On the number of solutions of the discretizable molecular distance geometry problem

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Abstract

The Generalized Discretizable Molecular Distance Geometry Problem is a distance geometry problems that can be solved by a combinatorial algorithm called “Branch-and-Prune”. It was observed empirically that the number of solutions of YES instances is always a power of two. We give a proof that this event happens with probability one.

Keywords: distance geometry, symmetry, Branch-and-Prune, power of two.

1 Introduction

We consider the following problem arising in the analysis of Nuclear Magnetic Resonance (NMR) data for general molecules.

Molecular Distance Geometry Problem (MDGP).
Given an undirected graph $G = (V, E)$ and a function $d : E \to \mathbb{R}$, decide whether there is an embedding $x : V \to \mathbb{R}^3$ such that

$$\forall \{u, v\} \in E \ (||x_u - x_v|| = d_{uv}) \quad (1)$$

The MDGP is usually cast as a nonconvex unconstrained mathematical program $\min \sum_{(u, v) \in E} (||x_u - x_v||^2 - d_{uv}^2)^2$, which can be solved using continuous Global Optimization techniques [1]. See [2, 3] for surveys.

If the NMR data is obtained from a protein, it is usually possible to distinguish between backbone atoms and atoms of side chains. We can then attempt to place the backbone first [4] and the side chains later [5]. We therefore assume that $G$ is the graph of the backbone. If a total order is given on $V$ such that for each atom $v$ there are at least three atoms that are adjacent to it in $E$ and preceding it in the order (these are called the adjacent predecessors of $v$), if strict triangle inequality holds for $d$ restricted to at least one triplet of adjacent predecessor for each vertex, and if spatial positions are given for the first
three atoms, there is only a finite number of possible embeddings compatible with the given distances, which can all be found using the so-called Branch-and-Prune (BP) algorithm [4]. The subset of MDGP instances for which the described atomic order exists is called Discretizable MDGP (DMDGP) [3] and is known to be NP-hard [6]. It was empirically observed that for any given practical instance, BP always finds a number of solution that is a power of two [4]. An isolated earlier counterexample, derived via a complexity reduction, given as Lemma 5.1 in [6], falsifies this conjecture. In this paper we give a formal description of the DMDGP in arbitrary dimensions (Sect. 2), of the BP algorithm and some of its theoretical properties (Sect. 3). We then study some geometrical aspects of the BP tree (Sect. 4), and prove that the number of solutions of feasible DMDGP instances is a power of two with probability one (Sect. 5). We also exhibit a family of counterexamples (Sect. 5) that are much more intuitive than the one given in [6].

2 The Discretizable Molecular Distance Geometry Problem

The generalization of the MDGP to arbitrary dimensions asks for an embedding of $G$ in $\mathbb{R}^K$ satisfying (1) and is called the Distance Geometry Problem (DGP). The generalization of the DMDGP to $\mathbb{R}^K$ replaces triplets with $K$-uples of adjacent predecessors and strict triangle with strict simplex inequalities (2). For a set $U = \{x_i \in \mathbb{R}^K \mid i \leq K + 1\}$ of points in $\mathbb{R}^K$, let $D$ be the symmetric matrix whose $(i, j)$-th component is $|x_i - x_j|^2$ for all $i, j \leq K + 1$ and let $D'$ be $D$ bordered by a left $(0, 1, \ldots, 1)^T$ column and a top $(0, 1, \ldots, 1)^T$ row (both of size $K + 2$). Then the Cayley-Menger formula states that the volume $\Delta_K(U)$ of the $K$-simplex on $U$ is given by $\Delta_K(U) = \sqrt{\frac{(−1)^{K+1}}{2^K}} |D'|$. The strict simplex inequalities are given by $\Delta_K(U) > 0$. For $K = 3$, these reduce to strict triangle inequalities. We remark that only the distances of the simplex edges are necessary to compute $\Delta_K(U)$, rather than the actual points in $U$; the needed information can be encoded as a complete graph $K_{K+1}$ on $K + 1$ vertices with edge weights as the distances.

Let $n = |V|$ and $m = |E|$. For all $v \in V$, let $\mathcal{N}(v) = \{u \in V \mid \{u, v\} \in E\}$ be the star of vertices around $v$ (also called the adjacencies of $v$); for a directed graphs $(V, A)$, where $A \subseteq V \times V$, we denote the outgoing star by $\mathcal{N}^+(v) = \{u \in V \mid (v, u) \in A\}$. For an order $< v$ on $V$, let $\gamma(v) = \{u \in V \mid u < v\}$ be the set of predecessors of $v$, and let $\rho(v) = |\gamma(v)| + 1$ the rank of $v$ in $<$. For $V' \subseteq V$, we denote by $G[V']$ the subgraph of $G$ induced by $V'$. For a finite set $M$, let $\mathcal{P}(M)$ be its power set. We call an embedding $x$ of $G$ valid if (1) holds for $G$. For a sequence $x = (x_1, \ldots, x_n)$ and a subset $U \subseteq \{1, \ldots, n\}$ we let $x(U)$ be the subsequence of $x$ indexed by $U$. If $x$ is an initial subsequence of $y$, then $y$ is an extension of $x$.

Generalized DMDGP (GDMDGP). Given an undirected graph $G = (V, E)$, an edge weight function $d : E \to \mathbb{R}^+$, an integer $K > 0$, a subset $V_0 \subseteq V$ with $|V_0| = K$, a partial embedding $\hat{x} : V_0 \to \mathbb{R}^K$ valid for $G[V_0]$, and a total order $<$ on $V$ such that:

\begin{align*}
\forall v \in V \mid \rho(v) \leq K & \quad = \quad V_0; \tag{2} \\
\forall v \in V \mid (\rho(v) > K \to |\mathcal{N}(v) \cap \gamma(v)| \geq K); \tag{3} \\
\forall v \in V \setminus V_0 \exists U_v \subseteq \mathcal{N}(v) \cap \gamma(v) (G[U_v] = K) \land \\
\Delta_{K-1}(U_v) > 0 \land \forall u \in U_v (\rho(u) - K \leq \rho(u) \leq \rho(v) - 1)), \tag{4}
\end{align*}

decide whether there is a valid extension $x : V \to \mathbb{R}^K$ of $\hat{x}$.

