

Distance geometry on the sphere

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Abstract. The Distance Geometry Problem asks whether a given weighted graph has a realization in a target Euclidean space \mathbb{R}^K which ensures that the Euclidean distance between two realized vertices incident to a same edge is equal to the given edge weight. In this paper we look at the setting where the target space is the surface of the sphere \mathbb{S}^{K-1} . We show that the DGP is almost the same in this setting, as long as the distances are Euclidean. We then generalize a theorem of Gödel about the case where the distances are spherical geodesics, and discuss a method for realizing cliques geodesically on a K -dimensional sphere.

1 Introduction

The Distance Geometry Problem (DGP), discussed at length in the surveys [16, 10, 14], is as follows. Given a positive integer K and a simple undirected graph $G = (V, E)$ weighted by an edge weight function $d : E \rightarrow \mathbb{R}_+$, determine whether there is a realization $x : V \rightarrow \mathbb{R}^K$ such that:

$$\forall \{u, v\} \in E \quad \|x_u - x_v\|_2 = d_{uv}. \quad (1)$$

The DGP is relevant to many applications: determining the shape of proteins from nuclear magnetic resonance data, localizing mobile sensors in wireless networks, designing efficient time synchronization protocols, controlling fleets of unmanned underwater vehicles, and more. It is auxiliary to other problems, such as the control of a multi-joint robotic arm, the rigidity of a bar-and-joint architecture structure, the completion of a matrix so that it is positive semidefinite, the visualization of high-dimensional data points [22].

The aim of this paper is to discuss the DGP on the sphere \mathbb{S}^{K-1} . Specifically, we emphasize two relatively straightforward observations which have a very high impact in realizing graphs on spheres using both Euclidean and geodesic distances, and use them to derive a method for realizing cliques geodesically on a sphere.

^{*} Partly supported by the French national research agency ANR under the “Bip:Bip” project.

^{**} The support of FAPESP and CNPq is gratefully acknowledged.

The DGP problem was shown to be **NP**-hard [24] in \mathbb{R}^K where $K = 1$, by reduction from **PARTITION**, and even for any fixed K with only a handful of edge weight values, by reduction from **3-SATISFIABILITY**. A similar reduction from **PARTITION** was also used to show **NP**-hardness of the subclass consisting of certain Henneberg type 1 graphs, namely graphs with a vertex order ensuring that:

- the first K vertices form a clique;
- every vertex v of rank greater than K in the order is adjacent to the vertices of ranks $v - 1, \dots, v - K$.

This class, also called ^kDMDGP, is relevant in the study of protein conformation [9].

The ^kDMDGP is usually solved using a worst-case exponential time Branch-and-Prune (BP) [12] algorithm, which is precise, reliable and efficient notwithstanding the **NP**-hardness of the problem. It was shown in [17] that the structure of the symmetry group of the partial reflections in the realizations of a given problem instance can be found efficiently. In [11] it was shown that this group can be used to count the number of incongruent realizations of a given ^kDMDGP graph. In [15] the latter result was used to show that the BP is actually Fixed-Parameter Tractable (FPT) on protein graphs, and that the parameter could be fixed at a very low value for all tested proteins. This essentially yields a polynomial time behaviour of the BP when used to realize protein graphs in \mathbb{R}^3 , and explains the efficiency of the BP on these graphs.

Instances from other applications have different structures which can also be exploited. Mobile sensor networks usually have at least two or three “anchors”, i.e. sensors which are actually fixed, and whose position is known; most often, anchor locations are likely to be evenly distributed among the mobile sensors, in order to control load peaks. This appears to have a good numerical effect on Semidefinite Programming (SDP) algorithms when solving an SDP formulation of the DGP [7].

Flexible graphs can be realized using a plethora of heuristic and approximate approaches, some of which are based on local Nonlinear Programming (NLP) solution algorithms [20, 13], and some others on different paradigms, see e.g. [1, 26].

Given the wealth of knowledge on solving the DGP in a Euclidean space \mathbb{R}^K , it would be desirable to be able to extend some of this knowledge to other spaces or manifolds. One specific application-related motivation for looking at the sphere \mathbb{S}^{K-1} is that it is a natural setting for the problem of completing partial correlation or covariance matrices, which arises in the financial sector [25].

