Classical and Quantum Iterative Optimization Algorithms Based on Matrix Legendre-Bregman Projections

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Abstract

We consider Legendre-Bregman projections defined on the Hermitian matrix space and design iterative optimization algorithms based on them. A general duality theorem is established for Bregman divergences on Hermitian matrices and it plays a crucial role in proving the convergence of the iterative algorithms. We study both exact and approximate Bregman projection algorithms. In the particular case of Kullback-Leibler divergence, our approximate iterative algorithm gives rise to the non-commutative versions of both the generalized iterative scaling (GIS) algorithm for maximum entropy inference and the AdaBoost algorithm in machine learning as special cases. As the Legendre-Bregman projections are simple matrix functions on Hermitian matrices, quantum algorithmic techniques are applicable to achieve potential speedups in each iteration of the algorithm. We discuss several quantum algorithmic design techniques applicable in our setting, including the smooth function evaluation technique, two-phase quantum minimum finding, and NISQ Gibbs state preparation.

1 Introduction

Bregman divergence is a quantity introduced in [9] to solve convex optimization problems under linear constraints. It is a distance-like measure defined for a convex function and generalizes the Euclidean distance. An important example of Bregman divergence beyond the squared Euclidean distance is the Kullback-Leibler information divergence. Bregman divergence and several related concepts play a crucial role in many areas of study, including optimization theory [10], statistical learning theory [34, 19, 24, 6], and information theory [20].

Given a convex optimization problem over a convex set \( C = \bigcap_j C_j \) specified as the intersection of potentially simpler convex sets \( C_j \), Bregman’s method iteratively projects the initial point to different \( C_j \)'s using Bregman’s divergence as the measure of distance. This method, referred to as Bregman’s projection algorithm [9], is one of the most influential iterative algorithms for solving convex optimization problems under linear constraints [10]. It generalizes the orthogonal projection algorithms in the Euclidean space and the Euclidean distance is replaced by the Bregman divergence for certain underlying convex functions. Many important convex optimization algorithms are special cases of Bregman’s iterative projection algorithm by choosing different divergence measures. When Bregman’s divergence is chosen to be the Kullback-Leibler divergence, Bregman’s projection is also known
as information projection [20] and several iterative algorithms, including the generalized iterative scaling algorithm [21] (also known as the SMART algorithm [29]), are information projection algorithms [20].

Bregman’s algorithm iteratively computes the Bregman’s projection on convex sets, the exact computation of which is a complicated task and usually does not have explicit formulas even in the simple case of linear constraints. Several different ideas have been proposed to compute the Bregman’s projection approximately [12, 23, 13, 14, 15, 19, 24, 25]. Of great importance to this work is the auxiliary function method [24, 19, 25] that designs an auxiliary function to bound the progress of the iterative update procedure measured by Bregman divergence. Important learning algorithms including the improved iterative scaling algorithm [24] and the AdaBoost algorithm [26, 19, 25] can be analyzed using the auxiliary function method and shown to converge to the correct optimizer.

This paper considers non-commutative analogs of Bregman’s projection algorithms where Bregman divergence is defined for Hermitian matrices. For a real convex function \( f \), and two matrices \( X, Y \), we consider the Bregman divergence \( D_f(X, Y) = \text{tr}(f(X) - f(Y) - f'(Y)(X - Y)) \). Even though generalizing the Bregman’s projection and related concepts to the matrix case is straightforward, analyzing their behavior is a challenging task. This is primarily due to two reasons. On the one hand, matrices are generally non-commutative, so inequalities used in the analysis become much harder to establish. On the other hand, the proof of convergence in the classical case relied on the continuity of Bregman divergence, while Bregman divergence for matrices is usually discontinuous. A natural question we ask here is: “Are there natural generalizations of the iterative Bregman projection algorithms that converge correctly given the difficulty posed in the non-commutative case?” We answer the question in the positive by establishing two main results in the paper.

First, we prove a general duality theorem in the non-commutative case. The duality theorem is concerned with the optimization of \( D_f(X, Y) \) in two situations. On one hand, we minimize \( D_f(X, Y_0) \) over \( X \) in a linear family defined as \( \mathcal{L} = \{ X \mid \langle F_j, X \rangle = \langle F_j, X_0 \rangle, \text{ for } j = 1, 2, \ldots, k \} \). That is, we compute the projection of \( Y_0 \) to the linear family under the Bregman divergence \( D_f \). On the other hand, we consider minimization \( D_f(X_0, Y) \) over \( Y \) in a family of Hermitian matrices called the Legendre-Bregman projection family \( \mathcal{P} = \{ Y \mid Y = \mathcal{L}_f(Y_0, \lambda \cdot F) \} \) where \( \mathcal{L}_f(Y, \Lambda) = (f^*)(f'(Y) + \Lambda) \). The duality theorem states that optimizers in the above two situations coincide under simple and easy-to-verify conditions on \( f \). An important special case of the duality theorem when \( f(x) = x \ln x - x \) is the well-known result that the linear family and the closure of the exponential family intersect at a point that maximizes the entropy function under linear constraints [20, 3]. This special case is well-known as the Jaynes’ maximum entropy principle [32], which states that the maximum entropy state satisfying linear constraints is the unique intersection of the linear family defined by the constraints and the closure of the exponential family. The duality theorem is the key to proving the convergence of our exact (and approximate) matrix Bregman projection algorithms.

Second, we prove a matrix inequality that is essential for analyzing the approximate information projection algorithms. In the classical case, Jensen’s inequality suffices to establish the properties we require for the auxiliary function. In the non-commutative case, the corresponding inequality is much harder to establish. In fact, the inequality is not always true for all convex functions. Fortunately for us, we can prove the inequality for Kullback-Leibler divergence by employing a strengthened version of Golden-Thompson inequality recently established by Carlen and Lieb [11]. This new inequality, together with the duality
theorem, guarantees the convergence of approximate information projection algorithms.

Important examples of this algorithm include the matrix AdaBoost algorithm and the matrix generalized iterative scaling (GIS) algorithm as special cases. The matrix AdaBoost algorithm has a physical interpretation. It is an iterative algorithm that minimizes the partition function of the linear family of Hamiltonians. The matrix GIS algorithm is an algorithm for maximum entropy inference and can be applied in understanding many-body quantum systems [16, 1]. The convergence of these algorithms follows as they are special cases of the information projection algorithm.

Several potential quantum speedups are identified for the iterative algorithms proposed in the paper. As the computation in each iterative step of our algorithms boils down to the computation of a matrix $Y' = \mathcal{L}_f(Y, \Lambda)$ and then an update of parameters based on average values of the matrix $Y'$ with respect to given operators $F_j$. We can represent $Y$ as a quantum state and then employ quantum algorithmic techniques such as singular value transformation [28, 27] and smooth function evaluation [4] to compute $Y'$, the updated version of $Y$.

Thanks to the flexibility of the auxiliary function framework, we can update the parameters either in parallel or sequentially, and the analysis of them can be treated uniformly. The sequential update variant has the advantage of utilizing the fast quantum OR lemma for searching a violation with low sample complexity of the states representing the matrix $Y' = \mathcal{L}_f(Y, \Lambda)$. As this state preparation is usually the most expensive part of the computation, the saving in samples could lead to substantial speedups.

When the state preparation for $Y' = \mathcal{L}_f(Y, \Lambda)$ can be done on a near-term quantum device, our algorithms can also be performed on the same near-term device because of the intrinsic iterative structure and simple update rules. This gives rise to near-term applications for certain convex optimization problems.

1.1 Techniques

To prove the general duality theorem, we followed the approach in [25] with important changes to avoid the problems caused by the discontinuity of $D_f(X, Y)$ and to simplify the assumptions on $f$. Assumption A.3 in [25] requires that $D_f(X, Y)$ is continuous with respect to $X$ and $Y$, a condition holds in the classical case but fails in the quantum case where $X, Y$ are matrices. In fact, an explicit example is given in [7, Example 7.29] showing that $\lim_{t \to \infty} D(Y, Y_t) \neq 0$ for a sequence $(Y_t)_t$ converging to $Y$. We get around the difficulty by extending the domain of the Bregman divergence carefully and establishing the required properties directly for the extended versions without using continuity of $D_f(X, Y)$. We also identify one simple condition that supersedes the five assumptions A.1–A.5 of [25]. The simple condition requires that the underlying convex function $f$ has an open conjugate domain $\text{dom} \ f^*$.

The key consequence for a convex function having an open conjugate domain is that we can show $D_f(X, Y)$ is coercive with respect to $Y$. That is, the set \( \{Y \mid D_f(X, Y) \leq c\} \) is bounded for any constant $c$, a condition key to show compactness and convergence later on. Such a condition is equivalent to the function being a so-called Bregman-Legendre function [7] for real functions. However, it is also shown in the same paper that when the function is extended to Hermitian matrices, the function is not Bregman-Legendre because of the discontinuity issue. We use techniques from matrix perturbation theory to prove that such a condition suffices to guarantee the validity of the duality theorem. There are many interesting convex functions that satisfy the condition, and we have
listed a few important ones in Table 1 [7].

The continuity of $L_f(Y, \Lambda)$ is still essential for our proof of the convergence analysis, and it is one of the main technical parts of our proof. In the end, the problem is roughly a matrix perturbation problem where we have a block matrix $\begin{pmatrix} A_0 & B \\ B^\dagger & A_1 \end{pmatrix}$ where $A_0$ has small eigenvalues and $A_1$ has large eigenvalues and $\|B\| \leq 1$. We need to show that the perturbation of the spectrum by $B$ becomes arbitrarily smaller when the eigenvalues of $A_0$ go to infinity. For this, we make use of two results from perturbation theory that take care of the perturbation of the eigenvalues (a result by Mathias [37]) and the perturbation of the eigenprojections (Davis-Kahan $\sin(\Theta)$ theorem [22]).

For the second result about information projection algorithms, the main difficulty we encounter is to show appropriate matrix inequalities so that we can bound the improvement measured by the change in the Bregman divergence using the auxiliary function. We are able to show the inequality for an important case when the divergence is Kullback-Leibler information divergence. The resulting iterative update algorithm has a very similar flavor to the matrix multiplicative weight update method (MMWU) [33, 5]. It is an adaptive version where the update step size is not fixed as in MMWU, but depends on the violation at the current step. MMWU is proved to be a powerful framework in designing both classical and quantum algorithms for semi-definite programming (SDP) problems. The QIS algorithm are applicable as a replacement for MMWU in some cases and provide possible speedups thanks to its adaptive nature of the QIS algorithm. The technical inequality for the MMWU analysis is the Golden-Thompson inequality. In contrast, the Golden-Thompson inequality does not seem to be powerful enough any more for the information projection algorithms, even in combination with Jensen’s operator and trace inequalities. Luckily for us, an improved Golden-Thompson inequality established recently by Carlen and Lieb [11] fits our analysis perfectly.

Jaynes’ maximum entropy principle was a crucial fact that recent studies [2, 3, 30] on the Hamiltonian learning problems heavily rely on. The QIS algorithm serves as a candidate algorithm that solves a related problem that we call the Hamiltonian inference problem. Both problem tries to learn information about the Hamiltonian. In the Hamiltonian learning problem, the algorithm is provided copies of the Gibbs state of the true Hamiltonian. While in the Hamiltonian inference problem, the algorithm does not have access to the true Gibbs state, but only has information about the local information of it and is allowed to make adaptive queries to the Gibbs state of candidate Hamiltonians in the linear family of the Hamiltonians. For local Hamiltonians, it is likely that the QIS algorithm can solve the Hamiltonian inference problem with not only polynomial sample complexity but with polynomial time complexity as well. We leave the analysis to future work.

2 Preliminary

We will need the following concepts from convex analysis. In convex analysis, functions are defined on all of $\mathbb{R}^m$ and take values from $\mathbb{R} \cup \{\pm \infty\}$. The (effective) domain of a function $\phi : \mathbb{R}^m \to \mathbb{R} \cup \{\pm \infty\}$ is the set
\[
\text{dom} \phi = \{x \in \mathbb{R}^m \mid \phi(x) < +\infty\}.
\]
A function $\phi$ is convex if its domain $\text{dom} \phi$ is a convex set and it satisfies
\[
\phi(tx + (1-t)y) \leq t\phi(x) + (1-t)\phi(y)
\]
Then define $C$ given above. Let $A$ be the eigenvalues of $\sum_{i=1}^{m} x_i y_i$. For matrices $A, B$, define $\langle A, B \rangle = \text{tr}(A^T B)$.

The Fenchel conjugate $\phi^*$ of a convex function $\phi$ is defined as

$$\phi^*(y) = \sup \{ x \cdot y - \phi(x) | x \in \mathbb{R}^m \}. \tag{1}$$

Let $f$ be a smooth real function and $A(x)$ a matrix whose entries are functions of $x$. Then

$$\frac{d}{dx} \text{tr} f(A(x)) = \left< f'(A(x)), \frac{d}{dx} A(x) \right>. \tag{2}$$

We will need several results from matrix perturbation theory in our proofs. Let $A$ be an Hermitian matrix of size $m + n$ by $m + n$ and has a block form $A = \begin{pmatrix} A_0 & 0 \\ 0 & A_1 \end{pmatrix}$, where $A_0$ and $A_1$ are $m$ by $m$ and $n$ by $n$ Hermitian matrices respectively. Let $\tilde{A} = \begin{pmatrix} A_0 & B \\ B^\dagger & A_1 \end{pmatrix}$ be a perturbation of $A$. We have the following two eigenvalue and eigenvector perturbation bounds.