Conditions (2) and (4) allow the search for vertex $v$ to only depend on the $K$ vertices of rank preceding $\rho(v)$, as $x_u$ is the intersection of at least $K$ spheres centered at $x_u$ and with radius $d_{uv}$ for all $u \in U_v$. This, in particular, implies that the predecessors of $v$ are placed before $v$, so that all of the distances between all predecessors are known when placing $v$. Thus, we can replace the condition $G[U_v] = K_0$ in (1) by $|U_v| = K$. We remark that eliminating the condition $\forall u \in U_v (\rho(v) - K \leq \rho(u) \leq \rho(v) - 1)$ from (1) and fixing $K$ gives rise to a problem called the Discretizable Distance Geometry Problem in $K$.
dimensions (DDGP$_K$), discussed in [8], which is itself a subset of instances of the DDGP, where the number of dimensions is not fixed. The DMDGP is therefore the subset of the GDMDGP for which $K = 3$ [6]. In summary, we have the following diagram (where arrows represent the $\subset$ relation).

A polynomial reduction from Subset-Sum to the DMDGP shows that the GDMDGP is NP-hard. Even restricting the range of $d$ to the set of rational numbers, it is not clear whether there are YES certificates for the DDGP that have polynomially bounded size.

In the following, we assume that the probability of any point of $\mathbb{R}^K$ belonging to any given subset of $\mathbb{R}^K$ having Lebesgue measure zero is equal to zero.

### 3 Branch-and-Prune

The BP algorithm for the DMDGP, presented in [4], can easily be generalized to the GDMDGP. As mentioned above, once the vertices of $U_v$ have been embedded in $\mathbb{R}^K$, the known distances from vertices in $U_v$ to a given $v$ will enforce the position of $v$ as the intersection of $K$ spheres. Under strict simplex inequalities, this intersection consists of at most two distinct points. The BP exploits this fact to recursively generate a binary search tree of height at most $n$ where a node at level $i$ represents a possible placement in $\mathbb{R}^K$ of the vertex of $G$ with rank $i$ in $\subset$. Paths of length $n$ correspond to valid embeddings.

Let $G$ be a GDMDGP instance. Consider $v \in V$ with rank $\rho(v) = i > K$, let $G^v = G[\gamma(v) \cup \{v\}]$ and $x$ be a valid embedding of $G[\gamma(v)]$. We characterize the number of extensions of $x$ valid for $G^v$ in the following lemmata (which also hold for the DDGP); the proof technique for Lemma 3.1 is well known [9] [10]; we restate the proof here because we believe the explicit form [7] is unpublished.

#### 3.1 Lemma

If $|N(v) \cap \gamma(v)| = K$ then there are at most two distinct extensions of $x$ that are valid for $G^v$. If one valid extension exists, then with probability $1$ there are exactly two distinct valid extensions.

**Proof.** Since $|N(v) \cap \gamma(v)| = K$, $U_v = N(v) \cap \gamma(v)$ and $v$ is at the intersection of exactly $K$ spheres in $\mathbb{R}^K$ (each centered at $x_u$ with radius $d_{uv}$, where $u \in U_v$). The position $z \in \mathbb{R}^K$ of $v$ must then satisfy:

$$\forall u \in U_v \quad \|z - x_u\| = d_{uv} \Rightarrow \|z\|^2 - 2x_u \cdot z + \|x_u\|^2 = d_{uv}^2. \tag{5}$$

As in [11], we choose an arbitrary $w \in U_v$, say $w = \max_{\subset} U_v$, and subtract from the Eq. (5) indexed by $w$ the other equations of (5), obtaining the system:

$$\forall u \in U_v \setminus \{w\} \quad 2(x_u - x_w) \cdot z = (\|x_u\|^2 - d_{uw}^2) - (\|x_w\|^2 - d_{uw}^2) \tag{6}$$

The system (6) consists of a set of $K - 1$ linear equations and a single quadratic equation in the $K$-vector $z$. We write the linear equations as the system $Az = b$, where the $(u,j)$-th component of $A$ is $2(x_{uj} - x_{w})$, the $u$-th component of $b$ is $\|x_u\|^2 - \|x_w\|^2 - d_{uw}^2 + d_{uw}^2$. A is $(K - 1) \times K$ and $b \in \mathbb{R}^{K-1}$. By strict simplex inequality, $A$ has full rank (for otherwise $\sum_{u \neq w} \lambda_u (x_u - x_w) = 0$ implies that $x_w$ is in the span of $\{x_u \mid u \in U_v\}$, and hence that $\Delta_{K-1}(U_v) = 0$); so without loss of generality assume that the square matrix $B$ formed by the first $K - 1$ columns of $A$ is invertible. Let $z_B$ be the vector consisting of the first $K - 1$ components of $z$; then the linear part (first $K - 1$ equations) of (6) yields
Let $z_B = B^{-1}(b - Nz_K)$, where $N = 2(x_{wK} - x_{wk} \mid u \in U_v \setminus \{w\}) \in \mathbb{R}^{K-1}$. After replacement of $z_B$ in (6) with $z_B(z_K)$, we obtain the following quadratic equation in $z_K$:

$$((\bar{N}^2 + 1)z_K^2 - 2((\bar{b} + x_{wB})\bar{N} + x_{wK})z_K + ((\|x_{wB} - \bar{b}\|^2 + x_{wK}^2 - d_{wv}^2)) = 0,$$  \hspace{1cm} (7)

where $\bar{b} = B^{-1}b$ and $\bar{N} = B^{-1}N$. If the discriminant of (7) is negative then no extension of $x$ to $v$ is possible and the result follows. If the discriminant is nonnegative, (7) has solutions $z' = (z_B(z_K), z_K')$ and $z'' = (z_B(z''_K), z''_K) \in \mathbb{R}^K$, which are distinct with probability 1 because the discriminant is zero with probability 0. The extended embeddings, distinct with probability 1, are given by $(x, z')$ and $(x, z'')$.

