\ell-1}}$ and bias vectors $b_\ell \in \mathbb{R}^{k_\ell}$, and the activation φ acts component-wise as $\varphi(x_1, \ldots, x_k) = (\varphi(x_1), \ldots, \varphi(x_k))$. For $M \in \mathbb{R}_{\geq 0}$, let $\mathcal{F}^{\mathrm{NN}}(L, K, M, m, \varphi)$ be the set of all such f with $\max_{0 \leq \ell \leq L} k_\ell \leq K$ and $\max_{1 \leq \ell \leq L} \|A_\ell\|_{\max} \vee \|b_\ell\|_{\max} \leq M$, where $\|A\|_{\max} \coloneqq \max_{i,j} |A_{i,j}|$ is the maximum of the absolute values of the entries of A. Henceforth, we take φ as the ReLU function $\varphi_{\mathrm{R}}(x) \coloneqq x \vee 0$ unless specified otherwise, and set $\mathcal{F}^{\mathrm{NN}}(L, K, M, m) \coloneqq \mathcal{F}^{\mathrm{NN}}(L, K, M, m, \varphi_{\mathrm{R}})$.

Performance Guarantees with Shallow Nets

We start by treating the shallow neural class, $\mathcal{F}^{\mathrm{SNN}}(K, M, m) \coloneqq \mathcal{F}^{\mathrm{NN}}(2, K, M, m)$, with the canonical embedding $e_d\colon i \mapsto |i\rangle$, where $|i\rangle$ is a d-dimensional vector with 1 in the i^{th} position and 0 elsewhere. Consider the following shallow neural class with d neurons in the hidden layer:

$$\tilde{\mathcal{F}}^{\mathrm{SNN}}(d, M) \coloneqq \left\{ f(x) = \sum_{j=1}^{d} \beta_j \varphi_{\mathrm{R}}(\langle j, x \rangle),\ x \in \mathbb{R}^d : |\beta_j| \leq M,\ j \in [1:d] \right\} \subseteq \mathcal{F}^{\mathrm{SNN}}(d, M, d).$$

The next corollary bounds the expected absolute error achieved by the QNE with such a neural net.

Corollary 2 (Performance guarantees with shallow nets)**.** *The following hold for $\mathcal{S} \subseteq \mathcal{S}_d(b)$ with $a(\delta, b) \coloneqq 2\delta(b + \log b)$:*

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{E}\left[\left|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\Theta(\delta,\mathcal{S}),\tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b)}\right|\right] \leq a(\delta, b) + 96(\log b)(b+1)d^{\frac{1}{2}}n^{-\frac{1}{2}}, \tag{22a}$$

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{P}\left(\left|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\Theta(\delta,\mathcal{S}),\tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b)}\right| \geq a(\delta, b) + 128(\log b)(b+1)\left(2d^{\frac{1}{2}}n^{-\frac{1}{2}} + z\right)\right)$$
$$\leq 2e^{-nz^2}, \quad \forall\ z \geq 0. \tag{22b}$$

The proof of Corollary 2 is given in Section 5.2, and it follows from Theorem 1 by showing that $\varepsilon(\tilde{\mathcal{F}}^{\mathrm{SNN}}(d, \log b), \mathcal{S}_d(b)) = 0$ and $\kappa(\tilde{\mathcal{F}}^{\mathrm{SNN}}(d, \log b)) \leq 2\sqrt{d}$. From (22a), we observe that given n copies of the quantum states ρ, σ, the expected absolute error of the QNE for estimating $\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)$ over $(\rho, \sigma) \in \mathcal{S}_d(b)$ with neural class $\mathcal{F}^{\mathrm{SNN}}(d, \log b)$ and quantum circuit $\mathcal{U}(\delta, \mathcal{S})$ is $O(b(\log b + 1)(\delta + D^{1/2}n^{-1/2}))$, where $D \coloneqq d\,\Theta(\delta, \mathcal{S}_d(b))$.

Remark 2 (Lower bound on minimax risk)**.** *It is instructive to compare the expected absolute error of QNE with the following lower bound on the expected minimax risk for estimating classical relative entropy which holds when $db \lesssim n \log d$ and $b \geq (\log d)^2 \vee 2$:*

$$R^\star_n(\mathcal{S}_d(b)) \gtrsim \frac{\sqrt{b}}{\sqrt{n}} + \frac{db}{n \log d}. \tag{23}$$

This bound can be distilled from the results in [83] and [84] by slightly modifying the proofs therein to account for the class $\mathcal{S}_d(b)$ considered herein (see Appendix B). From (22a) and (23), it thus follows that the expected minimax risk over $\mathcal{S}_d(b)$ has a parametric rate of convergence in n (independent of d), and moreover that it is achieved by the QNE with a shallow net. However, there is a mismatch in the dependence on d in (22a) and (23) as the second term in the lower bound scales as $\Omega_b(d \log d/n)$ for $d \log d/n \lesssim 1$ whereas the upper bound is $O_b(d^{1/2} n^{-1/2})$ with $\delta = 0$ (applicable in the classical setting). That said, this mismatch is not unexpected as achieving the optimal dependence on d requires explicit bias-correction mechanisms even in the classical case, which is not performed by the QNE.

Performance Guarantees with Deep Nets

We next derive performance guarantees for QNEs realized by deep neural nets. For this purpose, we consider the one-dimensional embedding into $\mathbb{R}$ given by $e_1 \colon i \mapsto i/d$. Let

$$\mathcal{P}_k(a) \coloneqq \left\{ p(x) = \sum_{i=0}^{k} a_i x^i,\ x \in \mathbb{R} : \|\boldsymbol{a}\|_\infty \leq a \right\},$$

denote the class of univariate polynomials of degree at most k and magnitude of coefficients, $\boldsymbol{a} \coloneqq (a_0, \ldots, a_k)$, bounded by a. We define the following class of density operator pairs for $\alpha > 0$:

$$\tilde{\mathcal{S}}_{k,d,\alpha}(b, a, \varepsilon) \coloneqq \left\{ (\rho, \sigma) \in \mathcal{S}_d(b) : \begin{array}{c} \text{for any enumeration } \Lambda^\star_\alpha(\rho,\sigma) = \{\lambda^\star_{i,\alpha}\}_{i=1}^d, \\ \exists\ p \in \mathcal{P}_k(a) \text{ s.t. } \max\limits_{i \in [1:d]} \left| p(e_1(i)) - \lambda^\star_{i,\alpha} \right| \leq \varepsilon \end{array} \right\}. \tag{24}$$

In other words, $\tilde{\mathcal{S}}_{k,d,\alpha}(b, a, \varepsilon)$ is the class of density operator pairs $(\rho, \sigma) \in \mathcal{S}_d(b)$ such that any ordering of the eigenvalues $\Lambda^\star_\alpha(\rho, \sigma)$ of the optimizer $H^\star_\alpha(\rho, \sigma)$, embedded into the interval $[0, 1]$ in a uniformly spaced manner, can be approximated within ε precision by a real polynomial of degree at most k and absolute value of coefficients bounded by a.

While $\tilde{\mathcal{S}}_{k,d,\alpha}(b, a, \varepsilon) \subseteq \mathcal{S}_d(b)$ by definition, Proposition 3 below shows that $\tilde{\mathcal{S}}_{k,d,\alpha}(b, a, \varepsilon) = \mathcal{S}_d(b)$ for k, a, and ε sufficiently large.

Proposition 3 (Relation between classes of density operators)**.** *The following hold for all $\alpha > 0$:*

(i) For all $k \geq d - 1$, $a \geq ((3e)^d \log b)/(2\pi)$, and $\varepsilon \geq 0$,

$$\tilde{\mathcal{S}}_{k,d,\alpha}(b, a, \varepsilon) = \mathcal{S}_d(b).$$

(ii) For all $k \in \mathbb{N}$, $a \geq 2^k k! \log b$, and $\varepsilon \geq (2d + 0.5)\, k^{-\frac{1}{3}} \log b$,

$$\tilde{\mathcal{S}}_{k,d,\alpha}(b, a, \varepsilon) = \mathcal{S}_d(b).$$

See Appendix C for a proof. For proving Proposition 3 (i), given $\{\lambda_i\}_{i=1}^d$ such that $\max_{1 \leq i \leq d} |\lambda_i| \leq \log b$, we simply construct a polynomial p of degree $d-1$ such that $p(i/d) = \lambda_i$ for $i \in [1 : d]$ and obtain an upper bound on its coefficients. For a proof of Part (ii), we consider an intermediate Lipschitz continuous function $\hat{f}$ such that $\hat{f}(i/d) = \lambda_i$ and quantify the error of approximating this function via Bernstein polynomials of degree at most k whose coefficients are bounded as given therein. The next proposition provides an upper bound on the expected absolute error (along with a deviation inequality) for

estimating the measured relative entropy, achieved by a QNE that employs a fixed width deep neural net with appropriately chosen parameters. Let

$$\tilde{\mathcal{F}}^{\mathrm{NN}}(L,K,M,1) \coloneqq \left\{ \begin{matrix} \tilde{f}(x) = f(x)\mathbb{1}_{|f(x)|\leq \log b} + (\log b)\big(\mathbb{1}_{f(x)>\log b} - \mathbb{1}_{f(x)<-\log b}\big) \\ : f \in \mathcal{F}^{\mathrm{NN}}(L,K,M,1) \end{matrix} \right\}. \tag{25}$$

That is, $\tilde{\mathcal{F}}^{\mathrm{NN}}(L,K,M,1)$ is the neural network class $\mathcal{F}^{\mathrm{NN}}(L,K,M,1)$ (see Definition 3) with the function values saturated at $\pm \log b$. Set $\tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon) \coloneqq \tilde{\mathcal{S}}_{k,d,1}(b,a,\varepsilon)$.

Proposition 4 (Performance guarantees with deep nets)**.** *There exists a constant $c>0$ such that setting*

$$L_{\varepsilon,k,a} \coloneqq ck\left(\log(\varepsilon^{-1}) + \log k + \log a\right), \tag{26a}$$

$$B_{\varepsilon,k,a,b} \coloneqq 24 L_{\varepsilon,k,a}\log b + 13\sqrt{L_{\varepsilon,k,a}\log b}, \tag{26b}$$

$\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a}) \equiv \tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a},9,1,1)$ *and* $\mathcal{S} \subseteq \tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon)$*, the following hold for all* $z \geq 0$*:*

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{E}\Big[\Big|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}^{n}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a})}\Big|\Big] \leq 2(b+1)\varepsilon + 2\delta(b+\log b) + 48(b+1)B_{\varepsilon,k,a,b}n^{-\frac{1}{2}}. \tag{27}$$

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{P}\Bigg(\Big|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}^{n}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a})}\Big| \geq 2(b+1)\varepsilon + 2\delta(b+\log b) + 128(b+1)\left(B_{\varepsilon,k,a,b}n^{-\frac{1}{2}} + z\log b\right)\Bigg) \leq 2e^{-nz^2}. \tag{28}$$

The proof of Proposition 4 (see Section 5.3) follows from Theorem 1 by using the neural class $\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a})$, which is rich enough to approximate polynomials of degree k and coefficients uniformly bounded by a, up to an error of ε, thanks to the results in [85]. The unspecified constant c in the definition of $L_{\varepsilon,k,a}$ is the same one that appears in [85, Proposition III.5]. Leveraging this approximation result and upper bounding $\kappa(\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a}))$ leads to the claim in (28). The advantage of Proposition 4 compared to Corollary 2 is that the bounds are independent of the dimension d, albeit over a sub-class, $\tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon)$, of $\mathcal{S}_d(b)$.

3.2 Measured Rényi Relative entropy

The following analogue of Theorem 1 holds for the measured Rényi relative entropy.

Theorem 5 (Performance guarantees for measured Rényi relative entropy)**.** *Let $\alpha \in (0,1)\cup(1,\infty)$. Consider a QNE for estimating $\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma)$ with classical neural net $\mathcal{F} \subseteq \mathcal{F}_b$ satisfying Assumption 1 and a PQC $\mathcal{U}_\alpha(\delta,\mathcal{S})$ parametrized by $\Theta_\alpha(\delta,\mathcal{S})$. Setting*

$$\xi_{\mathcal{F},\mathcal{S},\delta,b,\alpha} \coloneqq \alpha\left(b^{|\alpha-1|} + b^{\alpha}\right)\varepsilon_\alpha(\mathcal{F},\mathcal{S}) + 2\left(\frac{\alpha}{|\alpha-1|}b^{|\alpha-1|} + b^{\alpha}\right)\delta,$$

we have for $\mathcal{S} \subseteq \mathcal{S}_d(b)$ and $z \geq 0$ that

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{E}\Big[\Big|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \hat{\mathsf{D}}^{n}_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\mathcal{F}}\Big|\Big] \leq \xi_{\mathcal{F},\mathcal{S},\delta,b,\alpha} + 48\alpha\big(b^{\alpha}+b^{|\alpha-1|}\big)(\log b)\,\kappa(\mathcal{F})n^{-\frac{1}{2}}, \tag{29}$$

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{P}\Bigg(\Big|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \hat{\mathsf{D}}^{n}_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\mathcal{F}}\Big| \geq \xi_{\mathcal{F},\mathcal{S},\delta,b,\alpha} + 128\alpha\big(b^{\alpha}+b^{|\alpha-1|}\big)(\log b) \times \left(\kappa(\mathcal{F})n^{-\frac{1}{2}} + z\right)\Bigg) \leq 2e^{-nz^2}. \tag{30}$$

The proof of Theorem 5 is analogous to that of Theorem 1, and is given in Section 5.4 below.

Specializing Theorem 5 to a QNE employing the shallow neural net used in Corollary 2, we obtain the result stated below (proof is omitted as it is similar to Corollary 2).

Corollary 6 (Performance guarantees with shallow neural net)**.** *Let $\alpha \in (0,1) \cup (1,\infty)$. The following hold with $\mathcal{S} \subseteq \mathcal{S}_d(b)$ for all $z \geq 0$:*

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{E}\Big[\Big|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b)}\Big|\Big] \leq 2\left(\frac{\alpha}{|\alpha-1|}b^{|\alpha-1|} + b^\alpha\right)\delta + 96\alpha(b^\alpha + b^{|\alpha-1|})(\log b) d^{\frac{1}{2}} n^{-\frac{1}{2}}, \quad (31a)$$

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{P}\left(\left|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b)}\right| \geq 2\left(\frac{\alpha}{|\alpha-1|}b^{|\alpha-1|} + b^\alpha\right)\delta + 128\alpha(b^\alpha + b^{|\alpha-1|})(\log b)(2d^{\frac{1}{2}} n^{-\frac{1}{2}} + z)\right) \leq 2e^{-nz^2}. \quad (31b)$$

To benchmark the above performance guarantees, one may compare it with the following lower bound on the minimax which holds when $db^\alpha \lesssim n \log d$, $b \geq (\log d)^2 \vee 2$ and $\alpha > 1$:

$$R^\star_{n,\alpha}(\mathcal{S}_d(b)) \gtrsim_\alpha \frac{\sqrt{b}}{\sqrt{n}} + \frac{db}{n \log d}. \quad (32)$$

This claim (see Appendix B for a proof) follows from the lower bound on the minimax risk for classical α-divergence estimation obtained in [84], by tweaking the proof therein to account for the class $\mathcal{S}_d(b)$ and noting that $R^\star_{n,\alpha}(\mathcal{S}_d(b))$ can be lower bounded in terms of this minimax risk (up to multiplicative constants which depend on α and b). On the other hand, given n copies of the quantum states ρ, σ, the expected absolute error achieved by QNE for estimating $\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma)$ as quantified in (31a) is $O_{\alpha,b}(D^{1/2}n^{-1/2})$, where $D = \Theta_\alpha(\delta, \mathcal{S}_d(b))\, d$. Comparing these two bounds, it follows that the QNE achieves the parametric rate of convergence in n, meaning it is minimax optimal for estimating measured Rényi relative entropy over $\mathcal{S}_d(b)$.

The next proposition also follows from Theorem 5 by specializing to a QNE realized by the deep neural net from Proposition 4.

Proposition 7 (Performance guarantees with deep neural net)**.** *Let $\alpha \in (0,1)\cup(1,\infty)$, let $\tilde{\mathcal{S}}_{k,d,\alpha}(b,a,\varepsilon)$ be the class of density operator pairs defined in (24), and let $\tilde{\mathcal{F}}^{\mathrm{NN}}(L,K,M,1)$ be the neural class given in (25). With $L_{\varepsilon,k,a}$, $B_{\varepsilon,k,a,b}$ as defined in (26a) and $\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a}) \equiv \tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a},9,1,1)$, the following holds for all $\mathcal{S} \subseteq \tilde{\mathcal{S}}_{k,d,\alpha}(b,a,\varepsilon)$ and $z \geq 0$:*

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{E}\Big[\Big|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a})}\Big|\Big] \leq 2\alpha(b^\alpha + b^{|\alpha-1|})(\varepsilon + 24B_{\varepsilon,k,a,b}n^{-\frac{1}{2}}) + 2\left(\frac{\alpha}{|\alpha-1|}b^{|\alpha-1|} + b^\alpha\right)\delta,$$

$$\sup_{(\rho,\sigma)\in\mathcal{S}} \mathbb{P}\left(\left|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a})}\right| \geq 2\left(\frac{\alpha}{|\alpha-1|}b^{|\alpha-1|} + b^\alpha\right)\delta + 2\alpha\Big(b^\alpha + b^{|\alpha-1|}\Big)\Big(\varepsilon + 64B_{\varepsilon,k,a,b}n^{-\frac{1}{2}} + 64z\log b\Big)\right) \leq 2e^{-nz^2}.$$

The proof of Proposition 7 follows similarly to the proof of Proposition 4, and hence is omitted.

