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Francis Bach. Sum-of-Squares Relaxations for Information Theory and Variational Inference. 2022. hal-03703475v1

HAL Id: hal-03703475

https://hal.science/hal-03703475v1

Preprint submitted on 24 Jun 2022 (v1), last revised 15 Sep 2023 (v3)

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Sum-of-Squares Relaxations for Information Theory and Variational Inference

Francis Bach

June 24, 2022

Abstract

We consider extensions of the Shannon relative entropy, referred to as f-divergences. Three classical related computational problems are typically associated with these divergences: (a) estimation from moments, (b) computing normalizing integrals, and (c) variational inference in probabilistic models. These problems are related to one another through convex duality, and for all them, there are many applications throughout data science, and we aim for computationally tractable approximation algorithms that preserve properties of the original problem such as potential convexity or monotonicity. In order to achieve this, we derive a sequence of convex relaxations for computing these divergences from non-centered covariance matrices associated with a given feature vector: starting from the typically non-tractable optimal lower-bound, we consider an additional relaxation based on "sums-of-squares", which is is now computable in polynomial time as a semidefinite program, as well as further computationally more efficient relaxations based on spectral information divergences from quantum information theory. For all of the tasks above, beyond proposing new relaxations, we derive tractable algorithms based on augmented Lagrangians and first-order methods, and we present illustrations on multivariate trigonometric polynomials and functions on the Boolean hypercube.

1 Introduction

Tools from information theory are ubiquitous in data science. Starting with the notion of Shannon entropy, other notions have emerged, in particular f-divergences [1, 2], which are defined as

$$D(p\|q) = \int_{\mathcal{X}} f\Big(\frac{dp}{dq}(x)\Big) dq(x), \tag{1}$$

where p and q are two finite positive measures on an arbitrary measurable set $\mathcal{X}$, $\frac{dp}{dq}$ is the density of p with respect to q, and $f : \mathbb{R}_+^* \to \mathbb{R}$ is a convex function. A classical example is $f(t) = t \log t - t + 1$, where $D(p\|q)$ is the usual Kullback-Leibler divergence, associated with Shannon information theory [3], which we will use as a running example. These divergences have been used in many areas in machine learning, signal processing or statistics, such as within message passing and variational inference [4], PAC-Bayes analysis [5], independent component analysis [6], information theory [7], differential privacy [8], design of surrogate losses for classification [9], and optimization [10]. We review f-divergences and their basic properties in Section 2, see [11, 12, 13] for a more complete treatment.

Three classical related computational problems are typically associated with f-divergences, which have to be estimated or optimized in some way, a task that can become difficult in multivariate settings. For

all them, there are many applications throughout data science, and we aim for computationally tractable algorithms that preserve properties of the original problem (such as potential convexity or monotonicity).

(1) **Estimation of divergences from moments:** Given some function T from $\mathcal{X}$ to some vector space, the goal is to estimate $D(p\|q)$ only from the knowledge of the integrals $\int_{\mathcal{X}} T(x)dp(x)$ and $\int_{\mathcal{X}} T(x)dq(x)$. Our aim in this paper is to estimate $D(p\|q)$ from below, and to obtain the largest possible lower bound. We focus on particular functions T of the form $T(x) = \varphi(x)\varphi(x)^*$, where $\varphi : \mathcal{X} \to \mathbb{C}^d$ is some complex-valued feature map, and where M^* denotes the conjugate transpose of the matrix M. Thus T takes values in the set $\mathbb{H}_d^+$ of positive semi-definite Hermitian matrices of size $d \times d$.

For this particular form of moments as non-centered covariance matrices, we first provide in Section 4 a characterization of the tightest such lower bound. This formulation involves the maximization on $\mathcal{X}$ of functions of the form $x \mapsto \varphi(x)^* M \varphi(x)$, where $M \in \mathbb{H}_d$ (the set of Hermitian matrices).

Our first contribution is to replace the exact maximization of such quadratic forms of $\varphi(x)$ by "sum-of-squares" relaxations, that is, relaxations based on semi-definite programming and the representation of non-negative functions as positive-semidefinite quadratic forms in $\varphi(x)$ [14, 15] (see review in Section 3). This relaxation is developed in Section 5 and allows to bring to bear the well-developed area of sum-of-squares optimization with its computational tools and extensive analyses. We also provide in Section 6 a further relaxation which is based on information divergences from quantum information theory (which are reviewed in Section 2.6).

Note that a related interesting task is to estimate estimation divergences directly from samples [16, 17]. We could use our algorithms with increasingly large feature vectors and use empirical estimates, but a detailed analysis is left for future research.

(2) **Computing integrals:** We consider the task of computing $\int_{\mathcal{X}} f^*(h(x))dq(x)$, where q is a finite positive measure on $\mathcal{X}$, f^* is the Fenchel conjugate of f, and $h : \mathcal{X} \to \mathbb{R}$ an arbitrary function (such that the integral is finite). For $f(t) = t \log t - t + 1$, we have $f^*(u) = e^u - 1$, and we there aim at estimating integrals of exponential functions, a classical task in probabilistic modelling (see [18, 19] and references therein).

This computational task can be classically related to f-divergences by Fenchel duality as:

$$\int_{\mathcal{X}} f^*(h(x))dq(x) = \sup_{p \text{ positive measure on } \mathcal{X}} \int_{\mathcal{X}} h(x)dp(x) - D(p\|q).$$

In Section 7.3, we show that for functions $h(x)$ which are quadratic forms in $\varphi(x)$, we can replace $D(p\|q)$ by the lower-bound we just defined above, and obtain a computable upper bound of the integral.

(3) **Variational inference in probabilistic models:** One classical inference task in probabilistic modelling is to compute moments of some distributions from which we know the density. In our f-divergence context, we consider a density (with respect to q) proportional to $(f^*)'(h(x) - \rho)$, where $\rho \in \mathbb{R}$ is a normalizing constant. This density happens to be exactly the maximizer in

$$c_q(h) = \sup_{p \text{ probability measure on } \mathcal{X}} \int_{\mathcal{X}} h(x)dp(x) - D(p\|q).$$

The optimal quantity $c_q(h)$ is referred to as the f-partition-function, and for $f(t) = t\log t - t + 1$, we recover the usual log-partition function, and densities proportional to $e^{h(x)}$.

When we restrict h to be a quadratic form in $\varphi(x)$, that is of the form $\varphi(x)^* H \varphi(x)$ for some $H \in \mathbb{H}_d$, then the gradient with respect to H of the f-partition function ends up being exactly the moment of $T(x) = \varphi(x)\varphi(x)^* \in \mathbb{H}_d$ for the desired distribution. This relaxation is presented in Section 7.

Contributions. In this paper, we first derive a sequence of three convex formulations of f-divergences based on covariance matrices. Starting from the typically non-tractable optimal lower-bound, we consider an additional relaxation based on "sums-of-squares", which is is now computable in polynomial time as a semidefinite program, as well as further computationally more efficient relaxations based on spectral information divergences from quantum information theory. For all of the tasks above, beyond proposing new relaxations, we derive tractable algorithms based on augmented Lagrangians and first-order methods, and we present illustrations on multivariate trigonometric polynomials and functions on the Boolean hypercube.

2 Review of f-divergences and quantum information theory

We consider f-divergences, where $f : \mathbb{R}_+^* \to \mathbb{R}_+$ is a convex function such that $f(1) = 0$. We assume that f is strictly convex and differentiable, so that the Fenchel conjugate f^* is differentiable and non-decreasing, with $(f^*)'(u) \geqslant 0$ on the domain of f^*. Moreover, we assume that $f(1) = 0$, and thus 1 is the minimizer of f, leading to $f'(1) = 0$ and $(f^*)'(0) = 1$. Moreover, we then have $f^*(0) = 0$. Our running example is $f(t) = t\log t - t + 1$ with $f^*(u) = e^u - 1$ (see more examples below).

On the set $\mathcal{X}$, we consider several sets of finite measures: $\mathcal{M}_+(\mathcal{X})$ the set of finite *positive* measures on $\mathcal{X}$, $\mathcal{M}(\mathcal{X})$ the set of finite *signed* measures on $\mathcal{X}$, and $\mathcal{P}(\mathcal{X})$ the set of *probability* measures on $\mathcal{X}$ (that is, positive measures in $\mathcal{M}_+(\mathcal{X})$ that integrates to one).

For two finite positive measures p, q in $\mathcal{M}_+(\mathcal{X})$, we can define

$$D(p\|q) = \int_{\mathcal{X}} f\Big(\frac{dp}{dq}(x)\Big) dq(x),$$

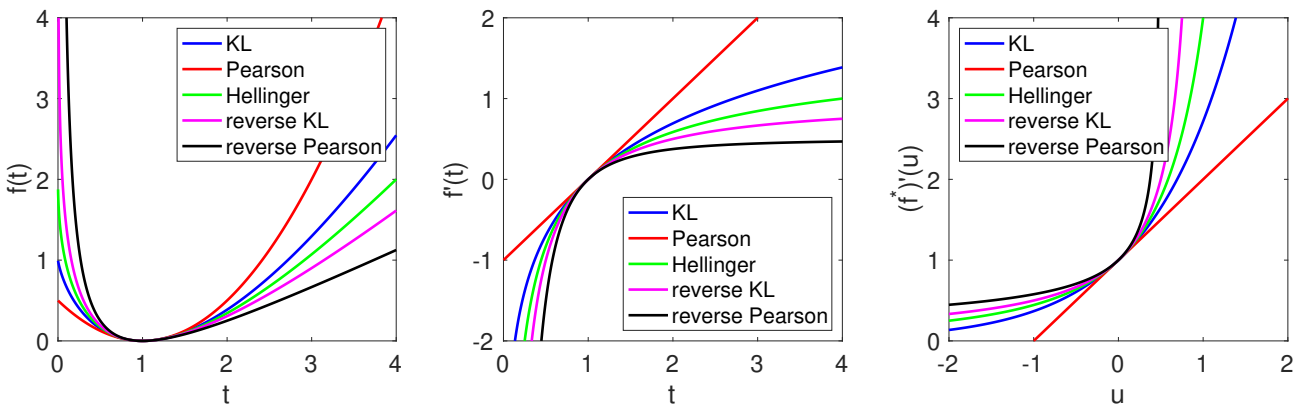
for all non-negative measures (possibly non normalized), assuming that $\frac{dp}{dq}(x)$ exists for all $x \in \mathcal{X}$ and that the integral is finite. We now review several properties and examples, see [1, 13, 5] for more results.

Classical properties. Given our assumption that 1 is a global minimizer of f and $f(1) = 0$, $D(p\|q) \geqslant 0$ with equality if and only if $p = q$. Moreover, $D(p\|q)$ is jointly convex in p and q.

Examples. We have the following classical examples, with the usual "reversion" of f-divergences: if we define $g(t) = tf(1/t)$, swapping p and q in $D(p\|q)$ is equivalent to replacing f by g (for α-divergences below, this corresponds to $\alpha \to 1-\alpha$). All of the approximations that we consider in this paper will satisfy this reversibility: swapping p and q (and later moment matrices A and B) is equivalent to replacing f by g.

Note that the total variation case, where $f(t) = |t-1|$ is excluded from most developments because it is neither differentiable nor strictly convex (nor operator convex), but many results (except the quantum ones) would apply as well. We normalize all functions f so that $f''(1) = 1$. See table and plots below.

Divergence	$f(t)$	$f^*(u)$	$(f^*)'(u)$
α-Rényi	$\frac{1}{\alpha(\alpha-1)}\left[t^\alpha - \alpha t + (\alpha-1)\right]$	$\frac{1}{\alpha}\left[-1+(1+(\alpha-1)u)^{\alpha/(\alpha-1)}\right]$	$(1+(\alpha-1)u)^{1/(\alpha-1)}$
Kullback-Leibler, $\alpha = 1$	$t\log t - t + 1$	$e^u - 1$	e^u
Reverse KL, $\alpha = 0$	$-\log t + t - 1$	$-\log(1-u)$	$\frac{1}{1-u}$
squared Hellinger, $\alpha = \frac{1}{2}$	$2(\sqrt{t}-1)^2$	$\frac{u}{1-u/2}$	$\frac{1}{(1-u/2)^2}$
Pearson χ^2, $\alpha = 2$	$\frac{1}{2}(t-1)^2$	$\frac{1}{2}(u+1)_+^2 - \frac{1}{2}$	$(u+1)_+$
Reverse Pearson, $\alpha = -1$	$\frac{1}{2}\left(\frac{1}{t}+t\right) - 1$	$1 - \sqrt{1-2u}$	$\frac{1}{\sqrt{1-2u}}$
Le Cam	$\frac{(t-1)^2}{t+1}$	$2 - u - 2\sqrt{1-2u}$	$\frac{2}{\sqrt{1-2u}} - 1$
Jensen-Shannon	$2t\log\frac{2t}{t+1} + 2\log\frac{2}{t+1}$	$-2\log(2-e^{u/2})$	$\frac{1}{2\exp(-u/2)-1}$



2.1 Variational representations

The f-divergence has a variational representation obtained from the Fenchel conjugate of perspective functions [20]. Indeed, the function $(p,q) \mapsto qf\left(\frac{p}{q}\right)$ defined on $\mathbb{R}_+^2$ is referred to as the *perspective function* of f, and has the variational representation for $p, q \in \mathbb{R}_+$:

$$qf\left(\frac{p}{q}\right) = \sup_{v,w\in\mathbb{R}} \; vp + wq \;\text{ such that }\; \forall r \geqslant 0,\; rv + w \leqslant f(r),$$

where for $p, q \in \mathbb{R}_+^*$, the optimal values v^* and w^* of v and w are obtained as follows: $v^* = f'\left(\frac{p}{q}\right)$, and $w^* = -f^*(v^*) = f\left(\frac{p}{q}\right) - \frac{p}{q}f'\left(\frac{p}{q}\right)$.

Following [21], for $p, q \in \mathcal{M}_+(\mathcal{X})$, this leads to a variational representation of $D(p\|q)$ as the supremum of linear functions

$$D(p\|q) = \sup_{v,w:\mathcal{X}\to\mathbb{R}} \int_{\mathcal{X}} v(x)dp(x) + \int_{\mathcal{X}} w(x)dq(x) \;\text{ such that }\; \forall x \in \mathcal{X}, \forall r \geqslant 0,\; rv(x) + w(x) \leqslant f(r). \quad (2)$$

The optimal functions w and v are such that $v(x) = f'\left(\frac{dp}{dq}(x)\right)$, and $w(x) = f\left(\frac{dp}{dq}(x)\right) - \frac{dp}{dq}(x)f'\left(\frac{dp}{dq}(x)\right) = -f^*(v(x))$. Note that in this representation, the non-negativity of the measures p and q is automatically satisfied (the value of the optimization problem in Eq. (2) is infinite otherwise). Optimizing with respect to $w(x)$ in closed form as above then leads to the representation from [16] as the supremum with respect to $v : \mathcal{X} \to \mathbb{R}$ of $\int_{\mathcal{X}} v(x)dp(x) - \int_{\mathcal{X}} f^*(v(x))dq(x)$.

