

A Differential Geometric Approach to Equidistributed Knots on Riemannian Manifolds

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Abstract. We introduce a differential geometric approach to the numerical generation of equidistributed knots on closed compact Riemannian manifolds. The algorithms are based on minimization of a potential function by intrinsic versions of gradient or BFGS methods. Our approach finds also applications to equidistribution on spheres and is able to reproduce already known results. Numerical examples are given at the end of the paper.

§1. Introduction

The problem of finding equidistributed knot sets on a sphere has a long history. Applications of such knots can be found, e.g., in interpolation or numerical quadrature on spheres, in geophysics, meteorology, astrophysics, and elsewhere.

A common way to generate equidistributed points on spheres is the minimization of a given potential function E (see, e.g., [3, 7, 8, 11]) which is motivated by physics. In case of the 2-sphere $S^2 \subset \mathbb{R}^3$, this potential is the electromagnetic potential

$$E(x_1, \dots, x_N) = \sum_{1 \leq i < j \leq N} \|x_i - x_j\|_2^{-1}, \quad (1)$$

where the points can be interpreted as electrons influenced by repulsing forces. For optimal points an equilibrium position is reached (in physics, this problem is known as **Thomson's problem** [10]). Here, $x_i \in \mathbb{R}^3$ are the coordinates of the electrons and $\|\cdot\|_2$ is the usual Euclidean norm in \mathbb{R}^3 . Because all electrons should stay on the sphere, we have the additional constraints $\|x_i\|_2 = 1$ with $i = 1, \dots, N$, and minimization of E is a constrained optimization problem.

Note that in this approach the distance between two points $\|x_i - x_j\|_2$ is measured in Euclidean space \mathbb{R}^3 .

The numerical minimization of E is usually done by mapping the sphere first on some flat 2-dimensional parameter space (e.g., on \mathbb{R}^2 when using the stereographic projection, or on a rectangle $[0, \pi] \times [0, 2\pi]$ when using spherical coordinates), and applying a numerical minimization scheme then. Therefore, minimization does not take place on the sphere S^2 itself, but on some flat subset of \mathbb{R}^2 . Note that the topological structure of these parameter spaces is different from the topological structure of the sphere (e.g., the plane \mathbb{R}^2 is not compact and the rectangle $[0, \pi] \times [0, 2\pi]$ has a boundary, while the sphere does not). Further, some methods (like the stereographic projection) are restricted to the 2-sphere and cannot be generalized to higher dimensional spheres S^n with $n > 2$.

In our new method we avoid these problems by formulating everything intrinsically, i.e., we work in terms of **Riemannian geometry**. We consider the sphere no longer as a subset of a Euclidean space, but as a closed compact Riemannian manifold. Using this approach, all points stay on the manifold by definition (yielding an unconstrained optimization problem) and distances are measured *inside* the manifold. Denoting the intrinsic distance between two points p, q by $d(p, q)$, the intrinsic version of (1) reads

$$E(x_1, \dots, x_N) = \sum_{1 \leq i < j \leq N} d(x_i, x_j)^{-1}.$$

In case of the n -sphere $S^n \subset \mathbb{R}^{n+1}$, the intrinsic distance between two points $p, q \in \mathbb{R}^{n+1}$, $\|p\|_2 = \|q\|_2 = 1$, is the *spherical distance*, which can be written $d(p, q) = \arccos(p^T \cdot q)$, with $p^T \cdot q$ the usual inner product in \mathbb{R}^{n+1} .

Minimization of E now requires modified intrinsic minimization schemes. In this paper, we show how to adapt the *gradient* and the *BFGS method* to the Riemannian case. It is also possible (although very technical) to construct an intrinsic *Newton method*, but we will describe this in a forthcoming paper.

Because the starting point of our method is a closed compact Riemannian manifold, we are no longer restricted to spheres. Moreover, it is possible to apply these algorithms directly to other manifolds, e.g., tori or ellipsoids, in any finite dimension.

