Convergence Rate Analysis of the Multiplicative Gradient Method for PET-Type Problems

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Abstract

We analyze the convergence rate of the multiplicative gradient (MG) method for PET-type problems with \( m \) component functions and an \( n \)-dimensional optimization variable. We show that the MG method has an \( O(\ln(n)/t) \) convergence rate, in both the ergodic and the non-ergodic senses. Furthermore, we show that the distances from the iterates to the set of optimal solutions converge (to zero) at rate \( O(1/\sqrt{t}) \). Our results show that, in the regime \( n = O(\exp(m)) \), to find an \( \varepsilon \)-optimal solution of the PET-type problems, the MG method has a lower computational complexity compared with the relatively-smooth gradient method and the Frank-Wolfe method for convex composite optimization involving a logarithmically-homogeneous barrier.

1 Introduction

We consider the following optimization problem:

\[
\begin{align*}
  f^* := \max_{x \in \Delta_n} \left\{ f(x) := \sum_{j=1}^{m} p_j \ln(a_j^\top x) \right\},
\end{align*}
\]

where \( \Delta_n := \{x \in \mathbb{R}^n : x \geq 0, \sum_{i=1}^{n} x_i = 1\} \) denotes the (standard) unit simplex in \( \mathbb{R}^n \), \( p_j > 0 \) for all \( j \in [m] \), and \( a_j \in \mathbb{R}_+^n \) for all \( j \in [m] \). (Here \( \mathbb{R}_+^n := \{x \in \mathbb{R}^n : x_i \geq 0, \forall i \in [n]\} \), namely the nonnegative orthant in \( \mathbb{R}^n \).) We assume without loss of generality that \( \sum_{j=1}^{m} p_j = 1 \). For well-posedness, we further assume that \( a_j \neq 0 \) for every \( j \in [m] \), from which it follows that \( \text{dom } f \cap \Delta_n \neq \emptyset \) and hence (P) has an optimal solution.

1.1 Applications

The problem (P) subsumes many diverse applications, including most notably the positron emission tomography (PET) problem in medical imaging [1], computing the rate distortion in information theory [2], maximum likelihood estimation for mixture models in statistics [3], the log-optimal investment problem [4], and the maximum-likelihood inference of the multi-dimensional Hawkes processes [5]. For motivation and clarity we now briefly describe the PET problem; for an expanded description we also refer the reader to [6, Section 1.1] and [7].

PET is a medical imaging technique that measures the metabolic activities of human tissues and organs. In a typical setting radioactive materials are injected into the organ of interest, and

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these materials emit (radioactive) events that can be detected by PET scanners. The mathematical model behind this process is described as follows. Suppose that an emission object (for example a human organ) has been discretized into \( n\) voxels. The number of events emitted by voxel \( i \) (\( i \in [n] \)) is a Poisson random variable \( X_i \) with unknown mean \( x_i \geq 0 \), and so \( X_i \sim \text{Poiss}(x_i) \), and furthermore \( \{X_i\}_{i=1}^n \) are assumed to be independent. We also have a scanner array comprised of \( m \) bins. Each event emitted by voxel \( i \) has a known probability \( p_{ij} \) of being detected by bin \( j \) (\( j \in [m] \)), and we assume that \( \sum_{j=1}^m p_{ij} = 1 \), i.e., the event will be detected by exactly one bin. Let \( \tilde{Y}_j \) denote the total number of events detected by bin \( j \), whereby

\[
\mathbb{E}[\tilde{Y}_j] := y_j := \sum_{i=1}^n p_{ij} x_i .
\]

By Poisson thinning and superposition, it follows that \( \{\tilde{Y}_j\}_{j=1}^m \) are independent random variables and \( \tilde{Y}_j \sim \text{Poiss}(y_j) \) for all \( j \in [m] \).

We seek to perform maximum-likelihood (ML) estimation of the unknown means \( \{x_i\}_{i=1}^n \) based on observations \( \{Y_j\}_{j=1}^m \) of the random variables \( \{\tilde{Y}_j\}_{j=1}^m \). From the model above, we easily see that the log-likelihood of observing \( \{Y_j\}_{j=1}^m \) given \( \{X_i\}_{i=1}^n \) is (up to some constants)

\[
l(x) := -\sum_{i=1}^n x_i + \sum_{j=1}^m Y_j \ln \left( \sum_{i=1}^n p_{ij} x_i \right) ,
\]

and therefore an ML estimate of \( \{x_i\}_{i=1}^n \) is given by an optimal solution \( x^* \) of

\[
\max_{x \geq 0} l(x) .
\]

It follows from the first-order optimality conditions that any optimal solution \( x \) must satisfy

\[
\sum_{i=1}^n x_i = S := \sum_{j=1}^m Y_j .
\]

By incorporating (4) into (3), and re-scaling both the objective function \( l \) and the optimization variable \( x \) by a factor of \( S^{-1} \), (3) can be equivalently written as

\[
\max_{z \in \Delta_n} \sum_{j=1}^m p_j \ln \left( \sum_{i=1}^n p_{ij} z_i \right) ,
\]

where \( p_j := Y_j/S \) for all \( j \in [m] \). The maximization problem (5) is easily seen to be an instance of (P) with \( a_j := (p_{j1}, \ldots, p_{jn})^\top \) for \( j \in [m] \).

