An Alternative to EM for Gaussian Mixture Models: Batch and Stochastic Riemannian Optimization

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Abstract

We consider maximum likelihood estimation for Gaussian Mixture Models (GMMs). This task is almost invariably solved (in theory and practice) via the Expectation Maximization (EM) algorithm. EM owes its success to various factors, of which is its ability to fulfill positive definiteness constraints in closed form is of key importance. We propose an alternative to EM by appealing to the rich Riemannian geometry of positive definite matrices, using which we cast GMM parameter estimation as a Riemannian optimization problem. Surprisingly, such an out-of-the-box Riemannian formulation completely fails and proves much inferior to EM. This motivates us to take a closer look at the problem geometry, and derive a better formulation that is much more amenable to Riemannian optimization. We then develop (Riemannian) batch and stochastic gradient algorithms that outperform EM, often substantially. We provide a non-asymptotic convergence analysis for our stochastic method, which is also the first (to our knowledge) such global analysis for Riemannian stochastic gradient. Numerous empirical results are included to demonstrate the effectiveness of our methods.

1 Introduction

Gaussian Mixture Models are extensively used across many tasks in machine learning, signal processing, and other areas [6, 13, 14, 21, 24, 26, 30]. For a vector $x \in \mathbb{R}^d$, the density of a Gaussian Mixture Model (GMM) is given by

$$p(x) := \sum_{j=1}^{K} \alpha_j p_N(x; \mu_j, \Sigma_j), \quad (1.1)$$

where $p_N$ is a Gaussian with mean $\mu \in \mathbb{R}^d$ and covariance $\Sigma > 0$, i.e.,

$$p_N(x; \mu, \Sigma) := \det(\Sigma)^{-1/2} (2\pi)^{-d/2} \exp \left(-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right).$$

Given i.i.d. samples $\{x_1, \ldots, x_n\}$ drawn from (1.1), we seek maximum likelihood estimates $\{\hat{\mu}_j \in \mathbb{R}^d, \hat{\Sigma}_j > 0\}_{j=1}^{K}$ and $\hat{\alpha} \in \Delta_K$ of the parameters of the GMM. This estimation is cast as the following log-likelihood maximization problem:

$$\max_{\alpha \in \Delta_K, \{\mu_j, \Sigma_j > 0\}_{j=1}^{K}} \sum_{i=1}^{n} \log \left( \sum_{j=1}^{K} \alpha_j p_N(x_i; \mu_j, \Sigma_j) \right). \quad (1.2)$$

A quick literature search reveals that (1.2) is most frequently solved via the Expectation Maximization (EM) algorithm [12] or its variants. Although other optimization methods have also been considered [29], for solving practical instances of (1.2) usual methods such as conjugate gradients, quasi-Newton, Newton, are typically regarded as inferior to EM [41].

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Difficulties and Motivation. The primary reason why standard nonlinear methods have difficulties in solving (1.2) is the positive definiteness constraint on the covariance matrices. Since this constraint defines an open subset of Euclidean space, in principle, if the iterates remain in the interior, standard unconstrained Euclidean optimization methods could be used. The iterates may, however, approach the boundary of the constraint set, especially in higher dimensions, which can lead to very slow convergence. One approach is to formulate the positive definite constraint via a set of smooth convex inequalities \[37\] and use interior-point methods. It was observed in \[34\] that using such sophisticated methods can be vastly slower (on some closely related statistical problems) than simpler EM-like fixed-point methods, especially with growing problem dimensionality.

Another “natural” approach to handle the positive definite constraint is to use the Cholesky decomposition, as was exploited for semidefinite programming in \[10\], and more recently in \[5\]. In general, this decomposition can add spurious local maxima and stationary points to the objective function of general optimization problems, even for semidefinite programs \[37\]. Remarkably, it can be shown that such a decomposition does not add spurious local maxima to (1.2). Nevertheless, we observed (empirically) that the convergence speed of standard nonlinear solvers for estimating parameters of (1.2) using Cholesky decomposition is considerably slower than EM.

Motivated by the success of non-Euclidean optimization for some problems with positive definite variables \[34, 35\], we consider an alternative approach to EM. In particular, we solve (1.2) via Riemannian optimization. Surprisingly, a naïve use of Riemannian methods completely fails to compete with EM, while their use on a careful reformulation\(^1\) of (1.2) demonstrably succeeds.

We describe this reformulation in Section 3, and remark here informally on why a naïve use of manifold optimization fails: The negative log-likelihood for a single Gaussian is Euclidean convex (the key property that makes the “M-step” of EM easy), but not geodesically convex. Reformulating the problem to remove this geometric mismatch might therefore be fruitful, i.e., if we reformulate the single Gaussian likelihood to be geodesically convex, manifold optimization may benefit. This intuition turns out to have remarkable empirical consequences as will become apparent from the paper.

Contributions. The present paper goes substantially beyond our preliminary work \[17\] in several important aspects. Let us therefore outline our main contributions below.

- We develop reformulations not only for GMMs, but also for richer likelihood models that incorporate conjugate priors.
- We present both batch and stochastic optimization algorithms; the latter greatly enhances the scalability of our methods. Moreover, our methods permit the use of retractions (beyond the usual exponential map) and vector transport, which enables further scalability.
- We provide an iteration complexity analysis of stochastic gradient on manifolds, obtaining a \(O(1/\sqrt{T})\) bound. To our knowledge, this is the first non-asymptotic convergence analysis for stochastic gradient on manifolds. Subsequently, we present analysis that outlines why Riemannian SGD applies to penalized GMM-likelihood maximization.

We provide experimental evidence on several real-data comparing manifold optimization to EM. As may be gleaned from our results, manifold optimization performs well across a wide range of parameter values and problem sizes, while being much less sensitive to overlapping data than EM, and while displaying less variability in running times.

We review key concepts of first-order deterministic manifold optimization. We also include the design and specific implementation choices of our line-search procedure. These choices ensure convergence, and are instrumental to making our Riemannian-LBFGS solver outperform both EM and Riemannian conjugate gradients. This solver should be of independent interest too.

\(^{1}\) A preliminary version of this work appeared at the Advances in Neural Information Processing Systems (NIPS 2015), wherein this reformulation was originally introduced.
We will also release a MATLAB implementation of the methods developed in this paper. The manifold CG method that we use is directly based on the excellent toolkit MANOPT [8].

1.1 Related work

EM is such a widely studied method, that we have no hope of summarizing all the related work, even if we restrict to just GMMS. Let us instead mention a few lines of related work. Xu and Jordan [41] examine several aspects of EM for GMMS and counter the claims of Redner and Walker [29], who thought EM to be inferior to general purpose nonlinear programming methods, especially second-order methods. However, it is well-known (see e.g., [29, 41]) that EM can attain good likelihood values rapidly, and that it scales to larger problems than amenable to second-order methods. Local convergence analysis of EM is available in [41], with more refined and precise results in [23], who formally show that when data have low overlap, EM can converge locally superlinearly. Our paper uses manifold LBFGS, which being a quasi-Newton method can also display local superlinear convergence, though this capability is not the focus of our paper.

Parameter fitting using gradient-based methods has also been suggested [27, 33]. Here, to satisfy positive definiteness, the authors suggest using Cholesky decompositions. These works report results only for low-dimensional problems and spherical (near spherical) covariance matrices.

Beyond EM, there is also substantial work on theoretical analysis of GMMS [3, 11, 15, 25]. These studies are theoretically valuable (though sometimes limited to either low-dimensional, or small number of mixture components, or spherical Gaussians, etc.), but orthogonal to our work which focuses on practical numerical algorithms for general GMMS.