§2. Notations

Many of our notations come from differential geometry. The reader who is not familiar with the concepts addressed below may consult [2, 4, 6].

We denote by (M, g) the Riemannian manifold M with metric tensor (first fundamental form) g and finite dimension n . For $p \in M$, the **tangent space** at p is written $T_p M$. $T_p M$ is a linear space and has the same dimension as M . Because we restrict ourselves to real manifolds, $T_p M$ is isomorphic to \mathbb{R}^n . The **inner product** of two vectors $v, w \in T_p M$ is written $\langle v, w \rangle := g_p(v, w)$, where g_p is the metric tensor at the point p (therefore, $T_p M$ is in general not isometric to \mathbb{R}^n). The length or **norm** of a vector $v \in T_p M$ is $\|v\| := \sqrt{\langle v, v \rangle}$.

Let $\gamma : [a, b] \rightarrow M$ be a smooth path in M . Differentiating γ results in the vector field $\dot{\gamma}$. For every $t \in [a, b]$, we have $\dot{\gamma}(t) \in T_{\gamma(t)}M$. If γ is parameterized by arclength, then $\|\dot{\gamma}\| \equiv 1$. The length of γ is

$$L(\gamma) = \int_a^b \|\dot{\gamma}\| dt.$$

The distance $d(p, q)$ between two points $p, q \in M$ is defined as the length of the shortest path in M joining p and q . $d : M \times M \rightarrow \mathbb{R}$ is a metric in the usual sense.

Given two vector fields X and Y on M , the covariant derivative of Y in the direction X is $\nabla_X Y$. Here ∇ is the Riemannian connection. For three vector fields X, Y, Z , the Riemannian curvature tensor is $R(X, Y, Z) = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X, Y]} Z$, with $[X, Y] := XY - YX$ the Lie bracket. A vector field Y along the path γ is said to be **parallel** along γ if $\nabla_{\dot{\gamma}} Y \equiv 0$. The path γ is called a **geodesic** if $\dot{\gamma}$ is parallel along γ , i.e., $\nabla_{\dot{\gamma}} \dot{\gamma} \equiv 0$. Geodesics will play an important role in our approach. In Euclidean space, geodesics are straight lines; on spheres, geodesics are the great circles. Unfortunately, on most manifolds there are no explicit formulas for geodesics. But in principle they can always be calculated (at least numerically) by solving the nonlinear differential equation $\nabla_{\dot{\gamma}} \dot{\gamma} \equiv 0$. Public domain software for doing this is available in the internet [1].

If $p \in M$ and $X \in T_p M$, $\|X\| = 1$, there exists a unique geodesic γ (parameterized by arclength) with $\gamma(0) = p$ and $\dot{\gamma}(0) = X$. In general, γ is defined only in a neighborhood of 0, i.e., $\gamma : (-\varepsilon, \varepsilon) \rightarrow M$, with some $\varepsilon > 0$. If γ is defined in all of \mathbb{R} , M is said to be **complete**. Because we only consider closed compact Riemannian manifolds, our manifolds are always complete. Thus, we can define the **exponential map** at $p \in M$ as follows:

$$\exp|_p : T_p M \rightarrow M, \quad \exp|_p(X) := \gamma_{p, \frac{X}{\|X\|}}(\|X\|),$$

where $\gamma_{p, \frac{X}{\|X\|}}$ is the unique geodesic with $\gamma_{p, \frac{X}{\|X\|}}(0) = p$ and $\dot{\gamma}_{p, \frac{X}{\|X\|}}(0) = \frac{X}{\|X\|}$.

