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New methods for the Distance Geometry Problem

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Abstract

Given an integer K and a simple edge-weighted undirected graph $G = (V, E)$, the Distance Geometry Problem questions the existence of a vertex realization function $V \to \mathbb{R}^K$ such that each vertex pair adjacent to an edge is placed at a distance which is equal to the edge weight. This problem has many applications to science and engineering, and many methods have been proposed to solve it. We propose some new formulation-based methods.

Keywords: DGP, Semidefinite Programming, Diagonally dominant matrices.

1 Introduction

The problem studied in this paper is the

Distance Geometry Problem (DGP). Given an integer $K \geq 1$ and a simple, edge-weighted, undirected graph $G = (V, E, d)$, where $d : E \to \mathbb{R}_+$, verify the existence of a vertex *realization* function $x : V \to \mathbb{R}^K$ such that:

$$\forall \{i, j\} \in E \quad \|x_i - x_j\| = d_{ij}. \tag{1}$$

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A recent survey on the DGP with the Euclidean norm is given in [2]. The DGP is **NP**-hard, by reduction from PARTITION. Three well-known applications are to clock synchronization ($K = 1$), sensor network localization ($K = 2$), and protein conformation ($K = 3$). A related problem, the DISTANCE MATRIX COMPLETION PROBLEM (DMCP), asks whether a partially defined matrix can be completed to a distance matrix. The difference is that while K is part of the input in the DGP, it is part of the output in the DMCP, in that a realization into *any* Euclidean space which allows the computation of the missing distances provides a certificate. It is remarkable that, by virtue of this seemingly minor difference, it is not known whether the Euclidean DMCP (EDMCP) is in **P** or **NP**-hard. It is currently thought to be "between the two classes".

In this short paper we sketch several new formulation-based methods for solving the DGP.

2 MILP formulations for 1- and ∞-norms

To the best of our knowledge, no method for solving DGPs with the 1- and ∞-norm currently exists.[3] Yet, since both norms can be linearized exactly, it is not difficult to derive Mixed-Integer Linear Programming (MILP) formulations for either. We first re-write Eq. (1) as follows:

$$\min_x \sum_{\{i,j\}\in E} |\, \|x_i - x_j\|_\ell - d_{ij}\,|, \tag{2}$$

for $\ell \in \{1, \infty\}$. Then, for $\ell = 1$ we write:

$$\min_x \sum_{\{i,j\}\in E} \left| \sum_{k\le K} |x_{ik} - x_{jk}| - d_{ij} \right|,$$

and equivalently for $\ell = \infty$. For $\ell = 1$, we apply some standard absolute value reformulations to obtain a MILP. The case $\ell = \infty$ is slightly more involved, but still easy to model. These formulations can be solved using any off-the-shelf MILP solver.

[3] We shall gladly take corrections to this statement!