Variational formulation as an infimum. We can consider the Lagrangian dual of Eq. (2), by introducing a Lagrange multiplier λ for the infinite-dimensional constraint $\forall x \in \mathcal{X}, \forall r \geqslant 0,\ rv(x)+w(x) \leqslant f(r)$ in the form of a positive finite measure λ on $\mathbb{R} \times \mathcal{X}$ [22]. We then obtain:

$$D(p\|q) \quad = \quad \inf_{\lambda \in \mathcal{M}_+(\mathbb{R}\times\mathcal{X})} \int_{\mathcal{X}} \int_{\mathbb{R}_+} f(r) d\lambda(x,r) \tag{3}$$

$$\text{such that } \int_{\mathbb{R}_+} d\lambda(\cdot, r) = dq(\cdot) \text{ and } \int_{\mathbb{R}_+} r d\lambda(\cdot, r) = dp(\cdot).$$

2.2 Piecewise affine approximation from below

In this paper, we will approximate maximization of quadratic forms with respect to $x \in \mathcal{X}$ using sums-of-squares (see Section 3), and we will need to take care of the constraint obtained from the infinitely many positive reals r's in Eq. (2). While tools derived from [23] could be used get low approximation errors, we prefer to preserve our lower-bounding properties, and thus we will use approximations $\widehat{D}(p\|q)$ which are always*smaller* than $D(p\|q)$. We now consider a simple piecewise affine approximation. This will be only needed for the sum-of-squares relaxations, while for the ones based on quantum divergences, we will be able to use spectral representations that are significantly more efficient, as they do not need such approximations.

We consider an approximation of f on $\mathbb{R}_+$ from m of its tangents, at $r_1 < \cdots < r_m$, that is, we consider, for $r \in \mathbb{R}_+$:

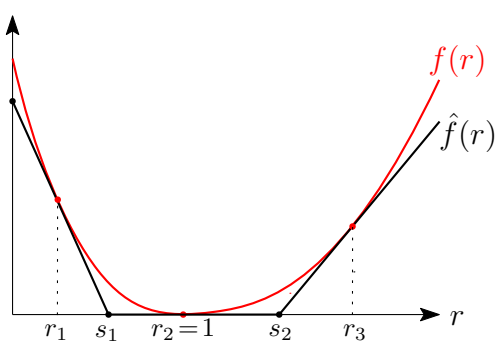
$$\hat{f}(r) = \sup_{i \in \{1,\ldots,m\}} f(r_i) + f'(r_i)(r - r_i).$$

By adding sufficiently many r_i's, we can get an approximation of f which is as tight as desired (quantitative statements could be made on compact intervals based on regularity properties of f).

We can then represent $\hat{f}$ as the convex envelope of the function equal to $\hat{f}(s_i)$ at well-chosen points $0 = s_0 < s_1 < \cdots < s_m = +\infty$ (see illustration below), with for $i \in \{1, \ldots, m-1\}$, $s_i = \frac{f(r_i) - r_i f'(r_i) - f(r_{i+1}) + r_{i+1} f'(r_{i+1})}{f'(r_{i+1}) - f'(r_i)} = \frac{f^*(f'(r_{i+1})) - f^*(f'(r_i))}{f'(r_{i+1}) - f'(r_i)}$ and $\hat{f}(s_i) = -f^*(f'(r_i)) + [f^*(f'(r_{i+1})) - f^*(f'(r_i))]\frac{f'(r_i)}{f'(r_{i+1}) - f'(r_i)}$, and $\hat{f}(0) = f(r_1) - r_1 f'(r_1) = -f^*(f'(r_1))$, while $\hat{f}(s_m) \sim f'(r_m) s_m$, when s_m tends to infinity. We then normalize $w(x) + s_i v(x) \leqslant \hat{f}(s_i)$ as $\frac{1}{\sqrt{1+s_i^2}} w(x) + \frac{s_i}{\sqrt{1+s_i^2}} v(x) \leqslant \frac{\hat{f}(s_i)}{\sqrt{1+s_i^2}}$, so that we (inner) approximate the set of $w(x), v(x)$ such that $\forall r \in \mathbb{R}_+$, $rv(x) + w(x) \leqslant f(r)$ by the constraints:

$$\forall i \in \{0, \ldots, m\},\ a_i w(x) + b_i v(x) \leqslant f_i, \tag{4}$$

with $a_i = \frac{1}{\sqrt{1+s_i^2}}$, $b_i = \frac{s_i}{\sqrt{1+s_i^2}}$, and $f_i = \frac{\hat{f}(s_i)}{\sqrt{1+s_i^2}}$, which satisfy $a_i^2 + b_i^2 = 1$ for all $i \in \{0, \ldots, m\}$.



This leads to the two equivalent primal-dual formulations of a *lower bound* on $D(p\|q)$, based on the constraints from Eq. (4):

$$\begin{aligned}\widehat{D}(p\|q) &= \sup_{v,w:\mathcal{X}\to\mathbb{R}} \int_{\mathcal{X}} v(x)dp(x) + \int_{\mathcal{X}} w(x)dq(x) \text{ such that } \forall i \in \{0,\ldots,m\}, \forall x \in \mathcal{X},\ a_i w(x) + b_i v(x) \leqslant f_i \\ &= \inf_{\lambda_0,\ldots,\lambda_m \in \mathcal{M}_+(\mathcal{X})} \sum_{i=0}^{m} f_i \int_{\mathcal{X}} d\lambda_i(x) \text{ such that } \sum_{i=0}^{m} b_i\lambda_i = q, \text{ and } \sum_{i=0}^{m} a_i\lambda_i = p.\end{aligned}$$

They will be used extensively in our approximation algorithms in later sections.

2.3 f-partition function

Given a function $h : \mathcal{X} \to \mathbb{R}$, and q a fixed positive measure not necessarily summing to one (that is, in $\mathcal{M}_+(\mathcal{X})$), we can define the "$f$-partition function" as

$$c_q(h) = \sup_{p\in\mathcal{P}(\mathcal{X})} \int_{\mathcal{X}} h(x)dp(x) - D(p\|q). \tag{5}$$

Using the variational formulation in Eq. (2), introducing a Lagrange multiplier ρ for the constraint $\int_{\mathcal{X}} dp(x) = 1$, using strong duality, and optimizing w out, we get (see [5] for similar derivations in the context of PAC-Bayes analysis):

$$\begin{aligned}c_q(h) &= \sup_{p\in\mathcal{M}(\mathcal{X})} \inf_{v:\mathcal{X}\to\mathbb{R}} \int_{\mathcal{X}} h(x)dp(x) - \int_{\mathcal{X}} v(x)dp(x) + \int_{\mathcal{X}} f^*(v(x))dq(x) \text{ such that } \int_{\mathcal{X}} dp(x) = 1 \\ &= \sup_{p\in\mathcal{M}(\mathcal{X})} \inf_{\rho\in\mathbb{R},\ v:\mathcal{X}\to\mathbb{R}} \int_{\mathcal{X}} h(x)dp(x) - \int_{\mathcal{X}} v(x)dp(x) + \int_{\mathcal{X}} f^*(v(x))dq(x) - \rho\Big(\int_{\mathcal{X}} dp(x) - 1\Big) \\ &= \inf_{\rho\in\mathbb{R}} \ \rho + \int_{\mathcal{X}} f^*(h(x)-\rho)dq(x),\end{aligned}$$

since the supremum with respect to $p \in \mathcal{M}(\mathcal{X})$ leads to the constraint $v = h - \rho$. The optimality condition for ρ is that $\int_{\mathcal{X}} (f^*)'(h(x)-\rho)dq(x) = 1$. Moreover, the set of functions $h : \mathcal{X} \to \mathbb{R}$ such that $c_q(h)$ is finite is a convex set.

This means that we can define a probability distribution with density $(f^*)'(h(x)-\rho)$ with respect to q, which we denote $p(x|h)$. For $f(t) = t\log t - t + 1$, where $(f^*)'(u) = e^u$, we recover classical exponential families (see [18, 19] and references therein), and $c_q(h) = \log\Big(\int_{\mathcal{X}} e^{h(x)}dq(x)\Big) + 1 - \int_{\mathcal{X}} q(x)$, which is the traditional log-partition function.

Alternatively, we can use the variational formulation in Eq. (2), but now optimize v out, still using strong duality:

$$\begin{aligned}
c_q(h) &= \sup_{p\in\mathcal{P}(\mathcal{X})} \int_{\mathcal{X}} h(x)dp(x) - D(p\|q) \\
&= \sup_{p\in\mathcal{M}(\mathcal{X})} \inf_{v,w:\mathcal{X}\to\mathbb{R}} \int_{\mathcal{X}} h(x)dp(x) - \int_{\mathcal{X}} v(x)dp(x) - \int_{\mathcal{X}} w(x)dq(x) \text{ such that } \int_{\mathcal{X}} dp(x) = 1 \\
&\qquad\qquad \text{such that } \forall x\in\mathcal{X}, \forall r \geqslant 0,\ rv(x) + w(x) \leqslant f(r) \\
&= \sup_{p\in\mathcal{M}(\mathcal{X})} \inf_{\rho,\ v,w:\mathcal{X}\to\mathbb{R}} \int_{\mathcal{X}} h(x)dp(x) - \int_{\mathcal{X}} v(x)dp(x) - \int_{\mathcal{X}} w(x)dq(x) - \rho\Big(\int_{\mathcal{X}} dp(x) - 1\Big) \\
&\qquad\qquad \text{such that } \forall x\in\mathcal{X}, \forall r \geqslant 0,\ rv(x) + w(x) \leqslant f(r) \\
&= \inf_{\rho,\ w:\mathcal{X}\to\mathbb{R}} \rho - \int_{\mathcal{X}} w(x)dq(x) \ \text{ such that } \forall x\in\mathcal{X}, \forall r \geqslant 0,\ rh(x) + w(x) \leqslant f(r) + \rho r. \qquad (6)
\end{aligned}$$

Finally, we also have an expression as a supremum, rather than as an infimum above:

$$\begin{aligned}
c_q(h) &= \sup_{\lambda\in\mathcal{M}_+(\mathbb{R}\times\mathcal{X})} \int_{\mathcal{X}}\int_{\mathbb{R}_+} \big[rh(x) - f(r)\big] d\lambda(x,r) \\
&\qquad\qquad \text{such that } \int_{\mathbb{R}_+} d\lambda(\cdot,r) = dq(\cdot) \text{ and } \int_{\mathcal{X}}\int_{\mathbb{R}_+} r d\lambda(x,r) = 1.
\end{aligned}$$

In Section 4, we will obtain similar representations with covariance matrices obtained from the feature vector $\varphi : \mathcal{X} \to \mathbb{C}^d$.

Computing integrals. The tools derived in this paper can also provide a way to approximate integrals of the form $\int_{\mathcal{X}} f^*(h(x))dq(x)$ as we have (only maximizing with respect to positive measures that may not sum to one):

$$\begin{aligned}
\sup_{p\in\mathcal{M}_+(\mathcal{X})} \int_{\mathcal{X}} h(x)dp(x) - D(p\|q) &= \sup_{p\in\mathcal{M}_+(\mathcal{X})} \int_{\mathcal{X}} h(x)\frac{dp}{dq}(x) - f\Big(\frac{dp}{dq}(x)\Big)dq(x). \\
&= \int_{\mathcal{X}} f^*(h(x))dq(x).
\end{aligned}$$

We also have the representation that will be useful later:

$$\int_{\mathcal{X}} f^*(h(x))dq(x) = \inf_{w:\mathcal{X}\to\mathbb{R}} -\int_{\mathcal{X}} w(x)dq(x) \ \text{ such that } \ \forall x\in\mathcal{X}, \forall r \geqslant 0,\ rh(x) + w(x) \leqslant f(r). \qquad (7)$$

There exist many ways of estimating integrals, in particular in compact sets in small dimensions, where various quadrature rules, such as the trapezoidal or Simpson's rule, can be applied to compute integrals based on function evaluations, with well-defined convergence rates [24]. In higher dimensions, still based on function evaluations, Bayes-Hermite quadrature rules [25], and the related kernel quadrature rules [26, 27] come with precise convergence rates linking approximation error and number of function evaluations [28]. An alternative in our context is Monte-Carlo integration from samples from q [29], with convergence rate in $O(1/\sqrt{n})$ from n function evaluations.

In this paper, we follow [30] and consider computing integrals given a specific knowledge of the integrand, here of the form $f^*(h(x))$, where h is a known quadratic form in a feature vector $\varphi(x)$. While we also use a sum-of-squares approach as in [30], we rely on different tools (link with f-divergences and partition functions rather than integration by parts).

2.4 Variational inference

In this section, we extend the notion of exponential families, which is classical for $f(t) = t \log t - t + 1$, to all f-divergences. These are also called "q-exponential families" for α-divergences [31].

f-family of probability distributions. Following Section 2.3, given the matrix feature map $x \mapsto \varphi(x)\varphi(x)^* \in \mathbb{H}_d$, we define the distribution $p(\cdot|H)$ with density with respect to q of the form $(f^*)'\big(\varphi(x)^* H \varphi(x) - \rho\big)$ for a certain Hermitian matrix $H \in \mathbb{H}_d$, and with the normalizing constant $\rho = \rho(H) \in \mathbb{R}$ that makes the density sum to one. We can then define

$$C_q(H) = \sup_{p \in \mathcal{P}(\mathcal{X})} \int_{\mathcal{X}} \varphi(x)^* H \varphi(x) dp(x) - D(p\|q) = c_q\big(\varphi(\cdot)^* H \varphi(\cdot)\big), \tag{8}$$

with the optimal probability distribution p exactly being the one above. The set of $H \in \mathbb{H}_d$ such that $C_q(H)$ is finite is convex. From the representation above, we obtain that the gradient $C_q'(H)$ is equal to $\displaystyle\int_{\mathcal{X}} p(x|H)\varphi(x)\varphi(x)^* dq(x)$, that is, exactly the expectation of $\varphi(x)\varphi(x)^*$ under $p(\cdot|H)$. Thus, a classical task in variational inference is to compute $C_q'(H)$ [18].

We can then define the Fenchel conjugate C_q^* of C_q as:

$$C_q^*(\Sigma) = \sup_{H \in \mathbb{H}_d} \operatorname{tr}[H\Sigma] - C_q(H).$$

The domain of C_q^* is then exactly the set of attainable moments (denoted $\mathcal{K}$ later in Section 3), and the moment $\Sigma(H) = C_q'(H)$ is exactly the maximizer in

$$\sup_{\Sigma \in \mathbb{H}_d} \operatorname{tr}[H\Sigma] - C_q^*(\Sigma).$$

Note that in the future approximations of C_q^* or C_q, there is both an approximation of the value *and* potentially of the domain.

