The Referenced Vertex Order Problem : Recent Advances and Future Works

Antonio Mucherino and Jérémy Omer

IRISA, INSA, University of Rennes 1, Rennes, France

jeremy.omer@insa-rennes.fr

antonio.mucherino@irisa.fr

Mots-clés : *Vertex orders, distance geometry, Revorder.*

Given a simple undirected graph $G = (V, E)$, a positive integer K and a subset S of V with cardinality at least K, the Referenced Vertex Order (Revorder) problem asks whether a vertex order $\sigma : V \to \{1, 2, \ldots, |V|\}$ exists such that $\sigma^{-1}(S) = \{1, 2, \ldots, |S|\}$ and every vertex $v \notin S$ admits at least K predecessors in the given order σ [12]. The Revorder may appear, at first sight, to be similar to classical scheduling but it is essentially different. We have, first of all, no orientation on the edges, so that the relationship "predecessor" vs. "successor" between two given vertices u and v is not a priori given. Moreover, there is a minimal number of predecessors that every vertex $v \notin S$ must have in the order, but more predecessors are allowed. The initial set S of vertices defining the beginning of the order σ plays an important role for the construction of the remaining part, because they are the initial potential predecessors for the first vertices of the order among those that are not in S.

Our interest in the Revorder has began when it was found out that it is an important preprocessing step for the solution of a particular subclass of instances of the Distance Geometry Problem (DGP) [4], whose search space can be subject to a discretization process [10]. In this case, K is the dimension of the Euclidean space where the DGP solutions are embedded, and there is an additional requirement for the the initial set S : its vertices need to form a clique of G. It's the choice of this initial clique, therefore, that sets the basis for the definition of the order σ, and it was observed empirically that several orders satisfying the Revorder assumptions can be defined for real life instances [5]. We focus here only on the DGP for lack of space, but we point out that this is not the only use of the Revorder [12].

For a given DGP instance, the greedy algorithm proposed in [4] is able to find, when it exists, one suitable vertex order for each possible choice of the initial clique. This algorithm was subsequently extended to graphs G having uncertain real weights (represented by intervals instead of singletons) in [8]. For a certain time, people working on the Revorder [1] believed that the inclusion of another constraint, named the *consecutivity assumption*, would have made the basic Revorder problem NP-hard for all dimensions K [1]. It was shown subsequently, however, that the NP-hardness holds only for dimension $K = 1$, whereas there exists a simple polynomial algorithm that is able to find Revorders with the additional requirement that the consecutivity assumption is satisfied [6] when working in dimension $K > 1$. However, we believe that those orders have no practical use, and that other approaches should instead to be taken into consideration in the applications.

The consecutivity assumption basically requires that the K references for every $v \in V$ with $\sigma(v) > K$ have their ranks in the set $\{\sigma(v) - K, \sigma(v) - K + 1, \ldots, \sigma(v) - 1\}$. Even if not strictly necessary for performing the discretization [10], this additional requirement can imply some interesting properties on the resulting search tree [7]. For this reason, a lot of attention has been given to this particular case. The use of linear programming was for example intensively

1. The authors of those articles do not refer to the problem as the "Revorder" because it was formally defined thereafter, but we now know that the problems they considered are instances of the Revorder.

investigated ; the interested reader can make reference to [11] and [2]. An alternative approach based on the definition of a de-Brujin graph was instead proposed in [9].

It was empirically observed that several orders, for a given DGP instance, are able to satisfy the required assumptions. For this reason, part of the recent works on the REVORDER have been focusing on the idea of selecting, among the different feasible orders, those that are able to optimize some criteria, such as the number of nodes composing the search tree. We refer to such orders as "optimal vertex orders", and we point out that finding such orders is always NP-hard [12]. In [3], the greedy algorithm mentioned above was extended in order to find approximated solutions. More recently, in [12], a branch-and-bound algorithm was proposed for performing a more efficient exploration of the space of feasible orders.

This extended abstract is not meant to give an exhaustive survey on the REVORDER, but only to mention to the main research lines around this problem. Current research is exploring the possibility to optimize alternative criteria in the definition of optimal vertex orders, with the main aim of selecting orders implying search domains that can be more easily explored by our current solvers for the DGP.

Références

[1] A. Cassioli, O. Günlük, C. Lavor, L. Liberti, *Discretization Vertex Orders in Distance Geometry*, Discrete Applied Mathematics **197**, 27–41, 2015.

[2] C. D'Ambrosio, L. Liberti, *Distance Geometry in Linearizable Norms*, Lecture Notes in Computer Science **10589**, F. Nielsen, F. Barbaresco (Eds.), Proceedings of Geometric Side of Information (GSI17), Paris, 830–837, 2017.

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

[4] 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.

[5] C. Lavor, L. Liberti, A. Mucherino, *The interval Branch-and-Prune Algorithm for the Discretizable Molecular Distance Geometry Problem with Inexact Distances*, Journal of Global Optimization **56**(3), 855–871, 2013.

[6] C. Lavor, M. Souza, L.M. Carvalho, L. Liberti, *On the Polynomiality of Finding ^{K}DMDGP re-orders*, Discrete Applied Mathematics **267**, 190–194, 2019.

[7] L. Liberti, B. Masson, J. Lee, C. Lavor, A. Mucherino, *On the Number of Realizations of Certain Henneberg Graphs arising in Protein Conformation*, Discrete Applied Mathematics **165**, 213–232, 2014.

[8] A. Mucherino, *On the Identification of Discretization Orders for Distance Geometry with Intervals*, Lecture Notes in Computer Science **8085**, F. Nielsen and F. Barbaresco (Eds.), Proceedings of Geometric Science of Information (GSI13), Paris, France, 231–238, 2013.

[9] A. Mucherino, *A Pseudo de Bruijn Graph Representation for Discretization Orders for Distance Geometry*, Lecture Notes in Computer Science **9043**, Lecture Notes in Bioinformatics series, F. Ortuño and I. Rojas (Eds.), Proceedings of the 3^{rd} International Work-Conference on Bioinformatics and Biomedical Engineering (IWBBIO15), Granada, Spain, 514–523, 2015.

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

[11] J. Omer, D.S. Gonçalves, *An Integer Programming Approach for the Search of Discretization Orders in Distance Geometry Problems*, Optimization Letters **14**(2), 439–452, 2020.

[12] J. Omer, A. Mucherino, *The Referenced Vertex Ordering Problem : Theory, Applications and Solution Methods*, Open Journal of Mathematical Optimization **2**, article no. 6, 29 pages, 2021.