Quantum relative entropy optimization

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based on joint works with James Saunderson (Monash Univ.),
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Entropy

Classical information theory If $p \geq 0$,

- Entropy $H(p) = -\sum_{i=1}^{n} p_i \log p_i$ (**Concave**).
- Kullback-Leibler divergence (or relative entropy)

$$D(p\|q) = \sum_{i=1}^{n} p_i \log(p_i/q_i)$$

Convex jointly in (p, q).

Matrix logarithm function

- X symmetric matrix with positive eigenvalues (positive definite)

$$X = U \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} U^T \quad \rightarrow \quad \log(X) = U \begin{pmatrix} \log(\lambda_1) & & \\ & \ddots & \\ & & \log(\lambda_n) \end{pmatrix} U^T$$

where U orthogonal.

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- Matrix (von Neumann) entropy of X:

$$H(X) = -\operatorname{Tr}[X \log X] = -\sum_{i=1}^{n} \lambda_i(X) \log(\lambda_i(X))$$

Concave in X. (Spectral function)

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  Concave in X. (Spectral function)

- (Umegaki) quantum relative entropy:

$$\boxed{D(X \| Y) = \operatorname{Tr}[X(\log X - \log Y)]}$$

  Convex in (X, Y) [Lieb-Ruskai, 1973]. Cornerstone result in quantum information. ($D(X\|Y)$ *not* spectral function!)

Applications

- Many problems in quantum information involve the quantum relative entropy function (quantum cryptography, computing quantum channel capacities, quantum many-body systems, ...)

  - Convex:

$$\min_{X,Y} \; D(X\|Y) \quad \text{s.t. } \mathcal{A}(X,Y)=b, \;\; X,Y \succeq 0.$$

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  - Nonconvex:

$$\max_{X,Y} \; D(X\|Y) \text{ s.t. } \mathcal{A}(X,Y) = b, \;\; X, Y \succeq 0.$$

Outline

This talk: algorithmic tools to solve quantum relative entropy optimization problems

1. Review of convexity of $D(X\|Y)$
2. Convex problems: a self-concordant barrier for the quantum relative entropy cone with optimal parameter
3. Nonconvex problems: a method to derive semidefinite relaxations

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Operator relative entropy

- Belavkin-Staszewski operator relative entropy

$$D_{op}(X\|Y) = X^{1/2}\log(X^{1/2}Y^{-1}X^{1/2})X^{1/2}$$

- Jointly operator convex in (X, Y), i.e.,

$$\mathrm{epi}(D_{op}) = \{(X, Y, T) : D_{op}(X\|Y) \preceq T\}$$

is a convex set.

Integral representation of log

$$\log(Y) = \int_0^1 \left(1 - \frac{1}{1+s(Y-1)}\right) \frac{ds}{s}$$

- Consequence:

$$D_{op}(X\|Y) = \int_0^1 \psi_s(X,Y) ds/s$$

where

$$\psi_s(X,Y) = X\left[(1-s)X + sY\right]^{-1} X - X$$

is jointly operator convex, since

$$\psi_s(X,Y) \preceq T \iff \underbrace{\begin{bmatrix} (1-s)X + sY & X \\ X & X+T \end{bmatrix} \succeq 0}_{\text{linear matrix inequality}}.$$

- $\implies$ $D_{op}(X\|Y)$ is convex as an (infinite) sum of convex functions.

Umegaki relative entropy

- Key observation [Pusz-Woronowicz, Ando, Petz, Effros, ...]:

$$D(X\|Y) = \phi(D_{op}(X \otimes I\|I \otimes Y))$$

where $\phi(Z) = \langle \mathrm{vec}(I_n), Z\mathrm{vec}(I_n)\rangle$ is a positive linear map.
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- Interpretation:
  - $X \otimes I \in \mathbb{R}^{n^2 \times n^2}$, seen as a linear operator $\mathcal{R}_X : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$, corresponds to right multiplication by X, i.e., $\mathcal{R}_X(a) = aX$.

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  - Similarly $I \otimes Y \in \mathbb{R}^{n^2 \times n^2}$ corresponds to left multiplication by Y, $\mathcal{L}_Y : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$, $\mathcal{L}_Y(a) = Ya$.