Estimation. Given some data $x_1, \dots, x_n \in \mathcal{X}$, we can form $\widehat{\Sigma} = \frac{1}{n}\sum_{i=1}^n \varphi(x_i)\varphi(x_i)^*$, and estimate $H \in \mathbb{H}_d$ by minimizing $D(p\|q)$ such that $\Sigma_p = \widehat{\Sigma}$. For $f(t) = t \log t - t + 1$, this is exactly maximum entropy estimation, which is classsicaly equivalent to finding the exponential family distributions with feature $x \mapsto \varphi(x)\varphi^*(x)$ and matching moment. This happens to be true for all f-divergences, that is, the optimal distribution p is exactly $p = p(\cdot|H)$ for H maximizing $\operatorname{tr}[H\widehat{\Sigma}] - C_q(H)$, and with matching moments. Note however that the formulation as the minimum (right) Kullback-Leibler divergence does not readily generalize beyond the Shannon entropy.

Computing integrals. Like in Section 2.3, if we maximize above with respect to $p \in \mathcal{M}_+(\mathcal{X})$ instead of $p \in \mathcal{P}(\mathcal{X})$ (that is, without the unit integral constraint), we get:

$$\int_{\mathcal{X}} f^*\big(\varphi(x)^* H \varphi(x)\big) dq(x) = \sup_{p \in \mathcal{M}_+(\mathcal{X})} \int_{\mathcal{X}} \varphi(x)^* H \varphi(x) dp(x) - D(p\|q). \tag{9}$$

2.5 Operator convexity

Some of the convex functions proposed in Section 2 are also "operator convex", meaning that for two positive semi-definite Hermitian matrices A, B, and any $\lambda \in [0,1]$,

$$f(\lambda A + (1-\lambda)B) \preccurlyeq \lambda f(A) + (1-\lambda) f(B),$$

where $\preccurlyeq$ defines the Löwner order between Hermitian matrices ($A \preccurlyeq B$ if and only if $B - A$ is positive semi-definite), and $f(A)$ is the spectral function defined as $f(A) = \sum_{i=1}^d \lambda_i u_i u_i^*$ when $A = \sum_{i=1}^d \lambda_i u_i u_i^*$ is the eigenvalue decomposition of A.

A classical necessary and sufficient condition for f being operator-convex is the existence of a representation of f as

$$f(t) = \beta(t-1)^2 + (t-1)^2 \int_0^{+\infty} \frac{1}{\lambda + t} d\nu(\lambda), \tag{10}$$

for some $\beta \in \mathbb{R}_+$ and a positive measure ν on $\mathbb{R}_+$ [32]. When the function f is extendable to an analytic function on $\mathbb{C}$, then the measure $\beta\delta_0 + \nu$ can be obtained from the Stieltjes inversion formula [33], as the limit of the measure with density $\frac{1}{\pi}\mathrm{Im}\Big(\frac{f(-\lambda - it)}{(\lambda + it + 1)^2}\Big)$ when $t \to 0^+$. In Appendix A, we provide this decomposition for the examples from the beginning of Section 2.

Operator convexity is crucial for the quantum information divergences that we now consider.

2.6 Quantum information divergences

We consider two Hermitian positive semi-definite matrices A and B in $\mathbb{H}_d^+$. If A and B commute, then they are jointly diagonalizable, and we can naturally define a divergence as

$$\sum_{i=1}^d \lambda_i(B) f\Big(\frac{\lambda_i(A)}{\lambda_i(B)}\Big),$$

where $\lambda_i(A)$ and $\lambda_i(B)$ are the corresponding eigenvalues of A and B (with the same eigenvectors). When A and B are not commuting, there are several notions of f-information divergences that reduce to the formula above when matrices commute [34]. Among the several candidates [21, 35, 36], two are particularly interesting in our context.

The so-called *maximal divergence* is equal to

$$D_{\max}^{\mathrm{QT}}(A\|B) = \mathrm{tr}\left[B^{1/2} f(B^{-1/2} A B^{-1/2}) B^{1/2}\right] = \mathrm{tr}\left[B f(B^{-1/2} A B^{-1/2})\right],$$

while the *standard divergence* is equal to:

$$D_{\mathrm{standard}}^{\mathrm{QT}}(A\|B) = \mathrm{vec}(B^{1/2})^* f(A \otimes B^{-1}) \mathrm{vec}(B^{1/2}), \tag{11}$$

with the usual Kronecker product notation between matrices and $\mathrm{vec}(M)$ the column vector obtained by stacking the columns of M [37]. It is equal to

$$\sum_{i,j=1}^{d} \lambda_i f\Big(\frac{\mu_j}{\lambda_i}\Big)(u_i^* v_j)^2,$$

where $A = \sum_{j=1}^{d} \mu_j v_j v_j^*$ and $B = \sum_{i=1}^{d} \lambda_i u_i u_i^*$ are eigenvalue decompositions of A and B. An important feature of these divergences is that they can both be computed in closed form from spectral decompositions. This will give a strong computation advantage for the relaxations that are based on these.

Examples of the standard divergence. We have the following classical examples below, with simpler formulas than Eq. (11).

Divergence	$f(t)$	$D^{\mathrm{QT}}_{\mathrm{standard}}(A\|B)$
α-Rényi	$\frac{1}{\alpha(\alpha-1)}\big[t^\alpha - \alpha t + (\alpha-1)\big]$	$\frac{1}{\alpha(\alpha-1)}\big[\,\mathrm{tr}[B^{1-\alpha}A^\alpha] - \alpha\,\mathrm{tr}[A] + (\alpha-1)\,\mathrm{tr}[B]\big]$
Kullback-Leibler, $\alpha = 1$	$t\log t - t + 1$	$\mathrm{tr}\,\big[A\log A - A\log B\big]$
squared Hellinger, $\alpha = \frac{1}{2}$	$2(\sqrt{t}-1)^2$	$2\,\mathrm{tr}\,A + 2\,\mathrm{tr}\,B - 4\,\mathrm{tr}\,\big[A^{1/2}B^{1/2}\big]$
Pearson χ^2, $\alpha = 2$	$\frac{1}{2}(t-1)^2$	$\frac{1}{2}\,\mathrm{tr}\,\big[B^{-1}(B-A)^2\big]$

From the representation of operator convex functions in Eq. (10), we can infer properties of these divergences from $f(t) = \frac{(t-1)^2}{\lambda+t}$, for which we have

$$D^{\mathrm{QT}}_{\mathrm{standard}}(A\|B) = \mathrm{vec}(A-B)^*(A\otimes I + \lambda\cdot B\otimes I)^{-1}\mathrm{vec}(A-B),$$

and

$$D^{\mathrm{QT}}_{\mathrm{max}}(A\|B) = \mathrm{tr}\,\big[(A-B)(A+\lambda B)^{-1}(A-B)\big].$$

This shows immediately that the two quantum divergences are jointly convex in A and B. A less direct property is that for all A and B (see proof in [36, Prop. 4.1]):

$$D^{\mathrm{QT}}_{\mathrm{standard}}(A\|B) \leqslant D^{\mathrm{QT}}_{\mathrm{max}}(A\|B).$$

Thus, in our context of lower bounds, we get a tighter result with $D^{\mathrm{QT}}_{\mathrm{max}}$, and a strict improvement over [38] which uses $D^{\mathrm{QT}}_{\mathrm{standard}}$ in the same context. Moreover, the key property outlined by [38] that $D^{\mathrm{QT}}_{\mathrm{standard}}(A\|B) \leqslant D(p\|q)$ for $A = \int_{\mathcal{X}} \varphi(x)\varphi(x)^* dp(x)$ and $B = \int_{\mathcal{X}} \varphi(x)\varphi(x)^* dq(x)$ as soon as for all $x \in \mathcal{X}$, $\|\varphi(x)\|^2 \leqslant 1$, is preserved for $D^{\mathrm{QT}}_{\mathrm{max}}$ (this is a direct consequence of Jensen's inequality).

Variational formulation. As shown in [21, Section 9.1], there is a representation of $D^{\mathrm{QT}}_{\mathrm{max}}$ with similar terms as in Eq. (2), that is:

$$D^{\mathrm{QT}}_{\mathrm{max}}(A\|B) = \sup_{M,N\in\mathbb{H}_d} \mathrm{tr}[MA] + \mathrm{tr}[NB] \;\text{ such that } rM + N \preccurlyeq f(r)I. \tag{12}$$

The optimal matrices may be found from the singular value decomposition of $B^{-1/2}A^{1/2} = \sum_{i=1}^{d} s_i^{1/2} u_i v_i^\top = U\,\mathrm{Diag}(s)^{1/2}V^\top$, as $M = \sum_{i,j=1}^{d} \frac{f(s_i)-f(s_j)}{s_i - s_j} u_i^\top B u_j \cdot B^{-1/2} u_i u_j^\top B^{-1/2}$, and $N = \sum_{i,j=1}^{d} \frac{s_i^{-1}f(s_i) - s_j^{-1}f(s_j)}{s_i^{-1} - s_j^{-1}} v_i^\top A v_j \cdot$

$A^{-1/2} v_i v_j^\top A^{-1/2}$, where by convention, when $s = t$, $\frac{f(s)-f(t)}{s-t} = f'(t)$. Note that swapping A and B is equivalent to replacing $f(t)$ by $g(t) = tf(1/t)$.

While the Fenchel conjugate of $D^{\mathrm{QT}}_{\mathrm{standard}}(A\|B)$ with respect to A can be computed in closed form in most cases, this is not the case for $D^{\mathrm{QT}}_{\max}(A\|B)$. Thus, some of the algorithms from [38] cannot be extended.

Special case of von Neumann relative entropy. When $f(t) = t\log t - t + 1$, for the standard divergence $D^{\mathrm{QT}}_{\mathrm{standard}}(A\|B)$, we get $\operatorname{tr}\big[A\log A - A\log B\big]$, which is the Bregman divergence associated with the von Neumann entropy $A \mapsto \operatorname{tr}[A\log A]$. Note that this is different from seeing that A and B are covariance matrices, and considering the Kullback-Leibler between zero-mean Gaussian distributions with these covariance matrices (which would lead to $\frac{1}{2}\operatorname{tr}[AB^{-1}] - \frac{1}{2}\log\det[AB^{-1}] - \frac{d}{2}$). For an approach linking semi-definite programming and Gaussian entropies, see [39].

3 Sum-of-squares relaxation

In this section, we assume that φ is bounded on $\mathcal{X}$. We consider the task of computing

$$\Gamma(M) = \sup_{x\in\mathcal{X}} \ \varphi(x)^* M \varphi(x), \tag{13}$$

for some matrix $M \in \mathbb{H}_d$. Since φ is bounded, then Γ is a positively homogeneous everywhere finite convex function on $\mathbb{H}_d$. We know introduce necessary tools and notations for presenting the sum-of-squares (SOS) relaxations.

Let $\mathcal{K}$ be the closure of the convex hull, $\mathcal{C}$ the closure of the conic hull of all $\varphi(x)\varphi(x)^*$, $x \in \mathcal{X}$, and $\mathcal{V}$ its linear span. We assume that we know one positive semidefinite Hermitian matrix $U \in \mathbb{H}_d^+$ such that $\varphi(x)^* U \varphi(x) = 1$ for all $x \in \mathcal{X}$ (there are typically many as two such matrices U and U' are such that $U - U' \in \mathcal{V}^\perp$). Note that all developments are not always independent of the choice of U, and bounds may depend on U, but the definition of the affine subspace $\{\Sigma \in \mathcal{V},\ \operatorname{tr}[U\Sigma] = 1\}$ is independent of that choice.

From the definition above, we have $\mathcal{K} \subset \mathcal{C} \subset \mathcal{V}$, and

$$\Sigma \in \mathcal{K} \quad \Leftrightarrow \quad \Sigma \in \mathcal{C} \text{ and } \operatorname{tr}[\Sigma U] = 1.$$

By definition of Γ in Eq. (13), and by properties of convex hulls, we have

$$\Gamma(M) = \sup_{x\in\mathcal{X}} \ \varphi(x)^* M \varphi(x) = \max_{\Sigma\in\mathcal{K}} \ \operatorname{tr}[\Sigma M],$$

that is, the function Γ is the support function of $\mathcal{K}$. Moreover, using our notations for finite measures from Section 2, we have $\mathcal{C} = \big\{ \int_{\mathcal{X}} \varphi(x)\varphi(x)^* dp(x),\ p \in \mathcal{M}_+(\mathcal{X})\big\}$ and $\mathcal{K} = \big\{ \int_{\mathcal{X}} \varphi(x)\varphi(x)^* dp(x),\ p \in \mathcal{P}(\mathcal{X})\big\}$.

3.1 Outer approximations of convex hulls

In order to obtain an *upper-bound* on $\Gamma(M)$ defined in Eq. (13), we will look for *outer* approximations of the set $\mathcal{K}$. By construction, the convex hull is included in the affine hull, that is, if $\Sigma \in \mathcal{K}$, then $\operatorname{tr}[\Sigma U] = 1$ and $\Sigma \in \mathcal{V}$. The extra condition we will use in this paper follows [14, 15], and is simply that Σ is positive semi-definite, which is a direct consequence of $\varphi(x)\varphi(x)^* \in \mathbb{H}_d^+$ for all $x \in \mathcal{X}$.

We thus consider outer approximations of $\mathcal{K} = \mathcal{C} \cap \{\Sigma,\ \mathrm{tr}[\Sigma U] = 1\}$, through the outer approximation of $\mathcal{C}$ as $\widehat{\mathcal{C}} = \mathcal{V} \cap \mathbb{H}_d^+$, which corresponds to $\widehat{\mathcal{K}} = \mathcal{V} \cap \mathbb{H}_d^+ \cap \{\Sigma,\ \mathrm{tr}[U\Sigma] = 1\}$, with $\mathbb{H}_d^+$ the set of PSD Hermitian matrices. This leads to our approximation of $\Gamma(M)$ as:

$$\widehat{\Gamma}(M) \quad = \quad \max_{\Sigma \in \widehat{\mathcal{K}}} \mathrm{tr}[\Sigma M] \quad = \quad \max_{\Sigma \in \mathbb{H}_d} \quad \mathrm{tr}[\Sigma M] \quad \text{such that} \quad \mathrm{tr}[\Sigma U] = 1,\ \Sigma \in \mathcal{V},\ \text{and}\ \Sigma \succcurlyeq 0,$$

which satisfies $\Gamma(M) \leqslant \widehat{\Gamma}(M)$ for all $M \in \mathbb{H}_d$.

