Quantum relative entropy optimization

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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)

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

where $U$ orthogonal.
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where $U$ orthogonal.

- Matrix (von Neumann) entropy of $X$:

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

**Concave** in $X$. (Spectral function)
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**Concave** in $X$. (Spectral function)

- (Umegaki) quantum relative entropy:

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

**Convex** in $(X, Y)$ [Lieb-Ruskai, 1973]. Cornerstone result in quantum information. ($D(X\|Y)$ *not* spectral function!)
Many problems in quantum information involve the quantum relative entropy function (quantum cryptography, computing quantum channel capacities, quantum many-body systems, ...)

Convex:

$$\min_{X,Y} \quad D(X\|Y) \quad \text{s.t.} \quad \mathcal{A}(X, Y) = b, \quad X, Y \succeq 0.$$
Many problems in quantum information involve the quantum relative entropy function (quantum cryptography, computing quantum channel capacities, quantum many-body systems, ...)

- Convex:
  \[
  \min_{X,Y} D(X\|Y) \quad \text{s.t. } A(X, Y) = b, \; X, Y \succeq 0.
  \]

- Nonconvex:
  \[
  \max_{X,Y} D(X\|Y) \quad \text{s.t. } A(X, Y) = b, \; X, Y \succeq 0.
  \]
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.,

\[ \text{epi}(D_{op}) = \{(X, Y, T) : D_{op}(X\|Y) \preceq T\} \]

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

\[
\psi_s(X, Y) \preceq T \iff \begin{bmatrix} (1 - s)X + sY & X \\ X & X + T \end{bmatrix} \preceq 0.
\]

- \( \implies D_{op}(X \| Y) \) 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 \( \phi(Z) = \langle \text{vec}(I_n), Z \text{vec}(I_n) \rangle \) is a positive linear map.

\[ \implies D(X \| Y) \text{ is convex} \]
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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., \( \mathcal{R}_X(a) = aX \).
Umegaki relative entropy

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

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  - Similarly \( I \otimes Y \in \mathbb{R}^{n^2 \times n^2} \) corresponds to left multiplication by \( Y \), \( \mathcal{L}_Y : \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n} \), \( \mathcal{L}_Y(a) = Ya \).
Key observation [Pusz-Woronowicz, Ando, Petz, Effros, ...]:

\[ D(X\|Y) = \phi(D_{\text{op}}(X \otimes I \| I \otimes Y)) \]

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Interpretation:

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

\[ D(X\|Y) = \langle I, D_{\text{op}}(\mathcal{R}_X \| \mathcal{L}_Y)(I) \rangle_{HS} \]
1. Review of convexity of $D(X \parallel Y)$

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

\[ r_m(X \parallel Y) \leq D(X \parallel Y) \leq \bar{r}_m(X \parallel Y) \]

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

Drawback: size of the semidefinite representation is \( \approx mn^2 \) (\( X, Y \in S^n \)).
Semidefinite approximations

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

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

\[ \rightarrow \text{Interior-point methods for the quantum relative entropy cone} \]
Interior-point methods

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

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

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

- Interior-point methods follow central path

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

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

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

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

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

- Formally, $F$ is self-concordant if

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

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


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

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

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

- Goal: construct a s.c. barrier for

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

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

of optimal parameter \(2n + 1\).

- Logarithmically homogeneous with parameter \(\nu\):
  \[ F(\lambda x) = F(x) - \nu \log \lambda \]

- “Natural” logarithmic barrier, first proposed by [Karimi, Tunçel]
Compatibility condition of Nesterov

- Assume $\psi : \text{dom}(\psi) \to S^m$ is matrix convex so that
  \[
  \text{epi}(\psi) = \{(Z, T) : \psi(Z) \preceq T\}
  \]
is a convex set.

- A natural candidate for a self-concordant barrier of $\text{epi}(\psi)$ is
  \[
  (Z, T) \mapsto -\log \det(T - \psi(Z)) + G(Z)
  \]
  where $G$ is a s.c. barrier of $\text{dom}(\psi)$.
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where $G$ is a s.c. barrier of $\text{dom}(\psi)$
- Nesterov: This is true provided the following compatibility condition is true:
  \[ D^3\psi(z)[h] \preceq 3 (D^2 G(z)[h])^{1/2} D^2\psi(z)[h] \quad \forall z \in \text{dom}(\psi), h \]
Compatibility condition of Nesterov

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

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- Key fact about condition: it is \textit{linear} in $\psi$!
  - If $\psi_1, \psi_2$ 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 $\text{epi}(\psi_1 + \psi_2)$ from s.c. barriers of $\text{epi}(\psi_1)$ and $\text{epi}(\psi_2)$. 
Proof

- Recall
  \[
  D(X\|Y) = \int_0^1 \phi(\psi_s(X \otimes I, I \otimes Y)) \, ds / s
  \]
  where \(\psi_s\) 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 \( \mathcal{K}_f = \text{epi}(P_f) \).

