On the complexity of discretization vertex orders for distance geometry problems.

PGMO's Days 2013

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a joint work with

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Outline

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2. DGP instances can be represented as graphs.
3. Under suitable assumptions the feasible set becomes finite and discrete.
4. A key point of the *discretization* is the availability of a suitable vertex order.

Distance Geometry Problem (DGP)

Given

- $K > 0$;
- a simple, undirected, nonnegatively weighted graph $G = (V, E)$;
- a function $d : E \to \mathbb{R}^+$;

find a realization $x : V \to \mathbb{R}^K$ such that:

$$\forall \{u, v\} \in E \quad \|x_u - x_v\|^2 = d_{uv}.$$

Vertex Order (VO)

Given a graph $G = (V, E)$, a total vertex order can be seen as

- a vertex permutation;
- a function (labeling) $\rho : V \to \mathbb{N}$ that induces a total order on V;

Applications: scheduling, labeling-based algorithm,...

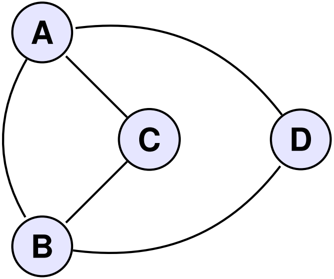
Assumptions and Notation

- we focus on **simple, connected and undirected** graphs;
- **adjacent vertices**: $N_v = \{w \in V : (v, w) \in E\}$
- **predecessor set**: $U_v = \{w \in V : w < v\}$
- we investigate the problem of determining the **existence of discretization vertex orders**

^{K}DDGP Order Definition

A ^{K}DDGP order for $G, K > 0$ is defined as follows:

- $\{v \in V | v \leq K\}$ is a $K-$clique;
- $\forall v \in V$ with $v > K, |U_v \cap N_v| \geq K$.

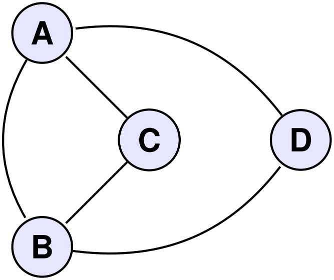


^{K}DDGP Orders for $K = 2$: ABCD, ABDC, ACBD,...

^{K}DMDGP Order Definition

A ^{K}DMDGP order for $G, K > 0$ is defined as follows:

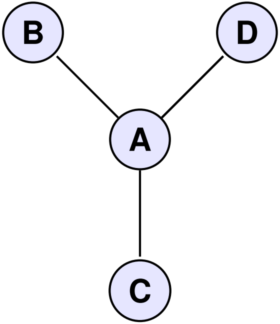
- $\{v \in V | v \leq K\}$ is a $K-$clique;
- $\forall v \in V$ with $v > K, v - K \leq w < v$ then $w \in N_v$.



^{K}DMDGP Orders for $K = 2$: DBAC, CBAD,...

^{K}DDGPO$\equiv{}^{K}$DMDGPO ?

Some graphs are YES for ^{K}DDGPO but NO for ^{K}DMDGPO:



The $S(K, n)$ family

We define for $K > 0$ and $n \leq K + 3$ a family of graphs $S(K, n)$ with n vertices $\{1, 2, \ldots, n\}$ and edges

$$\{\{u, v\} | u < v \leq K\} \cup \{\{u, v\} | u \leq K \vee v > K\}$$

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(in the previous slide $S(1, 4)$ is depicted.)

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(in the previous slide $S(1, 4)$ is depicted.)

Lemma

For a positive integer K and $n \geq K + 3$, no graph $S(K, n)$ can have a ^{K}DMDGP order.

^{K}DDGPO Properties

- DDGPO is trivially in *NP*;
- for fixed K a polynomial time algorithm exists [1].