These relaxations are often referred to as "sum-of-squares" (SOS) relaxations, through the following dual interpretation. Introducing Lagrange multipliers, $c \in \mathbb{R}$ for the constraint $\mathrm{tr}[\Sigma U] = 1$, $A \in \mathcal{V}^\perp$ for $\Sigma \in \mathcal{V}$, and $B \succcurlyeq 0$ for $\Sigma \succcurlyeq 0$, we get, using strong duality:

$$\begin{aligned}
\widehat{\Gamma}(M) \quad &= \quad \sup_{\Sigma \in \mathbb{H}_d} \ \inf_{c \in \mathbb{R},\ A \in \mathcal{V}^\perp,\ B \succcurlyeq 0} \ \mathrm{tr}[\Sigma M] + c(1 - \mathrm{tr}[\Sigma U]) + \mathrm{tr}\, A\Sigma + \mathrm{tr}\, B\Sigma \\
&= \quad \inf_{c \in \mathbb{R},\ A \in \mathcal{V}^\perp,\ B \succcurlyeq 0} \ \sup_{\Sigma \in \mathbb{H}_d} \ \mathrm{tr}[\Sigma M] + c(1 - \mathrm{tr}[\Sigma U]) + \mathrm{tr}\, A\Sigma + \mathrm{tr}\, B\Sigma \\
&= \quad \inf_{c \in \mathbb{R},\ A \in \mathcal{V}^\perp,\ B \succcurlyeq 0} \ c \quad \text{such that} \quad M = cU - A - B \\
&= \quad \inf_{c \in \mathbb{R},\ B \succcurlyeq 0} \ c \quad \text{such that} \quad \forall x \in \mathcal{X},\ c - \varphi(x)^* M \varphi(x) = \varphi(x)^* B \varphi(x).
\end{aligned}$$

This can be interpreted as finding the lowest upper-bound c on the function $x \mapsto \varphi(x)^* M \varphi(x)$ by relaxing the non-negativity of $c - \varphi(x)^* M \varphi(x)$ by the existence of $B \succcurlyeq 0$ such that $c - \varphi(x)^* M \varphi(x) = \varphi(x)^* B \varphi(x)$ (which is indeed non-negative). Finally, using the eigendecomposition of B, $\varphi(x)^* B \varphi(x)$ can be written as a sum of square functions, hence the denomination. Note that it is common to add extra conic constraints to further restrict $\widehat{\mathcal{C}}^*$, often leading to hierarchies of relaxations (see examples below and [14]), which makes the relaxations tighter and tighter.

Throughout the paper, we will often use the following statements based on dual cones (using that the dual of the intersection of cones is the sum of their duals [20]):

$$\begin{aligned}
\Gamma(M) \leqslant t \quad &\Leftrightarrow \quad \Gamma(tU - M) \leqslant 0 \quad \Leftrightarrow \quad tU - M \in \mathcal{C}^* \\
\widehat{\Gamma}(M) \leqslant t \quad &\Leftrightarrow \quad \widehat{\Gamma}(tU - M) \leqslant 0 \quad \Leftrightarrow \quad tU - M \in \widehat{\mathcal{C}}^* = \mathbb{H}_d^+ + \mathcal{V}^\perp.
\end{aligned} \tag{14}$$

3.2 Examples

Finite set with injective embedding. If $\mathcal{X}$ is finite and the Gram matrix of all features for all values of $\mathcal{X}$ is invertible, then the SOS relaxation is tight. Indeed, assuming (potentially after applying an invertible linear transformation to φ) that $\varphi(x)^*\varphi(y) = 1_{y=x}$, $\mathcal{K}$ is the set of diagonal matrices with a diagonal belonging to the simplex.

Trigonometric polynomials on $[-1,1]$. We consider $\mathcal{X} = [-1,1]$ and $\varphi(x) \in \mathbb{C}^{2r+1}$, with $\varphi(x)_\omega = e^{i\pi\omega x}$ for $\omega \in \{-r, \dots, r\}$. Then $(\varphi(x)\varphi(x)^*)_{\omega\omega'} = e^{i\pi(\omega-\omega')x}$, and thus $\mathcal{V}$ is the set of Hermitian Toeplitz matrices, and we can take $U = \frac{1}{d} I$. It turns out that the sum-of-squares relaxation is tight, see [40, Theorem 1.2.1] and [41].

Trigonometric polynomials on $[-1,1]^n$. We consider $\mathcal{X} = [-1,1]^n$ and $\varphi(x)_\omega = e^{i\pi\omega^\top x} \in \mathbb{C}$ for ω in a certain set $\Omega \subset \mathbb{Z}^n$, typically $\Omega = \{\omega \in \mathbb{Z}^n,\ \|\omega\|_\infty \leqslant r\}$. We then have $(\varphi(x)\varphi(x)^*)_{\omega\omega'} = e^{i\pi(\omega-\omega')^\top x}$,

which depends only on $\omega - \omega'$, which defines a set of linear constraints defining $\mathcal{V}$. The relaxation is then not tight, but by embedding Ω in a larger set, we can make the relaxation as tight as desired (see [41]).

Affine functions on the Euclidean unit sphere. We consider $\mathcal{X}$ the unit sphere in $\mathbb{R}^{d-1}$, with $\varphi(x) = \begin{pmatrix} 1 \\ x \end{pmatrix} \in \mathbb{R}^d$. Then $\mathcal{V}$ is the set of matrices $\begin{pmatrix} \alpha & x^\top \\ x & X \end{pmatrix}$ such that $\mathrm{tr}(X) = \alpha$. This is another situation where the sum of squares relaxation is tight [42].

Polynomials in $[-1,1]$. We consider $\mathcal{X} = [-1,1]$, and $\varphi(x) = (1, x, x^2, \dots, x^{d-1})^\top \in \mathbb{R}^d$. We have: $(\varphi(x)\varphi(x)^*)_{ij} = x^{i+j}$. Thud $\mathcal{V}$ is the set of $d \times d$ Hankel matrices. The SOS relaxation is not tight without extra constraints. In one dimension, it takes a simple form [43], as adding the constraint $\Sigma_{1:d-1,1:d-1} - \Sigma_{2:d,2:d} \succcurlyeq 0$ makes it tight. This can be generalized to polynomials in higher dimensions, and has been extensively in many numerical analysis tasks (see [14]).

Boolean hypercube. We consider $\mathcal{X} = \{-1,1\}^n$ with feature vectors composed of Boolean Fourier components of increasing orders [44]. This corresponds to features $\varphi_A(x) = \prod_{i \in A} x_i \in \{-1,1\}$, where A is a subset of $\{1,\dots,n\}$. Moreover, given two sets A and B, we have $\varphi_A(x)\varphi_B(x) = \varphi_{A\Delta B}(x)$, where $A\Delta B$ is the symmetric difference between A and B.

If we consider a set $\mathcal{A}$ of subsets of $\{1,\dots,n\}$, then, the element indexed (A,B) of $\varphi(x)\varphi(x)^*$ only depends on $A\Delta B$, and this defines a set of linear constraints defining $\mathcal{V}$. The relaxation is not tight in general, but if we see our moment matrix as a submatrix obtained from a sufficiently larger set of subsets, then we obtain a tight formulation (see [45, 46, 47] and references therein).

Note that for all of our examples, a simple algorithm exists for the orthogonal projection on $\mathcal{V}$, which will be useful for our estimation algorithms.

4 Exact lower bounds based on moments

We consider the optimal lower bound on $D(p\|q)$ given the integrals $\Sigma_p = \int_{\mathcal{X}} \varphi(x)\varphi(x)^* dp(x)$ and $\Sigma_q = \int_{\mathcal{X}} \varphi(x)\varphi(x)^* dq(x)$, that is,

$$D^{\mathrm{OPT}}(A\|B) = \inf_{p,q \in \mathcal{M}_+(\mathcal{X})} D(p\|q) \ \text{ such that } \ \Sigma_p = A \text{ and } \Sigma_q = B. \tag{15}$$

By construction, $D^{\mathrm{OPT}}(\Sigma_p\|\Sigma_q) \leqslant D(p\|q)$. Moreover, we have some immediate properties for the function defined in Eq. (15), which preserves similar properties of $D(p\|q)$. For other potential properties such as used within multivariate probabilistic modeling, see [38]:

- If A or B is not in $\mathcal{C}$ (the closure of the convex full of all $\varphi(x)\varphi(x)^*$, then value is infinite since the optimization problem is infeasible.
- if $\mathrm{tr}[AU] = \mathrm{tr}[BU]$, then the optimal measures p and q are probability measures.

- $D^{\mathrm{OPT}}(A\|B)$ is jointly convex in A and B, as the optimal value of a jointly convex problem in A, B, p, q.
- If φ is replaced by $T\varphi$ for an injective linear map T, the quantity $D^{\mathrm{OPT}}(\Sigma_q\|\Sigma_q)$ is unchanged.
- If φ is replaced by $T\varphi$ for a (potentially non-injective) linear map T, the quantity $D^{\mathrm{OPT}}(\Sigma_q\|\Sigma_q)$ is reduced. Therefore, to have tighter lower-bounds on $D(p\|q)$, we need to use high-dimensional features. In other words, apart from a maximizing pair (p, q), the approximation is typically tight, that is, $D(p\|q)$ close to $D^{\mathrm{OPT}}(\Sigma_p\|\Sigma_q)$ only if the feature $\varphi : \mathcal{X} \to \mathbb{C}^d$ is rich enough. For approximation capabilities when the feature size grows, see [38].

Variational representation. We have, using the representation of the f-divergence $D(p\|q)$ from Eq. (2), and strong convex duality:

$$\begin{aligned}
& D^{\mathrm{OPT}}(A\|B) \\
= & \inf_{p,q\in\mathcal{M}(\mathcal{X})} \sup_{M,N\in\mathbb{H}_d,\ v,w:\mathcal{X}\to\mathbb{R}} \mathrm{tr}[MA] + \mathrm{tr}[NB] - \int_{\mathcal{X}} \varphi(x)^* M\varphi(x) dp(x) - \int_{\mathcal{X}} \varphi(x)^* N\varphi(x) dq(x) \\
& \qquad + \int_{\mathcal{X}} v(x)dp(x) + \int_{\mathcal{X}} w(x)dq(x) \text{ such that } \forall x \in \mathcal{X}, \forall r \geqslant 0,\ rv(x) + w(x) \leqslant f(r) \\
= & \sup_{M,N\in\mathbb{H}_d} \mathrm{tr}[MA] + \mathrm{tr}[NB] \text{ such that } \forall x \in \mathcal{X}, \forall r \geqslant 0,\ r\varphi(x)^* M\varphi(x) + \varphi(x)^* N\varphi(x) \leqslant f(r) \\
= & \sup_{M,N\in\mathbb{H}_d} \mathrm{tr}[MA] + \mathrm{tr}[NB] \text{ such that } \forall r \geqslant 0,\ \Gamma(rM + N) \leqslant f(r). \qquad (16)
\end{aligned}$$

The representation above shows that being able to compute D^{OPT} requires the computability of Γ, that is, maximizing quadratic forms in $\varphi(x)$, which is exactly what SOS methods presented in Section 3 are taylored to approximate, and that will be used in Section 5 below.

Algorithms to compute $D^{\mathrm{OPT}}(A\|B)$. This tightest lower bound can only be approximated tightly, if we consider an approximation of f by a piecewise affine function with sufficiently many kinks (as done in Section 2.1), *and* we can compute Γ arbitrarily precisely. This is typically only easily possible without brute force enumeration with sum-of-squares relaxations which are asymptotically tight (thus using hierarchies). In our experiments where we compare all bounds, we consider the case of uni-dimensional trigonometric polynomials, for which our simplest relaxation is already tight. Computable lower bounds are considered in Section 5 (based on SOS relaxations) and Section 6 (based on quantum information divergences).

5 Relaxed f-divergence based on SOS

We consider replacing Γ in the optimal relaxation $D^{\mathrm{OPT}}(A\|B)$ in Eq. (16) by its approximation $\widehat{\Gamma}$ based on sums-of-squares, as defined in Section 3. This leads to, using that $\widehat{C} = \mathbb{H}_d^+ \cap \mathcal{V}$, and thus $\widehat{C}^* = \mathbb{H}_d^+ + \mathcal{V}^\perp$, with Eq. (14):

$$\begin{aligned}
D^{\mathrm{SOS}}(A\|B) &= \sup_{M,N\in\mathbb{H}_d} \mathrm{tr}[AM] + \mathrm{tr}[BN] \text{ such that } \forall r \geqslant 0,\ \widehat{\Gamma}(rM + N) \leqslant f(r) \qquad (17) \\
&= \sup_{M,N\in\mathbb{H}_d} \mathrm{tr}[AM] + \mathrm{tr}[BN] \text{ such that } \forall r \geqslant 0,\ f(r)U - rM - N \in \widehat{\mathcal{C}}^* = \mathbb{H}_d^+ + \mathcal{V}^\perp.
\end{aligned}$$

Since $\Gamma \leqslant \widehat{\Gamma}$, we have by construction $D^{\mathrm{SOS}} \leqslant D^{\mathrm{OPT}}$. Moreover, it is now finite if only if $A, B \in \widehat{\mathcal{C}} = \mathbb{H}_d^+ \cap \mathcal{V}$ (rather than $\mathcal{C}$). Note that the relaxation is independent of the particular choice of $U \in \mathbb{H}_d$ such that $\varphi(x)^* U \varphi(x) = 1$ for all $x \in \mathcal{X}$. It turns out that this is not the simplest formulation to consider, and that we can use Lagrangian duality, akin to Eq. (3). This requires to introduce a Lagrange multiplier of the constraint $\forall r \geqslant 0,\ f(r)U - rM - N \in \widehat{\mathcal{C}}^*$, which is a $\widehat{\mathcal{C}}$-valued finite measure on $\mathbb{R}_+$ [22]: to get:

$$\begin{aligned}
& D^{\mathrm{SOS}}(A\|B) \\
= & \inf_{\Lambda\ \widehat{\mathcal{C}}-\text{valued measure on } \mathbb{R}_+} \sup_{M,N \in \mathbb{H}_d} \operatorname{tr}[AM] + \operatorname{tr}[BN] + \int_0^{+\infty} \operatorname{tr}\left[d\Lambda(r)(f(r)U - rM - N)\right] \\
= & \inf_{\Lambda\ \widehat{\mathcal{C}}-\text{valued measure on } \mathbb{R}_+} \int_0^{+\infty} f(r) \operatorname{tr}\left[d\Lambda(r)U\right] \text{ such that } \int_0^{+\infty} d\Lambda(r) = B \text{ and } \int_0^{+\infty} r d\Lambda(r) = A. \quad (18)
\end{aligned}$$

Note that like D^{OPT}, D^{SOS} is jointly convex, and invariant by invertible linear transforms φ, and by construction for all $A, B \in \widehat{\mathcal{C}}$, $D^{\mathrm{SOS}}(A\|B) \leqslant D^{\mathrm{OPT}}(A\|B)$.