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  - $\mathcal{R}_X, \mathcal{L}_Y$ are self-adjoint (wrt Hilbert-Schmidt inner product), positive, and commute

$$D(X\|Y) = \langle I, D_{op}(\mathcal{R}_X \| \mathcal{L}_Y)(I) \rangle_{HS}.$$

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3. Nonconvex problems: a method to derive semidefinite relaxations

Semidefinite approximations

- In previous work [Fawzi, Saunderson, Parrilo] we derived semidefinite approximations of the quantum relative entropy function:

$$\underline{r}_m(X\|Y) \leq D(X\|Y) \leq \bar{r}_m(X\|Y)$$

  where $\underline{r}_m$ and $\bar{r}_m$ have a semidefinite representation, and converge to $D(X\|Y)$.

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- Goal: optimize over the quantum relative entropy cone without paying the quadratic dependence on n

- $\rightarrow$ Interior-point methods for the quantum relative entropy cone

Interior-point methods

Conic programming over $\mathcal{K}$ (a convex cone)

$$\min\ \langle c, x \rangle \quad \text{s.t.} \quad Ax = b,\ x \in \mathcal{K}.$$

- A *barrier function* for $\mathcal{K}$ is a strictly convex function $F : \mathrm{int}(\mathcal{K}) \to \mathbb{R}$ such that $F(x) \to +\infty$ as $x \to \partial\mathcal{K}$.

- Interior-point methods follow *central path*

$$x^*(t) = \underset{t}{\operatorname{argmin}}\{t\,\langle c, x \rangle + F(x) \ \text{ s.t. } \ Ax = b\}$$

  as $t \to \infty$, via Newton's method.

- Nesterov-Nemirovski: if F is self-concordant (s.c.) with parameter ν, then interior-point method solves conic program in $\approx \sqrt{\nu}\log(1/\epsilon)$ Newton steps (where ϵ is the desired objective function accuracy).

Self-concordant functions

- Self-concordance is a condition that governs the variation of $\nabla^2 F(x)$ wrt the local norm induced by F

$$\|h\|_x = \sqrt{\langle h, \nabla^2 F(x) h \rangle}$$

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- Formally, F is self-concordant if

$$\boxed{|D^3 F(x)[h]| \leq 2\|h\|_x^{3/2} \qquad \forall x \in \mathrm{dom}(F), h \in \mathbb{R}^n}$$

where $D^3 F(x)[h] = \frac{d^3}{dt^3} F(x + th)|_{t=0}$.

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- If F is self-concordant, then λF for $\lambda \geq 1$ is, and so is $x \mapsto F(Ax + b)$.

Self-concordant barriers

- Typical examples of barriers:
  - $\mathcal{K} = \mathbb{R}^n_+$: $F(x) = -\sum_{i=1}^n \log x_i$
  - $\mathcal{K} = \mathbf{S}^n_+$: $F(X) = -\log\det X$

- Goal: construct a s.c. barrier for

$$\mathcal{K}_{qre} = \{(X, Y, t) : D(X\|Y) \leq t\} = \text{epigraph of } D.$$

Main theorem

Theorem (Fawzi, Saunderson)

The function

$$F(X, Y, t) = -\log(t - D(X\|Y)) - \log\det X - \log\det Y$$

is a (logarithmically homogeneous) self-concordant barrier for

$$\mathcal{K}_{qre} = \{(X, Y, t) \in (\mathbf{S}_+^n)^2 \times \mathbb{R} : D(X\|Y) \leq t\}$$

of optimal parameter $2n+1$.

- Logarithmically homogeneous with parameter ν:

$$F(\lambda x) = F(x) - \nu \log \lambda$$

- "Natural" logarithmic barrier, first proposed by [Karimi, Tunçel]

Compatibility condition of Nesterov

- Assume $\psi : \mathrm{dom}(\psi) \to \mathbf{S}^m$ is *matrix convex* so that

$$\mathrm{epi}(\psi) = \{(Z, T) : \psi(Z) \preceq T\}$$

  is a convex set.