2 Realizing cliques in \mathbb{R}^K

The fundamental “building block” for realizing graphs in \mathbb{R}^K are cliques on $K + 1$ vertices. In general, a 1-clique is a vertex, which can be realized in zero

dimensions; a 2-clique is an edge, which can be realized in one dimension; a 3-clique is a triangle, which can be realized in two dimensions, as long as the edge weights satisfy the triangular inequality; a 4-clique is a tetrahedron, which can be realized in three dimensions, as long as the triangular and simplex inequalities are satisfied; larger cliques can be realized as long as the corresponding Cayley-Menger determinant [2, 18], which is proportional to the square of the signed volume, is appropriately signed.

2.1 Recursive realization process

We can obtain a $(K + 1)$ -clique from a K clique by adding a new vertex v to V , and edges of the form $\{u, v\}$ (for $u \in V$) to E . This recursive construction of cliques can be exploited to define a realization algorithm for $(K + 1)$ -cliques in \mathbb{R}^K : number the vertices so that $V = \{v_1, \dots, v_{K+1}\}$, assume (inductively) that the positions for v_1, \dots, v_K in \mathbb{R}^K are known to be x_1, \dots, x_K , and find the position y for v_{K+1} using K -lateration; the induction starts by setting x_1 at the origin.

2.2 K -lateration

The fundamental building block for the algorithm in Sect. 2.1 is the (well known) process of K -lateration is a generalization of trilateration, i.e. the process of computing one of the vertices of a triangle from the two other vertices and the side lengths. Whereas K -lateration is usually applied to realizations in \mathbb{R}^{K-1} [3, 4], we apply it here to \mathbb{R}^K , which requires a further step [8]. We start with the squared distance system:

$$\forall i \leq K \quad \|y - x_i\|_2^2 = d_{i,K+1}^2, \quad (2)$$

where $x_i \in \mathbb{R}^K$ and $d_{i,K+1}$ are known. Eq. (2) is trivially obtained by squaring Eq. (1). We re-write Eq. (2) as follows:

$$\|y\|_2^2 - 2x_1 y = d_{1,K+1}^2 - \|x_1\|_2^2 \quad ([1])$$

$$\vdots$$

$$\|y\|_2^2 - 2x_i y = d_{i,K+1}^2 - \|x_i\|_2^2 \quad ([i])$$

$$\vdots$$

$$\|y\|_2^2 - 2x_K y = d_{K,K+1}^2 - \|x_K\|_2^2 \quad ([K]),$$

where we denote the i -th equation of the system by $[i]$. We can now eliminate the square terms $\|y\|_2^2$ by forming the surrogate system $[i] - [j]$, where j is any given number in $\{1, \dots, K\}$. If we fix $j = K$ without loss of generality, we obtain:

$$2(x_K - x_1) y = d_{1,K+1}^2 - d_{K,K+1}^2 - \|x_1\|_2^2 + \|x_K\|_2^2 \quad ([1] - [K])$$

$$\vdots$$

$$2(x_K - x_{K-1}) y = d_{K-1,K+1}^2 - d_{K,K+1}^2 - \|x_{K-1}\|_2^2 + \|x_K\|_2^2 \quad ([K-1] - [K]),$$

which is a linear system which can be written as $Ay = b$ for appropriate A, b , where A is a $(K - 1) \times K$ matrix, and $b \in \mathbb{R}^K$.

The locus of points for y can be obtained by intersecting the affine space $Ay = b$ and one of the K spheres described by the equations in Eq. (2). Without loss of generality, we again take the K -th sphere:

$$\left. \begin{array}{l} Ay = b \\ \|y - x_K\|^2 = d_{K,K+1}^2 \end{array} \right\} \quad (3)$$

2.3 Assumptions on the rank of A

If A has full rank, then $\text{rk}(A) = K - 1$. Since A has K columns, $Ay = b$ describes a line in \mathbb{R}^K . Hence, the intersection Eq. (3) can either be empty (if the line is disconnected from the sphere), consist of exactly one point (if the line is tangent to the sphere), or consist of two points otherwise. If the application warrants the assumption that solutions do exist (as in the case of proteins), then Eq. (3) has either one or two solutions. If we have no further knowledge of the data at hand, then we can reasonably assume that Eq. (3) has two solutions almost surely.

