Discretizable Distance Geometry

Getting started

Let $G = (V, E, d)$ be a simple weighted undirected graph representing an instance of the Distance Geometry Problem (DGP) in dimension 3. In the following exercises, our focus will be on instances of the DGP consisting of exact distances only. When this is the case, we can say that the graph G represents an instance of the Discretizable DGP (DDGP) if and only if, by definition, there exists a vertex order for the vertices of G such that

A1 The first 3 vertices in the order from a clique;

A2 $\forall v \in V \ : \ v > K, \quad \exists\, u_1, u_2, u_3 \ :$

$$\begin{array}{ll} \textbf{A2.1} & u_1 < v,\ u_2 < v,\ u_3 < v, \\ \textbf{A2.2} & \{(u_1, v), (u_2, v), (u_3, v)\} \subset E, \\ \textbf{A2.3} & A(u_1, u_2, u_3) > 0, \end{array}$$

where A is the area of a possible triangle realizing the vertices u_1, u_2 and u_3 so that the distances in the clique are satisfied [3, 4]. The vertex order allowing for the discretization is named *discretization order* [1, 2]. Our analysis will be restricted to discretization orders that are total orders.

The assumptions of the DDGP make it possible to discretize the search domain of the DGP represented by the graph G. In fact, assumption **A1** allows us to fix the positions of the first 3 vertices in the vertex order, avoiding this way to generate the solutions that can be obtained by rotations, translations and total reflections of other solutions. Assumption **A2** ensures that, for every vertex v that does not belong to the initial clique, at least 3 vertices exist that can play the role of "reference" for v. In particular, assumption **A2.1** ensures that all vertices u_j (for $j \in \{1, 2, 3\}$) always precede v in the ordering, while assumption **A2.2** ensures that the distance between every vertex u_j and v is known. Finally, assumption **A2.3** ensures that the vertices u_j are not aligned (notice however that this last assumption can fail to be satisfied with probability 0). Under these assumptions, the search space is reduced to a tree, which can be explored by employing a branch-and-prune (BP) algorithm.

A *total order* for V is a sequence $r : \mathbb{N} \to V \cup \{0\}$ with length $|r| \in \mathbb{N}$ (for which $r_i = 0$ for all $i > |r|$) such that, for each $v \in V$, there is an index $i \in \mathbb{N}$ for which $r_i = v$. Given an order, r_i represents the vertex of V having rank i in the ordering. Let $\alpha(r_i)$ be the counter of adjacent predecessors of r_i, for each $r_i \in V$, that is:

$$\alpha(r_i) = \mathrm{card}\{(u, v) \in E \,|\, \exists j \in \mathbb{N} : u = r_j,\ v = r_i \text{ and } j < i\}.$$

In terms of α, a discretization order in dimension 3 is an order r for which

$$\begin{array}{ll} \textbf{C1} & G[\{r_1, r_2, r_3\}] \text{ is a clique}, \\ \textbf{C2} & \forall i > 3,\ \alpha(r_i) \geq 3, \end{array}$$

where $G[\cdot]$ is the subgraph induced by a subset of vertices in V. Notice that we suppose that assumption **A2.3** is always satisfied.

Greedy algorithm for identifying discretization (input: G, K; output: r)

find a 3-clique C in the graph G
let $n = 0$
for (each vertex $v \in C$, in any internal order) **do**
  let n++
  let $r_n = v$
end for
for ($i = n+1, \ldots, |V|$) **do**
  let $W = V \setminus \bigcup_{j=1}^{i-1} \{r_j\}$
  let $u = \arg\max_{v \in W} \alpha(v)$
  if ($\alpha(u) \geq 3$) **then**
    let $r_i = u$
  else
    abort: no order exists with initial clique C
  end if
end for

Exercise 1

Suppose we replace the discretization assumption **A2** with the following assumption:

B2 $\forall v \in V \;:\; v > K$,

B2.2 $\{(v-3,v),(v-2,v),(v-1,v)\} \subset E$,
B2.3 $A(v-3,v-2,v-1) > 0$.

What impact has this change on the discretization order? Which is the strongest assumption, the assumption **A2** or the assumption **B2**? Find a small instance of the DGP in dimension 3 for which either **A2** or **B2** is satisfied, while the other is not.

Exercise 2

Given G in dimension 3, what is the minimal cardinality for E that is necessary for V to admit a discretization order?

1. Express this minimal cardinality in function of the cardinality n of V.
2. Give an example where the cardinality of E is the minimal one but the instance is not discretizable.

Exercise 3

Given the two graphs G_1 and G_2 below, verify whether they represent instances of the DDGP in dimension 2 (it is not necessary to verify explicitly whether assumption **A2.3** is satisfied or not). In case some of them do not belong to the DDGP class, verify whether there exists a different order for the vertices of the corresponding graph for which the discretization assumptions are satisfied. The details about the two graphs follow:

$$G_1 = (V_1, E_1) : \quad |V_1| = 4, \quad E_1 = \{(1,2),(1,4),(2,3),(2,4),(3,4)\},$$
$$G_2 = (V_2, E_2) : \quad |V_2| = 4, \quad E_2 = \{(1,2),(2,3),(2,4),(3,4)\}.$$

Draw the two graphs by taking the vertices in the appropriate order.

Exercise 4

Apply the greedy algorithm for finding a discretization order for the following graph $G = (V, E)$ in dimension 2:

$$|V| = 6, \quad E = \{(1,2),(1,3),(1,6),(2,3),(3,4),(3,5),(3,6),(4,5),(4,6),(5,6)\}.$$

Exercise 5

Given the graph $G = (V, E)$:

vertex	adjacent vertices
1	2 3 7
2	1 3 4 5 7
3	1 2 5 7
4	2 5 6 7
5	2 3 4 6 7
6	4 5 7
7	1 2 3 4 5 6

verify whether the current vertex ordering allows for the discretization in dimension 3. If not, apply the greedy algorithm for reordering the vertices of the graph. Select as initial clique the triplet $(2,3,5)$ and find one possible discretization order. Then, try again with the clique $(5,6,7)$. In the two obtained orders, how many times, for a given vertex, there are more than 3 reference vertices?

References

[1] D.S. Gonçalves, A. Mucherino, *Optimal Partial Discretization Orders for Discretizable Distance Geometry*, International Transactions in Operational Research **23**(5), 947–967, 2016.

[2] C. Lavor, J. Lee, A. Lee-St.John, L. Liberti, A. Mucherino, M. Sviridenko, *Discretization Orders for Distance Geometry Problems*, Optimization Letters **6**(4), 783–796, 2012.

[3] L. Liberti, C. Lavor, N. Maculan, A. Mucherino, *Euclidean Distance Geometry and Applications*, SIAM Review **56**(1), 3–69, 2014.

[4] A. Mucherino, C. Lavor, L. Liberti, *The Discretizable Distance Geometry Problem*, Optimization Letters **6**(8), 1671–1686, 2012.