A new algorithm for a class of DGP[1]

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joint work with: M. Souza, L. M. Carvalho, C. Lavor, L. Liberti

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[1]Partially supported by CNPq and CAPES/PrInt/UFSC

Distance Geometry problem

DGP

Given a simple undirected graph $G = (V, E)$, a distance function $d : E \to \mathbb{R}_+$ and an integer $K > 0$, the Distance Geometry Problem (DGP) consists in finding (if possible) a *realization* $x : V \to \mathbb{R}^K$ such that

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

For an incomplete set of distances:

- $K = 1$, NP-complete (subset sum)
- Saxe (1979), NP-Hard for $K > 1$

A global optimization problem

$$\min_{X \in \mathbb{R}^{KN}} f(X) \equiv \sum_{\{u,v\} \in E} \left(\|x_u - x_v\|^2 - d_{uv}^2 \right)^2$$

X^* is a realization iff $f(X^*) = 0$.

Proposed approaches:

- general-purpose global optimization methods, heuristics
- (Moré, Wu, 1997) **DGSOL**, homotopy continuation method
- (Reams et al., 1999) **APA**, alternating projection
- (N. Krislock, H. Wolkowicz, 2010) **SDP** formulation
- (Lavor, Liberti, Maculan, Mucherino, 2012) **Discrete** formulation

K-laterative graphs

There exists an order $(<)$ on V ensuring:

1. An initial $(K+1)$-clique
2. For each $v > K+1$, there are at least $K+1$ adjacent predecessors

Geometric build-up (Dong, Wu, **J. Global Optim., 26**, 2003)

$$
\begin{aligned}
\|x_k - x_1\| &= d_{k,1},\\
\|x_k - x_2\| &= d_{k,2},\\
\|x_k - x_3\| &= d_{k,3},\\
\|x_k - x_4\| &= d_{k,4}.
\end{aligned}
$$

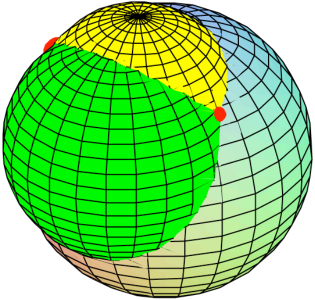
$$Ax = b,$$

$$A = \begin{bmatrix} (x_1 - x_2)^\top \\ (x_1 - x_3)^\top \\ (x_1 - x_4)^\top \end{bmatrix}$$

* coordinates obtained in $O(N)$.

$(K-1)$-laterative graphs

C. Lavor, L. Liberti, N. Maculan, A. Mucherino, **Comput. Optim. Appl., 52** (2012)



$$
\begin{aligned}
\|x_{i-1} - x_i\|^2 &= d_{i-1,i}^2 \\
\|x_{i-2} - x_i\|^2 &= d_{i-2,i}^2 \\
\|x_{i-3} - x_i\|^2 &= d_{i-3,i}^2
\end{aligned}
$$

Assumption. Initial K-clique, $\forall v > K$ there are at least K adjacent predecessors (whose realization vectors are affine independent).

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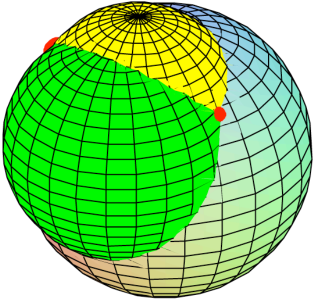

$$\begin{aligned} \|x_{i-1} - x_i\|^2 &= d^2_{i-1,i} \\ \|x_{i-2} - x_i\|^2 &= d^2_{i-2,i} \\ \|x_{i-3} - x_i\|^2 &= d^2_{i-3,i} \end{aligned}$$

No solution

Assumption. Initial K-clique, $\forall v > K$ there are at least K adjacent predecessors (whose realization vectors are affine independent).

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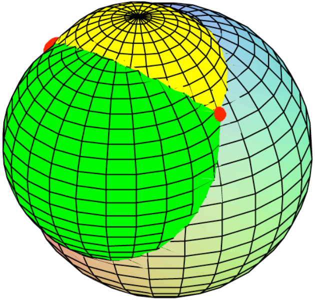

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No solution

One solution

Assumption. Initial K-clique, $\forall v > K$ there are at least K adjacent predecessors (whose realization vectors are affine independent).

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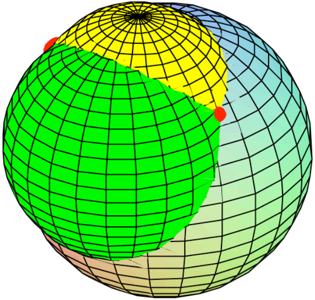

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No solution

One solution

Two solutions

Assumption. Initial K-clique, $\forall v > K$ there are at least K adjacent predecessors (whose realization vectors are affine independent).