If $\text{rk}(A) = K - 2$ or less, then $Ay = b$ describes a plane or hyperplane in \mathbb{R}^K . The intersection of a hyperplane with a sphere could be empty, or consist of only one point, or consist of uncountably many points. Since we are realizing a clique, and cliques are not flexible graphs, we can discount the latter possibility. If it consists of only one point, then the realization can be shown to be rigid, but infinitesimally flexible (think e.g. of a “flat triangle” realized in the plane as part of a line, which happens whenever the triangular inequality is satisfied at equality). Since the set of rank deficient $(K - 1) \times K$ matrices has Lebesgue measure zero in the set of all $(K - 1) \times K$ matrices, if we have no further knowledge of the data at hand, we can again reasonably assume that A has full rank almost surely [14].

2.4 Finding the intersection of a line and a sphere

We now assume that A has full rank. We use $Ay = b$ as a dictionary: we identify a $(K - 1) \times (K - 1)$ nonsingular submatrix B of A , and partition the columns of A as $(B|N)$, where N is a single column. For simplicity of notation we identify the columns with their indices, and thus correspondingly partition y into (y_B, y_N) , where y_N , called a *nonbasic variable*, is a single scalar. The linear system $Ay = b$ can therefore be written as $By_B + Ny_N = b$, which allows us to write the *basic variables* y_B in function of the nonbasic y_N :

$$y_B = B^{-1}b - B^{-1}Ny_N. \quad (4)$$

Now we use Eq. (4) to replace y_B in the sphere equation $\|y - x_K\|^2 = d_{K,K+1}^2$ in Eq. (3), and obtain a quadratic equation in the single variable y_N . The discriminant of this equation could be either negative, or zero, or positive. The first case corresponds to Eq. (3) having an empty intersection; the second to

a single intersection point (the line is tangent to the sphere) and the third to two intersection points. In terms of realizing the $(K + 1)$ -st clique vertex, the realization does not exist in the first case, corresponds to a “flat simplex” in the second case (i.e. a simplex which is realized in a lower dimensional space, see Fig. 1, right), or to two possible positions y^+, y^- for x_{K+1} , leading to two possible clique realizations x^+, x^- , which turn out to be reflection of each other w.r.t. the hyperplane spanned by x_1, \dots, x_K (see Fig. 1, left).

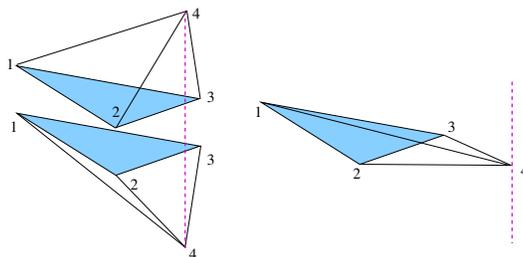


Fig. 1. Two reflected realizations of a 4-clique in \mathbb{R}^3 (left), which may coincide for certain values of the edge weights (right).

2.5 An efficient algorithm

The algorithm for realizing $(K - 1)$ -cliques in \mathbb{R}^K should now be clear: when x_1, \dots, x_K are known, we compute y : if it does not exist, the clique cannot be realized; if there are two distinct points, any of them can be chosen; if they coincide, the realization occurs in an affine lower dimensional subspace. Now x_1, \dots, x_K can be computed recursively, and we set $x_1 = \mathbf{0}$. To make this algorithm deterministic, we can give any rule to choose between the two points for x_{K+1} (for example, we can always choose y_N^+). This is a polynomial time algorithm in K . Note that, in most applications, K is fixed, so we can treat this as an $O(1)$ algorithm.

3 The Branch-and-Prune algorithm

The BP algorithm applies a similar idea to k DMDGP graphs, defined on page 2. The initial K -clique is realized in \mathbb{R}^K in $O(1)$ as per Sect. 2.5. Thereafter, the order ensures that each later vertex v is adjacent to at least its K immediate predecessors. Therefore v can be realized according to Sect. 2.4 in two points x_v^+, x_v^- which are reflections of each other w.r.t. x_{v-1}, \dots, x_{v-K} . We check whether the points x_v^+, x_v^- are feasible with respect to any further edge distance to vertices $u < v - K$, and remove the infeasible ones. We then recurse the process on $v + 1$ on the set of feasible points: we do not recurse at all if neither x^+, x^- are feasible;

we recurse once if only one point is feasible, and we recurse twice if both are feasible. The algorithm terminates when $v = |V|$ [12, 9].

In practice, BP is currently the only algorithm which can find all incongruent solutions to a given κ DMDGP graph. Moreover, it is the fastest, and is also very reliable. It scales up to realize protein backbone graphs tens of thousands of vertices, which it can realize in a few seconds of a common last generation laptop [23].