- A natural candidate for a self-concordant barrier of $\mathrm{epi}(\psi)$ is

$$(Z, T) \mapsto -\log\det(T - \psi(Z)) + G(Z)$$

  where G is a s.c. barrier of $\mathrm{dom}(\psi)$

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- Nesterov: This is true provided the following *compatibility condition* is true:

$$\boxed{D^3\psi(z)[h] \;\; \preceq \;\; 3\,(D^2G(z)[h])^{1/2}\; D^2\psi(z)[h]} \quad \forall z \in \mathrm{dom}(\psi), h$$

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- Key fact about condition: it is linear in ψ!
  - If ψ_1, ψ_2 compatible with G, then so is $\psi = \psi_1 + \psi_2$
  - Note: it is not in general easy to get a s.c. barrier for $\mathrm{epi}(\psi_1 + \psi_2)$ from s.c. barriers of $\mathrm{epi}(\psi_1)$ and $\mathrm{epi}(\psi_2)$.

Proof

- Recall
$$D(X\|Y) = \int_0^1 \phi(\psi_s(X \otimes I, I \otimes Y))ds/s$$
where ψ_s is a "nice" rational function.

- One can check "by hand" that the integrand
$$(X, Y) \mapsto \psi_s(X \otimes I, I \otimes Y)$$
satisfies the compatibility condition wrt $F(X, Y) = -\log\det X - \log\det Y$

- Thus $D(X\|Y)$ satisfies the compatibility condition too, and this proves that
$$(X, Y, t) \mapsto -\log(t - D(X\|Y)) - \log\det X - \log\det Y$$
is a s.c. barrier for $\mathcal{K}_{qre}$.

General result

- Löwner: any operator convex function $f : (0, \infty) \to \mathbb{R}$ has an integral representation similar to the one for logarithm.

Theorem (Fawzi, Saunderson)

If $f : (0, \infty) \to \mathbb{R}$ is operator convex and $P_f(X, Y) = X^{1/2} f(X^{-1/2} Y X^{-1/2}) X^{1/2}$ is its matrix perspective, then

$$F(X, Y, T) = -\log\det(T - P_f(X, Y)) - \log\det X - \log\det Y$$

is a s.c. barrier for $\mathcal{K}_f = \mathrm{epi}(P_f)$.

- Similar theorem can be proved for the epigraph of

$$(X, Y) \mapsto \phi(P_f(X \otimes I, I \otimes Y))$$

  where ϕ is any positive linear map.
- Allows us to get s.c. barriers for the quantum Rényi entropies

$$\mathrm{tr}[X^\alpha Y^{1-\alpha}], \ \ X^{1/2}(X^{-1/2} Y X^{-1/2})^\alpha X^{1/2}$$

Discussion

- Similar proof technique was used by Faybusovich and Zhou to obtain self-concordant barriers for $X \mapsto \mathrm{tr}(C \log(X))$ (i.e., one of the arguments of $D(X\|Y)$ is fixed).

- Basic path-following method of Nesterov & Nemirovski is too slow in practice. Primal-dual predictor-corrector methods are much faster. Can we use recent techniques used e.g., in MOSEK's exponential cone solver?

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Nonconvex relative entropy optimization

- We consider nonconvex problems, where the goal is to maximize the quantum relative entropy, e.g.,

$$\max_{X \succeq 0, \operatorname{tr} X = 1} D(\mathcal{A}(X) \| \mathcal{B}(X))$$

  where $\mathcal{A}, \mathcal{B}$ are two positive maps (i.e., $\mathcal{A}(X) \succeq 0, \ \forall X \succeq 0$).

- Nonpolynomial problem! Cannot use sum-of-squares/NPA, etc.

- **Goal:** derive semidefinite relaxations for this problem

Main idea

- Since $D(X\|Y)$ is convex and 1-homogeneous, it must have a variational formulation of the form

$$D(X\|Y) = \max_{(M,N)\in\mathcal{C}} \langle X, M\rangle + \langle Y, N\rangle$$

  for some complicated set $\mathcal{C}$

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- We will see such a formula holds and takes the more precise form

$$\boxed{D(X\|Y) = \max_{a} \langle X, P(a)\rangle + \langle Y, Q(a)\rangle}$$

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- Our original problem can thus be written as

$$\max_X D(\mathcal{A}(X)\|\mathcal{B}(X)) = \boxed{\max_{X,a} \mathrm{tr}[XS(a)]}$$

  where $S(a) = \mathcal{A}^*(P(a)) + \mathcal{B}^*(Q(a))$ is a polynomial.