3.2 Lemma
If $|N(v) \cap \gamma(v)| > K$ then, with probability 1, there is at most one extension of $x$.

Proof. Consider a subset $S \subseteq N(v) \cap \gamma(v)$ such that $|S| = K + 1$ and $S \supseteq U_v$. Either there is at least one point $x_v$ such that $(x, x_v)$ is an embedding of $G[S \cup \{v\}]$ that is valid w.r.t. the system:

$$\forall u \in S \sum_{k \leq K} (x_{uk}^2 - 2x_{uk}x_{vk} + x_{vk}^2) = d_{uv}^2,$$  \hspace{1cm} (8)

or the system has no solution. In the latter case, the result follows, so we assume now that there is a point $x_v$ satisfying (8). Since the points $x_u$ are known for all $u \in S$, (8) is a quadratic system with $K$ variables and $K + 1$ equations. As in the proof of Lemma 3.1, we derive an equivalent linear system from (8). Since $d$ satisfies the strict simplex inequalities on $U_v$ with probability 1 and $S \supseteq U_v$, by (12) the points of $U_v$ are not co-planar and the system has exactly one solution.

3.3 Lemma
With the notation of Lemma 3.1, if $\bar{x}$ is a valid embedding for $G[U_v]$, then $z''$ is a reflection of $z'$ with respect to the hyperplane through the $K$ points of $\bar{x}$.

Proof. Any sphere in $\mathbb{R}^K$ is symmetric with respect to any hyperplane through its center; so the intersection of up to $K$ spheres in $\mathbb{R}^K$ is symmetric with respect to the hyperplane containing all the centers.

Reflections with respect to hyperplanes are isometries, and can therefore be represented by linear operators. If $a \in \mathbb{R}^K$ is the unit normal vector to a hyperplane $H$ containing the origin, then the reflection operator $R_0$ w.r.t. $H$ can be expressed in function of the standard basis by the matrix $I - 2aa^\top$, where $I$ is the $K \times K$ identity matrix. If $H$ is a hyperplane with equation $a^\top x = a_0$, with $a_0 \neq 0$, s.t. $x$ is ordered and $a_i$, for some $1 \leq i \leq K$, is the nonzero coefficient of smallest index in $a$. Then, the reflection operator $R$ acting on a point $p \in \mathbb{R}^K$ w.r.t. $H$ is given by $R(p) = R_0(p - \frac{a_0}{a_i}e_i) + \frac{a_0}{a_i}e_i$, where $e_i \in \mathbb{R}^K$ is the unit vector with 1 at index $i$ and 0 elsewhere: we first we translate $p$ so that we can reflect it using $R_0$ w.r.t. the translation of $H$ containing the origin, then we perform the inverse translation of the reflection.

A formal description of the BP algorithm for the GDMGDGP (which also holds for the DDGP) is given in Alg. 1. It builds a binary search tree $T = (\mathcal{V}, \mathcal{A})$, directed from the root to the leaves, whose nodes are triplets $a = (x(a), \lambda(a), \mu(a))$. For $a \in T$ we denote by $p(a)$ the unique path from the root node $v$ of $T$ to $a$; $x(a)$ is an extension of the embedding $x^-$ found on $p(a^-)$, where $a^-$ is the unique parent node of $a$. Next, $\lambda(a) \in \{0, 1\}$ distinguishes whether $a$ is a “left” or a “right” subnode of $a^-$. More precisely, let $a$ be a node at level $i$ in $T$, $v = \rho^{-1}(i)$, $\bar{x}$ be a partial embedding of $G[U_v]$, and $a_v^\top x = a_v$ be the equation of the $((K-1))$-dimensional hyperplane through the points of $\bar{x}$. Assuming $u = \rho^{-1}(i - 1)$, $a_v \in \mathbb{R}^K$ is oriented so that $a_v \cdot a_u \geq 0$; then:

$$\lambda(a) = \begin{cases} 0 & \text{if } a_v^\top x(a)_i \leq a_v \phi \\ 1 & \text{if } a_v^\top x(a)_i > a_v \phi \end{cases},$$  \hspace{1cm} (9)
Lastly, $\mu(\alpha) = \Box$ if $x$ is a valid extension of $x^-$, in which case the node is said to be feasible, and $\mu = \Box$ otherwise. This allows us to retrieve the set $X$ of all valid embeddings of $G$ by simply traversing $T$ backwards from the leaf nodes marked $\Box$ up to $r$.

Algorithm 1 The Branch and Prune algorithm.

Require: Partial embedding $\bar{x}$ of first $K$ vertices of $G$

Ensure: $X$ of valid embeddings of $G$

1: Let $\alpha = (\bar{x}_1, 0, \Box)$ and $\alpha' = (\bar{x}_1, 1, \Box)$
2: Initialize $V = \{\alpha, \alpha'\}$ and $A = \{(r, \alpha), (r, \alpha')\}$
3: for $1 < i \leq K$ do
4: Let $\alpha = (\bar{x}_i, 0, \Box)$, $\alpha' = (\bar{x}_i, 1, \Box)$, $\beta = (\bar{x}_{i-1}, 0, \Box)$
5: Let $V \leftarrow V \cup \{\alpha, \alpha'\}$ and $A \leftarrow A \cup \{(\beta, \alpha), (\beta, \alpha')\}$
6: end for
7: $\text{BranchAndPrune}(K + 1, (\bar{x}_K, 0, \Box))$
8: Let $X = \{x(\theta) \mid \theta \in V \land |N^+(\theta)| = 0 \land \mu(\theta) = \Box\}$
9: stop
10: function $\text{BranchAndPrune}(i, \beta)$:
11: if $i > n \lor \mu = \Box$ then
12: return
13: end if
14: Let $v = \rho^{-1}(i)$
15: Choose $U_v$ such that Eq. (4) holds
16: Compute the equation $a_v^\top x = a_{v0}$ of the hyperplane through $x[U_v]$
17: Let $Z = \{z', z''\}$ be extensions of $x(\beta)$ to $v$, and $Z' = Z$
18: for $z \in Z$ do
19: if $\exists(u, v) \in E \parallel x(\beta)_u - z \parallel \neq d_{uv}$ then
20: Let $Z = Z \setminus \{z\}$
21: end if
22: end for
23: if $Z = \{z', z''\}$ then
24: if $a_v^\top z' \leq a_{v0}$ then
25: Let $\alpha = (z', 0, \Box)$, $\alpha' = (z'', 1, \Box)$
26: else
27: Let $\alpha = (z'', 0, \Box)$, $\alpha' = (z', 1, \Box)$
28: end if
29: else if $Z = \{z\}$ then
30: if $a_v^\top z \leq a_{v0}$ then
31: Let $\alpha = (z, 0, \Box)$, $\alpha' = (Z' \setminus \{z\}, 1, \Box)$
32: else
33: Let $\alpha = (z, 1, \Box)$, $\alpha' = (Z' \setminus \{z\}, 0, \Box)$
34: end if
35: else
36: return
37: end if
38: Let $V \leftarrow V \cup \{\alpha, \alpha'\}$ and $A \leftarrow A \cup \{(\beta, \alpha), (\beta, \alpha')\}$
39: for $\theta \in N^+(\beta)$ such that $\mu(\theta) = \Box$ do
40: $\text{BranchAndPrune}(i + 1, \theta)$
41: end for
42: return
43: end

