Euclidean distance and maximum likelihood retractions by homotopy continuation
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Abstract

We define a new second-order retraction map for statistical models. We also compute retractions using homotopy continuation. Riemannian optimization uses local methods to solve optimization problems whose constraint set is a smooth manifold. A linear step along some descent direction usually leaves the constraint set, and hence retraction maps are used to approximate the exponential map, and return to the manifold. For many common matrix manifolds, retraction maps are available, with more or less explicit formulas. For other implicitly-defined manifolds or varieties, suitable retraction maps are difficult to compute. We therefore develop Algorithm 1, which uses homotopy continuation to compute the Euclidean distance retraction for any implicitly-defined submanifold of $\mathbb{R}^n$.

We also consider statistical models as Riemannian submanifolds of the probability simplex with the Fisher metric. After defining an analogous maximum likelihood retraction, Algorithm 2 computes it using homotopy continuation. In Theorem 2, we prove that the resulting map is a second-order retraction; with the Levi-Civita connection associated to the Fisher metric, it approximates geodesics to second-order accuracy.

1 Introduction

We consider constrained optimization in the case where the constraint set is an implicitly-defined manifold or real algebraic variety $\mathcal{M} \subset \mathbb{R}^n$. We also consider statistical models $\mathcal{M} \subset \Delta_{n-1} \subset \mathbb{R}^n$ in Section 3. The algorithms we develop are local, motivated by examples which are too large for global methods like Lagrange multipliers. In Riemannian optimization, the basic idea of local methods is simple. To find the argmin, start somewhere on the manifold and move along a descent direction in the tangent space. This (usually) takes you off the manifold, so you must retract (see Definition 1) back to the manifold, and repeat. Eventually you hope to find $p \in \mathcal{M}$ locally minimizing $f$. Robust techniques and theoretical results accompany a well-chosen Riemannian metric and retraction map [2, 7, 22]. However, such methods require prior knowledge of a suitable retraction map, ideally with an explicit formula. These are available for many common matrix manifolds, making Riemannian optimization a powerful tool in applications. However, for less common, implicitly-defined manifolds or algebraic varieties, there are no readily available formulas for retractions. Therefore, retraction maps applicable to an arbitrary manifold are desirable.

To construct retraction maps on embedded manifolds or algebraic varieties, intuition suggests retracting to the closest point on the manifold. Such maps are called metric projections in [7, p.111]. When we step linearly off a sphere, we can normalize the resulting point. When we leave the manifold of fixed rank matrices, we can apply the singular value decomposition. However, for most implicitly-defined manifolds, retracting to the closest point does not admit an explicit formula or easy solution, and “it is difficult to compute in general” [7,
p.164]. However, if we can compute metric projections, it has been shown [3] that they are second-order retractions [7, Def. 5.41], a desirable property since they match geodesics on the manifold up to second-order. After all, retractions should approximate the exponential map, which is useful provided that retraction is easier to compute in practice.

On the one hand this is an obvious choice; retract to the closest point on the manifold. Upon further reflection an absurdity is noted: We begin with a constrained optimization problem on $\mathcal{M}$, to minimize some function $f$. Then we suggest solving another constrained optimization problem on $\mathcal{M}$ repeatedly, at every local step, with the goal of finding the closest point. In particular, we do not have an explicit formula. Have we replaced one hard problem with many hard problems? The absurdity is resolved by use of a small trick. As we explain in Section 2, we can use homotopy continuation methods [6, 9, 23] to easily find the closest point at each local step. We do this by creating a system of equations whose solutions we know, and deforming them via a homotopy. To be clear, without this tool, the metric retraction might be an absurd choice, since we cannot compute it easily. Note that, in contrast to [24], we use homotopy continuation locally, rather than globally. In other words, we only use homotopy continuation to compute the retraction map at each local step.

In Section 2 we describe Algorithm 1, which uses homotopy continuation to compute the Euclidean distance retraction (see Theorem 1) for any implicitly-defined submanifold of $\mathbb{R}^n$. In Section 3, we view statistical models as Riemannian submanifolds of the probability simplex equipped with the Fisher metric. In this setting, we prove Theorem 2, which shows that ideas from maximum-likelihood estimation may be used to create a second-order retraction applicable to arbitrary statistical models at smooth points. To show second-order, we use geodesics and covariant derivatives with the Levi-Civita connection on $\mathcal{M}$ corresponding to the Fisher metric. Theorem 2 shows that replacing the linear step $p + tv$ from Algorithm 1 by the quadratic curve $\left( p_i + tv_i + t^2 \frac{v_i^2}{4p_i} \right)_{i=1}^n$ in the usual coordinates on $\mathbb{R}^n$ allows the resulting retraction $R_p(tv)$ to follow geodesics on $\mathcal{M} \subset \Delta_{n-1} \subset \mathbb{R}_{>0}^n$ to second-order accuracy. We also describe Algorithm 2, which again uses homotopy continuation to compute this retraction. Section 4 describes a Julia package which implements Algorithm 1 and briefly demonstrates its usage, while Section 5 lists a few questions for future research.

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2 Euclidean distance retraction by homotopy

We begin by considering submanifolds $\mathcal{M} \subset \mathbb{R}^n$ with the usual Euclidean metric, and which are implicitly-defined, meaning a smooth function $g : \mathbb{R}^n \to \mathbb{R}^m$ is known such that $\mathcal{M} = g^{-1}(0)$. Since our methods are local, we also consider real algebraic varieties $\mathcal{M} \subset \mathbb{R}^n$, which are smooth manifolds outside the singular locus. Given any smooth function $f : \mathbb{R}^n \to \mathbb{R}$ our main objective is to solve the constrained optimization problem of minimizing $f$ restricted to $\mathcal{M}$.

Consider the smooth manifold structure on $\mathbb{R}^n$ induced by viewing the identity map as a global chart. For all of our computations we will use the coordinates denoted $(x_i)$ for this global chart. The chart-induced global frame for the tangent bundle over $\mathbb{R}^n$ is denoted
(∂₁, . . . , ∂ₙ). Recall, a global frame of a smooth vector bundle is an ordered tuple of global sections whose values at every point yield a basis. The values at a point \( x \in \mathbb{R}^n \) will be denoted \( ∂_i |_x \), so that the vectors \( (∂_1 |_x, . . . , ∂_n |_x) \) form a basis for \( T_x \mathbb{R}^n \). We view \( \mathbb{R}^n \) as a Riemannian manifold whose metric is given by the identity matrix in the global coordinates.