[1] Lavor, C., Lee, J., Lee-St. John, A., Liberti, L., Mucherino, A., Sviridenko, M.: Discretization orders for distance geometry problems. Optimization Letters (2012)

^{K}DDGPO Properties

- DDGPO is trivially in *NP*;
- for fixed *K* a polynomial time algorithm exists [1].

Proposition

[1] *DDGPO is equivalent to Spanning-Tree on an undirected simple graph.*

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^{K}DDGPO Problem

Proposition

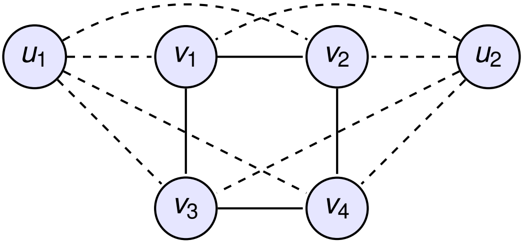
The ^{K}DDGPO problem is **NP***-complete.*

The proof uses a reduction from $K-$Clique problem.

^{K}DDGPO Problem – Reduction

Given $G = (V, E)$ we construct a ^{K}DDGPO instance G' using the following mapping:

- $V' = V \cup U$ with $U = \{u_1, u_2, \ldots, u_K\}, U \cap V = \emptyset$;
- $E' = E \cup \{(u, v) : v \in V \vee u \in U\}$

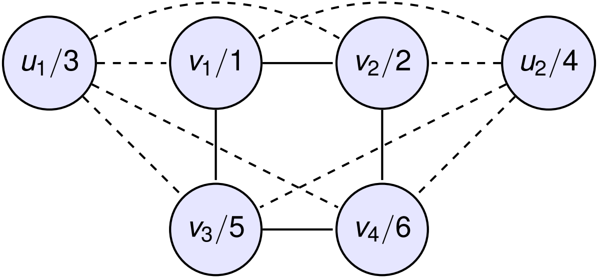


G' for $K = 2$

^{K}DDGPO Problem – Reduction

Let $\{v_1, \ldots, v_K\}$ be a K-clique in G. Then we can construct a ^{K}DDGPO:

1. postponing any permutation of U;
2. adding greedly vertices in $V \setminus \{v_1, \ldots, v_K\}$.



^{K}DDGPO Problem – Reduction

Let assume G is NO for K-clique but YES for ^{K}DDGPO.

1. the initial $K-$clique must contain one vertex w from U and $K-1$ from V.

2. the $K+1th$ vertex z cannot be in U because it is connected to w.
3. z is connected to all the other vertices of the initial K-clique.

Therefore G contains a $K-$clique and we got a contraddiction. Thus the reduction maps YES to YES.

^{K}DMDGPO Problem

- It is trivially in **NP**.

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- ^{K}DMDGPO is **NP**-complete.
- A ^{K}DMDGPO order is symmetric
- A graph G is YES for ^{K}DMDGPO only if it is for ^{K}DDGPO.

^{K}DMDGPO Problem

Proposition

The ^{1}DMDGPO is **NP***-complete.*

Proof.

The definition of ^{1}DMDGPO is equivalent of that HP.

□

^{K}DMDGPO Problem

Theorem

The ^{K}DMDGPO is **NP***-complete for any* $K > 1$

Proof idea:

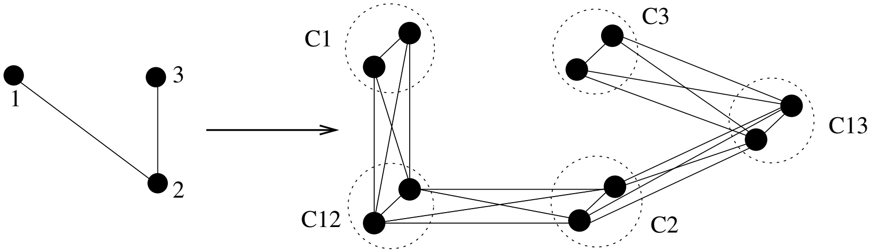
- consider a restriction with given initial $K-$clique (rDMDGPO);
- reduce from Hamiltonian Path with a given starting vertex (rHP);
- repeat for all possible $K-$cliques.