$(K-1)$-laterative graphs

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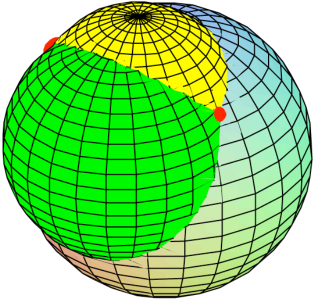

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\end{aligned}
$$

No solution

One solution

Two solutions

Infinite solutions

Assumption. Initial K-clique, $\forall v > K$ there are at least K adjacent predecessors (whose realization vectors are affine independent).

$(K-1)$-laterative graphs

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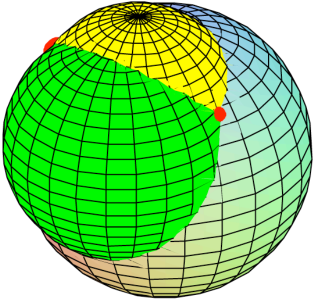

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~~No solution~~

One solution

Two solutions

~~Infinite solutions~~

Assumption. Initial K-clique, $\forall v > K$ there are at least K adjacent predecessors (whose realization vectors are affine independent).

Discretizable Molecular Distance Geometry Problem

Definition(DMDGP)

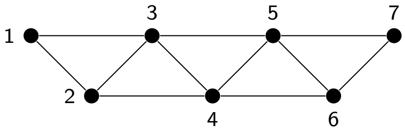
Formally, we say that a DGP instance (G, d, K) is a Discretizable Molecular Distance Geometry Problem if there exists a vertex order $(v_1, \ldots, v_n)$ such that

(a) $G[\{v_1, v_2, \ldots, v_K\}]$ is complete;

(b) $\forall i \in \{K+1, \ldots, |V|\}$:

1. $\forall j \in \{i-1, i-2, \ldots, i-K\} : \{v_j, v_i\} \in E$,
2. $CM(\{v_{i-K}, \ldots, v_{i-1}\})^2 > 0$,

- Assumptions ensure a chain of $(K+1)$-cliques.

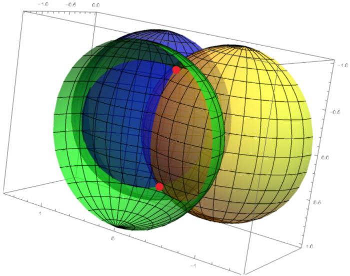


$(K = 2)$

Exact distances: a branch-and-prune approach

By DMDGP assumptions we have that coordinates x_i for each vertex v_i are obtained by intersecting K spheres:

$$
\begin{aligned}
\|x_{i-1} - x_i\|^2 &= d_{i-1,i}^2 \\
\|x_{i-2} - x_i\|^2 &= d_{i-2,i}^2 \\
&\vdots \\
\|x_{i-K} - x_i\|^2 &= d_{i-K,i}^2
\end{aligned}
$$



which leads to at most 2 candidate positions **(branching)**.

Pruning: Direct Distance Feasibility(DDF)

$$|\|x_h - x_i\| - d_{hi}| < \epsilon, \quad \forall h : \{h, i\} \in E \text{ and } h < i - K$$

(Lavor et al., **Comp. Optim. App., 52**, 2012)

BP Algorithm

Algorithm 1 BP

BP(i, n, G, x) *# $(i > K)$*

if $(i > n)$ **then**

  return x

else

  Find solutions $\{x_i^+, x_i^-\}$ for: $\|x_\ell - x_i\|^2 = d_{\ell,i}^2, \ell = i - K, \ldots, i - 1.$

  if x_i^+ is feasible **then**

    Set $x_i = x_i^+$ and call BP$(i + 1, n, G, x)$. *# 1st candidate position*

  end if

  if x_i^- is feasible **then**

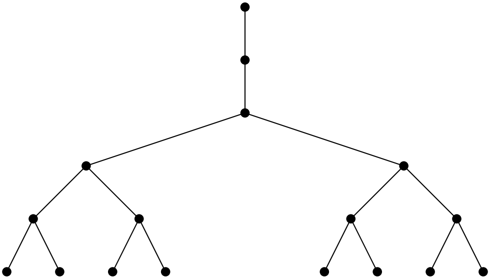
    Set $x_i = x_i^-$ and call BP$(i + 1, n, G, x)$. *# 2nd candidate position*

  end if

end if

Branch-and-Prune

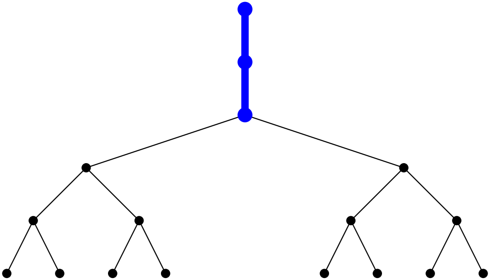
Discrete search space: binary tree



Pruning distances: $$|\|x_h - x_i\| - d_{hi}| < \epsilon, \quad \forall (h,i) \in E, h < i$$