4 Copy Complexity for Quantum Neural Estimation of Entropies

Here, we examine the copy complexity of QNE, focusing on measured relative entropy. The case of measured Rényi relative entropy is similar. As mentioned earlier, the number of copies of ρ and σ consumed by QNE in the worst case scales proportionally to $|\Theta(\delta, \mathcal{S})|$. Hence, it is of interest to understand how the number of parameters of efficient PQCs scales as δ shrinks, since this dependence directly affects the copy complexity. To get more insight into this aspect, consider the setting where $d = 2^N$, with N denoting the number of qubits. An application of the Solovay–Kitaev theorem (see Appendix E) shows that, for all $\mathcal{S} \subseteq \mathbb{S}_d \times \mathbb{S}_d$, there exists a PQC $\mathcal{U}(\delta, \mathcal{S})$ with $|\Theta(\delta, \mathcal{S})| = O\Big(\big(N^2 4^N \delta^{-1}\big)^{N^2 4^N}\Big)$. The super-exponential dependence of $|\Theta(\delta, \mathcal{S})|$ on N is a consequence of the requirement that the quantum circuit be able to universally approximate the whole unitary group uniformly. Moreover, when $\mathcal{S} = \mathbb{S}_d \times \mathbb{S}_d$, a lower bound based on a covering argument shows that such a dependence on N is unavoidable (see, e.g., [86, Section 4.5.4]).

Given that an exponential dependence on N is undesirable for practically realistic algorithms, it is of interest to determine conditions on $\mathcal{S}$ under which $|\Theta(\delta, \mathcal{S})|$ or the QNE copy complexity scales more efficiently, say polynomially or poly-logarithmically in N. The aforementioned determination is challenging for two reasons. First, the projectors $\{P_i^\star\}_{i=1}^d$ appearing in the spectral decomposition of $H^\star(\rho, \sigma)$, and consequently in the definition of $\mathcal{U}(\delta, \mathcal{S})$, do not have a closed-form expression. Second, even if such a characterization is available, determining the sets $\mathcal{S}$ for which (17) holds with an efficiently realizable PQC is known to be a hard problem. In fact, it is closely related to the problem of characterizing the classes of unitaries which can be efficiently approximated. Given this, a pertinent approach is to fix a PQC $\mathcal{U}$, as is the case in practice, and consider the classes $\mathcal{S}$ for which efficient QNEs exist.

To this end, let us recall the necessary and sufficient condition that the optimizer $H^\star(\rho, \sigma) = \log \omega^\star(\rho, \sigma)$ should satisfy, which can be obtained as the limit $\alpha \to 1$ of (10) (see Appendix A):

$$\sigma = \int_0^\infty \left(\omega^\star(\rho,\sigma) + sI\right)^{-1} \rho \left(\omega^\star(\rho,\sigma) + sI\right)^{-1} ds.$$

Solving this equation analytically to determine $\omega^\star(\rho, \sigma)$ appears challenging. Nevertheless, we can leverage it to determine a class of density operator pairs over which our copy complexity results hold. For a given $\rho \in \mathbb{S}_d$, unitary U on $\mathbb{H}_d$ and $b \geq 1$, let

$$\Omega(b, \rho, U) \coloneqq \left\{ \omega = \sum_{i=1}^d \frac{\mathrm{Tr}\left[U|i\rangle\langle i|U^\dagger \rho\right]}{v_i} U|i\rangle\langle i|U^\dagger : \begin{array}{l} \mathbf{v} \in (0,1]^d,\ \sum_{i=1}^d v_i = 1 \text{ and} \\ \dfrac{1}{b} \leq \dfrac{\mathrm{Tr}\left[U|i\rangle\langle i|U^\dagger \rho\right]}{v_i} \leq b,\ \forall\ i \in [1:d] \end{array} \right\}.$$

Setting $\sigma(\rho, \omega) \coloneqq \int_0^\infty \left(\omega + sI\right)^{-1} \rho \left(\omega + sI\right)^{-1} ds$ for $\omega \in \Omega(b, \rho, U)$, it is easy to see that $\sigma(\rho, \omega) \in \mathbb{S}_d$ since $\rho \mapsto \sigma(\rho, \omega)$ is a completely positive map and $\mathrm{Tr}[\sigma(\rho, \omega)] = \mathrm{Tr}\left[\rho \omega^{-1}\right] = \sum_{i=1}^d v_i = 1$. Hence, for a given PQC $\mathcal{U}$, define

$$\bar{\mathcal{S}}_d(\delta, b, \mathcal{U}) \coloneqq \left\{ (\rho, \sigma(\rho,\omega)) \in \mathcal{S}_d(b) : \begin{array}{l} \omega \in \Omega(b, \rho, U) \text{ for } U \text{ s.t. } \exists\, U(\boldsymbol{\theta}) \in \mathcal{U} \\ \text{satisfying } \|U - U(\boldsymbol{\theta})\| \leq \delta \end{array} \right\}, \tag{33}$$

i.e., $\bar{\mathcal{S}}_d(\delta, b, \mathcal{U})$ is the class of density operator pairs within $\mathcal{S}_d(b)$ such that the eigenbasis of the optimizer $H^\star(\rho, \sigma)$ (or $\omega^\star(\rho, \sigma)$) can be approximated by the PQC $\mathcal{U}$ within an

accuracy of δ. Given a PQC $\mathcal{U}$, $\bar{\mathcal{S}}_d(\delta, b, \mathcal{U})$ can be determined in principle by computing $(\rho, \sigma(\rho, \omega))$ pairs over $\omega \in \Omega(b, \rho, U)$ as in (33) and ascertaining if the pair lies within $\mathcal{S}_d(b)$.

The next result provides a copy complexity bound for the QNE with a shallow net and a PQC $\mathcal{U}$ with parameter set $\Theta(\mathcal{U})$.

Proposition 8 (Copy complexity of QNE)**.** *Let $\epsilon \geq 0$ and $b \geq 1$. With probability at least $p \in [0, 1)$, QNE with shallow net $\tilde{\mathcal{F}}^{\mathrm{SNN}}(d, \log b)$ and PQC $\mathcal{U}$ estimates $\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)$ between $(\rho, \sigma) \in \bar{\mathcal{S}}_d(\epsilon_b, b, \mathcal{U})$ within an error of ϵ given $O(c_{b,p}^2 d|\Theta(\mathcal{U})|\epsilon^{-2})$ copies each of ρ and σ, where $\epsilon_b = \epsilon/(4b + 4\log b)$ and $c_{b,p} \coloneqq (1 + \sqrt{-\log(1-p)})(b+1)\log b$.*

The proof of Proposition 8 follows immediately from Corollary 2 and can be found in Section 5.5. An analogous claim for QNE with a deep net and a quantum circuit $\mathcal{U}$ can be obtained by using Proposition 4 in place of Corollary 2, after setting $k = d - 1$, $a = ((3e)^d \log b)/(2\pi)$ according to Proposition 3(*i*).

Note that the copy complexity bound of QNE given in Proposition 8 is proportional to d, which scales exponentially in the number of qudits. We next show that a better copy complexity can be achieved by QNE when the states have additional symmetry, namely, permutation invariance. To state this result, let $d = m^N$ for some $m, N \in \mathbb{N}$, and take the underlying Hilbert space as $\mathbb{H}_d = \mathbb{H}_m^{\otimes N}$. Let S_N denote the symmetric group on $\{1, \ldots, N\}$, and let SU_d denote the special unitary group on $\mathbb{H}_d$. For a permutation $\pi \in \mathsf{S}_N$, define the permutation operator $V_m(\pi)$ to be the unitary operator such that

$$V_m(\pi)|i_1\rangle \otimes \cdots \otimes |i_N\rangle = |i_{\pi^{-1}(1)}\rangle \otimes \cdots \otimes |i_{\pi^{-1}(N)}\rangle, \tag{34}$$

for all $|i_1\rangle, \ldots, |i_N\rangle \in \mathbb{H}_m$. A state $\rho \in \mathcal{S}_d$ is permutation invariant if $V_m(\pi)\rho V_m(\pi)^\dagger = \rho$ for all $\pi \in \mathsf{S}_N$. Let $\mathfrak{P}(\mathbb{H}_m^{\otimes N})$ denote the class of all permutation-invariant states acting on $\mathbb{H}_m^{\otimes N}$.

The symmetries within the class $\mathfrak{P}(\mathbb{H}_m^{\otimes N})$ can be leveraged to construct a QNE whose copy complexity scales polynomially in N. The intuition for this improvement stems from the fact that the number of degrees of freedom of permutation-invariant operators acting on $\mathbb{H}_m^{\otimes N}$ scales polynomially in N. To utilize the underlying symmetries in the construction of QNE, we will rely on Schur–Weyl duality, which states that $\mathbb{H}_m^{\otimes N}$ can be written as (see, e.g., [87, Section 6.2]):

$$\mathbb{H}_d = \mathbb{H}_m^{\otimes N} = \bigoplus_{\kappa \in Y_m^N} \mathcal{W}_\kappa \otimes \mathcal{V}_\kappa, \tag{35}$$

where κ indexes the Young frames Y_m^N (with depth at most m and number of boxes N), and $\mathcal{W}_\kappa$ (resp. $\mathcal{V}_\kappa$) denotes the corresponding irreducible space of SU_d (resp. S_N). Let $\mathcal{K}_{m,N} \coloneqq \bigoplus_\kappa \mathcal{W}_\kappa$, and let P_κ denote the projection onto $\mathcal{W}_\kappa \otimes \mathcal{V}_\kappa$. Consider the completely positive trace preserving (CPTP) map $\bar{\mathcal{N}} \colon \mathcal{L}(\mathbb{H}_d) \to \mathcal{L}(\mathcal{K}_{m,N})$ given by

$$\bar{\mathcal{N}}(\rho) \coloneqq \sum_\kappa \mathrm{Tr}_{\mathcal{V}_\kappa}[P_\kappa \rho P_\kappa], \tag{36}$$

where $\mathrm{Tr}_{\mathcal{V}_\kappa}[\cdot]$ denotes the partial trace with respect to $\mathcal{V}_\kappa$. The quantum channel $\bar{\mathcal{N}}$ will be used below as a pre-processing channel for QNE, which can be realized by applying the Schur transform in conjunction with the partial trace operation.

For a PQC $\mathcal{U}$ acting on $\mathcal{K}_{m,N}$, let $\bar{\mathcal{S}}_{|\mathcal{K}_{m,N}|}(\delta, b, \mathcal{U})$ denote the set of density operator pairs on $\mathcal{K}_{m,N}$ as defined by (33), where $|\mathcal{K}_{m,N}|$ denotes the dimension of the Hilbert space $\mathcal{K}_{m,N}$. With $\bar{P}_\kappa$ denoting the projection onto $\mathcal{W}_\kappa$, let $\bar{\mathcal{M}} \colon \mathcal{L}(\mathcal{K}_{m,N}) \to \mathcal{L}(\mathbb{H}_d)$ denote the CPTP map defined as

$$\bar{\mathcal{M}}(\bar{\rho}) = \sum_\kappa \bar{P}_\kappa \bar{\rho} \bar{P}_\kappa \otimes \pi_\kappa, \tag{37}$$

where $\pi_\kappa = I/|\mathcal{V}_k|$ denotes the maximally mixed state on $\mathcal{V}_\kappa$. Consider the following class of density operator pairs on $\mathbb{H}_m^{\otimes N}$:

$$\hat{\mathcal{S}}_{m,N}(\delta, b, \mathcal{U}) \coloneqq \left\{ (\bar{\mathcal{M}}(\bar{\rho}), \bar{\mathcal{M}}(\bar{\sigma})) : (\bar{\rho}, \bar{\sigma}) \in \bar{\mathcal{S}}_{|\mathcal{K}_{m,N}|}(\delta, b, \mathcal{U}) \right\}.$$

The next proposition shows that QNE achieves a polynomial (in the number of qudits) copy complexity for density operator pairs within $\hat{\mathcal{S}}_{m,N}(\delta, b, \mathcal{U})$.

Proposition 9 (Copy complexity with permutation invariant states)**.** *Let $\epsilon \geq 0$ and $b \geq 1$. With probability at least $p \in [0, 1)$, QNE with $\mathcal{N} = \bar{\mathcal{N}}$ as given in (36), shallow neural net $\tilde{\mathcal{F}}^{\mathrm{SNN}}(\bar{d}_{m,N}, \log b)$ and a PQC $\mathcal{U}$ acting on $\mathcal{K}_{m,N}$, estimates $\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)$ for $(\rho, \sigma) \in \hat{\mathcal{S}}_{m,N}(\epsilon_b, b, \mathcal{U})$ within an error ϵ given $O(c_{b,p}^2 \bar{d}_{m,N} |\Theta(\mathcal{U})| \epsilon^{-2})$ copies each of ρ and σ, where $\bar{d}_{m,N} \coloneqq (N+1)^{m-1} N^{\frac{m(m-1)}{2}}$ and $\epsilon_b, c_{b,p}$ are as given in Proposition 8.*

The proof of Proposition 9 is given in Section 5.6 and is based on the observation that the quantum channel $\bar{\mathcal{N}}$ in (36) preserves the measured relative entropy between two output states when the corresponding inputs are permutation-invariant. Hence, the QNE can be run on i.i.d. copies of $\bar{\mathcal{N}}(\rho)$ and $\bar{\mathcal{N}}(\sigma)$, which are density operators on a much smaller Hilbert space $\mathcal{K}_{m,N}$ whose dimension is polynomial in N. To show that neural net $\tilde{\mathcal{F}}^{\mathrm{SNN}}(\bar{d}_{m,N}, \log b)$ suffices for QNE on this smaller space, we will use the fact that the Thompson metric $T(\rho, \sigma)$ contracts under application of a quantum channel. Combining these observations, the claim follows via Corollary 2. Note that the copy complexity in Proposition 9 is proportional to $\bar{d}_{m,N}$, which is an exponential improvement over that given in Proposition 8. We conclude this section by noting that analogous statements as given in Propositions 8 and 9 can be obtained for measured Rényi relative entropy via Corollary 6 in place of Corollary 2.

5 Proofs

5.1 Proof of Theorem 1

We will use the following lemma, whose proof is given in Appendix D.

Lemma 10 (Eigenvalues of optimizer)**.** *If $(\rho, \sigma) \in \mathcal{S}_d(b)$, then $|\lambda| \leq \log b$ for $\lambda \in \Lambda_\alpha^\star(\rho, \sigma)$, where $\Lambda_\alpha^\star(\rho, \sigma)$ is the set of eigenvalues of $H_\alpha^\star(\rho, \sigma)$.*

Proceeding with the proof of Theorem 1, fix $(\rho, \sigma) \in \mathcal{S}$. Let

$$\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) \coloneqq \sup_{\boldsymbol{\theta} \in \Theta(\delta,\mathcal{S})} \mathsf{D}_{\mathsf{M},\boldsymbol{\theta},\mathcal{F}}(\rho\|\sigma),$$

where

$$\mathsf{D}_{\mathsf{M},\boldsymbol{\theta},\mathcal{F}}(\rho\|\sigma) \coloneqq \sup_{H \in \mathcal{H}(\boldsymbol{\theta},\mathcal{F})} \mathrm{Tr}[H\rho] - \mathrm{Tr}[e^H \sigma] + 1, \tag{38}$$

and

$$\mathcal{H}(\boldsymbol{\theta}, \mathcal{F}) \coloneqq \left\{ H = \sum_{i=1}^{d} f(i) U(\boldsymbol{\theta}) |i\rangle\langle i| U^\dagger(\boldsymbol{\theta}),\ f \in \mathcal{F} \right\}, \tag{39}$$

is the class of Hermitian operators realized by the classical neural net for a fixed quantum circuit with parameter $\boldsymbol{\theta}$. Then, the triangle inequality implies that

$$\left| \mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}} \right| \leq \left| \mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) \right|$$

$$+\left|\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)-\hat{\mathsf{D}}^{n}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}\right|, \tag{40}$$

where the first and second terms on the right-hand side are referred to as the approximation error and estimation error, respectively. Note that the estimation error is random, due to $\hat{\mathsf{D}}^{n}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}$ being dependent on the measurement outcomes.

We first upper bound the approximation error. Since $\rho,\sigma>0$, the supremum in (2) is achieved for some $H^\star := H^\star(\rho,\sigma)$ [34]. From the definition of the set $\mathcal{U}(\delta,\mathcal{S})$, there exists a unitary $U(\boldsymbol{\theta}^\star)$ for some $\boldsymbol{\theta}^\star\in\Theta(\delta,\mathcal{S})$ and an enumeration $\mathbf{P}:=\{P_i^\star\}_{i=1}^d$ of rank-one orthogonal eigen-projectors of $H^\star$ such that (17) holds with $U^\star=U^\star(\mathbf{P})$ and $U(\boldsymbol{\theta})=U(\boldsymbol{\theta}^\star)$. Let $H^\star=\sum_{i=1}^d\lambda_i^\star P_i^\star$ be a spectral decomposition of $H^\star$. By definition of $\varepsilon(\mathcal{F},\mathcal{S})$ given in (18), there exists $f^\star\in\mathcal{F}$ such that

$$\max_{i\in[1:d]}|f^\star(e_m(i))-\lambda_i^\star|\le\varepsilon(\mathcal{F},\mathcal{S}), \tag{41}$$

This further yields

$$\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)=\mathrm{Tr}[H^\star\rho]-\mathrm{Tr}[e^{H^\star}\sigma]+1=\sum_{i=1}^d\lambda_i^\star\,\mathrm{Tr}[P_i^\star\rho],$$

where the last equality follows from (5). Set

$$P_{i,\boldsymbol{\theta}^\star}:=U(\boldsymbol{\theta}^\star)|i\rangle\langle i|U(\boldsymbol{\theta}^\star)^\dagger, \tag{42a}$$

$$F^\star:=\sum_{i=1}^d f^\star(e_m(i))\,|i\rangle\langle i|, \tag{42b}$$

$$H_{f^\star,\boldsymbol{\theta}^\star}:=\sum_{i=1}^d f^\star(e_m(i))\,P_{i,\boldsymbol{\theta}^\star}=U(\boldsymbol{\theta}^\star)F^\star U(\boldsymbol{\theta}^\star)^\dagger. \tag{42c}$$

We can bound the approximation error as follows:

$$\begin{aligned}\left|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)-\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)\right|&\overset{(a)}{=}\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)-\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)\\&=\mathrm{Tr}[H^\star\rho]-\mathrm{Tr}[e^{H^\star}\sigma]+1-\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)\\&\overset{(b)}{\le}\mathrm{Tr}\big[(H^\star-H_{f^\star,\boldsymbol{\theta}^\star})\rho\big]+\Big(\mathrm{Tr}\big[e^{H_{f^\star,\boldsymbol{\theta}^\star}}\sigma\big]-\mathrm{Tr}\big[e^{H^\star}\sigma\big]\Big)\\&\overset{(c)}{\le}\left\|H^\star-H_{f^\star,\boldsymbol{\theta}^\star}\right\|+\left\|e^{H^\star}-e^{H_{f^\star,\boldsymbol{\theta}^\star}}\right\|,\end{aligned} \tag{43}$$

where

(a) follows because $\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)\le\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)$ since the supremum over H (see (38)) is over a subset $\cup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\mathcal{H}(\boldsymbol{\theta},\mathcal{F})$ of the class of all Hermitian operators;

(b) follows by noting that $H_{f^\star,\boldsymbol{\theta}^\star}\in\mathcal{H}(\boldsymbol{\theta}^\star,\mathcal{F})$ (since $f^\star\in\mathcal{F}$ and $\boldsymbol{\theta}^\star\in\Theta(\delta,\mathcal{S})$), thus implying that

$$\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)\ge\mathsf{D}_{\mathsf{M},\boldsymbol{\theta}^\star,\mathcal{F}}(\rho\|\sigma)\ge\mathrm{Tr}[H_{f^\star,\boldsymbol{\theta}^\star}\rho]-\mathrm{Tr}[e^{H_{f^\star,\boldsymbol{\theta}^\star}}\sigma]+1;$$

(c) uses operator Hölder's inequality.