### 1.2 The Multiplicative Gradient (MG) Method

One of the earliest algorithms for solving (P) is the MG method, which seems to be first proposed by information theorists in the 1970s for computing channel capacity and rate-distortion functions [2, 8, 9]. The MG method is very simple and can be described as follows. Let \( x^0 \in \text{ri} \Delta_n \) be the initial point, where \( \text{ri} \Delta_n := \{x \in \mathbb{R}^n : x > 0, \sum_{i=1}^n x_i = 1\} \) denotes the relative interior of \( \Delta_n \). Then at each iteration \( t \geq 0 \) of the MG method we first compute the gradient of \( f \) at \( x^t \):

\[
\nabla_i f(x^t) = \sum_{j=1}^m p_j \frac{a_{ji}}{a_j} x^t , \quad \forall i \in [n] ,
\]

where \( \nabla_i f(x^t) \) denotes the \( i \)-th entry of \( \nabla f(x^t) \), and \( a_{ji} \) denotes the \( i \)-th entry of \( a_j \). We construct the next iterate \( x^{t+1} \) by simply multiplying the current iterate’s coefficients by their respective gradient coefficients, namely

\[
x_i^{t+1} := x_i^t \nabla_i f(x^t) , \quad \forall i \in [n] .
\]
Let us make two immediate (but important) observations about the MG method in (6). Define the \( m \times n \) (nonnegative) data matrix

\[
A := [a_1 \cdots a_m]^\top = [A_1 \cdots A_n],
\]

(i.e., \( a_j^\top \) denotes the \( j \)-th row of \( A \) for \( j \in [m] \) and \( A_i \) denotes the \( i \)-th column of \( A \) for \( i \in [n] \)), and let \( \mathcal{I} := \{ i \in [n] : A_i \neq 0 \} \) denote the “support pattern” of the columns of \( A \). Then we know that

(O1) the sequence \( \{x^t\}_{t \geq 0} \subseteq \Delta_n \) (namely, \( \{x^t\}_{t \geq 0} \) are feasible) and

(O2) for all \( t \geq 1 \), \( \mathcal{I}(x^t) = \mathcal{I} \), where \( \mathcal{I}(x) := \{ i \in [n] : x_i \neq 0 \} \) denotes the support of \( x \) (for any \( x \in \mathbb{R}^n \)).

To see (O1), note that \( x^0 \in \Delta_n \), and if \( x^t \in \Delta_n \) for some \( t \geq 0 \), then \( x^{t+1} \geq 0 \) since \( \nabla f(x^t) \geq 0 \) and

\[
\sum_{i=1}^n x_{i}^{t+1} = \sum_{i=1}^n x_{i}^{t} \sum_{j=1}^m p_j a_{ij} x^t_j = \sum_{j=1}^m p_j = 1.
\]

This shows that \( x^{t+1} \in \Delta_n \). To see (O2), note that \( \mathcal{I}(x^1) = \mathcal{I} \) since \( x^0 > 0 \) and \( \mathcal{I}(\nabla f(x^0)) = \mathcal{I} \), and if \( \mathcal{I}(x^t) = \mathcal{I} \) for some \( t \geq 1 \), then \( a_j^\top x^t > 0 \) for all \( j \in [m] \) and hence \( \mathcal{I}(\nabla f(x^t)) = \mathcal{I} \). As a result, we have \( \mathcal{I}(x^{t+1}) = \mathcal{I} \).

1.3 Motivation

As mentioned in Section 1.1, although the problem \( (P) \) appears to be structurally simple, it includes many important applications across a variety of fields. Unfortunately, due to the presence of \( \ln(\cdot) \), the objective function \( f \) is neither Lipschitz nor has Lipschitz gradient on the constraint set \( \Delta_n \), and this prohibits us from applying most of the traditional first-order methods \([10, 11]\) to solve \( (P) \).

In the literature, the standard choice for solving \( (P) \) is the MG method, and it has been long known that the sequence of iterates generated by the MG method has a unique limit point that is an optimal solution of \( (P) \) (see e.g., \([1, 12, 13]\)). However, the convergence rate of this method has remained unclear for almost fifty years. Recently, some “unconventional” first-order methods have been proposed to minimize certain differentiable functions whose gradients are not Lipschitz on the constraint set. Among them, two methods are applicable to \( (P) \), namely, the relatively-smooth gradient method (RSGM) \([14, 15]\) and the Frank-Wolfe method for convex composite optimization involving a logarithmically-homogeneous barrier (FW-LHB) \([6, 16]\).

Given the methods mentioned above, a natural question is to determine which method is “best suited” for solving \( (P) \). Numerically, the extensive experimental results in \([6, \text{Section 4.2}]\) indicate that the MG method significantly and consistently outperforms RSGM and FW-LHB across different values of \( m \) and \( n \), and regardless of the location of the initial point \( x^0 \) (namely, whether \( x^0 \) lies at the center of \( \Delta_n \) or lies close to the relative boundary of \( \Delta_n \)). The extraordinary numerical performance of the MG method is rather surprising and somewhat mysterious, for two reasons. First, the structure of the MG method is extremely simple. Indeed, compared with the other two methods, the MG method does not require selecting step-sizes, solving a projection sub-problem onto the constraint set \( \Delta_n \), or solving a linear minimization sub-problem over \( \Delta_n \). Second, unlike the other two methods with known convergence rates, the MG method has only been known to converge asymptotically (i.e., without any convergence rate guarantees).

