On Implementation of Long-Step Path-Following Algorithms for Convex Optimization Problems in Quantum Information Theory

Leonid Faybusovich*1 and Cunlu Zhou†2

1,2Department of Mathematics, University of Notre Dame, IN

Abstract

We consider computational aspects of the long-step path-following algorithm developed in our previous work. We show that a broad class of complicated optimization problems arising in quantum information theory can be solved using this approach. As a very difficult example, we consider one important optimization problem in quantum key distribution (QKD) and show that our method allows one to solve problems of this type much faster in comparison with (very few) available options.

Keywords: long-step path-following algorithm, self-concordant functions, matrix monotone functions, quantum information theory, quantum key distribution

1 Introduction

In [7] we developed a long-step path-following algorithm to deal with a broad class of symmetric programming problems with nonlinear objective functions. In our recent work [6] we noticed that this class includes a number of (difficult) convex optimization problems arising in quantum information theory. The main goal of this paper is to present some computational details of our long-step path-following algorithm essential for solving optimization problems of this type. Unlike [6, 7], we completely avoid using the language of Euclidean Jordan algebras and concentrate on examples with semidefinite constraints [12]. By doing this, we hope our results will reach a broader research community.

The plan of the paper is as follows. In section 2 we describe the major features of our algorithm in a broad setting. We then discuss in detail the structure of the algorithm for two concrete cases involving semidefinite constraints. In particular, the calculation of Newton

*lfaybuso@nd.edu
†czhou3@nd.edu
directions are discussed. In section 4 we consider a class of objective functions constructed with the help of matrix monotone functions. The structure of arising Hessians is described in detail. Several important practical aspects of implementation are discussed. The vectorization procedure which is crucial for performance and scalability of the algorithm is described. It is shown that several classes of optimization problems arising in quantum information theory (quantum entanglement problem, problems involving so-called fidelity objective function and relative Rényi entropy objective function) fit into this class. In section 4 we describe an important (and very difficult) optimization problem in quantum key distribution (QKD) [2, 11]. The objective function here involves the quantum relative entropy function. The proposed approach is somewhat heuristic in nature but obtained numerical results are quite stunning. For example, we compared our numerical results to one of the most competitive existing methods for quantum relative entropy optimization [4, 5]. For most of the test examples the other method simply cannot solve the problem, and for one of the cases it solved, our method is 20000 times faster! We conclude the paper by discussing some conjectures regarding possible generalization of our approach.

2 Long-Step Path-Following Algorithm

Let $(\mathbb{E}, \langle , \rangle)$ be a Euclidean real vector space with scalar product $\langle , \rangle$. Let $a + \mathcal{X}$ be an affine space of $\mathbb{E}$, $\Omega \subseteq \mathbb{E}$ be an open convex set and $\overline{\Omega}$ be its closure. Let $B(x)$ be a self-concordant barrier on $\Omega$ with barrier parameter $r$. For a discussion of self-concordant barriers, see [9, section 5.3].

Recall that the gradient $\nabla f(x) \in \mathbb{E}$ and Hessian $H_f(x) : \mathbb{E} \rightarrow \mathbb{E}$ are defined as follows:

$$
\begin{align*}
D f(x)(\xi) &= \langle \nabla f(x), \xi \rangle, \ x \in \Omega, \ \xi \in \mathbb{E}, \\
D^2 f(x)(\xi, \eta) &= \langle H_f(x)\xi, \eta \rangle, \ x \in \Omega, \ \xi, \eta \in \mathbb{E},
\end{align*}
$$

(1)

where $D^k f(x)$ is the $k$-th Fréchet derivative of $f$ at $x$.

Denote by $C^k(\Omega)$ the vector space of $k$ times continuously differentiable real-valued functions on $\Omega$.

**Definition 2.1.** Let $F : \Omega \rightarrow \mathbb{R}$, $F \in C^3(\Omega)$, be a convex function on $\Omega$. We say that $F$ is $\kappa$-self-concordant, if $\exists \kappa \geq 0$ such that

$$
|D^3 F(x)(\xi, \xi, \xi)| \leq 2\kappa \left[ D^2 F(x)(\xi, \xi) \right]^\frac{3}{2}, \ x \in \Omega, \ \xi \in \mathbb{E}.
$$

(2)

We assume that

$$
F(x) \rightarrow +\infty, \ x \rightarrow \partial \Omega.
$$

(3)

We also assume that the Hessian $H_F(x)$ is a positive definite symmetric linear operator on $\mathbb{E}$ for all $x \in \Omega$. Given $\xi \in \mathbb{E}$, $x \in \Omega$, we define norm

$$
\|\xi\|_x = \langle H_F(x)\xi, \xi \rangle^\frac{1}{2} = [D^2 F(x)(\xi, \xi)]^\frac{1}{2}.
$$

(4)
Under assumptions of definition 2.1 and (3), at any point $x \in \Omega$, there exists a so-called Dikin ellipsoid inside $\Omega$ [9, theorem 5.1.5]:

$$W_r(x) = \{y \in \Omega : \|y - x\|_x \leq r\} \subset \Omega, \ \forall r < \frac{1}{\kappa}. \quad (5)$$

Now consider the following conic programming problem:

$$f(x) \to \min, \quad x \in \overline{\Omega} \cap (a + \mathcal{X}), \quad (6)$$

where $f \in C^3(\Omega)$, $f$ is continuous on $\overline{\Omega}$ and convex. The feasible set is bounded and has a nonempty (relative) interior.

**Definition 2.2.** $f$ is said to be $\nu$-compatible with $B(x)$ if $\exists \nu \geq 1$ such that

$$|D^3 f(x)(\xi, \xi, \xi)| \leq 2\nu D^2 f(x)(\xi, \xi)|D^2 B(x)(\xi, \xi)|^{\frac{1}{2}}, \ \forall \xi \in \mathbb{E}. \quad (7)$$

Subsequent results are proved in [7] for the case where $\Omega$ is the cone of squares of a Euclidean Jordan algebra and $B(x) = -\ln \det(x), \ x \in \Omega$. However, for understanding of this paper, no knowledge of Jordan algebras is necessary. We will formulate two special cases in section 2.2 and show concrete calculations of the so-called Newton direction and Newton decrement.