Estimation algorithms. In order to approximate $D^{\mathrm{SOS}}(A\|B)$ in Eq. (16) or Eq. (17), we consider $\hat{f}$ defined in Section 2.2 instead of f, and consider

$$\widehat{D}^{\mathrm{SOS}}(A\|B) = \inf_{\Lambda_0,\ldots,\Lambda_m \in \widehat{\mathcal{C}} = \mathbb{H}_d^+ \cap \mathcal{V}} \sum_{i=0}^m f_i \operatorname{tr}\left[\Lambda_i U\right] \text{ such that } \sum_{i=0}^m b_i \Lambda_i = B \text{ and } \sum_{i=0}^m a_i \Lambda_i = A, \quad (19)$$

with the following dual formulation:

$$\widehat{D}^{\mathrm{SOS}}(A\|B) = \sup_{M,N \in \mathbb{H}_d} \operatorname{tr}[AM] + \operatorname{tr}[BN] \text{ such that } \forall i \in \{0,\ldots,m\}, f_i U - a_i M - b_i N - Z_i \in \mathcal{V}^\perp, Z_i \succcurlyeq 0.$$

In order to have a valid lower-bound on $D(p\|q)$, we need a feasible pair (M, N). In order to compute $\widehat{D}^{\mathrm{SOS}}(A\|B)$, we can first consider a generic interior-point method [48, 49] adapted to the semi-definite program defined above. Given that there are m matrices of size $d \times d$, we get an overall complexity of $O((md^2)^{3.5})$, which is not scalable for large problems. We consider a augmented Lagrangian method [50] applied to Eq. (19), which is detailed in Appendix B.1, with a complexity per iteration of $O(md^3)$. Note that we can get a good spectral initializer from the next section.

Tightness. In this paper, we focus on the computation of upper-bounds of the partition function. The study of the approximation capabilities when the feature vector grows is left for future work.

6 Relaxed f-divergence based on quantum information theory

In the expression in Eq. (16), the matrix U only has to satisfy $\varphi(x)^* U \varphi(x)$ for all $x \in \mathcal{X}$, and the expression does not depend on the choice of such an U. We now also implose that it is positive semi-definite, and we denote it as V. We defined $\mathcal{U}$ as the set of such matrices V (which we have assumed to be non-empty).

Starting from Eq. (18), and recalling that $\widehat{\mathcal{C}} = \mathcal{V} \cap \mathbb{H}_d^+$, we further relax the optimization problem by removing the constraint that the measure has values in $\mathcal{V}$ (the span of all $\varphi(x)\varphi(x)^*$), and just keep values in $\mathbb{H}_d^+$. It turns out that the solution may be obtained in closed form, and related to the quantum information divergences from Section 2.6.

Lemma 1 *Assume $A, B \succcurlyeq 0$, and $V \succcurlyeq 0$, and f is operator-convex. Then*

$$\inf_{\Lambda\ \mathbb{H}_d^+-\text{valued measure on } \mathbb{R}_+} \int_0^{+\infty} f(r)\,\mathrm{tr}\left[d\Lambda(r)V\right] \text{ such that } \int_0^{+\infty} d\Lambda(r) = B \text{ and } \int_0^{+\infty} r d\Lambda(r) = A$$

is equal to $\mathrm{tr}\left[B^{1/2}VB^{1/2}f\big(B^{-1/2}AB^{-1/2}\big)\right]$ *(see proof for minimizer).*

Proof Given the eigendecomposition $B^{-1/2}AB^{-1/2} = \sum_{i=1}^d \lambda_i u_i u_i^*$, we consider $\Lambda = \sum_{i=1}^d B^{1/2}u_i u_i^* B^{1/2}\delta_{\lambda_i}$, where δ_{λ_i} is the Dirac measure at λ_i, so that we get a feasible measure Λ, and an objective equal to $\mathrm{tr}\left[B^{1/2}VB^{1/2}f\big(B^{-1/2}AB^{-1/2}\big)\right]$. Thus the infimum is less than $\mathrm{tr}\left[B^{1/2}VB^{1/2}f\big(B^{-1/2}AB^{-1/2}\big)\right]$.

The other direction is a direct consequence of the operator Jensen's inequality [51]; for any feasible measure Λ approached by an empirical measure $\sum_{i=1}^d M_i\delta_{r_i}$, we have $\displaystyle\sum_{i=1}^d (M_i^{1/2}B^{-1/2})^*(M_i^{1/2}B^{-1/2}) = I$, and thus

$$\begin{aligned}\int_{\mathbb{R}_+} f(r)d\Lambda(r) &= B^{1/2}\Big(\sum_{i=1}^d (M_i^{1/2}B^{-1/2})^* f(rI)(M_i^{1/2}B^{-1/2})\Big)B^{1/2}\\ &\succcurlyeq B^{1/2}f\Big(\sum_{i=1}^d (M_i^{1/2}B^{-1/2})^*(rI)(M_i^{1/2}B^{-1/2})\Big)B^{1/2} = B^{1/2}f\big(B^{-1/2}AB^{-1/2}\big)B^{1/2}.\end{aligned}$$

The lower bound follows by using $V \succcurlyeq 0$. Note that a sufficient condition to get a tight solution to $D^{\mathrm{SOS}}(A\|B)$, is $B^{1/2}u_i u_i^* B^{1/2} \in \mathcal{V}$ for all $i \in \{1, \dots, d\}$. ■

Since we have a lower-bound on $D^{\mathrm{SOS}}(A\|B)$ for all $V \in \mathcal{U}$, we can maximize with respect to V, and define the quantity

$$D^{\mathrm{QT}}(A\|B) = \sup_{V\in\mathcal{U}}\ \mathrm{tr}\left[B^{1/2}VB^{1/2}f\big(B^{-1/2}AB^{-1/2}\big)\right]. \tag{20}$$

By construction $D^{\mathrm{SOS}}(A\|B) \leqslant D^{\mathrm{OPT}}(A\|B)$.

Maximimizing with respect to V. For $Q = B^{1/2}f\big(B^{-1/2}AB^{-1/2}\big)B^{1/2} \succcurlyeq 0$, considering a matrix $U \in \mathbb{H}_d$ such that $\varphi(x)^*U\varphi(x) = 1$ for all $x \in \mathcal{X}$:

$$\begin{aligned}\max_{V\in\mathcal{U}}\ \mathrm{tr}[QV] &= \max_V\ \mathrm{tr}[QV] \text{ such that } V \succcurlyeq 0 \text{ and } \forall x \in \mathcal{X},\ \varphi(x)^*V\varphi(x) = 1\\ &= \max_V\ \mathrm{tr}[QV] \text{ such that } V \succcurlyeq 0 \text{ and } V - U \in \mathcal{V}^\perp\\ &= \min_{\Sigma\in\mathcal{V}}\ \mathrm{tr}[\Sigma U] \text{ such that } \Sigma \succcurlyeq Q, \text{ by Lagrange duality.}\end{aligned}$$

Note that the expression above is independent of the choice of U. We have thus another expression:

$$D^{\mathrm{QT}}(A\|B) = \min_{\Sigma\in\mathcal{V}}\ \mathrm{tr}[\Sigma U] \text{ such that } \Sigma \succcurlyeq B^{1/2}f\big(B^{-1/2}AB^{-1/2}\big)B^{1/2}.$$

Note that like D^{OPT} and D^{SOS}, D^{QT} is jointly convex, and $D^{\mathrm{QT}}(\Sigma_p\|\Sigma_q)$ is invariant by invertible linear transform of φ (which would not be the case without optimizing with respect to V). Moreover, $D^{\mathrm{QT}}(A\|B)$ is finite only if A and B are positive semi-definite (as opposed to be also in $\mathcal{V}$ for $D^{\mathrm{SOS}}(A\|B)$).

In terms of algorithms to approximate $D^{\mathrm{QT}}(A\|B)$, we can either use interior-point methods to solve Eq. (20) for small problems, or consider an augmented Lagrangian method detailed in Appendix B.2.

6.1 Link with quantum information theory and metric learning

Given a feature map $\varphi : \mathcal{X} \to \mathbb{C}^d$ and an invertible matrix $T \in \mathbb{C}^{d\times d}$, such that $V = T^*T \in \mathcal{U}$. Writing $\tilde{A} = TAT^*$, and $\tilde{B} = TBT^*$, we get, using the *maximal divergence* defined in Section 2.6:

$$D^{\mathrm{QT}}_{\max}(TAT^*\|TBT^*) = D^{\mathrm{QT}}_{\max}(\tilde{A}\|\tilde{B}) = \mathrm{tr}(\tilde{B}^{1/2} f(\tilde{B}^{-1/2}\tilde{A}\tilde{B}^{-1/2})\tilde{B}^{1/2}).$$

Since $\tilde{B}^{1/2}$ and $TB^{1/2}$ are two square roots of $\tilde{B}$, there exists a unitary matrix R such that $\tilde{B}^{1/2} = TB^{1/2}R$. We then get $\tilde{B}^{-1/2}\tilde{A}\tilde{B}^{-1/2} = R^*B^{-1/2}AB^{-1/2}R$, leading to $f(\tilde{B}^{-1/2}\tilde{A}\tilde{B}^{-1/2}) = R^*f(B^{-1/2}AB^{-1/2})R$, which in turn leads to

$$\begin{aligned} D^{\mathrm{QT}}_{\max}(\tilde{A}\|\tilde{B}) &= \mathrm{tr}(\tilde{B}^{1/2} f(\tilde{B}^{-1/2}\tilde{A}\tilde{B}^{-1/2})\tilde{B}^{1/2}) = \mathrm{tr}\left[TB^{1/2} f(B^{-1/2}AB^{-1/2})B^{1/2}T^*\right] \\ &= \mathrm{tr}\left[T^*TB^{1/2} f(B^{-1/2}AB^{-1/2})B^{1/2}\right] = \mathrm{tr}\left[VB^{1/2} f(B^{-1/2}AB^{-1/2})B^{1/2}\right], \end{aligned}$$

which is exactly the objective function maximized to define $D^{\mathrm{QT}}(A\|B)$ in Eq. (20).

As observed in [38], we have $D^{\mathrm{QT}}_{\max}(TAT^*\|TBT^*) \leqslant D(p\|q)$ for any $p, q \in \mathcal{M}_+(\mathcal{X})$ such that $\Sigma_p = A$ and $\Sigma_q = B$, as soon as $T^*T \in \mathcal{U}$. Our new relaxation is thus equivalent to estimating the best feature vector in a linear model defined by φ. A simple consequence is that, while $D^{\mathrm{QT}}_{\max}$ is not invariant by invertible linear transforms, D^{QT} is (just like D^{OPT} and D^{SOS}).

6.2 Direct relationship with the SOS relaxation

We can also provide a dual formulation to $D^{\mathrm{QT}}(A\|B)$ in Eq. (20), by applying the representation of quantum divergences from Eq. (12) to $\tilde{A} = TAT^*$ and $\tilde{B} = TBT^*$:

$$\begin{aligned} D^{\mathrm{QT}}(A\|B) &= \sup_{M,N\in\mathbb{H}_d,\ T\in\mathbb{C}^{d\times d}} \mathrm{tr}[\tilde{M}TAT^*] + \mathrm{tr}[\tilde{N}TBT^*] \text{ such that } \forall r \geqslant 0, r\tilde{M} + \tilde{N} \preccurlyeq f(r)I, \text{ and } T^*T \in \mathcal{U} \\ &= \sup_{M,N,V\in\mathbb{H}_d} \mathrm{tr}[MA] + \mathrm{tr}[NB] \text{ such that } \forall r \geqslant 0, rM + N \preccurlyeq f(r)V,\ V \in \mathcal{U}, \end{aligned}$$

with the changes of variables $M = T^*\tilde{M}T$ and $N = T^*\tilde{N}T$.

Once $V \in \mathbb{H}_d^+$ is obtained, and a square root $T \in \mathbb{C}^{d\times d}$, we can obtain estimates of M and N as follows. We first consider the singular value decomposition of $\tilde{B}^{-1/2}\tilde{A}^{1/2} = \sum_{i=1}^d s_i^{1/2} u_i v_i^* = U\,\mathrm{Diag}(s)^{1/2}V^*$, for $\tilde{A} = TAT^*$, and $\tilde{B} = TBT^*$. We then take $M = \sum_{i,j=1}^d \frac{f(s_i)-f(s_j)}{s_i - s_j} u_i^*\tilde{B}u_j \cdot T^*\tilde{B}^{-1/2}u_i u_j^*\tilde{B}^{-1/2}T$, and $N = \sum_{i,j=1}^d \frac{s_i^{-1}f(s_i)-s_j^{-1}f(s_j)}{s_i^{-1}-s_j^{-1}} v_i^*\tilde{A}v_j \cdot T^*\tilde{A}^{-1/2}v_i v_j^*\tilde{A}^{-1/2}T$. The corresponding measure is then equal to $\Lambda = \sum_{i=1}^n T^{-1}\tilde{B}^{1/2}u_i u_i^*\tilde{B}^{1/2}T^{-*}\delta_{s_i}$, for which we have $\int_{\mathbb{R}_+} d\Lambda(r) = B$, $\int_{\mathbb{R}_+} r d\Lambda(r) = A$, and $\int_{\mathbb{R}_+} f(r)\,\mathrm{tr}[V d\Lambda(r)] = D^{\mathrm{QT}}(A\|B)$. This can thus be used as an initializer for the previous section.

Dual formulation. We also have a formulation akin to Eq. (18), that is,

$$\begin{aligned} D^{\mathrm{QT}}(A\|B) &= \inf_{\Lambda\ \mathbb{H}_d^+\text{-valued measure on } \mathbb{R}_+} \int_0^{+\infty} f(r)\,\mathrm{tr}\left[d\Lambda(r)U\right] \\ &\qquad \text{such that } \int_0^{+\infty} d\Lambda(r) = B, \int_0^{+\infty} r d\Lambda(r) = A, \text{ and } \int_0^{+\infty} f(r) d\Lambda(r) \in \mathcal{V}, \end{aligned}$$

which shows the additional relaxation compared to $D^{\mathrm{SOS}}(A\|B)$, for which Λ is a measure (almost everywhere) valued in $\mathcal{V}$.

7 Relaxed f-partition function

Given the three lower bounds on the f-divergence $D^{\mathrm{OPT}} \geqslant D^{\mathrm{SOS}} \geqslant D^{\mathrm{QT}}$, we get a sequence of upper-bounds for $C_q(H)$ defined in Eq. (8), for any Hermitian matrix $H \in \mathbb{H}_d$. We start by using D^{OPT} and define

$$C_q^{\mathrm{OPT}}(H) = \sup_{A \in \mathbb{H}_d} \quad \mathrm{tr}[AH] - D^{\mathrm{OPT}}(A\|B) \ \text{ such that } \ \mathrm{tr}[AU] = 1. \tag{21}$$

We use the variational representation in Eq. (16), as well as convex duality, to get:

$$\begin{aligned}
& C_q^{\mathrm{OPT}}(H) \\
= & \sup_{A \in \mathbb{H}_d} \inf_{M,N \in \mathbb{H}_d} \quad \mathrm{tr}[AH] - \mathrm{tr}[MA] - \mathrm{tr}[NB] \text{ such that } \forall r \geqslant 0,\ \Gamma(rM+N) \leqslant f(r) \text{ and } \mathrm{tr}[AU] = 1 \\
= & \sup_{A \in \mathbb{H}_d} \inf_{M,N \in \mathbb{H}_d,\ \rho \in \mathbb{R}} \mathrm{tr}[AH] - \mathrm{tr}[MA] - \mathrm{tr}[NB] - \rho\big(\mathrm{tr}[AU] - 1\big) \text{ such that } \forall r \geqslant 0,\ \Gamma(rM+N) \leqslant f(r) \\
= & \inf_{N \in \mathbb{H}_d,\ \rho \in \mathbb{R}} \quad \rho - \mathrm{tr}[NB] \text{ such that } \forall r \geqslant 0,\ \Gamma(rH+N) \leqslant f(r) + \rho r.
\end{aligned}$$

This corresponds to the formulation in Eq. (6).