To control the terms in the right hand side of (43), we will use the following lemma.

Lemma 11 (Bound on operator norm)**.** *Let H_1 and H_2 be Hermitian operators with spectral decompositions $H_1 = U_1\Lambda_1 U_1^\dagger$ and $H_2 = U_2\Lambda_2 U_2^\dagger$. Then*

$$\|H_1 - H_2\| \leq \|\Lambda_1 - \Lambda_2\| + \big(\,\|\Lambda_1\| + \|\Lambda_2\|\,\big)\,\|U_1 - U_2\|\,.$$

For completeness, the proof is given in Appendix F and relies on sub-multiplicativity of the spectral norm.

Applying Lemma 11 with $H_1 = H^\star = U^\star(\mathbf{P})\Lambda^\star U^\star(\mathbf{P})^\dagger$ and $H_2 = H_{f^\star,\boldsymbol{\theta}^\star} = U(\boldsymbol{\theta}^\star)F^\star U(\boldsymbol{\theta}^\star)^\dagger$ yields

$$\|H^\star - H_{f^\star,\boldsymbol{\theta}^\star}\| \leq \varepsilon(\mathcal{F},\mathcal{S}) + 2\delta\log b, \tag{44}$$

where we used $\|U^\star(\mathbf{P}) - U(\boldsymbol{\theta}^\star)\| \leq \delta$ due to (17), $\|\Lambda_1\| = \|\Lambda^\star\| \leq \log b$ by Lemma 10, $\|\Lambda_2\| = \|F^\star\| = \|f^\star\|_{\infty,\mathcal{X}} \leq \log b$, and

$$\|\Lambda_1 - \Lambda_2\| = \max_{i\in[1:d]} |f^\star(e_m(i)) - \lambda_i^\star| \leq \varepsilon(\mathcal{F},\mathcal{S}),$$

which follows from (41). Similarly, applying Lemma 11 with $H_1 = U^\star(\mathbf{P})e^{\Lambda^\star}U^\star(\mathbf{P})^\dagger$ and $H_2 = U(\boldsymbol{\theta}^\star)e^{F^\star}U(\boldsymbol{\theta}^\star)^\dagger$ yields

$$\left\|e^{H^\star} - e^{H_{f^\star,\boldsymbol{\theta}^\star}}\right\| = \left\|U^\star(\mathbf{P})e^{\Lambda^\star}U^\star(\mathbf{P})^\dagger - U(\boldsymbol{\theta}^\star)e^{F^\star}U^\dagger(\boldsymbol{\theta}^\star)\right\| \leq b\,\varepsilon(\mathcal{F},\mathcal{S}) + 2b\delta, \tag{45}$$

where we used $\left\|e^{F^\star}\right\| = \left\|e^{f^\star}\right\|_{\infty,\mathcal{X}} \leq b$, $\left\|e^{\Lambda^\star}\right\| \leq b$, and

$$\left\|e^{F^\star} - e^{\Lambda^\star}\right\| = \max_{i\in[1:d]} \left|e^{\lambda_i^\star} - e^{f^\star(e_m(i))}\right| \overset{(a)}{\leq} b \max_{i\in[1:d]} |\lambda_i^\star - f^\star(e_m(i))| \leq b\,\varepsilon(\mathcal{F},\mathcal{S}).$$

In the above, (a) is due to the fact that e^x is Lipschitz[3] for all $x \in [-\log b, \log b]$, with the Lipschitz constant bounded by b. Combining (43)-(45) the approximation error can be bounded as

$$\left|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)\right| \leq \varepsilon(\mathcal{F},\mathcal{S})(1+b) + 2\delta(b+\log b). \tag{46}$$

We next obtain an upper bound on the expected estimation error. First observe that

$$\begin{aligned}
&\left|\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}\right| \\
&\leq \sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})} \left|\mathsf{D}_{\mathsf{M},\theta,\mathcal{F}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\theta,\mathcal{F}}\right| \\
&\leq \sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})} \sup_{f\in\mathcal{F}} \left|\frac{1}{n}\sum_{\ell=1}^n f(i_\ell(\boldsymbol{\theta})) - \frac{1}{n}\sum_{\ell=1}^n e^{f(j_\ell(\boldsymbol{\theta}))} - \mathbb{E}_{p^\rho_{\boldsymbol{\theta}}}[f] + \mathbb{E}_{q^\sigma_{\boldsymbol{\theta}}}[e^f]\right| \\
&\leq \sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})} \sup_{f\in\mathcal{F}} \left|\frac{1}{n}\sum_{\ell=1}^n \big(f(i_\ell(\boldsymbol{\theta})) - \mathbb{E}_{p^\rho_{\boldsymbol{\theta}}}[f]\big)\right| + \sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})} \sup_{f\in\mathcal{F}} \left|\frac{1}{n}\sum_{\ell=1}^n e^{f(j_\ell(\boldsymbol{\theta}))} - \mathbb{E}_{q^\sigma_{\boldsymbol{\theta}}}[e^f]\right|. \\
&\leq \sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})} \sup_{f\in\mathcal{F}} \left|\frac{1}{n}\sum_{\ell=1}^n \big(f(i_\ell(\boldsymbol{\theta})) - \mathbb{E}_{p^\rho_{\boldsymbol{\theta}}}[f]\big)\right| + b \sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})} \sup_{f\in\mathcal{F}} \left|\frac{1}{n}\sum_{\ell=1}^n \big(f(j_\ell(\boldsymbol{\theta})) - \mathbb{E}_{q^\sigma_{\boldsymbol{\theta}}}[f]\big)\right|,
\end{aligned} \tag{47}$$

[3]Recall that, by definition, f is L-Lipschitz on $[a,b]$ if $|f(x) - f(y)| \leq L\,|x-y|$ for all $x, y \in [a,b]$.

where to obtain the first inequality, we used that for arbitrary functionals $f\colon \Omega \mapsto \mathbb{R}$ and $g\colon \Omega \mapsto \mathbb{R}$ such that at least $\sup_{\omega\in\Omega} f(\omega)$ or $\sup_{\omega\in\Omega} g(\omega)$ is finite,

$$\left|\sup_{\omega\in\Omega} f(\omega) - \sup_{\omega\in\Omega} g(\omega)\right| \leq \sup_{\omega\in\Omega} |f(\omega) - g(\omega)|\,, \tag{48}$$

and the final inequality again follows from the Lipschitz property of e^x mentioned above. Now, note that each term in (47) is a separable random process indexed by (f,θ) since the neural net class has a finite number of bounded parameters with continuous activation and each parameter can be approximated by rational-valued parameters, and the unitary group on $\mathbb{H}_d$ is separable (e.g., with respect to the trace norm). Hence, the suprema above are measurable. Taking expectations, we obtain

$$\begin{aligned}
&\mathbb{E}\Big[\Big|\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}\Big|\Big] \\
&\leq \mathbb{E}\left[\sup_{\substack{f\in\mathcal{F},\\ \boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}} \left|\frac{1}{n}\sum_{\ell=1}^n \left(f(i_\ell(\boldsymbol{\theta})) - \mathbb{E}_{p^\rho_{\boldsymbol{\theta}}}[f]\right)\right|\right] + b\,\mathbb{E}\left[\sup_{\substack{f\in\mathcal{F},\\ \boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}} \left|\frac{1}{n}\sum_{\ell=1}^n \left(f(j_\ell(\boldsymbol{\theta})) - \mathbb{E}_{q^\sigma_{\boldsymbol{\theta}}}[f]\right)\right|\right] \\
&\leq 2\mathbb{E}\left[\sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{\ell=1}^n R_\ell f(i_\ell(\boldsymbol{\theta}))\right|\right] + 2b\mathbb{E}\left[\sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{\ell=1}^n R_\ell (f(j_\ell(\boldsymbol{\theta}))\right|\right],
\end{aligned} \tag{49}$$

where the final step is due to the symmetrization inequality [88, Lemma 2.3.1] using i.i.d. Rademacher variables $\{R_\ell\}_{\ell=1}^n$, i.e., $\mathbb{P}(R_\ell = 1) = \mathbb{P}(R_\ell = -1) = 0.5$, independent of $\cup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\{i_\ell(\boldsymbol{\theta}), j_\ell(\boldsymbol{\theta})\}_{\ell=1}^n$.

Let

$$Z^{(n)}_{f,\boldsymbol{\theta}} \coloneqq \frac{1}{\sqrt{n}}\sum_{\ell=1}^n R_\ell f(i_\ell(\boldsymbol{\theta})) \quad \text{and} \quad \tilde{Z}^{(n)}_{f,\boldsymbol{\theta}} \coloneqq \frac{1}{\sqrt{n}}\sum_{\ell=1}^n R_\ell f(j_\ell(\boldsymbol{\theta})).$$

Let μ_n and ν_n be the empirical probability measures corresponding to $\{i_\ell(\boldsymbol{\theta})\}_{\ell=1}^n$ and $\{j_\ell(\boldsymbol{\theta})\}_{\ell=1}^n$, respectively. Note that for fixed $(f,\boldsymbol{\theta},\{i_\ell(\boldsymbol{\theta}), j_\ell(\boldsymbol{\theta})\}_{\ell=1}^n)$, $Z^{(n)}_{f,\boldsymbol{\theta}}$ and $\tilde{Z}^{(n)}_{f,\boldsymbol{\theta}}$, being weighted sums of i.i.d. Rademacher variables, are centered and sub-Gaussian random variables with respect to pseudo-metrics $\|\cdot\|_{2,\mu_n}$ and $\|\cdot\|_{2,\nu_n}$ on $\mathcal{F}\times\Theta(\delta,\mathcal{S})$, respectively. Hence, they both are also centered and sub-Gaussian random variables with respect to the pseudometric $\|\cdot\|_{\infty,\mathcal{X}}$ on $\mathcal{F}\times\Theta(\delta,\mathcal{S})$, which does not depend on $\boldsymbol{\theta}$. For instance, we have via an application of Hoeffding's lemma that for all $(f,\boldsymbol{\theta}),\ (f',\boldsymbol{\theta}') \in \mathcal{F}\times\Theta(\delta,\mathcal{S})$,

$$\begin{aligned}
&\mathbb{E}_{\{R_\ell\}_{\ell=1}^n}\left[Z^{(n)}_{f,\boldsymbol{\theta}}\right] = 0,\ \forall\ (f,\boldsymbol{\theta}) \in \mathcal{F}\times\Theta(\delta,\mathcal{S}), \\
\text{and}\quad &\mathbb{E}_{\{R_\ell\}_{\ell=1}^n}\left[e^{t\left(Z^{(n)}_{f,\boldsymbol{\theta}} - Z^{(n)}_{f',\boldsymbol{\theta}'}\right)}\right] \leq e^{\frac{t^2\|f-f'\|_{2,\mu_n}}{2}} \leq e^{\frac{t^2\|f-f'\|_{\infty,\mathcal{X}}}{2}}.
\end{aligned}$$

Then, using the law of iterated expectations by first taking conditional expectation with respect to $\{R_\ell\}_{\ell=1}^n$ given the samples $\cup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\{i_\ell(\boldsymbol{\theta}), j_\ell(\boldsymbol{\theta})\}_{\ell=1}^n$ and then with respect to these samples, we obtain

$$\begin{aligned}
&\mathbb{E}\Big[\Big|\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}\Big|\Big] \\
&\leq 2\,\mathbb{E}_{\mathsf{P}_n}\left[\mathbb{E}_{\left|\cup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\{i_\ell(\boldsymbol{\theta}),j_\ell(\boldsymbol{\theta})\}_{\ell=1}^n}\left[\sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{\ell=1}^n R_\ell f(i_\ell(\boldsymbol{\theta}))\right|\right]\right] \\
&\qquad + 2b\,\mathbb{E}_{\mathsf{Q}_n}\left[\mathbb{E}_{\left|\cup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\{i_\ell(\boldsymbol{\theta}),j_\ell(\boldsymbol{\theta})\}_{\ell=1}^n}\left[\sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{\ell=1}^n R_\ell f(j_\ell(\boldsymbol{\theta}))\right|\right]\right]
\end{aligned} \tag{50}$$

$$\overset{(a)}{\leq} 24n^{-\frac{1}{2}}\mathbb{E}_{\mathsf{P}_n}\left[\int_0^\infty \sqrt{\log N(\epsilon,\mathcal{F},\|\cdot\|_{\infty,\mathcal{X}})}d\epsilon\right] + 24b\mathbb{E}_{\mathsf{Q}_n}\left[\int_0^\infty \sqrt{\log N(\epsilon,\mathcal{F},\|\cdot\|_{\infty,\mathcal{X}})}d\epsilon\right]$$
$$\leq 48n^{-\frac{1}{2}}(b+1)\log b\int_0^1 \sqrt{\log N\big(2\epsilon\log b,\mathcal{F},\|\cdot\|_{\infty,\mathcal{X}}\big)}d\epsilon$$
$$\overset{(b)}{\leq} 48(b+1)\log b\ \kappa(\mathcal{F})n^{-\frac{1}{2}}, \tag{51}$$

where the outer expectations in the first and second terms in (50) are with respect to probability measures $\mathsf{P}_n := \bigotimes_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}(p^\rho_{\boldsymbol{\theta}})^{\otimes n}$ and $\mathsf{Q}_n := \bigotimes_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}(q^\sigma_{\boldsymbol{\theta}})^{\otimes n}$, respectively, and

(a) follows by applying the standard maximal inequality for bounding the expectation of a separable sub-Gaussian process with respect to the $\|\cdot\|_{\infty,\mathcal{X}}$ pseudometric on $\mathcal{F}\times\Theta(\delta,\mathcal{S})$ (see e.g. [88, Corollary 2.2.8.] and [78, Corollary 5.25]) as given below:

$$\mathbb{E}_{\{R_\ell\}_{\ell=1}^n}\left[Z^{(n)}_{f,\boldsymbol{\theta}}\right] \leq 12\int_0^\infty \sqrt{\log N(\epsilon,\mathcal{F},\|\cdot\|_{\infty,\mathcal{X}})}d\epsilon.$$

(b) follows from (15).

From (46) and (51), (19) follows via the triangle inequality and noting that the resulting bound holds uniformly for $(\rho,\sigma)\in\mathcal{S}$.

To prove (20), we will use the theorem stated below[4], which gives a tail probability bound for the deviation of the supremum of a sub-Gaussian process from its associated entropy integral.

Theorem 12. *[78, Theorem 5.29] Let $(X_\theta)_{\theta\in\Theta}$ be a separable sub-Gaussian process on a pseudometric space (Θ,d). Then, for all $\theta_0\in\Theta$ and $z\geq 0$, we have*

$$\mathbb{P}\left(\sup_{\theta\in\Theta} X_\theta - X_{\theta_0} \geq 32\int_0^\infty \sqrt{\log N(\epsilon,\Theta,\mathsf{d})}d\epsilon + z\right) \leq 2e^{-\frac{z^2}{72\,\mathsf{diam}(\Theta,\mathsf{d})^2}}, \tag{52}$$

where $\mathsf{diam}(\Theta,\mathsf{d}) := \sup_{\theta,\tilde\theta\in\Theta}\mathsf{d}(\theta,\tilde\theta)$.