**Proposition 2.1** (Eigenvalue Perturbation Bound [37]). Let $A$ and $\tilde{A}$ be Hermitian matrices given above. Let $\lambda_k$ and $\tilde{\lambda}_k$ be the $k$-th largest eigenvalue of $A$ and $\tilde{A}$ respectively. Suppose the eigenvalues of $A_0$ and $A_1$ are separated in the sense that $\lambda_{\min}(A_1) - \lambda_{\max}(A_0) \geq \eta > 0$. Then for all $k = 1, 2, \ldots, m + n$,

$$|\lambda_k - \tilde{\lambda}_k| \leq \frac{\|B\|^2}{\eta}.$$ 

**Proposition 2.2** (Davis-Kahan $\sin(\Theta)$ Theorem [22]). Let $A$ and $\tilde{A}$ be Hermitian matrices in $\text{Herm}(\mathcal{X})$ given above. Let $V_0$ and $V_1$ be two isometries mapping into $\mathcal{X}$ whose ranges are two orthogonal eigenspaces of $\tilde{A}$ and let $V = (V_0 \ V_1)$. Write $\tilde{A} = V \begin{pmatrix} A_0 & 0 \\ 0 & A_1 \end{pmatrix} V^\dagger$. Define $C_0, S_0, C_1, S_1$ to be the submatrices of $V$ as $V = \begin{pmatrix} C_0 & -S_1 \\ S_0 & C_1 \end{pmatrix}$. Suppose the eigenvalues of $A_0$ and $A_1$ are separated in the sense that $\lambda_{\min}(A_1) - \lambda_{\max}(A_0) \geq \eta > 0$. Then

$$\|S_0\| \leq \frac{\|B\|}{\eta}.$$ 

### 2.1 Inequalities

**Lemma 2.1** (Jensen’s operator inequality). For operator convex function $f$, operators $A_i$ satisfying $\sum_i A_i^\dagger A_i = \mathbb{1}$ and $X_i \in \text{Herm}(\mathcal{X})$, the following inequality holds

$$f\left(\sum_i A_i^\dagger X_i A_i\right) \leq \sum_i A_i^\dagger f(X_i) A_i.$$ 

**Lemma 2.2** (Jensen’s trace inequality). For convex function $f$, operators $A_i$ satisfying $\sum_i A_i^\dagger A_i = \mathbb{1}$ and $X_i \in \text{Herm}(\mathcal{X})$, the following inequality holds

$$\text{tr} f\left(\sum_i A_i^\dagger X_i A_i\right) \leq \text{tr} \sum_i A_i^\dagger f(X_i) A_i.$$
Lemma 2.3 (Golden-Thompson inequality). For Hermitian matrices $A$ and $B$, it holds that
\[ \text{tr } e^{A+B} \leq \text{tr}(e^A e^B). \]

Lemma 2.4 (Carlen-Lieb inequality). Suppose $H$ is an Hermitian matrix, $Y > 0$. Then the following inequality holds
\[ \text{tr } \exp(\ln(Y) + H) \leq \exp(\inf \{ \lambda_{\max}(H - \ln Q) : Q > 0, \text{tr}(YQ) = 1 \}). \] (3)

We remark that Carlen-Lieb is a strengthening of Golden-Thompson as pointed out in [11]. This can be seen by choosing $Y = e^A$, $H = B$, and $Q = e^B / \text{tr}(e^A e^B)$ in Carlen-Lieb.

2.2 Bregman Divergence

Bregman divergence is an important quantity in convex analysis and information theory. In this section, we recall its definition, and discuss the definition of Legendre functions for which the Bregman divergence behaves nicely.

Definition 2.1. Let $\phi$ be a convex function such that $\phi$ is differentiable on $\text{int}(\text{dom } \phi)$. The Bregman divergence $D_\phi: \text{dom } \phi \times \text{int}(\text{dom } \phi) \to [0, +\infty)$ is defined as
\[ D_\phi(x, y) = \phi(x) - \phi(y) - \nabla \phi(y) \cdot (x - y). \] (4)

The Bregman divergence is sometimes also known as the Bregman distance because $D_\phi(x, y)$ is a natural measure of the distance between $x, y$ even though it is not necessarily a distance in the sense of metric topology (e.g., $D_\phi(x, y)$ is in general not symmetric with respect to $x, y$). For example, when $\phi(x) = \|x\|^2$, $D_\phi(x, y)$ recovers the squared Euclidean distance $\|x - y\|^2$. It also holds that $D_\phi(x, y) \geq 0$ and equality holds if and only if $x = y$ for strictly convex $\phi$.

We now define the Bregman projection of a point to a convex set. The definition is natural in the geometric picture that Bregman divergence generalizes the squared Euclidean distance.

Definition 2.2 (Bregman Projection). Let $C$ be a closed convex set in $\mathbb{R}^m$ such that $C \cap \text{dom } \phi$ is not empty. Then the Bregman projection of $y$ to $C$ is defined as
\[ y^* = \arg\min_{x \in C \cap \text{dom } \phi} D_\phi(x, y). \]

Next, we will define an important family of functions called Legendre functions. For this, we need the following technical definitions about convex functions. A convex function is proper if never takes the value $-\infty$ and takes a finite value for at least one $x$. Most of the time, we work with proper convex functions. A convex function $\phi$ is closed if its epigraph $\text{epi } \phi = \{(x, t) \in \mathbb{R}^{m+1} \mid x \in \text{dom } \phi, \phi(x) \leq t\}$ is closed. A proper convex function $\phi$ is essentially smooth if it is everywhere differentiable on the interior of the domain $\text{int}(\text{dom } \phi)$ and if $\|\nabla \phi(x_j)\|$ diverges for every sequence $(x_j)$ in $\text{int}(\text{dom } \phi)$ converging to a point on the boundary of $\text{dom } \phi$.

Definition 2.3. A function $\phi$ is Legendre if it is a proper closed convex function that is essentially smooth and strictly convex on the interior of its domain.
A fundamental fact about Legendre convex functions is recorded below.

**Proposition 2.3** (Theorem 26.5 of [41]). *If \( \phi \) is Legendre then \( \nabla \phi : \text{int}(\text{dom } \phi) \to \text{int}(\text{dom } \phi^*) \) is a bijection, continuous in both directions, and \( \nabla \phi^* = (\nabla \phi)^{-1} \).

The Fenchel conjugate of a closed convex function is again a closed convex function. For proper closed convex function \( \phi \), \((\phi^*)^* = \phi \). A convex function is Legendre if and only if its conjugate is.

As an example, consider the extended real function \( \phi_H : \mathbb{R} \to \mathbb{R} \cup \{\pm \infty\} \)

\[ \phi_H(x) = \begin{cases} x \ln x - x & \text{for } x > 0, \\ 0 & \text{for } x = 0, \\ +\infty & \text{otherwise.} \end{cases} \]

It is easy to verify that \( \phi_H \) is Legendre and has domain \( \text{dom } \phi_H = [0, +\infty) \). The conjugate \( \phi_H^* \) of \( \phi_H \) is \( \phi_H^*(y) = e^y \) with domain \( \text{dom } \phi_H^* = \mathbb{R} \). The derivative \( \nabla \phi_H(x) = \ln(x) \) is a bijection between \((0, +\infty)\) and \( \mathbb{R} \) and is the inverse function of \( \nabla \phi_H^* \). More examples of Legendre functions, their conjugates and effective domains are given in Table 1.

| \( f \)    | \( \text{dom } f \) | \( f^* \)    | \( \text{dom } f^* \) | Remarks       |
|------------|-------------------|-------------|---------------------|--------------|
| \( x^2/2 \)   | \( \mathbb{R} \)  | \( y^2/2 \)  | \( \mathbb{R} \)       | Euclidean     |
| \( -\sqrt{1-x^2} \) | \([-1, 1]\)  | \( \sqrt{1+y^2} \) | \( \mathbb{R} \)       | Hellinger     |
| \( x \ln x - x \)   | \([0, \infty)\) | \( e^y \)   | \( \mathbb{R} \)       | Boltzmann/Shannon |
| \( x \ln x + (1-x) \ln(1-x) \) | \([0, 1]\) | \( \ln(1+e^y) \) | \( \mathbb{R} \)       | Fermi/Dirac   |
| \( -\ln x \)       | \((0, \infty)\) | \( 1 - \ln(-y) \) | \((-\infty, 0)\)     | Burg          |

Table 1: Examples of Legendre convex functions

The importance of Legendre functions is highlighted in [7] where it is shown that when \( \phi \) is Legendre, the Bregman projection defined above exists, is unique, and belongs to the interior \( \text{int}(\text{dom } \phi) \). The fact that for Legendre functions, the Bregman projection is in \( \text{int}(\text{dom } \phi) \) is crucial for iterative Bregman projection algorithms considered in the literature and in this paper because we will project \( y^* \) again and \( D_\phi(x, y^*) \) is only defined for \( y^* \in \text{int}(\text{dom } \phi) \). This was previously guaranteed by the additional requirement called “zone consistency” and the use of Legendre functions is a great simplification.

**Lemma 2.5.** *Let \( \phi \) be a Legendre convex function. Then for \( y \in \text{int}(\text{dom } \phi) \),

\[ \phi^*(y) = y \cdot \nabla \phi^*(y) - \phi(\nabla \phi^*(y)). \]

**Proof.** For fixed \( y \in \text{int}(\text{dom } \phi) \), the function \( x \mapsto x \cdot y - \phi(x) \) is concave and has zero gradient at \( x^* = \nabla \phi^*(y) \) and, therefore, achieves the maximum at \( x^* \). The lemma follows by evaluating the function \( x \mapsto x \cdot y - \phi(x) \) at \( x^* \). \( \square \)

We will also extensively use Legendre-Bregman conjugate and Legendre-Bregman projections from [25].

**Definition 2.4.** For a convex function \( \phi \) of Legendre type defined on \( \mathbb{R}^m \), the *Legendre-Bregman conjugate* of \( \phi \) is \( \ell_\phi : \text{int}(\text{dom } \phi) \times \mathbb{R}^m \to \mathbb{R} \cup \{\pm \infty\} \)

\[ \ell_\phi(y, \lambda) = \sup_{x \in \text{dom } \phi} (\lambda \cdot x - D_\phi(x, y)), \quad (5) \]
The Legendre-Bregman projection $L_\phi : \text{int(dom } \phi) \times \mathbb{R}^m \to \text{dom } \phi$ is
\[
L_\phi(y, \lambda) = \arg\max_{x \in \text{dom } \phi} (\lambda \cdot x - D_\phi(x, y)).
\]

By the definition of $\ell_\phi(y, \lambda)$ as the conjugate of function $D_\phi(\cdot, y)$, it is convex with respect to $\lambda$ for all fixed $y$, a property useful in later analysis.

The following proposition is crucial for this work and, as $\nabla \phi$ and $\nabla \phi^*$ are inverse to each other, the proposition gave $L_\phi(y, \lambda)$ the meaning of updating of the parameter by first mapping $y$ to the parameter space and pulling it back after the update using $\nabla \phi^*$.

**Proposition 2.4** (Proposition 2.6 of [25]). Let $\phi$ be a function of Legendre type. Then for $y \in \text{int(dom } \phi)$ and $\lambda \in \text{int(dom } \phi^*) - \nabla \phi(y)$, the Legendre-Bregman projection is given explicitly by
\[
L_\phi(y, \lambda) = (\nabla \phi^*)(\nabla \phi(y) + \lambda).
\]

Moreover, it can be written as a Bregman projection
\[
L_\phi(y, \lambda) = \arg\min_{x \in \text{dom } \phi \cap H_\phi} D_\phi(x, y)
\]
for the hyperplane $H = \{x \in \mathbb{R}^m | \lambda \cdot (x - L_\phi(y, \lambda)) = 0\}$.

An important corollary of the proposition and Proposition 2.3 is the following.

**Corollary 2.1.** $L_\phi(y, \lambda)$ is additive in $\lambda$. Namely, for $\lambda_1, \lambda_1 + \lambda_2 \in \text{int(dom } \phi^*) - \nabla \phi(y)$,
\[
L_\phi(L_\phi(y, \lambda_1), \lambda_2) = L_\phi(y, \lambda_1 + \lambda_2).
\]

**Lemma 2.6.** Suppose $f$ is a Legendre real convex function with domain $\Delta \subseteq \mathbb{R}$ and the domain $\text{dom } f^*$ is open. Let $a$ be a real number in $\text{cl}(\Delta) \setminus \Delta$ and $(y_t)$ be a sequence in $\Delta_{\text{int}}$ that converges to $a$. Let $(x_t)$ be a sequence in $\Delta$ that converges to $x \in \Delta$. Then
\[
\lim_{t \to \infty} D_f(x_t, y_t) = +\infty.
\]

**Proof.** As $f$ is a real convex function, it is possible to perform a case study for the domain $\Delta$. We will prove the claim for $\Delta = (a, \infty)$ and other cases can be dealt with similarly. Fix any $y \in (a, x)$, then eventually it will hold that $y_t < y$ for sufficiently large $t$. Thus,
\[
f'(y_t) \leq \frac{f(y_t) - f(y)}{y_t - y}.
\]

Hence, we have
\[
D_f(x_t, y_t) = f(x_t) - f(y_t) + f'(y_t)(y_t - x_t)
\]
\[
\geq f(x_t) - f(y_t) + \frac{f(y_t) - f(y)}{y_t - y}(y_t - x_t)
\]
\[
= f(x_t) - f(y) \frac{y_t - x_t}{y_t - y} + f(y_t) \frac{y - x_t}{y_t - y},
\]
where the first two terms converge and the third term goes to $+\infty$ when $t$ goes to $\infty$. \qed
3 Bregman Divergence for Hermitian Operators

Suppose $X$ is a finite dimensional Hilbert space and $f$ is an extended real convex function. In this section, we will always use $\Delta$ to denote the domain $\text{dom}\ f$ of $f$, the interval on which $f$ takes finite values. Then $f$ extends to all Hermitian operators in $\text{Herm}_\Delta(X)$ as

$$f(X) = \sum_k f(\lambda_k)\Pi_k$$

where $X = \sum_k \lambda_k\Pi_k$ is the spectral decomposition of $X$. In this paper, we focus on convex functions of the form $\phi = \text{tr} \circ f$. Denote the interior and boundary of $\Delta$ as $\Delta_{\text{int}}$ and $\Delta_{\text{bd}} = \Delta \setminus \Delta_{\text{int}}$ respectively. It is easy to see that the domain of $\phi$ is $\text{dom}\ \phi = \text{Herm}_\Delta(X)$, and the interior of the domain $\text{int}(\text{dom}\ \phi) = \text{Herm}_{\Delta_{\text{int}}}(X)$.

In this case, the Bregman divergence becomes

$$D_\phi(X, Y) = \text{tr}(f(X) - f(Y) - f'(Y)(X - Y)),$$

defined for $X \in \text{Herm}_{\Delta_{\text{int}}}(X)$ and $Y \in \text{Herm}_{\Delta_{\text{int}}}(X)$. The Legendre-Bregman projection can be written explicitly as

$$L_\phi(Y, \Lambda) = (f^+)'(f'(Y) + \Lambda)$$

for $Y \in \text{Herm}_{\Delta_{\text{int}}}(X)$ and $\Lambda \in \text{Herm}_{\Delta_{\text{int}}}(X) - f'(Y)$. Slightly abusing the notation, we use $D_f$, $\ell_f$ and $L_f$ to denote $D_{\text{tr} \circ f}$, $\ell_{\text{tr} \circ f}$, and $L_{\text{tr} \circ f}$ respectively.