**Proposition 2.3.** Let $f$ be $\nu$-compatible with $B(x)$. Then

$$F_{\beta}(x) = \beta f(x) + B(x), \ x \in \overline{\Omega}, \ \beta \geq 0, \quad (8)$$

is $\kappa$-self-concordant, where $\kappa = 1 + \frac{2}{3}\nu$.

This is easy to show and we omit the proof here.

Next we introduce the Newton direction $p_{\beta}(x)$ of $F_{\beta}$ at $x \in (a + \mathcal{X}) \cap \Omega$:

$$H_{F_{\beta}}(x)p_{\beta}(x) = -(\nabla F_{\beta}(x) + \mu_{\beta}(x)), \quad \mu_{\beta}(x) \in \mathcal{X}^\perp, \ p_{\beta}(x) \in \mathcal{X}, \quad (9)$$

and the Newton decrement of $F_{\beta}$ at $x$:

$$\delta_{\beta}(x) \triangleq \langle p_{\beta}(x), H_{F_{\beta}}(x)p_{\beta}(x) \rangle^{\frac{1}{2}}, \ x \in (a + \mathcal{X}) \cap \Omega. \quad (10)$$

Note that

$$\delta_{\beta}(x)^2 = -\langle \nabla F_{\beta}(x), p_{\beta}(x) \rangle. \quad (11)$$

Under the assumption of proposition 2.3, we have the following results.
Proposition 2.4. Given \( x \in (a + \mathcal{X}) \cap \Omega \), let \( \delta_\beta(x) \leq \frac{1}{3\kappa} \). Then

\[
F_\beta(x) - F_\beta(x(\beta)) \leq \frac{\delta_\beta(x)^2}{1 - \left[\frac{\kappa \delta_\beta(x)}{4}\right]^2}.
\] (12)

Proposition 2.5. Given \( x \in (a + \mathcal{X}) \cap \Omega \) and \( \delta_\beta(x) \leq \frac{1}{3\kappa} \), we have

\[
|f(x) - f(x(\beta))| \leq \left[\frac{\delta_\beta(x)}{1 - \frac{\kappa}{4} \delta_\beta(x)} \cdot \frac{1 + \kappa \delta_\beta(x)^2}{1 - \kappa \delta_\beta(x)}\right]^\frac{1}{2} \sqrt{r},
\] (13)

where \( r \) is the barrier parameter of \( B(x) \).

Algorithm 1: A Long-Step Path-Following Algorithm

1. Set \( \beta_0 > 0 \), and \( \theta > 0 \). Choose an accuracy \( \epsilon > 0 \) and initial point \( x_0 \in (a + \mathcal{X}) \cap \Omega \) such that

\[
\delta_{\beta_0}(x_0) \leq \frac{1}{3\kappa}.
\]

2. At \( i \)-th (outer) iteration \( (i \geq 0) \), set

\[
\beta_{i+1} = (1 + \theta)^i \beta_0.
\]

Find \( x_{i+1} \in (a + \mathcal{X}) \cap \Omega \) such that \( \delta_{\beta_{i+1}}(x_{i+1}) \leq \frac{4r}{\kappa} \) by performing several Newton steps (inner iteration) for the function \( F_{\beta_{i+1}} \), using \( x_i \) as the starting point:

\[
x_i = x_i + \alpha p_{\beta_{i+1}}(x_i).
\]

3. Stop the process if

\[
\beta_i \geq \frac{4r}{\epsilon}.
\]

Remark 2.6. Note that in the second step, \( \alpha \) is obtained by performing a line search for each inner iteration, where \( 0 < \alpha < \alpha_{\text{max}} \) and \( \alpha_{\text{max}} \) is the largest positive number such that

\[
x_i + \alpha p_{\beta_{i+1}}(x_i) > 0,
\]

i.e., the new point stays feasible.

2.1 Complexity Estimates

Theorem 2.7. Given \( \epsilon > 0 \) and

\[
i \geq \frac{\ln(\frac{4r}{\kappa \epsilon})}{\ln(1 + \theta)}.
\] (14)

Then

\[
f(x_i) - f(x^*) \leq \epsilon,
\]
where $x^*$ is an optimal solution to the problem (6).

**Theorem 2.8.** Each outer iteration requires at most

$$
\frac{22}{3} + 22\theta \left( \frac{5}{2} \kappa \sqrt{r} + \frac{\theta \kappa^2 r}{\theta + 1} \right)
$$

inner iterations.

Taking into account theorems 2.7 and 2.8, we get the following complexity result for our algorithm.

**Theorem 2.9.** An upper bound for the total number of Newton iterations is given by

$$
\frac{\ln \left( \frac{\kappa}{\kappa_0} \right)}{\ln(1 + \theta)} \left( \frac{22}{3} + 22\theta \left( \frac{5}{2} \kappa \sqrt{r} + \frac{\theta \kappa^2 r}{\theta + 1} \right) \right).
$$

**Remark 2.10.** Theorems 2.7 to 2.9 are proved in [7] under assumptions that $\Omega$ is a cone of squares in Euclidean Jordan algebras and $B(x) = -\ln \det(x)$.

### 2.2 Two Special Cases

We consider two special cases of the conic programming problem (6). Without loss of generality, let $\mathbb{E} = \mathbb{S}^n$, the real vector space of $n \times n$ symmetric matrices. We denote by $\mathbb{S}^n_+$ and $\mathbb{S}^n_{++}$ the convex cone of positive semidefinite matrices and positive definite matrices respectively. Let $\mathbb{R}^N_+$ denote the nonnegative orthant of $\mathbb{R}^N$.