From (47), it follows that

$$\left|\mathsf{D}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}\right| \leq \sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\sup_{f\in\mathcal{F}}\left|\bar{Z}^{(n)}_{f,\boldsymbol{\theta}}\right|, \tag{53}$$

where the above inequality again used (48) with

$$\bar{Z}^{(n)}_{f,\boldsymbol{\theta}} := \frac{1}{n}\sum_{\ell=1}^n f(i_\ell(\boldsymbol{\theta})) - \frac{1}{n}\sum_{\ell=1}^n e^{f(j_\ell(\boldsymbol{\theta}))} - \mathbb{E}_{p^\rho_{\boldsymbol{\theta}}}[f] + \mathbb{E}_{q^\sigma_{\boldsymbol{\theta}}}[e^f].$$

To apply Theorem 12, we will show that $\{\bar{Z}^{(n)}_{f,\boldsymbol{\theta}}\}_{(f,\boldsymbol{\theta})\in\mathcal{F}\times\Theta(\delta,\mathcal{S})}$ is a centered separable sub-Gaussian process with respect to an appropriate pseudo-metric defined on $\mathcal{F}\times\Theta(\delta,\mathcal{S})$. To see this, observe that $\mathbb{E}[\bar{Z}^{(n)}_{f,\boldsymbol{\theta}}]=0$ for all $(f,\boldsymbol{\theta})\in\mathcal{F}\times\Theta(\delta,\mathcal{S})$. Moreover,

$$\bar{Z}^{(n)}_{f,\boldsymbol{\theta}} - \bar{Z}^{(n)}_{\tilde f,\tilde{\boldsymbol{\theta}}} = \sum_{\ell=1}^n \frac{1}{n}\Big((f(i_\ell(\boldsymbol{\theta})) - f(i_\ell(\tilde{\boldsymbol{\theta}})) - (e^{f(j_\ell(\boldsymbol{\theta}))} - e^{\tilde f(j_\ell(\tilde{\boldsymbol{\theta}}))}) - (\mathbb{E}_{p^\rho_{\boldsymbol{\theta}}}[f] - \mathbb{E}_{p^\rho_{\tilde{\boldsymbol{\theta}}}}[\tilde f])$$

[4] While [78, Theorem 5.29] is stated without specifying explicit constants, a straightforward computation by following the proof therein yields the constants stated in (52).

$$+ \left(\mathbb{E}_{q^\sigma_{\boldsymbol{\theta}}}[e^f] - \mathbb{E}_{q^\sigma_{\tilde{\boldsymbol{\theta}}}}[e^{\tilde{f}}]\right)\Bigg).$$

Since $\{(i_\ell(\boldsymbol{\theta}), j_\ell(\boldsymbol{\theta}))\}_{\ell=1}^n$ are i.i.d. variables, the moment generating function of $\bar{Z}^{(n)}_{f,\boldsymbol{\theta}} - \bar{Z}^{(n)}_{\tilde{f},\tilde{\boldsymbol{\theta}}}$ is equal to the product of the moment generating function of each term within the sum above. Also, by using the Lipschitz property of e^x mentioned earlier, each term within that sum is upper bounded as follows:

$$\begin{aligned}
&\left|\frac{1}{n}\Bigg((f(i_\ell(\boldsymbol{\theta})) - \tilde{f}(i_\ell(\tilde{\boldsymbol{\theta}})) - (e^{f(j_\ell(\boldsymbol{\theta}))} - e^{\tilde{f}(j_\ell(\tilde{\boldsymbol{\theta}}))}) - (\mathbb{E}_{p^\rho_{\boldsymbol{\theta}}}[f] - \mathbb{E}_{p^\rho_{\tilde{\boldsymbol{\theta}}}}[\tilde{f}])\right.\\
&\qquad\qquad\left.+ \left(\mathbb{E}_{q^\sigma_{\boldsymbol{\theta}}}[e^f] - \mathbb{E}_{q^\sigma_{\tilde{\boldsymbol{\theta}}}}[e^{\tilde{f}}]\right)\Bigg)\right|\\
&\leq \frac{2(1+b)}{n}\|f - \tilde{f}\|_{\infty,\mathcal{X}}. \qquad (54)
\end{aligned}$$

Then, it follows from Hoeffding's lemma that

$$\mathbb{E}\left[e^{t\left(\bar{Z}^{(n)}_{f,\boldsymbol{\theta}} - \bar{Z}^{(n)}_{\tilde{f},\tilde{\boldsymbol{\theta}}}\right)}\right] \leq e^{\frac{1}{2}t^2 \mathsf{d}_{b,n}(f,\tilde{f})^2},$$

where $\mathsf{d}_{b,n}(f,\tilde{f})$ is the pseudo-metric on $\mathcal{F}\times\Theta(\delta,\mathcal{S})$ given by

$$\mathsf{d}_{b,n}(f,\tilde{f}) \coloneqq \mathsf{d}_{b,n}((f,\theta),(\tilde{f},\tilde{\theta})) \coloneqq 2(1+b)n^{-\frac{1}{2}}\|f-\tilde{f}\|_{\infty,\mathcal{X}}.$$

Thus, $\{\bar{Z}^{(n)}_{f,\boldsymbol{\theta}}\}_{(f,\boldsymbol{\theta})\in\mathcal{F}\times\Theta(\delta,\mathcal{S})}$ is a separable sub-Gaussian process on the pseudo-metric space $(\mathcal{F}\times\Theta(\delta,\mathcal{S}), \mathsf{d}_{b,n})$, where the separability follows from (54) and the fact that $\mathcal{F}\times\Theta(\delta,\mathcal{S})$ is totally bounded with respect to the pseudometric $\|\cdot\|_{\infty,\mathcal{X}}$ by (15) in Assumption 1. The total boundedness is because $N(\epsilon, \mathcal{F}\times\Theta, \|\cdot\|_{\infty,\mathcal{X}})$ is finite for all $\epsilon > 0$ due to (15) and the monotonically non-increasing property of covering number in ϵ. Also,

$$\mathsf{diam}(\mathcal{F}\times\Theta(\delta,\mathcal{S}), \mathsf{d}_{b,n}) = 4n^{-\frac{1}{2}}(1+b)\log b,$$

and

$$\begin{aligned}
\int_0^\infty \sqrt{\log N(\epsilon, \mathcal{F}\times\Theta(\delta,\mathcal{S}), \mathsf{d}_{b,n})}d\epsilon &= \int_0^{\mathsf{diam}(\mathcal{F}\times\Theta(\delta,\mathcal{S}),\mathsf{d}_{b,n})} \sqrt{\log N(\epsilon, \mathcal{F}\times\Theta(\delta,\mathcal{S}), \mathsf{d}_{b,n})}d\epsilon\\
&= 4n^{-\frac{1}{2}}(1+b)(\log b)\int_0^1 \sqrt{\log N(2\epsilon\log b, \mathcal{F}, \|\cdot\|_{\infty,\mathcal{X}})}d\epsilon\\
&= 4n^{-\frac{1}{2}}(1+b)(\log b)\,\kappa(\mathcal{F}),
\end{aligned}$$

where the first equality follows because in an arbitrary pseudometric space (Θ,d), $N(\epsilon,\Theta,\mathsf{d}) = 1$ for $\epsilon \geq \mathsf{diam}(\Theta,\mathsf{d})$, while the second equality uses a change of variables along with $N(a\epsilon,\Theta,a\mathsf{d}) = N(\epsilon,\Theta,\mathsf{d})$ for $a > 0$. Then, (52) in Theorem 12 (with $\bar{Z}^{(n)}_{0,\boldsymbol{\theta}} = 0$ which corresponds to $f = 0 \in \mathcal{F}$) yields

$$\mathbb{P}\left(\sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\sup_{f\in\mathcal{F}} \bar{Z}^{(n)}_{f,\boldsymbol{\theta}} \geq 128\,n^{-\frac{1}{2}}(1+b)\log b\,\kappa(\mathcal{F}) + \bar{z}\right) \leq 2\,e^{-\frac{n\bar{z}^2}{72(1+b)^2(\log b)^2}},\ \bar{z}\geq 0,$$

for some $c > 0$. Noting that the above also holds with $\bar{Z}^{(n)}_{f,\boldsymbol{\theta}}$ replaced by $-\bar{Z}^{(n)}_{f,\boldsymbol{\theta}}$, we obtain

$$\mathbb{P}\left(\sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})}\sup_{f\in\mathcal{F}} \left|\bar{Z}^{(n)}_{f,\boldsymbol{\theta}}\right| \geq 128\,n^{-\frac{1}{2}}(1+b)\log b\,\kappa(\mathcal{F}) + \bar{z}\right) \leq 2\,e^{-\frac{n\bar{z}^2}{72(1+b)^2(\log b)^2}}.$$

From (40) and (46), we have with $\xi_{\mathcal{F},\mathcal{S},\delta,b} \coloneqq \varepsilon(\mathcal{F},\mathcal{S})(b+1) + 2\delta(b+\log b)$ that

$$\mathbb{P}\left(\left|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma) - \hat{\mathsf{D}}^{n}_{\mathsf{M},\Theta(\delta,\mathcal{S}),\mathcal{F}}\right| \geq \xi_{\mathcal{F},\mathcal{S},\delta,b} + 128n^{-\frac{1}{2}}(1+b)\log b\,\kappa(\mathcal{F}) + \bar{z}\right) \leq 2e^{-\frac{n\bar{z}^2}{72(1+b)^2(\log b)^2}},$$

for some $c \geq 0$. Setting $\bar{z} = \sqrt{72}\,z(1+b)\log b$ and taking the supremum over $(\rho,\sigma) \in \mathcal{S}$ leads to the claim in (20), thus completing the proof.

5.2 Proof of Corollary 2

We will apply Theorem 1 with $\mathcal{F} = \tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b) \subseteq \mathcal{F}_b$ and $\mathcal{S} = \mathcal{S}_d(b)$. To this end, we first verify that Assumption 1 is satisfied as required therein. Note that $\mathcal{X} = \{|i\rangle, i \in [1:d]\}$ for the embedding $e_d : i \mapsto |i\rangle$. By Lemma 10, for all $(\rho,\sigma) \in \mathcal{S}_d(b)$ and $\Lambda^\star(\rho,\sigma) = \{\lambda_i^\star\}_{i\in[1:d]}$, we have $|\lambda_i^\star| \leq \log b$ for all $i \in [1:d]$. Hence,

$$f^\star(x) \coloneqq \sum_{i=1}^{d} \lambda_i^\star \varphi_{\mathrm{R}}(\langle i,x\rangle) \in \tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b),$$

satisfies $\max_{i\in[1:d]} |f^\star(e_d(i)) - \lambda_i^\star| = 0$. Further, observe that $\|f\|_{\infty,\mathcal{X}} \leq \log b$ for $f \in \tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b)$ and that for all $f = \sum_{i=1}^d \beta_i \varphi_{\mathrm{R}}(\langle i,x\rangle)$ and $\tilde{f} = \sum_{i=1}^d \tilde{\beta}_i \varphi_{\mathrm{R}}(\langle i,x\rangle)$, we have

$$\left\|f - \tilde{f}\right\|_{\infty,\mathcal{X}} = \max_{i\in[1:d]} |\beta_i - \tilde{\beta}_i|.$$

This implies that

$$N(\epsilon, \tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b), \|\cdot\|_{\infty,\mathcal{X}}) = N(\epsilon, [-\log b, \log b]^d, \|\cdot\|_\infty) \leq (3(\log b)\,\epsilon^{-1})^d, \forall\ \epsilon > 0,$$

where the second inequality used a standard upper bound on the ϵ-covering number of $\|\cdot\|_\infty$ ball of radius $\log b$ in $\mathbb{R}^d$. Hence

$$\log N(2\epsilon\log b, \tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b), \|\cdot\|_{\infty,\mathcal{X}}) \leq d\log(3\epsilon^{-1}) \leq 3d\epsilon^{-1}, \forall\ \epsilon > 0.$$

From the above, it follows that Assumption 1 holds with

$$\begin{aligned}
\varepsilon(\mathcal{F}^{\mathrm{SNN}}(d,\log b), \mathcal{S}_d(b)) &= 0,\\
\bar{\kappa}(\mathcal{F}^{\mathrm{SNN}}(d,\log b), \epsilon) &= d\epsilon^{-1},\\
\text{and } \kappa(\mathcal{F}^{\mathrm{SNN}}(d,\log b)) &= \int_0^1 \sqrt{d\epsilon^{-1}}d\epsilon = 2\sqrt{d}.
\end{aligned}$$

Substituting these in (19) and (20) leads to the desired claim.

5.3 Proof of Proposition 4

We will apply Theorem 1 with $\mathcal{F} = \tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a}) \subseteq \mathcal{F}_b$ and $\mathcal{S} = \tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon) \subseteq \mathcal{S}_d(b)$. We first verify that Assumption 1 is satisfied. Note that for the embedding $e_1 : i \mapsto i/d$, we have $\mathcal{X} = \{1/d, 2/d, \ldots, 1\}$. By definition, for any $(\rho,\sigma) \in \tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon)$ and any enumeration $\Lambda^\star(\rho,\sigma) = \{\lambda_i^\star\}_{i=1}^d$, there exists a polynomial $p \in \mathcal{P}_k(a)$ of degree at most k such that

$$\max_{i\in[1:d]} |p(e_1(i)) - \lambda_i^\star| \leq \varepsilon.$$

Now, suppose the neural class $\mathcal{F}^{\mathrm{NN}}(L,K,M,1)$ with depth L, width K, and parameter norm M appropriately chosen, is such that there exists $f \in \mathcal{F}^{\mathrm{NN}}(L,K,M,1)$ satisfying

$$\|f - p\|_{\infty,\mathcal{X}} \leq \varepsilon. \tag{55}$$

Then, we obtain via the triangle inequality that

$$\max_{i\in[1:d]} |f(e_1(i)) - \lambda_i^\star| \le 2\varepsilon. \tag{56}$$

Hence, (18) holds with $\varepsilon(\mathcal{F}^{\mathrm{NN}}(L,K,M,1),\tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon)) = 2\varepsilon$. For quantifying the error in approximating polynomials via neural nets in (55), we will use the error bounds from [85]. In particular, [85, Proposition III.5] implies that there exists $f \in \mathcal{F}^{\mathrm{NN}}(L_{\varepsilon,k,a},K,M,1)$ with $K = 9$, $M = 1$ and

$$L_{\varepsilon,k,a} \coloneqq ck\left(\log(\varepsilon^{-1}) + \log k + \log a\right), \tag{57}$$

such that (55) holds, where $c > 0$ is some constant. By considering the truncated neural class given in (25), we obtain that

$$\|f\|_{\infty,\mathcal{X}} \le \log b,\ \forall f \in \tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a},K,M,1). \tag{58}$$

Moreover, it is easy to see that (55) continues to hold with f replaced by the corresponding $\tilde{f}$ since $|p(i/d)| \le \log b$ for all $i \in [1:d]$.

Next, we obtain a bound on the covering entropy of $\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a},K,M,1)$. We have

$$N\Big(\epsilon,\tilde{\mathcal{F}}^{\mathrm{NN}}(L,K,M,1),\|\cdot\|_{\infty,\mathcal{X}}\Big) \le N\Big(\epsilon,\mathcal{F}^{\mathrm{NN}}(L,K,M,1),\|\cdot\|_{\infty,\mathcal{X}}\Big).$$

Applying the covering entropy bound[5] given in [89, Lemma 5] to the neural class $\tilde{\mathcal{F}}^{\mathrm{NN}}(L) \coloneqq \tilde{\mathcal{F}}^{\mathrm{NN}}(L,9,1,1)$ yields (with $p_0 = p_L = 1$ and $p_l = 9$ for $1 \le l \le L-1$ in the statement therein) that

$$\log N(\epsilon,\tilde{\mathcal{F}}^{\mathrm{NN}}(L),\|\cdot\|_{\infty,\mathcal{X}}) \le (28 + 81(L-2))\log\Big(32L10^{2(L-1)}\epsilon^{-1}\Big) \le 81L\log\Big(10^{3L}\epsilon^{-1}\Big).$$

From this, we obtain using $\log x \le x$ for all $x \ge 0$ and $\sqrt{x+y} \le \sqrt{x} + \sqrt{y}$ for all $x, y \ge 0$ that

$$\int_0^1 \sqrt{\log N(2\epsilon\log b,\tilde{\mathcal{F}}^{\mathrm{NN}}(L),\|\cdot\|_{\infty,\mathcal{X}})}\,d\epsilon \le 24L + 9\sqrt{\frac{L}{2\log b}}\int_0^1 \epsilon^{-\frac{1}{2}}\,d\epsilon \le 24L + 13\sqrt{\frac{L}{\log b}}. \tag{59}$$

Hence, from (56) and (59), we have that $\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a}) \subseteq \mathcal{F}_b$ and $\tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon) \subseteq \mathcal{S}_d(b)$ satisfies Assumption 1 with $\varepsilon(\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a}),\tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon)) = 2\varepsilon$ and $\kappa(\tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a})) \le B_{\varepsilon,k,a,b}/\log b$. Then, applying Theorem 1 with $\mathcal{F} = \tilde{\mathcal{F}}^{\mathrm{NN}}(L_{\varepsilon,k,a})$ and $\mathcal{S} = \tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon)$ yields the desired claims.

5.4 Proof of Theorem 5

The proof largely follows via steps similar to those in the proof of Theorem 1. So, we only highlight the differences. Fix $(\rho,\sigma) \in \mathcal{S}$. Let

$$\mathsf{D}_{\mathsf{M},\alpha,\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) \coloneqq \sup_{\boldsymbol{\theta}\in\Theta(\delta,\mathcal{S})} \mathsf{D}_{\mathsf{M},\alpha,\boldsymbol{\theta},\mathcal{F}}(\rho\|\sigma),$$

[5] This bound applies since covering number of a truncated function class is upper bounded by that of the original function class.

where

$$\mathsf{D}_{\mathsf{M},\alpha,\boldsymbol{\theta},\mathcal{F}}(\rho\|\sigma) \coloneqq \sup_{H\in\mathcal{H}(\boldsymbol{\theta},\mathcal{F})} \frac{\alpha}{\alpha-1}\log \mathrm{Tr}[e^{(\alpha-1)H}\rho] - \log \mathrm{Tr}[e^{\alpha H}\sigma], \tag{60}$$

and $\mathcal{H}(\boldsymbol{\theta},\mathcal{F})$ is as defined in (39). Then, the triangle inequality implies that

$$\begin{aligned}\left|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta(\delta,\mathcal{S}),\mathcal{F}}\right| \le{}& \left|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \mathsf{D}_{\mathsf{M},\alpha,\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)\right| \\ &+ \left|\mathsf{D}_{\mathsf{M},\alpha,\Theta(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta(\delta,\mathcal{S}),\mathcal{F}}\right|,\end{aligned} \tag{61}$$

where the first and second terms on the right-hand side are the approximation and estimation errors, respectively.

