Distance constraints in Euclidean geometry

Leo Liberti

IBM Research, Yorktown Heights

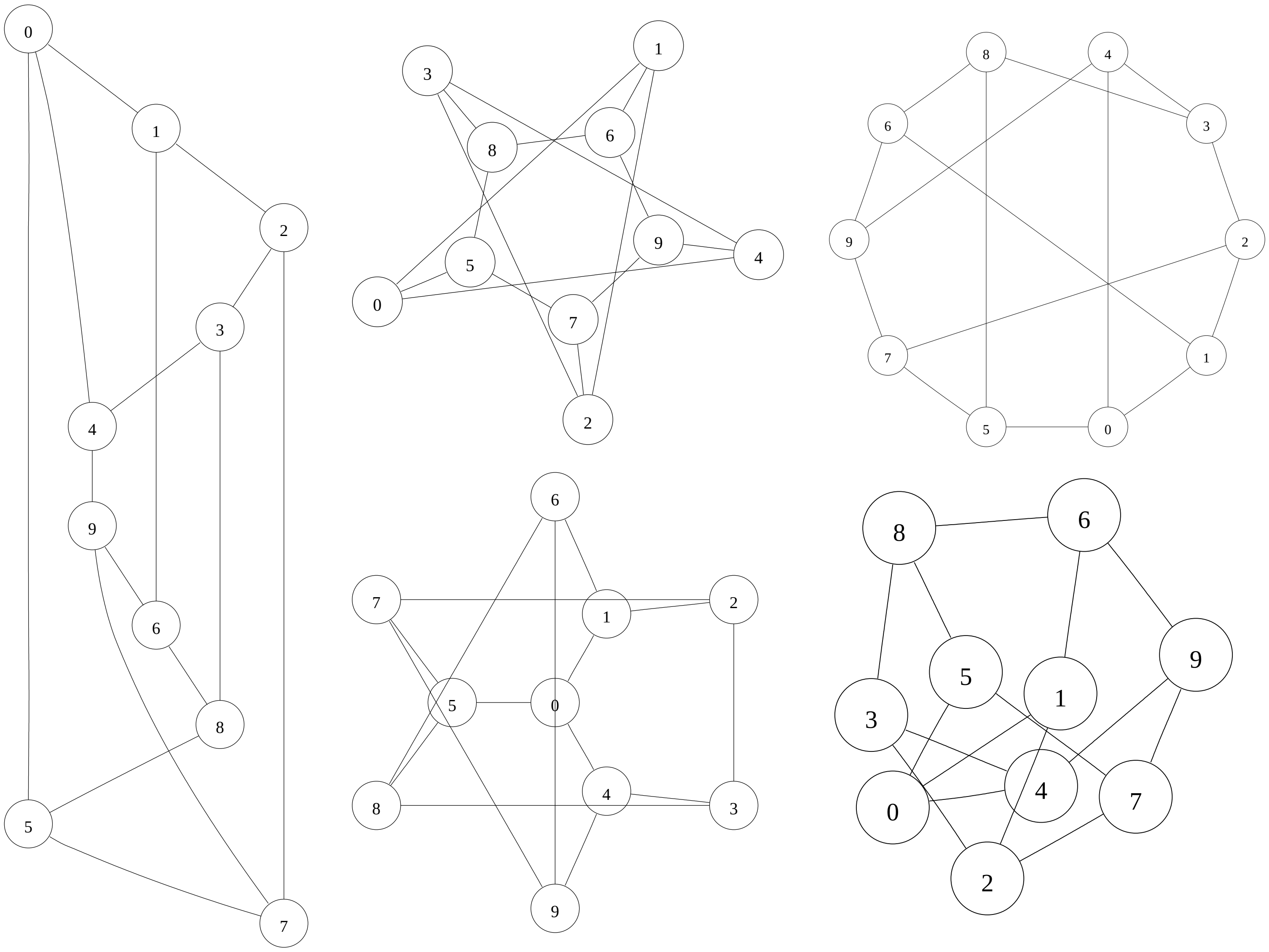
LIX, Ecole Polytechnique, France

Joint work with:

C. Lavor (IMECC-UNICAMP), N. Maculan (COPPE-UFRJ), A. Mucherino (Univ. Rennes)

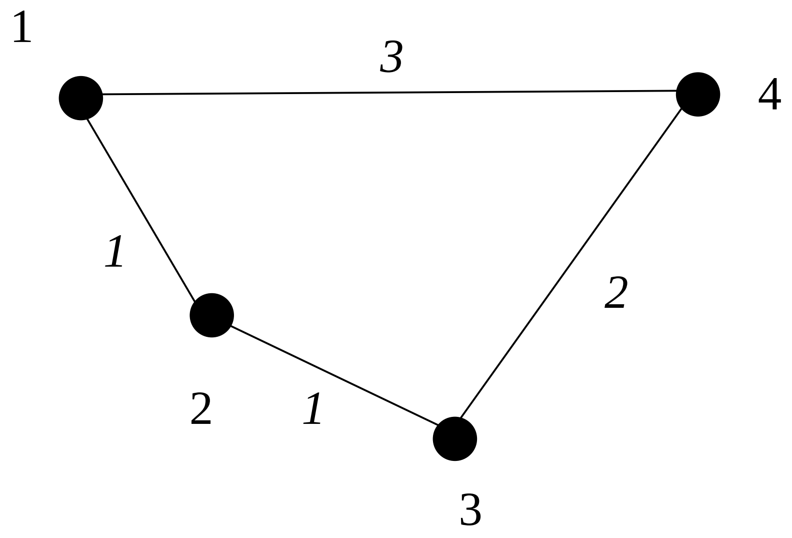
J. Lee (Univ. Michigan), B. Masson (INRIA), M. Nilges (Inst. Pasteur), T. Malliavin (Inst. Pasteur)

At a glance



Which graph has most symmetries?

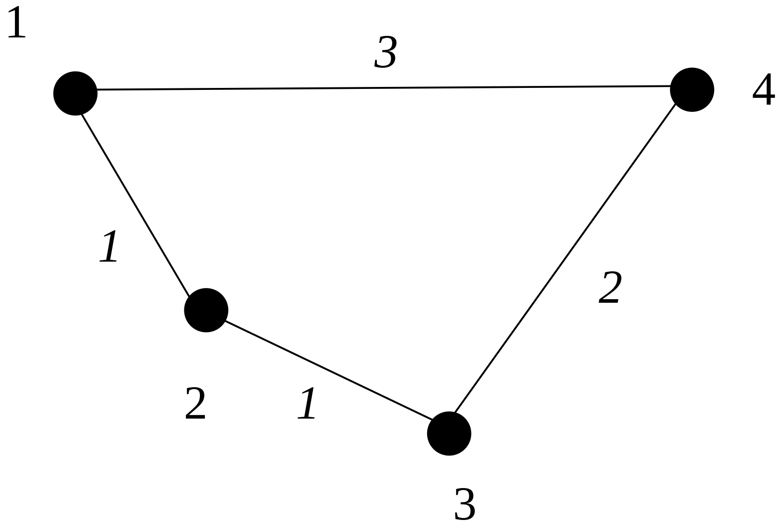
How does a weighted graph look?



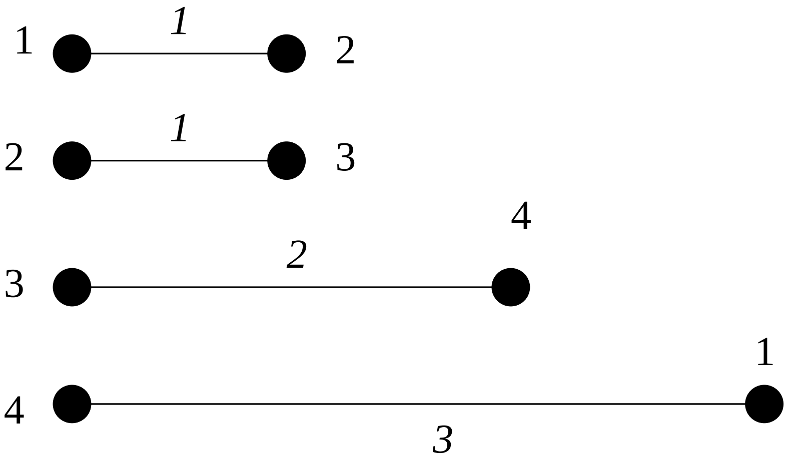
- Like this?

How does a weighted graph look?

- Like this?



- Perhaps like this?



Motivation I: Don’t confuse a graph with its drawing

Completing partial matrices

- Schoenberg's theorem:
  Euclidean Distance Matrix Completion Problem ⇔
  Positive Semidefinite Matrix Completion Problem
- Low-rank matrix completion relaxations
- Covariance/correlation matrix completions

Motivation II:
Drawing conclusions from partial data

Many applications

Applications:

- Phase retrieval — 1D
- Wireless sensor network localization — 2D
- Molecular conformation — 3D
- Multidimensional scaling — (whatever)D

Motivation III: Variety: a new dimension, a new application!

A nonlinear system

- Given a simple weighted undirected graph $G = (V, E)$ with a distance function $d : E \to \mathbb{R}_+$, solve the constraint system:

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

- Obtain an embedding $x : V \to \mathbb{R}^2$
- Computationally OK up to 5-10 vertices

Global optimization

- Reformulate (1) to

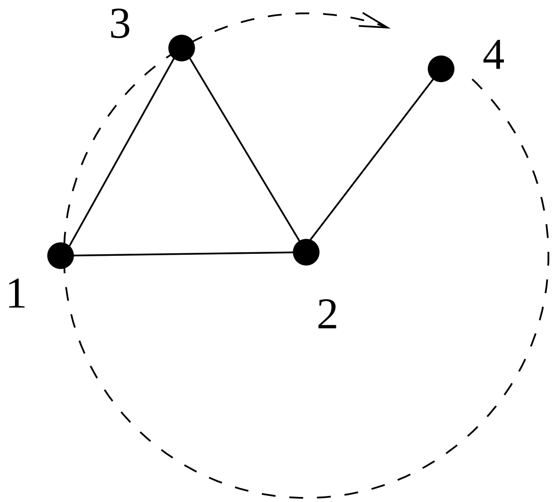
$$\min_{x} \sum_{\{u,v\}\in E} (\|x_u - x_v\|^2 - d_{uv}^2)^2 \tag{2}$$

- G has an embedding $\Leftrightarrow$ optimum x^* of (2) has value 0.
- Eq (2) is nonconvex in x
- Computationally OK up to 100 vertices
- Surveys: [ITOR(2010), EJOR(2012), SIREV(to appear)]

Large-scale methods: Exploiting the combinatorial structure

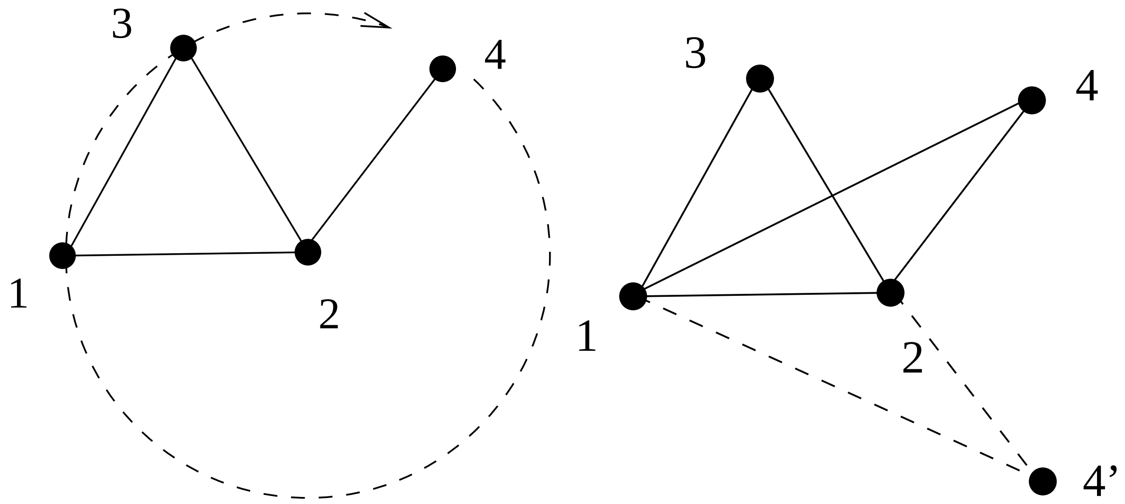
The number of embeddings

- Uncountably many (incongruent) embeddings



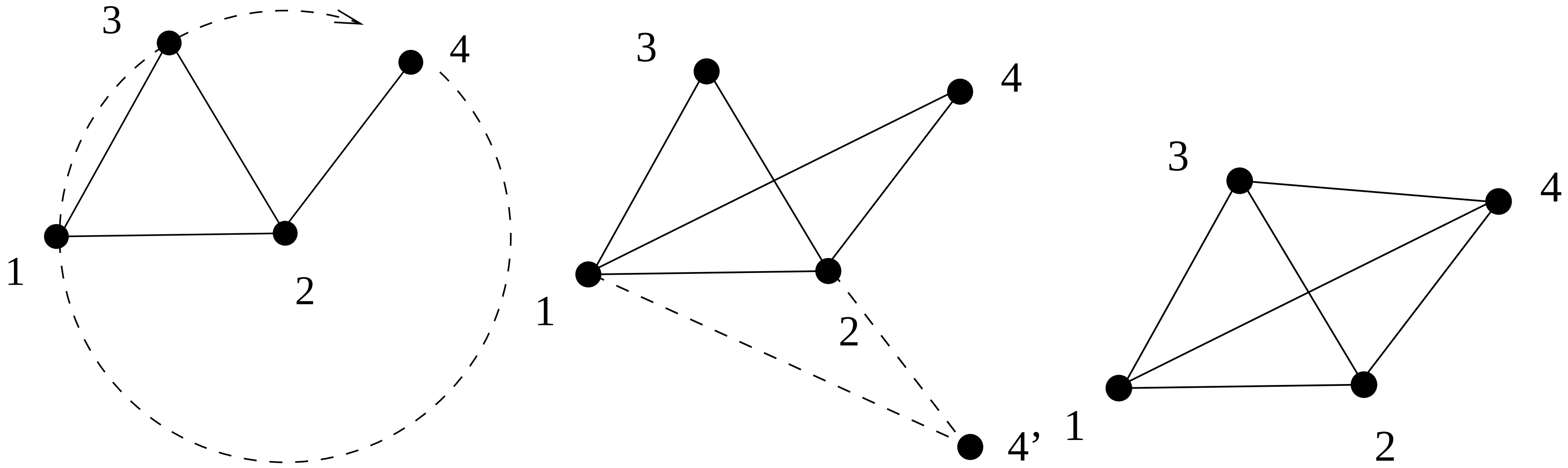
The number of embeddings

- Uncountably many (incongruent) embeddings
- Finitely many



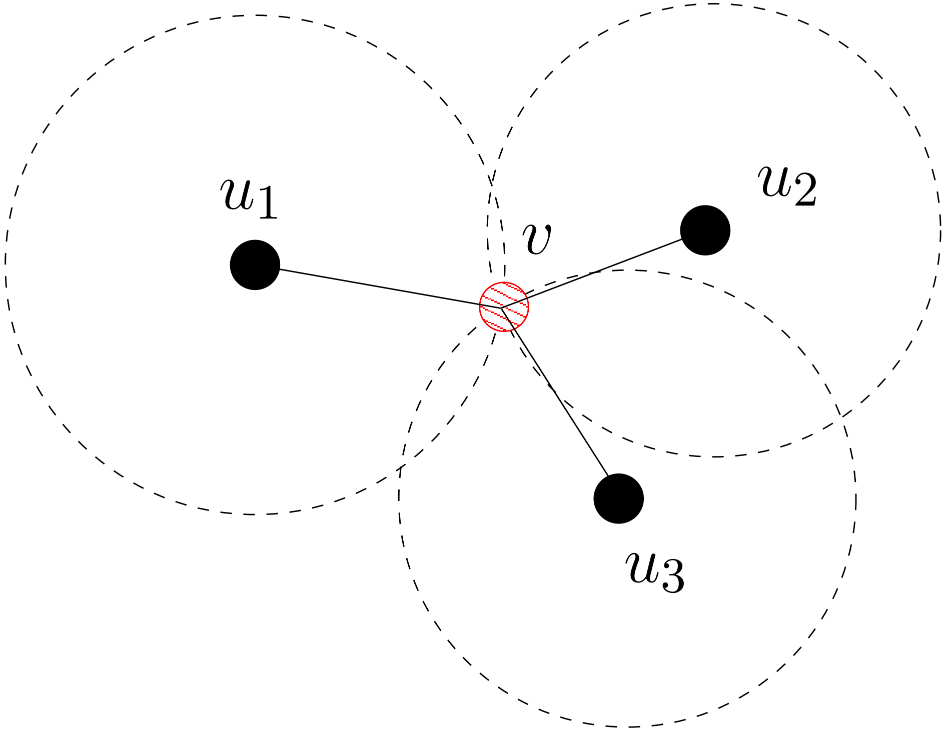
The number of embeddings

- Uncountably many (incongruent) embeddings
- Finitely many
- At most one



Cannot have countably infinitely many solutions

Trilateration



v has $\geq K+1$ adjacencies with known general positions $\Rightarrow$

If system has a solution, find x_v in polytime

A linear system

Let $v \in V$ be adjacent to $1, 2, 3$

x_1, x_2, x_3 known, find $x_v \in \mathbb{R}^2$

$$\begin{array}{rcl} \|x_v - x_1\|^2 & = & d^2_{1v} \\ \|x_v - x_2\|^2 & = & d^2_{2v} \\ \|x_v - x_3\|^2 & = & d^2_{3v} \end{array} \Rightarrow \begin{array}{rcl} \|x_v\|^2 - 2x_v \cdot x_1 + \|x_1\|^2 & = & d^2_{1v} \text{ (3)} \\ \|x_v\|^2 - 2x_v \cdot x_2 + \|x_2\|^2 & = & d^2_{1v} \text{ (4)} \\ \|x_v\|^2 - 2x_v \cdot x_3 + \|x_3\|^2 & = & d^2_{1v} \text{ (5)} \end{array}$$