We can also use the dual version of $D^{\mathrm{OPT}}(A\|B)$ similar to Eq. (18) to obtain, with $\Gamma(rH+N) \leqslant f(r)+\rho r$ being equivalent to $(f(r)+\rho r)U - rH - N \in \mathcal{C}^*$:

$$\begin{aligned}
C_q^{\mathrm{OPT}}(H) \quad = \quad & \sup_{\Lambda:\ \mathcal{C}-\text{valued measure on } \mathbb{R}_+} \int_0^{+\infty} \mathrm{tr}\left[d\Lambda(r)(rH - f(r)U)\right] \\
& \text{such that } \int_0^{+\infty} \mathrm{tr}\left[U d\Lambda(r) r\right] = 1 \text{ and } \int_0^{+\infty} d\Lambda(r) = B.
\end{aligned}$$

The function C_q^{OPT} is convex in H, and also non-decreasing in H, that is, if $H \succcurlyeq H'$, then $C_q^{\mathrm{OPT}}(H) \geqslant C_q^{\mathrm{OPT}}(H')$ (this will be applied to the relaxed versions below). As needed for variational inference, we can get the optimal $A \in \mathcal{C}$ in Eq. (21) as $A = \int_{\mathbb{R}^+} r d\Lambda(r)$. In terms of computability, like for D^{OPT}, this is possible when the SOS relaxation is tight.

Tightness. In this paper, we focus on the computation of upper-bounds of the partition function. The study of the approximation capabilities when the feature vector grows is left for future work. In particular, it would be interesting to compare to other convex upper-bounds on the log partition functions such as the "tree-reweighted representation" framework [18].

We now consider computable relaxations, first based on SOS in Section 7.1, then on quantum information divergences in Section 7.2.

7.1 Sum-of-squares relaxation

We get the SOS relaxation where Γ is replaced by $\widehat{\Gamma}$, with the following primal and dual formulations:

$$\begin{aligned} C_q^{\mathrm{SOS}}(H) &= \inf_{N\in\mathbb{H}_d,\ \rho\in\mathbb{R}} \ \rho - \mathrm{tr}[NB] \text{ such that } \forall r \geqslant 0,\ (f(r)+\rho r)U - rH - N \in \widehat{\mathcal{C}}^* \\ &= \sup_{\Lambda:\ \widehat{\mathcal{C}}-\text{valued measure on } \mathbb{R}_+} \int_0^{+\infty} \mathrm{tr}\left[d\Lambda(r)(rH - f(r)U)\right] \\ &\qquad\qquad \text{such that } \int_0^{+\infty} \mathrm{tr}\left[U d\Lambda(r) r\right] = 1 \text{ and } \int_0^{+\infty} d\Lambda(r) = B. \end{aligned}$$

This is now approximable in polynomial time and is an upper bound on $C^{\mathrm{OPT}}(H)$. Moreover, we can get the optimal $A \in \mathcal{C}$ as $A = \displaystyle\int_{\mathbb{R}^+} r d\Lambda(r) \in \widehat{\mathcal{C}}$.

Algorithms. We consider the approximation $\hat{f}$ of f from Section 2.1, and we solve

$$\begin{aligned} &\inf_{N\in\mathbb{H}_d,\ \rho\in\mathbb{R},\ Z_0,\dots,Z_m\succcurlyeq 0} \ \rho - \mathrm{tr}[NB] \ \text{ such that } \ \forall i \in \{0,\dots,m\},\ f_i U + a_i(\rho U - H) - b_i N - Z_i \in \mathcal{V}^\perp \\ = &\sup_{\Lambda_0,\dots,\Lambda_m\in\widehat{\mathcal{C}}} \sum_{i=0}^m \mathrm{tr}\left[\Lambda_i(a_i H - f_i U)\right] \ \text{ such that } \ \sum_{i=0}^m a_i \,\mathrm{tr}[U\Lambda_i] = 1 \text{ and } \sum_{i=0}^m b_i \Lambda_i = B. \end{aligned}$$

This can be solved empirically using either interior-point methods or an augmented Lagrangian method, as detailed in Appendix B.3.

7.2 Quantum relaxation

We now consider the quantum relaxation instead of the sum-of-squares relaxation, for $H \in \mathbb{H}_d$ (the constraint that $A \succcurlyeq 0$ is automatically satisfied but not the one that $A \in \mathcal{V}$), using convex duality:

$$C_q^{\mathrm{QT}}(H) = \sup_{A\in\mathcal{V}} \ \mathrm{tr}[AH] - D^{\mathrm{QT}}(A\|B) \ \text{ such that } \ \mathrm{tr}[AU] = 1.$$

This can expressed as follows, with the introduction of Lagrange multipliers, to only keep constraints that are easy to deal with algorithmically:

$$\begin{aligned} &C_q^{\mathrm{QT}}(H) \\ = &\sup_{A\in\mathcal{V}} \inf_{V\in\mathcal{U}} \ \mathrm{tr}[AH] - \mathrm{tr}\left[B^{1/2} V B^{1/2} f\big(B^{-1/2} A B^{-1/2}\big)\right] \ \text{ such that } \ \mathrm{tr}[AU] = 1, \text{ and } U - V \in \mathcal{V}^\perp \\ = &\sup_{A\succcurlyeq 0, \Sigma\in\mathcal{V}} \inf_{Y\in\mathcal{V}^\perp,\ V\succcurlyeq 0} \ \mathrm{tr}[AH] - \mathrm{tr}\left[B^{1/2} V B^{1/2} f\big(B^{-1/2} A B^{-1/2}\big)\right] + \mathrm{tr}[\Sigma(V-U)] + \mathrm{tr}[AY] \\ &\qquad\qquad \text{such that } \ \mathrm{tr}[AU] = 1. \end{aligned}$$

Note that we have $\mathrm{tr}[BV] = \displaystyle\int_{\mathcal{X}} dq(x)$, so that we can add the constraint to obtain a compact space for V.

Algorithm. Several algorithms could be considered. We could use the framework of [23] for high precisions and with a semi-definite programming solver, or use discretization techniques from Section 2.2. We could also consider stochastic gradient algorithms based on the representation in Eq. (10). We propose an alternative simple approach.

From now on, for simplicity and without loss of generality, we assume that $B = I$ and $\int_{\mathcal{X}} dq(x) = 1$. Therefore, at optimum we have the extra constraint $\operatorname{tr}[V] = 1$.

We smooth the problem by adding an von Neumann entropy regularizer on V and a square Frobenius penalty on V, which leads to the problem

$$\sup_{A \succcurlyeq 0, \Sigma \in \mathcal{V}} \operatorname{tr}[AH] - \varepsilon \log \operatorname{tr} \exp\Big(\frac{1}{\varepsilon}(f(A) - \sqrt{d}\Sigma)\Big) - \sqrt{d}\operatorname{tr}[\Sigma U] - \frac{1}{2\varepsilon} d(A, \mathcal{V})^2 \quad \text{such that} \quad \operatorname{tr}[AU] = 1,$$

and running mirror descent with the mirror map $(A, \Sigma) \mapsto \operatorname{tr}[f(A)] + \frac{1}{2}\|\Sigma\|_F^2$. In turns out that the function to optimize is relatively smooth with respect to this mirror map, with a constant to be computed, and thus we can apply mirror descent with convergence rate in $O(1/t)$ after t iterations [52]. See details in Appendix B.4 for $f(t) = t \log t - t + 1$.

The main advantage of this formulation is that compared to our other relaxations, there is no need to find an approximation of the function f, and that the running-time complexity of each iteration is $O(d^3)$.

Alternative formulation. We also have a formulation which can be used without the spectral formulation (and thus adapted to interior-point methods):

$$\begin{aligned} C_q^{\mathrm{QT}}(H) \quad &= \sup_{\Lambda:\ \mathbb{H}_d^+ \text{-valued measure on } \mathbb{R}_+} \int_0^{+\infty} \operatorname{tr}\big[d\Lambda(r)(rH - f(r)U)\big] \\ &\quad \text{such that } \int_0^{+\infty} \operatorname{tr}\big[U d\Lambda(r) r\big] = 1, \int_0^{+\infty} d\lambda(r) = B, \text{ and } \int_0^{+\infty} f(r) d\Lambda(r) \in \mathcal{V}, \int_0^{+\infty} r d\Lambda(r) \in \mathcal{V}. \end{aligned}$$

Note the similarity with Eq. (7).

7.3 Computing integrals

In order to compute integrals, we simply use the same technique but without the constraint that measures sum to one, that is, without the constraint that $\operatorname{tr}[AU] = 1$. Starting from Eq. (9), we get, with $B = \Sigma_q$:

$$\begin{aligned} \widetilde{C}_q(H) = \int_{\mathcal{X}} f^*\big(\varphi(x)^* H \varphi(x)\big) dq(x) \quad &= \sup_{p \in \mathcal{M}_+(\mathcal{X})} \int_{\mathcal{X}} \varphi(x)^* H \varphi(x) dp(x) - D(p\|q) \\ &\leqslant \sup_{A \in \mathcal{C}} \operatorname{tr}[HA] - D^{\mathrm{OPT}}(A\|B) = \widetilde{C}_q^{\mathrm{OPT}}(H) \\ &= \inf_{N \in \mathbb{H}_d} \ -\operatorname{tr}[NB] \text{ such that } \forall r \geqslant 0,\ \Gamma(rH + N) \leqslant f(r). \end{aligned}$$

Note that we only have an inequality here because we are not optimizing over q. We then get two computable relaxations by considering $D^{\mathrm{SOS}}(A\|B)$ and $D^{\mathrm{QT}}(A\|B)$ instead of $D^{\mathrm{OPT}}(A\|B)$, with the respective formulation:

$$\begin{aligned} \widetilde{C}_q^{\mathrm{SOS}}(H) \quad &= \inf_{N \in \mathbb{H}_d} \ -\operatorname{tr}[NB] \text{ such that } \forall r \geqslant 0,\ f(r)U - rH - N \in \widehat{\mathcal{C}}^* \\ \widetilde{C}_q^{\mathrm{QT}}(H) \quad &= \sup_{A \in \mathbb{H}_d} \inf_{V \in \mathcal{U}} \operatorname{tr}[AH] - \operatorname{tr}\big[B^{1/2} V B^{1/2} f\big(B^{-1/2} A B^{-1/2}\big)\big]. \end{aligned}$$

Dual formulations and algorithms can then easily be derived.

8 Experiments

In this section, we illustrate our various relaxations and algorithms presented in earlier sections. We illustrate our results with the function $f(t) = t \log t - t + 1$, and the estimation of relative Shannon entropies and log-partition functions.

8.1 Relative entropy lower bounds on $\mathcal{X} = [-1, 1]$

We consider trigonometric polynomials, and q the uniform distribution on $[-1, 1]$ (with density $1/2$ with respect to the Lebesgue measure), and p with density $\frac{2}{\pi}\sqrt{1 - x^2}$. We have the following moments:

$$\begin{aligned}
\int_{-1}^{1} e^{i\pi\omega x} dq(x) &= 1 \text{ if } \omega = 0, \text{ and } 0 \text{ otherwise,} \\
\int_{-1}^{1} e^{i\pi\omega x} dp(x) &= \frac{2}{\omega\pi} J_1(\omega\pi) \text{ if } \omega \text{ is even, and } 0 \text{ otherwise,}
\end{aligned}$$

where J_1 is the Bessel function of the first kind, as well as the relative entropy $D(p\|q) \approx 0.0484$.

We can then consider $\omega \in \{-r, \dots, r\}$, and compute the various bounds: OPT, SOS (which are equal here, and for which we sampled 200 values of $\log r$ between -4 and 4), and QT (with a version only optimized over diagonal V), and the old version of QT from [38], where we only learn diagonal matrices V). We see in Figure 1 that the optimal bound is numerically identical to the full quantum bound, and close to the one with diagonal V, but with a strong improvement over the bound from [38]. Results are obtained by an interior-point method [49]. We also display the optimal matrix V for the quantum approximation.

8.2 Log-partition functions on $\mathcal{X} = [-1, 1]$

We consider $h(x) = \cos(\pi x)$, with $\log \int_{-1}^{1} e^{\cos(2\pi x)} \frac{dx}{2} = \log I_0(1) \approx 0.2359$, where we use the same $\varphi : [-1, 1] \to \mathbb{C}^{2r+1}$ as before, which enables us to write $h(x) = \varphi(x)^* H \varphi(x)$ for some Hermitian H. We then compute the two approximations, $C_q^{\mathrm{SOS}}(H)$ (equal to $C_q^{\mathrm{OPT}}(H)$), as well as, $C^{\mathrm{QT}}(H)$. We sampled 200 values of $\log r$ between -4 and 4. Results are obtained by an interior-point method [49].

We see in the left plot of Figure 2 that the quantum relaxation is here numerically identical to the one based on SOS, with an advantage in learning a full matrix V.

8.3 Entropy estimation on $\mathcal{X} = [-1, 1]^n$

We consider the task of estimating entropies from moments on a simple example, where we consider x_1 uniform on $[-1, 1]$ and $x_{i+1} = x_i + \eta_{i+1} \mod 2$, where η_{i+1} is uniform on $[-\rho, \rho]$. When $\rho = 0$, all x_i's are equal almost surely, while when $\rho = 1$, all x_i's are independent and uniform.