Let $H^\star_\alpha \coloneqq H^\star_\alpha(\rho,\sigma)$ be an optimizer of (4) satisfying (5) and (6). Recall from the definition of the set $\mathcal{U}_\alpha(\delta,\mathcal{S})$ that there exists an enumeration $\mathbf{P}_\alpha \coloneqq \{P^\star_{i,\alpha}\}_{i=1}^d$ of orthogonal rank-one eigenprojectors of $H^\star_\alpha$, and $U(\boldsymbol{\theta}^\star)$ for some $\boldsymbol{\theta}^\star \in \Theta_\alpha(\delta,\mathcal{S})$ such that (17) holds with $U^\star = U^\star(\mathbf{P}_\alpha)$ and $U(\boldsymbol{\theta}) = U(\boldsymbol{\theta}^\star)$, where $U^\star(\mathbf{P}_\alpha)$ is the unitary such that $U^\star(\mathbf{P}_\alpha)|i\rangle\langle i|(U^\star(\mathbf{P}_\alpha))^\dagger = P^\star_{i,\alpha}$. Let $H^\star_\alpha = \sum_{i=1}^D \lambda^\star_{i,\alpha}P^\star_{i,\alpha}$ be the spectral decomposition of $H^\star_\alpha$ with $\Lambda^\star_\alpha \coloneqq \Lambda^\star_\alpha(\rho,\sigma)$ denoting the set of eigenvalues. By definition of $\varepsilon_\alpha(\mathcal{F},\mathcal{S})$, there exists $f^\star \in \mathcal{F}$ such that

$$\max_{i\in[1:d]} \left|f^\star(e_m(i)) - \lambda^\star_{i,\alpha}\right| \le \varepsilon_\alpha(\mathcal{F},\mathcal{S}). \tag{62}$$

Let $H_{f^\star,\boldsymbol{\theta}^\star}$ be as defined (42). Then, we can bound the approximation error as

$$\begin{aligned}&\left|\mathsf{D}_{\mathsf{M},\alpha}(\rho\|\sigma) - \mathsf{D}_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma)\right| \\ &\overset{(a)}{\le} \frac{\alpha}{|\alpha-1|}\left\|e^{(\alpha-1)H^\star_\alpha} - e^{(\alpha-1)H_{f^\star,\boldsymbol{\theta}^\star}}\right\| + \left\|e^{\alpha H^\star_\alpha} - e^{\alpha H_{f^\star,\boldsymbol{\theta}^\star}}\right\| \\ &\overset{(b)}{\le} \alpha\left(b^{|\alpha-1|}+b^\alpha\right)\varepsilon_\alpha(\mathcal{F},\mathcal{S}) + 2\left(\frac{\alpha}{|\alpha-1|}b^{|\alpha-1|}+b^\alpha\right)\delta,\end{aligned} \tag{63}$$

where (a) follows via similar steps leading to (43) and (b) is via an application of Lemma 11 as leading to (46). For instance,

$$\begin{aligned}\left\|e^{\alpha H^\star_\alpha} - e^{\alpha H_{f^\star,\boldsymbol{\theta}^\star}}\right\| &\le \left\|e^{\alpha\Lambda^\star_\alpha} - e^{\alpha F^\star}\right\| + \left(\left\|e^{\alpha\Lambda^\star_\alpha}\right\| + \left\|e^{\alpha F^\star}\right\|\right)\|U^\star(\mathbf{P}_\alpha) - U(\boldsymbol{\theta}^\star)\| \\ &\le \alpha b^\alpha \max_{i\in[1:d]}\left|\lambda^\star_{i,\alpha} - f^\star(e_m(i))\right| + 2b^\alpha\delta \\ &\le b^\alpha(\alpha\varepsilon_\alpha(\mathcal{F},\mathcal{S}) + 2\delta),\end{aligned}$$

where the first inequality is by application of Lemma 11, and second inequality uses that the Lipschitz constant of $e^{\alpha x}$ is bounded by $\alpha e^{\alpha\log b} = \alpha b^\alpha$ for $|x| \le \log b$ along with $\left\|e^{\alpha f^\star}\right\|_{\infty,\mathcal{X}} \le b^\alpha$. Similarly,

$$\left\|e^{(\alpha-1)H^\star_\alpha} - e^{(\alpha-1)H_{f^\star,\boldsymbol{\theta}^\star}}\right\| \le b^{|\alpha-1|}(\,|\alpha-1|\,\varepsilon_\alpha(\mathcal{F},\mathcal{S}) + 2\delta).$$

Also, following analogous steps leading to (51), we have

$$\begin{aligned}&\mathbb{E}\left[\left|\mathsf{D}_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\mathcal{F}}(\rho\|\sigma) - \hat{\mathsf{D}}^n_{\mathsf{M},\alpha,\Theta_\alpha(\delta,\mathcal{S}),\mathcal{F}}\right|\right] \\ &\le 24n^{-\frac{1}{2}}\alpha b^{|\alpha-1|}\int_0^\infty \sqrt{\log N(\epsilon,\mathcal{F},\|\cdot\|_{\infty,\mathcal{X}})}d\epsilon + 24n^{-\frac{1}{2}}\alpha b^\alpha\int_0^\infty\sqrt{\log N(\epsilon,\mathcal{F},\|\cdot\|_{\infty,\mathcal{X}})}d\epsilon\end{aligned}$$

$$\leq 48n^{-\frac{1}{2}}\alpha\big(b^{\alpha}+b^{|\alpha-1|}\big)\log b\int_0^1\sqrt{\log N\big(2\epsilon\log b,\mathcal{F},\|\cdot\|_{\infty,\mathcal{X}}\big)}d\epsilon$$

$$\overset{(c)}{\leq} 48\alpha\big(b^{\alpha}+b^{|\alpha-1|}\big)\log b\;\kappa(\mathcal{F})n^{-\frac{1}{2}}. \tag{64}$$

The claim in (29) then follows by substituting (63) and (64) in (61), and taking supremum over $(\rho,\sigma)\in\mathcal{S}$. The proof of (30) follows analogous to that of (20) and hence is omitted.

5.5 Proof of Proposition 8

Recalling that $a(\delta,b):=2\delta(b+\log b)$ and applying Corollary 2 yields that for every $(\rho,\sigma)\in\bar{\mathcal{S}}_d(\delta,b,\mathcal{U})$,

$$\mathbb{P}\left(\left|\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)-\hat{\mathsf{D}}^{n}_{\mathsf{M},\Theta(\mathcal{U}),\tilde{\mathcal{F}}^{\mathrm{SNN}}(d,\log b)}\right|\geq a(\delta,b)+128(\log b)(b+1)\left(2d^{\frac{1}{2}}n^{-\frac{1}{2}}+z\right)\right)\leq 2e^{-nz^2}.$$

Take $\delta=\epsilon_b:=\epsilon/(4b+4\log b)$. Setting $2e^{-nz^2}=1-p$ and solving for z yields $z=n^{-\frac{1}{2}}\sqrt{\log\left(2/(1-p)\right)}$. Then, taking

$$0.5\epsilon=c'n^{-\frac{1}{2}}(b+1)\Big(d^{\frac{1}{2}}+\sqrt{\log\left(2/(1-p)\right)}\Big)\log b,$$

for some constant $c'>0$, solving for n and multiplying this with the upper bound for $\big|\Theta(\mathcal{U})\big|$ yields the desired upper bound on copy complexity.

5.6 Proof of Proposition 9

Consider the Schur–Weyl decomposition, $\mathbb{H}_d=\mathbb{H}_m^{\otimes N}=\bigoplus_{\kappa\in Y_m^N}\mathcal{W}_\kappa\otimes\mathcal{V}_\kappa$, given in (35). Recall that P_κ denotes the projection onto $\mathcal{W}_\kappa\otimes\mathcal{V}_\kappa$ and $\mathcal{K}_{m,N}:=\bigoplus_\kappa\mathcal{W}_\kappa$. Consider the quantum channels $\bar{\mathcal{N}}(\cdot)$ and $\bar{\mathcal{M}}(\cdot)$ given in (36) and (37), respectively. Note that any $\rho\in\mathfrak{P}(\mathbb{H}_m^{\otimes N})$ has the representation

$$\rho=\bigoplus_{\kappa\in Y_m^N}\bar{\rho}_\kappa\otimes\pi_\kappa,$$

for some endomorphism $\bar{\rho}_\kappa$ on $\mathcal{W}_\kappa$. Hence, $(\rho,\sigma)\in\hat{\mathcal{S}}_{m,N}(\delta,b,\mathcal{U})$ implies that $\rho,\sigma\in\mathfrak{P}(\mathbb{H}_m^{\otimes N})$. Also observe that if $\rho>0$, then $\bar{\rho}_\kappa>0$ and for $\rho\in\mathfrak{P}(\mathbb{H}_m^{\otimes N})$, $\bar{\mathcal{M}}\circ\bar{\mathcal{N}}(\rho)=\rho$. By the data-processing inequality for measured relative entropy, we have for any $\rho,\sigma\in\mathfrak{P}(\mathbb{H}_m^{\otimes N})$:

$$\mathsf{D}_{\mathsf{M}}(\bar{\mathcal{N}}(\rho)\|\bar{\mathcal{N}}(\sigma))\leq\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)=\mathsf{D}_{\mathsf{M}}(\bar{\mathcal{M}}\circ\bar{\mathcal{N}}(\rho)\|\bar{\mathcal{M}}\circ\bar{\mathcal{N}}(\sigma))\leq\mathsf{D}_{\mathsf{M}}(\bar{\mathcal{N}}(\rho)\|\bar{\mathcal{N}}(\sigma)). \tag{65}$$

This yields

$$\mathsf{D}_{\mathsf{M}}(\bar{\mathcal{N}}(\rho)\|\bar{\mathcal{N}}(\sigma))=\mathsf{D}_{\mathsf{M}}(\rho\|\sigma),\ \forall\ (\rho,\sigma)\in\hat{\mathcal{S}}_{m,N}(\delta,b,\mathcal{U}).$$

The above observations provide a way to estimate the measured relative entropy between permutation invariant operators efficiently. Note that $\bar{\mathcal{N}}(\rho)$ and $\bar{\mathcal{N}}(\sigma)$ are density operators over a much smaller space $\mathcal{K}_{m,N}$, whose dimension $\bar{d}_{m,N}$ is bounded from above by $(N+1)^{m-1}N^{\frac{m(m-1)}{2}}$ (see e.g., [87, Equation 6.16]). By the variational form for measured relative entropy, we have

$$\mathsf{D}_{\mathsf{M}}(\rho\|\sigma)=\sup_H\mathrm{Tr}[H\bar{\mathcal{N}}(\rho)]-\mathrm{Tr}[e^H\bar{\mathcal{N}}(\sigma)]+1,$$

where the supremum is taken over Hermitian operators H on $\mathcal{K}_{m,N}$. Since $(\rho,\sigma) \in \hat{\mathcal{S}}_{m,N}(\delta,b,\mathcal{U})$ implies that $(\bar{\mathcal{N}}(\rho),\bar{\mathcal{N}}(\sigma)) \in \bar{\mathcal{S}}_{|\mathcal{K}_{m,N}|}(\delta,b,\mathcal{U})$, we have $T(\bar{\mathcal{N}}(\rho),\bar{\mathcal{N}}(\sigma)) \leq \log b$ by definition of $\bar{\mathcal{S}}_{|\mathcal{K}_{m,N}|}(\delta,b,\mathcal{U})$. From these, the claim in Proposition 9 follows by an application of Corollary 2 via similar steps as in the proof of Proposition 8. We also remark that since the Thompson metric contracts under application of a quantum channel, we have $T(\bar{\mathcal{N}}(\rho),\bar{\mathcal{N}}(\sigma)) = T(\rho,\sigma)$ for all $(\rho,\sigma) \in \hat{\mathcal{S}}_{m,N}(\delta,b,\mathcal{U})$ via analogous arguments as in (65).

6 Concluding Remarks

We studied the performance of the quantum neural estimator proposed in [29] for estimating measured relative entropy and its Rényi analogue. We obtained upper bounds on its expected absolute error and showed exponential deviation inequalities under regularity conditions on the underlying states, the neural class, and the parametrized quantum circuit. We then specialized our bounds to shallow and deep neural nets and derived concrete bounds using known results from the approximation theory of neural nets along with bounds on the covering entropy of the associated neural classes. We also established that, although the quantum neural estimator has a worst case copy complexity that scales exponentially in the number of qudits, this improves to polynomial when the underlying states are permutation invariant.

Several open questions remain in the context of quantum neural estimation of entropies. One such issue pertains to the quantification of the optimization error and an analysis of optimization dynamics such as the investigation of barren plateaus and local optima, which was neglected here. This would call for an in-depth study of the hybrid optimization landscape induced by the neural net and quantum circuit, and an analysis of specific parameterizations or architectures that lead to relatively fast convergence of the algorithm. Also relevant is the question of estimating the quantum relative entropy and its Rényi generalizations such as the sandwiched and Petz–Rényi relative entropies using quantum neural estimators. Recent progress on estimating quantum relative entropy has been reported in [28].

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References

[1] John von Neumann. "Thermodynamik quantenmechanischer gesamtheiten". Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische Klasse **1927**, 273–291 (1927). url: http://eudml.org/doc/59231.

[2] Claude E. Shannon. "A mathematical theory of communication". Bell System Technical Journal **27**, 379–423 (1948).

[3] Alfréd Rényi. "On measures of entropy and information". Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Contributions to the Theory of Statistics **4.1**, 547–561 (1961). url: https://digicoll.lib.berkeley.edu/record/112906.

[4] Solomon Kullback and Richard A. Leibler. "On information and sufficiency". The Annals of Mathematical Statistics **22**, 79–86 (1951).

[5] Hisaharu Umegaki. "Conditional expectations in an operator algebra IV (entropy and information)". Kodai Mathematical Seminar Reports **14**, 59–85 (1962).

[6] Dénes Petz. "Quasi-entropies for states of a von Neumann algebra". Publications of the Research Institute for Mathematical Sciences **21**, 787–800 (1985).

[7] Dénes Petz. "Quasi-entropies for finite quantum systems". Reports on Mathematical Physics **23**, 57–65 (1986).

[8] Martin Müller-Lennert, Frédéric Dupuis, Oleg Szehr, Serge Fehr, and Marco Tomamichel. "On quantum Rényi entropies: A new generalization and some properties". Journal of Mathematical Physics **54**, 122203 (2013).

[9] Mark M. Wilde, Andreas Winter, and Dong Yang. "Strong converse for the classical capacity of entanglement-breaking and Hadamard channels via a sandwiched Rényi relative entropy". Communications in Mathematical Physics **331**, 593–622 (2014).

[10] Tomohiro Ogawa and Hiroshi Nagaoka. "Strong converse and Stein's lemma in quantum hypothesis testing". IEEE Transactions on Information Theory **46**, 2428–2433 (2000).

[11] Tomohiro Ogawa and Masahito Hayashi. "On error exponents in quantum hypothesis testing". IEEE Transactions on Information Theory **50**, 1368–1372 (2004).

[12] Michael Nussbaum and Arleta Szkoła. "The Chernoff lower bound for symmetric quantum hypothesis testing". The Annals of Statistics **37**, 1040–1057 (2009).

[13] Koenraad M. R. Audenaert, Michael Nussbaum, Arleta Szkola, and Frank Verstraete. "Asymptotic error rates in quantum hypothesis testing". Communications in Mathematical Physics **279**, 251–283 (2008).

[14] Mario Berta, Fernando Brandao, and Christoph Hirche. "On composite quantum hypothesis testing". Communications in Mathematical Physics **385**, 55–77 (2021).

[15] Tongyang Li and Xiaodi Wu. "Quantum query complexity of entropy estimation". IEEE Transactions on Information Theory **65**, 2899–2921 (2017).

[16] Yigit Subasi, Lukasz Cincio, and Patrick J. Coles. "Entanglement spectroscopy with a depth-two quantum circuit". Journal of Physics A: Mathematical and Theoretical **52**, 44001 (2019).

[17] Jayadev Acharya, Ibrahim Issa, Nirmal V. Shende, and Aaron B. Wagner. "Estimating quantum entropy". IEEE Journal on Selected Areas in Information Theory **1**, 454–468 (2020).

[18] Sathyawageeswar Subramanian and Min-Hsiu Hsieh. "Quantum algorithm for estimating α-Rényi entropies of quantum states". Physical Review A **104**, 022428 (2021).

[19] András Gilyén and Tongyang Li. "Distributional property testing in a quantum world". In Thomas Vidick, editor, 11th Innovations in Theoretical Computer Science Conference (ITCS 2020). Volume 151 of Leibniz International Proceedings in Informatics (LIPIcs), pages 25:1–25:19. Dagstuhl, Germany (2020). Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik.

[20] Tom Gur, Min-Hsiu Hsieh, and Sathyawageeswar Subramanian. "Sublinear quantum algorithms for estimating von Neumann entropy" (2021). arXiv:2111.11139.

[21] Youle Wang, Benchi Zhao, and Xin Wang. "Quantum algorithms for estimating quantum entropies". Physical Review Applied **19**, 044041 (2023).

[22] Qisheng Wang, Ji Guan, Junyi Liu, Zhicheng Zhang, and Mingsheng Ying. "New quantum algorithms for computing quantum entropies and distances". IEEE Transactions on Information Theory **70**, 5653–5680 (2024). arXiv:2203.13522.

[23] András Gilyén and Alexander Poremba. "Improved quantum algorithms for fidelity estimation" (2022). arXiv:2203.15993.

[24] Youle Wang, Lei Zhang, Zhan Yu, and Xin Wang. "Quantum phase processing and its applications in estimating phase and entropies". Physical Review A **108**, 062413 (2023).

[25] Qisheng Wang, Zhicheng Zhang, Kean Chen, Ji Guan, Wang Fang, Junyi Liu, and Mingsheng Ying. "Quantum algorithm for fidelity estimation". IEEE Transactions on Information Theory **69**, 273–282 (2023).

[26] Xinzhao Wang, Shengyu Zhang, and Tongyang Li. "A quantum algorithm framework for discrete probability distributions with applications to Rényi entropy estimation". IEEE Transactions on Information Theory **70**, 3399–3426 (2024).

[27] Qisheng Wang and Zhicheng Zhang. "Time-efficient quantum entropy estimator via samplizer". IEEE Transactions on Information Theory **71**, 9569–9599 (2025).

[28] Yuchen Lu and Kun Fang. "Estimating quantum relative entropies on quantum computers". Communications Physics (2026). arXiv:2501.07292.

[29] Ziv Goldfeld, Dhrumil Patel, Sreejith Sreekumar, and Mark M. Wilde. "Quantum neural estimation of entropies". Physical Review A **109**, 032431 (2024).

[30] Myeongjin Shin, Junseo Lee, and Kabgyun Jeong. "Estimating quantum mutual information through a quantum neural network". Quantum Information Processing **23**, 57 (2024).

[31] Sangyun Lee, Hyukjoon Kwon, and Jae Sung Lee. "Estimating entanglement entropy via variational quantum circuits with classical neural networks". Physical Review E **109**, 044117 (2024).

[32] Dénes Petz. "A variational expression for the relative entropy". Communications in Mathematical Physics **114**, 345–349 (1988).

[33] Dénes Petz. "Quantum information theory and quantum statistics". Springer Science & Business Media. (2007).

[34] Mario Berta, Omar Fawzi, and Marco Tomamichel. "On variational expressions for quantum relative entropies". Letters in Mathematical Physics **107**, 2239–2265 (2015).

[35] Anthony C. Thompson. "On certain contraction mappings in a partially ordered vector space". Proceedings of the American Mathematical Society **14**, 438–443 (1963).

[36] Matthew J. Donald. "On the relative entropy". Communications in Mathematical Physics **105**, 13–34 (1986).

[37] Marco Piani. "Relative entropy of entanglement and restricted measurements". Physical Review Letters **103**, 160504 (2009).

[38] Fumio Hiai and Dénes Petz. "The proper formula for relative entropy and its asymptotics in quantum probability". Communications in Mathematical Physics **143**, 99–114 (1991).