We use $A \succeq 0$ for positive semidefiniteness (i.e., $x^T Ax \geq 0, \forall x \in \mathbb{R}^n$) and $A \succ 0$ for positive definiteness (i.e., $x^T Ax > 0, \forall x \in \mathbb{R}^n \setminus \{0\}$). Furthermore, we use notations

$$
A \succeq B \text{ if } A - B \succeq 0,
$$

and

$$
A \succ B \text{ if } A - B \succ 0.
$$

The scalar product $\langle A, B \rangle$, $A, B \in \mathbb{S}^n$, is defined as

$$
\langle A, B \rangle = \text{Tr}(AB) = \sum_{i,j} A_{ij} B_{ij}.
$$

Recall the following facts about $B(X) = -\ln \det(X)$, $X \in \mathbb{S}^n_{++}$ (see e.g. [12]):

$$
\nabla B(X) = -X^{-1}, \quad (15)
$$

$$
H_B(X) = P(X^{-1}), \quad (16)
$$

where

$$
P(X^{-1})Y = X^{-1} Y X^{-1}, \forall Y \in \mathbb{S}^n. \quad (17)
$$
I. We consider the following optimization problem:

\[ f(X) \rightarrow \min, \]
\[ \langle A_i, X \rangle \leq b_i, \ i = 1, \ldots, m, \]
\[ \langle A_i, X \rangle = b_i, \ i = m + 1, \ldots, N, \]
\[ X \succeq 0. \] \hfill (18)

Note that we can rewrite (18) in the following form:

\[ f(X) \rightarrow \min, \]
\[ \langle A_i, X \rangle + x_i = b_i, \ i = 1, \ldots, N, \]
\[ x_i \geq 0, \ i = 1, \ldots, m, \]
\[ x_i = 0, \ i = m + 1, \ldots, N, \]
\[ X \succeq 0. \] \hfill (19)

Notice that the closed convex cone \( \Omega \) in (6) is \( \mathbb{S}_+^n \times \mathbb{R}^N \) in this case.

Recall definition 2.2 and proposition 2.3. The \( \nu \)-compatibility (\( \nu \geq 1 \)) condition for \( f(x) \) in (19) and the corresponding auxiliary barrier family of optimization problems are given as follows:

\[ |D^3 f(X)(\xi, \xi, \xi)| \leq 2\nu D^2 f(X)(\xi, \xi)[D^2 B(X)(\xi, \xi)]^{\frac{1}{2}}, \ \forall \xi \in \mathbb{S}^n, \] \hfill (20)

and

\[ F_\beta(X; x) = \beta f(X) - \ln \det(X) - \sum_{i=1}^m \ln(x_i) \rightarrow \min, \]
\[ \langle A_i, X \rangle + x_i = b_i, \ i = 1, \ldots, N, \]
\[ x_i > 0, \ i = 1, \ldots, m, \]
\[ x_i = 0, \ i = m + 1, \ldots, N, \]
\[ X \succ 0. \] \hfill (21)

Next we show calculations of the Newton direction and Newton decrement. We first can rewrite the constraints into the following compact form:

\[ \left\langle \begin{bmatrix} A_i \\ e_i \end{bmatrix}, \begin{bmatrix} X \\ x \end{bmatrix} \right\rangle = \langle A_i, X \rangle + \langle e_i, x \rangle = b_i, \ i = 1, \ldots, N, \]

where \( e_i = [0, \ldots, 1, \ldots, 0]^T \) (with 1 at the \( i \)-th position) and for vectors of length \( N \) we use the standard Euclidean scalar product \( \langle , \rangle \) on \( \mathbb{R}^N \).

We have the gradient

\[ \nabla F_\beta(X; x) = \begin{bmatrix} \nabla F^{(1)}_\beta(X; x) \\ \nabla F^{(2)}_\beta(X; x) \end{bmatrix}, \] \hfill (22)
where
\[
\nabla F^{(1)}_\beta (X; x) = \beta \nabla f(X) - X^{-1},
\]
and
\[
\nabla F^{(2)}_\beta (X; x) = \left[ \frac{1}{x_1}, \ldots, \frac{1}{x_m}, 0, \ldots, 0 \right]^T.
\]
We have the Hessian
\[
H_{F_\beta} (X; x) = \begin{bmatrix}
H^{(1)}_{F_\beta} (X; x) & 0 \\
0 & H^{(2)}_{F_\beta} (X; x)
\end{bmatrix},
\]
where
\[
H^{(1)}_{F_\beta} (X; x) = \beta H_f(X) + P(X^{-1}),
\]
and
\[
H^{(2)}_{F_\beta} (X; x) = \text{diag} \left( \left[ \frac{1}{x_1^2}, \ldots, \frac{1}{x_m^2}, 0, \ldots, 0 \right] \right).
\]
From (9), we have the Newton direction \( p_\beta (X; x) \):
\[
H_{F_\beta} (X; x)p_\beta (X; x) = -\nabla F_\beta (X; x) + \sum_{j=1}^{N} \lambda_j \begin{bmatrix} A_j \\ e_j \end{bmatrix},
\]
where
\[
p_\beta (X; x) = \begin{bmatrix}
p^{(1)}_\beta (X; x) \\
p^{(2)}_\beta (X; x)
\end{bmatrix},
\]
and
\[
\left\langle \begin{bmatrix} A_j \\ e_j \end{bmatrix}, \begin{bmatrix} p^{(1)}_\beta (X; x) \\ p^{(2)}_\beta (X; x) \end{bmatrix} \right\rangle = 0.
\]
Using (22), (23), (24) and (25), we can assemble the following linear system of equations:
\[
\sum_{j=1}^{N} \lambda_j \left\langle A_i, H^{(1)}_{F_\beta} (X; x)^{-1} A_j \right\rangle + \lambda_i x_i^2
\]
\[
= \left\langle A_i, H^{(1)}_{F_\beta} (X; x)^{-1} \nabla F^{(1)}_\beta (X; x) \right\rangle - x_i, i = 1, \ldots, N.
\]
Solve for \( \lambda_j, j = 1, \ldots, N \) in (26), and then from (24) we obtain
\[
p^{(1)}_\beta (X; x) = H^{(1)}_{F_\beta} (X; x)^{-1} \left[ -\nabla F^{(1)}_\beta (X; x) + \sum_{j=1}^{N} \lambda_j A_j \right],
\]
and
\[
p_{\beta}^{(2)}(X; x) = H_{F_{\beta}}^{(2)}(X; x)^{-1} \begin{bmatrix} -\nabla F_{\beta}^{(2)}(X; x) + \sum_{j=1}^{N} \lambda_j e_j \\
\end{bmatrix}
\]
\[
= \begin{bmatrix}
x_1 + \lambda_1 x_1^2 \\
\vdots \\
x_m + \lambda_m x_m^2 \\
0 \\
\vdots \\
0
\end{bmatrix}.
\]