The use of Riemannian optimization for GM is relatively new, even though manifold optimization is by now a fairly well-developed branch of optimization. A classic reference is [36]; a more recent work is [1]; and even a MATLAB toolbox exists now [8]. In machine learning, manifold optimization has witnessed increasing interest, e.g., for low-rank optimization [20, 38], optimization based on geodesic convexity [34, 39], or for neural network training [40].

2 Background on manifold optimization

Manifolds are spaces that locally resemble a Euclidean space, and smooth manifolds have smooth transitions between locally Euclidean-like subsets [22]. The tangent space $T_x$ is an approximating vector space at each point $x$ of the manifold $\mathcal{M}$. The tangent bundle of a smooth manifold $\mathcal{M}$ is a manifold $T\mathcal{M}$, which assembles all the tangents in that manifold, $T\mathcal{M} = \bigsqcup_{x \in \mathcal{M}} T_x = \{(x,y)| x \in \mathcal{M}, y \in T_x \}$. If a smooth manifold is equipped with a smoothly-varying inner product on each of its tangent spaces, it is called Riemannian manifold.

This additional structure of a Riemannian manifold proves very useful in developing optimization techniques specific to manifolds [36]. Indeed, it is easy to extend unconstrained optimization techniques to smooth manifolds, at least from the perspective of asymptotic complexity analysis [1]; though the non-asymptotic case is considerably more complicated [42, 43].

The key manifold in this paper is $\mathbb{P}^d$, the manifold of $d \times d$ symmetric positive definite (PSD) matrices. At a point $\Sigma \in \mathbb{P}^d$, the tangent space $T_\Sigma$ is isomorphic to the entire set of symmetric matrices; and the Riemannian metric at $\Sigma$ between two vectors $\xi$ and $\eta$ in $T_\Sigma$ is given by $g_\Sigma(\xi, \eta) := \text{tr}(\Sigma^{-1}\xi \Sigma^{-1}\eta)$.

Riemannian manifolds have geodesics, which are curves that (locally) join points along shortest paths which depends on the choice of Riemannian metric. Geodesics help generalize the notion of convexity to manifolds.

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2Not to be confused with “manifold learning” a separate problem altogether.
2.1 Geodesic convexity

Let $\mathcal{M}$ be a Riemannian manifold and $\gamma_{xy}$ a geodesic from $x$ to $y$; that is

$$\gamma_{xy} : [0, 1] \rightarrow \mathcal{M}, \quad \gamma_{xy}(0) = x, \quad \gamma_{xy}(1) = y.$$ 

A set $A \subseteq \mathcal{M}$ is geodesically convex (henceforth g-convex) if for all $x, y \in A$ there is a geodesic $\gamma_{xy}$ contained within $A$. Further, a function $f : A \rightarrow \mathbb{R}$ is g-convex if for all $x, y \in A$, the composition $f \circ \gamma_{xy} : [0, 1] \rightarrow \mathbb{R}$ is convex in the usual Euclidean sense.

The Riemannian metric on $\mathbb{P}^d$ mentioned above induces a geodesic between two points $\Sigma_1$ and $\Sigma_2$ that has the well-known closed-form (see e.g., [4, Ch. 6]):

$$\gamma_{\Sigma_1, \Sigma_2}(t) := \Sigma_1^{1/2} \left( \Sigma_1^{-1/2} \Sigma_2 \Sigma_1^{-1/2} \right)^t \Sigma_1^{1/2}, \quad 0 \leq t \leq 1.$$ 

Thus, a function $f : \mathbb{P}^d \rightarrow \mathbb{R}$ if g-convex on $\mathbb{P}^d$ if it satisfies

$$f(\gamma_{\Sigma_1, \Sigma_2}(t)) \leq (1 - t)f(\Sigma_1) + tf(\Sigma_2), \quad t \in [0, 1], \quad \Sigma_1, \Sigma_2 \in \mathbb{P}^d.$$ 

The negative of a g-convex function is called g-concave. For a g-convex function, local optimality implies global optimality even if it is nonconvex in the Euclidean case. This remarkable property follows easily from g-convexity upon mimicking the corresponding Euclidean proof. This property has been investigated in some matrix theoretic applications [4, 35], and has been used in recent theoretical and applied works in nonlinear optimization [32, 34, 39, 42].

2.2 First-order methods for Riemannian optimization

At a high-level, first-order methods for manifold optimization methods operate iteratively as follows (see Fig. 1 for a conceptual demonstration):

i) Obtain a descent direction, namely, a vector in tangent space that decreases the cost function if we infinitesimally move along it;

ii) Perform a line-search along a smooth curve on the manifold to obtain sufficient decrease and ensure convergence.

Such a smooth curve that is parametrized by a point on the manifold and a (descent) direction is called retraction. A retraction is a smooth mapping $\text{Ret}$ from the tangent bundle $T\mathcal{M}$ to the manifold $\mathcal{M}$. The restriction of retraction to $T_x$, $\text{Ret}_x : T_x \rightarrow \mathcal{M}$, is a smooth mapping with

1) $\text{Ret}_x(0) = x$, where 0 denotes the zero element of $T_x$. 

2) $D \text{Ret}_x(0) = \text{id}_{T_x}$, where $D \text{Ret}_x$ denotes the derivative of $\text{Ret}_x$ and $\text{id}_{T_x}$ denotes the identity mapping on $T_x$.

One possible candidate for retraction on Riemannian manifolds is the exponential map. The exponential map $\text{Exp}_x : T_x \rightarrow M$ is defined as $\text{Exp}_x v = \gamma(1)$, where $\gamma$ is the geodesic satisfying the conditions $\gamma(0) = x$ and $\gamma'(0) = v$. The reader is referred to [1, 36] for more in depth discussion.

First-order methods are based on gradients. The gradient on a Riemannian manifold is defined as the vector $\nabla f(x)$ in tangent space such that

$$Df(x)\xi = \langle \nabla f(x), \xi \rangle,$$

for $\xi \in T_x$, where $\langle \cdot, \cdot \rangle$ is the inner product in the tangent space $T_x$.

Another important concept needed for methods like conjugate-gradient and LBFGS is **vector transport**. Vector transport is a smooth function that allows moving tangent vectors along retractions. A vector transport $T : M \times M \times TM \rightarrow TM_x(x, y, \xi) \mapsto T_{x, y}(\xi)$ is a mapping satisfying the following properties:

1) There exists an associated retraction $\text{Ret}$ and a tangent vector $\nu$ satisfying $T_{x, y}(\xi) \in T_{\text{Ret}(\nu)}$, for all $\xi \in T_x$.

2) $T_{x, y}(\xi) = \xi$, for all $\xi \in T_x$.

3) The mapping $T_{x, y}(\cdot)$ is linear.

An important special case of vector transport is parallel transport, which is defined as a differential map between tangent spaces at different points on the manifold with zero derivative along a smooth curve connecting the points. The differential map between tangent spaces on the manifold is a smooth vector field, where a vector field is an assignment of a tangent vector to each point on a manifold. For computing the derivative of such a map, one first needs to define a connection, which is a way to perform directional derivative of vector fields. Let $\mathcal{V}(M)$ be the set of smooth vector fields on $M$, a connection is a map $\nabla : \mathcal{V}(M) \times \mathcal{V}(M) \rightarrow \mathcal{V}(M)$ satisfying certain properties [1]. Given a smooth curve $\gamma : [0, 1] \rightarrow M$, transporting a vector $v_0 \in T_{\gamma(0)}$ to a vector $v(t) \in T_{\gamma(t)}$ can be done by solving the following initial value problem

$$\nabla_{\dot{\gamma}(t)} v = 0, \quad v(0) = v_0.$$

For $x = \gamma(0)$ and $y = \gamma(t)$, the parallel transport of $v_0 \in T_x$ to $v(t) \in T_y$ is a vector transport $v(t) = T_{x, y}v_0$.