[39] Masahito Hayashi. "Optimal sequence of quantum measurements in the sense of Stein's lemma in quantum hypothesis testing". Journal of Physics A: Mathematical and General **35**, 10759 (2002).

[40] Milán Mosonyi and Tomohiro Ogawa. "Quantum hypothesis testing and the operational interpretation of the quantum Rényi relative entropies". Communications in Mathematical Physics **334**, 1617–1648 (2015).

[41] Fernando Brandão, Aram W. Harrow, James R. Lee, and Yuval Peres. "Adversarial hypothesis testing and a quantum Stein's lemma for restricted measurements". IEEE Transactions on Information Theory **66**, 5037–5054 (2020).

[42] Tobias Rippchen, Sreejith Sreekumar, and Mario Berta. "Locally-measured Rényi divergences". IEEE Transactions on Information Theory **71**, 6105–6133 (2025).

[43] Sreejith Sreekumar, Christoph Hirche, Hao-Chung Cheng, and Mario Berta. "Distributed quantum hypothesis testing under zero-rate communication constraints". Annales Henri Poincaré (2025).

[44] Sergio Verdú. "Empirical estimation of information measures: A literature guide". Entropy **21**, 720 (2019).

[45] Sreejith Sreekumar and Kengo Kato. "Deviation inequalities for Rényi divergence estimators via variational expression" (2025). arXiv:2508.09382.

[46] Jeongwan Haah, Aram W. Harrow, Zhengfeng Ji, Xiaodi Wu, and Nengkun Yu. "Sample-optimal tomography of quantum states". IEEE Transactions on Information Theory **63**, 5628–5641 (2017).

[47] John Wright. "How to learn a quantum state". PhD thesis. Carnegie Mellon University. (2016). url: https://people.eecs.berkeley.edu/~jswright/papers/thesis.pdf.

[48] Ryan O'Donnell and John Wright. "Efficient quantum tomography". In Proceedings of the Forty-Eighth Annual ACM Symposium on Theory of Computing. Page 899–912. STOC '16, New York, NY, USA (2016). Association for Computing Machinery.

[49] Henry Yuen. "An improved sample complexity lower bound for (fidelity) quantum state tomography". Quantum **7**, 890 (2023).

[50] Jacob Biamonte, Peter Wittek, Nicola Pancotti, Patrick Rebentrost, Nathan Wiebe, and Seth Lloyd. "Quantum machine learning". Nature **549**, 195–202 (2017).

[51] Marco Cerezo, Alexander Poremba, Lukasz Cincio, and Patrick J. Coles. "Variational Quantum Fidelity Estimation". Quantum **4**, 248 (2020).

[52] M. Cerezo, Andrew Arrasmith, Ryan Babbush, Simon C. Benjamin, Suguru Endo, Keisuke Fujii, Jarrod R. McClean, Kosuke Mitarai, Xiao Yuan, Lukasz Cincio, and Patrick J. Coles. "Variational quantum algorithms". Nature Reviews Physics **3**, 625–644 (2021).

[53] Jonas Jäger and Roman V. Krems. "Universal expressiveness of variational quantum classifiers and quantum kernels for support vector machines". Nature Communications **14**, 576 (2023).

[54] XuanLong Nguyen, Martin J. Wainwright, and Michael I. Jordan. "Estimating divergence functionals and the likelihood ratio by convex risk minimization". IEEE Transactions on Information Theory **56**, 5847–5861 (2010).

[55] Sanjeev Arora, Rong Ge, Yingyu Liang, Tengyu Ma, and Yi Zhang. "Generalization and equilibrium in generative adversarial nets (GANs)". In Proceedings of the 34th International Conference on Machine Learning. Volume 70 of Proceedings of Machine Learning Research, pages 224–232. PMLR (2017). url: https://proceedings.mlr.press/v70/arora17a.html.

[56] Pengchuan Zhang, Qiang Liu, Dengyong Zhou, Tao Xu, and Xiaodong He. "On the discrimination-generalization tradeoff in GANs". In 6th International Conference on Learning Representations. (2018). url: https://openreview.net/forum?id=Hk9Xc_lR-.

[57] Mohamed Ishmael Belghazi, Aristide Baratin, Sai Rajeshwar, Sherjil Ozair, Yoshua Bengio, Aaron Courville, and Devon Hjelm. "Mutual information neural estimation". In Proceedings of the 35th International Conference on Machine Learning. Volume 80 of Proceedings of Machine Learning Research, pages 531–540. PMLR (2018). url: https://proceedings.mlr.press/v80/belghazi18a.html.

[58] Sreejith Sreekumar, Zhengxin Zhang, and Ziv Goldfeld. "Non-asymptotic performance guarantees for neural estimation of f-divergences". In Proceedings of the 24th International Conference on Artificial Intelligence and Statistics. Volume 130, pages 3322–3330. (2021). url: https://proceedings.mlr.press/v130/sreekumar21a.html.

[59] Sreejith Sreekumar and Ziv Goldfeld. "Neural estimation of statistical divergences". Journal of Machine Learning Research **23**, 1–75 (2022). url: https://www.jmlr.org/papers/v23/21-1212.html.

[60] Jeremiah Birrell, Paul Dupuis, Markos A. Katsoulakis, Luc Rey-Bellet, and Jie Wang. "Variational representations and neural network estimation of Rényi divergences". SIAM Journal on Mathematics of Data Science **3**, 1093–1116 (2021).

[61] Kok Chuan Tan and Tyler Volkoff. "Variational quantum algorithms to estimate rank, quantum entropies, fidelity, and Fisher information via purity minimization". Physical Review Research **3**, 033251 (2021).

[62] Jarrod R. McClean, Sergio Boixo, Vadim N. Smelyanskiy, Ryan Babbush, and Hartmut Neven. "Barren plateaus in quantum neural network training landscapes". Nature Communications **9**, 4812 (2018).

[63] Marco Cerezo, Akira Sone, Tyler Volkoff, Lukasz Cincio, and Patrick J. Coles. "Cost-function-dependent barren plateaus in shallow parameterized quantum circuits". Nature Communications **12**, 1791 (2021).

[64] Zoë Holmes, Kunal Sharma, Marco Cerezo, and Patrick J. Coles. "Connecting ansatz expressibility to gradient magnitudes and barren plateaus". PRX Quantum **3**, 010313 (2022).

[65] Johannes Jakob Meyer, Marian Mularski, Elies Gil-Fuster, Antonio Anna Mele, Francesco Arzani, Alissa Wilms, and Jens Eisert. "Exploiting symmetry in variational quantum machine learning". PRX Quantum **4**, 010328 (2023).

[66] Quynh T. Nguyen, Louis Schatzki, Paolo Braccia, Michael Ragone, Patrick J. Coles, Frédéric Sauvage, Martín Larocca, and Maciej Cerezo. "Theory for equivariant quantum neural networks". PRX Quantum **5**, 020328 (2024).

[67] Edward Grant, Leonard Wossnig, Mateusz Ostaszewski, and Marcello Benedetti. "An initialization strategy for addressing barren plateaus in parameterized quantum circuits". Quantum **3**, 214 (2019).

[68] Andrea Skolik, Jarrod R. McClean, Masoud Mohseni, Patrick van der Smagt, and Matthew Leib. "Layerwise learning for quantum neural networks". Quantum Machine Intelligence **3**, 1–19 (2021).

[69] Marco Cerezo, Martin Larocca, Diego García-Martín, N. L. Diaz, Paolo Braccia, Enrico Fontana, Manuel S. Rudolph, Pablo Bermejo, Aroosa Ijaz, Supanut Thanasilp, Eric R. Anschuetz, and Zoë Holmes. "Does provable absence of barren plateaus imply classical simulability?". Nature Communications **16**, 7907 (2025).

[70] Christopher Fuchs. "Distinguishability and accessible information in quantum theory". PhD thesis. University of New Mexico. (1996). arXiv:quant-ph/9601020.

[71] Zixin Huang and Mark M. Wilde. "Semi-definite optimization of the measured relative entropies of quantum states and channels" (2025). url: https://arxiv.org/abs/2406.19060.

[72] Liam Paninski. "Estimation of entropy and mutual information". Neural Computation **15**, 1191–1253 (2003).

[73] Nilanjana Datta. "Min- and max-relative entropies and a new entanglement monotone". IEEE Transactions on Information Theory **55**, 2816–2826 (2009).

[74] Dave Bacon, Isaac L. Chuang, and Aram W. Harrow. "Efficient Quantum Circuits for Schur and Clebsch-Gordan Transforms". Physical Review Letters **97**, 170502 (2006).

[75] Aram W. Harrow. "Applications of coherent classical communication and the Schur transform to quantum information theory". PhD thesis. Massachusetts Institute of Technology. (2005). arXiv:quant-ph/0512255.

[76] William M. Kirby and Frederick W. Strauch. "A practical quantum algorithm for the Schur transform". Quantum Information and Computation **18**, 0721–0742 (2018).

[77] Hari Krovi. "An efficient high dimensional quantum Schur transform". Quantum **3**, 122 (2019).

[78] Ramon Van Handel. "Probability in high dimension: Lecture notes-princeton university". [Online]. Available: https://web.math.princeton.edu/~rvan/APC550.pdf (2016).

[79] Andrey N. Kolmogorov and Vladimir M. Tikhomirov. "ε-entropy and ε-capacity of sets in functional spaces". Uspekhi Matematicheskikh Nauk **14**, 3–86 (1959). url: http://mi.mathnet.ru/eng/rm7289.

[80] Abhinav Kandala, Antonio Mezzacapo, Kristan Temme, Maika Takita, Matthias Brink, Jerry M. Chow, and Jay M. Gambetta. "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets". Nature **549**, 242–246 (2017).

[81] Seth Lloyd. "Quantum approximate optimization is computationally universal" (2018). arXiv:1812.11075.

[82] Mauro E. S. Morales, Jacob D. Biamonte, and Zoltán Zimborás. "On the universality of the quantum approximate optimization algorithm". Quantum Information Processing **19**, 291 (2020).

[83] Yihong Wu and Pengkun Yang. "Minimax rates of entropy estimation on large alphabets via best polynomial approximation". IEEE Transactions on Information Theory **62**, 3702–3720 (2016).

[84] Yanjun Han, Jiantao Jiao, and Tsachy Weissman. "Minimax estimation of divergences between discrete distributions". IEEE Journal on Selected Areas in Information Theory **1**, 814–823 (2020).

[85] Dennis Elbrächter, Dmytro Perekrestenko, Philipp Grohs, and Helmut Bölcskei. "Deep neural network approximation theory". IEEE Transactions on Information Theory **67**, 2581–2623 (2021).

[86] Michael A. Nielsen and Isaac L. Chuang. "Quantum computation and quantum information: 10th anniversary edition". Cambridge University Press. (2010).

[87] Masahito Hayashi. "A Group Theoretic Approach to Quantum Information". Springer. (2017).

[88] Aad W. van der Vaart and Jon A. Wellner. "Weak convergence and empirical processes". Springer, New York. (1996).

[89] Johannes Schmidt-Hieber. "Nonparametric regression using deep neural networks with ReLU activation function". The Annals of Statistics **48**, 1875–1897 (2020).

[90] Mark M. Wilde. "Quantum Fisher information matrices from Rényi relative entropies" (2025). arXiv:2510.02218.

[91] Sreejith Sreekumar and Mario Berta. "Limit distribution theory for quantum divergences". IEEE Transactions on Information Theory **71**, 459–484 (2025).

[92] Eric A. Carlen. "Trace inequalities and quantum entropy: An introductory course". In Contemporary Mathematics. Volume 529 of Entropy and the Quantum. American Mathematical Society (2010).

[93] Philip J. Davis. "Interpolation and approximation". Dover Publications, Inc. New York. (1975).

[94] Andrew C. Berry. "The accuracy of the Gaussian approximation to the sum of independent variates". Transactions of the American Mathematical Society **49**, 122–136 (1941).

[95] Carl-Gustav Esseen. "On the Liapunoff limit of error in the theory of probability". Arkiv för matematik, astronomi och fysik **28A**, 1–19 (1942).

[96] Neil J. Ross and Peter Selinger. "Optimal ancilla-free Clifford + T approximation of z-rotations". Quantum Information and Computation **16**, 901–953 (2016).

[97] Christopher M. Dawson and Michael A. Nielsen. "The Solovay-Kitaev algorithm". Quantum Information and Computation **6**, 81–95 (2006).

A Optimization of Measured Relative Entropies

For $\rho, \sigma > 0$, the optimizers $\omega_1^\star(\rho,\sigma)$ and $\omega_\alpha^\star(\rho,\sigma)$ of the RHSs of (7) and (9), respectively, are given by

$$\omega_\alpha^\star(\rho,\sigma) = \begin{cases} e^{(\alpha-1)H_\alpha^\star(\rho,\sigma)} = \sum_{i=1}^d \left(\frac{\mathrm{Tr}[P_{i,\alpha}^\star \rho]}{\mathrm{Tr}[P_{i,\alpha}^\star \sigma]}\right)^{\alpha-1} P_{i,\alpha}^\star, & \text{for } \alpha \in \left(0, \frac{1}{2}\right), \\ e^{\alpha H_\alpha^\star(\rho,\sigma)} = \sum_{i=1}^d \left(\frac{\mathrm{Tr}[P_{i,\alpha}^\star \rho]}{\mathrm{Tr}[P_{i,\alpha}^\star \sigma]}\right)^{\alpha} P_{i,\alpha}^\star, & \text{for } \alpha \in \left[\frac{1}{2}, \infty\right), \end{cases} \tag{66}$$

where $\{P_{i,\alpha}^\star\}_{i=1}^d$ are the orthogonal projectors in the spectral decomposition of $H_\alpha^\star(\rho,\sigma)$ from (5). This can be verified by substituting $\omega_\alpha^\star(\rho,\sigma)$ in (9) and noting that the RHS of (8) coincides with that obtained by substituting $H_\alpha^\star(\rho,\sigma)$ in the RHS of (4). The variational form in (8) and the relation (66) can be leveraged to show that $H_\alpha^\star(\rho,\sigma)$ is unique when $\rho, \sigma > 0$, and should satisfy the necessary (and sufficient) condition for optimality derived from it.

Proposition 13 (Necessary and sufficient condition for optimality)**.** *Suppose $\rho, \sigma > 0$. Then the optimal $\omega > 0$ in (7) is unique and determined by the following equation:*

$$\sigma = \int_0^\infty (\omega + sI)^{-1} \rho (\omega + sI)^{-1} ds. \tag{67}$$

The optimal $\omega > 0$ in (9) is unique and determined by the equations:

$$\rho = \left(\frac{1-\alpha}{\alpha}\right) \frac{\sin\left(\left(\frac{\alpha}{1-\alpha}\right)\pi\right)}{\pi} \int_0^\infty t^{\frac{\alpha}{\alpha-1}} (\omega + tI)^{-1} \sigma (\omega + tI)^{-1} dt, \quad \forall\ \alpha \in \left(0, \frac{1}{2}\right), \tag{68}$$

$$\sigma = \left(\frac{\alpha}{1-\alpha}\right) \frac{\sin\left(\left(\frac{1-\alpha}{\alpha}\right)\pi\right)}{\pi} \int_0^\infty t^{\frac{\alpha-1}{\alpha}} (\omega + tI)^{-1} \rho (\omega + tI)^{-1} dt, \ \forall\ \alpha \in \left[\frac{1}{2}, 1\right) \cup (1, \infty). \tag{69}$$

Proof. Let $A \in \mathcal{L}(\mathbb{H}_d)$, $\omega > 0$ and $r \in (-1, 0) \cup (0, 1)$. We will use the following expressions for the relevant matrix derivatives of interest (see [90] for a detailed derivation from first principles):

$$\frac{\partial}{\partial \omega} \operatorname{Tr}[A \log \omega] = \int_0^\infty (\omega + sI)^{-1} A (\omega + sI)^{-1} ds, \tag{70}$$

$$\frac{\partial}{\partial \omega} \operatorname{Tr}[A\omega^r] = \frac{\sin(r\pi)}{\pi} \int_0^\infty t^r (\omega + tI)^{-1} A (\omega + tI)^{-1} dt, \quad \forall r \in (-1, 0) \cup (0, 1). \tag{71}$$

The expressions in (70) and (71) also equal the directional derivatives of $\log \omega$ and ω^r, respectively, in the direction A (see [91, Proof of Theorem 1 and 5] for expressions of directional derivatives based on integral expressions given in [92, Lemma 2.8]).

To determine $\omega_1^\star(\rho, \sigma)$, we set the matrix derivative with respect to ω of the expression to be optimized in (7) to zero:

$$\begin{aligned} 0 = \frac{\partial}{\partial \omega} \left(\operatorname{Tr}[\rho \log \omega] + 1 - \operatorname{Tr}[\sigma\omega]\right) &= \frac{\partial}{\partial \omega} \operatorname{Tr}[\rho \log \omega] - \frac{\partial}{\partial \omega} \operatorname{Tr}[\sigma\omega] \\ &= \int_0^\infty (\omega + sI)^{-1} \rho (\omega + sI)^{-1} ds - \sigma, \end{aligned}$$

where we applied (70). We conclude that $\omega_1^\star(\rho, \sigma)$ should satisfy (67). Uniqueness of $\omega_1^\star(\rho, \sigma)$ and sufficiency of the above condition for optimality follows from the strict concavity of the function $\omega \mapsto \operatorname{Tr}[\rho \log \omega] + 1 - \operatorname{Tr}[\sigma\omega]$ for $\rho, \sigma > 0$, which in turn follows from strict operator concavity of log and the fact that $\operatorname{Tr}[AB] > 0$ for $A, B > 0$.