3.1 Domain Extension

In the previous discussion, $D_f(X, Y)$, $\ell_f(Y, \Lambda)$, and $L_f(Y, \Lambda)$, are only defined for $Y \in \text{Herm}_{\Delta_{\text{int}}}(X)$. For later discussions, it is necessary to extend the definition of them to all operators $Y \in \text{Herm}_\Delta(X)$, allowing the functions to take infinite values sometimes.

We first introduce several notations used in defining the extensions. For an operator $A \in \text{Herm}_\Delta(X)$, define $X_{\text{int}}(A)$ and $X_{\text{bd}}(A)$ as the spans of eigenspaces of $A$ corresponding to eigenvalues in $\Delta_{\text{int}}$ and $\Delta_{\text{bd}}$ respectively. Then the Hilbert space $X$ has decomposition $X = X_{\text{int}}(A) \oplus X_{\text{bd}}(A)$ and the operator $A$ has decomposition $A = A_{\text{int}} \oplus A_{\text{bd}}$ for $A_{\text{int}} \in \text{Herm}(X_{\text{int}}(A))$ and $A_{\text{bd}} \in \text{Herm}(X_{\text{bd}}(A))$ by grouping its eigenspaces depending on whether the corresponding eigenvalues are in $\Delta_{\text{int}}$ or in $\Delta_{\text{bd}}$ respectively. For operators $A, B \in \text{Herm}_\Delta(X)$, we write $B_{\text{int}}(A)$ as the restriction of $B$ to $X_{\text{int}}(A)$. For operators $A, B \in \text{Herm}_\Delta(X)$, define $X_{\text{bd}}(A \wedge B)$ as the span of common eigenvectors of $A, B$ with the same eigenvalues in $\Delta_{\text{bd}}$. Define $X_{\text{int}}(A \vee B)$ as the orthonormal complement of $X_{\text{bd}}(A \wedge B)$ in $X$. For $A, B \in \text{Herm}_\Delta(X)$ and all $t \in (0, 1)$, the restriction of $(1 - t)A + tB$ to $X_{\text{int}}(A \vee B)$ has all eigenvalues contained in $\Delta_{\text{int}}$. The support $\text{supp}(A)$ of an operator $A$ is defined to be $X_{\text{int}}(A)$. For a convex set $C \subseteq \text{Herm}_\Delta(X)$, it follows from the convexity of $C$ that there is an operator $A \in C$ whose support contains the support of all other operators in $C$. This is defined to be the support $\text{supp}(C)$ of the convex set $C$.

**Definition 3.1.** Let $f$ be a real convex function with domain $\Delta$. A pair of operators $X, Y \in \text{Herm}_\Delta(X)$ is said to be admissible (with respect to $f$), written as $X \triangleright Y$, if for all eigenvalues of $Y$ in $\Delta \setminus \Delta_{\text{int}}$, the corresponding eigenspace of $Y$ is contained in the eigenspace of $X$ of the same eigenvalue. Equivalently, $X \triangleright Y$ if and only if $X = X_{\text{int}}(Y) \oplus Y_{\text{bd}}$. 


The definition of $D_f(X,Y)$ is extended to all $X,Y \in \text{dom } \phi = \text{Herm}_\Delta(\mathcal{X})$ as follows.

**Definition 3.2.** Let $f$ be real convex function of Legendre type whose domain is $\Delta$. The (extended) Bregman divergence $D_f(X,Y)$ for all $X,Y \in \text{Herm}_\Delta(\mathcal{X})$ is defined as

$$D_f(X,Y) = \begin{cases} D_f(X_{\text{int}(Y)}, Y_{\text{int}}) & \text{if } X \succ Y, \\ +\infty & \text{otherwise}. \end{cases} \quad (11)$$

This extension follows the convention in information theory where for $f(x) = x \ln x - x$, $0 \cdot f'(0) = 0 \cdot \ln 0$ is defined to be 0 so that relative entropy $D(p||q)$ is defined as long as the support of $p$ is contained in that of $q$. The convention makes sense for general real convex functions of Legendre type as it is not hard to verify that $\lim_{x \to a} ((x-a)f'(x)) = 0$ for $x$ converging in $\text{int}_\Delta$ to $a \in \Delta \setminus \text{int}_\Delta$.

Similarly, we can extend the definition of the Legendre-Bregman projection $L_f(Y,\Lambda)$ to $Y \in \text{Herm}_\Delta(\mathcal{X})$.

**Definition 3.3.** The (extended) Legendre-Bregman projection $L_f(Y,\Lambda)$ is

$$L_f(Y,\Lambda) = L(Y_{\text{int}(Y)}, \Lambda_{\text{int}(Y)}) \oplus Y_{\text{bd}}, \quad (12)$$

which is defined for all $Y \in \text{Herm}_\Delta(\mathcal{X})$ and $\Lambda$ such that

$$\Lambda_{\text{int}(Y)} \in \text{Herm}_\Delta^*(\mathcal{X}) - f'(Y_{\text{int}}). \quad (13)$$

For convenience, we say that $\Lambda$ is *admissible* (with respect to $Y$) for $L_f$ if Eq. (13) holds.

The definition can be justified as follows.

$$L_f(Y,\Lambda) = \arg \max_{X \in \text{Herm}_\Delta(\mathcal{X})} \langle \Lambda, X \rangle - D_f(X,Y)$$

$$= \arg \max_{X \in \text{Herm}_\Delta(\mathcal{X})} \left( \langle \Lambda, X \rangle - D_f(X,Y) \right)_{X \succ Y} \quad \text{(By Eq. (11))}$$

$$= \arg \max_{X \in \text{Herm}_\Delta(\mathcal{X})} \left( \langle \Lambda_{\text{int}(Y)}, X_{\text{int}(Y)} \rangle - D_f(X_{\text{int}(Y)}, Y_{\text{int}}) \right)_{X=X_{\text{int}(Y)} \oplus Y_{\text{bd}}}$$

$$= L_f(Y_{\text{int}}, \Lambda_{\text{int}(Y)}) \oplus Y_{\text{bd}}. \quad (14)$$

Hence, the extended definition of $L_f$ is consistent with the requirement that it is the maximizer of $\langle \Lambda, X \rangle - D_f(X,Y)$. This also implies that $\text{supp}(L_f(Y,\Lambda)) = \text{supp}(Y)$ by Proposition 2.3.

### 3.2 Basic Properties

**Lemma 3.1** (Corollaries 3.2 and 3.3 of [35]). Convex function $\phi = \text{tr} \circ f$ is Legendre if and only if $f$ is Legendre.

**Proof.** This follows from the fact that $\phi = \text{tr} \circ f$ is the composition of $\hat{\phi}(x) = \sum_i f(x_i)$ and the spectrum map $\text{eig}$ that returns the ordered tuple of eigenvalues of Hermitian operators. The proposition follows from Corollaries 3.2 and 3.3 of [35] as $\hat{\phi}$ as the sum of Legendre functions is Legendre. \qed
Lemma 3.2. Suppose $f$ is a real convex of Legendre type and the domain of the conjugate $\text{dom } f^*$ is open. Then $D_f(X, \cdot)$ is coercive for all $X \in \text{Herm}_\Delta(\mathcal{X})$.

Proof. Theorem 5.8 of [7] states that for real convex functions, the condition that $\text{dom } f^*$ is open is equivalent to BL0 and BL1 defined there, and is therefore also equivalent to $f$ being coercive for all $x \in \text{dom } f$ by the discussion in Remark 5.3 in that paper. This shows that $D_f(x, \cdot)$ is coercive for all $x \in \Delta$. It remains to show that the coercive property remains true when lifting $f$ to $\text{tr} \circ f$. In other words, we need to prove that the set

$$\{ Y \mid D_f(X,Y) \leq c \}$$

is bounded for all $c$.

It suffices to consider the case where $\text{supp}(Y) = \mathcal{X}$ as the general case reduces to it by the definition of extended $D_f$. Let $Y = \sum_j y_j |\psi_j\rangle \langle \psi_j|$ be the spectrum decomposition of $Y$ where $\{|\psi_j\rangle\}$ is an orthonormal basis of $\mathcal{X}$. Define

$$\tilde{x}_j = \langle \psi_j | X | \psi_j \rangle,$$

the diagonal elements of $X$ in the basis $|\psi_j\rangle$ and

$$\tilde{X} = \sum_j \tilde{x}_j |\psi_j\rangle \langle \psi_j|.$$

It is obvious that $\tilde{x}_j \in \Delta$ for all $j$.

By the definition of $D_f(X,Y)$, we have

$$D_f(X,Y) = \text{tr} \left( f(X) - f(Y) - f'(Y)(X - Y) \right)$$

$$= \text{tr} f(X) - \sum_j f(y_j) - \sum_j f'(y_j)(\tilde{x}_j - y_j)$$

$$= \text{tr} f(X) - \text{tr} f(\tilde{X}) + \sum_j D_f(\tilde{x}_j, y_j).$$

Hence, $D_f(X,Y) \leq c$ implies that for all $j$

$$D_f(\tilde{x}_j, y_j) \leq c + \text{tr} f(\tilde{X}) - \text{tr} f(X),$$

which further implies that $y_j$ is bounded for all $j$ as $D_f(\tilde{x}_j, \cdot)$ is coercive.

Lemma 3.3. For all Legendre $f$, the Legendre-Bregman projection $L_f(Y, \Lambda)$ is continuous on its domain.

Proof. Using Eq. (10), we have $L_f(Y, \Lambda) = (f^*)'(f'(Y) + \Lambda)$. As $f$ is Legendre, both $(f^*)'$ and $f'$ are continuous in the interior of the domain $\Delta_{\text{int}}$ by Proposition 2.3. Let $(Y^{(n)}, \Lambda^{(n)})$ be a sequence that converges to $(Y, \Lambda)$. If $Y$ is in the interior $\text{Herm}_{\Delta_{\text{int}}}(\mathcal{X})$, the claim follows from the continuity of $f'$ and $(f^*)'$. Otherwise, suppose $Y = Y_{\text{int}} \oplus Y_{\text{bd}}$. Without loss of generality, assume $Y^{(t)} \in \text{Herm}_{\Delta_{\text{int}}}(\mathcal{X})$ and write

$$Y^{(t)} = Y_i^{(t)} \oplus Y_b^{(t)},$$
such that \( \lim_{t \to \infty} Y_i(t) = Y_{\text{int}} \) and \( \lim_{t \to \infty} Y_b(t) = Y_{\text{bd}} \). In the basis of the decomposition \( Y(t) = Y_i(t) \oplus Y_b(t) \), write \( \Lambda(t) = \begin{pmatrix} \Lambda_{00}(t) & \Lambda_{01}(t) \\ \Lambda_{10}(t) & \Lambda_{11}(t) \end{pmatrix} \). Hence,

\[
    f'(Y(t)) + \Lambda(t) = \begin{pmatrix} f'(Y_i(t)) + \Lambda_{00}(t) \\ \Lambda_{10}(t) f'(Y_b(t)) + \Lambda_{11}(t) \end{pmatrix} = \begin{pmatrix} A_0 \\ B \end{pmatrix} \left( \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right) \begin{pmatrix} A_0 \\ B \end{pmatrix},
\]

where we have omitted the dependence of \( A_0, A_1, \) and \( B \) on \( t \) for simplicity. Let \( V \) be the unitary that diagonalizes the matrix

\[
    \begin{pmatrix} A_0 & B \\ B^\dagger & A_1 \end{pmatrix} = V \begin{pmatrix} \Gamma_0 & 0 \\ 0 & \Gamma_1 \end{pmatrix} V^\dagger \tag{15}
\]

so that \( \Gamma_0 \) is a diagonal matrix that has all the small eigenvalues of \( \begin{pmatrix} A_0 & B \\ B^\dagger & A_1 \end{pmatrix} \) on its diagonal. Write \( V = \begin{pmatrix} C_0 & -S_1 \\ S_0 & C_1 \end{pmatrix} \) and expand the block matrix multiplication we have

\[
    A_0 = C_0 \Gamma_0 C_0^\dagger + S_1 \Gamma_1 S_1^\dagger, \\
    B^\dagger = S_0 \Gamma_0 C_0^\dagger - C_1 \Gamma_1 S_1^\dagger. \tag{16}
\]

The unitarity of \( V \) implies

\[
    C_0^\dagger C_0 + S_0^\dagger S_0 = 1, \\
    C_1^\dagger C_1 + S_1^\dagger S_1 = 1, \\
    S_1^\dagger C_0 - C_1^\dagger S_0 = 0. \tag{17}
\]

Using the above Eqs. (16) and (17),

\[
    S_1^\dagger A_0 - C_1^\dagger B^\dagger = (S_1^\dagger C_0 - C_1^\dagger S_0) \Gamma_0 C_0^\dagger + (S_1^\dagger S_1 + C_1^\dagger C_1) \Gamma_1 S_1^\dagger = \Gamma_1 S_1^\dagger. \tag{18}
\]

By the essential smoothness of the function \( f \) and Proposition 2.1, \( \Gamma_1 \) has eigenvalues that all go to \( \pm \infty \) when \( t \) goes to \( \infty \). And by Proposition 2.2, the norm \( \| S_0 \| \) (and \( \| S_1 \| \)) go to 0 as they are bounded by \( \| B \| / \eta \) where \( \eta \) is the gap between the eigenvalues of \( A_0 \) and \( \Gamma_1 (\Gamma_0 \) and \( A_1, \) respectively), a quantity that goes to \( +\infty \) when \( t \) goes to \( \infty \).