(5)-(3)
(5)-(4)

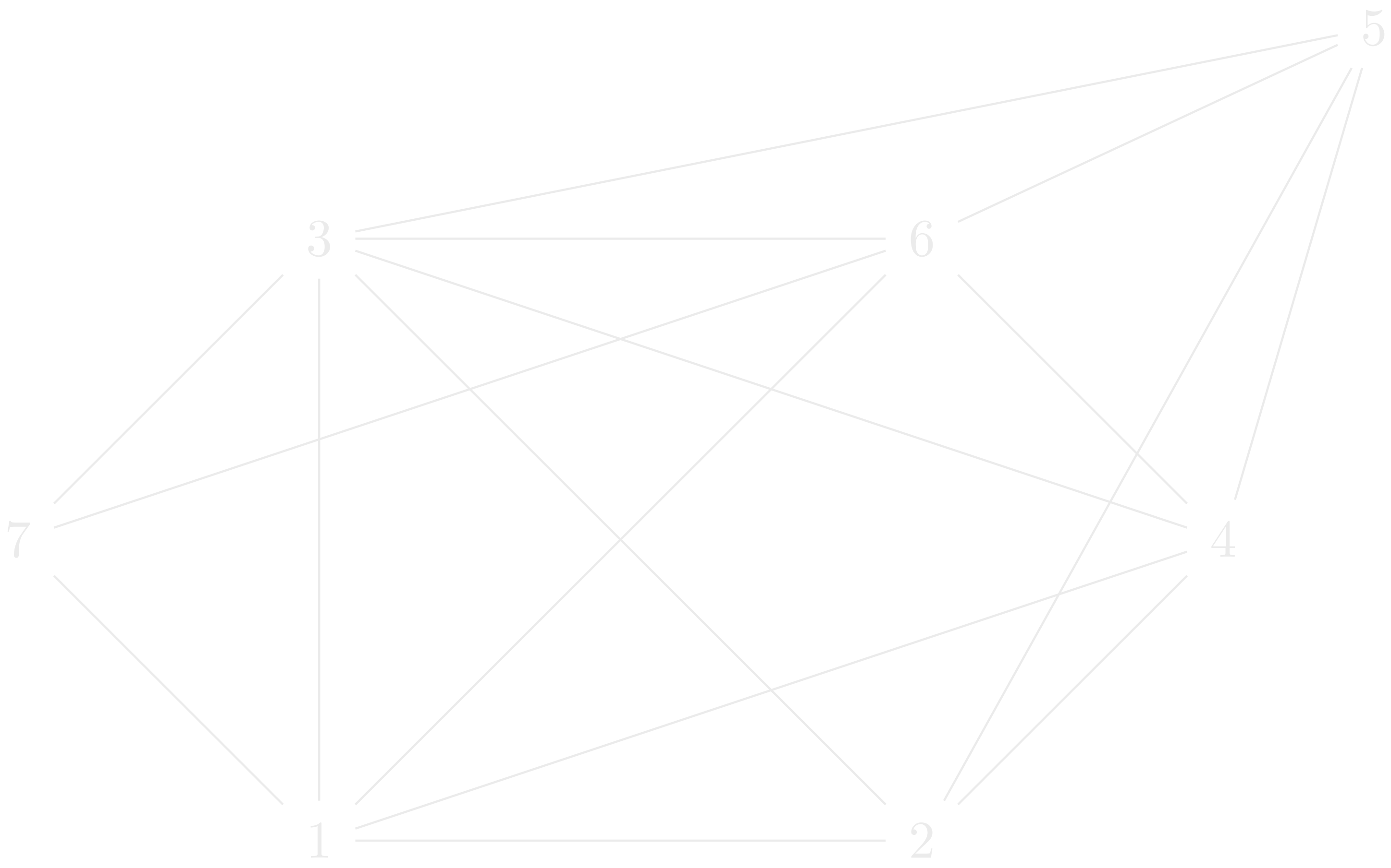
$$\Rightarrow \left(\begin{array}{c} 2(x_1 - x_3) \\ 2(x_2 - x_3) \end{array} \right) x_v = \left(\begin{array}{c} (\|x_1\|^2 - \|x_3\|^2) - (d^2_{1v} - d^2_{3v}) \\ (\|x_2\|^2 - \|x_3\|^2) - (d^2_{2v} - d^2_{3v}) \end{array} \right)$$