Table 1 summarizes the key quantities for $\mathbb{P}^d$. If the parameter space is a product space of several manifolds, the concepts can be easily defined based on individual manifolds. For example, the exponential map, gradient and parallel transport are defined as the Cartesian product of individual expressions, and the inner product is defined as the sum of inner product of the components in their respective manifolds.

Two typical line-search methods are used in practice, one is Armijo rule and the other is line-search algorithm satisfying Wolfe conditions. For the case of LBFGS method, it is more common to use Wolfe line-search because it can guarantee that each step of LBFGS creates a descent direction [32].

### 2.3 Wolfe line-search

The first Wolfe condition is a sufficient-decrease condition and is given by

$$f(\text{Ret}_{x_k}(a_k \xi_k)) \leq f(x_k) + c_1 a Df(x_k) \xi_k,$$

where $Df(x_k)$ is the derivative of $f$ at $x_k$. The Wolfe line-search algorithm requires that the function value decreases by a certain factor and the gradient norm decreases by a certain factor along the search direction. The algorithm terminates when these conditions are satisfied, or when a maximum number of iterations is reached.
The interpolation phase is chosen to be smaller than the actual interval so to have certain distances numerical stability, the interval wherein the minimum of the cubic polynomial is computed in the interval. For extrapolation, we use the function and gradient at 0 and at the end-point. To ensure cubic polynomial approximation to the function in an interval. For cubic polynomial interpolation, in \[28\] and zooming. In the bracketing phase, an interval is found that contains a point satisfying the Euclidean algorithm explained in \[28\].

\[Df (\text{Ret}_{\xi_k}(a\xi_k)) T_{\xi_k,\text{Ret}_{\xi_k}(a\xi_k)}(\xi_k) \geq c_2 Df(x_k)\xi_k,\]

where \(c_2 > c_1\) is a constant smaller than 1 (around 0.9 for LBFGS). Practical line-search algorithms usually satisfy strong Wolfe conditions, where (2.1) is replaced by the stronger condition:

\[|Df (\text{Ret}_{\xi_k}(a\xi_k)) T_{\xi_k,\text{Ret}_{\xi_k}(a\xi_k)}(\xi_k)| \leq c_2 |Df(x_k)\xi_k|.

Algorithm 1: Wolfe line-search

1: Given: Current point \(x_k\) and descent direction \(\xi_k\)
2: \(\phi(a) \leftarrow f(R_{\xi_k}(a\xi_k)); \phi'(a) \leftarrow aDf(x_k)\xi_k\)
3: \(a_0 \leftarrow 0, a_1 > 0\) and \(i \leftarrow 0\)
4: while \(i \leq i_{\text{max}}\) do
5: \(i \leftarrow i + 1\)
6: if \(\phi(a_i) > \phi(0) + c_1 a_i \phi'(0)\) or \(\phi(a_i) \geq \phi(a_{i-1}), i > 1\) then
7: \(a_{\text{low}} = a_{i-1}\) and \(a_{\text{hi}} = a_i\)
8: break
9: else if \(|\phi'(a_i)| \leq c_2 \phi'(0)\) then return \(a_i\)
10: else if \(|\phi'(a_i)| \geq 0\) then
11: \(a_{\text{low}} = a_i\) and \(a_{\text{hi}} = a_{i-1}\)
12: break
13: else
14: Extrapolate to find \(a_{i+1} > a_i\)
15: end if
16: end while
17: Call ZoomingPhase

Algorithm 2: Zooming Phase

1: while \(i \leq i_{\text{max}}\) do
2: \(i \leftarrow i + 1\)
3: Interpolate to find \(a_i \in (a_{\text{low}}, a_{\text{hi}})\)
4: if \(\phi(a_i) > \phi(0) + c_1 a_i \phi'(0)\) or \(\phi(a_i) \geq \phi(a_{\text{low}})\) then
5: \(a_{\text{hi}} \leftarrow a_i\)
6: else
7: if \(|\phi'(a_i)| \leq c_2 \phi'(0)\) then return \(a_i\)
8: else if \(\phi'(a_i)(a_{\text{hi}} - a_{\text{low}}) \geq 0\) then
9: \(a_{\text{hi}} \leftarrow a_{\text{low}}\)
10: end if
11: \(a_{\text{low}} \leftarrow a_i\)
12: end if
13: end while
14: return failure

Algorithm 1 summarizes a line-search algorithm satisfying strong Wolfe conditions based on the Euclidean algorithm explained in [28]. The algorithm is divided into two phases: bracketing and zooming. In the bracketing phase, an interval is found that contains a point satisfying the strong Wolfe condition. Next, in the zooming phase, the actual point is found. Theory behind why this algorithm is guaranteed to find a step-length satisfying (strong) Wolfe conditions can be found in [28].

For the interpolation and extrapolation steps of the line-search one can find the minimum of a cubic polynomial approximation to the function in an interval. For cubic polynomial interpolation, we approximate the function by a cubic polynomial so that the function \(\phi(\cdot)\) and its gradient \(\phi'(\cdot)\) matches the function value and the gradient of the cubic polynomial at the end-points of the interval. For extrapolation, we use the function and gradient at 0 and at the end-point. To ensure numerical stability, the interval wherein the minimum of the cubic polynomial is computed in the interpolation phase is chosen to be smaller than the actual interval so to have certain distances
from the end-points of the interval (we choose the distance to be 0.1 times the interval length). The interval for the extrapolation is assumed to be between 1.1 and 10 times the value of the current point.

The initial step-length \( \alpha_1 \) can be guessed using the previous function and gradient information. We propose the following choice that is quite effective:

\[
\alpha_1 = 2 \frac{f(x_k) - f(x_{k-1})}{Df(x_k) \xi_k}.
\]

Equation (2.2) is obtained by finding \( \alpha^* \) that minimizes a quadratic approximation of the function along the geodesic through the previous point (based on \( f(x_{k-1}) \), \( f(x_k) \) and \( Df(x_{k-1}) \xi_{k-1} \)):

\[
\alpha^* = 2 \frac{f(x_k) - f(x_{k-1})}{Df(x_{k-1}) \xi_{k-1}}.
\]

Then, assuming that first-order change will be the same as in the previous step, we write

\[
\alpha^* Df(x_{k-1}) \xi_{k-1} \approx \alpha_1 Df(x_k) \xi_k.
\]

Combining (2.3) and (2.4), we obtain our procedure of selection \( \alpha_1 \) expressed in (2.2). Nocedal and Wright [28] suggest using either \( \alpha^* \) of (2.3) as the initial step-length, or using (2.4) where \( \alpha^* \) is set equal to the step-length obtained in the line-search at the previous point. We observed the our choice (2.2) proposed above leads to substantially better performance than these other two approaches.

### 2.4 Stochastic optimization

If the objective function has the form

\[
\min_{x \in M} f(x) := \frac{1}{n} \sum_{i=1}^{n} f_i(x),
\]

then for large \( n \) each iteration of the first-order methods explained above becomes very expensive, as merely computing the gradient requires going through all \( n \) component functions. In this large-scale setting, one frequently passes to stochastic / incremental optimization methods such as stochastic gradient descent (SGD) that processes only a small batch of functions at each iteration. Note that SGD is actually not a descent method; it makes progress by replacing an exact descent direction by one which is a descent direction in expectation.