Using Eqs. (16) and (18), we expand \( A_0 \) as

\[
    A_0 = C_0 \Gamma_0 C_0^\dagger + S_1 \Gamma_1 S_1^\dagger = C_0 \Gamma_0 C_0^\dagger + S_1 S_1^\dagger A_0 - S_1 C_1^\dagger B^\dagger,
\]

and hence

\[
    \lim_{t \to \infty} A_0 = \lim_{t \to \infty} C_0 \Gamma_0 C_0^\dagger,
\]

12
because $A_0$ and $B^\dagger$ are finite and $\|S_i\|$ goes to 0 as $t$ goes to $\infty$. Define $L_0 = (f^*)'(\Gamma_0)$ and $L_1 = (f^*)'(\Gamma_1)$. It is easy to check that

\[
\lim_{t \to \infty} C_0 L_0 C_0^\dagger = \lim_{t \to \infty} (f^*)'(C_0 \Gamma_0 C_0^\dagger) = (f^*)'(f'(Y_{\text{int}}) + \Lambda_{\text{int}(Y)}) = \mathcal{L}_f(Y_{\text{int}}, \Lambda_{\text{int}(Y)}),
\]

and similarly

\[
\lim_{t \to \infty} C_1 L_1 C_1^\dagger = \lim_{t \to \infty} (f^*)'(f'(Y_{\text{int}}^{(t)})) = Y_{\text{bd}}.
\]

Finally, it follows from the definition of $\mathcal{L}_f$ that

\[
\mathcal{L}_f(Y^{(t)}, \Lambda^{(t)}) = V \begin{pmatrix} (f^*)'(\Gamma_0) & 0 \\ 0 & (f^*)'(\Gamma_1) \end{pmatrix} V^\dagger
\]

\[
= \begin{pmatrix} C_0 & -S_1 \\ S_0 & C_1 \end{pmatrix} \begin{pmatrix} L_0 & 0 \\ 0 & L_1 \end{pmatrix} \begin{pmatrix} C_0^\dagger & S_0^\dagger \\ -S_1^\dagger & C_1^\dagger \end{pmatrix}
\]

\[
= \begin{pmatrix} C_0 L_0 C_0^\dagger + S_1 L_1 S_1^\dagger & C_0 L_0 S_0^\dagger - S_1 L_1 C_1^\dagger \\ S_0 L_0 C_0^\dagger - C_1 L_1 S_1^\dagger & S_0 L_0 S_0^\dagger + C_1 L_1 C_1^\dagger \end{pmatrix},
\]

and hence,

\[
\lim_{t \to \infty} \mathcal{L}_f(Y^{(t)}, \Lambda^{(t)}) = \lim_{t \to \infty} \begin{pmatrix} C_0 L_0 C_0^\dagger & 0 \\ 0 & C_1 L_1 C_1^\dagger \end{pmatrix}
\]

\[
= \mathcal{L}_f(Y_{\text{int}}, \Lambda_{\text{int}(Y)}) \oplus Y_{\text{bd}}
\]

\[
= \mathcal{L}_f(Y, \Lambda),
\]

which completes the proof. □

Lemma 3.4. Suppose $f$ is a Legendre convex function. For all $X, Y \in \text{Herm}_\Delta(\mathcal{X})$ such that $X \triangleright Y$, and all admissible $\Lambda$, the following two identities hold

\[
D_f(X, Y) - D_f(X, \mathcal{L}_f(Y, \Lambda)) = \langle \Lambda, X \rangle - \ell_f(Y, \Lambda),
\]

\[
D_f(X, Y) - D_f(X, \mathcal{L}_f(Y, \Lambda)) = D_f(\mathcal{L}_f(Y, \Lambda), Y) + \langle \Lambda, X - \mathcal{L}_f(Y, \Lambda) \rangle.
\]

Proof. We first prove the lemma for the case when $\text{supp}(Y) = \mathcal{X}$. By expanding the definition of $D_f$ and abbreviating $\mathcal{L}_f(Y, \Lambda)$ as $L$, we have

\[
D_f(X, Y) - D_f(X, L)
\]

\[
= \text{tr}(f(L) - f(Y) + f'(L)(X - L) - f'(Y)(X - Y))
\]

\[
= \text{tr}(f(L) - f(Y) + (f'(Y) + \Lambda)(X - L) - f'(Y)(X - Y)) \quad \text{(Proposition 2.3)}
\]

\[
= \text{tr}(\Lambda(X - L) + f(L) - f(Y) - f'(Y)(L - Y))
\]

\[
= \text{tr}(\Lambda(X - L) + D_f(L, Y))
\]

\[
= \langle \Lambda, X \rangle - \ell_f(Y, \Lambda).
\]
In general, the definition of $D_f$ and $\mathcal{L}_f$ on the extended domain implies
\[
D_f(X, Y) - D_f(X, \mathcal{L}_f(Y, \Lambda)) = D_f(\hat{X}, \hat{Y}) - D_f(\hat{X}, \mathcal{L}_f(\hat{Y}, \hat{\Lambda})),
\]
where $\hat{X}$, $\hat{Y}$, and $\hat{\Lambda}$ are restrictions of $X$, $Y$, and $\Lambda$ to $\text{supp}(Y)$. By the calculation in Eq. (21), this further simplifies to
\[
\langle \hat{\Lambda}, \hat{X} \rangle - \ell_f(\hat{Y}, \hat{\Lambda}) = \langle \hat{\Lambda}, \hat{X} \rangle - \ell_f(Y, \Lambda) + \langle \Lambda, Y_{\text{bd}} \rangle = \langle \Lambda, X \rangle - \ell_f(Y, \Lambda).
\]
This proves Eq. (19). Equation (20) follows from Eq. (19) and the fact that $\mathcal{L}_f(Y, \Lambda)$ is the minimizer for $\ell_f(Y, \Lambda)$.

\[\square\]

**Lemma 3.5.** For Legendre convex function $f$ and $X, Y \in \text{Herm}_\Delta(\mathcal{X})$ such that $X \triangleright Y$, the mapping $t \mapsto D_f(X, \mathcal{L}_f(Y, t\Lambda))$ is differentiable at $t = 0$ with derivative
\[
\frac{d}{dt} D_f(X, \mathcal{L}_f(Y, t\Lambda)) \bigg|_{t=0} = \langle \Lambda, Y - X \rangle.
\]

**Proof.** We first compute the derivative
\[
\frac{d}{dt} D_f(\mathcal{L}_f(Y, t\Lambda), Y) \bigg|_{t=0} = \frac{d}{dt} \text{tr} \left( f(\mathcal{L}_f(Y, t\Lambda)) - f'(Y)\mathcal{L}_f(Y, t\Lambda) \right) \bigg|_{t=0} = \left( f'(\mathcal{L}_f(Y, t\Lambda)) - f'(Y), \frac{d}{dt} \mathcal{L}_f(Y, t\Lambda) \right) \bigg|_{t=0} = 0,
\]
where the third line uses Eq. (2) and the last line follows from $\mathcal{L}_f(Y, 0) = Y$. Using Eq. (20) of Lemma 3.4, we have
\[
\frac{d}{dt} D_f(X, \mathcal{L}_f(Y, t\Lambda)) \bigg|_{t=0} = \left( \langle t\Lambda, \mathcal{L}_f(Y, t\Lambda) - X \rangle - D_f(\mathcal{L}_f(Y, t\Lambda), Y) \right) \bigg|_{t=0} = \left( \langle \Lambda, \mathcal{L}_f(Y, t\Lambda) - X \rangle - \frac{d}{dt} D_f(\mathcal{L}_f(Y, t\Lambda), Y) \right) \bigg|_{t=0} = \langle \Lambda, Y - X \rangle.
\]
\[\text{(By Eq. (23))}\]

\[\square\]

**Lemma 3.6.** Let $f$ be a Legendre function and $\Lambda$ is admissible. $\ell_f(Y, \Lambda)$ has the following explicit form
\[
\ell_f(Y, \Lambda) = \text{tr} f^*(f'(Y) + \Lambda) - \text{tr} f^*(f'(Y)).
\]

**Proof.** Taking $X = Y$ in Eq. (19) and letting $R = f'(Y) + \Lambda$ and $L = \mathcal{L}_f(Y, \Lambda) = (f^*)'(R)$, we have
\[
\ell_f(Y, \Lambda) = \langle \Lambda, Y \rangle + D_f(Y, \mathcal{L}_f(Y, \Lambda)) = \langle \Lambda, Y \rangle + \text{tr} (f(Y) - f(L) - f'(L)(Y - L)) = \langle \Lambda, Y \rangle + \text{tr} (f(Y) - f((f^*)'(R)) - R(Y - L)) = \text{tr} (R(f^*)'(R) - f((f^*)'(R))) - \text{tr} (f'(Y)Y - f(Y)) = \text{tr} f^*(f'(Y) + \Lambda) - \text{tr} f^*(f'(Y)),
\]
where the last line follows from Lemma 2.5.

\[\square\]
Lemma 3.7. For Legendre convex function $f$ and a list of Hermitian matrices $F = (F_1, F_2, \ldots, F_k)$,
\[
\frac{\partial}{\partial \lambda_j} \ell_f(Y, \lambda \cdot F) = \langle F_j, \mathcal{L}_f(Y, \lambda \cdot F) \rangle.
\]

Proof. By Lemma 3.6, we can write
\[
\frac{\partial}{\partial \lambda_j} \ell_f(Y, \lambda \cdot F) = \frac{\partial}{\partial \lambda_j} \operatorname{tr} f^*(f(Y) + \lambda \cdot F)
= \langle F_j, (f^*)'(f(Y) + \lambda \cdot F) \rangle \quad \text{(By Eq. (2))}
= \langle F_j, \mathcal{L}_f(Y, \lambda \cdot F) \rangle.
\]

Lemma 3.8. Suppose $f$ is a Legendre convex function with domain $\Delta$ and the domain $\operatorname{dom} f^*$ is open. Let $c$ be a constant and a sequence $\{Y^{(t)}\}$ in $\operatorname{Herm}_\Delta(\mathcal{X})$ satisfies that $D_f(X, Y^{(t)}) \leq c$. Then $\{Y^{(t)}\}$ has a limiting point $\hat{Y}$ in $\operatorname{Herm}_\Delta(\mathcal{X})$.

Proof. As the domain $\operatorname{dom} f^*$ is open, Lemma 3.2 guarantees that $D_f(X, \cdot)$ is coercive for all $X \in \operatorname{Herm}_\Delta(\mathcal{X})$. That is, the sequence $\{Y^{(t)}\}$ is bounded. Hence, there must be a subsequence $\{Y^{(t_i)}\}$ of $\{Y^{(t)}\}$ that converges to $\hat{Y}$. We will show that $\hat{Y}$ is in $\operatorname{Herm}_\Delta(\mathcal{X})$. Assume to the contrary that $\hat{Y}$ is not in $\operatorname{Herm}_\Delta(\mathcal{X})$ and it has eigenvalues in $\operatorname{cl}(\Delta) \setminus \Delta$. Let $a \in \mathbb{R}$ be such an eigenvalue. $Y^{(t_i)} = \sum_j y_j^{(t_i)} \langle \psi_j^{(t_i)} \rangle \langle \psi_j^{(t_i)} \rangle$ be the spectrum decomposition of $Y^{(t_i)}$. Define $x_j^{(i)} = \langle \psi_j^{(t_i)} \rangle \langle X \psi_j^{(i)} \rangle$ and
\[
X^{(i)} = \sum_j x_j^{(i)} \langle \psi_j^{(i)} \rangle \langle \psi_j^{(i)} \rangle.
\]

As in the proof of Lemma 3.2, we have
\[
D_f(X, Y^{(t_i)}) = \operatorname{tr} f(X) - \operatorname{tr} f(X^{(i)}) + \sum_j D_f(x_j^{(i)}, y_j^{(i)}).
\]

Then we have $D_f(X, Y^{(t_i)})$ goes to $+\infty$ by Lemma 2.6, a contradiction with the assumption that $D_f(X, Y^{(t)}) \leq c$. \hfill \Box

3.3 Linear Families and Legendre-Bregman Projection Families

Definition 3.4. Given $X_0 \in \operatorname{Herm}_\Delta(\mathcal{X})$ and a tuple $F = (F_j)_{j=1}^k$ of Hermitian matrices $F_j$, the linear family for $X_0$ and $F$ is defined by
\[
\mathcal{L}(X_0, F) = \{ X \in \operatorname{Herm}_\Delta(\mathcal{X}) \mid \langle F_j, X \rangle = \langle F_j, X_0 \rangle, j = 1, 2, \ldots, k \}.
\]

For $Y_0 \in \operatorname{Herm}_\Delta$, the Legendre-Bregman projection family for $Y_0$ and $F$ is defined by
\[
\mathcal{P}(Y_0, F) = \{ Y \in \operatorname{Herm}_\Delta(\mathcal{X}) \mid Y = \mathcal{L}_f(Y_0, \lambda \cdot F) \}.
\]

We usually simply denote the two families of operators as $\mathcal{L}$ and $\mathcal{P}$ when $X_0, Y_0$, and $F$ is obvious from the context.

Lemma 3.9. Suppose $f$ is a real convex function of Legendre type and $\operatorname{dom} f^*$ is open. If $D_f(X_0, Y_0) < \infty$, then $\mathcal{L} \cap \operatorname{cl}(\mathcal{P})$ is nonempty.
Proof. By Lemma 3.2, $D_f(X_0, \cdot)$ is coercive, meaning that

$$\mathcal{R} = \{Y \mid D_f(X_0, Y) \leq D_f(X_0, Y_0)\}$$

is bounded. Hence, the minimization

$$\arg\min_{Y \in \text{cl}(\mathcal{R})} D_f(X_0, Y) = \arg\min_{Y \in \text{cl}(\mathcal{R} \cap \mathcal{L})} D_f(X_0, Y),$$

is obtained at a point $Y^*$ (not necessarily unique) in $\text{cl}(\mathcal{R} \cap \mathcal{L}) \subseteq \text{cl}(\mathcal{P})$. We will prove that $Y^* \in \mathcal{L}$.

Let $\overline{Y} \in \text{cl}(\mathcal{P})$ be such that $\overline{Y} = \lim_{j \to \infty} L_f(Y_0, \mu_j \cdot F)$. Then by the continuity of the $L_f$ proved in Lemma 3.3,

$$L_f(\overline{Y}, \lambda \cdot F) = \lim_{j \to \infty} L_f(L_f(Y_0, \mu_j \cdot F), \lambda \cdot F)$$

$$= \lim_{j \to \infty} L_f(Y_0, (\mu_j + \lambda) \cdot F) \in \text{cl}(\mathcal{P}).$$

Thus, for the limiting point $Y^* \in \text{cl}(\mathcal{P})$, $L_f(Y^*, \lambda \cdot F)$ is in $\text{cl}(\mathcal{P})$ for all admissible $\lambda$. By the optimality of $Y^*$, $D_f(X_0, L_f(Y^*, \lambda \cdot F))$ achieves a minimum at $\lambda = 0$. By Lemma 3.5, we conclude that $(F_j, Y^*) = (F_j, X_0)$ and $Y^* \in \mathcal{L}$. 

\[ \Box \]

Lemma 3.10. The Pythagorean identity

$$D_f(X, Y) = D_f(X, Y^*) + D_f(Y^*, Y) \quad (25)$$

holds for all $X \in \mathcal{L}$, $Y \in \text{cl}(\mathcal{P})$ and $Y^* \in \mathcal{L} \cap \text{cl}(\mathcal{P})$.