The discussion above motivates us to investigate the computational guarantees of the MG method, with the hope that the results could provide theoretical justification for the superior numerical performance of the MG method.
1.4 Contributions

Our contributions are summarized as follows.

i) We present the first (to our knowledge) convergence rate analysis for the MG method. We show – via a surprisingly simple proof – that the MG method has an $O(\ln(n)/t)$ convergence rate in both the ergodic and the non-ergodic cases. (Recall that $n$ denotes the dimension of the optimization variable $x$.)

ii) We provide an extremely short proof of the asymptotic convergence of $\{x^t\}_{t\geq 0}$ to an optimal solution of $(P)$, which is much simpler than the existing proofs in [1,12,13].

iii) We show that the distance from $x^t$ to the set of optimal solutions of $(P)$ converges to zero at rate $O(1/\sqrt{t})$, by constructing a quadratic error bound of $(P)$.

iv) We derive the computational complexities of RSGM and FW-LHB for finding an $\varepsilon$-optimal solution of $(P)$ with initial point $x_0 = (1/n)e$, where $e := (1,\ldots,1) \in \mathbb{R}^n$. This in turn enables us to conclude that the computational complexity of the MG method is always lower than that of RSGM, and is also lower than that of FW-LHB in the regime $n = O(\exp(m))$.

2 Convergence Rate Analysis

In this section we present the convergence analysis of the MG method, where we will prove an $O(\ln(n)/t)$ convergence rate for both the non-ergodic and the ergodic cases.

Before doing so, let us introduce some definitions and conventions. Let $\mathcal{X}^* \neq \emptyset$ be the set of optimal solutions of $(P)$, and let $x^*$ be any point in $\mathcal{X}^*$, so that $f^* = f(x^*)$. For any $x, y \geq 0$, define the Kullback-Leibler (KL) divergence

$$D_{KL}(y, x) := \sum_{i=1}^n y_i \ln(y_i/x_i),$$

where we use the following conventions:

$$0 \ln 0 := 0, \quad 0 \ln(0/0) := 0 \quad \text{and} \quad a \ln(a/0) := +\infty, \quad \forall a > 0. \quad (10)$$

Using these conventions and [17, Lemma 3], we know that

$$D_{KL}(y, x) \geq (1/2)\|y - x\|_1^2 \geq 0, \quad \forall y, x \in \Delta_n, \quad (11)$$

where $\| \cdot \|_1$ denotes the $\ell_1$-norm, namely, $\|x\|_1 := \sum_{i=1}^n |x_i|$ for $x \in \mathbb{R}^n$. (To see why (11) holds, note that if the support $\mathcal{I}(y) \not\subseteq \mathcal{I}(x)$, then $D_{KL}(y, x) = +\infty$ and (11) trivially holds; otherwise, we can restrict (11) to the “sub-simplex” $\Delta_{[\mathcal{I}(x)]}$ and apply [17, Lemma 3].)

Our main convergence results are stated as follows:

**Theorem 1.** Let $\{x^t\}_{t\geq 0}$ be the iterates of the MG method. Then for any $x^* \in \mathcal{X}^*$ and all $t \geq 0$:

(i) Non-ergodic rate: $f^* - f(x^t) \leq \frac{D_{KL}(x^*, x^0)}{t+1}$, and

(ii) Ergodic rate: $f^* - f(\bar{x}^t) \leq \frac{D_{KL}(x^*, x^0)}{t+1}$, where $\bar{x}^t := \frac{1}{t+1} \sum_{k=0}^t x^k$. \qed

Before proving Theorem 1, let us first state an important corollary.
Corollary 1. Let \( \{x^t\}_{t \geq 0} \) be the iterates of the MG method. The for all \( t \geq 0 \), we have

\[
f^* - f(x^t) \leq \frac{-\ln(x^0_{\min})}{t + 1} \quad \text{and} \quad f^* - f(x^t) \leq \frac{-\ln(x^0_{\min})}{t + 1}.
\] (12)

Consequently, if we choose \( x^0 = (1/n)e \), then for all \( t \geq 0 \), we have

\[
f^* - f(x^t) \leq \frac{\ln(n)}{t + 1} \quad \text{and} \quad f^* - f(x^t) \leq \frac{\ln(n)}{t + 1}.
\] (13)

Proof. Since \( D_{KL}(\cdot, x^0) \) is convex for any \( x^0 \in ri \Delta_n \), we have

\[
\max_{x \in \Delta_n} D_{KL}(x, x^0) = \max_{i \in [n]} D_{KL}(e_i, x^0) = \max_{i \in [n]} -\ln(x^0_i) = -\ln(x^0_{\min}),
\]

where \( e_i \) is the \( i \)-th standard coordinate vector in \( \mathbb{R}^n \) for \( i \in [n] \). Then based on Theorem 1, we arrive at (12). This completes the proof. \( \square \)

Remark 1. Note that in Theorem 1, we provide data-dependent convergence rates — this is because \( D_{KL}(x^*, x^0) \) depends on the optimal solution \( x^* \in \mathcal{X}^* \), which in turn depends on the data matrix \( A \) (cf. (7)). In contrast, in Corollary 1 we provide data-independent convergence rates. In fact, these rates only depend on the minimum element of the starting point \( x^0 \). From (12), it is clear that the optimal choice of \( x^0 \) should be \((1/n)e\), which yields \( O(\ln(n)/t) \) convergence rates in both the non-ergodic and the ergodic cases.

Towards the task of proving Theorem 1, we begin our analysis with the following simple but important observations about (P).