Riemannian SGD [7] runs the following iteration, where \( i_t \sim U(n) \), i.e. a random integer between 1 and \( n \):

\[
x_{t+1} \leftarrow \text{Ret}_{x_t}(-\eta_t \nabla f_i(x_t)), \quad t = 0, 1, \ldots,
\]

where \( \text{Ret}_x \) is a retraction at the point \( x \) and \( \eta_t \) is a suitable stepsize that typically satisfies \( \sum \eta_t = \infty \) and \( \sum \eta_t^2 < \infty \).

After this background on the Riemannian optimization methods that we will use for GMM parameter optimization, we are now ready to describe the problem reformulation and other important theoretical details.

### 3 Problem reformulation

Experience with mixture modeling shows that whenever an optimization method works well for a single component, the same optimization method also works well for the mixture model.
We begin, therefore, with parameter estimation for a single Gaussian. Although this problem has a closed-form solution that benefits EM, our goal is to tackle it in the context of manifold optimization.

Consider, maximum likelihood parameter estimation for a single Gaussian,

$$\max_{\mu, \Sigma > 0} \mathcal{L}(\mu, \Sigma) := \sum_{i=1}^{n} \log p_{\mathcal{N}}(x_i; \mu, \Sigma).$$  \hspace{1cm} (3.1)$$

This objective is concave in the Euclidean sense. But our aim is to apply manifold optimization and this objective is not g-concave on its domain $\mathbb{R}^{d} \times \mathbb{P}^{d}$, which makes it geometrically somewhat of a mismatch.

We invoke a simple transformation that turns (3.1) into a g-concave optimization problem. This transformation has a dramatic impact on the speed of the convergence for a single Gaussian, as seen in Fig. 2. Define new vectors $y_i^T = [x_i^T \ 1]$; then, the proposed transformed model is

$$\max_{S > 0} \hat{\mathcal{L}}(S) := \sum_{i=1}^{n} \log q_{\mathcal{N}}(y_i; S),$$  \hspace{1cm} (3.2)$$

where $q_{\mathcal{N}}(y_i; S) := 2\pi \exp(\frac{1}{2}y_i^T \Sigma^{-1} y_i) \mathbb{I}(y_i; S)$. Note that this new cost function is not just a reparametrization of (3.1). However, it becomes a reparametrization at a maximum. More precisely, Theorem 1 shows that solving the reformulation (3.2) also solves the original problem (3.1).

**Theorem 1.** If $\mu^*, \Sigma^*$ maximize (3.1), and if $S^*$ maximizes (3.2), then $\hat{\mathcal{L}}(S^*) = \mathcal{L}(\mu^*, \Sigma^*)$ and

$$S^* = \begin{pmatrix} \Sigma^* + \mu^* \mu^T & \mu^* \\ \mu^T & 1 \end{pmatrix}.$$

**Proof.** We express $S$ by new variables $U, t$ and $s$ by writing

$$S = \begin{pmatrix} U + st & t \\ st & s \end{pmatrix}.$$  \hspace{1cm} (3.4)$$

The objective function $\hat{\mathcal{L}}(S)$ in terms of the new parameters becomes

$$\hat{\mathcal{L}}(U, t, s) = \frac{n}{2} - \frac{d}{2} \log(2\pi) - \frac{n}{2} \log s - \frac{n}{2} \log \det(U) - \frac{1}{2} \sum_{i=1}^{n}(x_i - t)^T U^{-1} (x_i - t) - \frac{n}{2s}.$$ 

Optimizing $\hat{\mathcal{L}}$ over $s > 0$ we see that $s^* = 1$. Hence, the objective reduces to a $d$-dimensional Gaussian log-likelihood, for which $U^* = \Sigma^*$ and $t^* = \mu^*$.

In other words, Theorem 1 shows that our model transformation is “faithful” because it leaves the optimum unchanged. Figure 2 shows the unmistakable impact this transformation has on the convergence speed of Riemannian Conjugate-Gradient (CG) and Riemannian LBFGS.

Next, Proposition 3 proves another key property of this transformation: the objective in (3.2) becomes g-concave. For proving Proposition 3, we need the following lemma that is an easy consequence of [4, Thm. 4.1.3]:

**Lemma 2.** Let $S, R \succ 0$. Then, for a vector $x$ of appropriate dimension,

$$x^T (S^{-1/2} (S^{1/2} R^{-1} S^{1/2})^{1/2} S^{-1/2}) x \leq [x^T S^{-1} x]^{1/2} [x^T R^{-1} x]^{1/2}. \hspace{1cm} (3.5)$$

**Proposition 3.** The objective $\hat{\mathcal{L}}(S)$ in (3.2) is g-concave.
Proof. By continuity, it suffices to establish mid-point geodesic concavity:

\[ \hat{\mathcal{L}}(\gamma_{S,R}(\frac{1}{2})) \geq \frac{1}{2} \hat{\mathcal{L}}(S) + \frac{1}{2} \hat{\mathcal{L}}(R), \quad \text{for } S, R \in \mathbb{P}^d. \]

Denoting inessential constants by \( c \), the above inequality turns into

\[
\hat{\mathcal{L}}(\gamma_{S,R}(\frac{1}{2})) = -\log \det(S^{1/2}R^{1/2}) - c \sum_i y_i^T (S^{-1/2}(S^{-1/2}R^{-1}S^{-1/2})S^{-1/2}) y_i
\]

\[
\geq -\frac{1}{2} \log \det(S) - \frac{1}{2} \log \det(R) - c \sum_i |y_i^T S^{-1} y_i|^{1/2} |y_i^T R^{-1} y_i|^{1/2}
\]

\[
\geq -\frac{1}{2} \log \det(S) - \frac{c}{2} \sum_i y_i^T S^{-1} y_i - \frac{1}{2} \log \det(R) - \frac{c}{2} \sum_i y_i^T R^{-1} y_i,
\]

\[
= \frac{1}{2} \hat{\mathcal{L}}(S) + \frac{1}{2} \hat{\mathcal{L}}(R),
\]

where the first inequality is follows from Lemma 2.

\[ \blacksquare \]

**Theorem 4.** A local maximum of the reformulated GMM log-likelihood

\[
\hat{\mathcal{L}}(\{S_j\}_{j=1}^K) := \sum_{i=1}^n \log \left( \sum_{j=1}^K a_j \mathcal{N}(y_i; S_j) \right)
\]

is a local maximum of the original log-likelihood

\[
\mathcal{L}(\{\mu_j, \Sigma_j\}_{j=1}^K) := \sum_{i=1}^n \log \left( \sum_{j=1}^K a_j p_N(x_i; \mu_j, \Sigma_j) \right).
\]

Proof. Let \( S_1^*, \ldots, S_K^* \) be a local maximum of \( \hat{\mathcal{L}} \). Then, \( S_j^* \) is the maximum of the following cost function:

\[-\frac{1}{2} \sum_i w_i \log \det(S_j) - \frac{1}{2} \sum_i w_i y_i^T S_j^{-1} y_i,
\]

where for each \( i \in \{1, \ldots, n\} \) the weight

\[
w_i = \frac{q_N(y_i | S_j^*)}{\sum_{j=1}^K a_j q_N(y_i | S_j^*)}.
\]

(3.6)

Using an argument similar to that for Theorem 1, we see that \( s_j^* = 1 \), whereby \( q_N(y_i | S_j^*) = p_N(x_i; t_j^*, U_j^*) \). Thus, at a maximum the objective functions agree and the proof is complete. \( \blacksquare \)

Theorem 4 shows that we can replace (1.2) by a reformulated log-likelihood whose local maxima agree with those of (1.2). Moreover, the individual components of the reformulated log-likelihood are geodesically concave.