We remark that Alg. 1 differs from the original BP formulation [4] because it applies to $K$ dimensions and stores the binary search tree. In the rest of this section we list some of the elementary properties of the BP algorithm.
We now partition $\cal V$ in pairwise disjoint subsets $\cal V_1, \ldots, \cal V_n$ where for all $i \leq n$ the set $\cal V_i$ contains all the nodes of $\cal V$ at level $i$ of the tree $\cal T$.

### 3.5 Proposition
With probability 1, there is no level $i \leq n$ having two distinct feasible nodes $\beta, \theta \in \cal V_i$ such that $|\{\alpha \in N^+(\beta) \mid \mu(\alpha) = \Box\}| = 1$ and $|\{\alpha \in N^+(\theta) \mid \mu(\alpha) = \Box\}| = 2$.

**Proof.** We show that for all $i \leq n$ the event of having two distinct nodes $\beta, \theta \in \cal V_i$, with $\rho^{-1}(i) = v$, such that $\beta$ has one feasible subnode and $\theta$ has two has probability 0. Consider $T_v = N(v) \cap \gamma(v)$; if $|T_v| = K$ then by Lemma 3.1 $\beta$ should have exactly two feasible subnodes with probability 1; since it only has one, the event $|T_v| = K$ occurs with probability 0. Since $|T_v| \geq K$ by (4), the event $|T_v| > K$ occurs with probability 1. Thus by Lemma 3.2 there is at most one valid embedding extending the partial embedding at $v$, which means that the two feasible subnodes of $\theta$ represent the same embedding, an event that occurs with probability 0. □

### 4 Geometry in the BP Trees

Here we exhibit some geometrical symmetry properties between the valid embeddings of a GDMDGP instance. We prove in Thm 4.8 that for any valid embedding $y \in X$, if the BP tree branches at level $i$ on the path to $y$, then the embedding obtained by reflecting all the nodes after level $i$ is also valid.

To this aim, we need to emphasize those BP branchings which carry on to feasible leaf nodes along both branches. For $y \in X$ and a vertex $v \in V \setminus V_0$ we denote $\Upsilon(y, v)$ the following property:

$$\Upsilon(y, v): \text{there are feasible leaf nodes } \beta, \beta' \in \cal V_n \text{ such that } x(\beta) = y, \ p(\beta) \cap V_{\rho(v)}^{-1} = p(\beta') \cap V_{\rho(v)}^{-1} \text{ and } p(\beta) \cap V_{\rho(v)} = p(\beta') \cap V_{\rho(v)}.$$ 

If $\Upsilon(y, v)$ holds, it is easy to show that $p(\beta) \cap V_{\rho(v)}^{-1}$ contains a single feasible node with two feasible subnodes. With $\Upsilon(y, v)$ true, let $R^v$ be the Euclidean reflection operator with respect to the hyperplane through $y[U_v]$ (as defined on p. 4). Define $\tilde{R}^v = I^{\rho(v)^{-1}} \times (R^n)^{n-\rho(v)}$, i.e. $\tilde{R}^v y = (y_1, \ldots, y_{i-1}, R^n y_i, \ldots, R^n y_n)$. We remark that for all $i \leq \ell \leq n$ and for all $\alpha \in \cal V_{i\ell}$ the set $p(\alpha) \cap V_{i\ell}$ has a unique element.

#### 4.1 Corollary
Let $\alpha \in \cal V_{i\ell}$ for some $i > 1$, $v = \rho^{-1}(i)$ and $N^+(\alpha) = \{\eta, \beta\}$ with $\mu(\eta) = \mu(\beta) = \Box$. Then $x(\eta)_v = R^n x(\beta)_v$.

**Proof.** This is a corollary to Lemma 3.3 □

#### 4.2 Lemma
Let $\alpha \in \cal V_{i\ell}$ for some $i > 1$ such that $N^+(\alpha) = \{\eta', \beta'\}$, $u = \rho^{-1}(i)$; $v > u$ with $\rho(v) = \ell$, and consider two feasible nodes $\eta, \beta \in \cal V_i$ such that $\eta' = p(\eta) \cap \cal V_i$ and $\beta' = p(\beta) \cap \cal V_i$. Then, with probability 1, the following statements are equivalent:

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(i) \( \forall i \leq j \leq \ell, x(\beta''_w) = R^w x(\eta'')_w \), where \( \eta'' = p(\eta) \cap V_j \), \( \beta'' = p(\beta) \cap V_j \), and \( w = \rho^{-1}(j) \);

(ii) \( \forall i \leq j \leq \ell, \lambda(\eta'') = 1 - \lambda(\beta'') \), with \( \eta'' = p(\eta) \cap V_j \) and \( \beta'' = p(\beta) \cap V_j \).

**Proof.** Let \( a_i^0 \top x = a_i^0_0, a_i^1 \top x = a_i^1_0 \) be the equations of the hyperplanes \( H_{\alpha}, H_{\beta} \) defined respectively by \( x(\eta)[U_1] \) and \( x(\beta)[U_1] \), with the normals oriented as explained on page 4. We prove by induction on \( \ell - i \) that the following assumption is equivalent to (i) and (ii).

(iii) for all \( i \leq j \leq \ell, x(\beta''_w) = R^w x(\eta'')_w \) and \( a_u \cdot a_i^0 = a_u \cdot a_i^1 \), where \( \eta'' = p(\eta) \cap V_j \), \( \beta'' = p(\beta) \cap V_j \), \( w = \rho^{-1}(j) \), and \( a_i^0, a_i^1 \) are the normal vectors of the hyperplanes \( H_{\eta''} \) and \( H_{\beta''} \) oriented as usual.