Branch-and-Prune

Discrete search space: binary tree



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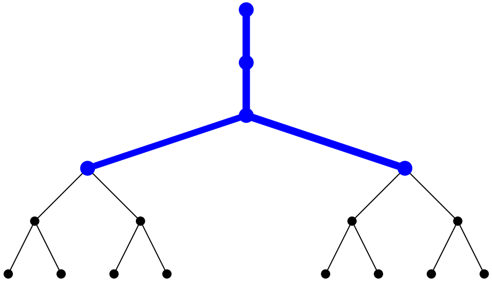

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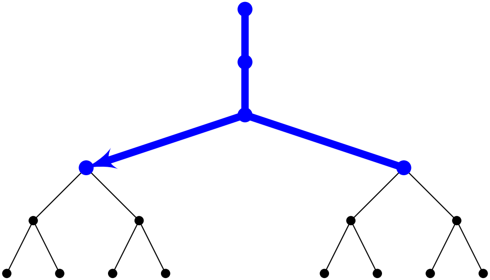

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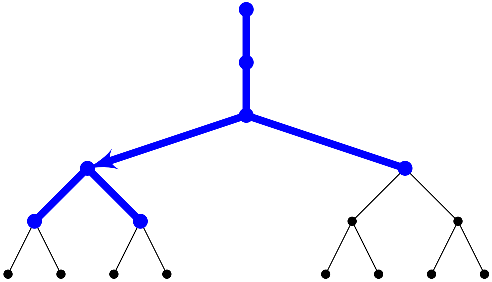

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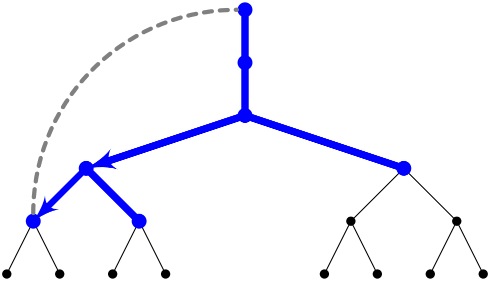

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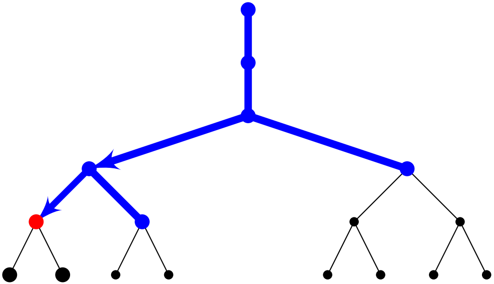

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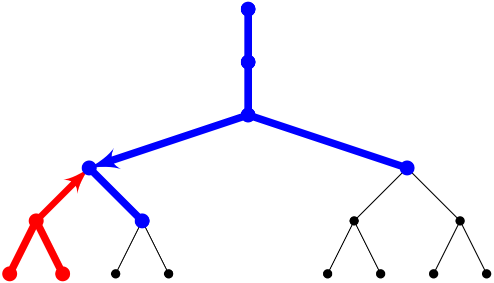

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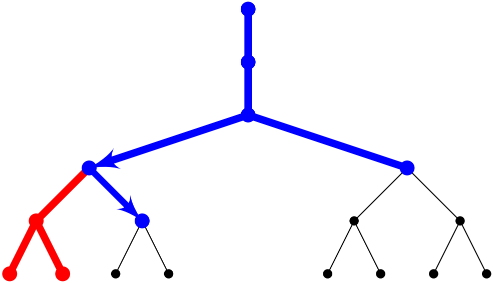

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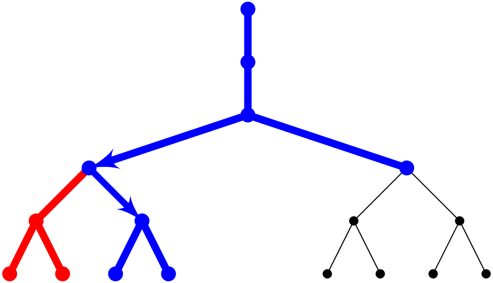