Lemma 1. There exists \( \nu \in \mathbb{R}^n_+ \) such that \( \nabla_i f(x^*) + \nu_i = 1 \) and \( \nu_i x^*_i = 0 \), for all \( i \in [n] \). In particular, if \( x^*_i > 0 \) for some \( i \in [n] \), then \( \nabla_i f(x^*) = 1 \).

Proof. First, let us observe that for any \( x \in \Delta_n \) we have

\[
\langle \nabla f(x), x \rangle = \sum_{i=1}^{n} x_i \sum_{j=1}^{m} p_j \frac{a_{ji}}{a_j} x = \sum_{j=1}^{m} p_j = 1,
\] (14)

where \( a_{ji} \) denotes the \( i \)-th entry of \( a_j \). The KKT conditions are necessary and sufficient for optimality for (P), and thus there exists \( \lambda \in \mathbb{R} \) and \( \nu \in \mathbb{R}^n_+ \) such that \( \nabla f(x^*) + \lambda e + \nu = 0 \), and \( \nu_i x^*_i = 0 \) for all \( i \in [n] \) (where recall that \( e \) denotes the vector of ones). Consequently

\[
1 + \lambda = \langle \nabla f(x^*), x^* \rangle + \lambda \langle e, x^* \rangle = 0,
\]

which implies that \( \lambda = -1 \) and hence \( \nabla f(x^*) + \nu = e \). \( \square \)

The next lemma, which is due to Cover [4, Theorem 1], presents a lower bound on the improvement of the objective value at each iteration of the MG method. For completeness, we include a short proof in Appendix A.

Lemma 2 (Cover [4, Theorem 1]). For all \( t \geq 0 \) we have

\[
f(x^{t+1}) - f(x^t) \geq D_{KL}(x^{t+1}, x^t) \geq 0.
\] \( \square \)
For convenience, let us define the objective gap at \( x \in \Delta_n \) as \( \delta(x) := f^* - f(x) \); then from Lemma 2 we see that \( \{\delta(x^t)\}_{t \geq 0} \) is a monotonically non-increasing sequence.

**Lemma 3.** For any \( x \in \Delta_n \) we have

\[
\delta(x) \leq \sum_{i=1}^{n} x^*_i \ln (\nabla_i f(x)).
\]  

(15)

**Proof.** Define \( I^* := \{i \in [n] : x^*_i > 0\} \), and from Lemma 1 it follows that for any \( i \in I^* \) we have

\[
\sum_{j=1}^{m} \frac{p_j a_{ji}}{a_j^* x^*} = \nabla_i f(x^*) = 1.
\]  

(16)

As a result we have

\[
\sum_{i=1}^{n} x^*_i \ln (\nabla_i f(x)) = \sum_{i \in I^*} x^*_i \ln (\nabla_i f(x))
\]

\[
= \sum_{i \in I^*} x^*_i \ln \left( \sum_{j=1}^{m} \frac{p_j a_{ji}}{a_j^* x^*} \right)
\]

\[
\geq \sum_{i \in I^*} x^*_i \sum_{j=1}^{m} \frac{p_j a_{ji}}{a_j^* x^*} \ln \left( \frac{a_j^* x^*}{a_j^* x^*} \right)
\]

\[
= \sum_{j=1}^{m} p_j \ln \left( \frac{a_j^* x^*}{a_j^* x^*} \right)
\]

\[
= f(x^*) - f(x) = \delta(x),
\]  

(17)

where the inequality above uses (16) and the concavity of \( \ln(\cdot) \).

Equipped with the above lemmas, we now prove Theorem 1.

**Proof of Theorem 1.** For any \( x^* \in X^* \), we have

\[
D_{KL}(x^*, x^t) - D_{KL}(x^*, x^{t+1}) = \sum_{i=1}^{n} x^*_i \ln \left( \frac{x^*_{i+1}}{x^*_i} \right) = \sum_{i=1}^{n} x^*_i \ln (\nabla_i f(x^t)) \geq \delta(x^t),
\]  

(18)

where the inequality on the right follows from Lemma 3. Telescoping over \( k = 0, \ldots, t \), we obtain

\[
D_{KL}(x^*, x^0) - D_{KL}(x^*, x^{t+1}) \geq \sum_{k=0}^{t} \delta(x^k).
\]

Using the convexity of \( \delta(\cdot) \), we have \( \sum_{k=0}^{t} \delta(x^k) \geq (t+1)\delta(x^t) \), which proves part (ii). Alternatively, using the property that \( \{\delta(x^t)\}_{t \geq 0} \) is a non-increasing sequence, we have \( \sum_{k=0}^{t} \delta(x^k) \geq (t+1)\delta(x^t) \), which then proves part (i).

**Remark 2.** Under the “normalization” assumption that \( \sum_{j=1}^{m} a_{ji} = 1 \) for all \( i \in [n] \), Iusem [13, Lemma 2.2] showed a recursion that is slightly more general than (18). In fact, the proof technique in [13] mainly leverages the joint convexity of the KL-divergence, which is quite different from our proof above. In addition, it is not clear (to us) if the technique in [13] can still be applied in the general setting where the normalization assumption is absent.
Next, we present an extremely short proof of the asymptotic convergence of \( \{x^t\}_{t \geq 0} \) to some \( x^* \in \mathcal{X}^* \), which is much simpler than the existing proofs in [1, 12, 13].