Solve $K \times K$ system in polytime

$\Rightarrow$ but $\not\Leftarrow$: Cannot detect infeasibility

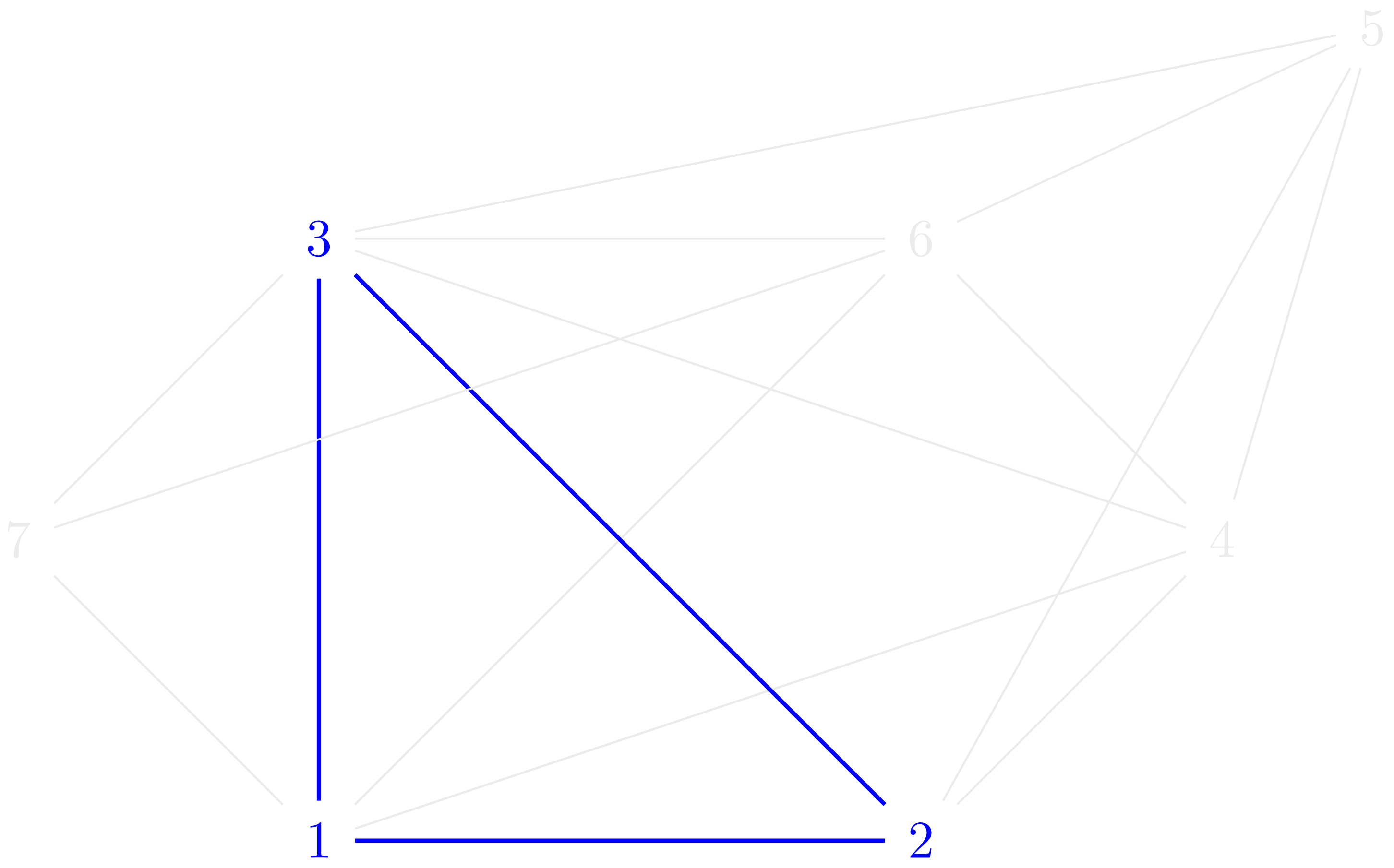
Combinatorial iterative approach

$$V = \{1, 2, 3, 4, 5, 6, 7\}$$



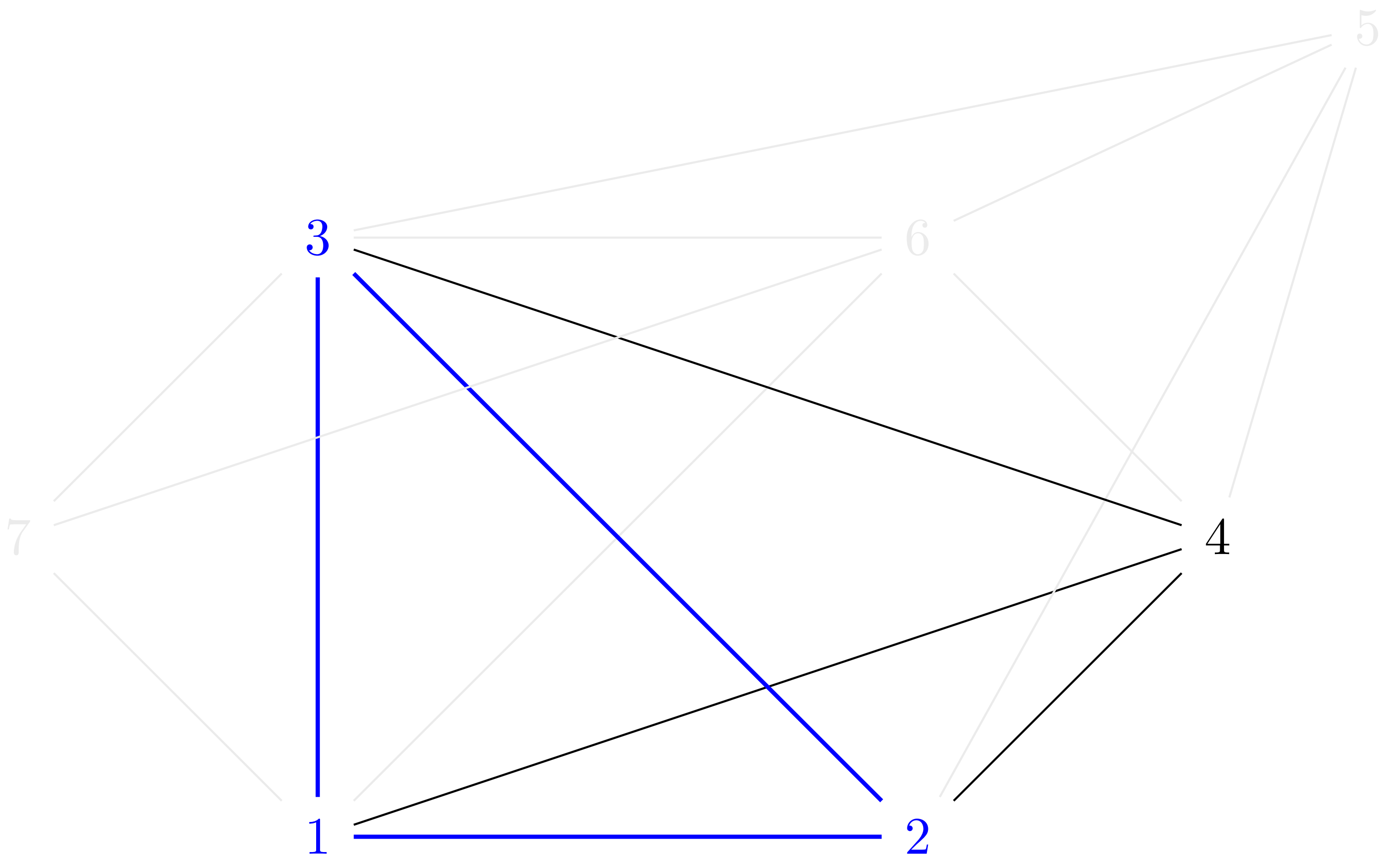
Combinatorial iterative approach

$$V = \{1,2,3,4,5,6,7\}$$



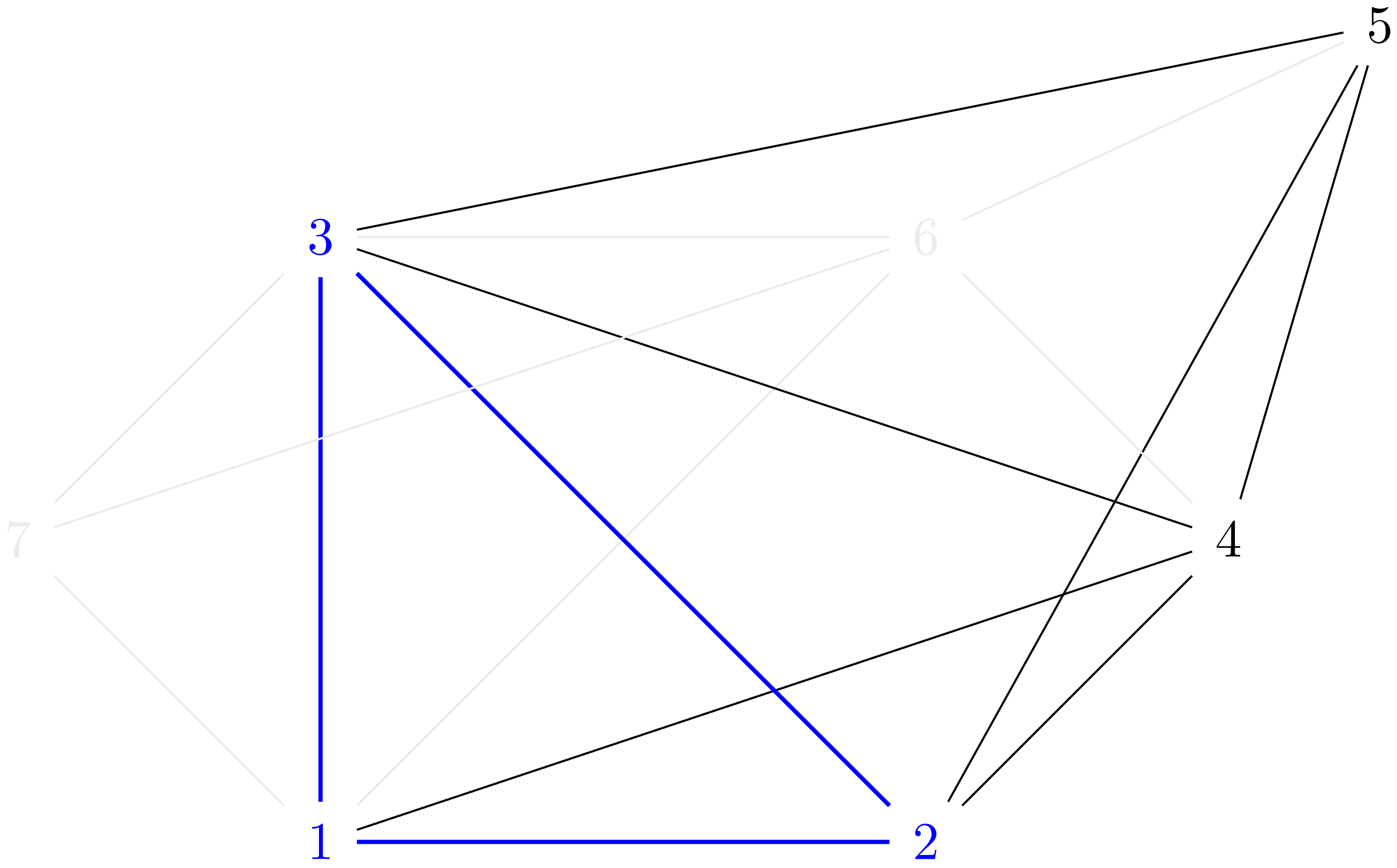
Combinatorial iterative approach

$$V = \{1, 2, 3, 4, 5, 6, 7\}$$



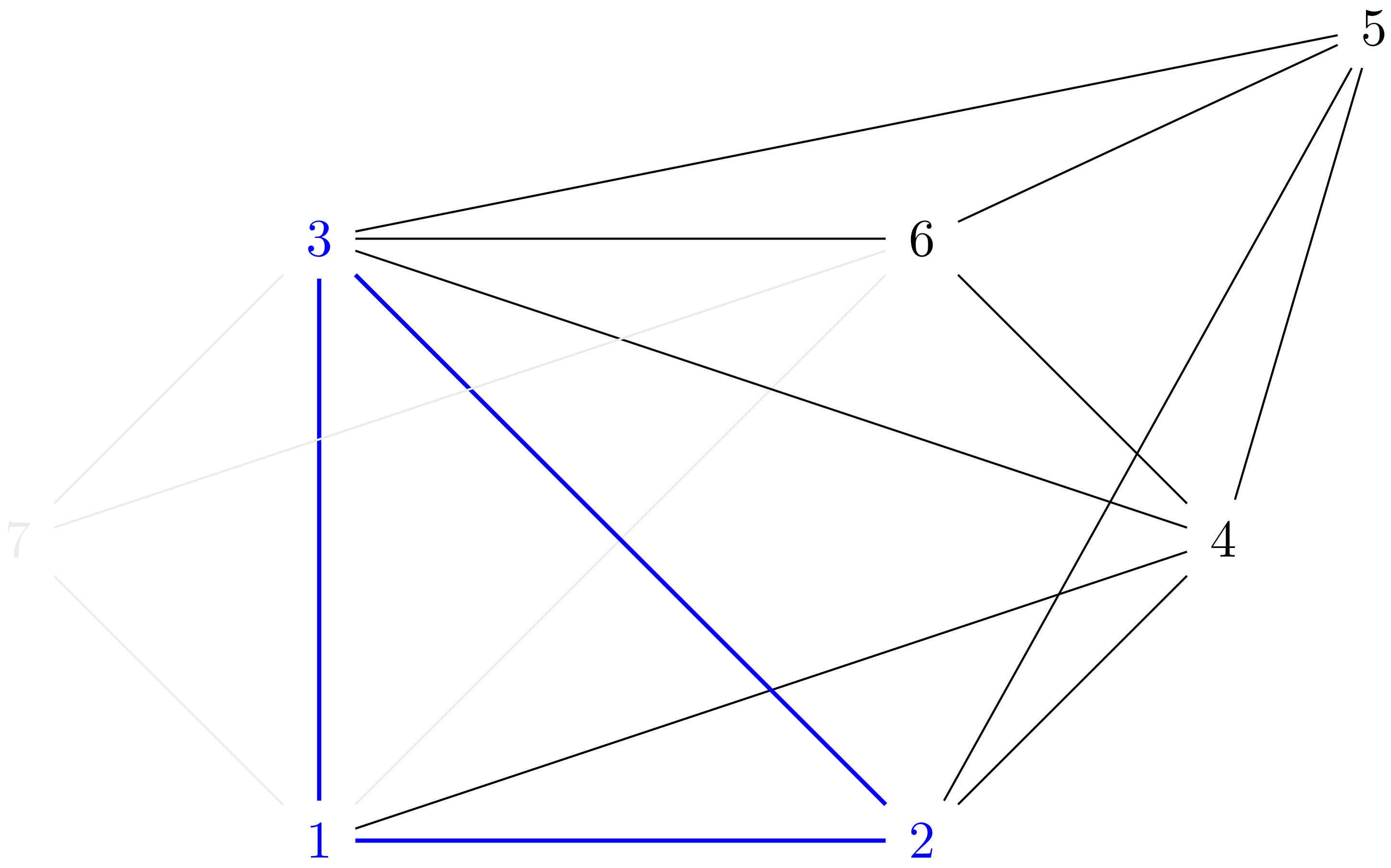
Combinatorial iterative approach

$$V = \{1, 2, 3, 4, 5, 6, 7\}$$



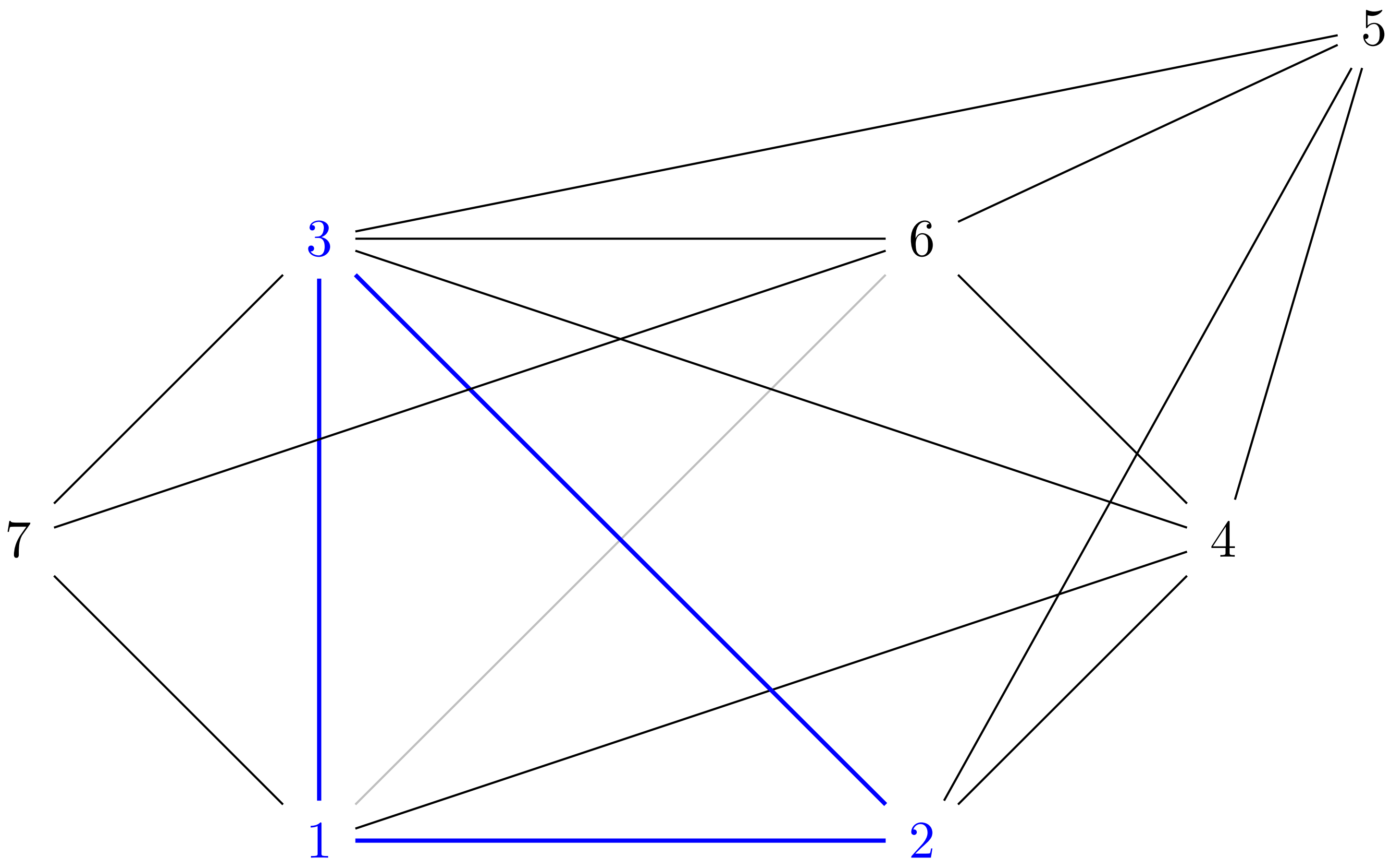
Combinatorial iterative approach

$$V = \{1, 2, 3, 4, 5, 6, 7\}$$



Combinatorial iterative approach

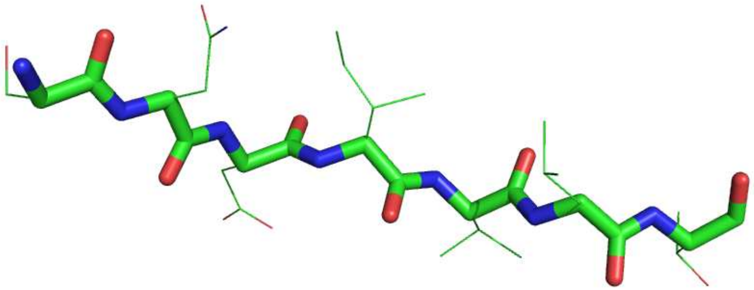
$$V = \{1, 2, 3, 4, 5, 6, 7\}$$



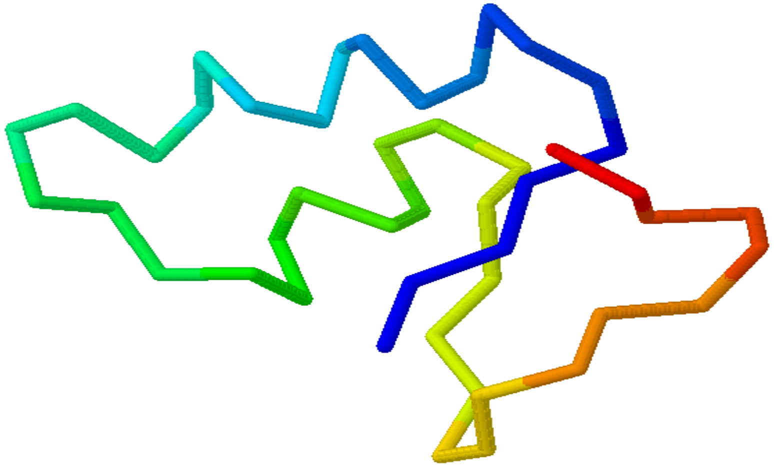
Does it work on my favourite application?

Proteins

- Proteins: *backbone* and *side chains*



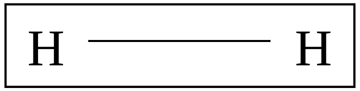
- Backbone: total order $<$ on a set V of atoms



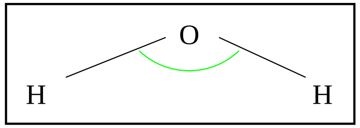
- Assume known embedding for backbone; embedding side chains is known as SIDE CHAIN PLACEMENT PROBLEM

Protein distances

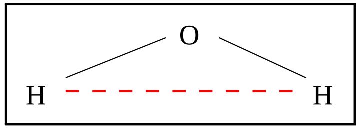
- Covalent bond distances $d_{v-1,v}$ are known



- Angles between covalent bonds are known



- $\Rightarrow d_{v-2,v}$ is known for all $v > 3$

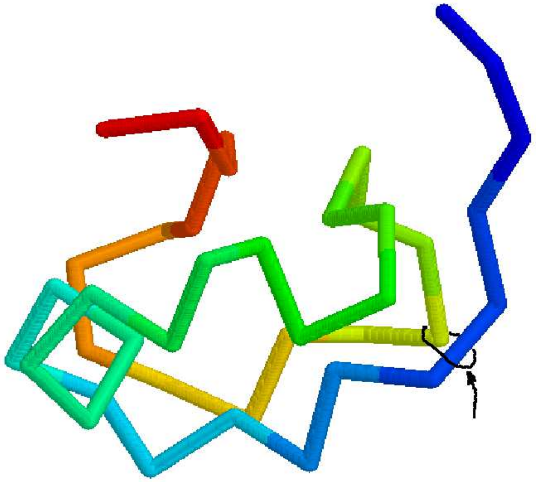


- Distances $d_{v-3,v}$ are always < 6Å, so they can be measured using NMR techniques

  We assume these distances are exact: this is false in practice, but we can find orders for which this assumption holds (see later if I have time)

- NMR might give other distances too

Atoms may be distant order-wise but closer than 6Å in space



Discretizable MDGP

- Protein backbones: 3 consecutive predecessors in 3D
- Weaken the condition $\geq K+1$ adjacent predecessors in $\mathbb{R}^K$ to:

$\geq K$ consecutive adjacent predecessors in $\mathbb{R}^K$

- DMDGP: complete an initial partial embedding in this setting
- **NP**-hard [Lavor et al. COAP 2012]

Adapt the iterative method?

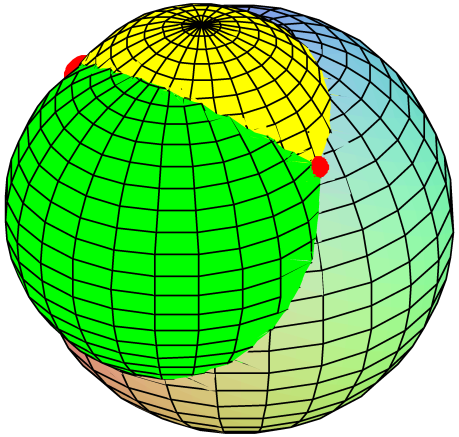
Sphere intersections

For given $v > 3$,

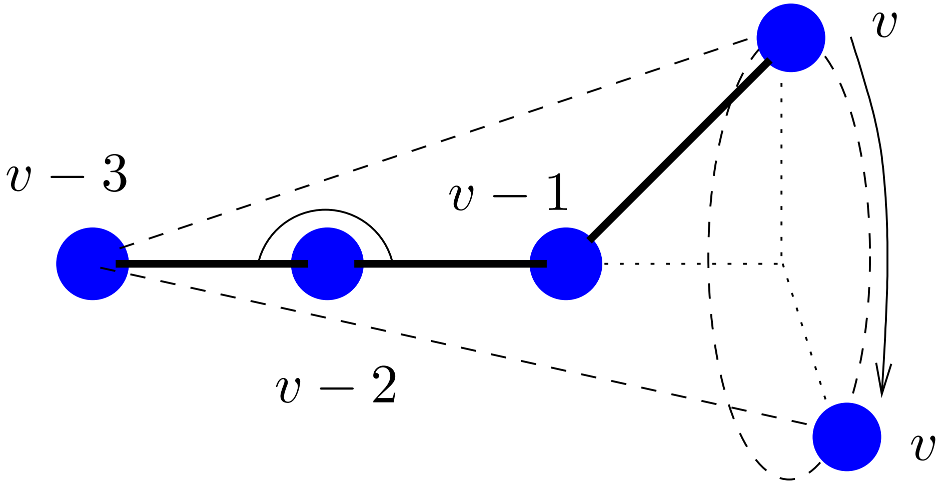
- $x_{v-3}, x_{v-2}, x_{v-1}$ are known
- $d_{v,v-1}, d_{v,v-2}, d_{v,v-3}$ are known

find x_v

Non-empty intersection of K spheres in $\mathbb{R}^K$ contains 2 points in general



When does it fail?