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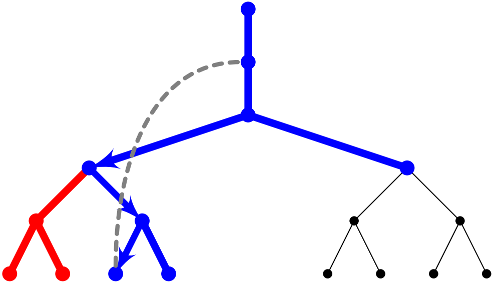

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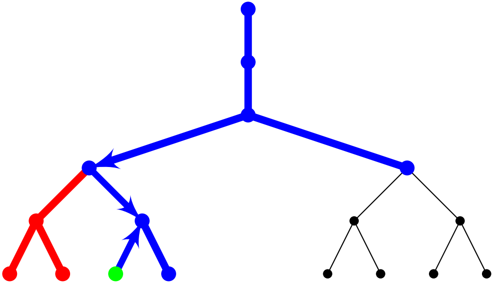

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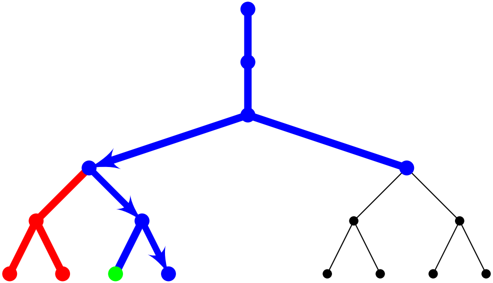

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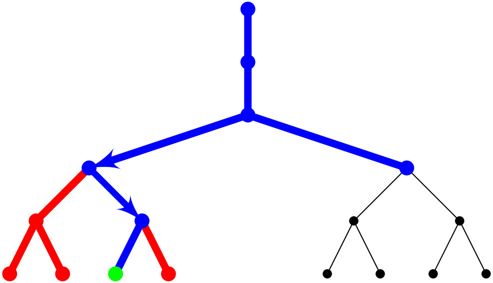

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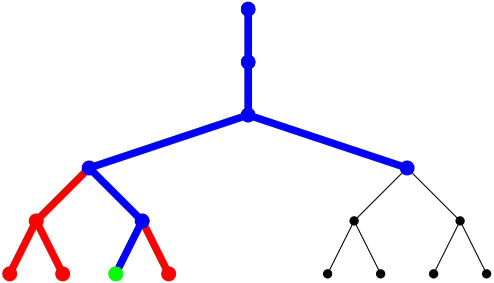

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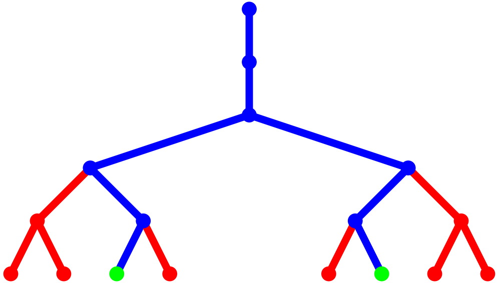

Pruning distances: $\quad |\|x_h - x_i\| - d_{hi}| < \epsilon, \quad \forall (h,i) \in E, h < i$

Numerical experiments

C. Lavor, L. Liberti, N. Maculan, A. Mucherino, **Comput. Optim. Appl., 52** (2012)

Instance			*BP-One*		*BP-All*		*DGSOL*	
Name	n	$\|E\|$	*CPU*	*LDE*	*CPU*	*#Sol*	*CPU*	*LDE*
1brv	57	476	0.00	1.54e-14	0.00	1	1.48	2.74e-01
1aqr	120	929	0.00	1.86e-09	0.00	2	7.77	4.88e-01
1ahl	147	1205	0.00	1.50e-09	0.00	8	6.95	1.46e-01
1brz	159	1394	0.00	3.53e-13	0.00	2	11.39	4.66e-01
1f39a	303	2660	0.00	2.68e-12	0.00	1	37.24	2.80e-01
1acz	324	3060	0.00	3.15e-12	0.02	4	35.97	3.97e-01
1mbn	459	4599	0.00	1.36e-09	0.00	1	124.24	4.46e-01
1rgs	792	7626	0.00	4.22e-13	0.01	1	237.93	4.69e-01
1bpm	1443	14292	0.02	2.85e-13	0.02	1	398.29	5.06e-01
1mqq	2032	19564	0.02	4.90e-12	0.06	1	451.58	5.40e-01
3b34	2790	29188	0.07	1.17e-11	0.07	1	940.95	6.47e-01
2e7z	2907	42098	0.08	4.26e-12	0.09	1	915.39	6.40e-01
1epw	3861	35028	0.16	3.19e-12	0.25	1	2037.86	4.92e-01