**Corollary 2.** There exists some \( x^* \in \mathcal{X}^* \) such that \( x^t \to x^* \).

**Proof.** Since \( \Delta_n \) is compact, there exists a sub-sequence of \( \{x^t\}_{t \geq 0} \), which we denote by \( \{x^{t_i}\}_{t \geq 0} \), that converges to some \( \bar{x} \in \Delta_n \). Using the conventions in (10), it is clear that \( D_{\text{KL}}(\bar{x}, x^{t_i}) \to 0 \) (as \( l \to +\infty \)). Since \( f(x^t) \to f^* \) (cf. Theorem 1(i)), we see that \( f(x^{t_i}) \to f^* \) and hence \( \bar{x} \in \mathcal{X}^* \). On the other hand, from (18), we know that the nonnegative sequence \( \{D_{\text{KL}}(\bar{x}, x^t)\}_{t \geq 0} \) is non-increasing, and hence \( D_{\text{KL}}(\bar{x}, x^t) \to d^* \) for some \( d^* \geq 0 \). Since \( D_{\text{KL}}(\bar{x}, x^t) \to 0 \), we know that \( d^* = 0 \), which implies that \( D_{\text{KL}}(\bar{x}, x^t) \to 0 \). Finally, since \( \bar{x} \in \Delta_n \) and \( x^t \in \Delta_n \) for all \( t \geq 0 \), we use (11) to conclude that \( \|x^t - x^*\|_1 \to 0 \). This completes the proof. \( \square \)

3 **Error Bound and Convergence Rate of the Distance to \( \mathcal{X}^* \)**

In this section we present an error bound for \( f \) on the constraint set \( \Delta_n \), which we then use to characterize the rate of convergence of the distances from \( \{x_t\}_{t \geq 0} \) to \( \mathcal{X}^* \). Let \( \|\cdot\| \) be any given norm on \( \mathbb{R}^n \), and define

\[
\text{dist}_{\|\cdot\|}(x, \mathcal{X}^*) := \min_{x^* \in \mathcal{X}^*} \|x - x^*\|, \quad \forall x \in \mathbb{R}^n.
\]  \((19)\)

Let us introduce some new notations. Let \( \mathcal{Y} := A(\Delta_n) \subseteq \mathbb{R}^m \), which is the image of \( \Delta_n \) under the linear operator \( A \) (cf. (7)). Note that we can write (P) equivalently as

\[
\max_{y \in \mathcal{Y}} [\tilde{f}(y) := \sum_{j=1}^{m} p_j \ln y_j] , \quad (P_y)
\]

where \( \text{dom} \tilde{f} = \mathbb{R}^m_+ := \{y \in \mathbb{R}^m : y > 0\} \). The strict concavity of \( \tilde{f} \) implies that (\( P_y \)) has a unique optimal solution \( y^* \in \mathcal{Y} \cap \text{dom} \tilde{f} = \mathcal{Y} \cap \mathbb{R}^m_+ \), and hence we have \( f^* = \tilde{f}(y^*) \) and

\[
\mathcal{X}^* := \{x \in \mathbb{R}^n_+ : e^\top x = 1, \ Ax = y^* \} . \quad (20)
\]

In particular, we can write

\[
\mathcal{X}^* = \Delta_n \cap \mathcal{L}, \quad \text{where} \quad \mathcal{L} := \{x \in \mathbb{R}^n : Ax = y^*\} . \quad (21)
\]

Let us define the following norm on \( \mathbb{R}^m \) induced by the Hessian of \( \tilde{f} \) at \( y^* \): \( \|\cdot\|_{y^*} \)

\[
\|y\|_{y^*} := \sqrt{\langle -\nabla^2 \tilde{f}(y^*) y, y \rangle} = \sqrt{\sum_{j=1}^{m} p_j (y_j/y^*_j)^2}, \quad \forall y \in \mathbb{R}^m
\]  \((22)\)

and define the “radius” of \( \mathcal{Y} \) centered at \( y^* \) as

\[
R_{y^*} := \max_{y \in \mathcal{Y}} \|y - y^*\|_{y^*} = \max_{x \in \Delta_n} \|Ax - y^*\|_{y^*} = \max_{i \in [n]} \|A_i - y^*\|_{y^*} . \quad (23)
\]

(Recall that \( A_i \) is the \( i \)-th column of \( A \) for \( i \in [n] \).) In addition, let \( p_{\min} := \min_{j \in [m]} p_j \), and note that since \( \sum_{j=1}^{m} p_j = 1 \), we have \( p_{\min} \in (0, 1/m] \). The next lemma uses the above notations and definitions to construct a lower bound of the optimality gap \( f^* - \tilde{f} \) on \( \mathcal{Y} \).
Lemma 4. For all \( y \in \mathcal{Y} \) we have
\[
f^* - \bar{f}(y) \geq \min \omega(p_{\min}^{-1/2}\|y - y^\ast\|_y^\ast),
\] (24)
where \( \omega(t) := t - \ln(1 + t) \) for \( t > -1 \).