Proof. Suppose that $X_1, X_2, Y_1, Y_2 \in \text{Herm}_\Delta(\mathcal{X})$ satisfying $X_j \triangleright Y_j$ for $j = 1, 2$ and $Y_2 = L_f(Y_1, \lambda \cdot F)$. By Eq. (19), we have

$$D_f(X_1, Y_1) - D_f(X_1, Y_2) = \langle \lambda \cdot F, X_1 \rangle - \ell_f(Y_1, \lambda \cdot F)$$

and

$$D_f(X_2, Y_1) - D_f(X_2, Y_2) = \langle \lambda \cdot F, X_2 \rangle - \ell_f(Y_1, \lambda \cdot F)$$

Taking the difference of the above two equations, we have

$$D_f(X_1, Y_1) - D_f(X_1, Y_2) - D_f(X_2, Y_1) + D_f(X_2, Y_2) = 0.$$

The lemma follows by choosing $X_1 = Y_1 = Y^*$. 

\[ \Box \]

3.4 Duality Theorem

Theorem 3.1. Suppose $f$ is a real convex function of Legendre type and $\text{dom} f^*$ is open. Let $\Delta$ be the domain of $f$ and $X_0, Y_0 \in \text{Herm}_\Delta(\mathcal{X})$ be two Hermitian operators satisfying $D_f(X_0, Y_0) < \infty$. Let $\mathcal{L}$ and $\mathcal{P}$ be the linear family of $X_0$ and the Legendre-Bregman projection family of $Y_0$ with respect to $F = (F_j)$. Then there is a unique $Y^* \in \text{Herm}_\Delta(\mathcal{X})$ such that

1. $Y^* \in \mathcal{L} \cap \text{cl}(\mathcal{P})$, 

2. $D_f(X, Y) = D_f(X, Y^*) + D_f(Y^*, Y)$ for any $X \in \mathcal{L}$ and $Y \in \text{cl} (\mathcal{P})$.
3. $Y^* = \arg\min_{X \in \mathcal{L}} D_f(X, Y_0)$.
4. $Y^* = \arg\min_{Y \in \text{cl}(\mathcal{P})} D_f(X_0, Y)$.

Moreover any one of these four conditions determines $Y^*$ uniquely.

Proof. Choose any point $Y^*$ in $\mathcal{L} \cap \text{cl} (\mathcal{P})$, whose existence is guaranteed by Lemma 3.9. It satisfies Item 1 by definition, Item 2 by Lemma 3.10. As a consequence of Item 2, it also satisfies Items 3 and 4. More specifically, Item 3 holds because for all $X \in \mathcal{L}$, it follows from Item 2 that

$$D_f(X, Y_0) = D_f(X, Y^*) + D_f(Y^*, Y_0) \geq D_f(Y^*, Y_0),$$

and equality holds if and only if $D_f(X, Y^*) = 0$, that is $X = Y^*$. Similarly, for all $Y \in \text{cl}(\mathcal{P})$, Item 2 implies that

$$D_f(X_0, Y) = D_f(X_0, Y^*) + D_f(Y^*, Y) \geq D_f(X_0, Y^*),$$

and equality holds if and only if $D_f(Y^*, Y) = 0$, or equivalently $Y = Y^*$. This proves Item 4.

It remains to show that each of the four Items 1 to 4 determines $Y^*$ uniquely. In other words, if $\tilde{Y}$ is an operator in $\text{Herm}_{\Delta}(\mathcal{X})$ satisfying any of the four Items, then $\tilde{Y} = Y^*$. Suppose first $\tilde{Y} \in \mathcal{L} \cap \text{cl}(\mathcal{P})$. It follows from Item 2 that

$$D_f(\tilde{Y}, Y^*) + D_f(Y^*, \tilde{Y}) = D_f(\tilde{Y}, \tilde{Y}) = 0,$$

which guarantees that $\tilde{Y} = Y^*$. If $\tilde{Y}$ satisfies Item 2, the same argument with the role of $\tilde{Y}$ and $Y^*$ reversed proves that $\tilde{Y} = Y^*$. If $\tilde{Y}$ is a minimizer for Item 3, we have by Item 2 that

$$D_f(X_0, Y^*) \geq D_f(X_0, \tilde{Y}) = D_f(X_0, Y^*) + D_f(Y^*, \tilde{Y}),$$

which implies $D_f(Y^*, \tilde{Y}) \leq 0$ and $\tilde{Y} = Y^*$. Similarly, if $\tilde{Y}$ is a minimizer for Item 4, we have by Item 2 that

$$D_f(Y^*, Y_0) \geq D_f(\tilde{Y}, Y_0) = D_f(\tilde{Y}, Y^*) + D_f(Y^*, Y_0).$$

This implies that $D_f(\tilde{Y}, Y^*) \leq 0$ and $\tilde{Y} = Y^*$. \qed

## 4 Iterative Algorithms

In this section, we present several iterative algorithms that are based on Bregman’s projection method. We start with an exact projection algorithm given in Meta-Algorithm 1. The fact this is indeed a Bregman projection algorithm will become obvious when we analyze the algorithm.

### 4.1 Exact Bregman Projection Algorithm

**Theorem 4.1.** Meta-Algorithm 1 outputs a sequence $\lambda^{(1)}, \lambda^{(2)}, \ldots$ such that

$$\lim_{t \to \infty} D_f(X_0, \mathcal{L}_f(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\lambda \in \mathbb{R}^k} D_f(X_0, \mathcal{L}_f(Y_0, \lambda \cdot F)).$$
Meta-Algorithm 1: Bregman’s Exact Iterative Projection Algorithm.

Proof. We consider the $t$-th iteration of the algorithm. The matrix $Y^{(t)}$ is our current estimate of the solution and the algorithms computes an update in Line 5 which can be understood as a Bregman’s projection as follows. Let $j_t$ be the index used in the algorithm and define the linear family

$$\mathcal{L}_{j_t} = \{ X \in \text{Herm}_\Delta(\mathcal{X}) \mid \langle F_{j_t}, X \rangle = \langle F_{j_t}, X_0 \rangle \},$$

and Legendre-Bregman projection family

$$\mathcal{P}_{j_t} = \{ Y \in \text{Herm}_\Delta(\mathcal{X}) \mid Y = \mathcal{L}_f(Y^{(t)}, \delta^{(t)} F_{j_t}) \}.$$

The projection of $Y^{(t)}$ onto $\mathcal{L}_{j_t}$ is in the intersection of $\mathcal{L}_{j_t}$ and $\mathcal{P}_{j_t}$, and therefore it can be written as $\mathcal{L}_f(Y^{(t)}, \delta^{(t)} F_{j_t})$ for some real parameter $\delta$. By the fact that is also in the linear family $\mathcal{L}_{j_t}$, we have that $\delta = \delta^{(t)}$ uniquely determined by the equation in Line 5 of Meta-Algorithm 1.

Define an auxiliary function

$$A(Y, \delta) = \langle \delta F_{j^*}, X_0 \rangle - \ell_f(Y, \delta F_{j^*})$$

for $j^* = \arg\max_j |\langle F_j, Y - X_0 \rangle|$. As $\ell_f(Y, \delta F_{j^*})$ is convex in $\delta$, $A(Y, \delta)$ is concave in $\delta$. In each step the algorithm makes progress measured by the quantity

$$D_f(X_0, Y^{(t)}) - D_f(X_0, Y^{(t+1)})$$

$$= D_f(X_0, Y^{(t)}) - D_f(X_0, \mathcal{L}_f(Y^{(t)}, \delta^{(t)} F_{j_t}))$$

$$= \langle \delta^{(t)} F_{j_t}, X_0 \rangle - \ell_f(Y^{(t)}, \delta^{(t)} F_{j_t})$$

$$= A(Y^{(t)}, \delta^{(t)}).$$

(By Eq. (19))
It is easy to verify that \( \mathcal{A}(Y, 0) = 0 \). From Lemma 3.7 and the concavity of \( \mathcal{A} \) in \( \delta \), the choice of \( \delta^{(t)} \) in the algorithm maximizes \( \mathcal{A}(Y^{(t)}, \delta) \) over \( \delta \) and we have

\[
\mathcal{A}(Y^{(t)}, \delta^{(t)}) \geq \mathcal{A}(Y^{(t)}, 0) = 0.
\]

Adding the above displayed equation together for \( t = 1, 2, \ldots, T - 1 \) gives

\[
D_f(X_0, Y^{(1)}) - D_f(X_0, Y^{(T)}) = \sum_{t=1}^{T-1} \mathcal{A}(Y^{(t)}, \delta^{(t)}).
\]

Since \( D_f(X_0, Y^{(1)}) = D_f(X_0, Y_0) < \infty \) and \( \mathcal{A}(Y^{(t)}, \delta^{(t)}) \geq 0 \) for all \( t \), it follows that \( D_f(X_0, Y^{(t)}) \) is bounded and, by Lemma 3.8, the sequence \( (Y^{(t)})^\infty_{t=1} \) has a subsequence \( (Y^{(t_i)}) \) converging to \( \hat{Y} \in \text{Herm}_\Delta(\mathcal{X}) \).

We claim that for the limiting point \( \hat{Y} \), \( \max_\delta \mathcal{A}(\hat{Y}, \delta) = 0 \). Otherwise, assume there exist a \( \delta \) and an \( \varepsilon > 0 \) such that \( \mathcal{A}(Y, \delta) = \varepsilon > 0 \). By the continuity of \( \mathcal{A} \) with respect to \( Y \), it follows that there is an integer \( m > 0 \) such that for all \( i \geq m \), \( \mathcal{A}(Y^{(t_i)}, \delta^{(t_i)}) \geq \mathcal{A}(Y^{(t_i)}, \delta) \geq \varepsilon/2 \). This is a contradiction with the fact that \( (\mathcal{A}(Y^{(t)}, \delta^{(t)}))_t \) converges to 0.

Finally, we show that the condition \( \max_\delta \mathcal{A}(\hat{Y}, \delta) = 0 \) implies that \( \hat{Y} \) is in \( \mathcal{L} \). Assume on the other hand that \( \hat{Y} \) is not in \( \mathcal{L} \) and, hence, for

\[
\hat{j^*} = \arg\max_j \left| \langle F_j, \hat{Y} - X_0 \rangle \right|,
\]

we must have

\[
\langle F_{\hat{j}^*}, \hat{Y} - X_0 \rangle \neq 0.
\] (26)

As

\[
\frac{d}{d\delta} \mathcal{A}(Y, \delta) = \langle F_{\hat{j}^*}, X_0 \rangle - \langle F_{\hat{j}^*}, \mathcal{L}_f(\hat{Y}, \delta F_{\hat{j}^*}) \rangle,
\]

the maximizer \( \hat{\delta}^* \) of \( \max_\delta \mathcal{A}(\hat{Y}, \delta) \) satisfies

\[
\langle F_{\hat{j}^*}, X_0 - \mathcal{L}_f(Y, \hat{\delta}^* F_{\hat{j}^*}) \rangle = 0.
\] (27)

Therefore,

\[
\max_\delta \mathcal{A}(\hat{Y}, \delta) = \mathcal{A}(\hat{Y}, \hat{\delta}^*)
\]

\[
= \langle \delta^* F_{\hat{j}^*}, X_0 \rangle - \ell_f(\hat{Y}, \delta^* F_{\hat{j}^*})
\]

\[
= \langle \delta^* F_{\hat{j}^*}, X_0 - \mathcal{L}_f(\hat{Y}, \delta^* F_{\hat{j}^*}) \rangle + D_f(\hat{Y}, \mathcal{L}_f(\hat{Y}, \delta^* F_{\hat{j}^*}))
\]

\[
= D_f(\hat{Y}, \mathcal{L}_f(\hat{Y}, \delta^* F_{\hat{j}^*})),
\]

where the third line uses the definition of \( \ell_f \) and the fourth uses Eq. (27). Now, \( \max_\delta \mathcal{A}(\hat{Y}, \delta) = 0 \) implies \( D_f(\hat{Y}, \mathcal{L}_f(\hat{Y}, \delta^* F_{\hat{j}^*})) = 0 \) and \( \hat{Y} = \mathcal{L}_f(\hat{F}, \delta^* F_{\hat{j}^*}) \). But then Eq. (27) becomes

\[
\langle F_{\hat{j}^*}, X_0 - \hat{Y} \rangle = 0,
\]

contradicting Eq. (26). Therefore \( \hat{Y} \in \mathcal{L} \) and by definition \( \hat{Y} \) is also in \( \text{cl} (\mathcal{P}) \). By the duality theorem in Theorem 3.1, \( \hat{Y} \) is the unique projection of \( X_0 \) to the projection family \( \mathcal{P} \). 

\( \square \)
4.2 Approximate Bregman Projection Algorithms

Most of the time, the exact Bregman projection equation (Line 5 in Meta-Algorithm 1) could be hard to solve. In the literature, a class of approximate projection algorithms are known whose corresponding equations are usually much easier to solve and sometimes have simple explicit formulas. We follow the auxiliary function approach [25, 19] to derive our approximate projection algorithms. Like in [19], both a parallel update algorithm (Meta-Algorithm 2) and a sequential update algorithm (Meta-Algorithm 3) are considered. Thanks to the generality of the auxiliary function method, we are able to prove the convergence for them in a uniform manner.

The equation in Line 5 of Meta-Algorithm 2 may seem complicated at first glance, but as we will see later in special examples, it is a simpler equation to solve. In the parallel projection algorithm, the parameters corresponding to \( F_j \) are updated simultaneously in each iteration. In this case, we require that \( \sum_{j=1}^{k} |F_j| \leq 1 \), a technical condition for the convergence proof to work in the parallel update algorithms.