3.1 Complexity

The BP defines a binary search tree. At level v , this tree contains all possible positions for vertex v . Every path from a leaf to the root defines a possible realization for the input graph. The complexity of the BP algorithm has the following extrema: if the number of calls which yield two feasible points is bounded by a polynomial in the instance size, then the search tree has a bounded tree width, and the BP is a polynomial time algorithm. Otherwise, is it exponential.

Typically, protein graphs have a combinatorial explosion at the beginning of the sequence, say up to the vertex having rank r . Then the folds of the protein ensure the that there are sufficiently many edges in the graph to guarantee that only polynomially many calls determine the feasibility of both points x_v^+, x_v^- at level v . This yields a complexity $O(2^r p(|(G, d)|))$, where p is a polynomial in the size of the input (G, d) , which causes BP to be FPT on a class of graphs which includes all proteins we tested .

3.2 Number of solutions

Since cliques are rigid graphs and κ DMDGP instances consist of sequences of rigidly connected cliques defined by the vertex order, κ DMDGP graphs are rigid. However, in view of the fact that there may be up to two positions for each vertex v in any branch of the BP tree, most κ DMDGP instances do not have unique realizations, but rather a finite set X of possible realizations modulo translations and rotations. We were able to explicitly describe the invariant group of X [17, 21], which is isomorphic to a certain cartesian product of copies of the cyclic group C_2 . We then used it to determine $|X|$ efficiently from the edge set E [11]. It turns out that $|X|$ is always a power of two, as long as the full rank assumptions given in Sect. 2.3 hold.

4 The DGP on the sphere

We now turn to the DGP on the sphere \mathbb{S}^{K-1} , meaning that we constrain any realization x to belong to the surface of the sphere. We first discuss the case where the edge weights are realized as Euclidean distances in \mathbb{S}^{K-1} embedded in \mathbb{R}^K , meaning that each edge is realized as a segment which crosses the interior of the sphere. We then discuss the case where the edge weights are realized as geodesic distances.

4.1 Euclidean distances

In this section we tackle the DGP where x is constrained to belong to the surface of the sphere \mathbb{S}^{K-1} , i.e.:

$$\forall v \in V \quad \|x_v\| = 1. \quad (5)$$

Since realize edges $\{u, v\}$ as segments of Euclidean length d_{uv} , the system in Eq. (1) holds. In particular, K -lateration can be simplified using Eq. (5):

$$\begin{aligned} \forall i \leq K \quad \|y - x_i\|_2^2 &= d_{i,K+1}^2 \\ \Rightarrow \|y\|^2 - 2x_i y + \|x_i\|^2 &= d_{i,K+1}^2 \\ (\text{by Eq. (5) applied to } y, x_i) \quad \Rightarrow \quad 2 - 2x_i y &= d_{i,K+1}^2 \\ \Rightarrow \quad x_i y &= 1 - \frac{1}{2}d_{i,K+1}^2, \end{aligned}$$

which is a linear system $Ay = b$, where A is a square $K \times K$ matrix and $y = x_{K+1}$.

As in Sect. 2.3, we can make assumptions on the rank of A being full, which brings us immediately to a spherical K -lateration process yielding $y = A^{-1}b$, which has a unique solution. Note that the algebraic derivation above holds even if the original system is infeasible, whereas $Ay = b$ always has a unique solution as long as A has full rank. This occurs because the derivation above is necessary but not sufficient, i.e. the linear system $Ay = b$ is implied by Eq. (1) and (5), but does not imply them univocally. For sufficiency, y needs to be verified feasible with respect to Eq. (1) and (5). If so, then y is a possible valid realization of the $(K + 1)$ -st vertex of the clique; otherwise, the input graph is a NO instance of the corresponding DGP.

With the full rank assumption, the difference between K -lateration in \mathbb{R}^K and \mathbb{S}^{K-1} is exactly the same as that between \mathbb{R}^K and \mathbb{R}^{K-1} : in the former case the linear system is undetermined, and describes a line in \mathbb{R}^K , whereas in the latter it only describes a point in \mathbb{R}^{K-1} . Accordingly, in \mathbb{R}^K we need to intersect the line with a sphere of Eq. (1) in order to obtain at most two points, whereas in \mathbb{R}^{K-1} and \mathbb{S}^{K-1} we do not.