Finally, we also need to replace the constraint \( \alpha \in \Delta_K \) to make the problem unconstrained. We do this via a commonly used change of variables [19]:

\[
\omega_k = \log \left( \frac{a_k}{a_K} \right), \quad k = 1, \ldots, K - 1.
\]

(3.7)

Assume \( \omega_K = 0 \) to be a constant; then the final optimization problem is:

\[
\max_{\{S_j \succ 0\}_{j=1}^K, \{\omega_j\}_{j=1}^{K-1}} \hat{\mathcal{L}}(\{S_j\}_{j=1}^K, \{\omega_j\}_{j=1}^{K-1}) := \sum_{i=1}^n \log \left( \sum_{j=1}^K \frac{\exp(\omega_j)}{\sum_{k=1}^K \exp(\omega_k)} q_N(y_i; S_j) \right)
\]

(3.8)

We solve (3.8) via Riemannian optimization problem in this paper; specifically, it is an optimization problem on the product manifold \((\prod_{j=1}^K \mathbb{P}^{d+1}) \times \mathbb{R}^{K-1}\).
3.1 Formulations for Penalized Likelihoods

One of the problems with ML estimation for GMMs is covariance singularity. There are several remedies to avoid this problem, and the most common approach is to use a penalized ML estimate [31]. We state the following generic results that helps choose priors amenable to our framework.

**Theorem 5.** Let $S$ be the block matrix defined in (3.4). Consider a regularizer that splits over the blocks of $S$, and has the form

$$
\psi(S) = \psi_1(U, t) + \psi_2(s),
$$

where $\psi_2(s)$ has a unique maximizer at $s = 1$. Let $S^*$ be the maximum of the penalized objective $\psi(S) + \tilde{L}(S)$, where $\tilde{L}(S)$ is the modified log-likelihood (3.2). Assume that $(\mu^*, \Sigma^*)$ maximizes the penalized log-likelihood $\psi_1(\Sigma, \mu) + L(\mu, \Sigma)$, where $L(\mu, \Sigma)$ is as in (3.1). Then, $S^*$ is related to $(\mu^*, \Sigma^*)$ via (3.3).

**Proof.** Similar to the proof of Theorem 1, it is easy to see that the penalized objective $\psi + \tilde{L}$ has its maximum at $s^* = 1$. Therefore, the objective reduces to a penalized log-likelihood of a Gaussian at its maximum. 

A widely used penalizer is obtained by placing an inverse Wishart prior on covariance matrices and using a maximum a priori estimate. The inverse Wishart prior is a conjugate prior for the covariance matrix, and is given by

$$
p(\Sigma; \Lambda, \nu) \propto \det(\Sigma)^{-1} \nu^{-d/2} \exp\left(-\frac{1}{2} \text{tr}(\Sigma^{-1} \Lambda)\right),
$$

where $\nu$ is a degree of freedom and $\Lambda$ is a scale parameter. The conjugate prior for the mean parameter is a Gaussian distribution conditioned on the covariance matrix; that is,

$$
p(\mu|\Sigma; \lambda, \kappa) \propto \det(\Sigma)^{-1} \exp\left(-\frac{1}{2} (\mu - \lambda)^T \Sigma^{-1} (\mu - \lambda)\right),
$$

where $\kappa$ is a so-called shrinkage parameter.

In the following, we propose a penalizer to our reformulated objective function. This penalized objective function converges to the penalized log-likelihood for GMM, when one uses the aforementioned conjugate priors for covariance matrices and means. Consider the penalizer

$$
\psi(S; \Psi) = -\frac{\rho}{2} \log \det(S) - \frac{\beta}{2} \text{tr}(\Psi S^{-1}),
$$

where $\Psi$ is the block matrix

$$
\Psi = \begin{pmatrix}
\frac{\rho}{\beta} \Lambda + \kappa \lambda T \\
\kappa \lambda T \\
\kappa T
\end{pmatrix},
$$

and the parameter $\rho = \alpha(d + \nu + 1) + \beta$. If we write $S$ as the block matrix

$$
S = \begin{pmatrix}
U + stt^T \\
st^T
\end{pmatrix},
$$

then the penalized cost function (3.9) becomes

$$
\psi(S; \Psi) = -\frac{\rho}{2} \left[ \log \det(U) + \log(s) \right] - \frac{\beta}{2} \left[ \frac{\rho}{\beta} \text{tr}(\Lambda U^{-1}) + \kappa T U^{-1} t + \kappa \lambda T U^{-1} \lambda - 2 \kappa \lambda T U^{-1} t + \kappa \right].
$$

Rearranging the terms, we thus obtain

$$
\psi(S; \Psi) = a \log p(U; \Lambda; \nu) + \beta \log p(t|U; \lambda, \kappa) - \frac{\rho}{2} \log(s) - \frac{\beta \kappa}{2s} + c,
$$

(3.11)
for some constant $c$. In order for this penalizer to satisfy the conditions of Theorem 5 we need the following condition:

$$\alpha = \beta \frac{k-1}{d+v+1}.$$ 

Using Proposition 3 one can again show that this penalizer is $g$-concave. We summarize these results as an informal corollary below.

**Corollary 6.** The penalizer given in (3.11) is $g$-concave and fulfills the structure required by Theorem 5. Hence, it can be used for penalized ML estimation.

It is easy to see that the single component results above extend to penalized maximum likelihood of GMMs. That is, Theorem 4 can be generalized to penalized maximum likelihood for GMMs.

Indeed, recall that a common prior on mixture weights is the symmetric Dirichlet prior that assumes the form

$$p(\alpha_1, \ldots, \alpha_K; \xi) \propto \prod_{i=1}^{K} \alpha_i \xi.$$ (3.12)

The penalizer for the mixture weights is the logarithm of (3.12), namely,

$$\varphi(\{\omega_j\}_{j=1}^{K-1}; \xi) := \xi \sum_{i=1}^{K} \log \left( \frac{\omega_j}{\sum_{k=1}^{K-1} \omega_k} \right) = \xi \sum_{i=1}^{K} \omega_i - K \xi \log \left( \sum_{k=1}^{K} \omega_k \right).$$ (3.13)

The final optimization problem for the penalized mixture model is

$$\max_{\{S_j\}_{j=1}^{K}, \{\omega_j\}_{j=1}^{K-1}} \tilde{L}(\{S_j\}_{j=1}^{K}, \{\omega_j\}_{j=1}^{K-1}) + \sum_{j=1}^{K} \psi(S_j; \Psi) + \varphi(\{\omega_j\}_{j=1}^{K-1}; \xi),$$ (3.14)

where $\tilde{L}(\{S_j\}_{j=1}^{K}, \{\omega_j\}_{j=1}^{K-1})$, $\psi(S; \Psi)$ and $\varphi(\{\omega_j\}_{j=1}^{K-1}; \xi)$ are given by (3.8), (3.9), and (3.13), respectively.

We have now presented our formulation of the main optimization problems of this paper, both GMM fitting, as well as a penalized version based on using an conjugate priors on means and covariance matrices combined with a Dirichlet model for mixture components weights. We can solve both these problems using Riemannian LBFGS procedure or a Riemannian SGD method for larger scale problems. The former method was also studied in [17]; we thus dedicate Section 4 to an general analysis Riemannian SGD before specializing it to our GMM problems in Section 5.