If \( \ell = i \), then (ii) and (iii) hold simultaneously. Indeed, \( \eta = \eta' \) and \( \beta = \beta' \), hence \( x(\beta)_v = R^w x(\eta)_v \) (Lemma 23.1) and \( \lambda(\eta) = 1 - \lambda(\beta) \) (Alg. 1 Steps 21 and 22). In addition, we have \( H_{\eta} = R^w H_{\beta} \), therefore \( \|a_u \cdot a^0_v\| = \|a_u \cdot a^1_v\| \). Because the orientation of \( a_i^0, a_i^1 \) is such that \( a_u \cdot a^0_v, a_u \cdot a^1_v \geq 0 \), the result holds.

Assume that the equivalence stated above holds for level \( \ell - 1 \), we show that it is still the case at level \( \ell \). In the sequel, denote \( t = \rho^{-1}(\ell - 1) \).

(i) \( \Leftrightarrow \) (ii) Suppose for all \( i \leq j < \ell, x(\beta''_w) = R^w x(\eta'')_w \) and \( \lambda(\eta'') = 1 - \lambda(\beta'') \) (by the induction hypothesis, both statements are equivalent). Hence, \( H_{\eta''} = R^w H_{\beta''} \) holds for all \( j \), because the \( K \) points generating the hyperplanes either belong to \( H_{\alpha} \), or are reflections of each other. This is true in particular if we choose \( \eta''_j, \beta''_j \in V_{t-1} \). In addition, if we use the induction hypothesis (i) \( \Rightarrow \) (iii), we have \( a_u \cdot a_i^0 = a_u \cdot a_i^1 \), so \( a_i^0, a_i^1 \) are directed similarly w.r.t \( a_u \), and \( \lambda(\eta) = 1 - \lambda(\beta) \) if and only if \( x(\beta)_v = R^w x(\eta)_v \) (see Fig. 4).

![Figure 1: Proof of Lemma 1.2. Case (ii) shows the contradiction deriving from \( \lambda(\eta) = \lambda(\beta) = 0 \) (or \( x(\beta)_v \neq R^w x(\eta)_v \)), and case (iii) the situation that actually occurs.](image-url)

(ii) \( \Rightarrow \) (iii) Suppose for all \( i \leq j \leq \ell, \lambda(\eta'') = 1 - \lambda(\beta'') \). By the previous result, we also know that \( i \leq j \leq \ell, x(\beta''_w) = R^w x(\eta'')_w \). It remains to prove that \( a_u \cdot a_i^0 = a_u \cdot a_i^1 \), i.e. that the angles \( \theta_i^0 \) and \( \theta_i^1 \) formed by these vectors have the same cosine. Notice once again that \( H_{\eta} = R^w H_{\beta} \). By induction, we know that the angles \( \theta_i^0, \theta_i^1 \) formed by \( a_u \) and respectively \( a_i^0, a_i^1 \), have same cosine. With probability 1, the hyperplanes \( H_{\eta}, H_{\beta} \) are not parallel, hence their normal vectors cannot be identical, therefore, \( \theta_i^0 = -\theta_i^1 \) (see the illustration on Fig. 2). Denote \( \theta^0, \theta^1 \) the angles formed respectively by \( a_i^0 \) and \( a_i^1 \), and by \( a_i^0 \) and \( a_i^1 \). We also have, \( H_{\eta''} = R^w H_{\beta''} \), where \( \eta''_j, \beta''_j \in V_{t-1} \), hence the normal vectors of these 4 hyperplanes are also symmetric, which implies \( \theta^0 = -\theta^1 \) or \( \theta^0 = \pi - \theta^1 \). By the definition of \( a_i^0 \)
4 GEOMETRY IN THE BP TREES

Figure 2: Proof of Lemma 1.2 illustration of the fact that $a_u \cdot a^0_v = a_u \cdot a^1_v$.

and $a^1_v$ (page 4), since the scalar products are positive, $-\pi/2 \leq \theta^0, \theta^1 \leq \pi/2$, thus $\theta^0 = -\theta^1$. Therefore, $\theta^0_0 = \theta^0 + \theta^0 = -\theta^1 - \theta^1 = -\theta^1$, which concludes this part of the proof. [iii] $\Rightarrow$ [i] Obvious. 

4.3 Proposition
Consider a subtree $T'$ of $T$ consisting of $K + 2$ consecutive levels $i - K - 1, \ldots, i$ (where $i \geq 2K + 1$), rooted at a single node $\eta$ and such that all nodes at all levels are marked $\exists$. Let $p = 2^{K+1}$ and consider the set $Y' = \{y_j \mid j \leq p\}$ of partial embeddings of $G$ at the leaf nodes $\{\alpha_j \mid j \leq p\}$ of $T'$. Let $u = \rho^{-1}(i - K - 1)$ and $v = \rho^{-1}(i)$. Then with probability 1 there are two distinct positive reals $r, r'$ such that $\|y_j(\alpha_j)_u - y_j(\alpha_j)_v\| \in \{r, r'\}$ for all $j \leq p$.

Proof. Fig. 3 shows a graphical proof sketch for $K = 2$. With a slight abuse of notation, for a vertex

Figure 3: Proof of Prop. 4.3 in $\mathbb{R}^2$. The arrangement of three segments gives rise, in general, to two distances $r, r'$ between root and leaves.

$w \in V$ in this proof we denote by $R^w$ the set of all reflections at level $w$. We order the $\alpha_j$ nodes so that the action of $R^w$ on $(\alpha_1, \ldots, \alpha_p)$ is the permutation $\prod_{j \mod 2=1} (j, j+1)$. Let $t = \rho^{-1}(i - 1)$. Since all nodes are feasible, $\|y_j(\alpha_j)_v - y_j(\alpha_j)_t\| = d_{tv}$ and $\|y_j(\alpha_j)_u - y_j(\alpha_j)_t\| = d_{ut}$ for all $j \leq p$ (we remark that $\{t, v\}$ and $\{u, t\}$ must be in $E$ by the definition of the GDMDGP). With probability 1, the segments through
Corollary 4.3 can be generalized to span an arbitrary number of levels by induction on

\[ \text{Let } d \in \mathbb{R}^n \]

\[ \text{Since } \Upsilon(\alpha_j) \]

\[ \text{then } \]

\[ \text{prune all feasible nodes due to } \]

\[ \text{Let } \]

\[ \text{Consider a subtree } \]

\[ \text{4.4 Example} \]