Integral representation

Recall integral representation of $D(X\|Y)$:

$$D(X\|Y) = \int_0^1 \underbrace{\phi(\psi_s(X \otimes I, I \otimes Y))}_{D_s(X\|Y)} ds/s$$

Key fact: each $D_s(X\|Y)$ has a simple variational formulation.

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Proposition

$$D_s(X\|Y) = \sup_{a \in \mathbb{R}^{n\times n}} \langle X, P_s(a)\rangle + \langle Y, Q_s(a)\rangle$$

where

$$\begin{cases} P_s(a) = -(I + a + a^T + (1-s)a^T a) \\ Q_s(a) = -saa^T \end{cases}$$

Proof of variational formula for D_s

$$\psi_s(X, Y) = X((1-s)X + sY)^{-1}X - X$$

Key ingredient:

- Schur complement corresponds to partial minimization of a quadratic form: for any block operator $\left[\begin{smallmatrix} A & B \\ B^T & C \end{smallmatrix}\right] \succ 0$ and any x,

$$\inf_y \left\langle \begin{bmatrix} x \\ y \end{bmatrix}, \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \right\rangle = \left\langle x, (A - BC^{-1}B^T)x \right\rangle.$$

$\implies$ Allows us to write $D_s(X\|Y) = \langle I, \psi_s(\mathcal{R}_X, \mathcal{L}_Y)(I)\rangle_{HS}$ as a supremum.

The variational formula for $D(X\|Y)$

$$\begin{aligned} D(X\|Y) &= \int_0^1 D_s(X\|Y) ds/s \\ &= \int_0^1 \sup_{a \in \mathbb{R}^{n\times n}} \langle X, P_s(a)\rangle + \langle Y, Q_s(a)\rangle \, ds/s \\ &= \sup_{\boldsymbol{a}=\{a(s)\}} \langle X, P(\boldsymbol{a})\rangle + \langle Y, Q(\boldsymbol{a})\rangle \end{aligned}$$

where

$$P(\boldsymbol{a}) = \int_0^1 P_s(a(s)) ds/s, \qquad Q(\boldsymbol{a}) = \int_0^1 Q_s(a(s)) ds/s.$$

This formula appeared in the works of [Kosaki, 1986] and [Donald, 1986]

Problem: infinite number of variables!

Discretizing the integral

$$\log(y) = \int_0^1 \underbrace{\frac{1}{s}\left(1 - \frac{1}{1+s(y-1)}\right)}_{f(s;y)} ds$$

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- Gaussian quadrature: choose $s_1, \ldots, s_m$ and weights $w_1, \ldots, w_m > 0$ such that
$$\int_0^1 p(s)ds = \sum_{i=1}^{m} w_i p(s_i) \;\; \forall \deg(p) \leq 2m - 1.$$
Resulting rational approximation $r_m(y)$ is the diagonal (m, m) Padé approximation of the log.

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- Gauss-Radau quadrature with one node fixed at $s = 1$:
$$\int_0^1 p(s)ds = \sum_{i=1}^{m-1} w_i p(s_i) + w_m p(1) \qquad \forall \deg(p) \leq 2m-2.$$
Resulting rational function $r_m(y)$ is a lower bound on $\log(y)$.

Putting things together

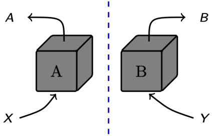
$$D(X\|Y) \le D^{(m)}(X\|Y) := \sup_{\boldsymbol{a}=(a_1,\ldots,a_m)} \left\langle X, P^{(m)}(\boldsymbol{a}) \right\rangle + \left\langle Y, Q^{(m)}(\boldsymbol{a}) \right\rangle$$

where

$$\begin{cases} P^{(m)}(\boldsymbol{a}) = \sum_{i=1}^{m} w_i P_{s_i}(a_i) \\ Q^{(m)}(\boldsymbol{a}) = \sum_{i=1}^{m} w_i Q_{s_i}(a_i). \end{cases}$$

Right-hand side converges to $D(X\|Y)$ as $m \to \infty$.