To determine the optimal choice of ω in (9) for $\alpha \in \left(0, \frac{1}{2}\right)$, we set the matrix derivative with respect to ω of the relevant expression to zero as follows:

$$\begin{aligned} 0 &= \frac{\partial}{\partial \omega} \left(\alpha \operatorname{Tr}[\rho\omega] + (1-\alpha) \operatorname{Tr}[\sigma\omega^{\frac{\alpha}{\alpha-1}}]\right) \\ &= \alpha\rho + (\alpha - 1) \frac{\sin\left(\left(\frac{\alpha}{1-\alpha}\right)\pi\right)}{\pi} \int_0^\infty t^{\frac{\alpha}{\alpha-1}} (\omega + tI)^{-1} \sigma (\omega + tI)^{-1} dt. \end{aligned}$$

Here, we used (71) with $r = \frac{\alpha}{\alpha-1} \in (-1, 0)$. Hence, $\omega_\alpha^\star(\rho, \sigma)$ satisfies (68). Uniqueness of $\omega_\alpha^\star(\rho, \sigma)$ and sufficiency of the above equation for optimality follows from the strict convexity of the function $\omega \mapsto \alpha \operatorname{Tr}[\rho\omega] + (1-\alpha) \operatorname{Tr}[\sigma\omega^{\frac{\alpha}{\alpha-1}}]$ for $\rho, \sigma > 0$, which in turn follows from strict operator convexity of $x \mapsto x^r$ for $r \in (-1, 0)$ and $\operatorname{Tr}[AB] > 0$ for $A, B > 0$.

To determine the optimal choice of ω in (9) for $\alpha \in \left[\frac{1}{2}, 1\right)$, we set the following matrix derivative to zero:

$$\begin{aligned} 0 &= \frac{\partial}{\partial \omega}\left(\alpha \operatorname{Tr}[\rho\omega^{1-\frac{1}{\alpha}}] + (1-\alpha)\operatorname{Tr}[\sigma\omega]\right) \\ &= (1-\alpha)\,\sigma - \alpha \frac{\sin\left(\left(\frac{1}{\alpha}-1\right)\pi\right)}{\pi} \int_0^\infty t^{\frac{\alpha-1}{\alpha}} (\omega + tI)^{-1} \rho\, (\omega + tI)^{-1}\, dt. \end{aligned}$$

Here, we applied (71) with $r = \frac{\alpha-1}{\alpha} \in (-1, 0)$. Hence, we conclude that $\omega_\alpha^\star(\rho, \sigma)$ should satisfy (69). Uniqueness of $\omega_\alpha^\star(\rho, \sigma)$ and sufficiency of the condition above for optimality follows from the strict convexity of $\omega \mapsto \alpha \operatorname{Tr}[\rho\omega^{1-\frac{1}{\alpha}}] + (1-\alpha)\operatorname{Tr}[\sigma\omega]$, which is a consequence of strict operator convexity of $x \mapsto x^r$ for $r \in (-1, 0)$ and $\operatorname{Tr}[AB] > 0$ for $A, B > 0$.

Finally, note that $\omega_\alpha^\star(\rho, \sigma)$ for $\alpha \in (1, \infty)$ should satisfy

$$\begin{aligned} 0 &= \frac{\partial}{\partial \omega}\left(\alpha \operatorname{Tr}[\rho\omega^{1-\frac{1}{\alpha}}] + (1-\alpha)\operatorname{Tr}[\sigma\omega]\right) \\ &= \alpha \frac{\sin\left(\left(\frac{\alpha-1}{\alpha}\right)\pi\right)}{\pi} \int_0^\infty t^{1-\frac{1}{\alpha}} (\omega + tI)^{-1} \rho\, (\omega + tI)^{-1}\, dt + (1-\alpha)\,\sigma, \end{aligned}$$

where we again applied (71) with $r = 1 - \frac{1}{\alpha} \in (0, 1)$. Hence, $\omega_\alpha^\star(\rho, \sigma)$ should satisfy (69). Uniqueness of $\omega_\alpha^\star(\rho, \sigma)$ and sufficiency of the above condition for characterizing $\omega_\alpha^\star(\rho, \sigma)$ follows from the strict concavity of the function $\omega \mapsto \alpha \operatorname{Tr}[\rho\omega^{1-\frac{1}{\alpha}}] + (1-\alpha)\operatorname{Tr}[\sigma\omega]$ for $\rho, \sigma > 0$, which in turn follows from strict operator concavity of $x \mapsto x^r$ for $r \in (0, 1)$. □

Remark 3 (Limit of optimality condition)**.** *The equation in* (67) *arises as the limit of* (69) *as* $\alpha \to 1$*. Indeed, this follows because*

$$\lim_{\alpha\to 1}\left(\frac{\alpha}{1-\alpha}\right)\frac{\sin\left(\left(\frac{1-\alpha}{\alpha}\right)\pi\right)}{\pi} = 1 \quad \textit{and} \quad \lim_{\alpha\to 1} t^{\frac{\alpha-1}{\alpha}} = 1,$$

so that

$$\lim_{\alpha\to 1}\left(\frac{\alpha}{1-\alpha}\right)\frac{\sin\left(\left(\frac{1-\alpha}{\alpha}\right)\pi\right)}{\pi}\int_0^\infty t^{\frac{\alpha-1}{\alpha}} (\omega + tI)^{-1} \rho\, (\omega + tI)^{-1}\, dt = \int_0^\infty (\omega + sI)^{-1} \rho\, (\omega + sI)^{-1}\, ds.$$

Here, the equality is justified by an application of the dominated convergence theorem.

B Lower Bound on Minimax Risk for Estimating Measured Relative Entropies

The proof of (23) and (32) relies on an application of Le Cam's two-point method and its generalized version with composite hypothesis, as done in the proof of [83, Proposition 2 and 3] and [84, Theorems 1 and 2] (see the arXiv version). Since the proofs are similar to those of the lower bounds in [84], we will only provide a sketch highlighting the differences in our case.

To prove (23), consider the following discrete probability distributions supported on $\{1, 2, \ldots, d\}$ with $\epsilon \in (0, 0.5)$ and $b \geq 2$:

$$Q_1 = \left(\frac{1-\epsilon}{b(d-1)}, \ldots, \frac{1-\epsilon}{b(d-1)}, 1 - \frac{(1-\epsilon)}{b}\right), \quad Q_2 = \left(\frac{1+\epsilon}{b(d-1)}, \ldots, \frac{1+\epsilon}{b(d-1)}, 1 - \frac{(1+\epsilon)}{b}\right), \tag{72a}$$

$$P = \left(\frac{1}{2(d-1)}, \ldots, \frac{1}{2(d-1)}, \frac{1}{2}\right). \tag{72b}$$

Denoting the i^{th} entry of P, Q_1, Q_2 by p_i, $q_{1,i}$ and $q_{2,i}$, respectively, we have

$$\max_{1 \leq i \leq d} \frac{p_i}{q_{1,i}} \vee \frac{p_i}{q_{2,i}} \vee \frac{q_{1,i}}{p_i} \vee \frac{q_{2,i}}{p_i} \leq b.$$

Hence, $(P, Q_1), (P, Q_2) \in \mathcal{S}_d(b)$ (when interpreted as quantum states diagonal in the same eigen-basis, say, the computational basis). Consequently, via an application of Le Cam's lemma as in the proof of [84, Theorem 2] yields $R_n^\star(\mathcal{S}_d(b)) \gtrsim b^{1/2} n^{-1/2}$, where $R_n^\star(\mathcal{S}_d(b))$ is the minimax risk defined in (11). This yields the first term on the RHS of (23).

It remains to show that $R_n^\star(\mathcal{S}_d(b)) \gtrsim db/(n \log d)$. For this purpose, consider the following distributions[6] supported on $\{1, 2, \ldots, d\}$ similar to that in [84, Theorem 2]:

$$P = \left(\frac{cb}{n \log d}, \ldots, \frac{cb}{n \log d}, 1 - \frac{c(d-1)b}{n \log d}\right), \tag{73a}$$

$$Q_1 = \left(q_{1,i}, \ldots, q_{1,d-1}, 1 - \sum_{i=1}^{d-1} q_{1,i}\right), \quad Q_2 = \left(q_{2,i}, \ldots, q_{2,d-1}, 1 - \sum_{i=1}^{d-1} q_{2,i}\right), \tag{73b}$$

where $c > 0$ is chosen such that P is a probability distribution (possible under the condition $db \lesssim n \log d$), and each of the first $d-1$ entries of Q_i, $i = 1, 2$, are chosen independently according to probability measure ν_i supported on $I = [c_1/(n \log d), c_2 \log d/n]$ satisfying $\mathbb{E}_{\nu_1}[\log X] - \mathbb{E}_{\nu_2}[\log X] \gtrsim d/(n \log d)$ and additional matching moment conditions as in [83]. The existence of such probability measures ν_1 and ν_2 has been shown in [83]. Since Q_1 and Q_2 are randomly generated, they need not be probability distributions, i.e., the entries need not sum to 1. However, one may restrict to approximate probability distributions with strictly positive entries such that $|\|q_i\|_1 - 1| \leq 1 + \epsilon$, with ϵ chosen appropriately and the constants c, c_1, c_2 adjusted, such that the probability distributions Q_1', Q_2' obtained after normalization by sum of its entries satisfy (almost surely)

$$\max_{1 \leq i \leq d} \frac{p_i}{q_{1,i}'} \vee \frac{p_i}{q_{2,i}'} \vee \frac{q_{1,i}'}{p_i} \vee \frac{q_{2,i}'}{p_i} \leq b \vee \frac{(\log d)^2}{b} \leq b.$$

In the last inequality, we used that $b \geq (\log d)^2$. The minimax risk can then be lower bounded by the minimax risk over the set of such approximate probability distributions under a Poisson sampling model up to an additive factor that vanishes as ϵ tends to zero. The minimax risk under the Poisson sampling model can in turn be further lower bounded (see [83, Proof of Lemma 2]) as $\Omega(db/(n \log d))$ via generalized Le Cam's method. Specifically, this can be done by taking the prior distributions used in generalized Le Cam's method to be the truncated measures obtained (via change of measure) by restricting support to

[6] We note that the distributions in (73) differs slightly from those used in the proof of lower bound in [84, Theorem 2], in that $\log d$ here is replaced by $\log n$ therein. This necessitates an additional condition $\log d \gtrsim \log n$ under which their lower bound holds. However, by using (73), it can be seen via essentially the same steps as in their proof that this constraint can be avoided.

distributions (P, Q_i') for $i = 1, 2$, such that $|\mathsf{D}_{\mathsf{M}}(P\|Q_1') - \mathsf{D}_{\mathsf{M}}(P\|Q_2')| = \Omega(db/(n \log d))$ for every (P, Q_1') and (P, Q_2'). This change of measure incurs an additive penalty on the lower bound that vanishes with an appropriately chosen large enough ϵ (that tends to zero at an appropriate rate). Finally, the total variation distance between the sufficient statistics (histogram) under these priors in the Poisson sampling model decays exponentially (see [83, Lemma 3]) due to the matching moments conditions under the priors ν_1 and ν_2, which can be used to obtain the desired lower bound via [83, Lemma 2]. To summarize, the above steps lead to $R_n^\star(\mathcal{S}_d(b)) \gtrsim db/(n \log d)$ given that $b \geq (\log d)^2$ and $db \lesssim n \log d$, thus concluding the proof sketch for the case of measured relative entropy.

To prove (32), we first observe that the minimax risk for estimating Rényi divergence of order α can be lower bounded in terms of the minimax risk for estimating the classical α-divergence, where α-divergence (see [84]) between two discrete distributions P and Q supported on $\{1, \ldots, d\}$ is

$$A_\alpha(P\|Q) \coloneqq \frac{1}{\alpha(\alpha-1)} \left(-1 + \sum_{i=1}^{d} p_i^\alpha q_i^{1-\alpha} \right).$$

Note that

$$A_\alpha(P\|Q) = \frac{e^{(\alpha-1)\mathsf{D}_{\mathsf{M},\alpha}(P\|Q)} - 1}{\alpha(\alpha-1)}.$$

Consider $\alpha > 1$. For $(P, Q) \in \mathcal{S}_d(b)$, we have

$$\mathsf{D}_{\mathsf{M},\alpha}(P\|Q) \coloneqq \frac{1}{\alpha-1} \log \left(\sum_{i=1}^{d} p_i^\alpha q_i^{1-\alpha} \right) \leq \frac{1}{\alpha-1} \log \left(\sum_{i=1}^{d} q_i b^{\alpha-1} \right) \leq \log b.$$

Hence, without loss of generality, it is sufficient to consider estimators $\hat{\mathsf{D}}_{n,\alpha}$ satisfying $\hat{\mathsf{D}}_{n,\alpha} \leq \log b$. Given such an estimator $\hat{\mathsf{D}}_{n,\alpha}$, a natural estimator for $A_\alpha(P\|Q)$ is

$$\hat{A}_{n,\alpha} = \frac{e^{(\alpha-1)\hat{\mathsf{D}}_{n,\alpha}} - 1}{\alpha(\alpha-1)}.$$

We can upper bound the absolute error for $\hat{A}_{n,\alpha}$ in terms of $\hat{\mathsf{D}}_{n,\alpha}$ as

$$\left| \hat{A}_{n,\alpha} - A_\alpha(P\|Q) \right| \leq \frac{\left| e^{(\alpha-1)\hat{\mathsf{D}}_{n,\alpha}} - e^{(\alpha-1)\mathsf{D}_{\mathsf{M},\alpha}(P\|Q)} \right|}{\alpha(\alpha-1)} \leq \frac{b^{\alpha-1} \left| \hat{\mathsf{D}}_{n,\alpha} - \mathsf{D}_{\mathsf{M},\alpha}(P\|Q) \right|}{\alpha}.$$

Hence

$$\left| \hat{\mathsf{D}}_{n,\alpha} - \mathsf{D}_{\mathsf{M},\alpha}(P\|Q) \right| \geq \alpha b^{1-\alpha} \left| \hat{A}_{n,\alpha} - A_\alpha(P\|Q) \right|.$$

Denoting the minimax risk for estimating classical α-divergence over the class $\mathcal{S}_d^{(\mathsf{c})}(b)$ of distributions (P, Q) satisfying $\max_{1 \leq i \leq d}(p_i/q_i) \vee (q_i/p_i) \leq b$ by $\bar{R}_{n,\alpha}^\star(\mathcal{S}_d^{(\mathsf{c})}(b))$, the above equation implies that $R_{n,\alpha}^\star(\mathcal{S}_d(b)) \geq \alpha b^{1-\alpha} \bar{R}_{n,\alpha}^\star(\mathcal{S}_d^{(\mathsf{c})}(b))$. Now, using Le Cam's two-point method and its generalized version with the distributions given in (72) and (73), it can be shown using similar steps as in the proof of the lower bound in [84, Theorem 1] that given $b \geq (\log d)^2 \vee 2$ and $db^\alpha \lesssim n \log d$:

$$\bar{R}_{n,\alpha}^\star\left(\mathcal{S}_d^{(\mathsf{c})}(b)\right) \gtrsim_\alpha \frac{b^{\alpha-\frac{1}{2}}}{\sqrt{n}} + \frac{db^\alpha}{n \log d},$$

which yields the desired lower bound

$$R_{n,\alpha}^\star(\mathcal{S}_d(b)) \gtrsim_\alpha \frac{\sqrt{b}}{\sqrt{n}} + \frac{db}{n \log d}.$$

C Proof of Proposition 3

We first consider Part (i). Since $\tilde{\mathcal{S}}_{k,d,\alpha}(b,a,\varepsilon) \subseteq \mathcal{S}_d(b)$ by definition, we only need to show that $\mathcal{S}_d(b) \subseteq \tilde{\mathcal{S}}_{k,d,\alpha}(b,a,\varepsilon)$ for k, a, and ε as in the statement of the proposition. We will only consider $\alpha = 1$ as the proof is exactly same for other α. Consider any $(\rho,\sigma) \in \mathcal{S}_d(b)$ and let $\Lambda^\star(\rho,\sigma) = \{\lambda_j^\star\}_{j=1}^d$ be any enumeration. By Lemma 10, we have $\left|\lambda_j^\star\right| \le \log b$ for all $j \in [1:d]$. Let

$$p(x) = \sum_{j=1}^{d} \lambda_j^\star \prod_{i\neq j} \frac{dx-i}{j-i}.$$

Note that $p(i/d) = \lambda_i^\star$ and that $p(x)$ is a polynomial of degree $d-1$, which can be written as

$$p(x) = \sum_{j=1}^{d} \tilde{\lambda}_j \tilde{p}_j(x), \quad \text{where} \quad \tilde{p}_j(x) \coloneqq \prod_{i\neq j}\left(x - \frac{i}{d}\right) \quad \text{and} \quad \tilde{\lambda}_j \coloneqq \frac{\lambda_j^\star d^{d-1}}{\prod_{i\neq j}(j-i)}.$$

Further, observe that $\tilde{p}_j(x)$ is a polynomial of the form $\sum_{l=0}^{d-1} \tilde{a}_{l,j} x^l$ with $|\tilde{a}_{l,j}| \le 1$ for all $j \in [1:d]$ and $l \in [0:d-1]$. Hence, $p(x)$ is a polynomial of the form $\sum_{l=0}^{d-1} a_l x^l$ with

$$|a_l| \le \sum_{j=1}^{d} |\tilde{\lambda}_j| = \sum_{j=1}^{d} \frac{\left|\lambda_j^\star\right| d^{d-1}}{\prod_{i\neq j}|j-i|} \overset{(a)}{\le} \sum_{j=1}^{d} \frac{d^{d-1}\log b}{\prod_{i\neq j}|j-i|} \overset{(b)}{\le} \frac{(3e)^d \log b}{2\pi},$$

where

(a) used that $\left|\lambda_j^\star\right| \le \log b$ for all $j \in [1:d]$;

(b) follows because for all $j \in [1:d]$,

$$\prod_{i\neq j}|j-i| \ge \min_{1\le m\le d}(m-1)!(d-m)! = \begin{cases} \left(\left(\frac{d-1}{2}\right)!\right)^2, & \text{if } d \text{ is odd,} \\ \left(\frac{d-2}{2}\right)!\left(\frac{d}{2}\right)!, & \text{if } d \text{ is even,} \end{cases} \ge 2\pi\left(\frac{d}{3e}\right)^d;$$

The last inequality can be verified to hold by computation for $1 \le d \le 4$, and for $d > 4$, we used $d-2 \ge 0.5d$, $(d-1)/2 \ge (d/3)$, and the DeMoivre–Stirling lower bound for the factorial given by $n! > \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$.

This implies that $\mathcal{S}_d(b) \subseteq \tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon)$ for k, a as in the statement of the proposition and $\varepsilon = 0$. Since $\tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon) \subseteq \tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon')$ for $\varepsilon' \ge \varepsilon$, the claim in Part (i) follows.