\[ \text{Consider a subtree } T' \text{ of } T \text{ like the one in Fig. 3 embedded in } \mathbb{R}^2, \text{ and suppose that all nodes at level } u, w, t \text{ are marked } \exists, \text{ and further that only one node within } \alpha_1, \alpha_2 \text{ is feasible, only one node within } \alpha_3, \alpha_4 \text{ is }

\[ \text{feasible, only one node within } \alpha_7, \alpha_8 \text{ is feasible, and } \alpha_5, \alpha_6 \text{ are both infeasible. This must be due to a distance } d_{u,v} \text{ with } u' \leq u. \text{ Consider now a circle } C \text{ completely determined by its center at } y_1(\alpha_1)_{uv} \text{ and its radius } d_{u,v}, \text{ if } C \text{ also contains the points at the nodes } \alpha_1, \alpha_4, \alpha_8 \text{ or the points at the nodes } \alpha_2, \alpha_3, \alpha_7 \text{ then we must have } u' = u, \text{ in which case also one of } \alpha_5, \alpha_6 \text{ will be feasible (against the hypothesis). And the probability that } C \text{ should contain the points at the nodes } \alpha_1, \alpha_3, \alpha_8 \text{ or } \alpha_2, \alpha_4, \alpha_7 \text{ is zero. Hence } T' \text{ can only occur with probability } 0. \]

\[ \text{4.5 Corollary} \]

\[ \text{Consider a subtree } T' \text{ of } T \text{ consisting of } K + q + 1 \text{ consecutive levels } i - K - q, \ldots, i \text{ (where } i \geq 2K + q \text{ and } q \geq 1), \text{ rooted at a single node } \eta \text{ and such that all nodes at all levels are marked } \exists. \text{ Let } p = 2K+q \text{ and consider the set } Y' = \{ y_j \mid j \leq p \} \text{ of partial embeddings of } G \text{ at the leaf nodes } \{ \alpha_j \mid j \leq p \} \text{ of } T'. \text{ Let } u = \rho^{-1}(i - K - q) \text{ and } v = \rho^{-1}(i). \text{ Then with probability } 1 \text{ there is a set } H^{uw} = \{ r_j \mid j \leq 2^q \} \text{ of } 2^q \text{ distinct positive reals such that } \| y_1(\alpha_i)_{uv} - y_i(\alpha_i)_{uv} \| \in H^{uw} \text{ for all } i \leq p. \]

\[ \text{Proof. The proof of Prop. 4.3 can be generalized to span an arbitrary number of levels by induction on } q. \text{ Two distances } r_1, r_2 \in H^{uw} \text{ can only be equal by collinearity of some subsets of points, an event occurring with probability } 0. \]

\[ \text{4.6 Corollary} \]

\[ \text{Let } y \in X \text{ and } v \in V - V_0 \text{ such that } \Upsilon(y, v) \text{ holds. If } \{ u, w \} \in E \text{ with } u < v < w \text{ and } \rho(w) - \rho(u) > K \text{ then } d_{uw} \in H^{uw} \text{ with probability } 1. \]

\[ \text{Proof. Since } \Upsilon(y, v) \text{ holds, then the GDMGDGP instance is YES and there must exist at least two feasible nodes at level } \rho(w) \text{ in } T. \text{ If } d_{uw} \notin H^{uw} \text{ the probability that a completely determined sphere contains two arbitrary points in } \mathbb{R}^K \text{ is zero. Since the instance is a YES one, however, the BP algorithm does not prune all feasible nodes due to } d_{uw}. \text{ By Cor. 4.5 the only remaining possibility (which therefore occurs with probability } 1) \text{ is that } d_{uw} \in H^{uw}. \]

\[ \text{4.7 Corollary} \]

\[ \text{Let } y \in X \text{ and } v \in V - V_0 \text{ such that } \Upsilon(y, v) \text{ holds. If } u \in V \text{ with } u > v \text{ then } R^y y_u \text{ belongs to a valid extension of } y|U_v. \]

\[ \text{Proof. If there is no edge } \{ w, u \} \in E \text{ with } \rho(u) - \rho(w) > K \text{ the result follows by Cor. 4.4. Otherwise, by Cor. 4.6 } d_{uw} \in H^{uw}. \text{ As in the proof of Prop. 4.3 all pairs of points that are feasible w.r.t. } d_{uw} \text{ are }\]
reflections of each other w.r.t. $R^v$.

\[ \square \]

4.8 Theorem
Let $y \in X$ and $v \in V \setminus V_0$ such that $\mathcal{T}(y, v)$ holds. Then $\hat{R}^v y \in X$ with probability 1.

Proof. We have to show that $\hat{R}^v y$ is a valid embedding for $G = (V, E)$. Partition $E$ into three subsets $E_1, E_2, E_3$, where $E_1 = \{ \{t, u\} \in E \mid t, u < v \}$, $E_2 = \{ \{t, u\} \in E \mid t, u \geq v \}$ and $E_3 = \{ \{t, u\} \in E \mid t < v \wedge u \geq v \}$. For $E_1$, by definition $||\hat{R}^v y_t - (\hat{R}^v y_u)|| = ||I y_t - I y_u|| = ||y_t - y_u|| = d_{tu}$ as claimed. For $E_2$, $||(\hat{R}^v y_t) - (\hat{R}^v y_u)|| = ||R^v y_t - R^v y_u|| = ||y_t - y_u|| = d_{tu}$ because $R^v$ is an isometry. For $E_3$, we aim to show that $||I y_t - R^v y_u|| = d_{tu}$. Since $y \in X$, by Lemma 3.4 there is a feasible leaf node $\alpha$ with $x(\alpha) = y$. Because $\mathcal{T}(y, v)$, $\exists \eta \in V_{\rho(v) - 1}$ such that $x(\eta) = y[\gamma(v)]$ and $N^+(\eta) = \{\beta, \beta'\}$ with $\rho(\beta) = \rho(\beta') = \uplus$; we can assume without loss of generality that $p(\alpha) \cap V_{\rho(v)} = \{\beta\}$; furthermore, again by $\mathcal{T}(y, v)$, there is at least one feasible leaf node $\alpha'$ such that $p(\alpha') \cap V_{\rho(v)} = \{\beta'\}$. Let $\omega = p(\alpha) \cap V_{\rho(v)}$ and $\omega' = p(\alpha') \cap V_{\rho(v)}$. Because $\omega'$ is feasible, $||x(\omega')' - x(\omega')u|| = d_{tu}$; because $\eta$ is an ancestor of both $\alpha$ and $\alpha'$ at level $\rho(v) - 1$ and $t < v$, $p(\alpha') \cap V_{\rho(v)} = p(\alpha) \cap V_{\rho(v)}$, which implies that $x(\omega')' = x(\omega)' = y_t$. Thus, $||y_t - y_u|| = d_{tu} = ||y_t - x(\omega')u||$. Furthermore, because $\beta' \in p(\omega') \cap V_{\rho(v)}$, $x(\omega')$ extends $x(\beta')$. By Alg. 1 Steps 26 and 28 $\lambda(\beta) = 1 - \lambda(\beta')$. Because $\alpha$ is feasible, at every level $\rho(u) \in V$ such that $v \leq u' < u$ the node $\theta \in p(\alpha) \cap V_{\rho(u)}$ has $f \in \{1, 2\}$ feasible subnodes; by Prop. 3.5 the node $\theta' \in p(\alpha') \cap V_{\rho(u)}$ also has $f$ feasible subnodes. If $f = 2$, by Cor. 1.7 it is possible to choose $\alpha'$ so that $\lambda(\theta') = 1 - \lambda(\theta)$ with probability 1; if $f = 1$ then by Alg. 1 Steps 32 and 33 all feasible nodes inherit the same $\lambda$ value as their parents, so $\lambda(\theta') = 1 - \lambda(\theta)$. By Lemma 1.2 $x(\omega')' = R^v y_u$ with probability 1. Hence $||y_t - R^v y_u|| = d_{tu}$ as claimed. $\square$