With (27), (28) and by (11), we have the Newton decrement
\[
\delta_{\beta}(X; x) = \sqrt{-\langle p_{\beta}(X; x), \nabla F_{\beta}(X; x) \rangle}
\]
\[
= \sqrt{-\left[\langle p_{\beta}^{(1)}(X; x), \nabla F_{\beta}^{(1)}(X; x) \rangle + \langle p_{\beta}^{(2)}(X; x), \nabla F_{\beta}^{(2)}(X; x) \rangle \right]}.
\]

II. We consider optimization problems of the following form:
\[
f(X) + g(Y) \to \min,
\]
\[
\langle A_i, X \rangle = b_i, i = 1, \ldots, m,
\]
\[
Y = L(X),
\]
\[
X \succeq 0,
\]
\[
Y \succeq 0.
\]

where \( L : S^n_+ \to S^k_+ \) is some linear operator. Note that \( \Omega = S^n \times S^k \) in this case.

The \( \nu \)-compatibility (\( \nu \geq 1 \)) condition for (30) and the corresponding auxiliary barrier family of optimization problems are given as follows:
\[
|D^3 f(X)(\xi, \xi, \xi) + D^3 g(Y)(h, h, h)| \leq 2\nu \left[|D^2 f(X)(\xi, \xi) + D^2 g(Y)(h, h)| \right]^\frac{1}{2},
\]
\[
\forall \xi \in S^n,
\]
(31)

where \( B_1(X) = -\ln \det(X) \) and \( B_2(Y) = -\ln \det(Y) \), and
\[
F_{\beta}(X) = \beta(f(X) + g(Y)) - \ln \det(X) - \ln \det(Y) \to \min,
\]
\[
\langle A_i, X \rangle = b_i, i = 1, \ldots, m,
\]
\[
Y = L(X),
\]
\[
X \succ 0,
\]
\[
Y \succ 0.
\]
(32)
Equivalently, we can rewrite (32) as follows

\[ F_{\beta}(X) = \beta(f(X) + g(\mathcal{L}(X))) - \ln \det(X) - \ln \det(\mathcal{L}(X)) \rightarrow \min, \]

\[ \langle A_i, X \rangle = b_i, \ i = 1, \ldots, m, \]

\[ X \succ 0, \]

\[ \mathcal{L}(X) \succ 0. \]  \hfill (33)

Next we show calculations of the Newton direction \( p_{\beta}(X) \) and Newton decrement \( \delta_{\beta}(X) \). By (9), we have

\[ H_{F_{\beta}}(X)p_{\beta}(X) = -\nabla F_{\beta}(X) + \sum_{j=1}^{m} \lambda_j A_j, \]  \hfill (34)

\[ \langle A_i, p_{\beta}(X) \rangle = 0, \]  \hfill (35)

from which we can assemble the following linear system of equations:

\[ \sum_{j=1}^{m} \lambda_j \langle A_i, H_{F_{\beta}}(X)^{-1}A_j \rangle = H_{F_{\beta}}(X)^{-1}\nabla F_{\beta}(X), \ i = 1, \ldots, m. \]  \hfill (36)

Solve for \( \lambda_j, j = 1, \ldots, m \), and we obtain the Newton direction

\[ p_{\beta}(X) = H_{F_{\beta}}(X)^{-1} \left( -\nabla F_{\beta}(X) + \sum_{j=1}^{m} \lambda_j A_j \right), \]  \hfill (37)

and the Newton decrement

\[ \delta_{\beta}(X) = \sqrt{ -\langle \nabla F_{\beta}(X), p_{\beta}(X) \rangle }. \]  \hfill (38)

For calculations of \( \nabla F_{\beta}(X) \) and \( H_{F_{\beta}}(X) \), note that \( h(X) = g(\mathcal{L}(X)) \) and \( \zeta(X) = B(\mathcal{L}(X)) = -\ln \det(\mathcal{L}(X)) \) need some special care. We have (by chain rule)

\[ Dh(X)(\xi) = Dg(\mathcal{L}(X))(\mathcal{L}(\xi)) \]

\[ = \langle \nabla g(\mathcal{L}(X)), \mathcal{L}(\xi) \rangle \]

\[ = \langle \mathcal{L}^T \nabla g(\mathcal{L}(X)), \xi \rangle \]  \hfill (39)

\[ = \langle \nabla h(X), \xi \rangle, \]

which implies that

\[ \nabla h(X) = \mathcal{L}^T \nabla g(\mathcal{L}(X)). \]  \hfill (40)
We further have
\[
D^2 h(X)(\xi, \xi) = D^2 g(\mathcal{L}(X))(\mathcal{L}(\xi), \mathcal{L}(\xi)) \\
= \langle H_g(\mathcal{L}(X))\mathcal{L}(\xi), \mathcal{L}(\xi) \rangle \\
= \langle \mathcal{L}^T H_g(\mathcal{L}(X))\mathcal{L}(\xi), \xi \rangle \\
= \langle H_h(X)\xi, \xi \rangle ,
\]
which implies that
\[
H_h(X) = \mathcal{L}^T H_g(\mathcal{L}(X))\mathcal{L}.
\]
Similarly, we have
\[
\nabla \zeta(X) = \mathcal{L}^T \nabla B(\mathcal{L}(X)) = \mathcal{L}^T (-\mathcal{L}(X)^{-1}).
\]
and
\[
H_\zeta(X) = \mathcal{L}^T H_B(\mathcal{L}(X))\mathcal{L} = \mathcal{L}^T P(\mathcal{L}(X)^{-1})\mathcal{L}.
\]