To prove Part (ii), let $\Lambda^\star(\rho,\sigma) = \{\lambda_i^\star\}_{i=1}^d$ be an (arbitrary) enumeration. We will consider approximation of a Lipschitz continuous function f satisfying $f(i/d) = \lambda_i^\star$ by polynomials of bounded degree and bounded coefficients. Specifically, with $\lambda_0^\star = 0$, let $\hat{f}\colon [0,1] \mapsto [-\log b, \log b]$ be the piecewise linear function given by $\hat{f}(x) = \lambda_{i+1}^\star(dx-i) - \lambda_i^\star(dx-i-1)$ for $i/d \le x \le (i+1)/d$ and $0 \le i \le d$. Note that $\hat{f}(i/d) = \lambda_i^\star$, $\|\hat{f}\|_{\infty,[0,1]} \le \log b$, and the Lipschitz constant of $\hat{f}$ is upper bounded by $2d\log b$ for $(\rho,\sigma) \in \mathcal{S}_d(b)$. We next consider Bernstein's approximation of $\hat{f}$ using polynomials of degree k, i.e., using

$$p_{k,\hat{f}}(x) = \sum_{m=0}^{k} B_{m,k}(x)\hat{f}\left(\frac{m}{k}\right), \quad x \in [0,1], \tag{74a}$$

$$\text{where} \quad B_{m,k}(x) \coloneqq \binom{k}{m} x^m (1-x)^{k-m}. \tag{74b}$$

Let $\ell \in \mathbb{N} \cup \{0\}$. By straightforward computation, the ℓ^{th} derivative of $B_{m,k}(x)$ at $x = 0$ is

$$B_{m,k}^{(\ell)}(0) = \frac{k!}{(k-\ell)!}\binom{\ell}{m}(-1)^{m+\ell}, \ \forall \ell \in \mathbb{N}. \tag{75}$$

Further, for any ℓ-times differentiable function f,

$$\left\|p_{k,f}^{(\ell)}\right\|_{\infty,(0,1)} \leq \left\|f^{(\ell)}\right\|_{\infty,(0,1)}. \tag{76}$$

We will use the following fact that bounds the error of approximating a Lipschitz f using its Bernstein's approximation.

Lemma 14 (Error in Bernstein's approximation, see e.g., [93])**.** *For all $f\colon [0,1] \mapsto \mathbb{R}$ and $k \in \mathbb{N}$, we have*

$$\|p_{k,f} - f\|_{\infty,[0,1]} \leq \left(\|f\|_{\mathrm{Lip},[0,1]} + 0.5\,\|f\|_{\infty,[0,1]}\right) k^{-\frac{1}{3}}, \tag{77}$$

where

$$\|f\|_{\mathrm{Lip},[0,1]} = \sup_{\substack{x,y\in[0,1]\\ x\neq y}} \frac{|f(x)-f(y)|}{|x-y|}.$$

Lemma 14 follows by optimizing δ in the expression stated below as given in [93, Page 111]:

$$\|p_{k,f} - f\|_{\infty,[0,1]} \leq \|f\|_{\mathrm{Lip},[0,1]}\,\delta + \frac{\|f\|_{\infty,[0,1]}}{2k\delta^2}, \ \forall\ \delta \geq 0. \tag{78}$$

An independent proof via an application of the Berry-Esseen theorem with the same approximation error rate in terms of k (albeit with slightly larger constants) is provided below, which was developed as we were initially unaware of (78).

Applying Lemma 14 to $\hat{f}$ as above, we obtain that

$$\left\|p_{k,\hat{f}} - \hat{f}\right\|_{\infty,[0,1]} \leq (2d+0.5)\,(\log b)k^{-\frac{1}{3}}.$$

Moreover, the coefficient $a_\ell(p_{k,\hat{f}})$ of x^ℓ in $p_{k,\hat{f}}$ is upper bounded by

$$\left|a_\ell(p_{k,\hat{f}})\right| = \left|p_{k,\hat{f}}^{(\ell)}(0)\right| \leq \sum_{m=0}^{k} \|\hat{f}\|_{\infty,[0,1]} \left|B_{m,k}^{(\ell)}(0)\right| \leq \log b \sum_{m=0}^{k} \left|B_{m,k}^{(\ell)}(0)\right|,$$

which yields via (75) that

$$\max_{\ell\in[0:k]} \left|a_\ell(p_{k,\hat{f}})\right| \leq 2^k k! \log b.$$

This implies by the definition of $\tilde{\mathcal{S}}_{k,d}(b,a,\varepsilon)$ that Part (ii) holds.

Alternative Proof of Lemma 14 with Different Constants

Since the bound is trivial if $\|f\|_{\infty,[0,1]} = \infty$ or $\|f\|_{\mathrm{Lip},[0,1]} = \infty$, we may assume that $\|f\|_{\infty,[0,1]} \vee \|f\|_{\mathrm{Lip},[0,1]} < \infty$. Recalling the definitions of $p_{k,f}$ and $B_{m,k}$ given in (74), note that $B_{m,k}(0) = 0$ for $m \in [1:k]$ and $B_{0,k}(0) = 1$. Similarly, $B_{m,k}(1) = 0$ for $m \in [0:k-1]$ and $B_{k,k}(1) = 1$ (by interpreting $0^0 = 1$). Hence, $p_{k,f}(0) = f(0)$ and $p_{k,f}(1) = f(1)$. Consequently, $|p_{k,f}(x) - f(x)| = 0$ for $x \in \{0,1\}$. Next, consider any $x \in (0,1)$ and $\epsilon > 0$. Then, we can bound the approximation error as follows:

$$
\begin{aligned}
&|p_{k,f}(x) - f(x)| \\
&= \left| \sum_{m=0}^{k} B_{m,k}(x) f\left(\frac{m}{k}\right) - f(x) \right| \\
&\overset{(a)}{=} \sum_{m=0}^{k} B_{m,k}(x) \left| f\left(\frac{m}{k}\right) - f(x) \right| \\
&= \sum_{\substack{0\le m\le k:\\ \left|x-\frac{m}{k}\right|\le\epsilon}} B_{m,k}(x) \left| f\left(\frac{m}{k}\right) - f(x) \right| + \sum_{\substack{0\le m\le k:\\ \left|x-\frac{m}{k}\right|>\epsilon}} B_{m,k}(x) \left| f\left(\frac{m}{k}\right) - f(x) \right| \\
&\overset{(b)}{\le} \epsilon \|f\|_{\mathrm{Lip},[0,1]} \sum_{0\le m\le k:\left|x-\frac{m}{k}\right|\le\epsilon} B_{m,k}(x) + 2\|f\|_{\infty,[0,1]} \sum_{0\le m\le k:\left|x-\frac{m}{k}\right|>\epsilon} B_{m,k}(x) \\
&\overset{(c)}{\le} \epsilon \|f\|_{\mathrm{Lip},[0,1]} + 2\|f\|_{\infty,[0,1]} \sum_{0\le m\le k:\left|x-\frac{m}{k}\right|>\epsilon} B_{m,k}(x),
\end{aligned} \tag{79}
$$

where

(a) and (c) are due to $B_{m,k}(x) \ge 0$ and $\sum_{m=0}^{k} B_{m,k}(x) = 1$ for all $x \in [0,1]$;

(b) follows by the definition of $\|f\|_{\mathrm{Lip},[0,1]}$ and $\|f\|_{\infty,[0,1]}$, and $|y-z| \le |y|+|z|$ for $y, z \in \mathbb{R}$.

To upper bound the summation in the right hand side of (79), we use the Berry-Esseen theorem [94, 95] (with refined constants) applied to an i.i.d. sum of Bernoulli random variables, $\{X_i\}_{i=1}^{k}$ with $\mathbb{P}(X_i = 1) = x$. This yields

$$
\mathbb{P}\left(\left| \sum_{i=1}^{k} X_i - kx \right| > y\sqrt{kx(1-x)} \right) \le \sqrt{\frac{2}{\pi}} \int_{y}^{\infty} e^{-\frac{z^2}{2}} dz + \frac{\mathbb{E}\left[|X_1 - x|^3 \right]}{2\sqrt{n}\mathbb{E}\left[(X_1-x)^2\right]},
$$

which in turn implies that

$$
\begin{aligned}
\sum_{0\le m\le k:\left|x-\frac{m}{k}\right|>\epsilon} B_{m,k}(x) &= \mathbb{P}\left(\left| \sum_{i=1}^{k} X_i - kx \right| > k\epsilon \right) \\
&\le \sqrt{\frac{2}{\pi}} \int_{\frac{\epsilon\sqrt{k}}{\sqrt{x(1-x)}}}^{\infty} e^{-\frac{z^2}{2}} dz + \frac{\mathbb{E}\left[|X_1 - x|^3 \right]}{2\sqrt{k}\left(\mathbb{E}\left[(X_1-x)^2\right]\right)^{\frac{3}{2}}} \\
&\le \sqrt{\frac{2x(1-x)}{k\pi}} \frac{1}{\epsilon} e^{-\frac{k\epsilon^2}{2x(1-x)}} + \frac{1-2x+2x^2}{2\sqrt{kx(1-x)}}.
\end{aligned}
$$

Let $k \ge 2$. For $x \in (k^{-1/3}, 1-k^{-1/3})$ and $\epsilon \ge k^{-\frac{1}{3}}$, observe that the right hand side of the above equation is upper bounded by

$$
\frac{k^{\frac{1}{6}}}{\sqrt{2\pi}} e^{-2k^{\frac{1}{3}}} + 2k^{-\frac{1}{3}} \le 3k^{-\frac{1}{3}}. \tag{80}
$$

On the other hand, for $x \in (0, k^{-1/3}]$, we have since $p_{k,f}(0) = f(0)$ that

$$\begin{aligned} |p_{k,f}(x) - f(x)| &= |p_{k,f}(x) - p_{k,f}(0) + f(0) - f(x)| \\ &\leq |p_{k,f}(x) - p_{k,f}(0)| + |f(0) - f(x)| \\ &\leq \left(\left\| p_{k,f}^{(1)} \right\|_{\infty,(0,1)} + \|f\|_{\mathrm{Lip},[0,1]} \right) k^{-1/3} \\ &\leq 2 \|f\|_{\mathrm{Lip},[0,1]} k^{-1/3}, \end{aligned} \tag{81}$$

where in the final inequality, we used $\|p_{k,f}^{(1)}\|_{\infty,(0,1)} \leq \|f\|_{\mathrm{Lip},[0,1]}$, which follows from (76) with $\ell = 1$ and the fact that a L-Lipschitz continuous function can be approximated arbitrarily well by a first-order differentiable function with derivative bounded by L. Similarly, for $x \in [1 - k^{-1/3}, 1)$, (81) holds. From (79), (80), (81) and the above discussion, it follows that for all $x \in [0, 1]$ and $k \geq 2$, we have

$$\|p_{k,f} - f\|_{\infty,[0,1]} \leq \left(2 \|f\|_{\mathrm{Lip},[0,1]} + 6 \|f\|_{\infty,[0,1]} \right) k^{-\frac{1}{3}}.$$

When $k = 1$, we obtain using (76) with $\ell = 0$ that

$$\|p_{k,f} - f\|_{\infty,[0,1]} \leq \|p_{k,f}\|_{\infty,[0,1]} + \|f\|_{\infty,[0,1]} \leq 2 \|f\|_{\infty,[0,1]}.$$

Hence, (77) holds for all $k \in \mathbb{N}$, thus completing the proof.

D Proof of Lemma 10

Consider the case $\alpha = 1$. As shown in [34], for $\rho, \sigma > 0$, the optimizer (Hermitian operator) $H^\star(\rho, \sigma)$ of (2) has the form

$$H^\star(\rho, \sigma) = \sum_{i=1}^{d} \lambda_i^\star P_i^\star, \qquad \text{with } \lambda_i^\star := \log\left(\frac{\mathrm{Tr}[P_i^\star \rho]}{\mathrm{Tr}[P_i^\star \sigma]} \right),$$

where $\{P_i^\star\}_{i=1}^d$ is some set of orthogonal rank-one projectors, so that

$$\mathsf{D}_{\mathsf{M}}(\rho \| \sigma) = \mathrm{Tr}[H^\star(\rho, \sigma)\rho] - \mathrm{Tr}[e^{H^\star(\rho,\sigma)}\sigma] + 1 = \sum_{i=1}^{d} \mathrm{Tr}[P_i^\star \rho] \log\left(\frac{\mathrm{Tr}[P_i^\star \rho]}{\mathrm{Tr}[P_i^\star \sigma]} \right).$$

Hence, the set of eigenvalues of $H^\star(\rho, \sigma)$ is

$$\Lambda^\star(\rho, \sigma) = \{\lambda_i^\star\}_{i=1}^d = \left\{ \log\left(\frac{\mathrm{Tr}[P_i^\star \rho]}{\mathrm{Tr}[P_i^\star \sigma]} \right) \right\}_{i=1}^{d}.$$

To obtain an upper bound on $|\lambda_i^\star|$, we will use the variational characterization of max-relative entropy given in [40, Lemma A.4]) as stated below:

$$D_{\max}(\rho \| \sigma) := \inf \left\{ \lambda \in \mathbb{R} : \rho \leq e^\lambda \sigma \right\} = \sup \left\{ \log\left(\frac{\mathrm{Tr}[M\rho]}{\mathrm{Tr}[M\sigma]} \right) : 0 \leq M \leq I \right\}.$$

From the last equation above, for every projector P, we have

$$\frac{\mathrm{Tr}[\rho P]}{\mathrm{Tr}[\sigma P]} \leq e^{D_{\max}(\rho \| \sigma)} = \inf \left\{ e^\lambda : \sigma^{-\frac{1}{2}} \rho \sigma^{-\frac{1}{2}} \leq e^\lambda I \right\} = \left\| \sigma^{-\frac{1}{2}} \rho \sigma^{-\frac{1}{2}} \right\|.$$

Similarly,

$$\frac{\mathrm{Tr}[\sigma P]}{\mathrm{Tr}[\rho P]} \leq e^{D_{\max}(\sigma\|\rho)} = \left\|\rho^{-\frac{1}{2}}\sigma\rho^{-\frac{1}{2}}\right\|.$$

Since $(\rho,\sigma) \in \mathcal{S}_d(b)$, we have for every (rank-one) projector P that

$$\frac{1}{b} \leq \frac{1}{\left\|\rho^{-\frac{1}{2}}\sigma\rho^{-\frac{1}{2}}\right\|} \leq \frac{\mathrm{Tr}[\rho P]}{\mathrm{Tr}[\sigma P]} \leq \left\|\sigma^{-\frac{1}{2}}\rho\sigma^{-\frac{1}{2}}\right\| \leq b.$$

Taking logarithms, we obtain the desired claim for $\alpha = 1$. The claim for $0 < \alpha \neq 1$ follows similarly by noting that $H^\star_\alpha(\rho,\sigma) = \sum_{i=1}^d \lambda^\star_{i,\alpha} P^\star_{i,\alpha}$ with $\lambda^\star_{i,\alpha} \coloneqq \log\left(\frac{\mathrm{Tr}[P^\star_{i,\alpha}\rho]}{\mathrm{Tr}[P^\star_{i,\alpha}\sigma]}\right)$.

E Solovay-Kitaev Theorem: Bound on Quantum Circuit Parameter Size

Let $\{P_i\}_{i=1}^d$ be an arbitrary set of orthogonal projectors on $\mathbb{H}_d$ such that $\sum_{i=1}^d P_i = I$. Let U be a unitary such that $P_i = U|i\rangle\langle i|U^\dagger$. Note that the determinant of U, $\det(U) = e^{i\omega}$, for some $\omega \in \mathbb{R}$. Hence, for $\tilde{U} = e^{-i\omega/d}U$, we have $\det(\tilde{U}) = 1$. Moreover, $\tilde{U}|i\rangle\langle i|\tilde{U}^\dagger = U|i\rangle\langle i|U^\dagger = P_i$. This implies that U satisfying $P_i = U|i\rangle\langle i|U^\dagger$ can be restricted (without loss of generality) to belong to the special unitary group $\mathsf{SU}(d)$, i.e., the subset of unitary operators on $\mathbb{H}_d$ with determinant one. Assume $d = 2^N$ for some $N \in \mathbb{N}$. Consider the universal gate set Univ composed of the Clifford group, i.e., the Hadamard gate, S gate, and CNOT gate, along with the T gate. Then, it is known from [96] that, for every $U \in \mathsf{SU}(d)$ acting on N qubits, there exists a quantum circuit $\bar{U}$ constructed by composition of at most $\ell(d,\delta) = O(N^2 4^N \log(N^2 4^N/\delta))$ gates selected from Univ such that $\|U - \bar{U}\| \leq \delta$. Since the number of possible configurations of quantum circuit composed of ℓ gates selected from Univ is $4^{\ell(d,\delta)}$, we obtain that there exists $\mathcal{U}(\delta,\mathcal{S})$ with $|\mathcal{U}(\delta,\mathcal{S})| \leq 4^{\ell(d,\delta)}$ such that (17) is satisfied. Similar claims can also be obtained for qudits, where $d = m^N$ for some positive integers m, N, by using a generalization of the Solovay-Kitaev algorithm to qudits as given in [97].

F Proof of Lemma 11

$$\begin{aligned}
\|H_1 - H_2\| &= \left\|U_1\Lambda_1U_1^\dagger - U_2\Lambda_2U_2^\dagger\right\| \\
&\overset{(a)}{\leq} \left\|U_1\Lambda_1U_1^\dagger - U_1\Lambda_1U_2^\dagger\right\| + \left\|U_1\Lambda_1U_2^\dagger - U_1\Lambda_2U_2^\dagger\right\| + \left\|U_1\Lambda_2U_2^\dagger - U_2\Lambda_2U_2^\dagger\right\| \\
&\overset{(b)}{\leq} \|U_1\|\,\|\Lambda_1\|\left\|U_1^\dagger - U_2^\dagger\right\| + \|U_1\|\,\|\Lambda_1 - \Lambda_2\|\left\|U_2^\dagger\right\| + \|U_1 - U_2\|\,\|\Lambda_2\|\left\|U_2^\dagger\right\| \\
&\overset{(c)}{=} (\,\|\Lambda_1\| + \|\Lambda_2\|\,)\,\|U_1 - U_2\| + \|\Lambda_1 - \Lambda_2\|,
\end{aligned}$$

where (a) is via triangle inequality for Schatten norms, (b) is due to sub-multiplicativity of Schatten norms, and (c) is because $\|U\| = \left\|U^\dagger\right\| = 1$ for a unitary U.