Branch-and-Prune

v: rank of current atom $x_{<v}$: partial embedding to rank $v-1$
G: instance X: current pool of embeddings
$S(y,r)$: $\mathbb{R}^K$ sphere centered at y with radius r

```
BranchAndPrune($v$, $x_{<v}$, $G$, $X$):
  Let $\mathcal{S} \leftarrow \bigcap_{i\in\{1,\ldots,K\}} S(x_{v-i}, d_{v-i,v})$ =($\{s_1, s_2\}$ or $\varnothing$)
  for $s \in \mathcal{S}$ do
    Extend current embedding to $x = (x_{<v}, s)$
    if $\forall u \in$ AdjPred($v$) $\|x_u - x_v\| = d_{uv}$ then
      if ($v = n$) then
        Let $X \leftarrow X \cup \{x\}$
      else
        BranchAndPrune($v+1$, $x$, $G$, $X$)
      end if
    end if
  end for
```

BP properties

- BP: worst-case exponential time
- With probability 1, find all incongruent embeddings of G extending initial partial embedding
- Performs very efficiently (speed and accuracy)

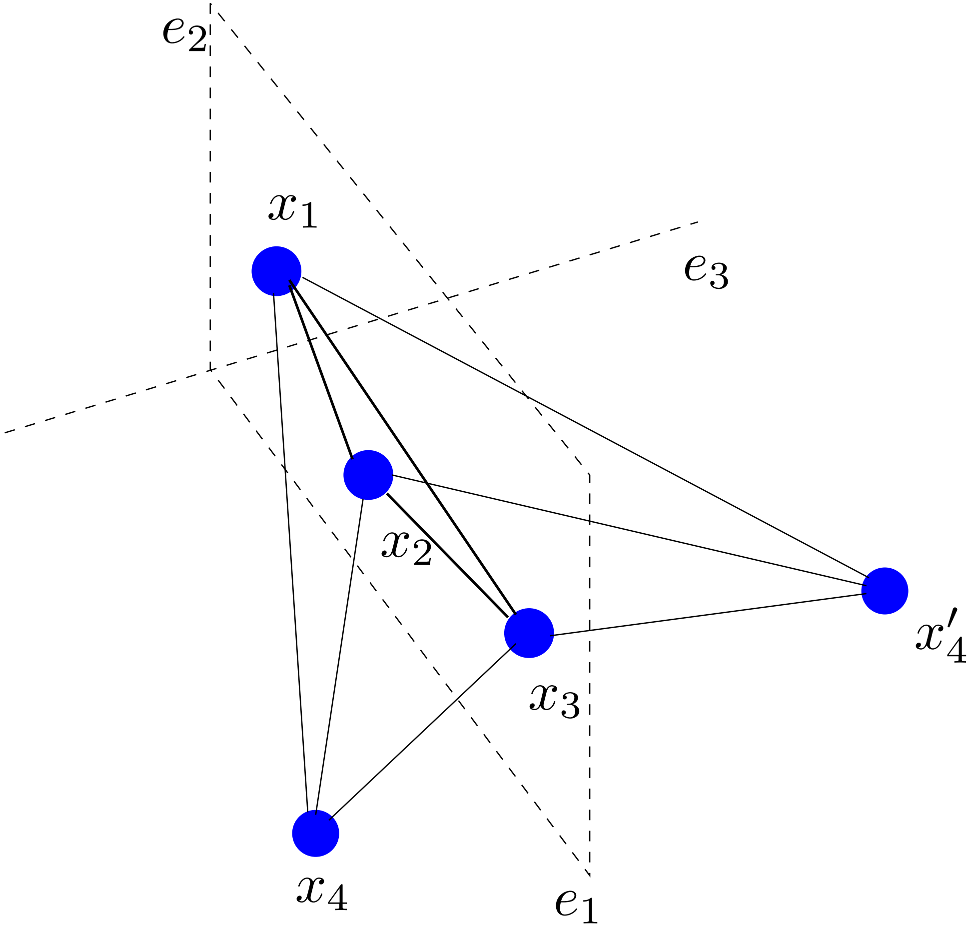
  Embed 10,000 vertices in a 13 seconds of CPU time
- Two empirical observations:
  1. **the number of solutions it finds is always a power of two**
  2. $|V|$ **versus CPU time plots are always linear-like for PDB**

Symmetry

BP root node symmetry

[Lavor et al. COAP, to appear]

- x'_4 is a reflection of x_4 w.r.t. the plane defined by x_1, x_2, x_3
- $\Rightarrow$ BP tree symmetric below level 3
- Start branching from level 4, not 3



Number of solutions

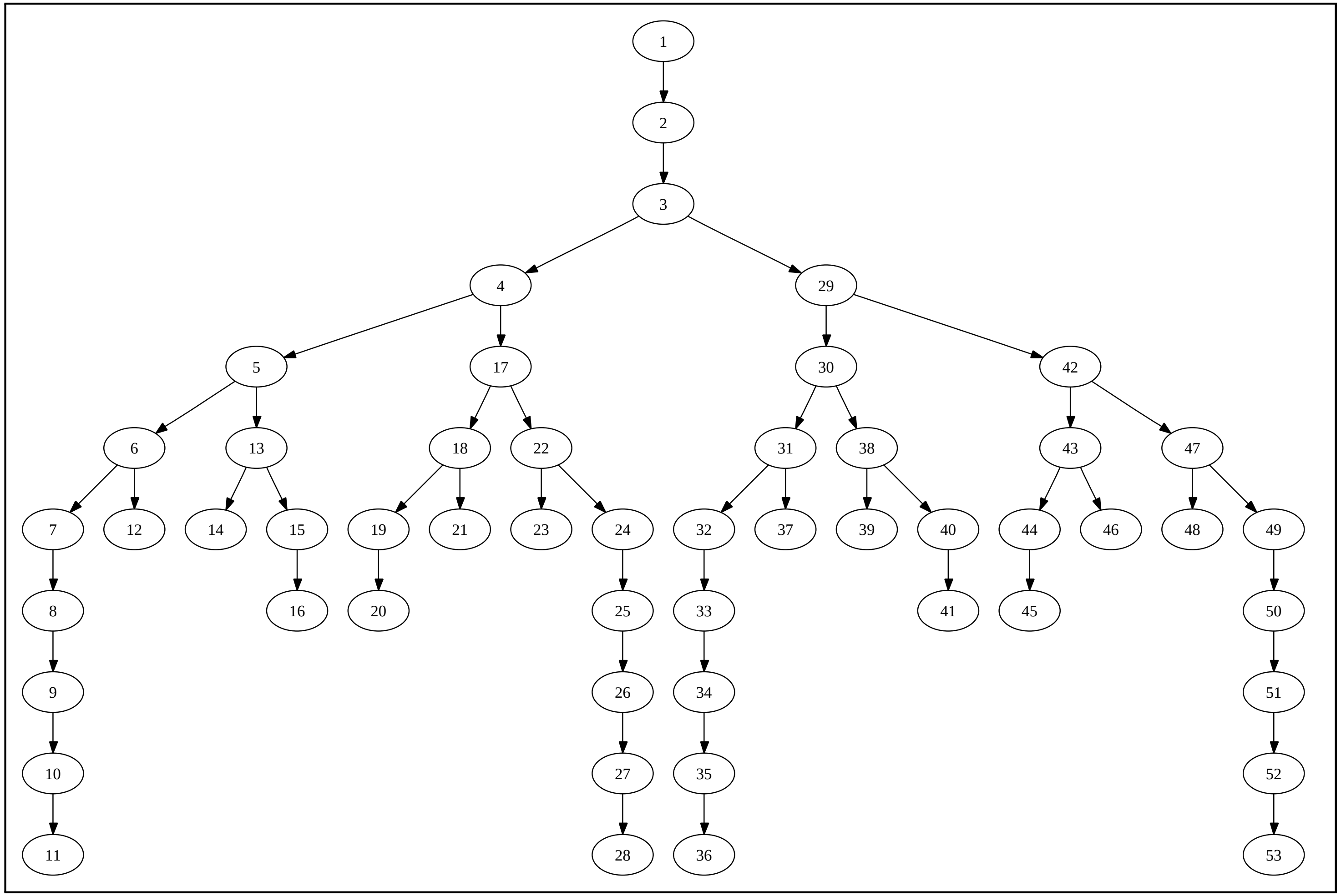
Instance	$\lvert X\rvert$
`mmorewu-2`	2
`mmorewu-3`	2
`mmorewu-4`	4
`mmorewu-5`	4
`mmorewu-6`	4
`lavor10_0`	4
`lavor15_0`	16
`lavor20_0`	8
`lavor25_0`	8
`lavor30_0`	2
`lavor35_0`	64
`lavor40_0`	2
`lavor45_0`	2
`lavor50_0`	4096
`lavor55_0`	64
`lavor60_0`	64

Instance	$\lvert X\rvert$
`1brv`	2
`1aqr`	4
`2erl`	2
`1crn`	2
`1ahl`	16
`1ptq`	2
`1brz`	4
`1hoe`	2
`1lfb`	2
`1pht`	2
`1jk2`	2
`1f39a`	2
`1acz`	8
`1poa`	2
`1fs3`	2
`1mbn`	2
`1rgs`	2
`1m40`	2
`1bpm`	2
`1n4w`	2
`1mqq`	2
`1rwh`	2
`3b34`	2
`2e7z`	2
`1epw`	2

For all tested DMDGP instances, $\exists \ell \in \mathbb{N}$ such that $|X| = 2^\ell$

A BP search tree example

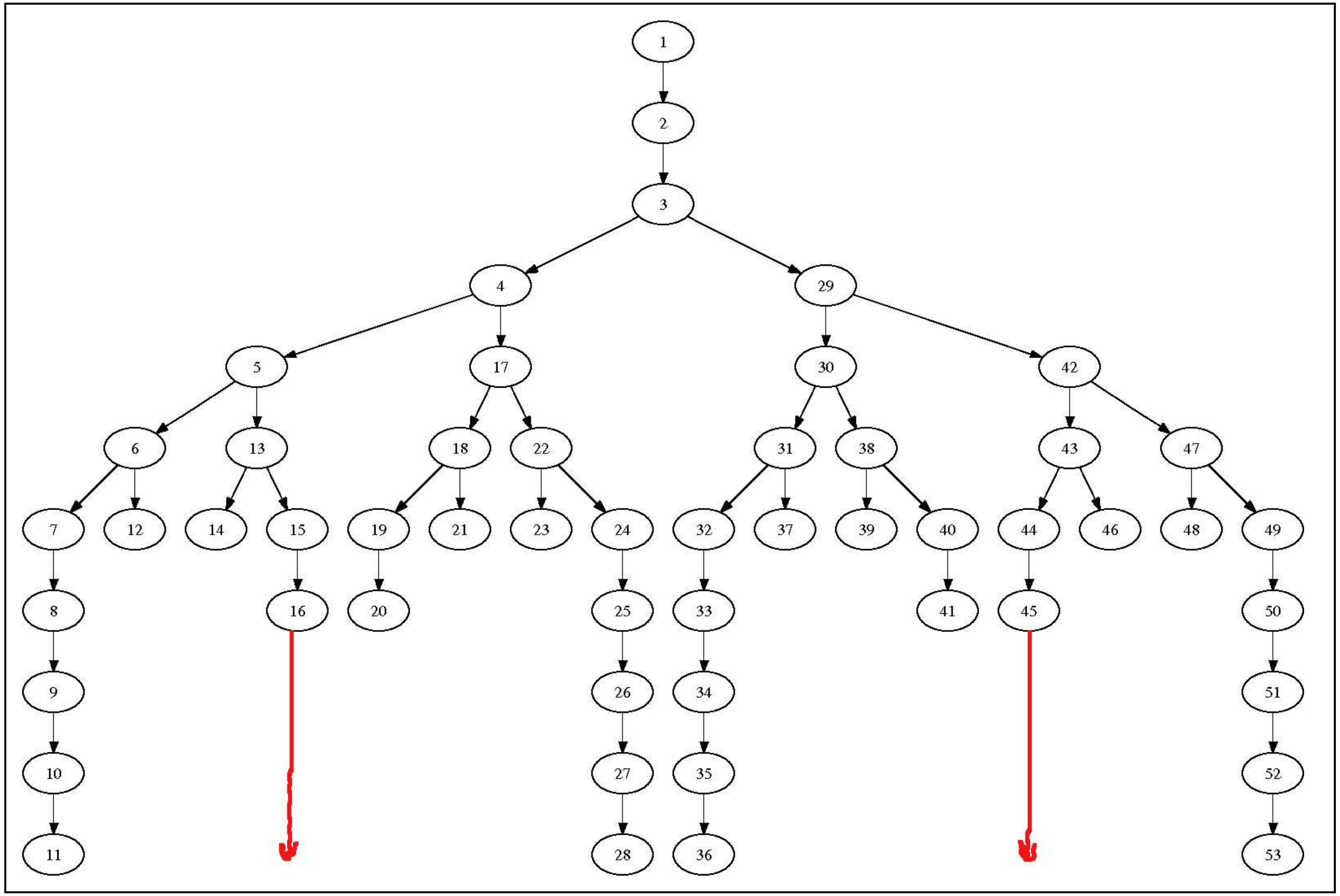
- Typical BP search tree (embeddings = paths root→leaves)



- Root node symmetry: $|X|$ is even
- No evident reason why $|X|$ should be a power of two

A BP search tree example

- Typical BP search tree (embeddings = paths root→leaves)



- Root node symmetry: $|X|$ is even
- No evident reason why $|X|$ should be a power of two (why not symmetric paths to level $|V|$ from nodes 16 and 45?)

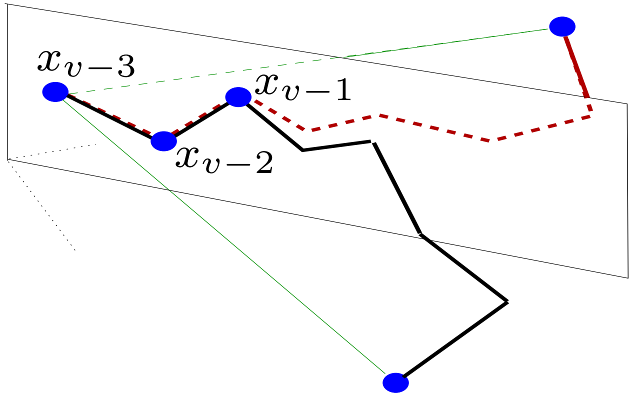
Discretization/pruning distances

- Let $E_D = \{\{u,v\} \mid |u-v| \le K\}$ and $E_P = E \smallsetminus E_D$
- E_D: **discretization distances**
  - they guarantee that the instance is a DMDGP
  - they allow the construction of the complete BP tree
  - this tree has $2^{|V|-3}$ leaves, $2^{|V|-4}$ if we consider root node symmetry
- E_P: **pruning distances**
  - they allow pruning of the BP tree
  - not clear why they should prune branches symmetrically

Symmetry by pruning distances

[Liberti et al., LNCS (COCOA), 2011]

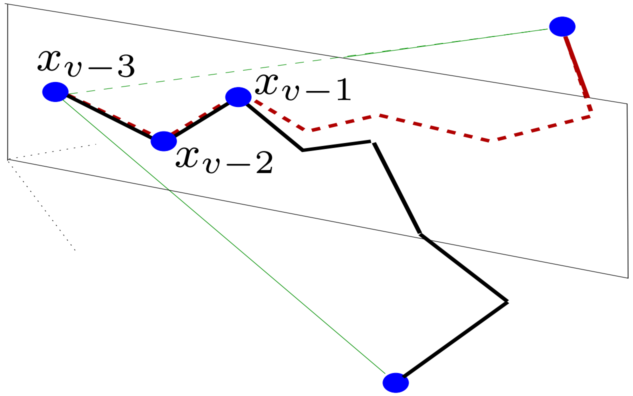
Given embedding x, $R_x^v =$ reflection w.r.t. hyperplane $x_{v-K}, \ldots, x_{v-1}$



Symmetry by pruning distances

[Liberti et al., LNCS (COCOA), 2011]

Given embedding x, $R^v_x =$ reflection w.r.t. hyperplane $x_{v-K}, \ldots, x_{v-1}$



Thm.