Proof. Define \( F := p_{\min}^{-1} \bar{f} \), and from standard results on self-concordant function theory (e.g., [18, Theorem 2.2.6]), we observe that \( -F \) is a (standard strongly non-degenerate) self-concordant function with \( \text{dom} F = \text{dom} \bar{f} = \mathbb{R}^n_{++} \). Therefore from [11, Theorem 4.1.7], we have for all \( y \in \mathcal{Y} \):
\[
-F(y) \geq -F(y^\ast) - \langle \nabla F(y^\ast), y - y^\ast \rangle + \omega\left(\sqrt{-\nabla^2 F(y^\ast)(y - y^\ast)}, y - y^\ast\right),
\] (25)
which is equivalent to
\[
\bar{f}(y) \leq \bar{f}(y^\ast) + \langle \nabla \bar{f}(y^\ast), y - y^\ast \rangle - \min \omega(p_{\min}^{-1/2}\|y - y^\ast\|_y^\ast)
\leq \bar{f}(y^\ast) - \min \omega(p_{\min}^{-1/2}\|y - y^\ast\|_y^\ast),
\]
where the last inequality uses \( \langle \nabla \bar{f}(y^\ast), y - y^\ast \rangle \leq 0 \) for all \( y \in \mathcal{Y} \). \( \square \)

Lemma 5. For any \( \bar{t} > 0 \) and any \( 0 < t \leq \bar{t} \), we have \( \omega(t) \geq \left(\omega(\bar{t})/\bar{t}^2\right) t^2 \).

Proof. It suffices to show the function \( \zeta(t) := \omega(t)/t^2 \) is non-increasing on \((0, +\infty)\), or equivalently, that \( \zeta'(t) \leq 0 \) for all \( t > 0 \). Indeed, we have \( \zeta'(t) = \frac{\xi(t)}{t^3} \), where \( \xi(t) := t^2/(1 + t) - 2\omega(t) \) for \( t > -1 \). Since \( \xi(0) = 0 \) and \( \xi'(t) = -t^2/(1 + t)^2 < 0 \) for all \( t > 0 \), we see that \( \zeta(t) < 0 \) for all \( t > 0 \), and hence \( \zeta'(t) \leq 0 \) for all \( t > 0 \). This completes the proof. \( \square \)

We also observe from (20) that \( X^\ast \) is the solution to the system of linear equalities and inequalities given therein, and hence there is a Hoffman constant \( C_H \) associated with \( X^\ast \), namely:

Lemma 6. There exists \( 0 < C_H < +\infty \) such that for all \( x \in \Delta_n \), we have
\[
\text{dist}_{\|\cdot\|}(x, X^\ast) \leq C_H\|Ax - y^\ast\|_{y^\ast}. \tag{26}
\]

Proof. This follows from Hoffman’s lemma [19], whereby there exists \( 0 < C_H < +\infty \) such that
\[
\text{dist}_{\|\cdot\|}(x, X^\ast) \leq C_H(\|x\|_\ast + e^\top x - 1 + \|Ax - y^\ast\|_{y^\ast}), \quad \forall x \in \mathbb{R}^n,
\] (27)
where \( (x)_\ast := (\min\{0, x_i\})_{i=1}^n \). However, since \( x \in \Delta_n \), we have \( (x)_\ast = 0 \) and \( e^\top x - 1 = 0 \), and this completes the proof. \( \square \)

Remark 3. Note that the Hoffman constant \( C_H \) depends on both the problem data (namely \( A \) and \( \{p_j\}_{j=1}^m \)) and the norm \( \|\cdot\| \) on \( \mathbb{R}^m \). However, for notational brevity, we omit such dependence.

Equipped with the above three lemmas, we now present our error bound for \( f \) on \( \Delta_n \).

Proposition 1 (An error bound for \( f \) on \( \Delta_n \)). For all \( x \in \Delta_n \) we have
\[
\text{dist}_{\|\cdot\|}(x, X^\ast) \leq \sqrt{p_{\min} \omega(p_{\min}^{-1/2} R_{y^\ast}) / C_H R_{y^\ast}} \sqrt{f^* - f(x)}, \tag{28}
\]
where \( R_{y^\ast}, \omega(\cdot), \) and \( C_H \) are defined in (23), Lemma 4, and Lemma 6, respectively.
Proof. Since \( f(x) = f(Ax) \) for all \( x \in \Delta_n \), we have
\[
\begin{align*}
    f^* &\geq f(x) + p_{\min} \omega(p_{\min}^{-1/2} (Ax - y^*)_y) \\
&\geq f(x) + p_{\min} \omega(p_{\min}^{-1/2} R_{y^*}) \frac{1}{p_{\min} R^2_{y^*}} \|Ax - y^*\|_y^2 \\
&\geq f(x) + p_{\min} \omega(p_{\min}^{-1/2} R_{y^*}) \frac{\text{dist}((x, x^*)^2}{R_y^2 C_H^2},
\end{align*}
\]
where the first inequality uses Lemma 4, the second inequality uses Lemma 5 and the definition of \( R_{y^*} \) in (23), and the third inequality uses Lemma 6. The proof is completed by rearranging and taking square roots.

By combining Theorem 1 and Proposition 1, we arrive at the following theorem, which shows that both \( \{\text{dist}((x^t, x^*)^{(i)}\}_{t \geq 0} \) and \( \{\text{dist}((\bar{x}^t, x^*)\}_{t \geq 0} \) converges to zero at \( O(1/\sqrt{t}) \) rate.

**Theorem 2.** Define \( \text{dist}_{KL}(x^0, x^*) := \min_{x \in X^*} D_{KL}(x, x^0) \) as the “KL-distance” from \( x^0 \) to \( x^* \). Then for all \( t \geq 0 \), we have
\[
\max\{\text{dist}((x^t, x^*), \text{dist}((\bar{x}^t, x^*)) \leq \sqrt{\frac{p_{\min} \omega(p_{\min}^{-1/2} R_{y^*}) \text{dist}_{KL}(x^0, x^*)}{C_H R_{y^*} \sqrt{t + 1}}},
\]
where \( R_{y^*}, \omega(\cdot) \), and \( C_H \) are defined in (23), Lemma 4, and Lemma 6, respectively.