Numerical experiments

C. Lavor, L. Liberti, N. Maculan, A. Mucherino, **Comput. Optim. Appl., 52** (2012)

Instance			*BP-One*		*BP-All*		*SDP-based*	
Name	n	$\|E\|$	*CPU*	*LDE*	*CPU*	*#Sol*	*CPU*	*LDE*
1brv	57	476	0.00	1.54e-14	0.00	1	0.03	1.24e-14
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1f39a	303	2660	0.00	2.68e-12	0.00	1	0.12	3.91e-13
1acz	324	3060	0.00	3.15e-12	0.02	4	0.13	3.04e-13
1mbn	459	4599	0.00	1.36e-09	0.00	1	0.22	9.67e-14
1rgs	792	7626	0.00	4.22e-13	0.01	1	0.42	1.58e-13
1bpm	1443	14292	0.02	2.85e-13	0.02	1	0.76	7.73e-13
1mqq	2032	19564	0.02	4.90e-12	0.06	1	1.22	6.17e-13
3b34	2790	29188	0.07	1.17e-11	0.07	1	1.68	3.00e-13
2e7z	2907	42098	0.08	4.26e-12	0.09	1	1.88	2.88e-13
1epw	3861	35028	0.16	3.19e-12	0.25	1	2.31	1.45e-12

Partial reflections

Notation:

- $E = E_D \cup E_P$
- $X := X(G) \neq \varnothing$ is the solution set of a DMDGP instance (G, K)
- $\hat{X}$ denotes the set of realizations considering E_D only.
- For $x \in \hat{X}$ and $i > K$, $R_x^i(y)$ is the reflection of $y \in \mathbb{R}^K$ through the plane containing x_{i-1}, $x_{i-2}, \ldots, x_{i-K}$.
- For all $i > K$, we defined partial reflection operators:

$$g_i(x) = (x_1, x_2, \ldots, x_{i-1}, R_x^i(x_i), R_x^i(x_{i+1}), \ldots, R_x^i(x_n)).$$

Partial reflections

Useful properties:

1. $\|R_x^i(y) - x_j\| = \|y - x_j\|, \forall j \in \{i-K, \ldots, i-1\}$.

2. All pairwise distances for $x_{i-K}, \ldots, x_{i-1}, x_i, \ldots, x_n$ from $x \in \hat{X}$ are preserved in $g_i(x)$.

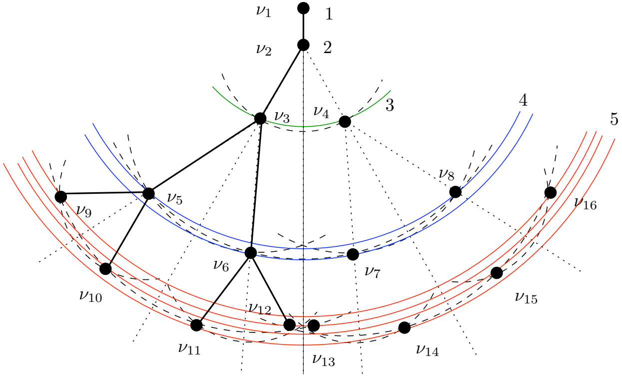
3. Partial reflections preserve distances related to discretization edges E_D, so that $g_i(x) \in \hat{X}$, for every $x \in \hat{X}$.

4. All realizations in $\hat{X}$ can be generated from a single $x \in \hat{X}$ by the composition of partial reflection operators g_i.

Partial reflections

Theorem 1 (Liberti et al., 2014)

With probability 1, for all $j > K + i$, there is a set H^{ij} of 2^{j-i-K} real positive values such that for each $x \in \hat{X}$, we have $\|x_j - x_i\| \in H^{ij}$. Furthermore, for all $x', x \in \hat{X}$ such that $x' \neq x$ and $x'_t = x_t$, for $t \leq i + K - 1$, $\|x_j - x_i\| = \|x'_j - x_i\|$ if and only if $x'_j = R_x^{i+K}(x_j)$.