We can then compute the Kullback-Leibler divergence to the uniform distribution by noticing that the sequence (x_i) forms a Markov chain, so that (using classical entropy decomposition results for tree-structured

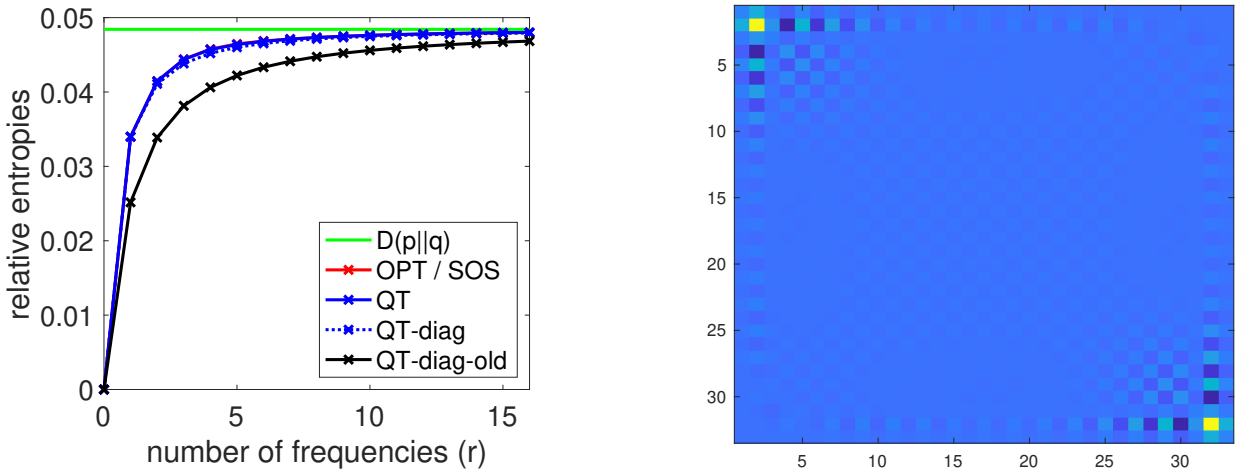


Figure 1: Comparison of relative entropy estimates for several numbers of frequencies. Left: effect of varying r; $D(p\|q)$ is the exact value, with moment-based approximations OPT/SOS (here equal), and the ones based on quantum information divergences, with full metric learning (QT) or diagonal metric learning (QT-diag), with also the use of the weaker quantum divergences done by [38]. Right: learned matrix V for the quantum bound.

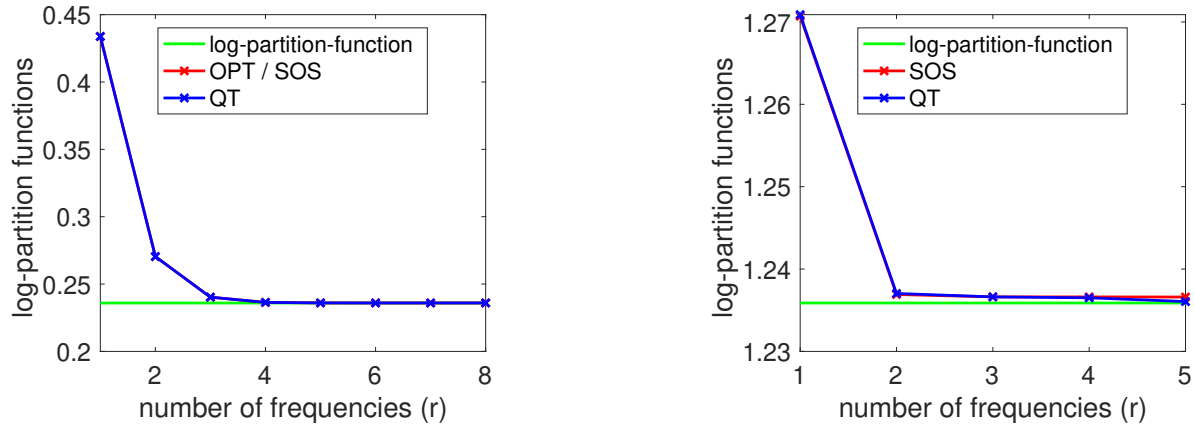


Figure 2: Comparison of log-partition function estimates for several numbers of frequencies. Left: $n = 1$, right: $n = 2$. For $n = 1$, the SOS relaxation is exactly the optimal lower bound.

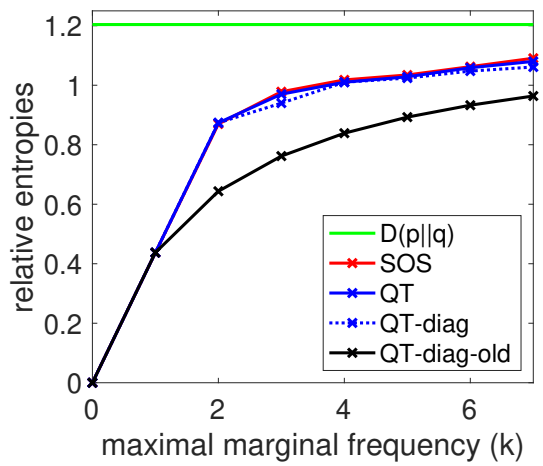


Figure 3: Comparison of relative entropy estimates for several numbers of maximal marginal frequency k, for $n = 2$. $D(p\|q)$ is the exact value, with moment SOS-based approximations, and the ones based on quantum information divergences, with full metric learning (QT) or diagonal metric learning (QT-diag), with also the use of the weaker quantum divergences done by [38].

graphical models [18]):

$$\begin{aligned} D(p\|q) &= \int_{[-1,1]^n} p(x)\log p(x)dx + n\log 2 \\ &= \sum_{i=1}^{n-1}\int_{[-1,1]^d} p(x_i,x_{i+1})\log p(x_i,x_{i+1})dx_i dx_{i+1} - \sum_{i=2}^{n-1}\int_{[-1,1]^d} p(x_i)\log p(x_i)dx_i + n\log 2 \\ &= -(n-1)\log(4\rho) + (n-2)\log 2 + n\log 2 = (n-1)\log\frac{1}{\rho}. \end{aligned}$$

We can also get all Fourier moments by introducing the $n \times (n-1)$ $\{0,1\}$-valued matrix M such that $x_i = (M\eta)_i + x_1$ for $i \in \{2,\ldots,n\}$. We then have

$$\mathbb{E}[e^{i\pi\omega^\top x}] = 1_{\omega^\top 1=0}\cdot\prod_{k=1}^{n-1}\frac{\sin\left[(M^\top\omega)_k\pi\rho\right]}{(M^\top\omega)_k\pi\rho}.$$

In order to estimate entropies, we consider $\|\omega\|_\infty \leqslant r$. See Figure 3, where we used an augmented Lagrangian method.

8.4 Log-partition functions on $\mathcal{X} = [-1,1]^n$

We consider task of computing the log-partition function. Given a function $h : [-1,1]^n \to \mathbb{R}$ that is expressed as $h(x) = \sum_{\omega\in\Omega} a_\omega e^{i\pi\omega^\top x}$, a simple strategy is to consider frequencies that contains $\Omega \cup \{0\}$. We could also find a smaller set Ω' such that $\Omega \subset \Omega' - \Omega'$.

For simplicity, we consider taking only frequencies such that $\|\omega\|_\infty \leqslant k$, leading to $d = (2k+1)^n$. We could also add random frequencies sampled from a geometric distribution.

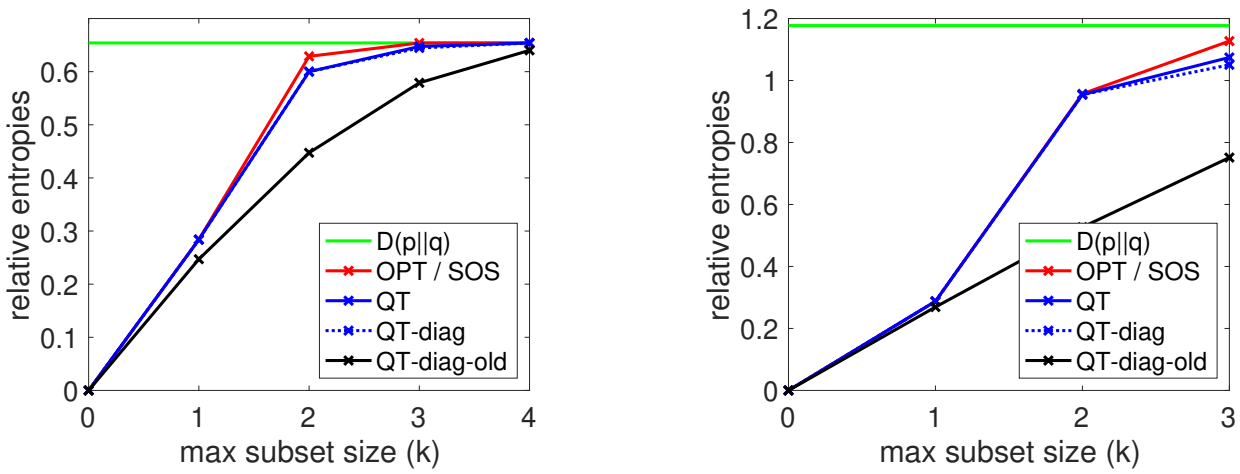


Figure 4: Comparison of relative entropy estimates for several numbers of frequencies for all subsets of cardinality less than k, for $n = 6$ (left, obtained with interior-point methods) and $n = 10$ (right, obtained with an augmented Lagrangian method). $D(p\|q)$ is the exact value, with moment SOS-based approximations, and the ones based on quantum information divergences, with full metric learning (QT) or diagonal metric learning (QT-diag), with also the use of the weaker quantum divergences done by [38].

In our experiments, we consider $h(x) = e^{i\pi \sum_{j=1}^n x_j}$. In order to compute the true partition function, we use sampling with many samples. See Figure 2.

8.5 Entropy estimation on $\mathcal{X} = \{-1, 1\}^n$

We consider the task of estimating entropies from moments on a simple example, where we consider x_1 uniform on $\{-1, 1\}$ and $x_{i+1} = x_i \eta_{i+1}$, where $\eta_{i+1} \in \{-1, 1\}$ is independent and equal to 1 with probability $1 - \rho/2$, and -1 otherwise. When $\rho = 0$, all x_i's are equal almost surely, while when $\rho = 1$, all x_i's are independent and uniform.

We can then compute the Kullback-Leibler divergence to the uniform distribution in the same way as for data in $[-1, 1]^n$, leading to $D(p\|q) = (n-1)\big[(1-\frac{\rho}{2})\log(2-\rho)+\frac{\rho}{2}\log\rho\big]$. We can also get all Fourier moments as $\mathbb{E}\big[\prod_{i\in A} x_i\big] = (1-(-1)^{|A|})\prod_{i=1}^{n-1}(1-\rho)^{1-(-1)^{(M^\top 1_A)_i}}$. In order to estimate entropies, we consider subsets of cardinality less then k. See Figure 4.

8.6 Log-partition functions on $\mathcal{X} = \{-1, 1\}^n$

We consider $h(x)$ a quadratic form in $x \in \{-1, 1\}^n$, and compare upper-bounds on the log-partition function using all subsets of cardinality less than a constant k. See Figure 5.

9 Conclusion

In this paper, we have proposed to combine tools from information theory, both classical such as f-divergences, and more recent, such as quantum information divergences, with sum-of-squares optimization.

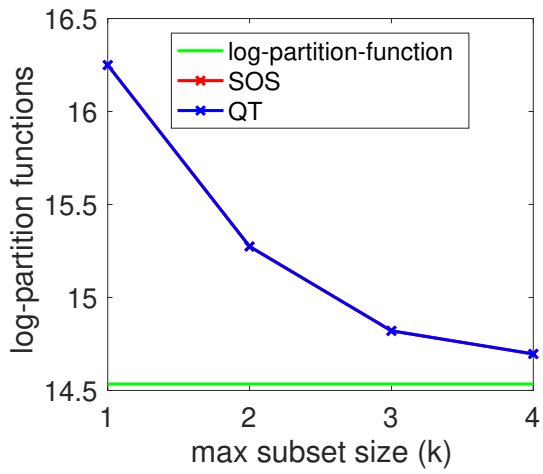


Figure 5: Comparison of log-partition function estimates for several numbers of frequencies for all subsets of cardinality less than k, for $n = 6$.

This leads to several relaxations of f-divergences based on sum-of-squares relaxations or quantum information divergences, together with efficient estimation algorithms for the tasks of divergence estimation from moments and the computation of log-partition functions. While the relaxation based on sum-of-squares is strictly superior, it is only mildly so in our experiments compared to the one based on quantum divergences, while being more costly to compute. This thus highlights the benefits of the quantum relaxation.

This quantum information relaxation takes its roots in earlier work [38] with a significant improvement of using a tighter quantum divergence. Several avenues are worth exploring: (a) check if the new notion of relative entropy with maximal divergence preserves properties from [38], in particular its use in probabilistic modelling and within graphical models, (b) potentially extend the positive definite kernel motivation that allows infinite-dimensional moments, (c) obtain convergence rates for entropies and log-partition function estimation to go with our encouraging empirical results, (d) develop algorithms to deal with larger scale problems using approximation techniques from kernel methods [53, 54] to go below the $O(d^3)$ complexity per iteration.

Acknowledgements

The author would like to thank Omar Fawzi for discussions related to quantum information divergences, as well as Adrien Taylor and Justin Carpentier for discussions on augmented Lagrangian algorithms. We also acknowledge support from the French government under the management of the Agence Nationale de la Recherche as part of the "Investissements d'avenir" program, reference ANR-19-P3IA-0001 (PRAIRIE 3IA Institute), as well as from the European Research Council (grant SEQUOIA 724063).

A Decomposition of operator-convex functions

We have the following particular cases from Section 2.

- α-divergences: $f(t) = \frac{1}{\alpha(\alpha-1)}\left[t^\alpha - \alpha t + (\alpha-1)\right] = \frac{1}{\alpha}\frac{\sin(\alpha-1)\pi}{(\alpha-1)\pi}(t-1)^2\int_0^{+\infty}\frac{1}{t+\lambda}\frac{\lambda^\alpha d\lambda}{(1+\lambda)^2}$ for $\alpha \in (-1,2)$. Other representations exist for $\alpha=-1$ and $\alpha=2$ (see below), but other cases are not operator-convex.
- KL divergence ($\alpha=1$): $f(t) = t\log t - t + 1 = \int_0^{+\infty}\frac{(t-1)^2}{t+\lambda}\frac{\lambda d\lambda}{(\lambda+1)^2}$.
- Rerverse KL divergence ($\alpha=0$): $f(t) = -\log t + t - 1 = \int_0^{+\infty}\frac{(t-1)^2}{t+\lambda}\frac{d\lambda}{(\lambda+1)^2}$.
- Pearson χ^2 divergence ($\alpha=2$): $f(t) = \frac{1}{2}(t-1)^2$ is operator convex.
- Reverse pearson χ^2 divergence ($\alpha=-1$): $f(t) = \frac{1}{2}\left(\frac{1}{t}+t\right) - 1 = \frac{1}{2}\frac{(t-1)^2}{t}$ is operator convex, with $d\nu(\lambda)$ proportional to a Dirac at $\lambda=0$.
- Le Cam distance: $f(t) = \frac{(t-1)^2}{t+1}$ is operator convex with $d\nu(\lambda)$ proportional to a Dirac at $\lambda=1$.
- Jensen-Shannon divergence: $f(t) = 2t\log\frac{2t}{t+1} + 2\log\frac{2}{t+1} = 2t\log t - 2(t+1)\log(t+1) + 2(t+1)\log 2 = 2t\log t - 4\frac{t+1}{2}\log\frac{t+1}{2}$ is operator convex, as it can be written $f(t) = 2(t-1)^2\int_0^{+\infty}\left(\frac{1}{t+\lambda} - \frac{1}{t+1+2\lambda}\right)\frac{\lambda d\lambda}{(1+\lambda)^2}$, which leads to $f(t) = 2(t-1)^2\int_0^{+\infty}\frac{1}{t+\lambda}\frac{\lambda d\lambda}{(1+\lambda)^2} - 2(t-1)^2\int_1^{+\infty}\frac{1}{t+\lambda}\frac{(\lambda-1)d\lambda}{(1+\lambda)^2}$.