Given a point \( p \in \mathcal{M} \), we can evaluate the Euclidean gradient of \( f \) at \( p \), obtaining a vector \( \nabla f |_p \in \mathbb{R}^n \). Projecting \( −\nabla f |_p \) onto the tangent space \( T_p \mathcal{M} \), we obtain a descent direction \( v = \sum v_i ∂_i |_p \in T_p \mathcal{M} \). There are (better) ways to produce descent directions as well, for example [7, Alg. 6.3 (Riemannian trust-region)] or [2, Alg. 5 (Riemannian Newton method)]. After obtaining a descent direction, the idea is to move from \( p \in \mathcal{M} \) to \( p + v / \in \mathcal{M} \), and then retract back to the manifold in such a way as to approximate the exponential map.

This leads us to the following

**Definition 1.** Let \( \mathcal{M} \subset \mathbb{R}^n \) be a manifold and \( p \in \mathcal{M} \) a point. A (first-order) retraction at \( p \) is a smooth map \( R_p : T_p \mathcal{M} \to \mathcal{M} \) satisfying

1. \( R_p(0) = p \), and
2. \( d(R_p)(0) : T_p \mathcal{M} \to T_p \mathcal{M} \) is the identity map.

Equivalently, for each curve \( c : (−\varepsilon, \varepsilon) \to \mathcal{M} \) with \( c(t) = R_p(tv) \) for some \( v \in T_p \mathcal{M} \) we have \( c'(0) = v \) and \( c(0) = p \). A local retraction at \( p \) is a retraction defined in some neighborhood of \( 0 \in T_p \mathcal{M} \), but satisfying the same two properties above.

A retraction is called second-order if, in addition, for all \( v \in T_p \mathcal{M} \)

\[
\frac{d^2}{dt^2} R_p(tv)|_{t=0} \in N_p \mathcal{M}.
\]

This implies that the curve \( R_p(tv) \) matches geodesics on \( \mathcal{M} \) up to second order at \( t = 0 \), i.e. \( R_p(tv) = \text{geodesic}(t; p, v) + O(t^3) \) as \( t \to 0 \) [3, Prop. 3].

We note that a retraction map has a different definition in topology, although they are related. Our Definition 1 is appropriate in the context of Riemannian optimization, and matches the definition in the textbook [7], for instance. Retractions were first defined in [4]. In the more general setting of Section 3 we consider Riemannian submanifolds of a Riemannian manifold which is not Euclidean space. In that case, the condition for a second-order retraction must instead be that the covariant derivative of the vector field defined by the velocity of the curve \( R_p(tv) \) lies in the normal space at \( t = 0 \) [7, Def. 8.64 and Eqn. 8.27]. We delay the additional details until Section 3.

By a result in [3], finding the closest point with respect to Euclidean distance defines a local retraction in the sense of Definition 1 on any submanifold of Euclidean space.

**Theorem 1** ([3]). Let \( \mathcal{M} \subset \mathbb{R}^n \) be a smooth manifold or real algebraic variety. For any smooth point \( p \in \mathcal{M} \), define the relation \( R_p \subset T_p \mathcal{M} \times \mathcal{M} \) by

\[
R_p = \{ (v, u) \in \mathbb{R}^n \times \mathbb{R}^n : u \in \text{argmin}_{y \in \mathcal{M}} |p + v - y| \}.
\]

There exists a neighborhood \( U \) of \( 0 \) in \( T_p \mathcal{M} \) such that \( R_p \) defines a local, second-order retraction. The curve \( t \mapsto R_p(tv) \) matches the geodesic for \( v \) up to second-order at \( p \).
Example 1. Denote the unit sphere in $\mathbb{R}^n$ by $S^{n-1}$. The expression

$$R_x(v) = \frac{x + v}{|x + v|}$$

provides a smooth map $R_x : T S^{n-1} \to S^{n-1}$. As can be easily checked, this formula defines a retraction, called the Euclidean distance retraction, which admits an explicit formula in this simple example. Consequently, we could rewrite

$$R_x(v) = \arg \min_{y \in S^{n-1}} |y - (x + v)|,$$

since the argmin is unique in every point except 0, which never equals $x + v$.

Example 2. Choose $\mathcal{M} = O_n$ the orthogonal group. Denote by $qr : GL_n(\mathbb{R}) \to O_n \times S^+_{n \times n}$ the QR decomposition of a real, invertible $n \times n$ matrix into an orthogonal matrix and an upper triangular matrix with strictly positive diagonal entries. Notice that $GL_n(\mathbb{R})$ is the complement of a hypersurface in $\mathbb{R}^n \times n$, cut out by $\{ A \in \mathbb{R}^{n \times n} | \det(A) \neq 0 \}$. Then, the map

$$R_X(\xi) = \pi_1(qr(X + \xi))$$

is a (local) retraction on the orthogonal group’s tangent bundle $TO_n$ with $\pi_1$ the projection onto its first argument. A proof can be found in [2, Ex. 4.1.2]

In general, the Euclidean distance retraction will not admit an explicit formula, except in special cases like those above. Therefore, it is desirable to develop techniques for computing the Euclidean distance retraction on arbitrary, implicitly-defined manifolds, in case an explicit formula is not available. This will be accomplished via Algorithm 1 below.

2.1 Homotopy continuation for the Euclidean distance retraction

In order to compute $R_p(v)$ for the Euclidean distance retraction of Theorem 1, we need to solve an optimization problem over the constraint set $\mathcal{M}$, namely, minimizing Euclidean distance. At first glance, this is absurd. We started with an optimization problem (minimizing some other function $f : \mathbb{R}^n \to \mathbb{R}$ restricted to $\mathcal{M}$), and now we suggest taking local steps by solving more optimization problems with the same constraints. However, we have tricks to solve these local optimization problems efficiently, so our proposal is surprisingly useful. In this section we describe how homotopy continuation allows us to easily compute the Euclidean distance retraction.