Symmetry vertices

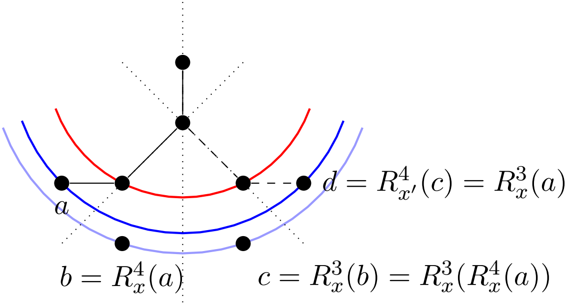
Symmetry vertices set:

$$S := \{v_\ell \in V \mid \nexists \{v_i, v_j\} \in E \text{ with } i + K < \ell \leq j\}.$$

Theorem 2

Let (G, K) be a feasible ^{K}DMDGP and S its set of symmetry vertices. Then, with probability 1, $|X| = 2^{|S|}$.

Corollary: If $\{v_1, v_n\} \in E$, then $|X| = 2$.



Reformulation

Given $x \in \hat{X}$, the DMDGP consists in finding a binary vector $s \in \{0,1\}^{n-K}$, such that

$$x(s) = U(x,s) := g_{K+1}^{s_1} \circ \cdots \circ g_n^{s_{n-K}}(x)$$

satisfies $||x_i(s) - x_j(s)|| = d_{ij}$, for all $\{i,j\} \in E = E_D \cup E_P$.

Lemma 3 (Other solutions)

Let $x(s)$ be a valid realization for (G,K). For every

$$s' \in B := \{s' \in \{0,1\}^{n-K} \mid s'_\ell = s_\ell \text{ if } v_{K+\ell} \notin S\},$$

$x(s') \in X$.

Pruning edges and sequence of subproblems

New Idea: Given $x \in \hat{X}$, include/handle one pruning edge at a time

- We assume an order for the edges in E_P
- The set of pruning edges preceding edge $\{i, j\}$:

$$P^{ij} := \{\{u, w\} \in E_P \mid \{u, w\} < \{i, j\}\}.$$

Subproblem: Find x such that $\|x_i - x_j\| = d_{ij}$,
subject to $\|x_u - x_w\| = d_{uw}, \forall \{u, w\} \in E_D \cup P^{ij}$.

Definition (Subproblem spanned by pruning edge)

Let (G, K) be a feasible ${}^K DMDGP$ with $G = (V, E, d)$. Let $G^{ij} = (V, E^{ij}, d_{|E^{ij}})$, where $E^{ij} = E_D \cup P^{ij} \cup \{i, j\}$, $\{i, j\} \in E_P$ and $d_{|E^{ij}}$ is the restriction of d to E^{ij}.

Remark: If $X \neq \varnothing$ and $\{u, w\} < \{i, j\}$, then $X(G^{uw}) \supset X(G^{ij})$.

Necessary symmetry vertices

- Let $s \in \{0,1\}^{n-K}$ such that $x(s)$ is valid for (G^{uw}, K), $\forall \{u,w\} \in P^{ij}$.
- The set of necessary symmetry vertices for subproblem (G^{ij}, K):

$$S^{ij} = \{v_\ell \in \{v_{i+K+1}, \ldots, v_j\} \mid \nexists \{u,w\} \in P^{ij}, u + K < \ell \leq w\}.$$

Reduced search space: the search space for the new $s' \in \{0,1\}^{n-K}$ is further reduced to

$$s' \in B^{ij} := \{s' \in \{0,1\}^{n-K} \mid s'_\ell = s_\ell \text{ if } v_{i+K+\ell} \notin S^{ij}\}.$$

Lemma 4

Let $S^{ij} \neq \emptyset$, $e_{k+1} = \{i,j\} > \{u,w\} = e_k$ and $x(s)$ be a valid realization for (G^{uw}, K). For every $s' \in B^{ij}$, $x(s') \in X(G^{uw})$.

Uniqueness of $s' \in B^{ij}$

1. If (G, K) is a ^{K}DMDGP instance, so is $(G[v_i, \ldots, v_j], K)$, for $j > K + i$.

2. Any DMDGP instance $(G[v_i, \ldots, v_j], K)$ spanned by $\{v_i, v_j\} \in E_P$ has only two solutions.

3. These two solutions correspond to a particular configuration of the components $s'_{i+K}, \ldots, s'_j$.

4. The only difference between the two is the first component s'_{i+K}.

5. Since $v_{i+K} \notin S^{ij}$ and the components of s'_ℓ with $\ell \leq i + K$ or $\ell > j$ are kept fixed, we conclude that $s' \in B^{ij}$ is unique.

New algorithm

Algorithm 2 New BP

NewBP$(G, K, (e_1, \dots, e_m), x \in \hat{X})$
Set $s = 0$, $x(0) = x$
for $k = 1, 2, \dots, m$ **do**
  $\{i, j\} = e_k$
  if $|S^{ij}| > 0$ **then**
    Find $s' \in B^{ij} \ : \ \|x_i(s') - x_j(s')\| = d_{ij}$
    Update $s = s'$ and $x(s) = U(x, s)$
  end if
end for
return a valid realization $x(s)$

Correctness

Proposition: Let $x(s)$ be a valid realization for (G^{uw}, K), for all $\{u, w\} \in P^{ij}$. If $S^{ij} = \varnothing$, then $x(s)$ is valid for (G^{ij}, K).