5 Symmetry and Number of Solutions

Our strategy for proving that feasible GDMDGP instances have power of two solutions with probability 1 is as follows. We map embeddings $y \in X$ to binary sequences $\chi \in \{0, 1\}^n$ describing the “branching path” in the tree $\mathcal{T}$. We define a symmetry operation on $\chi$ by flipping its tail from a given component $i$ to its end (this operation is akin to branching at level 1). We show that the cardinality of the group of all such symmetries is a power of two by bijection with a set of binary sequences. Finally we prove that the cardinality of the symmetry group is the same as $|X|$.

For all leaf nodes $\alpha \in V$ with $\mu(\alpha) = \boxplus$ let $\chi(\alpha) = (\lambda(\beta) \mid \beta \in p(\alpha))$; since embeddings in $X$ are also in correspondence with leaf $\boxplus$-nodes of $\mathcal{T}$ by Alg. 1 Step 8 $\chi$ defines a relation on $X \times \{0, 1\}^n$.

5.1 Lemma
With probability 1, the relation $\chi$ is a function.

Proof. For $\chi$ to fail to be well-defined, there must exist an embedding $x$ which is in relation with two distinct binary sequences $\chi', \chi''$, which corresponds to the discriminant of the quadratic equation in the proof of Lemma 5.1 taking value zero at some rank $> K$, which happens with probability 0. $\square$

Let $\Xi = \{\chi(y) \mid y \in X\}$. For $y \in X$ let $y^i$ be its subsequence $(x_1, \ldots, x_i)$. We extend $\chi$ to be defined on all such subsequences by simply setting $\chi^i = (\chi(y_1), \ldots, \chi(y_i))$; $\chi(y)$ is valid if $y$ is a valid embedding.

Let $N = \{1, \ldots, n\}$ and $g$ be the $n \times n$ binary matrix such that $g_{ij} = 1$ if $i \leq j$ and 0 otherwise (the upper triangular $n \times n$ all-1 matrix); let $g_i$ be its $i$-th row vector and $\Gamma = \{g_i \mid i \in N\}$. Consider the elementwise modulo-2 addition in the set $F_2^n$ (denoted $\oplus$): this endows $F_2^n$ with an additive group structure with identity $e = (0, \ldots, 0)$ where each element is idempotent. Thus, $\mathcal{G} = (F_2^n, \oplus) \cong C_2^g$. This group naturally acts on itself (and subsets thereof) using the same $\oplus$ operation. It is not difficult to
prove that $G$ is a set of group generators for $G$ and a linearly independent set of the vector space $V$ given by $G$ with scalar multiplication over $\mathbb{F}_2$. For all $S \subseteq N$, let

$$g_S = \bigoplus_{i \in S} g_i,$$

and define a mapping $\phi : \mathcal{P}(N) \to G$ given by $\phi(S) = g_S$.

**5.2 Lemma**

$\phi$ is injective.

**Proof.** We show that for all $S, T \subseteq N$, if $g_S = g_T$ then $S = T$.

$$\begin{align*}
g_S &= g_T \\
\Rightarrow \quad \bigoplus_{i \in S} g_i &= \bigoplus_{i \in T} g_i \\
\Rightarrow \quad \bigoplus_{i \in S} g_i \oplus \bigoplus_{i \in S} g_i &= \bigoplus_{i \in T} g_i \\
\text{idempotency} \quad \Rightarrow \quad \bigoplus_{i \in S \Delta T} g_i &= \bigoplus_{i \in S \Delta T} g_i \\
\Rightarrow \quad S \Delta T &= \emptyset \\
\Rightarrow \quad S &= T.
\end{align*}$$

This concludes the proof. \hfill \Box

**5.3 Lemma**

For all $H \subseteq \Gamma$, $|\langle H \rangle| = 2^{|H|}$.

**Proof.** The restriction of function $\phi$ to $\mathcal{P}(H)$ is injective by Lemma 5.2. Furthermore, each element $g$ of $\langle H \rangle$ can be written as $\bigoplus_{i \in S} g_i$ for some $S \subseteq H$ because $H$ is a spanning set for the vector space $H$ over $\mathbb{F}_2$, which is setwise equal to the group $\langle H \rangle$. Thus $\phi$ is surjective too. Hence $\phi$ is a bijection between $\mathcal{P}(H)$ and $\langle H \rangle$, which yields the result. \hfill \Box

Let $I$ be the set of levels of $T$ for which from all nodes with two valid children there is a path going to a feasible leaf through both children. Let $L = \{ g_i \in \Gamma \mid i \in I \}$ and $\Lambda = \langle L \rangle$ be the subgroup of $G$ generated by $L$.

**5.4 Theorem**

If $\Xi \neq \emptyset$, for all $\xi \in \Xi$ we have $\xi \oplus \Lambda = \Xi$ with probability 1.