### 4 Riemannian stochastic optimization

In this section, we consider the stochastic gradient descent algorithm

$$x_{t+1} \leftarrow \text{Ret}_{x_t}(-\eta_t \nabla f_{t_i}(x_t)), \quad t = 0, 1, \ldots,$$ (4.1)

where Ret$_x$ is a suitable retraction (to be specialized later). We assume for our analysis of (4.1) the following fairly standard conditions:

(i) The function satisfies the Lipschitz growth bound

$$f(\text{Ret}_x(\xi)) \leq f(x) + \langle \nabla f(x), \xi \rangle + \frac{L}{2} \| \xi \|^2.$$ (4.2)

(ii) The stochastic gradients in all iterations are unbiased, i.e.,

$$\mathbb{E}[\nabla f_{t_i}(x_t) - \nabla f(x_t)] = 0.$$
(iii) The stochastic gradients have bounded variance, so that
\[ \mathbb{E}[\|\nabla f_t(x_i) - \nabla f_t(x_i)\|^2] \leq \sigma^2, \quad 0 \leq \sigma < \infty. \]

When the retraction is the exponential map, condition (i) can be reexpressed as (provided that \(\text{Exp}_y^{-1}(\cdot)\) exists)
\[ f(x) - f(y) - \langle \nabla f(y), \text{Exp}_y^{-1}(x) \rangle \leq \frac{1}{2}d^2(x, y). \quad (4.3) \]

Given these conditions, the iterates produced by (4.1) satisfy the following:

**Lemma 7.** Assume conditions (i)-(iii) hold. Then, the gradients in SGD satisfy the bound
\[ \sum_{t=1}^{T} \left( \eta_t^2 - \frac{1}{2} \eta_t^2 \right) \mathbb{E}[\|\nabla f(x_t)\|^2] \leq f(x_1) - f^* + \frac{L^2}{2} \sum_{t=1}^{T} \eta_t^2. \quad (4.4) \]

**Proof.** Denote the stochastic error by \(\delta_i = \nabla f(x_t) - \nabla f_t(x_t)\); also, as a shorthand set \(g_t = \nabla f_t(x_t)\). Then, we have
\[
\begin{align*}
f(x_{t+1}) & \leq f(x_t) + \langle \nabla f(x_t), -\eta_t \nabla f_t(x_t) \rangle + \frac{1}{2} \|\eta_t \nabla f_t(x_t)\|^2 \\
& = f(x_t) - \eta_t \langle \nabla f(x_t), g_t \rangle + \frac{L^2}{2} \|g_t\|^2 \\
& = f(x_t) - \eta_t \|\nabla f(x_t)\|^2 - \eta_t \langle \nabla f(x_t), \delta_t \rangle + \frac{L^2}{2} \|\nabla f(x_t)\|^2 + 2 \langle \nabla f(x_t), \delta_t \rangle + \|\delta_t\|^2 \\
& = f(x_t) - \left( \eta_t^2 - \frac{1}{2} \eta_t^2 \right) \|\nabla f(x_t)\|^2 - (\eta_t - L \eta_t^2) \langle \nabla f(x_t), \delta_t \rangle + \frac{L^2}{2} \|\delta_t\|^2.
\end{align*}
\]

Summing over \(t = 1, \ldots, T\), using telescoping sums and rearranging we obtain
\[
\begin{align*}
\sum_{t=1}^{T} \left( \eta_t^2 - \frac{1}{2} \eta_t^2 \right) \|\nabla f(x_t)\|^2 & \leq f(x_1) - f(x_{T+1}) - \sum_{t=1}^{T} (\eta_t - L \eta_t^2) \langle \nabla f(x_t), \delta_t \rangle + \frac{L}{2} \sum_{t=1}^{T} \eta_t^2 \|\delta_t\| \|\delta_t\| \\
& \leq f(x_1) - f^* - \sum_{t=1}^{T} (\eta_t - L \eta_t^2) \langle \nabla f(x_t), \delta_t \rangle + \frac{L}{2} \sum_{t=1}^{T} \eta_t^2 \|\delta_t\| \|\delta_t\|,
\end{align*}
\]
where we used \(f^* \leq f(x_t)\) for all \(t\). Now taking expectations, and noting that by our assumption \(\mathbb{E}[\|\delta_t\|^2] \leq \sigma^2\) while by unbiasedness of the stochastic gradients we have \(\mathbb{E}[\langle \nabla f(x_t), \delta_t \rangle] = 0\). Thus, we obtain the bound (4.4).

By using a specific choice of parameter \(\eta_t\) and using Lemma 7, we can obtain a convergence rate result for SGD with a slight modification.

**Theorem 8.** Assume a slightly modified version of SGD which output a point \(x_d\) by randomly picking one of the iterates, say \(x_t\), with probability \(p_t := (2\eta_t - L \eta_t^2) / Z_T\), where \(Z_T = \sum_{t=1}^{T} (2\eta_t - L \eta_t^2)\). Furthermore, choose \(\eta_t = \min \{ L^{-1}, c\sigma \sigma^{-1} T^{-1/2} \}\) for a suitable constant \(c\). Then, we obtain the following bound on \(\mathbb{E}[\|\nabla f(x_d)\|^2]\), which measures the expected gap to stationarity:
\[ \mathbb{E}[\|\nabla f(x_d)\|^2] \leq \frac{2L \Delta T}{T} + (c + c^{-1} \Delta T) \frac{L \sigma}{\sqrt{T}} = O \left( \frac{1}{T} \right) + O \left( \frac{1}{\sqrt{T}} \right). \quad (4.5) \]

**Proof.** Using the definition of \(x_d\) and using Lemma 7, we immediately have
\[
\mathbb{E}[\|\nabla f(x_d)\|^2] = \sum_{t=1}^{T} p_t \mathbb{E}[\|\nabla f(x_t)\|^2] \leq \frac{2(f(x_1) - f^*)}{Z_T} + L \sigma^2 \sum_{t=1}^{T} \eta_t^2 / Z_T.
\]

Using the choice of \(\eta_t\) in the theorem, this bound yields (4.5).
Theorem 8 uses a randomized stopping rule, a choice motivated by [16]. If one wishes to avoid such a rule, then under a stronger assumption one can obtain the same rate. Specifically, in the theorem below we replace conditions (ii) and (iii) with the stronger condition (iv).

(iv) The function $f$ has a G-bounded gradient, that is $\|\nabla f_i(x)\| \leq G$ for all $i \in [n]$

Under this condition, we can obtain the following convergence rate.

**Theorem 9.** Assume conditions (i) and (iv) hold. Then, the gradient in SGD satisfies the following bound for a suitable choice of $\eta_t$:

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\|\nabla f(x_t)\|^2] \leq \frac{1}{\sqrt{T}} \left( \frac{f(x_1) - f(x^*)}{c} + \frac{Lc}{2}G^2 \right).$$

**Proof.** The Lipschitz smoothness condition yields

$$\mathbb{E}[f(x_{t+1})] \leq \mathbb{E}[f(x_t)] + \mathbb{E} \left[ (\nabla f(x_t), -\eta_t \nabla f_i(x_t)) + \frac{L}{2} \|\eta_t \nabla f_i(x_t)\|^2 \right]$$

$$\leq \mathbb{E}[f(x_t)] - \eta_t \mathbb{E}[\|\nabla f(x_t)\|^2] + \frac{LT}{2}G^2.$$

Rearranging the terms above we obtain

$$\mathbb{E}[\|\nabla f(x_t)\|^2] \leq \frac{1}{\eta_t} \mathbb{E}[f(x_t) - f(x_{t+1})] + \frac{L \eta_t}{2}G^2.$$

Choose $\eta_t = \frac{c}{\sqrt{T}}$ for some constant $c$ and sum over $t = 0$ to $T - 1$ to obtain

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\|\nabla f(x_t)\|^2] \leq \frac{1}{\sqrt{T}c} \mathbb{E}[f(x_1) - f(x_{T+1})] + \frac{Lc}{2\sqrt{T}}G^2$$

$$\leq \frac{1}{\sqrt{T}} \left( \frac{f(x_1) - f(x^*)}{c} + \frac{Lc}{2}G^2 \right).$$

By optimizing over the constant $c$, the following corollary is immediate.