In case of the n -sphere S^n , there is an explicit expression for the exponential map (see, e.g., [4], p. 117):

$$\exp|_p(X) = p \cos(\|X\|) + \frac{X}{\|X\|} \sin(\|X\|), \quad X \neq 0.$$

§3. Potential Function

For $N \in \mathbb{N}$ points (knots) $x_1, \dots, x_N \in M$ define the potential function

$$E(x_1, \dots, x_N) := \sum_{1 \leq i < j \leq N} U(d(x_i, x_j)), \quad (2)$$

with $U : (0, \infty) \rightarrow \mathbb{R}$ a nonnegative, strictly decreasing, smooth function. In our experiments we used $U(r) = r^{-1}$. Further, we require that there is one and

only one minimal length geodesic joining p and q (i.e., we avoid conjugated points). In case of the sphere, e.g., the north and south pole are conjugated points. In order to include conjugated points on the sphere, one has to employ a potential function which vanishes at π together with its first derivative.

Our aim is to solve the minimization problem

$$\min_{x_1, \dots, x_N \in M} E(x_1, \dots, x_N). \quad (3)$$

To develop numerical methods (like gradient or BFGS methods) we need the first derivative of E (the gradient). Due to linearity, it is enough to consider the first derivative of $U(d(p, q)) : M \times M \rightarrow \mathbb{R}$ (*two variables only*).

Proposition 1. *Let $p, q \in M$, $p \neq q$, two points in M which are not conjugated, $\ell := d(p, q)$, and $\gamma : [0, \ell] \rightarrow M$ the unique minimal length geodesic joining p and q , parameterized by arclength, $\gamma(0) = p$, $\gamma(\ell) = q$. With $f(p, q) := U(d(p, q))$ we have*

$$\frac{\partial f}{\partial p}(p, q) = -U'(d(p, q)) \cdot \dot{\gamma}(0) \quad \text{and} \quad \frac{\partial f}{\partial q}(p, q) = U'(d(p, q)) \cdot \dot{\gamma}(\ell).$$

Proof: For $v \in T_p M$ and $w \in T_q M$ ($v, w \neq 0$) we denote by Z the Jacobi field along γ (i.e., $\nabla_{\dot{\gamma}} \nabla_{\dot{\gamma}} Z + R(Z, \dot{\gamma}, \dot{\gamma}) \equiv 0$) with $Z(p) = v$ and $Z(q) = w$.

If $\varepsilon > 0$ is sufficiently small, we can define the *variation* of γ by

$$V(s, t) : [0, \ell] \times [-\varepsilon, \varepsilon] \rightarrow M, \quad V(s, t) := \exp|_{\gamma(s)}(t \cdot Z(\gamma(s))).$$

V satisfies $V(s, 0) = \gamma(s)$ for all $s \in [0, \ell]$, and

$$V(0, t) = \exp|_p(tv), \quad V(\ell, t) = \exp|_q(tw), \quad t \in [-\varepsilon, \varepsilon].$$

Further, we have $d(\exp|_p(tv), \exp|_q(tw)) = L(V(\cdot, t))$ with $L(V(\cdot, t))$ the length of $V(\cdot, t)$. Therefore

$$\frac{d}{dt} U(d(\exp|_p(tv), \exp|_q(tw)))|_{t=0} = U'(d(p, q)) \cdot \frac{d}{dt} L(V(\cdot, t))|_{t=0}.$$

But from [4, p. 122], we get

$$\frac{d}{dt} L(V(\cdot, t))|_{t=0} = \langle w, \dot{\gamma}(\ell) \rangle - \langle v, \dot{\gamma}(0) \rangle. \quad \square$$

We only remark, that the second derivative of $U(d(p, q))$ can be calculated in a similar way, giving the Hessian of U (which we need to develop Newton methods). Details of the computations will be given in a forthcoming paper by the authors.

Using the gradient as given in Proposition 1, we can build intrinsic gradient and BFGS methods.