rDMDGPO Problem – Reduction

Given $G = (V, E)$ we construct a rDMDGPO instance G' using the following mapping τ_K:

- a $K-$clique C_v for all $v \in V$
- a $K-$clique C_{ij} for each $(i, j) \in E$
- edges to have bicliques C_{ij}, C_i and C_{ij}, C_j for each $(i, j) \in E$

rDMDGPO Problem – Reduction



Transformation τ_2

rDMDGPO Problem – Preliminary Results (1)

Lemma

Let $(G = (V, E)\,, s)$ be a YES instance of rHP, and $K > 1$. Then $G' = \tau_K(G)$ has a consecutive ^{K}DMDGP order starting with C_s.

Proof.

Let $\beta = \{v_1, \dots, v_{|V|}\}$ a HP in G with $s \equiv v_1$, which corresponds to the clique order

$$\gamma = \{C_1, C_{12}, C_2, \dots\}.$$

Taking $C_i = \{u_{i1}, \dots, u_{iK}\}$ and expanding the cliques we get

$$\alpha = \{u_{11}, \dots, u_{1K}, u_{121}, \dots, u_{12K}, u_{21}, \dots, u_{2K}, \dots\},$$

which is a ^{K}*DMDGP* order in G'.

rDMDGPO Problem – Preliminary Results (2)

Lemma

Let $(G = (V, E)\ , s)$ *be an instance of rHP,* $K > 1$*, and* α *be a* ^{K}*DMDGP order in* $G' = \tau_K(G)$*. Then G is a YES instance for rHP.*

Proof.

If α spans the cliques of G' sequentially then $\tau^{-1}(\alpha)$ is a HP in G. By Lemma .. □

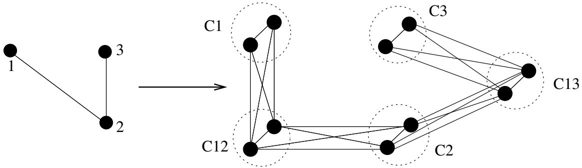
rDMDGPO Problem – Preliminary Results (3)

Lemma

Let C_1, C_2, C_3 be three $K-$cliques in $G' = \tau_K(G)$. There is no vertex triplet $v_1 \in C_1, v_2 \in C_2, v_3 \in C_3$ inducing a triangle in G'.

Proof.

Idea: only cliques of different types are connected on G', i.e. a triangle cannot be *closed*.



^{K}DMDGPO Problem

Theorem

The ^{K}DMDGPO is **NP***-complete for any* $K > 1$

Proof.

By the first two lemmata τ_K maps YES/NO instances to YES/NO instances between rHP and rDMDGPO. Then we can reduce rDMDGPO to ^{K}DMDGPO dropping the initial $K-$clique. □

^{K}DMDGPO ILP Formulation

$$\text{find } x \in \{0,1\}^{|V|\times|V|}$$

$$\sum_{i=1}^{|V|} x_{vi} = 1 \qquad \forall v \in V$$

$$\sum_{v \in V} x_{vi} = 1 \qquad \forall i \in \{1,\ldots,|V|\}$$

$$\sum_{u \in N_v} \sum_{j<i} x_{uj} \geq i x_{vi} \qquad \forall i \in \{1,\ldots,K\}$$

$$\sum_{u \in N_v} \sum_{i-K \leq j < i} x_{uj} \geq K x_{vi} \qquad \forall i > K, \forall v \in V$$

Computational Results (1)

5 random instances for $K \in \{1, 2, 3\}$ with 1 hour cpu time limit with CPLEX 12.5.