Given any smooth function $f : \mathbb{R}^n \to \mathbb{R}$ we consider the constrained optimization problem of minimizing $f$ restricted to $\mathcal{M} = g^{-1}(0)$, where $g : \mathbb{R}^n \to \mathbb{R}^m$ is a smooth map and $n - m = \dim(\mathcal{M})$. In what follows, let $dg_x$ denote the $m \times n$ Jacobian matrix of $g$ in the standard basis, evaluated at the point $x$, and let $dg_x^T$ denote the $n \times m$ transpose matrix. Given a point $p \in \mathcal{M}$, and a descent direction $v \in T_p \mathcal{M}$, the idea is to move from $p \in \mathcal{M}$ to $p + v$, which in general will not lie on the manifold $\mathcal{M}$. Subsequently, we want to retract back to the manifold in such a way as to approximate the exponential map. Theorem 1 shows that computing the Euclidean closest point $q = R_p(v) \in \mathcal{M}$ to the point $p + v \in \mathbb{R}^n$ achieves this goal.
**Homotopy Continuation.** Choose $\lambda_1 \in \mathbb{C}^m$ randomly, say, from a multivariate Gaussian distribution. Set $u_1 = dg_p^T \lambda_1 + p \in \mathbb{C}^n$. Let $G : \mathbb{C}^n \times \mathbb{C}^m \times \mathbb{C}^m \to \mathbb{C}^{m+n}$ be the map sending $(x, \lambda, u) \mapsto G(x, \lambda, u)$ whose first $m$ component functions are those of $g$ and the the last $n$ component functions of $G$ are those of $dg_x^T \lambda - u + x$, denoted $G(x, \lambda, u) = (g, dg_x^T \lambda - u + x)$. Fixing the parameters $u = u_1$, we know that $(p, \lambda_1)$ solves the system of equations $G(x, \lambda, u_1) = 0$ for the variables $(x, \lambda)$, by construction.

Now set $u_0 = p + v \in \mathbb{R}^n \subset \mathbb{C}^n$, and create a straight-line path $u(t) = tu_1 + (1-t)u_0$ so that $u(1) = u_1$ and $u(0) = u_0$. For the homotopy (1) defined below, certain parameter values $u(t) \in \mathbb{C}^m$ might correspond to a system of equations with singular Jacobian. Such problematic parameter values are called the *discriminant* in [23]. By Lemma 7.1.2 of [23], and since we chose $\lambda_1 \in \mathbb{C}^m$ randomly, this path avoids the discriminant in the parameter space $\mathbb{C}^m$ with probability one. Using $\mathbb{C}^m$ rather than $\mathbb{R}^m$ was crucial here, since the discriminant forms a subset of real codimension two in $\mathbb{C}^m$, and hence our straight line will avoid it with probability one. Therefore, the solution paths from the homotopy (1) below will consist of nonsingular solutions $H(x, \lambda, t)$ for all fixed $t \in (0, 1]$. We setup the homotopy to begin at $t = 1$ and end at $t = 0$ since the only singular solution can occur at $t = 0$, and there are more floating point numbers near zero.

Define the homotopy $H : \mathbb{C}^n \times \mathbb{C}^m \times \mathbb{R} \to \mathbb{C}^{m+n}$ by

$$H(x, \lambda, t) = G(x, \lambda, tu_1 + (1-t)u_0).$$

Consider the system of ordinary differential equations $\frac{d}{dt} H(x(t), \lambda(t), t) = 0$ with initial values $(x(1), \lambda(1)) = (p, \lambda_1) \in \mathbb{C}^n \times \mathbb{C}^m$. Then the solution path $(x(t), \lambda(t)) \in \mathbb{C}^n \times \mathbb{C}^m$ can be computed numerically from $t = 1$ to $t = 0$ to obtain the previously unknown solutions $(x(0), \lambda(0))$ to the equations $G(x, \lambda, u_0)$. By construction, $x(0) = q = R_p(v)$, and we will have successfully computed the Euclidean distance retraction. Note that although our solution path travels in complex space to ensure everywhere nonsingular Jacobians by avoiding the discriminant, the solution $q = x(0)$ we obtain at the end is again real-valued (See Remark 1 below).

A few remarks are in order. One could object that we are solving a system of ODEs to compute a retraction, so why don’t we simply solve the system of ODEs defining the exponential map? One reason is that for arbitrary implicitly-defined manifolds we do not have parametrizations, and hence even setting up the ODEs corresponding to geodesics becomes difficult. Another reason is that the ODEs arising in homotopy continuation are very easy to solve, since at every $t$ we know that $H(x(t), \lambda(t), t) = 0$. The errors that normally accumulate during the numerical solution of ODEs can be corrected by applying Newton’s method to the system of equations $H(x, \lambda, t') = 0$ in variables $(x, \lambda)$ at any fixed $t'$. Even a naive algorithm using Euler’s method to predict and Newton’s method to correct is surprisingly effective (see [23] for more details). Adaptive step sizes can be chosen so that we never leave the region of quadratic convergence of Newton’s method, and hence the corrector steps are accomplished with just a few linear system solves. Already there exists efficient software specially designed for solving the ODEs arising in homotopy continuation, see for example [6, 9, 11, 19, 25].

**Path-tracking.** Although in practice one can use the specialized software listed above, we will give a brief description of a naive path-tracking algorithm for the reader’s benefit.
To simplify notation, we lump the variables \((x, \lambda)\) into one symbol, \(x\), for this paragraph. Solving the system of ordinary differential equations

\[
\frac{d}{dt}H(x(t), t) = 0
\]

to numerically approximate the solution path \(x(t)\) is much easier than for an arbitrary system of ODEs. The main reason is that we can use Newton’s method to quickly correct any accumulated errors, since for any fixed \(t\) we know that the true solution point \(x(t)\) solves the square system of equations \(H(x(t), t) = 0\), and that its Jacobian will be nonsingular for all \(t \in (0, 1]\). By a first-order Taylor series, consider that

\[
H(x + \Delta x, t + \Delta t) \approx H(x, t) + \frac{\partial H}{\partial x}(x, t)\Delta x + \frac{\partial H}{\partial t}(x, t)\Delta t.
\]  

(2)

In (2), \(H(x, t)\) is a vector resulting from the map \(H\) evaluated at the current point \((x, t)\). \(\frac{\partial H}{\partial x}(x, t)\) is the square Jacobian matrix of partial derivatives in the \(x\) variables evaluated at \((x, t)\), and \(\frac{\partial H}{\partial t}(x, t)\) is a vector of derivatives in \(t\) evaluated at \((x, t)\). To predict the next point \(x + \Delta x\) on the solution path, choose \(\Delta t \neq 0\), set the left-side of (2) to zero, and solve the resulting system of linear equations for \(\Delta x\). This is essentially Euler’s method. If at some point \((x, t)\) we notice that \(H(x, t)\) is no longer zero, errors have begun to accumulate, and so we correct via Newton’s method: In (2), set \(\Delta t = 0\), set the left-side to zero, and solve the resulting linear system for \(\Delta x\). If the stepsizes \(\Delta t\) are chosen appropriately, we should never leave the region of quadratic convergence of Newton’s method, and hence the correction steps will quickly eliminate any errors in path-tracking.