3.1. Gradient Method

The simplest minimization procedure we can construct is the **gradient method**. The intrinsic version of the algorithm works as follows:

- (1) Set $k = 0$ and start with N different points $x_1^{(0)}, \dots, x_N^{(0)} \in M$ which are not conjugated.
- (2) For $i = 1, \dots, N$, compute $v_i := \frac{\partial E}{\partial x_i}(x_1^{(k)}, \dots, x_N^{(k)})$.
- (3) For $i = 1, \dots, N$, compute $x_i^{(k+1)} := \exp|_{x_i^{(k)}}(v_i)$.
- (4) If $E(x_1^{(k+1)}, \dots, x_N^{(k+1)})$ is not small enough, set $k := k + 1$ and go to step (2).

3.2. BFGS Method

To improve the convergence rate, we modify the gradient method to obtain a **BFGS method**.

Before starting, we need the notation of *parallel displacement* or *pullbacks*. To define this, fix $b \in M$. If $p \in M$, $p \neq b$, $v \in T_p M$, and $\gamma : [\alpha, \beta] \rightarrow M$ the minimal length geodesic with $\gamma(\alpha) = p$ and $\gamma(\beta) = b$, then there exists one and only one parallel vector field X along γ (i.e., $\nabla_{\dot{\gamma}} X \equiv 0$) with $X(p) = v$. We call $v^* := X(b)$ the **parallel displacement** or **pullback** of v (from $T_p M$ to $T_b M$). For $v \in T_b M$ (i.e., $p = b$) set $v^* := v$. Using this notation, we obtain the following BFGS algorithm, which is an intrinsic version of the Euclidean BFGS method (described e.g., in Stoer [9, p. 281]):

- (1) Start with N different points $x_1^{(0)}, \dots, x_N^{(0)} \in M$ which are not conjugated. Let $H^{(0)} := I$, the $(N \cdot \dim M) \times (N \cdot \dim M)$ identity matrix, b a fixed point in M , and

$$v_i^{(0)} := \frac{\partial E}{\partial x_i}(x_1^{(0)}, \dots, x_N^{(0)}), \quad i = 1, \dots, N.$$

- (2) For $k = 0, 1, 2, \dots$ iterate as follows:

(3)

$$\begin{pmatrix} w_1^{(k)} \\ \vdots \\ w_N^{(k)} \end{pmatrix} := H^{(k)} \cdot \begin{pmatrix} (v_1^{(k)})^* \\ \vdots \\ (v_N^{(k)})^* \end{pmatrix}$$

- (4) Let $u_i^{(k)}$ be the parallel displacement of $w_i^{(k)}$ from $T_b M$ to $T_{x_i^{(k)}} M$, $i = 1, \dots, N$ (i.e., $(u_i^{(k)})^* = w_i^{(k)}$).
- (5) Minimize (as a function of $\lambda \geq 0$)

$$E \left(\exp|_{x_1^{(k)}}(\lambda u_1^{(k)}), \dots, \exp|_{x_N^{(k)}}(\lambda u_N^{(k)}) \right),$$

and name the minimal solution $\lambda_{\min}^{(k)}$.

(6) Calculate the new points $x_i^{(k+1)} := \exp|_{x_i^{(k)}}(\lambda_{\min}^{(k)} u_i^{(k)})$, $i = 1, \dots, N$.
 If $E(x_1^{(k+1)}, \dots, x_N^{(k+1)})$ is small enough, then stop.

(7) Let $p_i^{(k)} := (\lambda_{\min}^{(k)} u_i^{(k)})^*$, $i = 1, \dots, N$, and set $p^{(k)} := \begin{pmatrix} p_1^{(k)} \\ \vdots \\ p_N^{(k)} \end{pmatrix}$.

(8) Calculate $v_i^{(k+1)} := \frac{\partial E}{\partial x_i}(x_1^{(k+1)}, \dots, x_N^{(k+1)})$, $i = 1, \dots, N$.

(9) Let $q_i^{(k)} := (v_i^{(k+1)})^* - (v_i^{(k)})^*$, $i = 1, \dots, N$, and $q^{(k)} := \begin{pmatrix} q_1^{(k)} \\ \vdots \\ q_N^{(k)} \end{pmatrix}$.