In view of Sect. 3, this difference translates to k DMDGP graphs realized in a Euclidean space as follows: if vertices are adjacent to K immediate predecessors but not necessarily $K + 1$, then we have to realize the graph using the BP algorithm, which has a worst-case exponential behaviour, and finds an exponential number of incongruent realizations. If vertices can be guaranteed to be adjacent to at least $K + 1$ immediate predecessors, the BP can be shown to work in polynomial time (in fact, linear in the number of recursion calls, each of which has polynomial complexity in K).

The procedure on the sphere which is analogous to K -lateration in \mathbb{R}^K (yielding exponential behaviour in the BP), is K -lateration in \mathbb{S}^K , embedded in \mathbb{R}^{K+1} . In this setting the system $Ay = b$ derived above is $K \times (K + 1)$, and therefore again describes a line in \mathbb{R}^{K+1} , which must be intersected with one of the spheres in either Eq. (1) or Eq. (5) (the latter giving rise to easier algebraic derivations), in order to obtain at most two points in \mathbb{R}^{K+1} .

4.1 Example

Realizing a tetrahedron on \mathbb{S}^2 with Euclidean distances by K -lateration yields a unique point, whereas realizing a triangle on \mathbb{S}^2 yields at most two points (see Fig. 2). Comparing with \mathbb{R}^3 , it would take the distances to four known points to

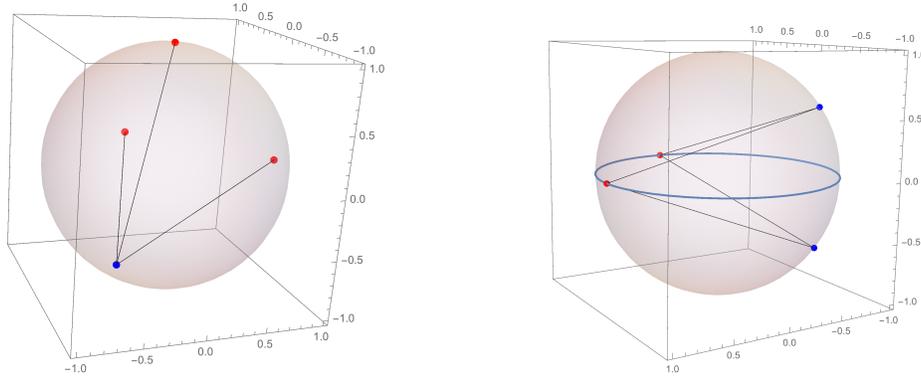


Fig. 2. A tetrahedron in a sphere (left) and two reflected triangles in a sphere (right).

determine the solution for the last point uniquely, whereas the distances to three known points only suffice to determine at most two positions, each of which is a reflection of the other. \square

Summarizing, in order to realize x_{K+1} from x_1, \dots, x_K on \mathbb{S}^{K-1} or \mathbb{S}^K using Euclidean distances, it suffices to remark that the norm constraints $\|x_K\|^2 = 1$ are quadratic constraints which can be used in conjunction with the original DGP system in Eq. (1).

4.2 Geodesic distances

Not many people know that Kurt Gödel performed research in Distance Geometry (DG) in his youth. Two of the talks he gave at Karl Menger's seminar [19] are about DG, and also appear in [5]. Specifically, we are interested in [6], titled *Über die metrische Einbettbarkeit der Quadrupel des R_3 in Kugelflächen*, translated as *On the isometric embeddability of quadruples of points of R_3 in the surface of a sphere*. Apparently, Gödel had been working to solve a question posed by Laura Klanfer in a previous *colloquium*, i.e. whether an affinely independent quadruplet of points in \mathbb{R}^3 can be realized on the surface of a scaling of \mathbb{S}^2 so that the geodesic distances between the realized points have the same length as the Euclidean distances between the given points. Gödel managed to reply in the positive by means of a clever fixed point argument in \mathbb{R}^3 and \mathbb{S}^2 .

In the following, we present a (rather trivial) generalization of Gödel's DG theorem to an arbitrary dimension K . We first remark that, for any $K > 1$,

there is a unique shortest curve, called *geodesic*, between any two points on the surface of \mathbb{S}^K . Moreover, by elementary trigonometry the length c of the chord subtending a geodesic of length α on a sphere of radius $\frac{1}{\rho}$ (for some $\rho > 0$) is given by

$$c_\rho(\alpha) = \frac{2}{\rho} \sin \frac{\alpha\rho}{2}. \quad (6)$$

4.2 Theorem

Any weighted $(K+1)$ -clique $G = (V, E, d)$, where $d : E \rightarrow \mathbb{R}_+$, which is realizable in \mathbb{R}^K but not in \mathbb{R}^{K-1} , can also be realized on $r\mathbb{S}^{K-1}$ (for some radius $r > 0$) with geodesic distances.