**Corollary 10.** Assume conditions (i) and (iv) hold, then for suitable $\eta_t$ we have

$$\min_{1 \leq t \leq T} \mathbb{E}[\|\nabla f(x_t)\|^2] \leq O \left( \frac{1}{\sqrt{T}} \right).$$

5 **SGD for GMM**

In this section, we investigate if SGD based on retractions satisfies the conditions needed for obtaining a global rate of convergence when applied to our GMM optimization problems. Since Euclidean retraction turns out to be computationally more effective than many other retractions, we perform the analysis below for Euclidean retraction.

Recall that we are maximizing a cost of the form $\frac{1}{n} \sum_{i=1}^{n} f_i(\cdot)$ using SGD. In a concrete realization, each function $f_i$ is set to the penalized log-likelihood for a batch of observations (data points). For simpler notation, assume that each $f_i$ corresponds to a single observation. Thus,

$$f_i(\{S_j \succ 0\}_{j=1}^{K}, \{\eta_j\}_{j=1}^{K-1}) = \log \left( \sum_{j=1}^{K} \frac{\exp(\eta_j)}{\sum_{k=1}^{K} \exp(\eta_k)} q_N(y_i; S_j) \right)$$

$$+ \frac{1}{n} \left( \sum_{j=1}^{K} \psi(S_j; \Psi) + \varphi(\{\eta_j\}_{j=1}^{K-1}; \zeta) \right).$$

(5.1)
where \( q, \psi \) and \( \varphi \) are as defined by (3.9) and (3.13), respectively. Since we are maximizing, the update formula for SGD is

\[
\left\{ \{ S_j > 0 \}_{j=1}^N, \{ \eta_j \}_{j=1}^{K-1} \right\} \leftarrow \text{Ret}_{\{ S_j > 0 \}_{j=1}^N, \{ \eta_j \}_{j=1}^{K-1}} \left( \eta_t \nabla f_i \left( \left\{ S_j > 0 \right\}_{j=1}^N, \{ \eta_j \}_{j=1}^{K-1} \right) \right),
\]

(5.2)

where \( i \) is a randomly chosen index between 1 and \( n \).

Note that, the conditions needed for a global rate of convergence are not satisfied on the entire set of positive definite matrices. In particular, to apply our convergence results for SGD we need to show that the iterates stay within a compact set. Theorem 11 below ensures this property.

**Theorem 11.** If the stepsize is smaller than one, then the iterates of SGD for the penalized likelihood of GMM stay within a compact set.

**Proof.** We write down the formula of the gradient and show that the update formula (5.2) guarantees that the variables remain in a bounded set. The Euclidean gradient of penalized log-likelihood with respect to one of the covariance matrices \( S_j \) for a single datapoint \( y_n \) is equal to

\[
\nabla_{E f_i}(S_j) = -\frac{w}{2} S_j^{-1} + \frac{w}{2} S_j^{-1} y_n y_n^T S_j^{-1} - \frac{\rho}{2 n} S_j^{-1} + \frac{\beta}{2 n} S_j^{-1} \Psi S_j^{-1},
\]

(5.3)

where \( w \), a weight calculated as in (3.6), is a positive number smaller than 1 and \( \rho \), a small constant that appears in \( \psi(S_j; \Psi) \), is of order of \( 10^{-2} \). Using the update formula (5.2), \( S_j \) is updated by

\[
S_j \leftarrow \left( 1 - \eta_t \frac{w + \rho n^{-1}}{2} \right) S_j + \eta_t \Psi',
\]

(5.4)

where

\[
\Psi' = \frac{w}{2} y_n y_n^T + \frac{\beta n^{-1}}{2} \Psi.
\]

If \( \eta_t \leq 1 \), then the first term in (5.4) remains positive definite. Assume \( \lambda \) and \( \lambda' \) to be the smallest eigenvalue of \( S_j \) before and after the update of (5.4). Furthermore, assume the smallest eigenvalue of \( S_j \) before update be \( \lambda_{\min}(S_j) = \tau \lambda_{\min}(\Psi) \). From the update rule (5.4) and knowing that the smallest eigenvalue of sum of two matrices with positive eigenvalues is not smaller than sum of smallest eigenvalue of two matrices, we have

\[
\lambda' \geq \lambda + \frac{\eta_t}{2} \lambda_{\min}(\Psi) \left( -\tau (w + \rho n^{-1}) + \beta n^{-1} \right).
\]

If \( \tau < \beta/(n + \rho) \), then \( \lambda' > \lambda \). Otherwise, \( \lambda' \geq \tau (1 - \frac{\eta_t}{2} (1 + \rho n^{-1})) \lambda_{\min}(\Psi) + \frac{\eta_t}{2} \beta n^{-1} \lambda_{\min}(\Psi) \). Since \( \frac{\eta_t}{2} (1 + \rho n^{-1}) < 1 \), the smallest eigenvalue of \( S_j \) can not become smaller than

\[
\lambda_{\min}(\Psi) \frac{\beta}{n + \rho}.
\]

Now, assume \( \lambda \) and \( \lambda' \) to be the largest eigenvalue of \( S_j \) before and after the update given in (5.4). Furthermore, assume the largest eigenvalue of \( S_j \) before update be \( \| S_j \| = \tau \| \Psi \| \). From the update rule (5.4) and knowing that the largest eigenvalue of sum of two matrices with positive eigenvalues is not larger than sum of largest eigenvalues of two matrices, we have

\[
\lambda' \leq \lambda + \frac{\eta_t}{2} \| \Psi \| \left( -\tau (w + \rho n^{-1}) + w \| y_n \| \| \Psi \| + \beta n^{-1} \right).
\]
If
\[ \tau > \max_{w \in [0,1]} \frac{w \max_i \{ \| y_i \| \}}{w + \rho n^{-1}} + \beta n^{-1}, \]
then \( \lambda' < \lambda \). Therefore, the largest eigenvalue of \( S_j \) remains smaller than
\[ \max_{w \in [0,1]} \frac{wn \max_i \{ \| y_i \| \} + \beta \| \Psi \|}{wn + \rho}. \]