3 Matrix Monotone Functions

Let
\[
g : [0, +\infty) \rightarrow \mathbb{R}
\]
be a real-valued function. We say that \(g\) is matrix monotone (anti-monotone) if for any real symmetric matrices of the same size such that \(A \succeq 0, B \succeq 0\) and \(A \succeq B\), we have
\[
g(A) \succeq g(B) \ (g(A) \preceq g(B)).
\]
It is obvious that if \(g\) is matrix monotone then \(-g\) is matrix anti-monotone and vice versa.

In [6], we proved that for any matrix anti-monotone function
\[
g : [0, +\infty) \rightarrow \mathbb{R},
\]
we have the following compatibility result (adapted for the case of symmetric matrices).

**Theorem 3.1.** Let \(C \in \mathbb{S}_+^n\) and \(B(X) = -\ln \det(X), X \in \mathbb{S}_+^{n+}\). Then
\[
|D^3 \varphi_c(X)(\xi, \xi, \xi)| \leq 3 D^2 \varphi_c(X)(\xi, \xi) \sqrt{D^2 B(X)(\xi, \xi)}, X \in \mathbb{S}_+^{n+}, \xi \in \mathbb{S}^n,
\]
where
\[
\varphi_c(X) = \langle C, g(X) \rangle .
\]
Hence, by proposition 2.3, we have the following self-concordance result.
Corollary 3.2. For any $\beta \geq 0$, the function

$$\Phi_\beta(X) = \beta \varphi_c(X) + B(X), \; X \in S^n_{++},$$

is $\kappa$-self-concordant on $S^n_{++}$ with $\kappa = 2$.

With theorem 3.1 and corollary 3.2, the long-step path-following algorithm discussed in section 2 can then be applied to optimization problems involving objective functions of the form

$$\varphi_c(X) = \langle C, g(X) \rangle = \text{Tr}(Cg(X)).$$

(46)

Next we will illustrate some important implementation details of the long-step path-following algorithm through examples. In [6], we showed calculations of the gradient and Hessian of $\varphi_c(X)$ for the case when $g(t) = -\ln(t)$, $t > 0$. Since the results are derived from the integral representation of $-\ln(X)$ and any matrix monotone function admits such an integral representation, we can derive the gradient and Hessian of $\varphi_c(X)$ for any matrix anti-monotone function $g(t), t \geq 0$. The only difference will be calculations of the first and second divided differences.

Now let

$$X = U\Lambda U^T$$

be a spectral decomposition of $X$, where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$ and $UU^T = I$. Let

$$D = (\Lambda + tI)^{-1}, \; \tilde{C} = U^T CU, \; \tilde{\xi} = U^T \xi U \; \text{and} \; d_i = (\lambda_i + t)^{-1}.$$

For a continuously differentiable function $h : [0, +\infty) \rightarrow \mathbb{R}$, we introduce the first divided difference $h^{[1]}$:

$$h^{[1]}(\lambda_i, \lambda_j) = \begin{cases} 
\frac{h(\lambda_i) - h(\lambda_j)}{\lambda_i - \lambda_j}, & \lambda_i \neq \lambda_j, \\
\frac{h'(\lambda_i)}{\lambda_i}, & \lambda_i = \lambda_j,
\end{cases}$$

and the second divided difference $h^{[2]}$:

$$h^{[2]}(\lambda_i, \lambda_j, \lambda_k) = \frac{h^{[1]}(\lambda_i, \lambda_j) - h^{[1]}(\lambda_i, \lambda_k)}{\lambda_j - \lambda_k}$$

(47)

for distinct $\lambda_i$, $\lambda_j$, and $\lambda_k$ while for other cases the function is defined by taking limits in (47), e.g.,

$$h^{[2]}(\lambda, \lambda, \lambda) = \frac{1}{2} h''(\lambda).$$

Lastly, recall the Schur product: for $m \times n$ matrices $A$ and $B$,

$$[A \circ B]_{ij} = A_{ij}B_{ij},$$

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and the vectorization operator \( \text{vec}(\cdot) \) for an \( n \times m \) matrix \( A = [a_{ij}] \):

\[
\text{vec}(A) = [a_{11}, \ldots, a_{n1}, a_{12}, \ldots, a_{n2}, \ldots, a_{1m}, \ldots, a_{nm}]^T.
\]

Now, we are ready to present expressions of the gradient and Hessian of \( \varphi_c(X) \).

\[
\nabla \varphi_c(X) = U \left( \tilde{C} \circ g^{[1]}(\Lambda) \right) U^T, \tag{48}
\]

where \( g^{[1]}(\Lambda) \) is the \( n \times n \) first divided difference matrix with \( [g^{[1]}(\Lambda)]_{ij} = g^{[1]}(\lambda_i, \lambda_j) \). The vectorized form of the gradient is given by

\[
\text{vec}(\varphi_c(X)).
\]

The Hessian in vectorized form is given as

\[
H_{\varphi_c(X)}(X) = (U \otimes U) \left( \int_0^{+\infty} ((D\tilde{C}D) \otimes D + D \otimes (D\tilde{C}D)) \, dt \right) (U \otimes U)^T. \tag{49}
\]

As discussed in [6], the middle part

\[
S = \int_0^{+\infty} ((D\tilde{C}D) \otimes D + D \otimes (D\tilde{C}D)) \, dt
\]

is a sparse block matrix with \((ij, kl)\)-th entry:

\[
S_{ij,kl} = \delta_{kl}\tilde{C}_{ij}\Gamma_{ijkl} + \delta_{ij}\tilde{C}_{kl}\Gamma_{jkl}, \tag{50}
\]

where

\[
\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases}
\]

and \( \Gamma_{ijk} = g^{[2]}(\lambda_i, \lambda_j, \lambda_k) \), from which we notice that the \( ij \)-th sub-block matrix is diagonal if \( i \neq j \).