We hope the brief explanation above has at least convinced the reader to learn more about homotopy continuation. We defer to either of the two excellent textbooks [6, 23] or the instructive tutorials at https://www.juliahomotopycontinuation.org/ for more details on how homotopy continuation works, and its many benefits. At this point, we record the main idea in the following algorithm.

By \(\alpha \in \mathbb{R}_{>0}\) we denote a step size, which may be chosen appropriately using back-tracking line search or many other methods.

**Algorithm 1:** Euclidean distance retraction homotopy

**Inputs:** \(g, p, v, \alpha\) as described above.

**Output:** \(q = R_p(\alpha v)\) from Theorem 1.

Choose \(\lambda_1 \in \mathbb{C}^m\) randomly.

Set \(u_1 = dg_p^T \lambda_1 + p\).

Set \(G(x, \lambda, u) = (g, dg_x^T \lambda + x - u)\)

Set \(u_\alpha = p + \alpha v\)

Set \(H(x, \lambda, t) = G(x, \lambda, (1 - t)u_\alpha + tu_1)\).

Use path-tracking (as described above) to discover the solution \((x(0), \lambda(0))\) at \(t = 0\) from the initial values \((x(1), \lambda(1)) = (p, \lambda_1)\) at \(t = 1\). Return \(q = x(0)\).

**Remark 1.** In general, the target system \(H(x, \lambda, 0) = G(x, \lambda, u_\alpha) = 0\) at \(t = 0\) will have many solutions, since there can be many critical points for minimizing Euclidean distance
from \( u_\alpha \) to \( \mathcal{M} \). One of these critical points is \( q = R_p(\alpha v) \), which should satisfy \( |p - q| \approx |\alpha v| \).

If the size \( |\text{dg}_T^p \lambda| \) is too large, the solution \((p, \lambda_1)\) of the start system at \( t = 1 \) may evolve into some far-away solution \((r, \lambda_r)\) of the target system \( G(x, \lambda, u_\alpha) = 0 \) with \( r \neq R_p(\alpha v) \). If we had all solutions to the start system, and tracked them, it is guaranteed that we would find \( R_p(\alpha v) \). For a precise statement of this theorem, see [23, Thm. 8.4.1]. However, we only start with one solution \((p, \lambda_1)\). This issue is easily identified in practice. If the solution \( r \) computed via homotopy is complex-valued rather than real, you know \( r \neq R_p(\alpha v) \). If the solution \( r \) is real-valued, but the distance \( |p - q| \) is much larger than expected based on \( |\alpha v| \), then \( r \neq R_p(\alpha v) \). In either case, one may choose another \( \lambda_1 \) or simply shorten \( |\lambda_1| \), making \( u_1 \) closer to \( p \). Running the algorithm again for this new, “shorter” homotopy, should solve the issue. In fact, in all examples we computed using the software described in Section 4, we never ran into this problem. We discuss this further in Section 5 in terms of future research.

3 Statistics: Maximum likelihood retraction

In this section we leave the setting of submanifolds of Euclidean space and instead consider statistical models as submanifolds of a more general Riemannian manifold whose metric varies from point to point. In this context, we will show that if minimizing Euclidean distance is replaced by maximizing likelihood, then we can define analogous retraction maps to optimize functions on statistical models \( \mathcal{M} \). Theorem 2 shows how to make these retractions second-order accurate for the Levi-Civita connection on \( \mathcal{M} \). Finally, Algorithm 2 describes how homotopy continuation may be used to compute these retraction maps on arbitrary, implicitly-defined statistical models.

Consider the smooth manifold structure on \( \mathbb{R}^n_{>0} \) induced by viewing the identity map as a global chart. We will use the coordinates denoted \((x_i)\) for this global chart for all of our computations. The chart-induced global frame for the cotangent bundle over \( \mathbb{R}^n_{>0} \) is denoted \((dx_1, \ldots, dx_n)\), while \((\partial_1, \ldots, \partial_n)\) will denote the chart-induced global frame for the tangent bundle. Recall, a global frame of a smooth vector bundle is an ordered tuple of global sections whose values at every point yield a basis. The values at a point \( x \in \mathbb{R}^n_{>0} \) will be denoted \( \partial_i|_x \), so that the vectors \((\partial_1|_x, \ldots, \partial_n|_x)\) form a basis for \( T_x \mathbb{R}^n_{>0} \).

Let \( \Delta_{n-1} \subset \mathbb{R}^n_{>0} \subset \mathbb{R}^n \) be the open probability simplex defined by

\[
\Delta_{n-1} = \left\{ (x_1, \ldots, x_n) \in \mathbb{R}^n_{>0} : \sum_{i=1}^n x_i = 1 \right\}.
\]

Given \( u \in \Delta_{n-1} \) we define the log-likelihood function \( \ell_u : \mathbb{R}^n_{>0} \to \mathbb{R} \) by

\[
(x_1, \ldots, x_n) \mapsto \sum_{i=1}^n u_i \log(x_i) = \log \left( \prod_{i=1}^n x_i^{u_i} \right).
\]

A smooth statistical model is a subset \( \mathcal{M} \subset \Delta_{n-1} \) which is also a smooth manifold. In contrast, an algebraic statistical model is a subset \( \mathcal{M} \subset \Delta_{n-1} \) which is also a real algebraic variety. Given a point \( u \in \Delta_{n-1} \) coming from the results of an experiment, maximum likelihood estimation seeks to find the point \( p \in \mathcal{M} \) which maximizes the likelihood of
observing the results $u$. Such a point also maximizes $\ell_u$ restricted to $\mathcal{M} \subset \Delta_{n-1}$. For more details, see [14, Ch. 6] or [21].

A Riemannian metric is a smooth symmetric covariant 2-tensor field that is positive definite at each point. In the global chart on $\mathbb{R}^n_{>0}$, the Fisher metric is defined by

$$g = \sum_{i,j=1}^{n} g_{ij} \, dx_i \otimes dx_j$$

where $g_{ii} = \frac{1}{x_i}$ and $g_{ij} = 0$ for any $i \neq j$ are smooth functions written in the global chart coordinates. Indeed, it is a Riemannian metric (see [5, p. 31]). In statistics and information geometry, the Fisher metric arises naturally, being the unique metric invariant under sufficient statistics [5, Thm 1.2]. In maximum likelihood estimation, one chooses the parameters of a model so as to maximize the likelihood of the observed data. Since the Fisher metric appears in the Cramér-Rao inequality [5, Thm 1.3], it is also related to the reliability of the estimator.