### 4 Complexity Comparison of MG, RSGM and FW-LHB

In this section, we compare the computational complexities of the MG method in (6) with two other principled first-order methods for finding an \( \epsilon \)-optimal solution of (P), which include RSGM and FW-LHB. Here an \( \epsilon \)-optimal solution of (P) refers to a feasible point \( x \in \Delta_n \) such that \( f^* - f(x) \leq \epsilon \). For simplicity, we presume that \( p_1 = \cdots = p_m = 1/m \) in (P), which then becomes
\[
f^* := \max_{x \in \Delta_n} \left\{ f(x) := (1/m) \sum_{j=1}^m \ln(a_j^\top x) \right\}. \tag{P_u}
\]
In addition, for comparison purpose, we presume that all the three methods share the same starting point \( x^0 = (1/n)e \), which is a common choice for each of the methods (see e.g., [1, 15, 20]).

Let us now derive the computational complexities of RSGM and FW-LHB. Before doing so, we first make the following simple but important observation.

**Lemma 7.** In (P_u), for any problem data \( \{a_j\}_{j=1}^m \subseteq \mathbb{R}^n_+ \setminus \{0\} \), we always have
\[
\delta(x^0) = f^* - f(x^0) = f^* - f((1/n)e) \leq \ln(n). \tag{29}
\]

**Proof.** Let \( x^* \in \Delta_n \) be any optimal solution of (P_u). Then we have
\[
f^* - f((1/n)e) = \frac{1}{m} \sum_{j=1}^m \ln \left( \frac{a_j^\top x^*}{a_j e/n} \right) \overset{(a)}{\leq} \frac{1}{m} \sum_{j=1}^m \ln \left( \frac{\max_{i \in [n]} a_{ji}}{\sum_{i=1}^n a_{ji}/n} \right) \overset{(b)}{\leq} \ln(n),
\]
where in (a) we use \( x^* \in \Delta_n \) and in (b) we use \( \max_{i \in [n]} a_{ji} \leq \sum_{i=1}^n a_{ji} \) (for all \( j \in [m] \)).
Remark 4. Note that the estimate in (29) is indeed tight. To see this, let \( a_1 = \ldots = a_m = \epsilon_1 \). Then \( f^* = 0 \) and \( f(x^0) = f((1/n)e) = -\ln(n) \), and hence \( \delta(x^0) = \ln(n) \).

Next, let us briefly describe the specific form of RSGM when applied to solving \((P_u)\). We first define the “reference” function
\[
r(x) := -\sum_{i=1}^n \ln(x_i) \quad \text{with} \quad \text{dom } r = \mathbb{R}^n_+,
\]
and its induced Bregman divergence
\[
D_r(y, x) := r(y) - r(x) - \langle \nabla r(x), y - x \rangle, \quad \forall y, x \in \mathbb{R}^n_+.
\]
Starting from \( x^0 = (1/n)e \), each iteration of RSGM solves the following (Bregman) projection problem:
\[
x^{t+1} := \operatorname{argmax}_{x \in \Delta_n} \langle \nabla f(x^t), x \rangle - D_r(x, x^t).
\]
(BP)
The computational complexity of RSGM for finding an \( \epsilon \)-optimal solution of \((P_u)\) is stated below.

**Proposition 2.** Starting from \( x^0 = (1/n)e \), RSGM finds an \( \epsilon \)-optimal solution of \((P_u)\) in at most
\[
O\left(\frac{(mn + n \ln(n))n}{\epsilon} \ln \left(\frac{\ln(n)}{\epsilon}\right)\right)
\]
arithmetic operations.

**Proof.** Since \( f \) is 1-smooth relative to \( r \) on \( \mathbb{R}^n_+ \) (cf. [14, Lemma 7]), from [15, Theorem 3.1] (see also [14, Theorem 1(iv)]), we know that for all \( x \in \mathbb{R}^n_+ \),
\[
f(x) - f(x^t) \leq D_r(x, x^0)/t, \quad \forall t \geq 1.
\]
(32)
Since it may happen that \( \mathbb{R} \Delta_n \cap L = \emptyset \) and hence \( \mathbb{R}^n_+ \cap \mathbb{R} \Delta_n = \emptyset \), similar to [15, Theorem 4.1], let us fix any \( x^t \in \mathbb{R}^n_+ \), and define \( \hat{x} := (1 - \alpha)x^* + \alpha x^0 \) with \( \alpha := \epsilon/(2\delta(x^0)) \). This ensures that
\[
\delta(\hat{x}) \leq (1 - \alpha)\delta(x^*) + \alpha \delta(x^0) = \epsilon/2.
\]
(33)
In addition, since \( x^0 = (1/n)e \), we have \( \nabla r(x^0) = -ne \) and hence
\[
D_r(\hat{x}, x^0) = r(\hat{x}) - r(x^0) \leq r(\alpha x^0) - r(x^0) = -n \ln(\alpha) = n \ln(2\delta(x^0)/\epsilon),
\]
(34)
where the inequality follows from that \( \hat{x} \geq \alpha x^0 \) and the function \( r \) is coordinate-wise decreasing.