**Example 3.3.** Consider the function

\[
g(t) = t^{-1}, \quad t > 0.
\]

Clearly, \( g \) is matrix anti-monotone. Therefore, we can apply the long-step path-following algorithm to the following optimization problem: for \( C \succeq 0 \),

\[
f(X) = \text{Tr}(CX^{-1}) \rightarrow \min,
\]

\[
\langle A_i, X \rangle \leq b_i, \quad i = 1, \ldots, m,
\]

\[
\langle A_i, X \rangle = b_i, \quad i = m + 1, \ldots, N,
\]

\[
X \succeq 0. \tag{51}
\]
Note that this is the optimization problem of type I discussed in section 2.2. Table 1 shows numerical results for solving (51).

Our algorithm is implemented in Matlab, and all the numerical experiments in this paper are performed on a personal 15-in Macbook Pro with Intel core i7 and 16 GB memory. Data are randomly generated with an initial interior feasible point \(^1\) and without loss of generality, \(\text{Tr}(X) = 1\) is imposed (we assume that the feasible set is bounded). In table 1, nNewton denotes the total number of Newton steps.

| \(n\) | \(m\) | \(N\) | \(f_{\text{min}}\) | nNewton | Time(s) |
|------|------|------|----------------|--------|-------|
| 4    | 2    | 4    | 27.3538       | 8      | 0.0095|
| 8    | 4    | 8    | 8.3264        | 39     | 0.0712|
| 16   | 8    | 16   | 18.4274       | 33     | 0.2078|
| 32   | 16   | 32   | 38.3216       | 43     | 2.3169|
| 64   | 32   | 64   | 83.0738       | 63     | 74.5580|

Remark. 1. We noticed that the most time consuming part when running the algorithm is assembling the linear system, e.g., (26) and (36).

2. In general, using vectorization greatly improves performance and scalability of the algorithm [1].

3. When solving linear systems, sparsity of the Hessian should also be exploited, e.g., in Matlab, if \(H\) is sparse, use \(H = \text{sparse}(H)\).

4. Avoid inverting a matrix directly. For example, in (26), (36), (24) and (37), one should solve linear systems instead of calculating the Hessian inverse; in Matlab one can use \(H \setminus a\) instead of \(\text{inv}(H) \ast a\) to obtain \(H^{-1}a\). Moreover, if \(A = [a_1, \ldots, a_m]\), where \(a_i\)'s are \(n \times 1\) column vectors, it is more efficient to use \(H \setminus A\) to obtain \([H^{-1}a_1, \ldots, H^{-1}a_m]\) in Matlab.

Example 3.4. In quantum information theory, the so-called relative Rényi entropy is defined as

\[
\varphi_\alpha(X,Y) = -\text{Tr}(X^\alpha Y^{1-\alpha}), \alpha \in (0,1),
\]

\(X,Y \in \mathcal{S}_n^{++}\).

The function \(\varphi_\alpha\) is jointly convex in \(X,Y\). For a fixed \(Y\), the function \(X \mapsto \varphi_\alpha(X,Y)\) is matrix anti-monotone, and for a fixed \(Y\), the function \(X \mapsto \varphi_\alpha(X,Y)\) is matrix anti-monotone. Therefore, for optimization problems involving the relative Rényi entropy, our

\(^1\)Data can be accessed here: https://doi.org/10.13140/RG.2.2.35488.43524
long-step path-following algorithm combined with an alternative minimization procedure (similar to the one used in [6]) can be applied.

**Example 3.5.** The relative entropy of entanglement (REE) problem described in [6] involves the following optimization problem which gives a lower bound to the REE of a quantum state $C$ (i.e., $C \succeq 0$ and $\text{Tr}(C) = 1$):

$$
\begin{align*}
  f(X) &= \text{Tr}(C \ln(C)) - \text{Tr}(C \ln(X)) \rightarrow \min, \\
  \text{Tr}(X) &= 1, \\
  \mathcal{L}(X) &\geq 0, \\
  X &\succeq 0,
\end{align*}
$$

where $\mathcal{L}(\cdot)$ is the so-called partial transpose operator. Note that the function $\lambda \mapsto -\ln(\lambda)$ is matrix anti-monotone and the REE optimization problem (53) is of type II discussed in section 2.2. Therefore, our long-step path-following is readily to be applied. For numerical results and more details regarding the REE problem, we refer to our previous work [6].

**Example 3.6.** The objective functions based on fidelity [3] have the form

$$
\varphi(X) = -\text{Tr}(\mathcal{L}(X)^\frac{1}{2}),
$$

where $X \in S^n_{++}$ and $\mathcal{L}(X) = Y^\frac{1}{2} X Y^\frac{1}{2}$ for some fixed $Y \in S^n_{++}$. Note that the function $\lambda \mapsto -\sqrt{\lambda}$ is matrix anti-monotone. It immediately follows that our path-following algorithm can be applied to this type of problems as well.

### 3.1 Some Important Observations

During our numerical experiments, we have the following important observations:

1. While conducting extensive numerical experiments with Newton’s method (with line search) applied to problems with semidefinite constraints, we noticed a striking difference between the cases of self-concordant and non-self-concordant functions. In the latter case the convergence of Newton’s method is rather slow (or there is no convergence to an optimal solution) even when the optimal solution lies in the interior of a feasible set.