Given a function $f$ on a manifold, the vector field $\text{grad} f$ is given in local coordinates [17, p. 27] by

$$\sum_{j=1}^{n} \left( \sum_{i=1}^{n} g^{ij} \partial_i f \right) \partial_j$$

where the $g^{ij}$ are smooth functions giving the inverse of the matrix $g_{ij}$ of the metric. For the Fisher metric, $g^{jj} = x_j$ and $g^{ij} = 0$ for $i \neq j$. Since $\partial_j \ell_u = u_j / x_j$ we see that

$$\text{grad} \ell_u = \sum_{j=1}^{n} \left( x_j \frac{u_j}{x_j} \right) \partial_j = \sum_{j=1}^{n} u_j \partial_j.$$ 

Compare this with the Euclidean gradient, which we denote $\nabla \ell_u$, given by

$$\nabla \ell_u = \sum_{j=1}^{n} \frac{u_j}{x_j} \partial_j$$

in the same global frame, but computed with the Euclidean metric $g_{ij} = \delta_{ij}$. The metrics themselves will be denoted by $\langle \cdot, \cdot \rangle^{(f)}_p$ and $\langle \cdot, \cdot \rangle^{(e)}_p$ when they act as inner products on the tangent space $T_p \mathbb{R}^n_{>0}$. Accordingly, $N_p^{(f)} \mathcal{M}$ and $N_p^{(e)} \mathcal{M}$ denote the normal spaces inside $T_p \mathbb{R}^n_{>0}$ with respect to to the Fisher and Euclidean metrics. Viewing $\mathcal{M}$ as a Riemannian submanifold of $\mathbb{R}^n_{>0}$, we will use the Levi-Civita connection (cf. [17, Ch. 5]) corresponding to the Fisher metric in our computations of covariant derivatives below.

**Theorem 2.** Let $\mathcal{M} \subset \Delta_{n-1} \subset \mathbb{R}^n_{>0}$ be a smooth statistical model. For $p \in \mathcal{M}$ and $v = \sum v_i \partial_i |_p \in T_p \mathcal{M}$, consider the relation $R_p \subset T_p \mathcal{M} \times \mathcal{M}$ defined by $\{(v, q^*) : v \in T_p \mathcal{M}, q^* \in \text{argmax}_{q \in \mathcal{M}} \ell_{u(p,v)}(q)\}$ where $u(p,v) \in \mathbb{R}^n$ has components $u_i = p_i + v_i + \frac{v_i^2}{4p_i}$. Then there exists a neighborhood $U \subset T_p \mathcal{M} \times 0$ where the argmax is unique and the relation $R_p|_U$ defines a function

$$R_p|_U : U \to \mathcal{M}$$

$$v \mapsto \text{argmax}_{q \in \mathcal{M}} \ell_{u(p,v)}(q),$$

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which is a first-order, local retraction on $\mathcal{M}$ at $p$.

Furthermore, viewing $\mathcal{M}$ as a Riemannian submanifold of $\mathbb{R}^n_{>0}$ with the Fisher metric and its Levi-Civita connection, $R_p|_U$ is a second-order retraction, so that the curve $t \mapsto R_p(tv)$ matches geodesics on $\mathcal{M}$ up to second-order at $t = 0$.

**Proof.** First we check that there exists a neighborhood $U$ of $0 \in T_p\mathcal{M}$ such that $R_p \cap (U \times \mathcal{M})$ actually defines a function $R_p : U \to \mathcal{M}$. Then we will check that this function is a retraction. Consider the normal bundle $N^{(f)}\mathcal{M}$ as a submanifold of $\mathbb{R}^n \times \mathbb{R}^n$ and define $E : N^{(f)}\mathcal{M} \to \mathbb{R}^n$ by $E(y, w) = (y_i + w_i)_{i=1}^n$ in the global coordinates, denoted $y + w$ for short. This is a smooth map, being the restriction of the addition map on $\mathbb{R}^n$. Its differential at $(p, 0)$ is bijective. To see this, consider $E$ restricted to the subset $\mathcal{M}_0 = \{(y, 0) : y \in \mathcal{M}\}$. Then $E|_{\mathcal{M}_0}$ is a diffeomorphism of $\mathcal{M}_0$ onto $\mathcal{M}$ and hence its differential at $(p, 0)$ is bijective to $T_p\mathcal{M}$. Restricting $E$ to $N_0 = \{(p, w) : w \in N^{(f)}\mathcal{M}\}$ gives a map onto the affine subspace $p + N^{(f)}\mathcal{M} \subset \mathbb{R}^n$ whose differential is also bijective. Since $\mathbb{R}^n = T_p\mathbb{R}^n_{>0} = T_p\mathcal{M} \oplus N^{(f)}\mathcal{M}$ we see that $dE|_{(p, 0)}$ is bijective. Therefore $E$ is a local diffeomorphism at $(p, 0)$ by the inverse function theorem for manifolds [16, Thm. 4.5]. In particular, there is a neighborhood $W$ of $(p, 0)$ in $N^{(f)}\mathcal{M}$ where $E$ is injective.

The image of this neighborhood under $E$ is an open neighborhood of $p$ in $\mathbb{R}^n$ for which the maximum likelihood problem has a unique solution. Say $w \in E(W)$ had two points $y, z \in \mathcal{M}$ which maximized the log-likelihood function $\ell_w$ restricted to $\mathcal{M}$. By the usual first-order criteria for local maxima constrained to a subset of $\mathbb{R}^n$, we know that the Euclidean gradients $\nabla \ell_w|_y$ and $\nabla \ell_w|_z$ lie in the Euclidean normal spaces $N_y^{(e)}\mathcal{M}$ and $N_z^{(e)}\mathcal{M}$, respectively. We claim that this forces both $\sum_i(w_i - y_i)\partial_i|_y$ and $\sum_i(w_i - z_i)\partial_i|_z$ to be in $N_y^{(f)}\mathcal{M}$ and $N_z^{(f)}\mathcal{M}$, respectively. To see this we calculate with an arbitrary tangent vector $\nu \in T_p\mathcal{M}$,

$$\langle \nu, w - y \rangle^{(f)} = \langle \nu, w \rangle^{(f)} - \langle \nu, y \rangle^{(f)} = \langle \nu, \nabla \ell_w|_y \rangle^{(e)} - \langle \nu, 1 \rangle^{(e)}.$$

The first term is zero by first-order criteria for local maxima, and the second term is zero because $\mathcal{M} \subset \Delta_{n-1}$ is a statistical model, and hence lives in an affine hyperplane whose Euclidean normal vector is the all ones vector, since probabilities sum to one. In this case, the symbol $1$ denotes the all ones vector $\sum_j \partial_j|_y$. Therefore $\sum_i(w_i - y_i)\partial_i|_y \in N_y^{(f)}\mathcal{M}$. Similarly, $\sum_i(w_i - z_i)\partial_i|_z \in N_z^{(f)}\mathcal{M}$. But then $E(y, w - y) = y + w - y = w$ and $E(z, w - z) = z + w - z = w$ contradicts the injectivity of $E$ on $W$. Therefore $E(W)$ is a neighborhood of $p \in \mathbb{R}^n$ for which the maximum likelihood problem has a unique solution. Let $u(p, \cdot) : T_p\mathcal{M} \to \mathbb{R}^n$ be the map sending a tangent vector $v = \sum v_i\partial_i|_p$ to the tuple $\left(p_i + v_i + \frac{v_i^2}{4p_i}\right)_{i=1}^n$, where all coordinates are in terms of the global chart. Then there exists a neighborhood $U$ of $0 \in T_p\mathcal{M}$ where $u(p, v) \in E(W)$ whenever $v \in U$, and hence the relation $R_p$ defines a function on $U$.