- Similar theorem can be proved for the epigraph of

\[
(X, Y) \mapsto \phi(P_f(X \otimes I, I \otimes Y))
\]

where \( \phi \) is any positive linear map.

- Allows us to get s.c. barriers for the quantum Rényi entropies

\[
\text{tr}[X^\alpha Y^{1-\alpha}], \quad X^{1/2}(X^{-1/2} Y X^{-1/2})^\alpha X^{1/2}
\]
Similar proof technique was used by Faybusovich and Zhou to obtain self-concordant barriers for $X \mapsto \text{tr}(C \log(X))$ (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.,

\[
\max_{X \succeq 0, \tr X = 1} D(A(X) \parallel B(X))
\]

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

- 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

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

for some complicated set $C$
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- We will see such a formula holds and takes the more precise form

$$D(X\|Y) = \max_a \langle X, P(a) \rangle + \langle Y, Q(a) \rangle$$

where $P, Q$ are quadratic polynomials
Main idea

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

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- Our original problem can thus be written as

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

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

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

$$D(X \parallel Y) = \int_0^1 \phi(\psi_s(X \otimes I, I \otimes Y)) \frac{ds}{s}$$

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

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

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

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

Proposition

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

where

$$
\begin{aligned}
P_s(a) &= -(I + a + a^T + (1 - s)a^T a) \\
Q_s(a) &= -sa a^T
\end{aligned}
$$
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 $\begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \succ 0$ 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 $D(X\|Y)$

$$D(X\|Y) = \int_0^1 D_s(X\|Y)ds/s$$

$$= \int_0^1 \sup_{a \in \mathbb{R}^{n \times n}} \langle X, P_s(a) \rangle + \langle Y, Q_s(a) \rangle \ ds/s$$

$$= \sup_{a=\{a(s)\}} \langle X, P(a) \rangle + \langle Y, Q(a) \rangle$$

where

$$P(a) = \int_0^1 P_s(a(s))ds/s, \quad Q(a) = \int_0^1 Q_s(a(s))ds/s.$$ 

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

Problem: infinite number of variables!
Discretizing the integral

\[ \log(y) = \int_0^1 \frac{1}{s} \left( 1 - \frac{1}{1 + s(y - 1)} \right) ds \]

Gaussian quadrature: choose \( s_1, \ldots, s_m \) and weights \( w_1, \ldots, w_m > 0 \) such that

\[ \int_0^1 p(s) \, ds = \sum_{i=1}^m w_i p(s_i) \quad \forall \deg(p) \leq 2m - 1. \]

Resulting rational approximation \( r_m(y) \) is the diagonal \((m, m)\) Padé approximation of \( \log \).

Gauss-Radau quadrature with one node fixed at \( s = 1 \):

\[ \int_0^1 p(s) \, ds = \sum_{i=1}^{m-1} w_i p(s_i) + w_m p(1) \quad \forall \deg(p) \leq 2m - 2. \]

Resulting rational function \( r_m(y) \) is a lower bound on \( \log(y) \).
Discretizing the integral

\[
\log(y) = \int_0^1 \frac{1}{s} \left( 1 - \frac{1}{1 + s(y - 1)} \right) ds \approx \sum_{i=1}^m w_i f(s_i; y) = r_m(y)
\]
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Resulting rational approximation \(r_m(y)\) is the diagonal \((m, m)\) Padé approximation of the log.
Discretizing the integral

\[
\log(y) = \int_{0}^{1} \frac{1}{s} \left(1 - \frac{1}{1 + s(y - 1)}\right) ds \approx \sum_{i=1}^{m} w_i f(s_i; y) = r_m(y)
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  \]

  Resulting rational function \(r_m(y)\) is a lower bound on \(\log(y)\).
Putting things together

\[ D(X \parallel Y) \leq D^{(m)}(X \parallel Y) := \sup_{a=(a_1, \ldots, a_m)} \left( \langle X, P^{(m)}(a) \rangle + \langle Y, Q^{(m)}(a) \rangle \right) \]

where

\[
\begin{align*}
P^{(m)}(a) &= \sum_{i=1}^{m} w_i P_{s_i}(a_i) \\
Q^{(m)}(a) &= \sum_{i=1}^{m} w_i Q_{s_i}(a_i).
\end{align*}
\]

Right-hand side converges to \( D(X \parallel Y) \) as \( m \to \infty \).
Quantum random number generators

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

$$\inf_{M,N,\rho} H(A|E)_\rho$$

s.t. observed statistics (nc polynomial constraints).

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

- **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**:

\[
\inf_{M,N,\rho} \text{tr}[\rho S(M, N, a_1, \ldots, a_m)]
\]

s.t. nc polynomial constraints.

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

- 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)