2. For some optimization problems of type II, such as the REE problem (53), the barrier term $-\ln \det(X)$ seems unnecessary when running our long-step path-following algorithm. We suspect that this is related to certain properties of the linear operator involved and it would be interesting to understand more about this phenomenon.
4 An Important Optimization Problem in Quantum Key Distribution

Key distribution is used to distribute security keys to two parties so they can securely share information. While traditional public key distribution is based on the computational intractability of hard mathematical problems, quantum key distribution (QKD) relies on the fundamental law of nature, or more precisely, on the theory of quantum mechanics. QKD has been shown to provide a quantum-secure method of sharing keys which in principle is immune to the power of an eavesdropper [10, 8].

One of the main theoretical problems in QKD is to calculate the secret key rate for a given QKD protocol, i.e., how much secret key can be distributed for a given protocol [2]. It turns out that the essential tool is to solve the following optimization problem involving the quantum relative entropy function [2, 11]:

\[
\begin{align*}
    f(\tilde{X}, \tilde{Y}) &= \text{Tr}(\tilde{X} \ln(\tilde{X})) - \text{Tr}(\tilde{X} \ln(\tilde{Y})) \rightarrow \min, \\
    \tilde{X} &= \sum_{j=1}^{l} K_j X K_j^*, \\
    \tilde{Y} &= \sum_{k=1}^{s} Z_k X Z_k, \\
    \text{Tr}(A_i X) &= b_i, \ i = 1, \ldots, m,
\end{align*}
\]

(55)

where \( X \) is a density matrix (i.e., \( X \succeq 0 \) and \( \text{Tr}(X) = 1 \)), \( K_j \)'s are \( k \times n \) matrices and \( \sum_{j=1}^{l} K_j^* K_j \leq I \), and \( Z_k \)'s are \( n \times n \) orthogonal projectors and \( \sum_{k=1}^{s} Z_k = I \). Note that \( k \) usually depends on \( n \) (e.g., \( k = 2n \)).

In [11], a conditional gradient method was used to calculate the key rate, however, the convergence is slow and the method is unstable. We are interested in applying our long-step path-following algorithm to (55).

First we can rewrite (55) in the following general form:

\[
\begin{align*}
    f(\tilde{X}, \tilde{Y}) &= \text{Tr}(\tilde{X} \ln(\tilde{X})) - \text{Tr}(\tilde{X} \ln(\tilde{Y})) \rightarrow \min, \\
    \tilde{X} &= \mathcal{L}_1(X), \\
    \tilde{Y} &= \mathcal{L}_2(X), \\
    \text{Tr}(A_i X) &= b_i, \ i = 1, \ldots, m, \\
    X &\succeq 0,
\end{align*}
\]

(56)
where $L_1$ and $L_2$ are two linear operators of the same type:

\[
L_1 : X \mapsto \sum_{j=1}^{r_1} K_j X K_j^*,
\]

\[
L_2 : X \mapsto \sum_{j=1}^{r_2} T_j X T_j^*,
\]

where $K_j$'s and $T_j$'s are $k \times n$ matrices.

Equivalently, we can consider the following optimization problem:

\[
f(X) = \text{Tr}(L_1(X) \ln(L_1(X))) - \text{Tr}(L_1(X) \ln(L_2(X))) \to \min,
\]

\[
\text{Tr}(A_i X) = b_i, \ i = 1, \ldots, m,
\]

\[
X \succeq 0.
\]

To guarantee the positive definiteness of $L_1(X)$ and $L_2(X)$, we perturb them a little bit in our algorithm, namely, use $L_1(X) + \epsilon$ and $L_2(X) + \epsilon$ instead, where $\epsilon$ is a very small positive number, e.g. $\epsilon = 1 \times 10^{-16}$.

4.1 Calculations of Gradient and Hessian

Note that without loss of generality, we again only consider the real vector space of symmetric matrices. The case of Hermitian matrices can be handled within the general Jordan algebraic scheme (see e.g. [7]).

Let

\[
f_1(X) = \text{Tr}(L_1(X) \ln(L_1(X))), \ f_2(X) = -\text{Tr}(L_1(X) \ln(L_2(X))),
\]

and

\[
B(X) = -\ln \det(X),
\]

then

\[
\nabla F_{\beta}(X) = \beta(\nabla f_1(X) + \nabla f_2(X)) + \nabla B(X),
\]
and
\[ H_{F_3}(X) = \beta(H_{f_1}(X) + H_{f_2}(X)) + H_B(X). \quad (60) \]

Next we will show calculations for the three components. Let
\[ \mathcal{L}_1(X) = O_1\Lambda_1O_1^T \]
be a spectral decomposition of \( \mathcal{L}_1(X) \), where \( \Lambda_1 = \text{diag}(\lambda^{(1)}_1, \ldots, \lambda^{(1)}_n) \) and \( O_1O_1^T = I \). Similarly, let
\[ \mathcal{L}_2(X) = O_2\Lambda_2O_2^T \]
be a spectral decomposition of \( \mathcal{L}_2(X) \). Let \( h(\lambda) = \ln(\lambda), \lambda > 0, \) and \( h^{[1]}(\Lambda_i), i = 1, 2, \) be the first divided difference matrix.

Further, note that the vectorization of \( \mathcal{L}_1 \) and \( \mathcal{L}_2 \) can be expressed as
\[ \mathcal{L}_1 = \sum_{j=1}^{r_1} K_j \otimes K_j, \]
\[ \mathcal{L}_2 = \sum_{j=1}^{r_2} T_j \otimes T_j. \quad (61) \]

By (40) and (42), we have (in vectorized form)
\[ \nabla f_1(X) = \text{vec} \left( \mathcal{L}_1^T (I + \ln(\mathcal{L}_1(X))) \right), \quad (62) \]

and
\[ H_{f_1}(X) = \mathcal{L}_1^T \mathcal{L}_1 + \mathcal{L}_1 \mathcal{L}_1^T. \]
\[ = \mathcal{L}_1^T \mathcal{D} \ln(\mathcal{L}_1(X)) \mathcal{L}_1 \]
[63]
\[ = \mathcal{L}_1^T (O_1 \otimes O_1) \text{diag}(\text{vec}(h^{[1]}(\Lambda_1)))(O_1 \otimes O_1)^T \mathcal{L}_1. \]