As a result of the previous discussion, for $p \in \mathcal{M}$ and $v \in U \subset T_p\mathcal{M}$ we can define the function

$$R_p(v) = \arg\max_{q \in \mathcal{M}} \ell_{u(p, v)}(q).$$

First we check that $R_p$ is smooth. Let $\pi : N^{(f)}\mathcal{M} \to \mathcal{M}$ be the projection onto $\mathcal{M}$, sending $(y, n) \mapsto y$. For $v \in U \subset T_p\mathcal{M}$ we have $u(p, v) \in E(W)$. Since $E$ is a diffeomorphism
between $W$ and $E(W)$ we know the inverse $E^{-1}$ exists and is smooth on $E(W)$. Since $R_p = \pi \circ E^{-1} \circ u(p, \cdot)$ is the composition of smooth maps, $R_p$ is also smooth.

Now we check that $R_p(0) = p$. But this follows since the argmax of the function $\ell_u$ for any $u \in \Delta_{n-1}$ over the larger domain $\Delta_{n-1}$ is unique and equal to $u$. This fact is well-known, and can be checked by noting that $u$ is the only critical point of $\ell_u$ on $\Delta_{n-1}$ and that the Hessian is negative definite since $\Delta_{n-1} \subset \mathbb{R}^n_{>0}$. Therefore since $M \subset \Delta_{n-1}$, when $v = 0$ we have a unique argmax at $u(0) = p + 0 = p \in M \subset \Delta_{n-1}$ as needed.

Finally, we check the conditions for a first-order and second-order retraction. We don’t need the Riemannian structure for first-order, but since we are proving second-order as well we treat both cases uniformly. Define $c(t) = R_p(tv)$ for $t$ in a small enough neighborhood $I \subset \mathbb{R}$ of zero, such that $Iv \subset U$. Then $c(t)$ is the unique point in $M$ which maximizes the log-likelihood function $\ell_{u(p, tv)}$ restricted to $M$. Let $\dot{c}$ be the vector field on the curve $c$ given in the global chart by $\dot{c} = \sum_{j=1}^n \dot{c}_j(t) \partial_j$, where $\dot{c}_j(t)$ denotes the derivative of the component function $c_j(t)$ of the curve $c : I \to M$. To show that $R_p$ is a first-order retraction we need to show that $v = \sum_j v_j \partial_j |_p$ is equal to $\dot{c}_p = \sum_j \dot{c}_j(0) \partial_j |_p$. To show that $R_p$ is a second-order retraction we need to show that $D_t \dot{c}_p \in N_{P}^f M$ [7, Def. 8.64 and Eqn 8.27]. Here, $D_t$ denotes the covariant derivative along the curve $c$, using the Levi-Civita connection for the Fisher metric on $M$ (See [17, Thm 4.24]).

Let $A$ be any vector field on the curve $c$ which is tangent to $M$, so that $A(t) = A|_{c(t)} \in T_{c(t)}M$ for all $t \in I$. By first-order criteria for local maxima we know that $\langle A(t), \nabla \ell_{u(t)} \rangle_{c(t)} = 0$ for all $t \in I$, since $A$ is everywhere tangent to $M$. We also know that $\langle A(t), 1 \rangle_{c(t)} = 0$ since $M \subset \Delta_{n-1}$. By $u(t) = u(p, tv)$ denote the curve in $E(W)$ with components $p_i + tv_i + t^2 \frac{v_i^2}{2p_i}$, and let $B = B(t)$ be the vector field along the curve $c$ given by $\sum_j B_j(t) \partial_j |_{c(t)}$ where $B_j(t) = u_j(t) - c_j(t) = p_j + tv_j + t^2 \frac{(v_i)^2}{4p_i} - c_j(t)$. Then, we have

$$0 = \langle A(t), \nabla \ell_{u(t)} \rangle_{c(t)} - \langle A(t), 1 \rangle_{c(t)}$$

$$= \langle A(t), \nabla \ell_{u(t)} - 1 \rangle_{c(t)}$$

$$= \langle A(t), \sum_{i=1}^n (u_i(t) - c_i(t)) \partial_i |_{c(t)} \rangle_{c(t)}$$

$$= \langle A(t), B(t) \rangle_{c(t)}.$$

Note that $B(t)$ is the orthogonal projection of $\nabla \ell_{u(p, tv)}$ onto $T_{c(t)} \Delta_{n-1}$ along the curve $c$ when using the Fisher metric. Applying $\frac{d}{dt}$ and $\frac{d^2}{dt^2}$ using [17, Prop 5.5] we find

$$0 = \frac{d}{dt} \langle A, B \rangle_{c(t)} = \langle D_tA, B \rangle_{c(t)} + \langle A, D_tB \rangle_{c(t)}$$

$$0 = \frac{d^2}{dt^2} \langle A, B \rangle_{c(t)} = \langle D_tD_tA, B \rangle_{c(t)} + 2 \langle D_tA, D_tD_tB \rangle_{c(t)} + \langle A, D_tD_tD_tB \rangle_{c(t)}.$$

Recall (see [17, p. 102]) the covariant derivative of a vector field along a curve $c$ is given by

$$D_tB(t) = \sum_k \left( \dot{B}_k(t) + \sum_i \sum_j \dot{c}_i(t)B_j(t)\Gamma^k_{ij}(c(t)) \right) \partial_k |_{c(t)}$$
where $\Gamma_{ij}^k$ are the Christoffel symbols of the metric in the given local frame. For the Fisher metric with the corresponding Levi-Civita connection in the global frame $\partial_k$ induced by the global chart, every $\Gamma_{ij}^k = 0$ except $\Gamma_{ij}^j(c(t)) = \frac{-1}{\epsilon_{ij}(t)}$, evaluating at the point $c(t)$ along the curve (cf. [17, p. 123]). Using this in our calculations, equation (5) becomes $D_t B(t) = \sum_k \left( \dot{B}_k(t) - \frac{\dot{c}_k(t)}{2\epsilon_k(t)} \right) \partial_k | c(t) | p$. Then, since $c(0) = p$ we have $B(0) = 0$, and since both $v$ and $\dot{c}$ are in the tangent space at $p$, equation (3) implies that $v_k = \dot{c}_k(0)$ and so $v = \dot{c} | p$, which completes the proof that $R_p$ is a first-order retraction.