Proof. Let $x = (x_1, \dots, x_{K+1})$ be an affinely independent realization of G in \mathbb{R}^K , and let \bar{r} be the radius of the sphere circumscribing the realization x (there is a unique sphere in \mathbb{R}^K whose surface contains $K+1$ given affinely independent points). Without loss of generality, we translate x so that the circumscribed sphere $\bar{r}\mathbb{S}^{K-1}$ is centered at the origin.

The idea is now to deform this sphere into a family $S(r) = r\mathbb{S}^{K-1}$ of spheres of continuously decreasing radius r , which also deforms the realization x to a continuous map of realizations on $S(r)$, until we find a value r^* which makes the lengths of the geodesics on $S(r^*)$ equal to the lengths of the chords in $S(\bar{r})$. The nontrivial part of the argument shows that such an r^* exists. Its existence will be implied by a fixed point argument on an appropriate function of the inverse ρ of the radius r .

Let $\tau(\rho)$ be the realization on $S(r)$ mapped from x as r decreases. More precisely, we let $\tau(\rho)$ be the realization of G with edges weighted by the function $c_\rho(d)$, meaning that the weight of the edge $\{u, v\} \in E$ is $c_\rho(d_{uv})$. We now define $\phi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ so that $\frac{1}{\phi(\rho)}$ is the radius of the sphere circumscribed about $\tau(\rho)$.

The parameter ρ is a measure of “how close the sphere is to being flat”: it is easy to see that, as ρ tends to zero, r tends to infinity (yielding a sphere with zero curvature, where the chord and the geodesic lengths are equal), which means that $c_\rho(d_{uv})$ tends to d_{uv} for all edges $\{u, v\} \in E$. This implies that $\tau(\rho)$ tends to the realization x of G in \mathbb{R}^K . Since x exists, we can define $\tau(0) = x$ and $\phi(0) = 1/\bar{r}$.

We now claim that ϕ has a fixed point in the open interval $I = (0, \pi/\alpha)$, where $\alpha = \max_{\{u, v\} \in E} d_{uv}$ (see Lemma 4.3 for the proof). So let ρ^* be the fixed point of ϕ , namely $\phi(\rho^*) = \rho^*$. What this means is that $r^* = \frac{1}{\rho^*}$ is the radius of the sphere circumscribed about $\tau(\rho^*)$. In turn, $\tau(\rho^*)$ is a realization of G where the edges are weighted by the length of the chords subtending geodesics of length d_{uv} (for all $\{u, v\} \in E$) with respect to a radius r^* . A moment’s reflection on this long sentence should convince the reader that this is the same as saying that $\tau(\rho^*)$ is a realization of G on the surface of a sphere $r^*\mathbb{S}^{K-1}$ where the edges are realized as geodesics of length d_{uv} . \square

4.3 Lemma

The function ϕ defined in the proof of Thm. 4.2 has a fixed point in the open interval $I = (0, \pi/\alpha)$, where α is the maximum edge weight of the given clique graph G .

Proof. First notice that $\tau(\rho)$ is defined in terms of c_ρ , and c_ρ is continuous over α for each $\rho > 0$ by definition (see Eq. (6)). Note that $\tau(0)$ exists since it is equal to x by definition. Since $\tau(\rho)$ is defined as the realization of G weighted by $c_\rho(d)$ over a sphere of radius $1/\rho$, τ is a continuous map in some open interval $J = (0, \varepsilon)$ for some $\varepsilon > 0$, since 0 is in the closure of J . Therefore $\bar{\rho} = \max\{\rho \in I \mid \tau(\rho) \text{ is defined}\}$ exists by continuity of τ . We look at two mutually exclusive cases: $\bar{\rho} = \pi/\alpha$ and $\bar{\rho} < \pi/\alpha$.