From (33), it is clear that if \( f(\hat{x}) - f(x^t) \leq \epsilon/2 \), then \( \delta(x^t) \leq \epsilon \), and from (34), we know that this happens in no more than
\[
\left\lfloor \frac{2(n/\epsilon) \ln(2\delta(x^0)/\epsilon)}{\epsilon} \right\rfloor = O((n/\epsilon) \ln(2\delta(x^0)/\epsilon)) = O((n/\epsilon) \ln(\ln(n)/\epsilon)) \quad \text{iterations.}
\]
(35)
Next, we analyze the complexity of arithmetic operations in each iteration. First, note that computing \( \nabla f(x^t) \) requires \( O(mn) \) arithmetic operations, for all \( t \geq 0 \). In addition, from [21, Section 7], we know that the projection problem in (BP) be reduced to finding the unique root of a strictly decreasing univariate function on \((0, +\infty)\), and the root can be computed to machine precision in \( O(n \ln(n)) \) arithmetic operations (see also [22, 23]). Therefore, each iteration of RSGM requires \( O(mn + n \ln(n)) \) arithmetic operations. This, together with (35), completes the proof.
Table 1: The computational complexities of MG, RSGM and FW-LHB for finding an \( \varepsilon \)-optimal solution of \((P_u)\).

| Method   | Complexity                                      |
|----------|-------------------------------------------------|
| RSGM     | \( O \left( \frac{(mn+n\ln(n))\ln n}{\varepsilon} \right) \) |
| FW-LHB   | \( O \left( m^2n \ln(n)(\ln(m) + \ln(n)) + \frac{m^2n}{\varepsilon} \right) \) |
| MG       | \( O \left( \frac{mn\ln(n)}{\varepsilon} \right) \) |

Now, let us switch our focus to FW-LHB. Note that FW-LHB cannot be directly applied to \((P_u)\), since the objective function \( f \) in \((P_u)\) is not self-concordant (cf. \cite[Section 2.1]{24}). Instead, we apply FW-LHB to an equivalent problem of \((P_u)\), namely

\[
\min_{x \in \Delta_n} - \sum_{j=1}^{m} \ln(a_j^\top x). \tag{P_s}
\]

Clearly, \( x \in \Delta_n \) is an \( \varepsilon \)-optimal solution of \((P_u)\) if and only if it is an \( \bar{\varepsilon} \)-optimal solution of \((P_s)\) for \( \bar{\varepsilon} = m\varepsilon \). Based on this, we state the computational complexity of FW-LHB for finding an \( \varepsilon \)-optimal solution of \((P_u)\) as follows:

**Proposition 3.** Starting from \( x^0 = (1/n)e \), FW-LHB finds an \( \varepsilon \)-optimal solution of \((P_u)\) in at most

\[
O\left( m^2n \ln(n)(\ln(m) + \ln(n)) + \frac{m^2n}{\varepsilon} \right) \text{ arithmetic operations.}
\]

**Proof.** From \cite[Remark 2.1]{6}, we know that to find an \( \bar{\varepsilon} \)-optimal solution of \((P_s)\), the iteration complexity of FW-LHB is

\[
O\left( m\delta(x^0) \ln(m\delta(x^0)) + m^2/\bar{\varepsilon} \right) = O\left( m\delta(x^0) \ln(m\delta(x^0)) + m/\varepsilon \right). \tag{36}
\]

Since \( \delta(x^0) \leq \ln(n) \) (cf. Lemma 7) and each iteration of FW-LHB requires \( O(mn) \) arithmetic operations (cf. \cite[Section 2]{6}), we complete the proof.

Finally, from Theorem 1, we can easily derive the computational complexity of MG for finding an \( \varepsilon \)-optimal solution of \((P_u)\) as follows:

**Proposition 4.** Starting from \( x^0 = (1/n)e \), MG finds an \( \varepsilon \)-optimal solution of \((P_u)\) in at most

\[
O\left( mn \ln(n)/\varepsilon \right) \text{ arithmetic operations.}
\]

For ease of comparison, we summarize the computational complexities of MG, RSGM and FW-LHB for finding an \( \varepsilon \)-optimal solution of \((P_u)\) in Table 1. From this table, we see that MG always has a lower complexity compared to RSGM. In addition, for sufficiently small accuracy \( \varepsilon \) — so that the computational complexity of FW-LHB becomes (essentially) \( O(m^2n/\varepsilon) \), MG has a lower complexity compared to FW-LHB as long as \( n = O(\exp(m)) \). This provides an explanation to the superior numerical performance of MG compared to RSGM and FW-LHB on the PET problem as observed in \cite[Section 4.2]{6}.
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A Proof of Lemma 2

The following proof is borrowed from Cover [4, Theorem 1]. We have

\[ f(x^{t+1}) - f(x^t) = \sum_{j=1}^{m} p_j \ln \left( \frac{a_j^\top x^{t+1}}{a_j^\top x^t} \right) \]
\[ = \sum_{j=1}^{m} p_j \ln \left( \sum_{i=1}^{n} \frac{a_{ji} x_i^t x_i^{t+1}}{a_j^\top x^t} \right) \]
\[ \geq \sum_{j=1}^{m} p_j \sum_{i=1}^{n} \frac{a_{ji} x_i^t}{a_j^\top x^t} \ln \left( \frac{x_i^{t+1}}{x_i^t} \right) \]
\[ = \sum_{i=1}^{n} x_i^t \nabla_i f(x^t) \ln \left( \frac{x_i^{t+1}}{x_i^t} \right) \]
\[ = \sum_{i=1}^{n} x_i^{t+1} \ln \left( \frac{x_i^{t+1}}{x_i^t} \right) = D_{KL}(x^{t+1}, x^t), \]

where the inequality follows from the concavity of \( \ln(\cdot) \), and the last equality uses (9). \( \square \)

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