Having proved first-order, both $B(0)$ and $D_t B(0)$ are zero, and the first two terms of equation (4) vanish at $t = 0$. A somewhat tedious calculation (which we omit) shows that $D_t D_t B(0) = \sum_k \left( \frac{(v_k)^2}{2\epsilon_k} - \dot{c}_k(0) \right) \partial_k | p$. Calculating $D_t \dot{c}(0)$ using equation 5, it is noted that $D_t D_t B(0) = -D_t \dot{c}(0)$. Therefore, equation (4) becomes

$$\langle A(0), -D_t \dot{c}(0) \rangle_p^{(f)} = 0.$$  

Since this is true for any vector field $A$ which is everywhere tangent to $\mathcal{M}$, and hence for any tangent vector $A(0) \in T_p \mathcal{M}$, we have $D_t \dot{c}(0) \in N_p(\mathcal{M})$, which completes the proof.

### 3.1 Maximum likelihood retraction by homotopy

Having established Theorem 2, we now describe how to use homotopy continuation to compute this new retraction map on statistical models.

Let $p \in \mathcal{M}$, $v = \sum v_i \partial_i | p \in T_p \mathcal{M}$, and a stepsize $\alpha \in \mathbb{R}_{>0}$ be given. Say that $\mathcal{M} \subset \Delta_{n-1} \subset \mathbb{R}^n$ is equal to the zeros of the smooth map $g : \mathbb{R}^n \to \mathbb{R}^m$. We will also assume that the dimension of $\mathcal{M}$ is equal to $n - m$. If not, standard techniques of randomization in numerical nonlinear algebra can be used to create a new map $\tilde{g} : \mathbb{R}^n \to \mathbb{R}^k$ so that $\mathcal{M} \subset \tilde{g}^{-1}(0)$, $\dim \mathcal{M} = n - k$, and the additional zeros of $\tilde{g}$ are well-controlled. See [23, Ch. 13.5]. In what follows, let $dg_x$ denote the $m \times n$ Jacobian matrix of $g$ in the standard basis, $dg_x^T$ denote its $n \times m$ transpose, and let $\text{diag}(p_i)$ denote the $n \times n$ diagonal matrix with entries $p_i$. Since $\mathcal{M} \subset \Delta_{n-1}$, we may assume that $g_1 = -1 + \sum x_i$ is the first component function of the map $g : \mathbb{R}^n \to \mathbb{R}^m$ implicitly defining $\mathcal{M}$. Choose $\lambda_1 \in \mathbb{C}^m$ randomly from a multivariate Gaussian distribution, and then set the first component to 1, producing $\lambda_1 = (1, \lambda_{12}, \lambda_{13}, \ldots, \lambda_{1m}) \in \mathbb{C}^m$. Then set $u_1 = \text{diag}(p_i) dg_x^T \lambda_1 \in \mathbb{C}^n$. Notice that since the first scalar in $\lambda_1$ equals 1, $u_1$ is equal to $p$ plus a random, small step in the complexified normal space $N_p(\mathcal{M})$. By construction, $p \in \mathbb{R}^n$ solves the equation $dg_x^T \lambda_1 = \nabla \ell_{u_1}$ for the variables $x$. These equations say that the Euclidean gradient of $\ell_{u_1}$ at $p$ is in the Euclidean normal space at $p$, making $p$ a critical point of $\ell_{u_1}$ restricted to $\mathcal{M}$. We will use $(p, \lambda_1)$ as a starting solution to a homotopy that begins with parameters $u_1$ and ends with parameters $u_\alpha = \left( p_i + \alpha v_i + \alpha^2 \frac{v_i^2}{4 \epsilon_i} \right)_{i=1}^n$.

Let $G : \mathbb{C}^n \times \mathbb{C}^m \times \mathbb{C}^n \to \mathbb{C}^{m+n}$ send $(x, \lambda, u) \mapsto G(x, \lambda, u)$, where the $m + n$ component functions of $G$ are those of $g$ plus those of $\text{diag}(x_i) dg_x^T \lambda - u$. Then let $H : \mathbb{C}^n \times \mathbb{C}^m \times \mathbb{R} \to \mathbb{C}^{m+n}$ be the homotopy defined by $H(x, \lambda, t) = G(x, \lambda, (1 - t) u_\alpha + tu_1)$. As is the convention in the homotopy continuation literature, and since there are more floating point numbers near zero than one, we begin our homotopy at $t = 1$ and end at $t = 0$. At $t = 1$ we have
by construction $H(p, \lambda_1, 1) = 0$. If $H(q, \lambda_0, 0) = 0$, then $q = R_p(\alpha v)$. We can compute $(q, \lambda_0)$ by homotopy continuation using the start solution $(p, \lambda_1)$ at $u_1$, though we only keep $q = R_p(\alpha v)$ and throw away $\lambda_0$. We record this idea in the following algorithm.

**Algorithm 2**: Maximum likelihood retraction by homotopy

**Inputs**: $g, p, v, \alpha$ as described above.

**Output**: $q = R_p(\alpha v)$ from Theorem 2.

Choose $(\lambda_{12}, \lambda_{13}, \ldots, \lambda_{1m}) \in \mathbb{C}^{m-1}$ randomly.

Set $\lambda_1 = (1, \lambda_{12}, \lambda_{13}, \ldots, \lambda_{1m}) \in \mathbb{C}^m$.

Set $u_1 = \text{diag}(p_i) d g_p^T \lambda_1$.

Set $G(x, \lambda, u) = (g, \text{diag}(x_i) d g_x^T \lambda - u)$

Set $u_\alpha = \left( \frac{p_i + \alpha v_i + \alpha^2 \frac{v_i^2}{4n}}{i=1} \right)$

Set $H(x, \lambda, t) = G(x, \lambda, (1 - t)u_\alpha + tu_1)$.