By (40), (48) and product rule, we have
\[ \nabla f_2(X) = \text{vec} \left( -\mathcal{L}_2 \ln(\mathcal{L}_2(X)) - \mathcal{L}_2^T O_2 \left( (O_2^T \mathcal{L}_1(X)O_2) \circ h^{[1]}(\Lambda_2) \right) O_2^T \right). \quad (64) \]

By (40), (42), (49), (63) and product rule, we have
\[ H_{f_2}(X) = -2\mathcal{L}_1^T \mathcal{D} \ln(\mathcal{L}_2(X)) \mathcal{L}_2 - \mathcal{L}_2^T H_{f_1}(X) \mathcal{L}_2 \]
\[ = -2\mathcal{L}_1^T (O_2 \otimes O_2) \text{diag}(\text{vec}(h^{[1]}(\Lambda_2)))(O_2 \otimes O_2)^T \mathcal{L}_2 \]
\[ + \mathcal{L}_2^T (O_2 \otimes O_2) \int_0^{+\infty} (D\tilde{C}D) \otimes D + D \otimes (D\tilde{C}D) \, dt \, (O_2 \otimes O_2)^T \mathcal{L}_2, \quad (65) \]
where $D = (\Lambda_2 + tI)^{-1}$ and $\tilde{C} = O_2^T L_1(X) O_2$. As mentioned earlier (see (49)),

$$S = \int_0^{+\infty} (D\tilde{C}D) \otimes D + D \otimes (D\tilde{C}D) \, dt$$

is a sparse block matrix with $(ij, kl)$-th entry:

$$S_{ij,kl} = \delta_{kl} \tilde{C}_{ij} \Gamma_{ijl} + \delta_{ij} \tilde{C}_{kl} \Gamma_{jkl},$$

where

$$\delta_{ij} = \begin{cases} 
1 & \text{if } i = j, \\
0 & \text{if } i \neq j,
\end{cases} \quad \text{and} \quad \Gamma_{ijk} = -h^{[2]}(\lambda_i, \lambda_j, \lambda_k).$$

Lastly, we have

$$\nabla B(X) = \text{vec}(-X^{-1}),$$

$$H_B(X) = X^{-1} \otimes X^{-1}. \quad (66)$$

### 4.2 Numerical Results

In this section, we present some of our numerical results. Data are randomly generated with an initial interior feasible point and without loss of generality, $\text{Tr}(X) = 1$ is imposed (we assume that the feasible set is bounded). Recall that the dimension of $X$ is $n \times n$. We use $k = 2n$ in our experiment. Table 2 shows numerical results for the QKD optimization problem (57) compared to the results obtained by using the `quantum_relnentr` function in `cvxquad` combined with SDP solver MOSEK [4] (one of the most competitive approaches available for optimization problems involving quantum relative entropy). In table 2, nNewton denotes the number of total Newton steps.

| $n$ | $k$ | $m$ | $r_1$ | $r_2$ | Time(s) | $f_{min}$ | nNewton | Time(s) | $f_{min}$ |
|-----|-----|-----|-------|-------|-------|--------|---------|--------|---------|
| 4   | 8   | 2   | 2     | 2     | 0.05  | 0.2744 | 7       | 40.39  | 0.2744   |
| 6   | 12  | 4   | 1     | 2     | 0.13  | 0.0498 | 8       | 2751.39| 0.0498   |
| 12  | 24  | 6   | 2     | 4     | 1.07  | 0.0440 | 17      | N/A    | failed   |
| 16  | 32  | 10  | 2     | 2     | 2.07  | 0.0511 | 9       | N/A    | failed   |
| 32  | 64  | 20  | 2     | 2     | 71.25 | 0.0332 | 11      | N/A    | failed   |

**Remark.**

1. Our numerical results are quite stunning. For example, for the second test sample when $n = 6$, our method is 20000 times faster! And for the larger dimensions, `cvxquad` with MOSEK simply cannot solve the problem.

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\(^2\)Data can be accessed here: https://doi.org/10.13140/RG.2.2.35488.43524
2. During our numerical experiments, we notice that for most of the cases omitting the barrier term $B(X) = -\ln \det(X)$ does not affect the convergence. We suspect this is due to the fact that $-\text{Tr}(C \ln(X))$, $X \succeq 0$ is a self-concordant barrier for $C > 0$ (see [6]). However, the barrier term $B(X)$ does increase stability and accuracy of the algorithm.

For a rigorous justification of our numerical scheme, we propose the following conjecture.

4.3 A Conjecture Regarding the QKD Optimization Problem
We conjecture that $F_\beta(X)$ in (58) is a self-concordant function for each $\beta > 0$ and such self-concordance depends on structure of the quantum relative entropy function and properties of the linear operators $L_1$ and $L_2$ involved.

5 Concluding Remarks
The difficulty of optimization problems arising in quantum information theory stems from the fact that their objective functions are rather complicated functions of several matrix arguments. In [6, 7] and this paper we noticed that many of these functions are compatible in the sense of Nesterov and Nemirovskii with standard self-concordant barriers associated with symmetric cones. This observation, in principle, allows one to use structured interior-point algorithms for solving such optimization problems. To implement such algorithms one needs to be able to deal with very complicated Hessians. Our extensive numerical experiments confirm that this is doable but certain limitations on the size of the problem definitely exist. To the best of our knowledge our work is the first systematic attempt to use second-order methods for problems arising in quantum information theory. In comparison with first-order methods, our approach solves comparable problems faster and with higher accuracy (asymptotic quadratic convergence!).

We formulated our algorithm in a very general setting (see theorems 2.7 to 2.9) but complexity estimates are available only for problems involving symmetric cones with standard self-concordant barrier functions. A natural question is whether it is possible to generalize complexity estimates for the setting involving arbitrary self-concordant barriers. Another interesting question is whether quasi-Newton versions of interior-point algorithms would allow to increase the size of the problems which can be realistically solved.

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