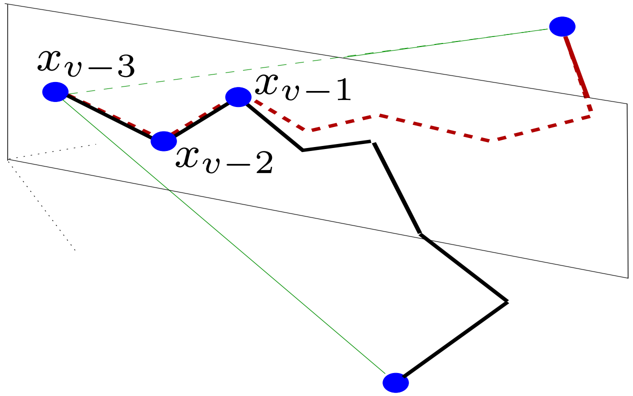
With prob. 1, for each $u, v \in V$ with $v > K, u < v - K$, $\exists$ a finite set $H^{uv} \subseteq \mathbb{R}_+$ with $|H^{uv}| = 2^{v-u-K}$ s.t.

$$\forall x \in X \; (\underbrace{\|x_u - x_v\|}_{\text{plays the role of pruning dist.}} \in H^{uv})$$

Symmetry by pruning distances

[Liberti et al., LNCS (COCOA), 2011]

Given embedding x, $R^v_x =$ reflection w.r.t. hyperplane $x_{v-K}, \ldots, x_{v-1}$



Thm.

With prob. 1, for each $u, v \in V$ with $v > K, u < v - K$, $\exists$ a finite set $H^{uv} \subseteq \mathbb{R}_+$ with $|H^{uv}| = 2^{v-u-K}$ s.t.

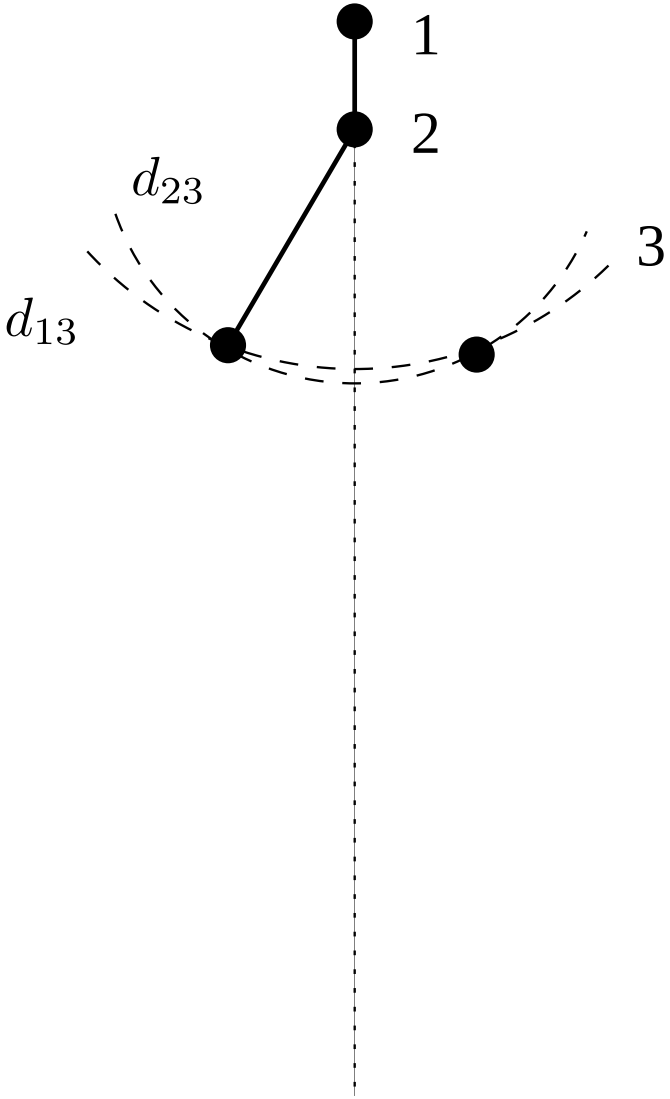
$$\forall x \in X \; (\underbrace{\|x_u - x_v\|}_{\text{plays the role of pruning dist.}} \in H^{uv})$$

Thm.

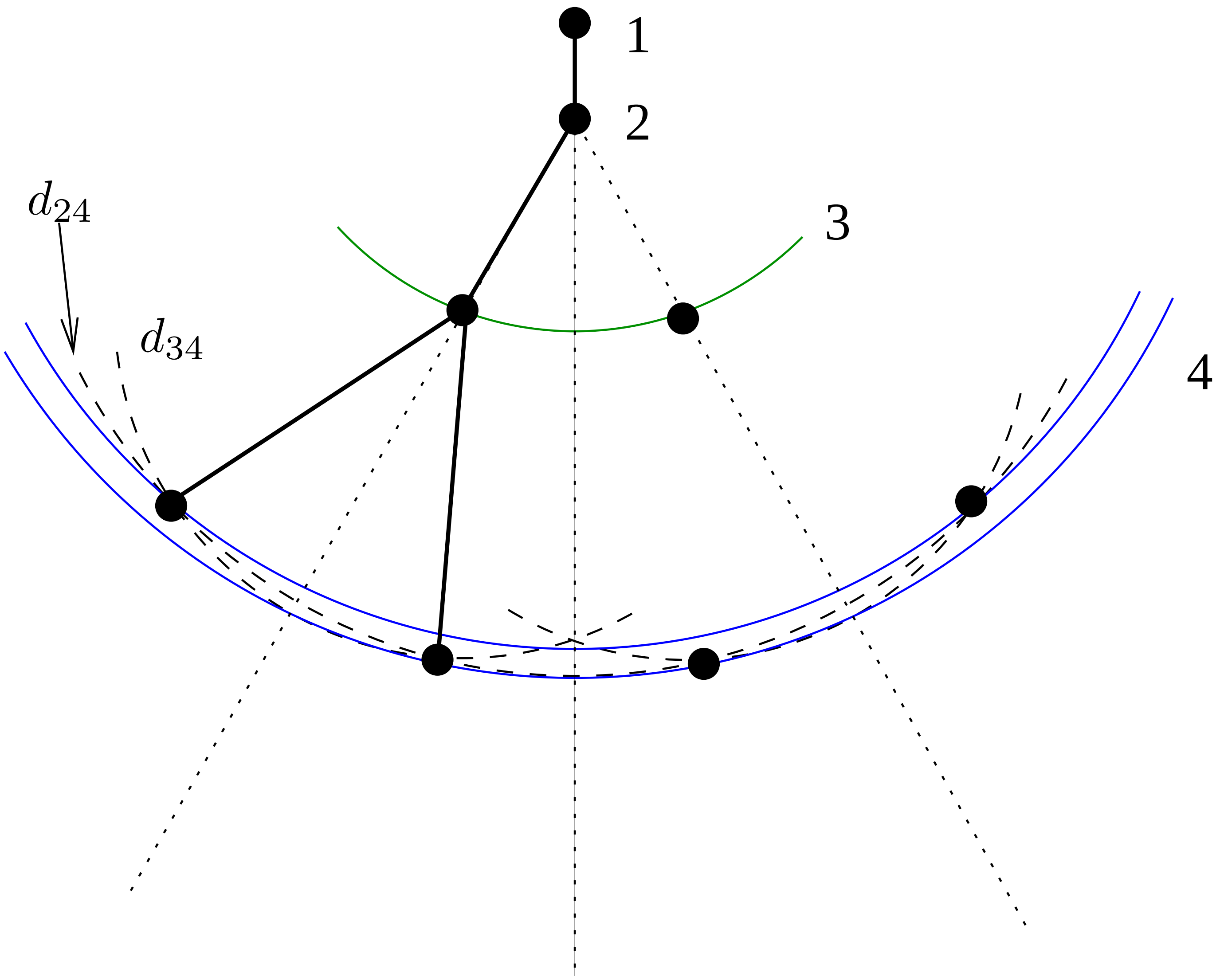
With prob. 1, for each $u, v \in V$ with $v > K, u < v - K$,

$$\forall x \neq x' \in X \quad \|x_u - x_v\| = \|x'_u - x'_v\| \Leftrightarrow x'_v = R^{u+K}_x(x_v)$$

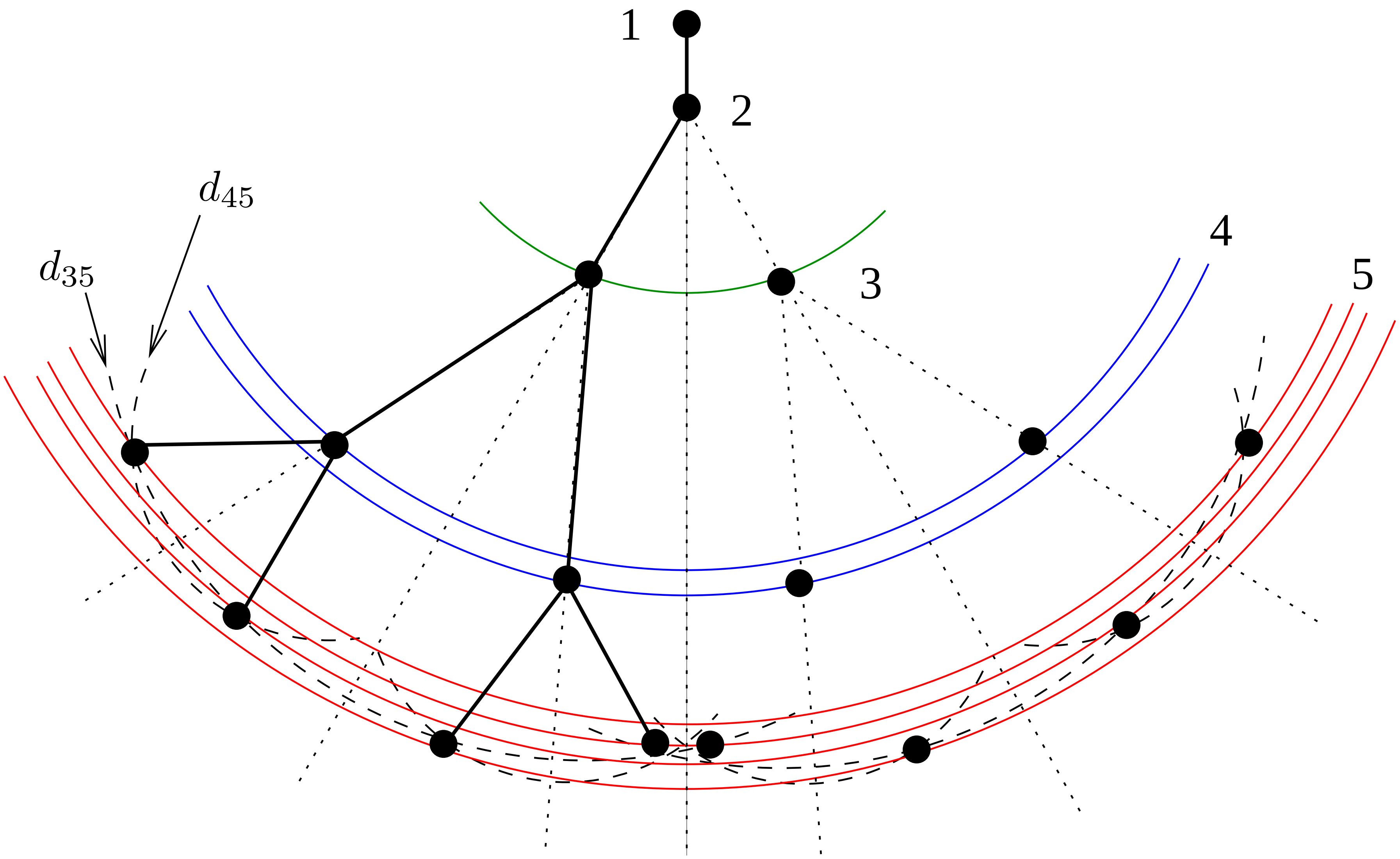
Structure of the BP tree ($\mathbb{R}^2$)



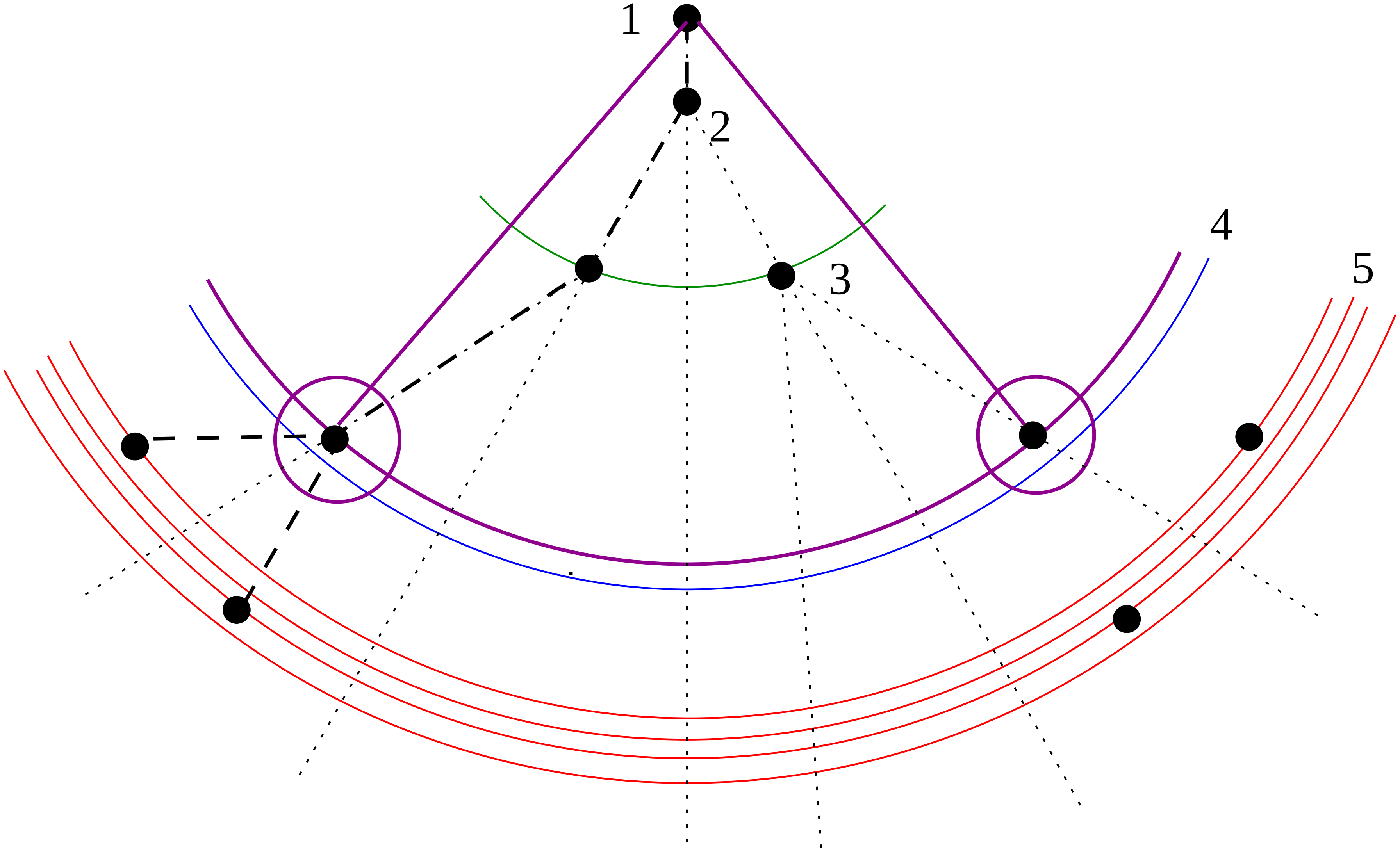
Structure of the BP tree ($\mathbb{R}^2$)