Unlike the classical case where the convergence of similar approximate projection algorithms always holds, in the non-commutative case, we require a strong convex condition of \( \ell_f \) to hold.

**Definition 4.1.** The Legendre-Bregman conjugate \( \ell_f(Y, \Lambda) \) is strongly convex if for operators \( F_j \succeq 0 \) and \( \sum_j F_j = 1 \),

\[
\ell_f(Y, \delta \cdot F) \leq \text{tr} \left( \sum_{j=1}^{k} \hat{\ell}_f(Y, \delta_j) F_j \right),
\]

where \( \hat{\ell}_f(Y, \delta_j) \) is the application of \( \ell_f(\cdot, \delta_j) \) to \( Y \).

**Lemma 4.1.** The Legendre-Bregman conjugate is strongly convex if and only if

\[
\text{tr} \ f^*(f'(Y) + \delta \cdot F) \leq \text{tr} \sum_{j=1}^{k} \left( f^*(f'(Y) + \delta_j) F_j \right).
\]

**Proof.** This directly follows from Lemma 3.6.

If \( f'(Y) \) and \( F_j \)'s are commuting, the inequality for strong convexity is always true and follows from Jensen’s trace inequality as long as \( f^* \) is convex. This is not the case however in the non-commutative case.

**Theorem 4.2.** Suppose \( \ell_f \) is strongly convex. Then Meta-Algorithm 2 outputs a sequence \( \lambda^{(1)}, \lambda^{(2)}, \ldots \) such that

\[
\lim_{t \to \infty} D_f(X_0, \mathcal{L}_f(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\Lambda \in \mathbb{R}^k} D_f(X_0, \mathcal{L}_f(Y_0, \lambda \cdot F)).
\]

**Proof.** For all \( \delta \in \mathbb{R} \) and Hermitian matrix \( Y \), define \( \hat{\ell}_f(Y, \delta) \) as the application of function \( \ell_f(\cdot, \delta) \) to matrix \( Y \). That is, if \( Y = \sum_i y_i \Pi_i \) is a spectrum decomposition of \( Y \),

\[
\hat{\ell}_f(Y, \delta) = \sum_i \ell_f(y_i, \delta) \Pi_i.
\]
This proves our claim about the optimality of $\delta$ to compute the derivative of $A$. The fact that $\hat{\delta}$ maximized over $(t; X)$ is open.

**Output:** $\lambda^{(1)}, \lambda^{(2)}, \cdots$ such that

$$\lim_{t \to \infty} D_f(X_0, L_f(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\lambda \in \mathbb{R}^k} D_f(X_0, L_f(Y_0, \lambda \cdot F)).$$

1: Initialize $\lambda^{(1)} = (0, 0, \ldots, 0)$.
2: for $t = 1, 2, \ldots$ do
3: Compute $Y^{(t)} = L_f(Y_0, \lambda^{(t)} \cdot F)$.
4: for $j = 1, 2, \ldots, k$ do
5: Solve the following equation of $\delta_j^{(t)}$:
   $$\text{tr} \left( F_j^+ L_f(Y^{(t)}, \delta_j^{(t)}) - F_j^- L_f(Y^{(t)}, -\delta_j^{(t)}) \right) = \langle F_j, X_0 \rangle.$$
6: end for
7: Update parameters $\lambda^{(t+1)} = \lambda^{(t)} + \delta^{(t)}$.
8: end for

Meta-Algorithm 2: Parallel Approximate Projection Algorithm.

Define an auxiliary function $A$ as

$$A(Y, \delta) = \langle \delta \cdot F, X_0 \rangle - \text{tr} \left( \hat{\ell}_f(Y, \delta_j) F_j^+ + \hat{\ell}_f(Y, -\delta_j) F_j^- \right). \quad (28)$$

We claim several properties of the auxiliary function $A$.

First, it is easy to verify that $A(Y, 0) = 0$. This follows from the definition of $A$ and the fact that $\hat{\ell}_f(Y, 0) = 0$ for all $Y$.

Second, the choice of $\delta_j^{(t)}$'s in the algorithm is exactly those so that $A(Y^{(t)}, \delta^{(t)})$ is maximized over $\delta^{(t)}$. To see this, we first notice that $\hat{\ell}_f(Y, \delta)$ is convex in $\delta$, $A$ is concave in $\delta^{(t)}$, and the maximum is achieved at the point with zero gradient. Next, we use Lemma 3.7 to compute the derivative of $A(Y^{(t)}, \delta^{(t)})$ with respect to $\delta_j^{(t)}$ as

$$\langle F_j, X_0 \rangle - \text{tr} \left( L_f(Y^{(t)}, \delta_j^{(t)}) F_j^+ - L_f(Y^{(t)}, -\delta_j^{(t)}) F_j^- \right).$$

This proves our claim about the optimality of $\delta_j^{(t)}$ and, in particular, it holds that $A(Y^{(t)}, \delta^{(t)}) \geq A(Y^{(t)}, 0) = 0$.

Third, if $\max_{\delta} A(Y, \delta) = 0$, then $Y \in \mathcal{L}$. Let $\delta^* = \arg\max_{\delta} A(Y, \delta)$ be the maximizer of $A(Y, \delta)$. It satisfies the equations

$$\langle F_j, X_0 \rangle - \text{tr} \left( L_f(Y, \delta_j^*) F_j^+ - L_f(Y, -\delta_j^*) F_j^- \right) = 0, \quad (29)$$

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for all $j$. We compute
\[
\mathcal{A}(Y, \delta^*) = \langle \delta^* \cdot F, X_0 \rangle - \text{tr} \sum_{j=1}^{k} \left( \ell_f(Y, \delta_j^*) F_j^+ + \ell_f(-\delta_j^*) F_j^- \right)
\]
\[
= \langle \delta^* \cdot F, X_0 \rangle - \text{tr} \sum_{j=1}^{k} \sum_{i} \left( \ell_f(y_i, \delta_j^*) \Pi_i F_j^+ + \ell_f(y_i, -\delta_j^*) \Pi_i F_j^- \right).
\]
By the definition of $\ell_f$, we have
\[
\ell_f(y_i, \delta_j^*) = \mathcal{L}_f(y_i, \delta_j^*) \delta_j^* - D_f(\mathcal{L}_f(y_i, \delta_j^*), y_i),
\]
and we can continue the calculation for $\mathcal{A}(Y, \delta^*)$ as
\[
\mathcal{A}(Y, \delta^*) = \langle \delta^* \cdot F, X_0 \rangle - \text{tr} \sum_{j=1}^{k} \left( \mathcal{L}_f(Y, \delta_j^*) F_j^+ \delta_j^* - \mathcal{L}_f(Y, -\delta_j^*) F_j^- \delta_j^* \right)
\]
\[
+ \text{tr} \sum_{j=1}^{k} \sum_{i} \left( D_f(\mathcal{L}_f(y_i, \delta_j^*), y_i) \Pi_i F_j^+ + D_f(\mathcal{L}_f(y_i, -\delta_j^*), y_i) \Pi_i F_j^- \right)
\]
\[
= \text{tr} \sum_{j=1}^{k} \sum_{i} \left( D_f(\mathcal{L}_f(y_i, \delta_j^*), y_i) \Pi_i F_j^+ + D_f(\mathcal{L}_f(y_i, -\delta_j^*), y_i) \Pi_i F_j^- \right).
\]
Therefore, $\mathcal{A}(Y, \delta^*) = 0$ implies that $D_f(\mathcal{L}_f(y_i, \delta_j^*), y_i) = 0$ (or equivalently, $y_i = \mathcal{L}_f(y_i, \delta_j^*)$) for all $i, j$ such that $\text{tr}(\Pi_i F_j^+) > 0$ and $D_f(\mathcal{L}_f(y_i, -\delta_j^*), y_i) = 0$ (or $y_i = \mathcal{L}_f(y_i, -\delta_j^*)$) for all $i, j$ such that $\text{tr}(\Pi_i F_j^-) > 0$. These conditions and Eq. (29) guarantee that
\[
\langle F_j, X_0 - Y \rangle = \langle F_j, X_0 \rangle - \text{tr} \left( \mathcal{L}_f(Y, \delta_j^*) F_j^+ - \mathcal{L}_f(Y, -\delta_j^*) F_j^- \right) = 0,
\]
for all $j = 1, 2, \ldots, k$ and $Y \in \mathcal{L}$.

Fourth, it is a lower bound on the improvement each iteration measured by the difference between
\[
D_f(X_0, Y^{(t)}) - D_f(X_0, Y^{(t+1)}) \geq \mathcal{A}(Y^{(t)}, \delta^{(t)}).
\]
More generally, we prove that for all $Y \in \text{Herm}_\Delta(\mathcal{X})$ such that $X_0 \triangleright Y$, and $\delta \in \mathbb{R}^k$ such that $\delta \cdot F$ is admissible with respect to $Y$,
\[
D_f(X_0, Y) - D_f(X_0, \mathcal{L}_f(Y, \delta \cdot F)) \geq \mathcal{A}(Y, \delta). \tag{30}
\]
The special condition follows from this more general form by choosing $Y = Y^{(t)}$ and noticing that $Y^{(t+1)} = \mathcal{L}_f(Y^{(t)}, \delta^{(t)} \cdot F)$. To prove the general bound in Eq. (30), we use Eq. (19) and the strong convexity assumption on $\ell_f$:
\[
D_f(X_0, Y) - D_f(X_0, \mathcal{L}_f(Y, \delta \cdot F))
\]
\[
= \langle \delta \cdot F, X_0 \rangle - \ell_f(Y, \delta \cdot F)
\]
\[
\geq \langle \delta \cdot F, X_0 \rangle - \text{tr} \sum_{j=1}^{k} \left( F_j^+ \hat{\ell}_f(Y, \delta_j) + F_j^- \hat{\ell}_f(Y, -\delta_j) \right)
\]
\[
= \mathcal{A}(Y, \delta).
\]

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This implies that for all \( t = 1, 2, \ldots \),
\[
D_f(X_0, Y^{(t)}) - D_f(X_0, Y^{(t+1)}) \geq \mathcal{A}(Y^{(t)}, \delta^{(t)}).
\]
Adding these inequalities together, we have for all \( T \geq 1 \),
\[
D_f(X_0, Y^{(1)}) - D_f(X_0, Y^{(T)}) \geq \sum_{t=1}^{T-1} \mathcal{A}(Y^{(t)}, \delta^{(t)}).
\]
As \( D_f(X_0, Y^{(1)}) = D_f(X_0, Y_0) < \infty \), and both \( D_f \) and \( \mathcal{A} \) are nonnegative, the sequence
\[
(\mathcal{A}(Y^{(t)}, \delta^{(t)}))_t
\]
converges to 0.

By Lemma 3.2 and the fact that \( D_f(X_0, Y^{(t)}) \) is a non-increasing sequence, it follows that the sequence \( Y^{(t)} \) is in a compact subset of \( \text{Herm}_\Delta(\mathcal{A}) \) and that there is subsequence \( Y^{(t_i)} \) converging to a limiting point \( \hat{Y} \).

We claim that \( \max_\delta \mathcal{A} (\hat{Y}, \delta) = 0 \). Otherwise, assume there exist a \( \delta \) and an \( \varepsilon > 0 \) such that \( \mathcal{A}(\hat{Y}, \delta) = \varepsilon > 0 \). By the continuity of \( \mathcal{A} \) with respect to \( Y \), it follows that there is an integer \( m > 0 \) such that for all \( i \geq m \),
\[
\mathcal{A}(Y^{(t_i)}, \delta^{(t_i)}) \geq \mathcal{A}(Y^{(t_i)}, \delta) \geq \varepsilon/2.
\]
This is a contradiction with the fact that \( (\mathcal{A}(Y^{(t)}, \delta^{(t)}))_t \) converges to 0. Hence the assumption is false and we conclude that \( \max_\delta \mathcal{A}(\hat{Y}, \delta) = 0 \).

This now implies that \( \hat{Y} \) is the intersection of \( \mathcal{L} \) and \( \mathcal{P} \) and we complete the proof using Theorem 3.1.

**Theorem 4.3.** Suppose \( \ell_f \) is strongly convex. Then Meta-Algorithm 3 outputs a sequence \( \lambda^{(1)}, \lambda^{(2)}, \ldots \) such that
\[
\lim_{t \to \infty} D_f(X_0, \mathcal{L}_f(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\lambda \in \mathbb{R}^k} D_f(X_0, \mathcal{L}_f(Y_0, \lambda \cdot F)).
\]

**Proof.** Thanks to the flexibility of the auxiliary function proof technique, the analysis is identical to that of Theorem 4.2 by choosing \( \delta_l^{(t)} = 0 \) for all \( l \neq j_t \) in the \( t \)-th iteration.

## 5 Approximate Information Projection Algorithms

In this section, we discuss several interesting special cases of the general framework when the convex function \( f \) is \( x \ln(x) - x \). For such a convex function, the Bregman divergence is known as Kullback–Leibler divergence and the Bregman projection is also known as the information projection for the central role Kullback–Leibler divergence plays in information theory. We will show that many important classical algorithms in learning theory generalize to the quantum (non-commutative) case nicely in this framework.
Require: $f$ is an extended real function with domain $\Delta \subseteq \mathbb{R}$ and domain of $f^*$ is open. $X_0, Y_0 \in \text{Herm}(\mathcal{X})$ such that $D_f(X_0, Y_0) < \infty$.
Input: $F = (F_1, F_2, \ldots, F_k) \in \text{Herm}(\mathcal{X})^k$ and $|F_j| \leq 1$ for all $j$.
Output: $\lambda^{(1)}, \lambda^{(2)}, \ldots$ such that
\[
\lim_{t \to \infty} D_f(X_0, \mathcal{L}_f(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\lambda \in \mathbb{R}^k} D_f(X_0, \mathcal{L}_f(Y_0, \lambda \cdot F)).
\]

1: Initialize $\lambda^{(1)} = (0, 0, \ldots, 0)$.
2: for $t = 1, 2, \ldots$, do
3: Compute $Y^{(t)} = \mathcal{L}_f(Y_0, \lambda^{(t)} \cdot F)$.
4: Compute $j_t = \text{argmax}_j |\langle F_j, Y^{(t)} - X_0 \rangle|$.
5: Solve the following equation of $\delta^{(t)}_j \in \mathbb{R}$:
\[
\text{tr} \left( F_{j_t}^+ \mathcal{L}_f(Y^{(t)}, \delta^{(t)}_j) - F_{j_t}^- \mathcal{L}_f(Y^{(t)}, -\delta^{(t)}_j) \right) = \langle F_{j_t}, X_0 \rangle.
\]
6: Update parameters $\lambda^{(t+1)}_j = \begin{cases} 
\lambda^{(t)}_j + \delta^{(t)}_j & \text{if } j = j_t, \\
\lambda^{(t)}_j & \text{otherwise.}
\end{cases}$
7: end for

Meta-Algorithm 3: Sequential Approximate Projection Algorithm.