$\|V\|$	10%	20%
10	5/0.2/1.676/4.06	5/0.1/1.186/3.22
20	5/20.43/104.578/207.72	5/7.13/116.242/232.02
30	2/7.46/767.415/1527.37	1/2294.5/2294.5/2294.5
40	0/-/-/-	0/-/-/-
50	0/-/-/-	0/-/-/-
60	0/-/-/-	0/-/-/-
70	0/-/-/-	0/-/-/-
80	0/-/-/-	0/-/-/-
90	0/-/-/-	0/-/-/-
100	0/-/-/-	0/-/-/-

Computational Results (2)

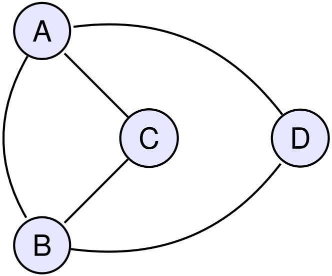
5 random instances for $K \in \{1, 2, 3\}$ with 1 hour cpu time limit with CPLEX 12.5.

$\lvert V \rvert$	50%	90%
10	5/0.02/0.094/0.14	5/0.02/0.022/0.03
20	5 / 4.43/15.998/38.77	5/0.1/0.194/0.3
30	5/109.25/351.612/829.44	5/0.29/0.606/1.03
40	1/1960.15/1960.15/1960.15	5/0.84/1.21/1.96
50	2/2244.54/2403.365/2562.19	5/1.62/4.098/6.54
60	0/-/-/-	5/3.52/8.586/17.87
70	0/-/-/-	5/7.4/17.708/28.75
80	0/-/-/-	5/20.94/31.368/52.05
90	0/-/-/-	5/38.96/57.918/78.25
100	0/-/-/-	5/69.85/132.258/165.43

^{K}DMDGPO ILP Formulation – Extensions (1)

Let π be any total order on V. Then, by the symmetry of any ^{K}DMDGP order it holds that

$$x_{\pi(w)0} \leq x_{\pi(v)|V|} \quad \forall v, w : \pi(v) < \pi(w)$$



$CBAD \equiv DABC$ (π as alphabetical order...)

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- $N_v \geq K$ for all $v \in V$;
- for $i \in \{K, \ldots, 2K-1\}$ it must hold that

$$|\{v \in V : |N_v| = i\}| \leq 2(i - K + 1);$$

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$$|\{v \in V : |N_v| = i\}| \leq 2(i - K + 1);$$

- a least K $(K + 1)$-cliques in G;
- G YES for the ^{K}DDGPO;

^{K}DMDGPO ILP Formulation – Extensions (2)

Let $\bar{C}_K$ the set of $K-$cliques for which a ^{K}DDGPO can be found. Let $y_c, w_c \in \{0,1\}$ indicates whether the clique c is used to start or end the order, respectively.

$$\sum_{i=1,\dots,K} \sum_{v \in c} x_{vi} \geq K y_c \qquad \forall c \in \bar{C}_K$$

$$\sum_{i=|V|-K,\dots,|V|} \sum_{v \in c} x_{vi} \geq K w_c \qquad \forall c \in \bar{C}_K$$

$$\sum_{c \in \bar{C}_K} y_c = \sum_{c \in \bar{C}_K} w_c = 1$$

$$y_c + w_c \leq 1 \qquad \forall c \in \bar{C}_K$$

^{K}DMDGPO ILP Formulation – Extensions (3)

Assuming $|V| \geq 2K$, we can ask that the first and last cliques to be disjoint. Let

$$\bar{C}_K(l) = \{w \in \bar{C}_k : l \cap w = \emptyset\}.$$

Then the following constraints hold:

$$\sum_{t \in C_K(l)} w_t \geq y_c \qquad \forall c \in \bar{C}_K$$

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Conclusions

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2. we proof ^{K}DMDGPO to be **NP**-complete for any fixed $K > 0$.
3. we provide an infinity family of instances that are YES for ^{K}DDGPO but NO for ^{K}DMDGPO.

Future Directions

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Thank You! Questions??