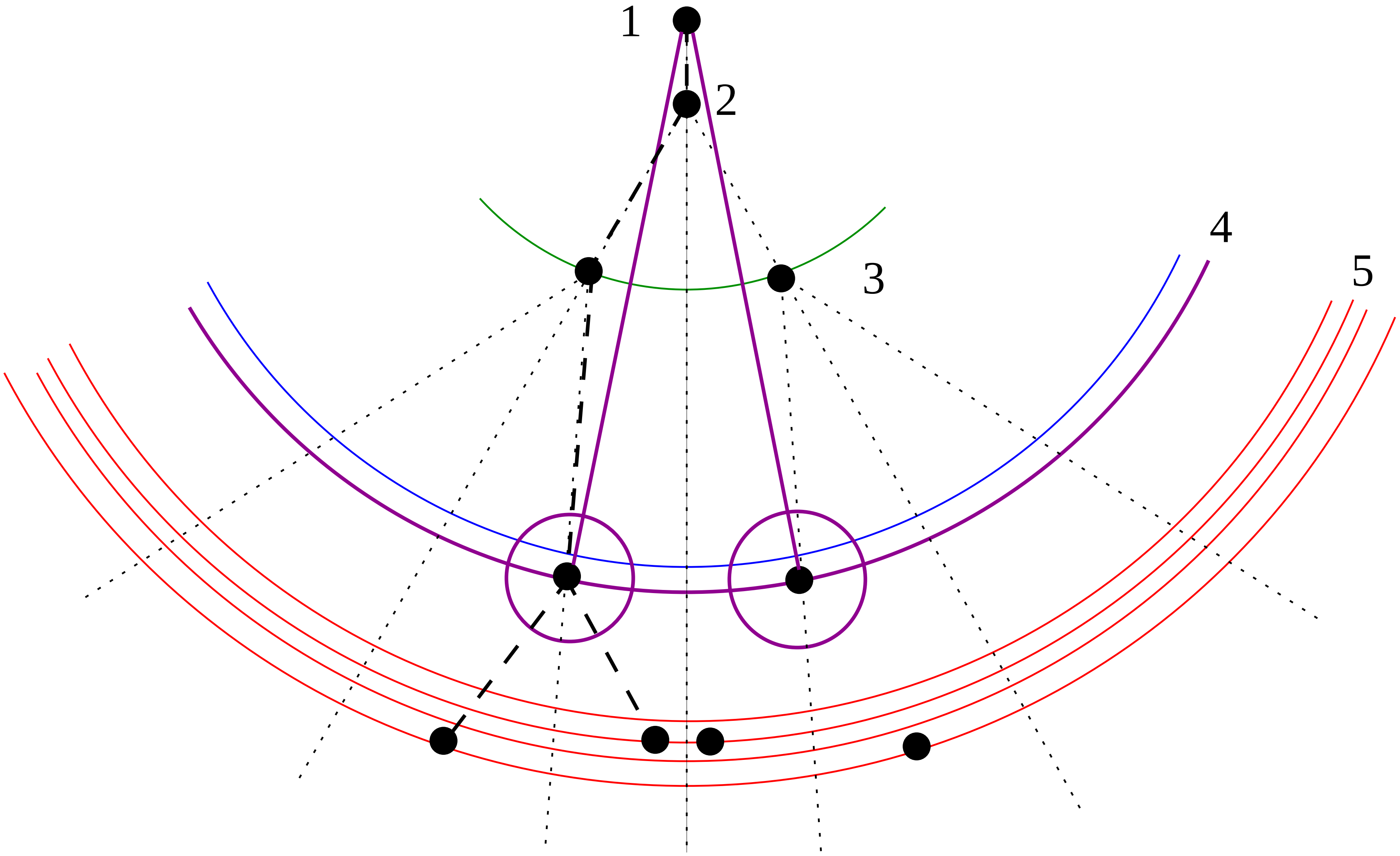
Structure of the BP tree ($\mathbb{R}^2$)