5.1 General Approximate Information Projection Algorithms

For $f(x) = x \ln(x) - x$, we compute the relevant functions and quantities as follows
\[
\begin{align*}
    f^*(x) &= \exp(x), \\
    f'(x) &= \ln(x), \\
    D_f(X, Y) &= \text{tr}(X \ln X - X \ln Y - X + Y), \\
    \mathcal{L}_f(Y, \Lambda) &= \exp(\ln(Y) + \Lambda), \\
    \ell_f(Y, \Lambda) &= \text{tr} \exp(\ln(Y) + \Lambda) - \text{tr} Y.
\end{align*}
\]

Because of the fundamental importance of this case, we may sometimes omit the subscript $f$ and use $D(X, Y)$, $\mathcal{L}(Y, \Lambda)$, and $\ell(Y, \Lambda)$ to denote $D_f(X, Y)$, $\mathcal{L}_f(Y, \Lambda)$, $\ell_f(Y, \Lambda)$ respectively. For density matrices $\rho$ and $\sigma$, $D(\rho, \sigma)$ reduces to the usual Kullback–Leibler divergence $D(\rho||\sigma) = \text{tr}(\rho \ln \rho - \rho \ln \sigma)$. We choose to work with the non-normalized Kullback-Leibler divergence as it is more flexible.

In this special case, it is possible to solve the equation in Line 5 of the algorithm analytically, which turns out to be a quadratic equation in $e^{\delta^{(t)}_j}$. The advantage of making approximate Bregman projection steps is now evident as the calculation of the update in each step is extremely simple. In light of Theorem 3.1, this algorithm leads to Algorithm 1 that minimizes the Kullback-Leibler divergence subject to linear constraints. In particular, the linear constraints are given by the matrix $X_0$ as $\langle F_j, X - X_0 \rangle = 0$ for all $j = 1, 2, \ldots, k$ and the problem is to compute the minimizer of $D(X, Y_0)$ for $X$ satisfying these linear constraints. Algorithm 1 is a parallel update algorithm, but as in Section 4.2, it is also straightforward to
Require: \( X_0, Y_0 \in \text{Herm}_\Delta(\mathcal{X}) \) such that \( D(X_0, Y_0) < \infty \).
Input: \( F = (F_1, F_2, \ldots, F_k) \in \text{Herm}(\mathcal{X})^k \) and \( \sum_{j=1}^k |F_j| \leq 1 \).
Output: \( \lambda^{(1)}, \lambda^{(2)}, \ldots \) such that
\[
\lim_{t \to \infty} D(X_0, \mathcal{L}(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\lambda \in \mathbb{R}^k} D(X_0, \mathcal{L}(Y_0, \lambda \cdot F)).
\]

1: Initialize \( \lambda^{(1)} = (0, 0, \ldots, 0) \).
2: for \( t = 1, 2, \ldots \) do
3: \( \text{Compute } Y^{(t)} = \exp(\ln Y_0 + \lambda^{(t)} \cdot F). \)
4: for \( j = 1, 2, \ldots, k \) do
5: \( \text{Solve the following equation of } \delta^{(t)}_j: } \)
\[
\left\{ \begin{array}{l}
\langle F_j^+, Y^{(t)} \rangle e^{\delta^{(t)}_j} - \langle F_j^-, Y^{(t)} \rangle e^{-\delta^{(t)}_j} = \langle F_j, X_0 \rangle.
\end{array} \right.
\]
6: end for
7: \( \text{Update parameters } \lambda^{(t+1)}_j = \begin{cases} 
\lambda^{(t)}_j + \delta^{(t)}_j & \text{if } j = j_t, \\
\lambda^{(t)}_j & \text{otherwise.}
\end{cases} \)
8: end for

Algorithm 1: Parallel Iterative Update Algorithm for Kullback-Leibler Divergence Minimization.

Require: \( X_0, Y_0 \in \text{Herm}_\Delta(\mathcal{X}) \) such that \( D(X_0, Y_0) < \infty \).
Input: \( F = (F_1, F_2, \ldots, F_k) \in \text{Herm}(\mathcal{X})^k \) and \( |F_j| \leq 1 \) for all \( j \).
Output: \( \lambda^{(1)}, \lambda^{(2)}, \ldots \) such that
\[
\lim_{t \to \infty} D(X_0, \mathcal{L}(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\lambda \in \mathbb{R}^k} D(X_0, \mathcal{L}(Y_0, \lambda \cdot F)).
\]

1: Initialize \( \lambda^{(1)} = (0, 0, \ldots, 0) \).
2: for \( t = 1, 2, \ldots \) do
3: \( \text{Compute } Y^{(t)} = \exp(\ln Y_0 + \lambda^{(t)} \cdot F). \)
4: Compute \( j_t = \text{argmax}_j \left| \langle F_j, Y^{(t)} - X_0 \rangle \right| \).
5: Compute \( \delta^{(t)}_j: \)
\[
\left\{ \begin{array}{l}
\langle F_j^+, Y^{(t)} \rangle e^{\delta^{(t)}_j} - \langle F_j^-, Y^{(t)} \rangle e^{-\delta^{(t)}_j} = \langle F_j, X_0 \rangle.
\end{array} \right.
\]
6: Update parameters \( \lambda^{(t+1)}_j = \begin{cases} 
\lambda^{(t)}_j + \delta^{(t)}_j & \text{if } j = j_t, \\
\lambda^{(t)}_j & \text{otherwise.}
\end{cases} \)
7: end for

Algorithm 2: Sequential Iterative Update Algorithm for Kullback-Leibler Divergence Minimization.

define and analyze a sequential version where only one entry of the parameter \( \lambda \) is updated.
each step. This is given in Algorithm 2.

We now prove the convergence of Algorithm 1 which follows directly from the general convergence theorem in Theorem 4.2 as long as we can prove that \( \ell \) is strongly convex.

**Lemma 5.1.** Function \( \ell(Y, \Lambda) = \text{tr} \exp(\ln(Y) + \Lambda) - \text{tr} Y \) is strongly convex as defined in Definition 4.1.

**Proof.** Let \( F_j \geq 0 \) be positive semi-definite matrices satisfying \( \sum_{j=1}^k F_i \leq 1 \), and let \( Y \) be positive. \( \delta_j \in \mathbb{R} \) are real numbers. By definition, we need to show that

\[
\ell\left(Y, \sum_{j=1}^k \delta_j F_j\right) \leq \sum_{j=1}^k \text{tr} \left(\hat{\ell}(Y, \delta_j) F_j\right). \tag{32}
\]

We first compute the right hand side as

\[
\sum_{j=1}^k \text{tr} \left(\hat{\ell}(Y, \delta_j) F_j\right) = \sum_{i=1}^k \sum_{j=1}^k \text{tr} \left(\ell(y_i, \delta_j) \Pi_i F_j\right) = \sum_{j=1}^k \sum_{i=1}^k \text{tr} \left(e^{\ln(y_i) + \delta_j} - y_i\right) \Pi_i F_j = \text{tr} \left(Y \sum_{j=1}^k e^{\delta_j} F_j\right) - \text{tr} \left(Y \sum_{j=1}^k F_j\right).
\]

The inequality in Eq. (32) then simplifies to

\[
\text{tr} \exp\left(\ln(Y) + \sum_{j=1}^k \delta_j F_j\right) \leq \text{tr} \left(Y \sum_{j=1}^k e^{\delta_j} F_j\right) + \text{tr} \left(Y \left(1 - \sum_{j=1}^k F_j\right)\right).
\]

Define \( F_0 = \mathbb{1} - \sum_{j=1}^k F_j \) and \( \delta_0 = 0 \). The above inequality can be written as

\[
\text{tr} \exp\left(\ln(Y) + \sum_{j=0}^k \delta_j F_j\right) \leq \text{tr} \left(Y \sum_{j=0}^k e^{\delta_j} F_j\right) \tag{33}
\]

for \( \sum_{j=0}^k F_j = \mathbb{1} \) and \( F_j \geq 0 \).

In the following we prove Eq. (33) using Lemma 2.4 and this will complete the proof.

By choosing \( H = \sum_{j=0}^k \delta_j F_j \) and

\[ Q = \sum_{j=0}^k e^{\delta_j} F_j / \text{tr} \left(Y \sum_{i=0}^k e^{\delta_i} F_i\right), \]

in the Carlen-Lieb inequality, we have

\[
\text{tr} \exp\left(\ln(Y) + \sum_{j=0}^k \delta_j F_j\right) \leq \exp \left(\lambda_{\text{max}} \left(\sum_{j=0}^k \delta_j F_j - \ln Q\right)\right) \tag{34}
\]

\[
\leq \text{tr} \left(Y \sum_{j=0}^k e^{\delta_j} F_j\right) \exp \left(\lambda_{\text{max}} \left(\sum_{j=0}^k \delta_j F_j - \ln \left(\sum_{j=0}^k e^{\delta_j} F_j\right)\right)\right).
\]

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By the operator concavity of the ln function and the operator Jensen’s inequality, we have
\[ \sum_{j=0}^{k} \delta_j F_j - \ln \left( \sum_{j=0}^{k} e^{\delta_j F_j} \right) \preceq 0, \]
and therefore
\[ \lambda_{\text{max}} \left( \sum_{j=0}^{k} \delta_j F_j - \ln \left( \sum_{j=0}^{k} e^{\delta_j F_j} \right) \right) \leq 0. \]
Together with Eq. (34), this completes the proof of the claimed inequality in Eq. (33) which is equivalent the statement of the lemma.

We mention that the inequality is not easy to establish without using the Carlen-Lieb inequality. For example, one may try to prove it using Golden-Thompson as it is already very close in the form. Yet, to complete the proof we would require that the exponential function is operator convex, which is not the case unfortunately. One may also try to use Jensen’s trace inequality, but the strategy fails to work because of the non-commutativity between the matrices.

**Theorem 5.1.** Let the sequence \( \lambda^{(1)}, \lambda^{(2)}, \ldots \) be generated by Algorithm 1. Then
\[ \lim_{t \to \infty} D(X_0, \mathcal{L}(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\Lambda \in \mathbb{R}^k} D(X_0, \mathcal{L}(Y_0, \lambda \cdot F)). \]

**Proof.** It has been explained in the main text that the algorithm is derived from Meta-Algorithm 2 by taking \( f = x \ln(x) - x \). By Lemma 5.1, the assumption that \( \ell_x \) is strong convex in this case is verified and the theorem follows from Theorem 4.2.

Similarly, Theorem 4.3 and Lemma 5.1 guarantee the following convergence theorem about the sequential version in Algorithm 2.

**Theorem 5.2.** Let the sequence \( \lambda^{(1)}, \lambda^{(2)}, \ldots \) be generated by Algorithm 2. Then
\[ \lim_{t \to \infty} D(X_0, \mathcal{L}(Y_0, \lambda^{(t)} \cdot F)) = \inf_{\Lambda \in \mathbb{R}^k} D(X_0, \mathcal{L}(Y_0, \lambda \cdot F)). \]

### 5.2 Quantum Partition Function Minimization and AdaBoost

In the following, we will discuss two important special cases of Algorithm 1 (and its sequential analog Algorithm 2).

The first case is given in Algorithm 3 presented in the sequential update form. It is an algorithm for minimizing the quantum partition function over a linear family of Hamiltonians and is the non-commutative analog the famous AdaBoost algorithm in learning theory. The input to the algorithm is a tuple of Hermitian matrices \( F = (F_1, F_2, \ldots, F_k) \), satisfying simple normalization conditions. An important example is that the tuple consists of all terms of a local Hamiltonian. The algorithm iteratively computes a \( \lambda \) so that the quantum partition function \( \text{tr}(\exp(\lambda \cdot F)) \) is minimized over the linear Hamiltonian family \( \sum_j \lambda_j F_j \) for \( \lambda_j \in \mathbb{R} \).

To see that this is indeed a special case of Algorithm 2, we choose \( X_0 = 0 \) and \( Y_0 = 1 \). In this case, the (non-normalized) Kullback-Leibler divergence \( D(X_0, \mathcal{L}(Y_0, \Lambda)) \) simplifies to
\[ D(0, \mathcal{L}(Y_0, \Lambda)) = \text{tr} \mathcal{L}(Y_0, \Lambda) = \text{tr} \exp(\Lambda), \]
Input: $F = (F_1, F_2, \ldots, F_k) \in \text{Herm}(\mathcal{X})^k$ and $|F_j| \leq 1$ for all $j$.
Output: $\lambda^{(1)}, \lambda^{(2)}, \ldots$ such that

$$\lim_{t \to \infty} \text{tr}(\exp(\lambda^{(t)} \cdot F)) = \inf_{\lambda \in \mathbb{R}^k} \text{tr}(\exp(\lambda \cdot F)).$$

1: Initialize $\lambda^{(1)} = (0, 0, \ldots, 0)$.
2: for $t = 1, 2, \ldots,$ do
3: Compute $Y^{(t)} = \exp(\lambda^{(t)} \cdot F)$.
4: Compute $j_t = \arg\max_j |\langle F_j, Y^{(t)} \rangle|$.
5: Compute $\delta^{(t)} = \frac{1}{2} \ln \frac{\langle F_{j_t}^-, Y^{(t)} \rangle}{\langle F_{j_t}^+, Y^{(t)} \rangle}$.
6: Update parameters $\lambda^{(t+1)}_j = \begin{cases} \lambda^{(t)}_j + \delta^{(t)} & \text{if } j = j_t, \\ \lambda^{(t)}_j & \text{otherwise.} \end{cases}$
7: end for

Algorithm 3: Sequential Iterative Update Algorithm for Quantum Partition Function Minimization.

and the equation in Line 5 of Algorithm 2 has solution

$$\delta^{(t)}_j = \frac{1}{2} \ln \frac{\langle F_{j_t}^-, Y^{(t)} \rangle}{\langle F_{j_t}^+, Y^{(t)} \rangle}.$$

These calculations explains the changes made in Algorithm 3 from Algorithm 2. The general convergence theorem Theorem 4.3 implies the following.