Theorem 5

Let (G, K) be a feasible ^{K}DMDGP instance. Considering exact arithmetic, Algorithm 2 finds $x \in X$.

Proof Sketch. Since $x(0) = x \in \hat{X}$, due to $x(s') \in X(G^{uw}), \forall s' \in B^{ij}$ and $X \neq \varnothing$, Step 6 is well-defined. Then, from the exhaustive search in Step 6, it follows that $x(s') \in X(G^{ij})$, for every $e_k = \{i, j\}$. □

Computational experiments

- Artificial instances generated from PDB: consider only the backbone $N - C_\alpha - C$, distances are included either when the atoms are separated by at most three covalent bonds or the distance between pairs of atoms is smaller than a certain cut-off value.
- The natural backbone order for instances generated in this way provides a vertex order satisfying the DMDGP assumptions.
- Quality measure: Mean Distance Error (MDE):

$$MDE(X,E,d) = \frac{1}{|E|} \sum_{\{i,j\} \in E} \frac{|\, \|x_i - x_j\|_2 - d_{ij} \,|}{d_{ij}}.$$

Remarks

- $|S^{ij}|$ is a good indicator of the computational cost for solving subproblem (G^{ij}, K). **Total work**:

$$W := \sum_{\{i,j\} \in \hat{E}} 2^{|S^{ij}|},$$

where $\hat{E} = \{\{v_i, v_j\} \in E_P \mid |S^{ij}| > 0\}$.

- Maximum work per subproblem: $\bar{W} = \max_{\hat{E}} 2^{|S^{ij}|}$.
- $|S^{ij}|$ depends on the order in which the pruning edges are handled
- Our codes and datasets: https://github.com/michaelsouza/sbbu
- classic Branch-and-Prune: https://github.com/mucherino/mdjeep

Results: cut-off 6 Å

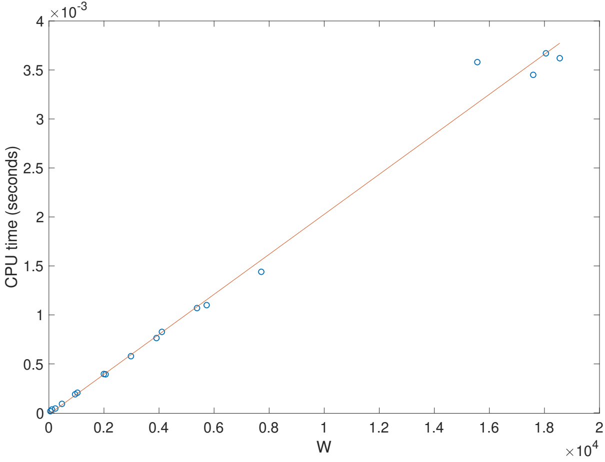
			BP		New BP				
ID	$\lvert V\rvert$	$\lvert E\rvert$	Time	MDE	Time	MDE	$\bar{W}_{ij}$	W	Speed-up
1N6T	30	236	7.60E-05	8.32E-05	1.77E-05	2.72E-12	2	52	4.29
1FW5	60	558	1.30E-04	1.51E-05	3.51E-05	4.22E-12	2	112	3.70
1ADX	120	1008	2.10E-04	5.62E-12	4.49E-05	3.78E-12	2	232	4.67
1BDO	241	2167	4.10E-04	3.79E-12	9.24E-05	1.39E-11	2	474	4.44
1ALL	480	4932	8.40E-04	8.91E-13	1.90E-04	3.80E-12	2	952	4.42
6S61	522	5298	8.70E-04	6.50E-13	2.06E-04	3.09E-12	2	1036	4.23
1FHL	1002	9811	2.00E-03	6.82E-12	3.97E-04	1.93E-11	2	1996	5.04
4WUA	1033	9727	1.80E-03	1.47E-11	3.94E-04	7.73E-12	8	2060	4.57
6CZF	1494	14163	2.60E-03	1.33E-12	5.79E-04	4.18E-12	2	2980	4.49
5IJN	1950	18266	3.40E-03	1.37E-12	7.64E-04	1.76E-11	16	3908	4.45
6RN2	2052	19919	3.70E-03	1.11E-12	8.27E-04	1.54E-11	16	4104	4.48
1CZA	2694	26452	4.90E-03	1.29E-12	1.07E-03	6.22E-11	2	5380	4.59
6BCO	2856	27090	7.90E-03	4.53E-13	1.10E-03	7.91E-12	16	5730	7.15
1EPW	3861	35028	7.80E-03	1.88E-11	1.44E-03	2.50E-10	2	7714	5.40
5NP0	7584	80337	3.10E-02	6.58E-12	3.58E-03	1.35E-10	256	15562	8.66
5NUG	8760	82717	2.40E-02	1.43E-06	3.45E-03	5.33E-10	16	17592	6.96
4RH7	9015	85831	2.50E-02	1.62E-12	3.67E-03	2.22E-10	16	18054	6.82
3VKH	9126	87621	2.70E+00	3.00E-08	3.62E-03	1.15E-09	256	18556	745.03