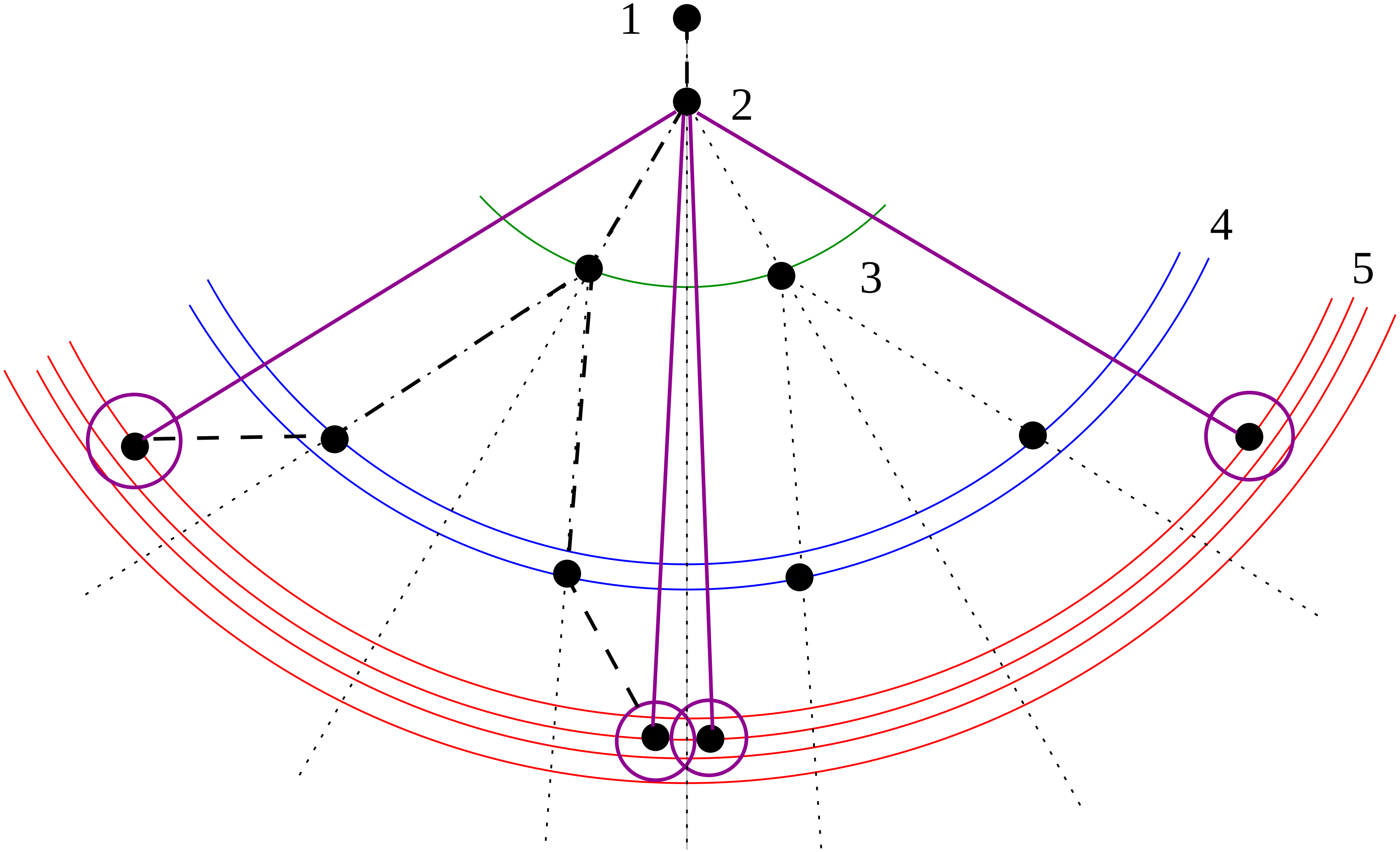
Effect of pruning distance d_{14}



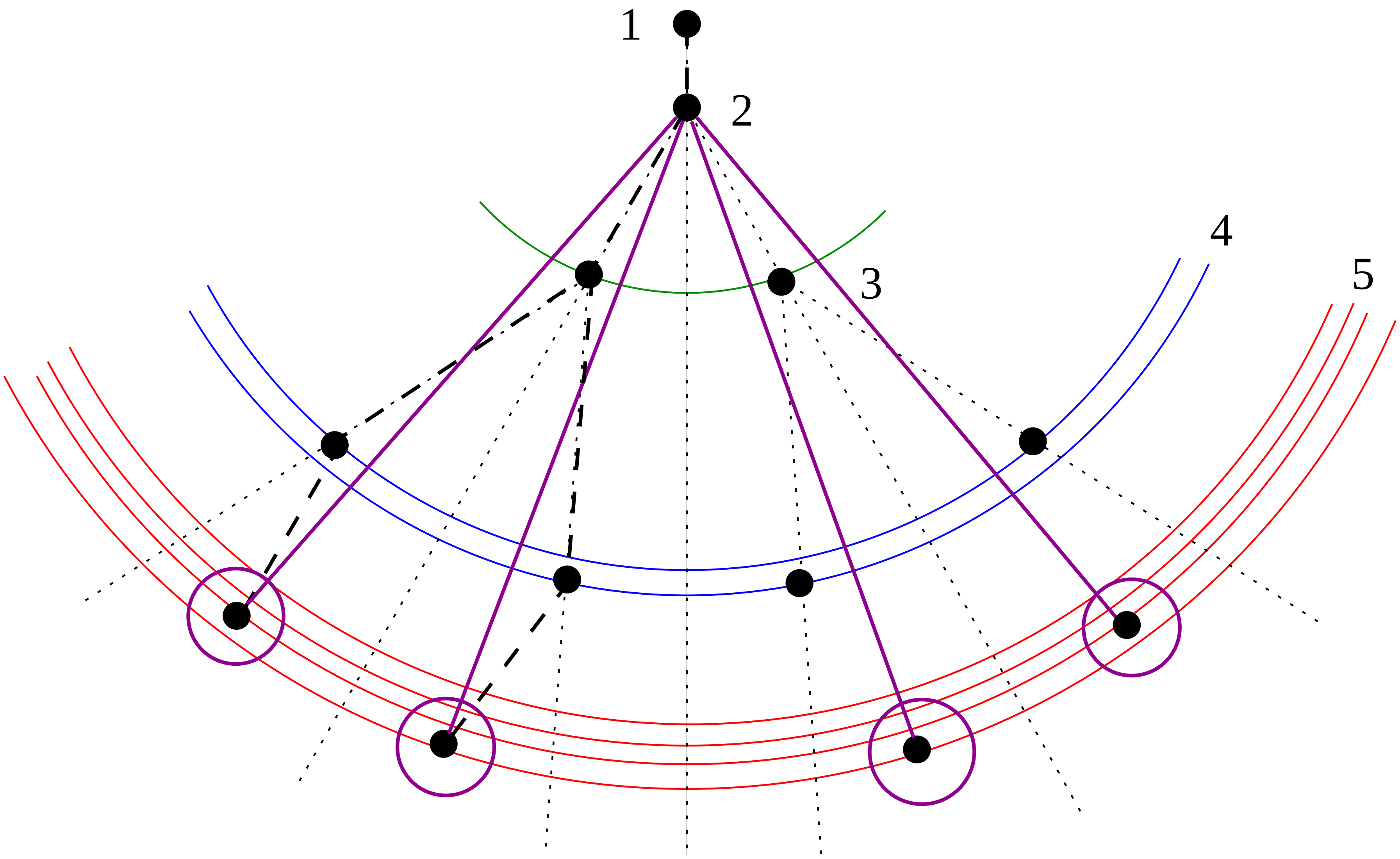
Effect of pruning distance d_{14}



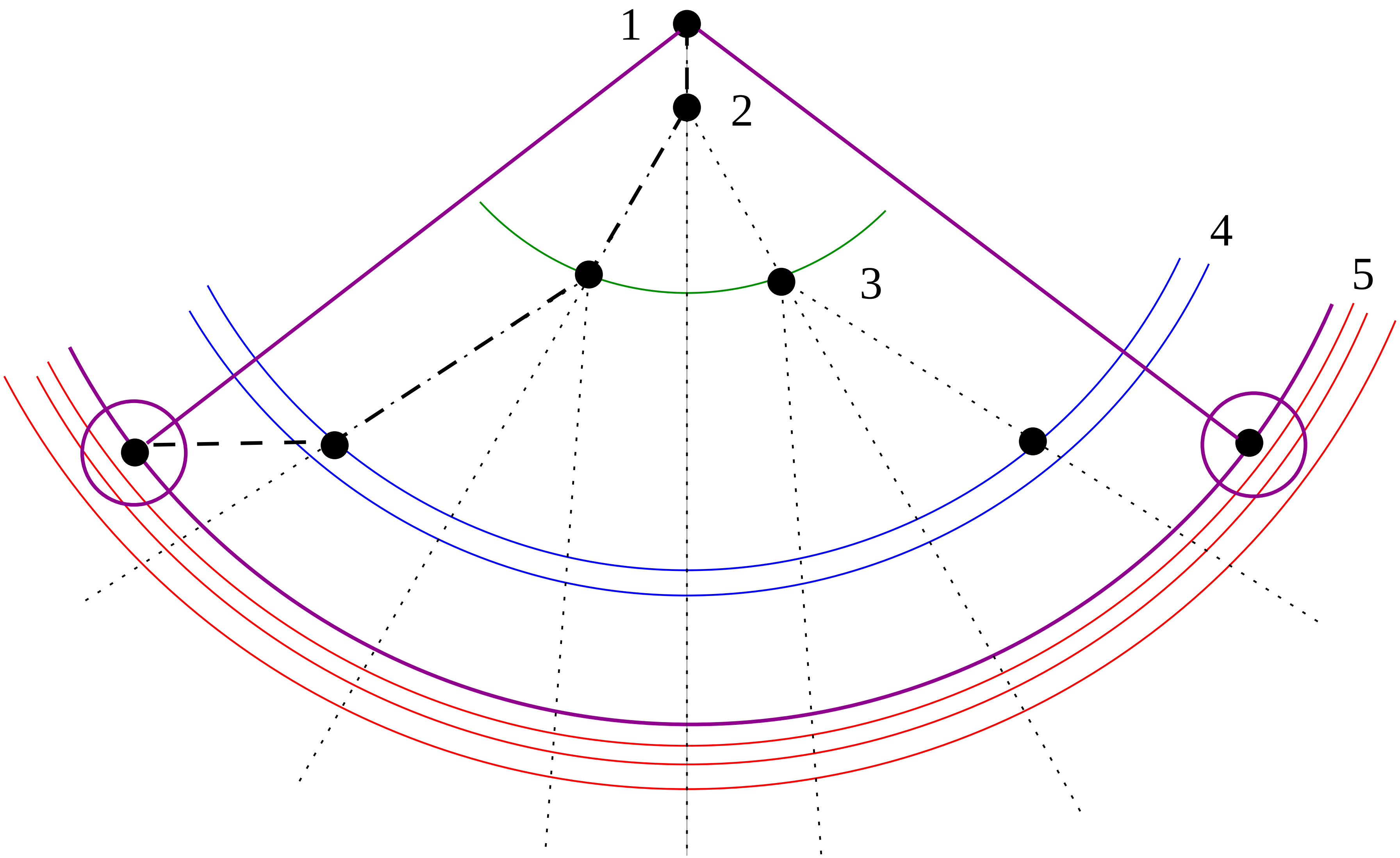
Effect of pruning distance d_{25}



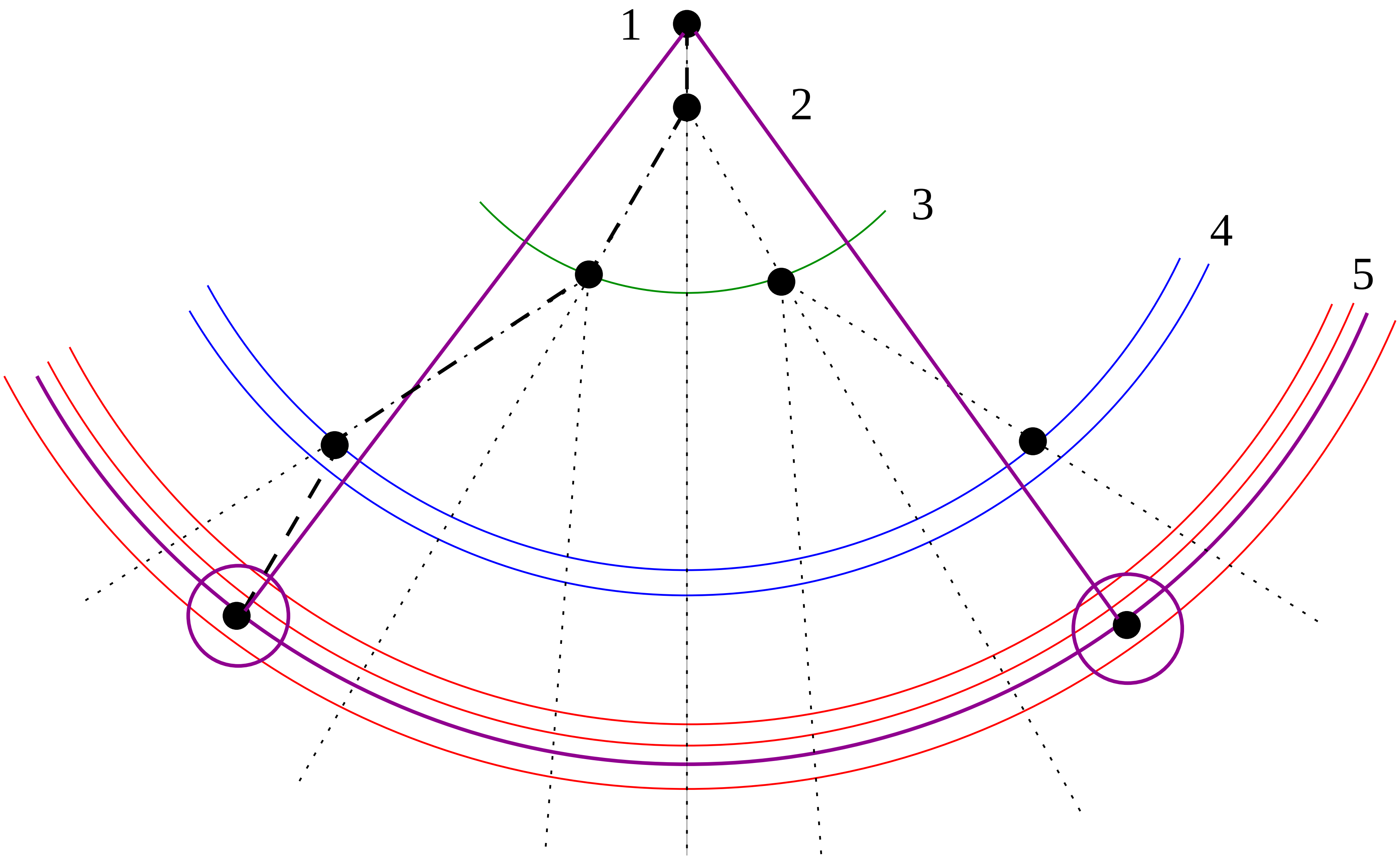
Effect of pruning distance d_{25}



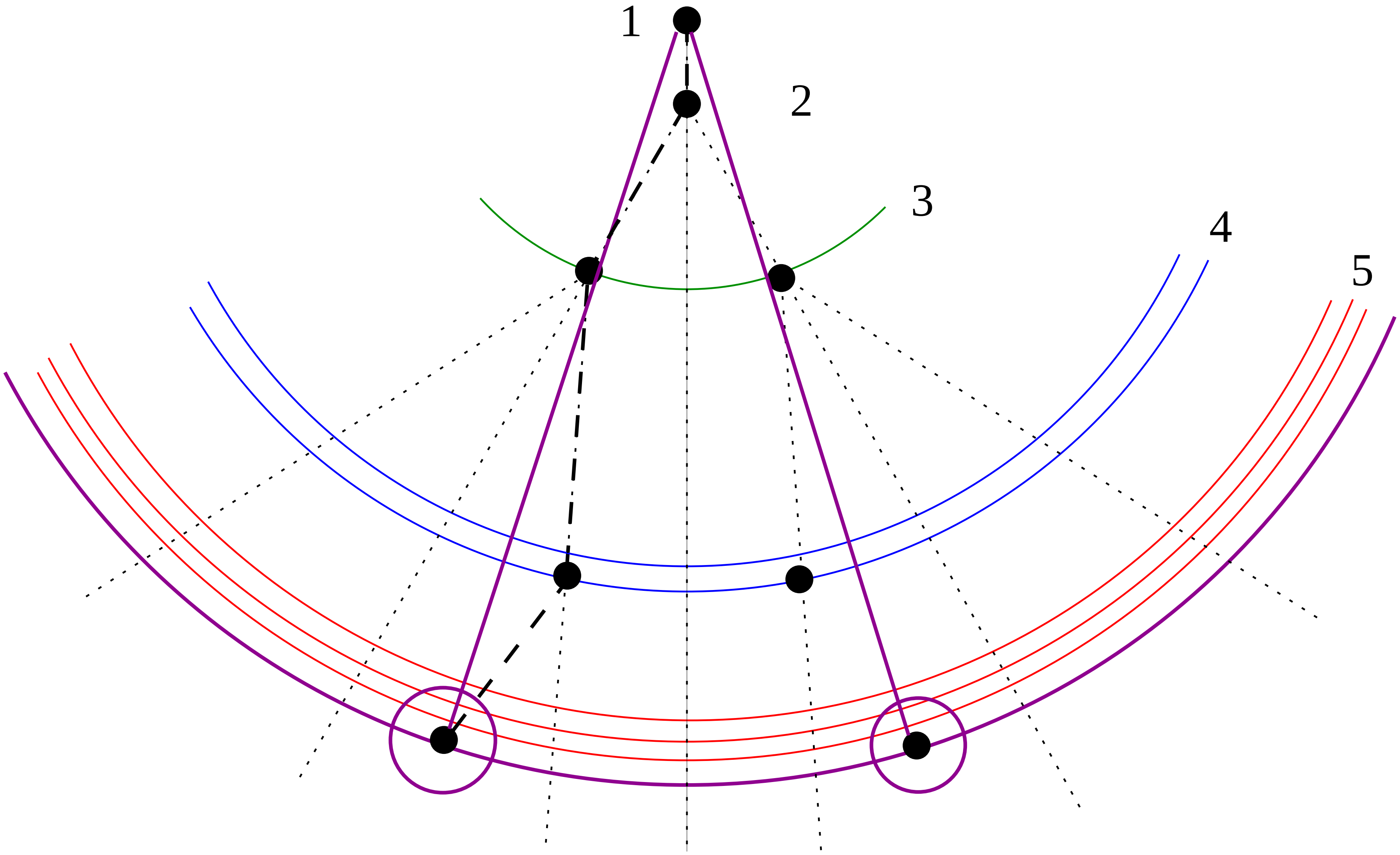
Effect of pruning distance d_{15}



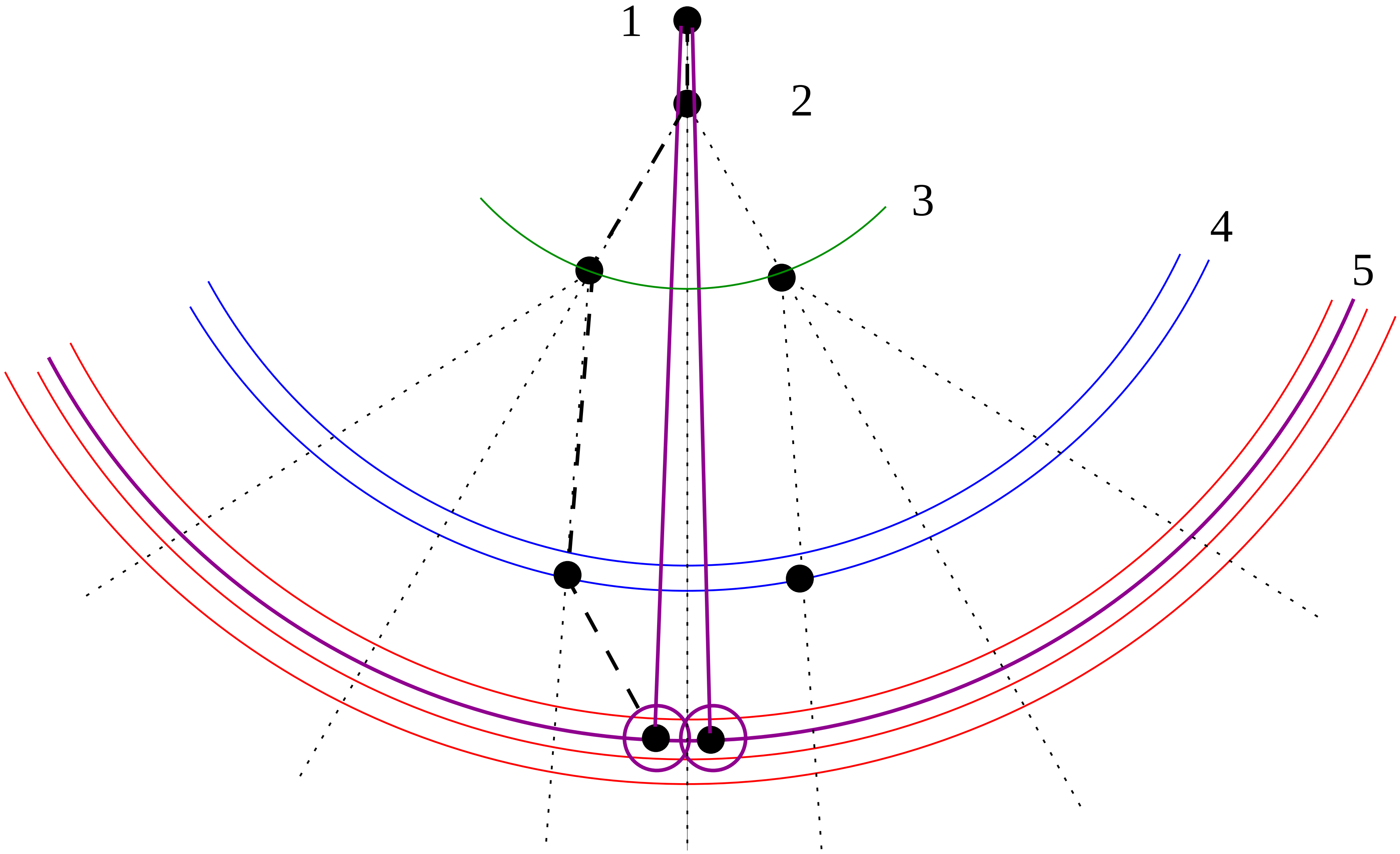
Effect of pruning distance d_{15}



Effect of pruning distance d_{15}

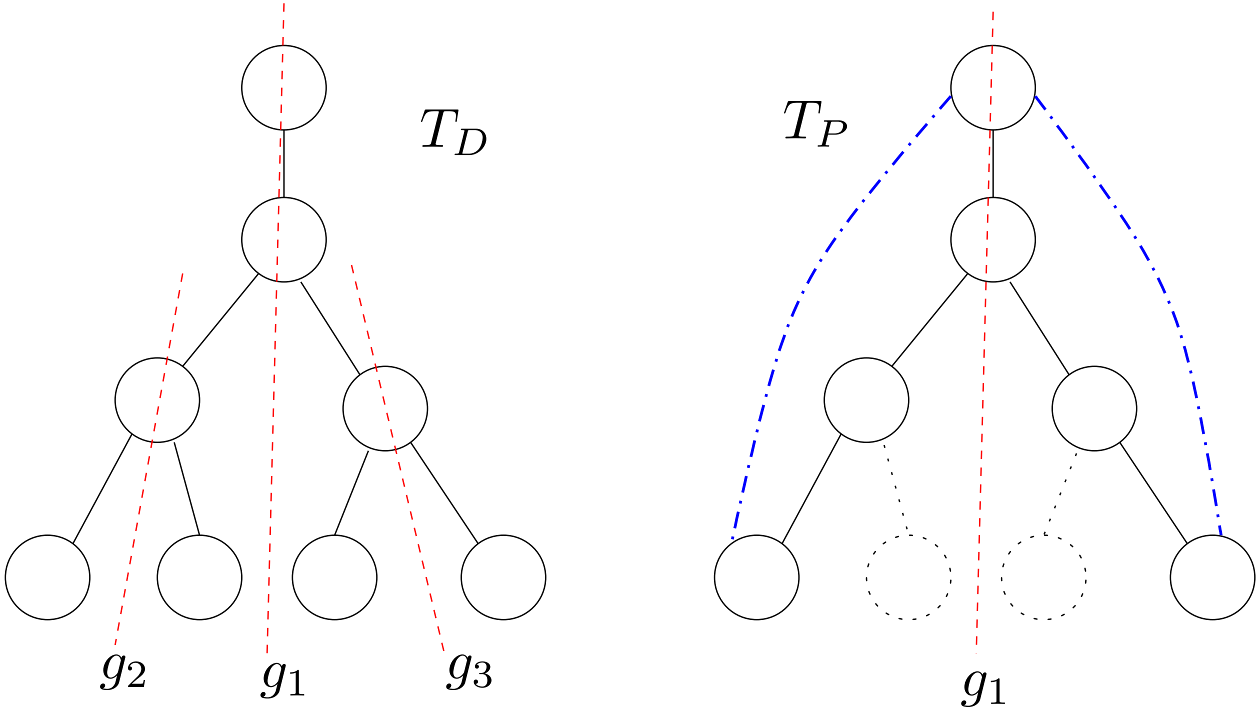


Effect of pruning distance d_{15}



Groups fixing the trees

- Let T_D be a full BP binary search tree
- Let T_P be the subtree of T_D representing only feasible branches
- Draw them so $T_P \subseteq T_P$
- Invariant group for T_D: all partial reflections (g_1, g_2, g_3)
- Invariant group for T_P: only some partial reflections (g_1)



Partial reflections

$$g_v(x) = (x_1, \ldots, x_{v-1}, R^v_x(x_v), \ldots, R^v_x(x_n))$$

Only reflect starting from vertex v

Discretization group

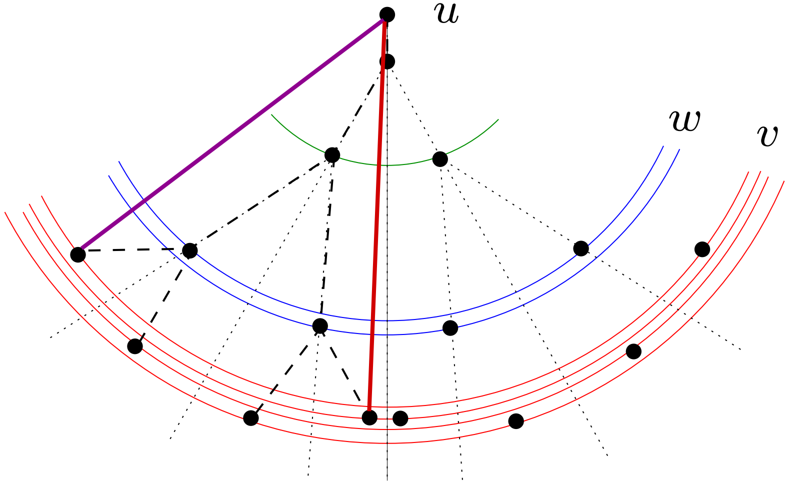
Group of partial reflections fixing the complete BP tree (no pruning distances)

- The following hold with probability 1 $\forall v > K$:
  1. **g_v is injective with probability 1 (by reflection)**
  2. **$\boxed{g_v \text{ is idempotent}}$ (by reflection)**
  3. **$\forall u > K, u \neq v$, g_u and g_v commute (nontrivial)**
- Thus, $\mathcal{G}_D = \langle g_v \mid v > K \rangle$ is an Abelian group under composition $\Rightarrow$ $\boxed{\text{isomorphic to } C_2^{n-K}}$
- By previous thm, discretization distances are invariant under $\mathcal{G}_D$
- The action of $\mathcal{G}_D$ on X is transitive, i.e. $\forall x, x' \in X \exists g \in \mathcal{G}_D \; (x' = g(x))$
- This action has only one orbit, i.e. $X = \mathcal{G}_D x$

Pruning group

Group of partial reflections fixing the actual BP tree (with pruning distances)

- Assume DMDGP instance is YES, consider $\{u,v\} \in E_P$
- With probability 1, $d_{uv} \in H^{uv}$ (otherwise the instance would be NO)
- Notice $d_{uv} = \|x_v - x_u\| \neq \|g_w(x)_v - g_w(x)_u\|$ for all $w \in \{u+K+1, \ldots, v\}$



- In order to keep invariance we remove such g_w's from the group
- **Pruning group**: $\mathcal{G}_P = \langle g_w \mid w > K \wedge \forall \{u,v\} \in E_P \; (w \notin \{u+K+1, \ldots, v\}) \rangle$
- $\boxed{\mathcal{G}_P \leq \mathcal{G}_D}$ and all distances are invariant w.r.t. the pruning group
- Again, $\boxed{\text{action of } \mathcal{G}_P \text{ on } X \text{ is transitive}}$ (nontrivial proof)

Power of two

Thm.