B Optimization algorithm

In this section, we provide algorithmic details for the first-order algorithms that can deal with larger scale problems, than can be dealt with by interior point methods.

B.1 Detailed computations for Section 5

We want to minimize the pair of primal/dual problems:

$$\begin{aligned}
\widehat{D}^{\mathrm{SOS}}(A\|B) &= \inf_{\Lambda_0,\dots,\Lambda_m \in \widehat{\mathcal{C}} = \mathbb{H}_d^+ \cap \mathcal{V}} \sum_{i=0}^m f_i \operatorname{tr}\left[\Lambda_i U\right] \text{ such that } \sum_{i=0}^m b_i\Lambda_i = B \text{ and } \sum_{i=0}^m a_i\Lambda_i = A, \\
&= \sup_{M,N\in\mathbb{H}_d, \forall i, \mathbb{Z}_i \succcurlyeq 0, Y_i \in \mathcal{V}^\perp} \operatorname{tr}[AM] + \operatorname{tr}[BN] \\
&\qquad\qquad \text{such that } \forall i \in \{0,\dots,m\}, f_i U - a_i M - b_i N - Z_i - Y_i = 0.
\end{aligned}$$

In order to have a valid lower-bound on $D(p\|q)$, we need a feasible pair (M, N). We consider the augmented Lagrangian method [50], which solves, at every iteration:

$$\sup_{M,N\in\mathbb{H}_d,\forall i,\ Z_i\succcurlyeq 0, Y_i\in\mathcal{V}^\perp} \operatorname{tr}[AM] + \operatorname{tr}[BN] - \frac{1}{2\varepsilon}\sum_{i=0}^m \left\|f_iU - a_iM - b_iN - Z_i - Y_i\right\|_F^2 + \sum_{i=0}^m \operatorname{tr}\left[\Lambda_i(f_iU - a_iM - b_iN - Z_i - Y_i)\right], \tag{22}$$

and updates the matrices Λ_i's as:

$$\Lambda_i = \Lambda_i - \frac{1}{\varepsilon}(f_iU - a_iM - b_iN - Z_i - Y_i).$$

Note the difference with traditional penalty methods that take $\Lambda_i = 0$ for all i, but then need ε to be small.

Solving the inner problem with a first-order method. In order to solve Eq. (22), we minimize out M and N and then do randomized coordinate descent (this can also be accelerated [55]). We write the objective function in Eq. (22). as (removing the part not depending on M and N):

$$\operatorname{tr}\left[M\Big(A - \sum_{i=0}^m a_i\Lambda_i + \frac{1}{\varepsilon}\sum_{i=0}^m a_i(f_iU - Z_i - Y_i)\Big)\right] + \operatorname{tr}\left[N\Big(B - \sum_{i=0}^m b_i\Lambda_i + \frac{1}{\varepsilon}\sum_{i=0}^m b_i(f_iU - Z_i - Y_i)\Big)\right] - \frac{1}{2\varepsilon}\sum_{i=0}^m \Big\{a_i^2\|M\|_F^2 + b_i^2\|N\|_F^2 + 2a_ib_i \operatorname{tr} MN\Big\},$$

with optimality condition for M and N, with $\Delta_A = A - \sum_{i=0}^m a_i\Lambda_i + \frac{1}{\varepsilon}\sum_{i=0}^m a_i(f_iU - Z_i - Y_i)$ and $\Delta_B = B - \sum_{i=0}^m b_i\Lambda_i + \frac{1}{\varepsilon}\sum_{i=0}^m b_i(f_iU - Z_i - Y_i)$, equal to:

$$\varepsilon\Delta_A - a^\top aM - a^\top bN = 0$$

$$\varepsilon\Delta_B - a^\top bM - b^\top bN = 0,$$

with solutions:

$$M = \varepsilon\frac{b^\top b\Delta_A - a^\top b\Delta_B}{a^\top ab^\top b - (b^\top a)^2}, \quad N = \varepsilon\frac{a^\top a\Delta_B - a^\top b\Delta_A}{a^\top ab^\top b - (b^\top a)^2}.$$

We can make an update on a single Y_i, Z_i (with i selected at random in $\{1, \ldots, m\}$) by projected gradient descent, or by "Gauss-Seidel" iterations.

The algorithm is updating M, N, Z_i, Y_i such that M, N is optimal given Z_i, Y_i, and (in parallel):

$$\begin{aligned} Z_i &= \Pi_{\mathbb{H}_d^+}\big(Z_i - \frac{\varepsilon}{2}(\frac{1}{\varepsilon}(Z_i + Y_i + a_iM + b_iN - f_iU) + \Lambda_i)\big) \\ Y_i &= \Pi_{\mathcal{V}^\perp}\big(Y_i - \frac{\varepsilon}{2}(\frac{1}{\varepsilon}(Z_i + Y_i + a_iM + b_iN - f_iU) + \Lambda_i)\big), \end{aligned}$$

or (sequentially):

$$\begin{aligned} Z_i &= \Pi_{\mathbb{H}_d^+}\big(Z_i - \varepsilon(\frac{1}{\varepsilon}(Z_i + Y_i + a_iM + b_iN - f_iU) + \Lambda_i)\big) \\ Y_i &= \Pi_{\mathcal{V}^\perp}\big(Y_i - \varepsilon(\frac{1}{\varepsilon}(Z_i + Y_i + a_iM + b_iN - f_iU) + \Lambda_i)\big), \end{aligned}$$

which in turns requires to update M and N, since $Y_i + Z_i$ is updated. Note that in the sequential update, we need to update M, and N between the two iterations.

In our experiments in Section 8, we perform a fixed number of iterations of randomized coordinate descent, but we could use finer stopping criteria based on primal-dual gaps [56].

Recovering feasible variables M, N, Y_i, Z_i. After each inner loop, and candidate variables M, N, Y_i, Z_i, we need to find feasible ones (at the expense of slightly higher cost). We define $\bar{Y}_i = \Pi_{\mathcal{V}^\perp}(f_i U - a_i M - b_i N - Z_i)$, and subtract αI to both M and N so that all $f_i U - a_i M - b_i N - \bar{Y}_i \succcurlyeq 0$ for all i, with the smallest possible α. This then moves down the objective function by$\alpha(\mathrm{tr}[A] + \mathrm{tr}[B])$.

Running-time complexity per inner iteration. There are $O(md^2)$ parameters, and $O(md^3)$ costs for the eigenvalue decompositions.

B.2 Detailed computations for Section 6

The goal is to solve the pair of primal-dual problems (we could also add an extra constraint on the trace of $\Sigma_q V$, which is always equal to $\int_{\mathcal{X}} dq(x)$ for any $q \in \mathcal{M}_+(\mathcal{X})$):

$$\min_{\Sigma \in \mathcal{V},\ \Delta \in \mathbb{H}_d^+} \mathrm{tr}[\Sigma U] \text{ such that } \Sigma = M + \Delta \quad = \quad \max_{V \in \mathbb{H}_d^+} \mathrm{tr}[VM] \text{ such that } U - V \in \mathcal{V}^\perp,$$

with iterations

$$\begin{aligned}(V, Y) &= \operatorname*{argmax}_{V \in \mathbb{H}_d^+,\ Y \in \mathcal{V}^\perp} \mathrm{tr}[VM] - \frac{1}{2\varepsilon}\|U - V - Y\|_F^2 + \mathrm{tr}[\Sigma(U - V - Y)] \\ \Sigma &= \Sigma - \frac{1}{\varepsilon}(U - V - Y).\end{aligned}$$

This can be initialized at $V = U$. This is closely related to the alternating direction method of multipliers (see, e.g., [57]).

In order to solve the subproblem, we consider the sequential iteration:

$$\begin{aligned}V &\leftarrow \Pi_{\mathbb{H}_d^+}(U - Y - \varepsilon\Sigma) \\ Y &\leftarrow \Pi_{\mathcal{V}^\perp}(U - V - \varepsilon\Sigma),\end{aligned}$$

and we could use acceleration (see, e.g., [58] and references therein).

Note that (a) if we restrict further the space where V is (e.g., diagonal matrix in Section 8, the solution is obtained in closed form by selecting the largest M_{ii}, and considering V with only a non-zero element at position (i, i), and (v) we can get a dual solution by considering $(1 - \alpha)(U - Y) + (1 - \alpha)U$ with the smallest positive α that makes it positive semi-definite.

B.3 Detailed computations for Section 7.1

We need to solve

$$\begin{aligned}
&\inf_{N,\rho,\ Z_0,\dots,Z_m \succcurlyeq 0} \ \rho - \operatorname{tr}[NB] \text{ such that } \forall i \in \{0,\dots,m\},\ f_i U + a_i(\rho U - H) - b_i N - Z_i \in \mathcal{V}^\perp \\
= &\sup_{\Lambda_0,\dots,\Lambda_m \in \widehat{\mathcal{C}}} \sum_{i=0}^m \operatorname{tr}\left[\Lambda_i(a_i H - f_i U)\right] \text{ such that } \sum_{i=0}^m a_i \operatorname{tr}[U\Lambda_i] = 1 \text{ and } \sum_{i=0}^m b_i \Lambda_i = B.
\end{aligned}$$

We consider the augmented Lagrangian method, which solves,

$$\begin{aligned}
\inf_{\rho, N \in \mathbb{H}_d, \forall i,\ Z_i \succcurlyeq 0, Y_i \in \mathcal{V}^\perp} \ \rho - \operatorname{tr}[NB] + \frac{1}{2\varepsilon} \sum_{i=0}^m \left\| f_i U + a_i(\rho U - H) - b_i N - Z_i - Y_i \right\|_F^2 \\
- \sum_{i=0}^m \operatorname{tr}\left[\Lambda_i(f_i U + a_i(\rho U - H) - b_i N - Z_i - Y_i)\right],
\end{aligned}$$

and updates the matrices Λ_i's as:

$$\Lambda_i = \Lambda_i - \frac{1}{\varepsilon}\big(f_i U + a_i(\rho U - H) - b_i N - Z_i - Y_i\big).$$

Solving the sub-problem. We simply need to optimize with respect to ρ and N in closed form. We can expand the cost function as (removing the part not depending on ρ and N):

$$\begin{aligned}
&\rho\Big(1 + \operatorname{tr}\Big[U\Big(-\sum_{i=0}^m a_i\Lambda_i + \frac{a^\top f}{\varepsilon}U - \frac{a^\top a}{\varepsilon}H - \frac{1}{\varepsilon}\sum_{i=0}^m a_i(Z_i + Y_i)\Big)\Big]\Big) \\
&+ \operatorname{tr}\Big[N\Big(-B + \sum_{i=1}^n b_i\Lambda_i - \frac{b^\top f}{\varepsilon}U + \frac{b^\top a}{\varepsilon}H + \frac{1}{\varepsilon}\sum_{i=0}^m b_i(Z_i + Y_i)\Big)\Big] \\
&+ \frac{a^\top a}{2\varepsilon}\rho^2\|U\|_F^2 + \frac{b^\top b}{2\varepsilon}\|N\|_F^2 - \frac{a^\top b}{\varepsilon}\rho \operatorname{tr}[UN].
\end{aligned}$$

This leads to optimality conditions (after zeroing gradients):

$$\begin{aligned}
\frac{a^\top a}{\varepsilon}\rho\|U\|_F^2 - \frac{a^\top b}{\varepsilon}\operatorname{tr}[UN] &= c_\rho = -\Big(1 + \operatorname{tr}\Big[U\Big(-\sum_{i=0}^m a_i\Lambda_i + \frac{a^\top f}{\varepsilon}U - \frac{a^\top a}{\varepsilon}H - \frac{1}{\varepsilon}\sum_{i=0}^m a_i(Z_i + Y_i)\Big)\Big]\Big) \\
-\frac{a^\top b}{\varepsilon}\rho U + \frac{b^\top b}{\varepsilon}N &= C_N = -\Big(-B + \sum_{i=1}^n b_i\Lambda_i - \frac{b^\top f}{\varepsilon}U + \frac{b^\top a}{\varepsilon}H + \frac{1}{\varepsilon}\sum_{i=0}^m b_i(Z_i + Y_i)\Big),
\end{aligned}$$

with solution

$$\begin{aligned}
\rho &= \varepsilon\frac{b^\top b \cdot c_\rho + a^\top b \cdot \operatorname{tr}[C_N U]}{a^\top a \cdot b^\top b - (b^\top a)^2} \\
N &= \varepsilon\frac{C_N}{b^\top b} + \frac{a^\top b}{\varepsilon}\rho U.
\end{aligned}$$

We can then do coordinate descent like in Section B.1.

B.4 Algorithms from Section 7.2

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We can compute the gradient with respect to Σ and A, by first computing the singular value decomposition of $A = \sum_{i=1}^d \lambda_i u_i u_i^*$, and of $f(A) - \sqrt{d}\Sigma = \sum_{i=1}^d \mu_i v_i v_i^*$, and computing $V = \frac{1}{\sum_{i=1}^d e^{\mu_i/\varepsilon}} \sum_{i=1}^d e^{\mu_i/\varepsilon} v_i v_i^*$, which is such that $V \succcurlyeq 0$ and $\mathrm{tr}[V] = 1$. The gradient with respect to A is $H - \frac{1}{\varepsilon}(A - \Pi_{\mathcal{V}}(A)) - \sum_{i=1}^d u_i^\top V u_j u_i u_j^\top \frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j}$, while the gradient with respect to Σ is $\sqrt{d}(-U + V)$. The update is, with step-size γ:

$$\begin{aligned} A &\leftarrow \operatorname*{argmin}_{A^+ \succcurlyeq 0, \mathrm{tr}[A^+U]=1} D(A^+ \| I) - \mathrm{tr}\left[(A^+ - A)\Big(H - \frac{1}{\varepsilon}(A - \Pi_{\mathcal{V}}(A)) - \sum_{i=1}^d u_i^\top V u_j u_i u_j^\top \frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j}\Big)\right] \\ \Sigma &\leftarrow \Sigma + \gamma\sqrt{d} \cdot \Pi_{\mathcal{V}}(V - U). \end{aligned}$$

We can compute the smoothness constant of the problem with respect to the mirror map $\mathrm{tr}[V \log V] + \frac{1}{2}\|\Sigma\|_F^2$ as

$$\max\{1 + \frac{2\alpha_d}{\varepsilon}, \frac{2d}{\varepsilon}\},$$

where $\alpha_d = \sup_{\lambda,\mu \in [0,d]} \frac{(f(\lambda) - f(\mu))^2}{(f'(\lambda) - f'(\mu))(\lambda - \mu)}$, which can be shown to be less than $\alpha_d \leqslant (d+1)\log(d+1)^2$ for the Shannon relative entropy.

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