Results: cut-off 5 Å

			BP		New BP				
ID	$\|V\|$	$\|E\|$	Time	MDE	Time	MDE	$\bar{W}_{ij}$	W	Speed-up
1N6T	30	176	7.60E-05	5.14E-05	1.04E-05	5.64E-12	2	52	7.31
1FW5	60	417	1.40E-04	7.99E-06	2.11E-05	3.08E-12	2	112	6.63
1ADX	120	659	4.70E-04	3.50E-06	3.49E-05	2.53E-12	2	232	13.48
1BDO	241	1345	3.60E-04	1.50E-07	7.05E-05	1.04E-11	2	474	5.11
1ALL	480	3443	9.80E-04	2.81E-06	1.67E-04	1.27E-12	2	952	5.88
6S61	522	3699	8.70E-04	8.10E-07	1.75E-04	1.39E-12	2	1036	4.98
1FHL	1002	6378	2.70E-03	2.56E-12	2.88E-04	1.17E-11	2	1996	9.38
4WUA	1033	6506	1.80E-03	5.34E-12	2.96E-04	2.94E-12	16	2066	6.08
6CZF	1494	9223	2.40E-03	4.62E-13	4.36E-04	2.33E-12	2	2980	5.51
5IJN	1950	11981	4.00E-03	4.43E-13	6.08E-04	4.23E-12	16	3908	6.58
6RN2	2052	13710	5.50E-03	3.89E-13	8.58E-04	9.35E-12	16	4112	6.41
1CZA	2694	17451	5.80E-03	4.51E-13	8.03E-04	3.06E-11	2	5380	7.22
6BCO	2856	18604	5.00E-03	6.00E-07	1.05E-03	6.96E-12	16	5706	4.75
1EPW	3861	23191	2.30E-02	3.00E-08	1.13E-03	9.78E-11	8	7716	20.29
5NP0	7584	59478	2.90E-01	2.56E-12	2.80E-03	4.11E-11	256	16138	103.55
5NUG	8760	56979	2.70E+00	3.60E-07	2.67E-03	1.05E-10	128	17700	1011.09
4RH7	9015	59346	3.10E-02	5.64E-13	2.97E-03	1.20E-10	32	18068	10.43
3VKH	9126	59592	–	–	2.45E-02	1.10E-09	65536	84066	

Computational cost

Total cost of New BP seems to vary linearly with the **total work** W.



Final remarks

- A new algorithm for DMDGP that efficiently employ symmetry properties to find the first solution more quickly
- It solves a sequence of nested DMDGP subproblems defined by pruning edges, in a specific order
- Numerical experiments indicate a non-trivial speed-up over the classical BP
- Future work: study the impact of different pruning edge orders on the total cost of New BP.

References

- C. Lavor, L. Liberti, N. Maculan, and A. Mucherino. *The discretizable molecular distance geometry problem*. Computational Optimization and Applications, 52:115–146, 2012.
- L. Liberti, C. Lavor, and A. Mucherino. *The Discretizable Molecular Distance Geometry Problem seems easier on proteins*. In Antonio Mucherino, Carlile Lavor, Leo Liberti, and Nelson Maculan, editors, Distance Geometry, pages 47–60. Springer New York, 2013.
- L. Liberti, B. Masson, J. Lee, C. Lavor, and A. Mucherino. *On the number of realizations of certain Henneberg graphs arising in protein conformation*. Discrete Applied Mathematics, 165:213–232, 2014.
- D. S. Gonçalves and A. Mucherino. *Discretization orders and efficient computation of cartesian coordinates for distance geometry*. Optimization Letters, 8:2111–2125, 2014.
- D. S. Gonçalves, C. Lavor, L. Liberti and M. Souza. *A new algorithm for the* ^{K}*DMDGP subclass of Distance Geometry Problems.* https://arxiv.org/abs/2009.05404