- (i) If $\bar{\rho} = \pi/\alpha$, then $\tau(\bar{\rho})$ is defined and its longest edge has length $c_{\bar{\rho}}(\alpha) = \frac{2\alpha}{\pi}$. Hence the radius of the sphere circumscribed around $\tau(\bar{\rho})$ is greater than $c_{\bar{\rho}}(\alpha)/2$, i.e. greater than $\alpha/\pi = 1/\bar{\rho}$, which implies $\phi(\bar{\rho}) < \bar{\rho}$. On the other hand, we have $\phi(0) = 1/\bar{r} > 0$, so the intermediate value theorem ensures that $\exists \rho^* \in (0, \bar{\rho})$ such that $\phi(\rho^*) = \rho^*$.
- (ii) Assume now $\bar{\rho} < \pi/\alpha$, and suppose that $\tau(\bar{\rho})$ is an affinely independent realization in \mathbb{R}^K . Then, for each $\tilde{\rho}$ in an arbitrary small neighbourhood around $\bar{\rho}$, $\tau(\tilde{\rho})$ must exist by continuity; then there must be some $\tilde{\rho} > \bar{\rho}$ where $\tau(\tilde{\rho})$ is defined, which contradicts the maximality of $\bar{\rho}$. So the realization $\tau(\bar{\rho})$ is affinely dependent, which means that its circumscribed sphere is flat, i.e. that $\phi(\bar{\rho}) = 0 < \bar{\rho}$. Together with $\phi(0) = 1/\bar{r} > 0$, this shows that there is $\rho^* < \pi/\alpha$ such that $\phi(\rho^*) = \rho^*$, which concludes the lemma. \square

4.3 Putting it all together

The results of Sect. 4.1 and Sect. 4.2 yield a method for realizing cliques in \mathbb{S}^{K-1} with geodesic distances: first realize the clique on a sphere using Euclidean distances, then solve the fixed point equations $\phi(\rho) = \rho$ and obtain a value of ρ^* numerically. This can then be used to compute the correct geodesic realization $\tau(\rho)$ (see Fig. 3).

5 Conclusion

This paper emphasizes two relatively easy observations about extending the considerable theoretical developments of the DGP to the setting of a spherical surface. The first observation applies to Euclidean distances, and amounts to noticing that the unit norm constraint can be exploited together with the DGP constraints. The second observation concerns geodesic distances, and yields an extension to \mathbb{S}^{K-1} of a result of Gödel's in \mathbb{S}^2 . The two observations yield a method for realizing cliques on a sphere with geodesic distances.

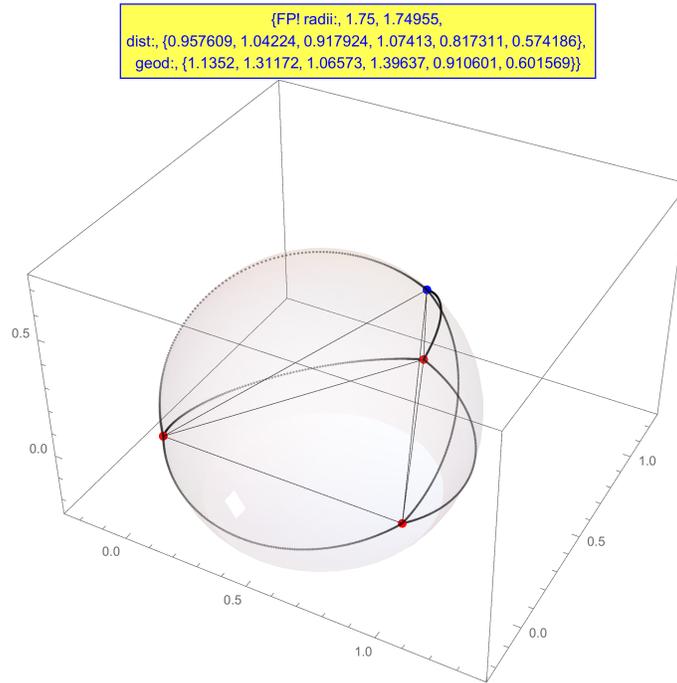


Fig. 3. Gödel's theorem yields a method for computing geodesic realizations. This picture shows the fixed point.