(10) Compute the matrix $H^{(k+1)} := \Psi(H^{(k)}, p^{(k)}, q^{(k)})$, where

$$\Psi(H, p, q) = H + \left(1 + \frac{q^T H q}{p^T q}\right) \cdot \frac{p p^T}{p^T q} - \frac{1}{p^T q} (p q^T H + H q p^T).$$

§4. Application to Spheres

Because most numerical results involve minimizing the (Euclidean) $1/r$ potential (1) of point sets on the 2-sphere S^2 , we apply our method to this special case. The algorithm also works for higher dimensional spheres S^n with $n > 2$. To compare our results with already known methods, we use a modified version of our intrinsic potential function U in (2), such that $U(d(p, q)) = 1/\|p - q\|_2$, with $\|\cdot\|_2$ the Euclidean norm in \mathbb{R}^3 .

The numerical computations were performed by a MatLab implementation of the intrinsic BFGS method. We always start with random points and perform 20 iteration steps. 192 points generated by this method are plotted in Figure 1.

We compare our results for $N = 50, 100, 192, 212, 272, 282$ points with results from a list of Hardin, Sloane, and Smith, which can be found in the internet [5]. The (conjecturally) minimal $1/r$ potentials found there are given in column ‘‘HSS’’ in Table 1. Our best results are listed in column ‘‘min E .’’

N Points	min E	HSS	Difference
50	1055.51281	1055.18231	0.0313 %
100	4449.80132	4448.35063	0.0326 %
192	16968.41162	16963.33838	0.0299 %
212	20773.49271	20768.05308	0.0262 %
272	34527.45917	34515.19329	0.0355 %
282	37160.01633	37147.29441	0.0342 %

Tab. 1. Numerical results after 20 iterations.

In Figure 2, we plotted the minimum potential E which was reached after $k = 1, \dots, 20$ iterations in case of 192 points. As can be seen in the figure, after only a few iteration steps we are quite near the optimal minimum.

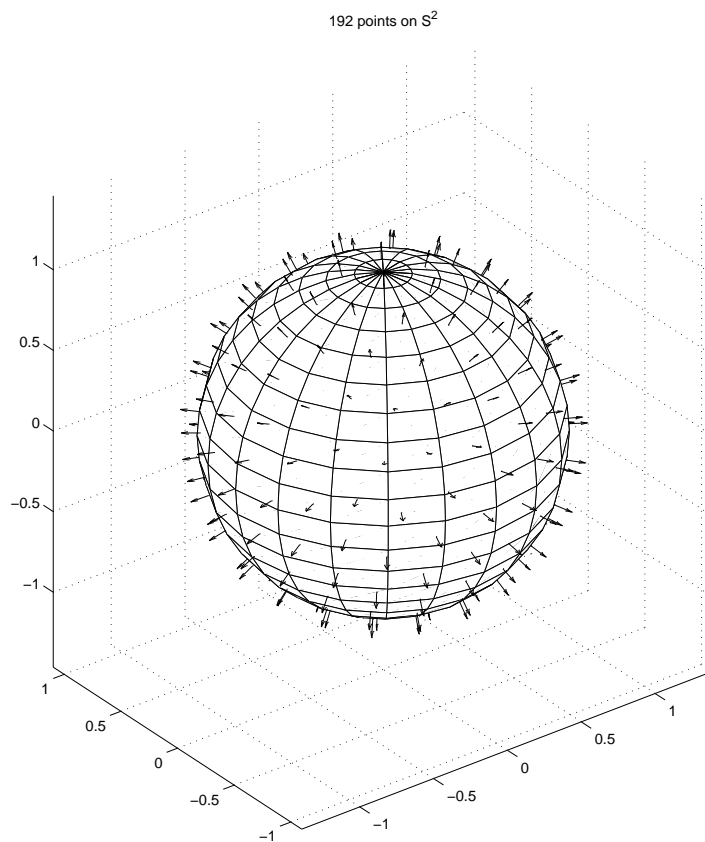


Fig. 1. 192 "equidistributed" points on S^2 .