Theorem 5.3. Let $\lambda^{(1)}, \lambda^{(2)}, \ldots$ be the sequence generated by Algorithm 3. Then

$$\lim_{t \to \infty} \text{tr}(\exp(\lambda^{(t)} \cdot F)) = \inf_{\lambda \in \mathbb{R}^k} \text{tr}(\exp(\lambda \cdot F)).$$

We now highlight the connection between the partition function minimization algorithm in Algorithm 3 and the well-known AdaBoost algorithm in learning theory. Let $(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)$ be a set of training examples where we assume for simplicity that each label $y_i$ is in $\{\pm 1\}$. There is also a set of features or base hypothesis $h_1, h_2, \ldots, h_T$ that predict the label $y_i$ when given $x_i$ as input. The AdaBoost algorithm maintains a distribution over the training examples and interacts with a weak learner. In each step, the algorithm query the weak learner with the distribution and the weak learner respond with a hypothesis $h_j$. The algorithm then evaluates the performs of $h_j$ on each example and increase the weight of the examples that are not correctly predicted by $h_j$ so that the weak learner is forced to focus more on those misclassified examples. Finally, the algorithm computes the parameters $\lambda \in \mathbb{R}^n$ based on the error of each hypothesis $h_j$ and outputs a final hypothesis

$$H(x) = \text{sign} \left( \sum_{j=1}^T \lambda_j h_j(x) \right).$$
We refer the readers to [26] for more details.

It is well known in the literature that the parameters $\lambda$ computed by the AdaBoost algorithm actually minimizes the exponential loss defined as

$$\sum_{i=1}^{m} \exp \left( -y_i \sum_{j=1}^{T} \lambda_j h_j(x_i) \right).$$  \hfill (35)

Define diagonal matrices

$$F_j = \sum_{i=1}^{m} -y_i h_j(x_i) |i\rangle\langle i|,$$

for $j = 1, 2, \ldots, T$. The corresponding partition function is then

$$\text{tr} \exp(\lambda \cdot F) = \text{tr} \exp \left( \sum_{j=1}^{T} \lambda_j F_j \right),$$

which is the same as the exponential loss in Eq. (35). In this sense, our algorithm generalizes the iterative update procedure of AdaBoost to the non-commutative setting.

### 5.3 Quantum Iterative Scaling

**Require:** $\rho_0, \sigma_0 \in \text{D}(X)$ such that $D(\rho_0, \sigma_0) < \infty$.

**Input:** $F = (F_1, F_2, \ldots, F_k) \in \text{Pos}(X)^k$ and $\sum_{j=1}^{k} F_j \leq 1$.

**Output:** $\lambda^{(1)}, \lambda^{(2)}, \ldots$ such that

$$\lim_{t\to\infty} D\left(\rho_0, \mathcal{L}(\sigma_0, \lambda^{(t)} \cdot F)\right) = \inf_{\lambda \in \mathbb{R}^k} D\left(\rho_0, \mathcal{L}(\sigma_0, \lambda \cdot F)\right).$$

1: Initialize $\lambda^{(1)} = (0, 0, \ldots, 0)$.
2: for $t = 1, 2, \ldots,$ do
3: Compute $Y^{(t)} = \exp(\ln \sigma_0 + \lambda^{(t)} \cdot F)$.
4: for $j = 1, 2, \ldots, k$ do
5: $\delta^{(t)}_j = \ln \langle F_j, \rho_0 \rangle - \ln \langle F_j, Y^{(t)} \rangle$.
6: end for
7: Update parameters $\lambda^{(t+1)} = \lambda^{(t)} + \delta^{(t)}$.
8: end for

Algorithm 4: Quantum iterative scaling algorithm.

In the second special case, we consider the case where $F_j$ form a POVM and $X_0 = \rho_0$, $Y_0 = \sigma_0$ are density matrices. In that case, the solution of the equation in Line 5 of Algorithm 1 can be computed as

$$\delta^{(t)}_j = \ln \langle F_j, \rho_0 \rangle - \ln \langle F_j, Y^{(t)} \rangle.$$

The quantum iterative scaling algorithm given in Algorithm 4 then follows naturally as a special case of Algorithm 1.
The convergence proved in Theorem 4.2 then implies the following theorem about the convergence of the quantum iterative scaling algorithm. It is a non-commutative analog of the generalized iterative scaling algorithm (also known as the SMART algorithm) as stated in Theorem 5.2 of [20]. As in the commutative case, the intermediate matrices \(Y^{(t)}\) are not normalized to have trace one. In fact, using the inequality in Lemma 5.1, it is easy to show \(\text{tr} \ Y^{(t)} \leq 1\) for all \(t\). Yet in the limit of \(t \to \infty\), \(Y^{(t)}\) converges to a density matrix.

**Theorem 5.4.** Let \(L\) be the linear family defined by \(\langle F_i, \rho \rangle = \alpha_i\) where \(F_i \geq 0\), \(\sum_{i=1}^{k} F_i = 1\), and \(\alpha_i = \langle F_i, \rho_0 \rangle\). Let \(\rho_0, \sigma_0\) be two density matrices such that \(D(\rho_0 \| \sigma_0) < +\infty\). Define a sequence of operators as

\[
Y^{(1)} = \sigma_0, \quad Y^{(t+1)} = \exp \left( \ln Y^{(t)} + \sum_{i=1}^{k} (\ln \alpha_i - \ln \beta_{n,i}) F_i \right),
\]

where \(\beta_{n,i} = \langle F_i, Y^{(t)} \rangle\). Then the limit \(\lim_{n \to \infty} Y^{(t)}\) converges to the information projection \(\rho^*\) of \(\sigma_0\) to linear family \(L\).

An important special case is when \(\sigma_0 = 1/d\) where \(d\) is the dimension and \(D(\rho, \sigma_0) = \ln(d) - S(\rho)\). The Bregman projection of \(\sigma_0\) to the linear family of \(\rho_0\) and \(\{F_j\}\) is therefore the solution of the maximum entropy inference problem formulated as

\[
\text{maximize: } S(\rho) \\
\text{subject to: } \langle F_j, \rho \rangle = \langle F_j, \rho_0 \rangle, \\
\rho \in D(\mathcal{X}).
\]

The sequence \(Y^{(1)}, Y^{(2)}, \ldots\) computed in Algorithm 4 converges to the solution of the above convex programming problem. This shows that the quantum iterative scaling algorithm is an algorithm for computing the maximum entropy inference given linear constraints of the density matrix. By Jaynes’ maximum entropy principle, the maximum entropy state is the exponential of a Hamiltonian of the form \(\sum_j \lambda_j F_j\). We call this problem of finding the Hamiltonian given local information of the state as the Hamiltonian inference problem. The general framework above proves the convergence of the algorithm for the Hamiltonian inference problem and we leave the more detailed analysis of its convergence rate as future work.

### 6 Quantum Algorithmic Speedups

In the previous discussions, the algorithms we presented are classical algorithms that require matrix computations such as \(Y^{(t)} = \exp(\lambda^{(t)} \cdot F)\). We will consider several ideas that can speedup the computation using techniques from quantum algorithm design.

#### 6.1 Implement Matrix Functions on Quantum Computers

The first natural attempt to quantize the algorithm is to implement the matrix computations using techniques such as quantum singular value transformation [28, 27] and smooth function evaluation [4].

We start with the exact Bregman projection algorithm in Meta-Algorithm 1. Notice that \(Y^{(t)}\) in the algorithm is an intermediate quantity that are used in later steps to approximate
\( \langle F_j, Y^{(t)} \rangle \) and \( \langle F_j, \mathcal{L}_f (Y^{(t)}, \delta^{(t)} F_j^t) \rangle \). It therefore suffices to have a subroutine Average that can compute the average value \( \langle F_j, \mathcal{L}_f (Y_0, \lambda \cdot F) \rangle \) given \( F_j, Y_0, \) and \( \lambda \) as input or certain oracle access. We emphasize that it is not necessary to compute the matrix \( \mathcal{L}_f \) explicitly. Numerical algorithms can then be employed to search for the solution of \( \delta^{(t)} \) in Line 5 of Meta-Algorithm 1 as it is an equation only involving a single real variable.

In the case of approximate Bregman projection algorithms, the situation is much simpler as the equation involved is usually explicitly solvable and no numerical search is necessary. For example, in the case of approximate information projection algorithms (Algorithms 1 and 2), each iteration amounts to the computation of \( \langle F_j, Y^{(t)} \rangle \) and \( \langle F_j^t, Y^{(t)} \rangle \) where \( Y^{(t)} \) has the exponential form \( \exp(\log Y_0 + \lambda^{(t)} \cdot F) \). All these average values are in the form of the subroutine call to Average.

Quantum algorithms that implement the subroutine Average are known. As

\[
\mathcal{L}_f (Y_0, \lambda \cdot F) = (f^\dagger)' (f^\dagger (Y_0) + \lambda \cdot F),
\]

it is a matrix function of matrix \( f^\dagger (Y_0) + \lambda \cdot F \). Hence, under the condition that \( f^\dagger (Y_0) + \lambda \cdot F \) is sparse, we can apply the quantum algorithms for evaluating smooth functions of Hamiltonians [4, Appendix B]. In the special case of Kullback-Leibler information projection algorithms, the Bregman-Legendre projection is the exponential function \( \exp(\lambda \cdot F) \) and their algorithm for approximating the average value \( \langle F_j, \exp(\lambda \cdot F) \rangle \) runs in time \( \tilde{O}(\frac{\sqrt{nKd}}{\theta}) \)

where \( n \) is the size of the matrices, \( K \) is the upper bound of \( \| \lambda \cdot F \| \), \( d \) is the sparsity of \( \lambda \cdot F \), and \( \tilde{O} \) suppresses the polynomial dependence on the parameters. The quantum running time is sometimes advantageous as classical algorithms for computing the same quantity will run in time at least linear in \( n \). One caveat is that the quantum running time depends on the upper bound of the Hamiltonian norm \( K \). In our case, \( \lambda^{(t)} \) is being updated each iteration and the norm \( \| \lambda^{(t)} \cdot F \| \) may even go to infinity for some problem instances. This prevents us to claim general time bounds using the techniques in [4] but the quantum implementation could be advantageous in many practical situations. Other quantum algorithms for preparing the quantum Gibbs states [39, 18, 38] are also known with different assumptions and performance guarantees and may be applicable as subroutines in our information projection algorithms.

### 6.2 Quantum Search for the Maximum Violation

The second possible approach to speedup the iterative algorithms presented in Section 4 is to employ the fast quantum OR lemma as in [31, 8] in sequential iterative algorithms.

Quantum implementations of \( Y^{(t)} \) in the algorithm usually represent the matrix as a quantum density matrix. As quantum measurements may disturb the state they measure, a trivial approach to estimate \( \langle F_j, Y^{(t)} \rangle \) requires a fresh copy of the state representing \( Y^{(t)} \) each time. This could be very expensive as the preparation of \( Y^{(t)} \) can be the hardest step among the computations needed in each iteration. The use of fast quantum OR lemma solves the problem by saving the number of copies of states required. Following the approach as in [8, 4, 42], we show similar ideas are applicable to our sequential update algorithms.

To be more specific, we will consider the case of the partition function minimization algorithm (Algorithm 3) and focus on the cost of Line 4 in that algorithm. We assume that there is a unitary \( U_j \) that estimates the value of \( \langle F_j, \rho^{(t)} \rangle \) to precision \( \eta_j \) using \( n_t^{(t)} \) copies.
of the state $\rho(t) = Y(t) / \text{tr}(Y(t))$. Further assume that the access to $U_j$ is provided by a unitary $U$ such that

$$U|j\rangle\langle \psi\rangle = |j\rangle U_j |\psi\rangle.$$  

A straightforward implementation of Line 4 has to use fresh copies of $\rho(t)$ for different $j$ and the cost is

$$\Omega\left(mT(U) + mn(t)T_{\text{State}}(\rho(t))\right),$$

where $T_{\text{State}}(\rho(t))$ is the time complexity of preparing the Gibbs state $\rho(t)$ and $m = k$ is the number of constraints. Applying the two-phase quantum minimum finding algorithm from [42, Lemma 7], the time complexity is improved to

$$\tilde{O}\left(\sqrt{mT(U) + \log^4(m) \log(1/\delta)n(t)} T_{\text{State}}(\rho(t))\right),$$

where $\delta$ is the precision parameter.

6.3 NISQ Applications

We now briefly mention potential applications of the above algorithms in the context of designing algorithms on noisy intermediate scale quantum devices [40].

Assume that there are NISQ algorithms for approximately preparing a quantum state representing the matrix $Y(t)$ in the algorithm. For the preparation of quantum Gibbs states, it is shown in [17, 36] that a variational quantum algorithm for preparing the Gibbs state can be derived using a gradient descent method optimizing the free energy. Then Algorithms 1 and 2 can also be efficiently implemented on a NISQ device as our iterative algorithm has the structure of hybrid quantum algorithms with a quantum part for the preparation of the quantum state for $Y(t)$ and classical part that updates the parameters using a simple rule based on the average values of the current state. In some sense, it is a variational quantum algorithm in which the quantum part is a Gibbs state preparation subroutine and the classical update rules are given by our algorithmic framework. In the case of quantum iterative scaling, this approach lifts the entropy estimation algorithm in [17] to a solver for maximum entropy problem with linear constraints.

7 Summary

In this paper, we prove a general duality theorem for Bregman divergence on Hermitian matrices under simple assumptions of the underlying convex function. Several iterative update algorithms are designed based on the idea of exact and approximate Bregman projections and the convergence is proved using the duality theorem and the auxiliary function method.

There are many interesting questions left open and we leave them as future work. First, we have only been able to prove the strong convex inequality for Kullback-Leibler divergence. Can we have a more general theory about the condition under which the strong convex is true? Better understanding of related inequalities will lead to, for example, the non-commutative analog of logistic regression based on Fermi/Dirac convex function (Line 4 of Table 1) [7, 19]. Second, we have only been able to work with linear equality constraints and it is an interesting problem to further generalize the framework so that we can handle linear inequality constraints. Finally, it is an interesting problem to establish quantitative bounds on the class and quantum time complexity of the algorithms introduced in the paper.
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