Quantum random number generators



- Goal: generate shared randomness between two parties
- Amount of randomness generated, secure against adversary:

$$\begin{array}{ll} \inf\limits_{M,N,\rho} & H(A|E)_\rho \\ \text{s.t.} & \text{observed statistics (nc polynomial constraints).} \end{array}$$

where $H(A|E)$ is the conditional entropy.

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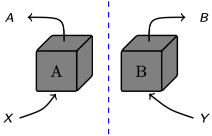

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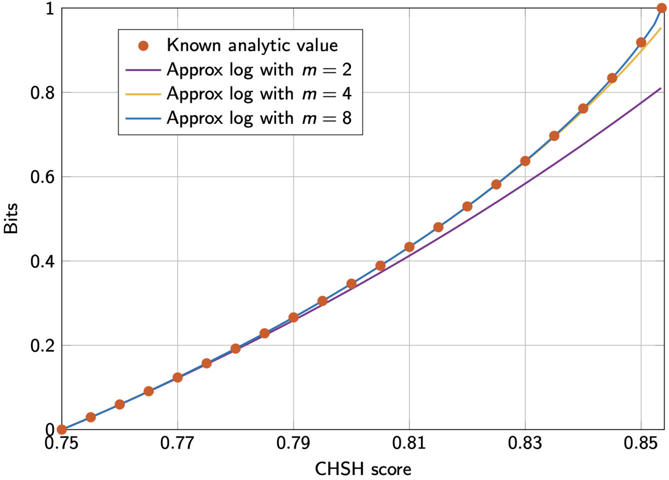
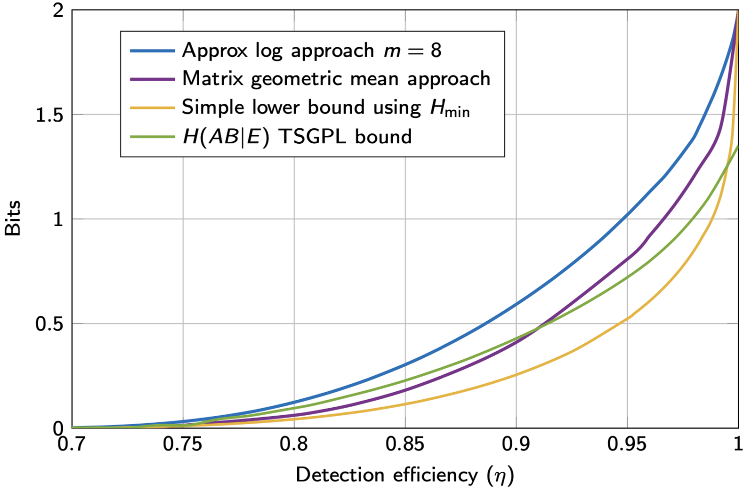
- **Approach:** Replace $H(A|E)$ by $H_{(m)}(A|E) \leq H(A|E)$ which has a variational expression with a polynomial objective
- Lower bound on rate of the protocol:

$$\begin{array}{ll} \inf\limits_{\substack{M,N,\rho \\ a_1,\dots,a_m}} & \mathrm{tr}[\rho S(M,N,a_1,\dots,a_m)] \\ \text{s.t.} & \text{nc polynomial constraints.} \end{array}$$

- Can apply NPA hierarchy to this problem. Method we obtain is computationally faster and more accurate than previous methods



[P. Brown, H. Fawzi and O. Fawzi, Device-independent lower bounds on the conditional von Neumann entropy, arXiv:2106.13692]



[P. Brown, H. Fawzi and O. Fawzi, Device-independent lower bounds on the conditional von Neumann entropy, arXiv:2106.13692]

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- Practical interior-point methods for quantum relative entropy cone
- Other applications of nonconvex quantum relative entropy optimization: squashed entanglement, ...

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Thank you!

`arXiv:2106.13692` (joint with P. Brown and O. Fawzi)

`arXiv:2205.04581` (joint with J. Saunderson)