**Proof.** ($\Rightarrow$) We show that $\xi \oplus \Lambda \subseteq \Xi$ with probability 1; because $\langle L \rangle = \Lambda$ it suffices to show that $\xi \oplus g_i \in \Xi$ for an arbitrary $g_i \in L$, i.e. that there exists a valid embedding $w \in X$ such that $\chi(w) = \xi \oplus g_i$. Let $y \in \chi^{-1}(\xi)$ and $v = \rho^{-1}(i)$ such that $\Upsilon(y, v)$, and define $w = \tilde{R}^y v$ (where $\tilde{R}^y$ is defined in Thm. 4.8 above); by Thm. 4.8 $w \in X$. Let $\alpha'$ be the leaf node of $T$ such that $x(\alpha') = y$; by Lemma 3.3 there is a leaf node $\beta'$ such that $x(\beta') = w$. We have to show that for all $\ell \geq i$ the node $\beta \in p(\beta') \cap V_i$ is such that $\lambda(\beta) = 1 - \lambda(\alpha)$, where $\alpha$ is the node in $p(\alpha') \cap V_i$. We proceed by induction on $\ell$. For $\ell = i$ this holds by Lemma 3.2. For $\ell > i$, the induction hypothesis allows us to apply Lemma 4.2 and conclude that the event $\lambda(\alpha) = 1 - \lambda(\beta)$ occurs with probability 1.

($\Leftarrow$) Now we show that $\Xi \subseteq \xi \oplus \Lambda$ with probability 1, i.e. for any $\eta \in \Xi$ there is $g \in \Lambda$ with $\xi \oplus g = \eta$. We proceed by induction on $n$, which starts when $n = K + 1$: if $K + 1 \not\in I$ then $|\Xi| = 1$, $L = \emptyset$ and the
theorem holds; if \( K + 1 \in I \) then \(|\Xi| = 2, L = \{g_{K+1}\}\) and the theorem holds. Now let \( n > K + 1 \); for all \( j \in \{K + 1, \ldots, n - 1\}\) define \( \Xi^j = \{x \mid x \in \Xi\} \) and \( L^j = \{g_{\ell} \mid \ell \in I \land \ell \leq j\} \). By the induction hypothesis, for all \( \xi^j \in \Xi^j \) \( (\xi^j \oplus (L^j) = \Xi^j) \). Now, either \( n \not\in I \) or \( n \in I \); by Prop. 5.5 with probability 1 if \( n \not\in I \) then nodes in \( \mathcal{V}_{n-1} \) can only have zero or one feasible subnode (let \( B^n_1 \) be the set of all such feasible subnodes), and if \( n \in I \) then nodes in \( \mathcal{V}_{n-1} \) can only have zero or two feasible subnodes \( \beta \) (let \( B^n_2 \) be the set of all such feasible subnodes). In the former case we let \( \Xi^n = \{\xi(x(\beta)) \mid \beta \in B^n_1\} \) and \( L^n = L^{n-1} \); in the latter we let \( \Xi^n = \{\xi(x(\beta)) \mid \beta \in B^n_2\} \) and \( L^n = L^{n-1} \cup \{g_n\} \). In both cases it is easy to verify that the theorem holds for \( \Xi^n, L^n \); in the former case it follows by the induction hypothesis, and in the latter case it follows because \( g_n = (0, \ldots, 0, 1) \), namely, if \( \eta \in \Xi \) and \( n \in I \) then take \( \xi = \eta \oplus g_n \) (the result follows by idempotency of \( g_n \)).

5.5 Corollary
If a GDMDGP instance is feasible, \(|X|\) is a power of two with probability 1.

Proof. By Lemma 5.1 \( \chi \) is a function with probability 1. Let \( x, x' \in X \) be distinct; then by Alg. 1 Steps 26, 28, 32, and 34, the map \( \chi : X \rightarrow \Xi \) is injective. By definition of \( \Xi \) it is also surjective, hence \(|X| = |\Xi| \). By Thm. 5.4 \( \Xi = |\chi \oplus A| \) for all \( \chi \in \Xi \) with probability 1. It is easy to show that \(|\chi \oplus A| = |A|\), so by Lemma 5.3 \(|X|\) is a power of two with probability 1.

6 Counterexamples

We discuss a class of counterexamples to the conjecture that all GDMDGP instances have a number of solutions which is a power of two (also see Lemma 5.1 in [4]). All these counterexamples are hand-crafted and have the property that two distinct embeddings \( x, x' \) have at least a level \( i \) where \( x_i = x'_i \), which is an event which happens with probability 0. For any \( K \geq 1 \), let \( n = K + 3, V = \{1, \ldots, n\}, E = \{\{i, j\} \mid 0 < i - j \leq K\} \cup \{\{1, n\}\} \) and \( d_{ij} = 1 \) for all \( \{i, j\} \in E \). The first \( n - 2 = K + 1 \) points can be embedded in the vertices of a regular simplex in dimension \( K \); then either \( x_{n-1} = x_1 \) or \( x_{n-1} \) is the symmetric position from \( x_1 \) with respect to the hyperplane through \( \{x_2, \ldots, x_{n-2}\} \). In the first case, the two positions for \( x_n \) are valid, in the second only \( x_n = x_2 \) is possible (see Fig. 4 for the 2-dimensional case), yielding a YES instance where \(|X| = 6\).

![Figure 4: The counterexample in the case \( K = 2 \). Embeddings \( x_5^{(00)}, x_5^{(01)}, \) and \( x_5^{(1)} \) are valid, while \( x_5^{(10)} \) is not.](image)

Lastly, Fig. 5 shows an example where the \((4) \Rightarrow (i)\) implication of Lemma 4.2 fails for instances in
DDGP \ GDMDGP. This shows that any generalization of our result to the DDGP is not trivial. Let $V = \{1, \ldots, 6\}$ (the graph drawing is the same as the embedding in $\mathbb{R}^2$). The nodes $5', 6'$ linked with dashed lines show alternative node placements. Let $U_5 = \{3, 4\}$ and $U_6 = \{1, 2\}$. The line through the points $3, 4$ does not provide a valid reflection mapping $6$ to $6'$. This happens because $U_6$ does not consist of the two immediate predecessors of $6$.

Figure 5: A counterexample to Lemma 4.2 applied to DDGP \ GDMDGP.

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