Use path-tracking (as described in Section 2.1) to discover the solution $(x(0), \lambda(0))$ at $t = 0$ from the initial values $(x(1), \lambda(1)) = (p, \lambda_1)$ at $t = 1$. Return $q = x(0)$.

4 Description of the software

The software package HomotopyOpt.jl has been written in Julia, a high-level, dynamic programming language. In particular, this gives us access to HomotopyContinuation.jl [9], a numerical algebraic geometry package. Note that because we use this package, the map $g : \mathbb{R}^n \rightarrow \mathbb{R}^m$ defining $\mathcal{M}$ must have polynomial component functions, while the objective function can be anything smooth. Assume now that we want to optimize the smooth function $f(x_1, x_2, x_3) = 2(x_2 - 1)^2$ subject to the constraint set

$$g = \begin{bmatrix} x_1^2 + x_2^2 + x_3^2 - 1 \\ x_3 - x_1^3 \end{bmatrix}.$$

To solve this optimization problem with initial point $(0, -1, 0) \in \mathcal{M}$ we write:

using HomotopyOpt # load package

```julia
p = [0, -1, 0]
f = x -> 2^((x[2] - 1)^2)
g = x -> [x[1]^2 + x[2]^2 + x[3]^2 - 1, x[3] - x[1]^3]
M = ConstraintVariety(g, 3, 1) # M embedded in R^3 with dim 1
res = findminima(p, 1e-5, M, f) # Set the tolerance to 10^(-5)
```

Now, we can use Lagrange multipliers to calculate analytically that the minimum of $f$ on $\mathcal{V}(g)$ is at $(0, 1, 0)$. Indeed, by typing `res.computedpoints[end]` in the command prompt the final point can be examined, revealing the vector

$$[-0.0012328615227131664, 0.9999992400259441, -1.8738848314414474e-9],$$

which is a solid approximation of the true optimum.
As described in Section 2, to solve this optimization problem the software takes several local steps (maxlocalsteps), running Riemannian gradient descent [7, p. 62]. First, it calculates a descent direction \( v \) in \( T_xV \), given by the negative Riemannian gradient obtained by projecting \( f \)'s gradient onto \( T_xV \). Afterwards, the algorithm uses backtracking line search with Wolfe conditions to compute a feasible step size corresponding to the previously chosen descent direction (see [15, 22]). These conditions provide a lower and an upper bound on admissible step sizes and come alongside convenient theoretical guarantees, such as existence of open intervals of step sizes satisfying the Wolfe conditions [15]. Furthermore, provided a sequence of step sizes satisfying the Wolfe conditions and well-chosen descent directions, Zoutendijk’s Theorem (cf. [22]) guarantees convergence in a large class of Riemannian optimization algorithms. After having chosen a step size \( \alpha \) and a descent direction \( v \), the linear steps \( p + \alpha v \) are corrected to the variety using the Euclidean Distance Retraction Algorithm.

Having completed maxlocalsteps local steps, we check if the first-order criterion for optimality \( \text{grad}(x_k) \approx 0 \) is satisfied, or whether the algorithm is stuck in a saddle point or singularity. Our method recognizes saddle points by looking for insufficient decrease in the objective function and singularities by comparing the current Jacobian’s (numerical) rank to the previous Jacobian’s rank. If it changed, we need to assume that the iteration is currently in or close to a singularity. In either of these cases, we proceed to check whether current iterate is a minimum by employing the second-order criterion on optimality (see [7, Prop. 6.3]). If it is inconclusive or finds that the current point is not optimal, the algorithm continues. In the case of a singularity, additionally we try to resolve the singularity by intersecting the variety with a sphere centered at the current iterate (and possibly additional hyperplanes) and choosing the intersection point with the smallest objective function value to continue the optimization. Otherwise, if the second-order criterion has a positive result, the current point is returned to the user as optimal. Finally, if the algorithm was inconclusive and exceeds the prescribed maximal amount of time maxseconds, the current point is returned with the additional information lastpointisminimum=false.

There are a few additional ways to interact with this package that deserve mentioning. The method watch animates the optimization procedure’s steps on the manifold, draw produces a static picture of both the local steps and a global picture and setequationsatp! randomizes the equations at a specific point, so there are only codimension-many left. For this, the dimension is calculated at the specified point by checking the constraint system’s Jacobian rank.

5 Questions

In this section, we briefly mention a few areas for future research.

1. As discussed in Remark 1, one may worry that the solution obtained at the end of the homotopy is not \( R_p(v) \), since there can be many solutions to the target system, and using Algorithms 1 and 2 only finds one of them. In practice we have found that this issue rarely happens. One explanation would be that under certain conditions, nearby solutions evolve to nearby solutions. Say we are given a homotopy between a start
system and target system, both with $N$ solutions. Let $p$ be one solution to the start system, and say that among the $N$ solutions to the target system, $q$ is closest to $p$. Under what conditions can it be expected that $p$ evolves into $q$ under the homotopy? There are many similar and interesting questions to answer along these lines of thought.

2. Theorem 4.3 of [10] calculates the condition number of critical points of the Euclidean distance function, which is related to the extrinsic curvature of the embedding of the manifold in $\mathbb{R}^n$ via the Riemannian Hessian. Corollary 5.5 of [10] implies that for points $u$ nearby $M$ in the ambient $\mathbb{R}^n$, the effect of curvature on the sensitivity of the Euclidean distance problem can essentially be ignored. Do similar results hold for the maximum likelihood retraction in the statistical setting?

3. Investigate the computational aspects of Algorithm 1, giving special attention to how it compares to existing software for Riemannian optimization (e.g. [8]). This should include a study of methods for finding descent directions and step sizes.

4. Examine the quality of Algorithm 2 as compared to other statistical methods solving the same problem, potentially contained in software environments like $\mathbb{R}$. In this context, the MLDegree may be worth exploring as the statistical analogous to the EDDegree (see also [12, p. 2]).

5. Explore prescribing a maximal step length using tools from metric algebraic geometry. This bound may for example be informed by invariants like the reach, medial axis, Voronoi tube, the Euclidean Distance Degree, or the size of the smallest bottleneck. While these properties are global in nature and as such may be too difficult to compute in practice, some have local analogues such as the empirical or local reach [1]. These could inform an upper bound on the step size.

6. A distinctive feature of algebraic varieties in comparison with smooth manifolds is the existence of singularities. While singularities can be resolved (cf. [13]), this procedure is usually computationally expensive and involves a significant increase in the ambient-space dimension. Investigating heuristics to cope with singularities may therefore vastly improve the algorithm’s runtime. There has been some recent progress in this area (cf. [18, 20]), but a general study of algebraic heuristics may be beneficial.

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