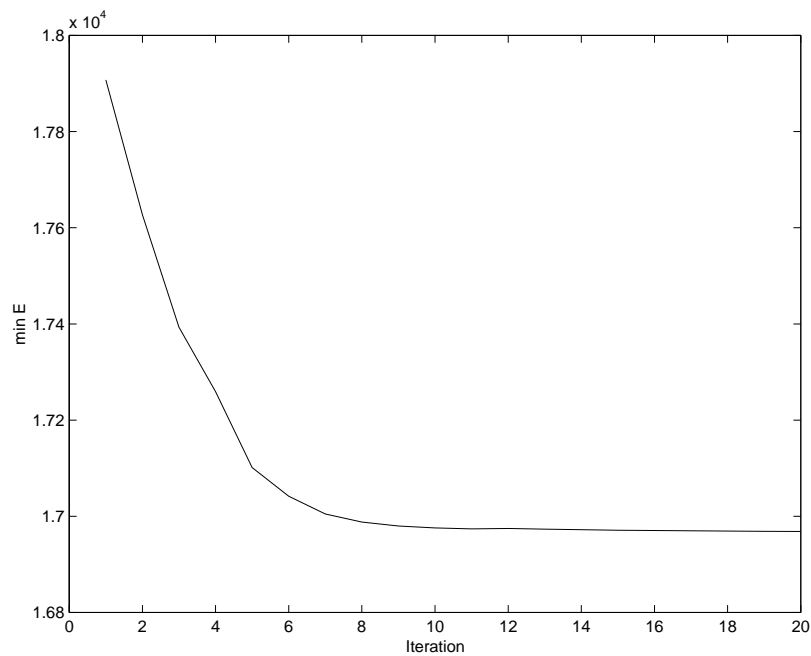


Fig. 2. Minimal potential E after $k = 1, \dots, 20$ iterations (192 points).

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References

1. Anderson, W. L., *geodes* software, Elements Research, Charlotte, NC, Web address: <http://www.netcom.com/~elements/>, 1997.
2. do Carmo, M. P., *Differential Geometry of Curves and Surfaces*, New Jersey, 1976.
3. Fliege, J. and U. Maier, A two-stage approach for computing cubature formulae for the sphere, *Ergebnisberichte Angewandte Mathematik* Nr. 139T, Universität Dortmund, 1996.
4. Gromoll, D., W. Klingenberg, and W. Meyer, *Riemannsche Geometrie im Großen*, Lecture Notes in Mathematics 55, Springer, Berlin, 1967.
5. Hardin, R. H., N. J. A. Sloan, and W. D. Smith, Minimal energy arrangements of points on a sphere, WWW page available in the internet, <http://www.research.att.com/~njas/electrons/index.html>, 1994.
6. Kobayashi, S. and K. Nomizu, *Foundations of Differential Geometry*, vol. I and II, Wiley, New York, 1996.
7. Saff, E. B. and A. B. J. Kuijlaars, Distributing many points on a sphere, *Math. Intelligencer* **19**(1) (1997), 5–11.
8. Steinacker, J., E. Thamm, and U. Maier, Efficient integration of intensity functions on the sphere, *J. Quantitative Spectroscopy and Radiative Transfer* **56**(1) (1996), 97–107.
9. Stoer, J. S., *Einführung in die Numerische Mathematik I*, Springer, Berlin, 1983.
10. Thomson, J. J., *Philos. Mag.* **41** (1921), p. 510.
11. Zhou, Y., *Arrangements of Points on the Sphere*, Ph.D. Thesis, University of South Florida, Tampa, 1995.

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