Till now, we have shown that the \( S_j \)s remain in a compact set. We use the same procedure to show that \( \omega_j \)s also remain in a bounded interval. The Euclidean gradient of the objective with respect to \( \omega_j \) for a single data-point is given by:
\[ \nabla_{E_f} f_i(\omega_j) = w - \alpha_j + \frac{\zeta}{n} - \frac{K\zeta}{n} \alpha_j. \]
If \( \alpha_j < \frac{\zeta n^{-1}}{1 + K\zeta n^{-1}} \), then the gradient is positive and \( \omega_j \) is increased after update. From (3.7), it is clear that \( \log(\alpha_j) \leq \omega_j \). Using the update formula \( \omega_j^{\text{new}} = \omega_j + \eta_t \nabla_{E_f} f_i(\omega_j) \), we get the following lower bound:
\[ \omega_j^{\text{new}} \geq \min_{\omega_j \geq \log(\frac{\zeta n^{-1}}{1 + K\zeta n^{-1}})} \left[ \omega_j + \eta_t \left( w - \alpha_j + \frac{\zeta}{n} - \frac{K\zeta}{n} \alpha_j \right) \right] \]
\[ \geq \min_{\omega_j \geq \log(\frac{\zeta n^{-1}}{1 + K\zeta n^{-1}})} \left[ \omega_j + \eta_t \left( 1 - \exp(\omega_j) + \frac{\zeta}{n} - \frac{K\zeta}{n} \exp(\omega_j) \right) \right] \]
\[ = \log(\frac{\zeta n^{-1}}{1 + K\zeta n^{-1}}). \]

From the definition (3.7), we have \( \log(\alpha_j) = \omega_j - \log(\sum_{k=1}^{K} \exp(\omega_k)) \). Using Jensen inequality, we obtain \( \omega_j \leq -\sum_{k=1}^{K} \omega_k \). Therefore, we obtain the following upper bound for \( \omega_j \):
\[ \omega_j \leq \log(\alpha_i) - \sum_{k=1}^{n} \omega_k_{k \neq i, k \neq j} \]
\[ \leq -(K - 2) \log(\frac{\zeta n^{-1}}{1 + K\zeta n^{-1}}). \]

Therefore, one sees that all the parameters (\( S_j \)s and \( \omega_j \)s) remain in a bounded set. 

Since the parameters remain bounded, we may invoke the following theorem:

**Theorem 12** (Boumal et al. [9]). Let \( M \) be a compact Riemannian submanifold of a Euclidean space. Let \( \text{Ret} \) be a retraction on \( M \). If \( f \) has a Euclidean Lipschitz continuous gradient in the convex hull of \( M \), then the function satisfies the Lipschitz growth bound with some constant \( L \) for all retractions.

We have shown above that the iterations of SGD for penalized log-likelihood stay within a compact set. It is also easy to see that the objective has a Euclidean Lipschitz continuous gradient on this set. Therefore, we can invoke Theorem 12 to show that the objective function satisfies condition (i) needed by Theorems 8 and 9. Furthermore, the objective function has a G-bounded gradient in this compact set and the iterations stay within it. Therefore, condition (iv) needed for Theorem 9 also holds. We summarize this result in the following corollary.
Corollary 13. Assume SGD is used for optimizing the penalized log-likelihood of GMM, which is given by
\[
f_i(\{S_j > 0\}_{j=1}^K, \{\eta_j\}_{j=1}^{K-1}) = \frac{1}{n} \sum_{i=1}^n f_i(\{S_j > 0\}_{j=1}^K, \{\eta_j\}_{j=1}^{K-1}),
\]
where \(f_i\) is as in (5.1). Then, the gradient of the objective after \(T\) iterations with constant step-size equal to \(\eta_t = c/\sqrt{T}\) satisfies
\[
\min_{1 \leq t \leq T} \mathbb{E} \left[ \| \nabla f_t(\{S_j > 0\}_{j=1}^K, \{\eta_j\}_{j=1}^{K-1}) \|_2 \right] \leq \frac{1}{\sqrt{T}} \left( \frac{f^* - f^0}{c} + \frac{Lc}{2} G^2 \right) = O\left( \frac{1}{\sqrt{T}} \right),
\]
where \(f^t\) is the penalized objective evaluated at the value of parameters after \(t\) iterations; \(f^*\) is the value of penalized objective at its optimum; \(f^0\) is the value of the objective at its initial point; \(L\) is the Lipschitz-growth bound constant; and \(G\) is the constant for the \(G\)-bounded condition of the gradient.

6 Experiments

![Figure 2: The effect of reformulation in convergence speed of manifold CG and manifold LBFGS methods (\(d = 35\)); note that the X-axis (time) is on a logarithmic scale [17].](image)

In all experiments, the parameters of the penalizer in (3.9) are \(\rho = \kappa = 0.01\) and \(\alpha = \beta = 1\). The parameter \(\Lambda\) is set to 0.01 of sample covariance of the data and \(\lambda\) is sample mean of the data. The parameter \(\zeta\) of the penalizer in (3.13) is set to 1. We initialize the mixture parameters using \(k\)-means++ [2] by testing 30 different initial candidate and choosing the one with the best cost function. All methods stop when the difference between cost functions falls below \(10^{-6}\).

In order to show the efficacy of SGD, we fix the step-size rule in all experiments. We use exponential decay for the step-size. Given the maximum number of epochs, we set the starting step-size to 1 and the last step-size to \(10^{-3}\). The batch size is set to be equal to the dimensionality of data.

For the deterministic Riemannian optimization methods, we use exponential map and parallel transport as they lead to superior performance compared to other kinds of retractions and vector transports. For Riemannian SGD, we report the result of using Euclidean retraction. We also tested a more expensive exponential map and a different positivity-preserving retraction [18]. However, we observed no difference in cost function decrease as a function of gradient evaluations.

In the first experiment, the effect of the problem reformulation of Section 3 is investigate. This effect is shown if Figure 2. The left plot is the result of optimization for a single Gaussian and the
In the next experiments, we compare the performance of manifold optimization methods on the reformulated problem and EM on some real datasets. One of the datasets is a dataset of natural images \cite{17}. The other three datasets called ‘corel’, ‘yearpredict’ and ‘wine’ data are taken from UCI machine learning dataset repository\cite{3}. The results are shown in Figure 3-6. The dimensionality \(d\) of data and number of data-points \(n\) are given in the figure legends.

It can be seen than deterministic manifold optimization methods achieve and outperforms the EM algorithm. The manifold SGD shows remarkable performance. This method leads to fast increase of the objective function in early iterations.

\footnote{Available via https://archive.ics.uci.edu/ml/datasets}{

\textbf{Figure 3:} Comparison of optimization methods on natural image data (\(d = 35, n = 200000\)). Y-axis: best cost minus current cost values. X-axis: number of function and gradient evaluations. Right: 3 number of components. Left: 7 number of components.

\textbf{Figure 4:} Comparison of optimization methods on year predict data (\(d = 90, n = 515345\)). Y-axis: best cost minus current cost values. X-axis: number of function and gradient evaluations. Right: 3 number of components. Left: 7 number of components.
Figure 5: Comparison of optimization methods on corel data ($d = 57$, $n = 68040$). Y-axis: current objective values minus best objective. X-axis: number of function and gradient evaluations. Right: 3 number of components. Left: 7 number of components.

Figure 6: Comparison of optimization methods on wine data ($d = 11$, $n = 6497$). Y-axis: current objective values minus best objective. X-axis: number of function and gradient evaluations. Right: 3 number of components. Left: 7 number of components.

7 Conclusions and future work

In this paper, we proposed a reformulation for the GMM problem that can make Riemannian manifold optimization a powerful alternative to the EM algorithm for fitting Gaussian mixture models. The deterministic manifold optimization methods can either match or outperform EM algorithm. Furthermore, we developed a global convergence theory for SGD on manifolds. We applied this theory to the GMM modeling. Experimentally Riemannian SGD for GMM shows remarkable convergence behavior, making it a potential candidate for large scale mixture modeling.

There are several venues for future works, including extension of Riemannian optimization to estimation in hidden Markov models, an exploration of manifold optimization for non-Gaussian mixture models, and a study of richer priors for GMMs beyond the usual conjugate priors.
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