References

1. Agrafiotis, D., Bandyopadhyay, D., Young, E.: Stochastic proximity embedding (SPE): A simple, fast and scalable algorithm for solving the distance geometry problem. In: Mucherino et al. [22]
2. Cayley, A.: A theorem in the geometry of position. *Cambridge Mathematical Journal II*, 267–271 (1841)
3. Dong, Q., Wu, Z.: A geometric build-up algorithm for solving the molecular distance geometry problem with sparse distance data. *Journal of Global Optimization* 26, 321–333 (2003)
4. Eren, T., Goldenberg, D., Whiteley, W., Yang, Y., Morse, A., Anderson, B., Belhumeur, P.: Rigidity, computation, and randomization in network localization. *IEEE Infocom Proceedings* pp. 2673–2684 (2004)
5. Feferman, S., Dawson, J., Kleene, S., Moore, G., Solovay, R., van Heijenoort, J. (eds.): *Kurt Gödel: Collected Works, vol. I*. Oxford University Press, Oxford (1986)
6. Gödel, K.: On the isometric embeddability of quadruples of points of r_3 in the surface of a sphere. In: Feferman et al. [5], pp. (1933b) 276–279
7. Krislock, N., Wolkowicz, H.: Explicit sensor network localization using semidefinite representations and facial reductions. *SIAM Journal on Optimization* 20, 2679–2708 (2010)

8. Lavor, C., Lee, J., Lee-St. John, A., Liberti, L., Mucherino, A., Sviridenko, M.: Discretization orders for distance geometry problems. *Optimization Letters* 6, 783–796 (2012)
9. Lavor, C., Liberti, L., Maculan, N., Mucherino, A.: The discretizable molecular distance geometry problem. *Computational Optimization and Applications* 52, 115–146 (2012)
10. Lavor, C., Liberti, L., Maculan, N., Mucherino, A.: Recent advances on the discretizable molecular distance geometry problem. *European Journal of Operational Research* 219, 698–706 (2012)
11. Liberti, L., Lavor, C., Alencar, J., Abud, G.: Counting the number of solutions of k DMDGP instances. In: Nielsen, F., Barbaresco, F. (eds.) *Geometric Science of Information*. LNCS, vol. 8085, pp. 224–230. Springer, New York (2013)
12. Liberti, L., Lavor, C., Maculan, N.: A branch-and-prune algorithm for the molecular distance geometry problem. *International Transactions in Operational Research* 15, 1–17 (2008)
13. Liberti, L., Lavor, C., Maculan, N., Marinelli, F.: Double variable neighbourhood search with smoothing for the molecular distance geometry problem. *Journal of Global Optimization* 43, 207–218 (2009)
14. Liberti, L., Lavor, C., Maculan, N., Mucherino, A.: Euclidean distance geometry and applications. *SIAM Review* 56(1), 3–69 (2014)
15. Liberti, L., Lavor, C., Mucherino, A.: The discretizable molecular distance geometry problem seems easier on proteins. In: Mucherino et al. [22]
16. Liberti, L., Lavor, C., Mucherino, A., Maculan, N.: Molecular distance geometry methods: from continuous to discrete. *International Transactions in Operational Research* 18, 33–51 (2010)
17. Liberti, L., Masson, B., Lavor, C., Lee, J., Mucherino, A.: On the number of realizations of certain Henneberg graphs arising in protein conformation. *Discrete Applied Mathematics* 165, 213–232 (2014)
18. Menger, K.: New foundation of Euclidean geometry. *American Journal of Mathematics* 53(4), 721–745 (1931)
19. Menger, K. (ed.): *Ergebnisse eines Mathematischen Kolloquiums*. Springer, Wien (1998)
20. Moré, J., Wu, Z.: Global continuation for distance geometry problems. *SIAM Journal of Optimization* 7(3), 814–846 (1997)
21. Mucherino, A., Lavor, C., Liberti, L.: Exploiting symmetry properties of the discretizable molecular distance geometry problem. *Journal of Bioinformatics and Computational Biology* 10, 1242009(1–15) (2012)
22. Mucherino, A., Lavor, C., Liberti, L., Maculan, N. (eds.): *Distance Geometry: Theory, Methods, and Applications*. Springer, New York (2013)
23. Mucherino, A., Lavor, C., Liberti, L., Talbi, E.G.: A parallel version of the branch & prune algorithm for the molecular distance geometry problem. In: *ACS/IEEE International Conference on Computer Systems and Applications (AICCSA10)*. pp. 1–6. IEEE, Hammamet, Tunisia (2010)
24. Saxe, J.: Embeddability of weighted graphs in k -space is strongly NP-hard. *Proceedings of 17th Allerton Conference in Communications, Control and Computing* pp. 480–489 (1979)
25. van der Schans, M., Boer, A.: A heuristic for completing covariance and correlation matrices. *Tech. Rep. 2013-01, ORTEC Finance* (2013)
26. Tenenbaum, J., de Silva, V., Langford, J.: A global geometric framework for nonlinear dimensionality reduction. *Science* 290, 2319–2322 (2000)