$\exists \ell \in \mathbb{N}\ (|X| = 2^\ell)$

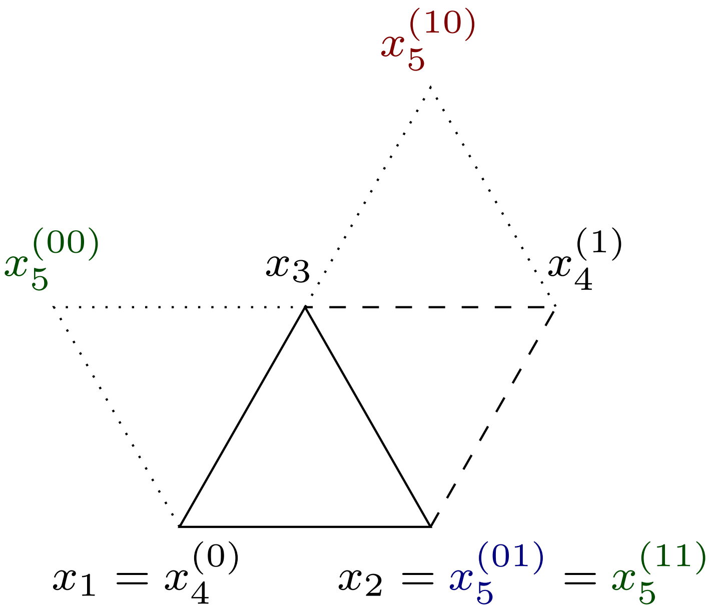
Proof

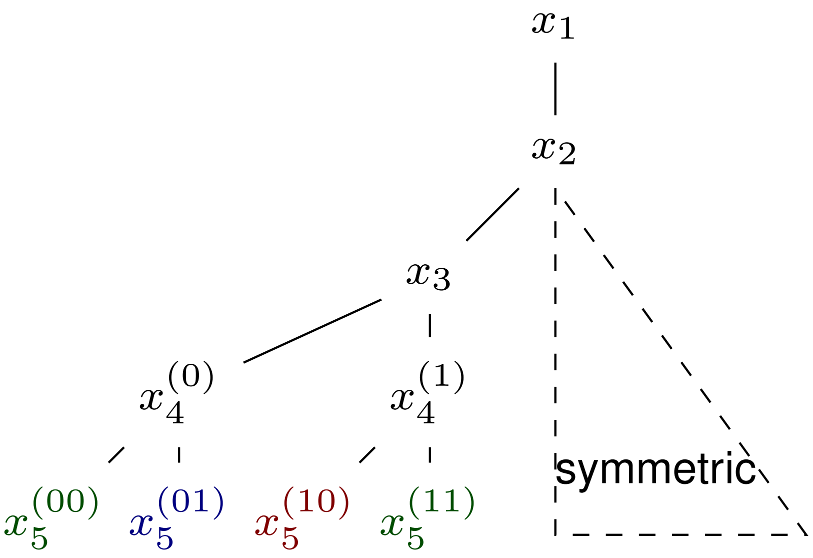
With probability 1:

- $\mathcal{G}_D \cong C_2^{n-K} \Rightarrow |\mathcal{G}_D| = 2^{n-K}$
- $\mathcal{G}_P \le \mathcal{G}_D \Rightarrow |\mathcal{G}_P| \mid |\mathcal{G}_D| \Rightarrow \exists \ell \in \mathbb{N}\ |\mathcal{G}_P| = 2^\ell$
- Action of $\mathcal{G}_P$ on X is transitive $\Rightarrow \mathcal{G}_P x = X$
- Idempotency $\Rightarrow$ for $g, g' \in \mathcal{G}_P$, if $gx = g'x$ then $g = g' \Rightarrow |\mathcal{G}_P x| = |\mathcal{G}_P|$
- Thus, $|X| = |\mathcal{G}_P x| = |\mathcal{G}_P| = 2^\ell$

Why the “probability 1”?

- Not all “YES” DMDGP instances have $|X| = 2^\ell$
- But the set of such instances (with real data) has Lebesgue measure zero in the set of all DMDGP instances





Happens when > 1 vertices are embedded in the same position

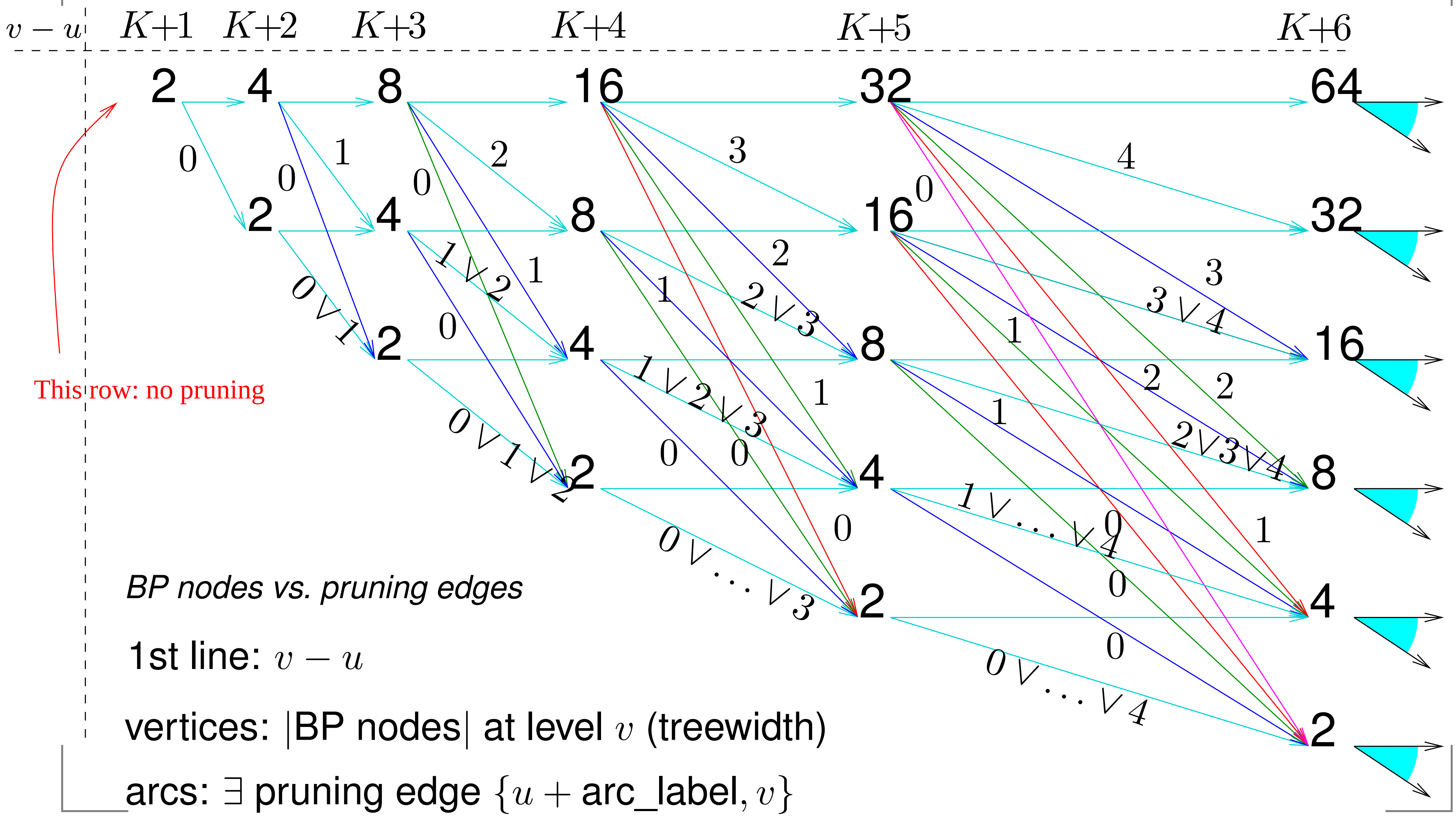
$x_5^{(01)}$ **should** be infeasible, but $x_5^{(01)} = x_5^{(11)}$ (event with prob. 0)

FPT behaviour

A polynomial BP?

- Empirically: never an exponential-time increase behaviour in our experiments (instances generated from PDB files)
- Embed 10000-atom protein backbones in 10-15s on one core
- Easy to show that BP has worst-case exponential complexity
- Are proteins a polynomial case of the DMDGP?
- Complexity depends on BP nodes; since height$\leq |V|$, only need to consider treewidth
- A pruning edge $\{u, v\}$ with $u < v - K$ reduces the number of nodes at level v from 2^{v-K} to $2^{v-K-(u-1)}$ (by symmetry)

BP subtree rooted at u



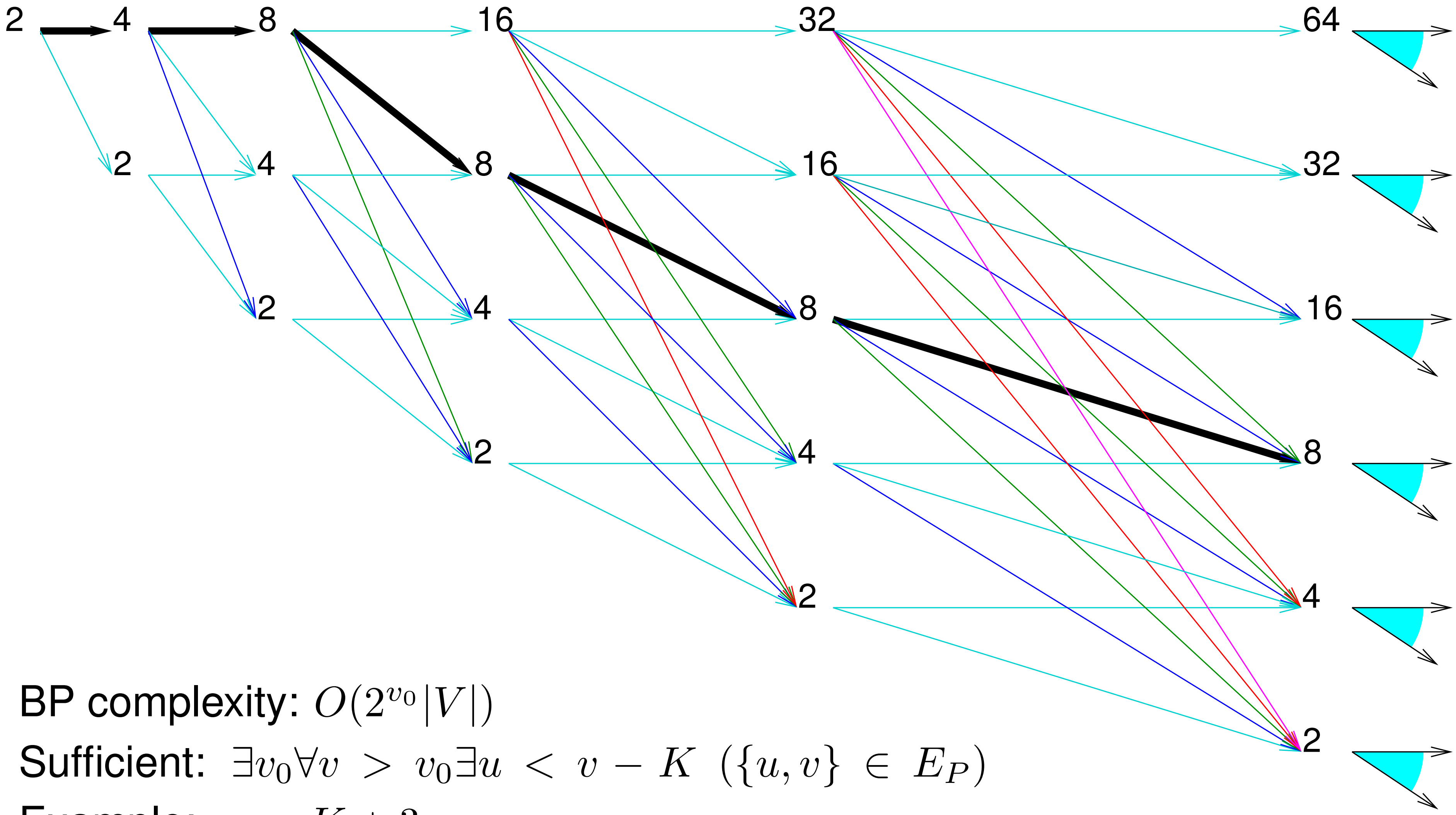
BP nodes vs. pruning edges

1st line: $v-u$

vertices: $|$BP nodes$|$ at level v (treewidth)

arcs: $\exists$ pruning edge $\{u+\text{arc\_label}, v\}$

Constant treewidth

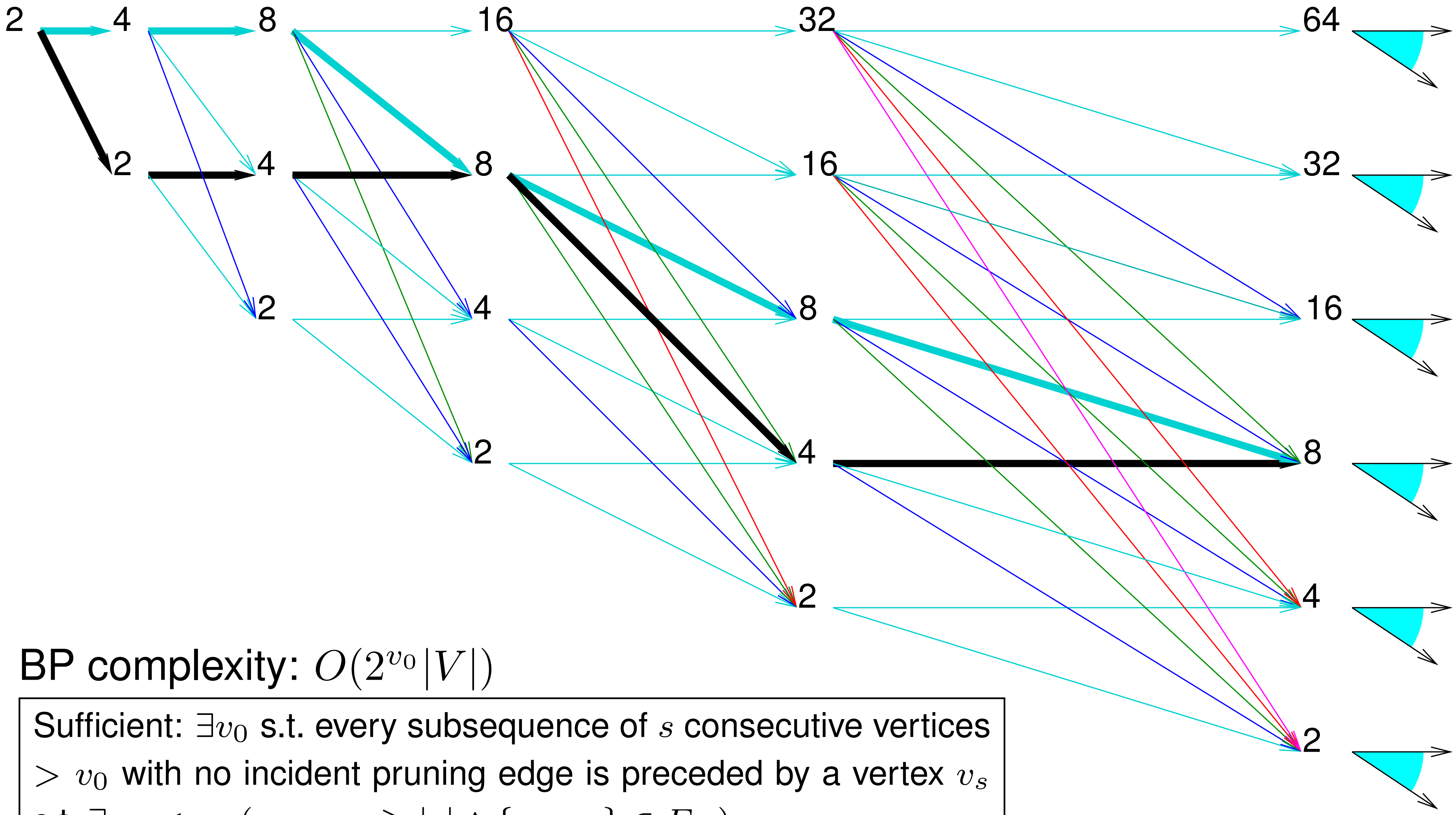


BP complexity: $O(2^{v_0}|V|)$

Sufficient: $\exists v_0 \forall v > v_0 \exists u < v - K \ (\{u,v\} \in E_P)$

Example: $v_0 = K + 3$

Constant-bounded treewidth



BP complexity: $O(2^{v_0}|V|)$

Sufficient: $\exists v_0$ s.t. every subsequence of s consecutive vertices $> v_0$ with no incident pruning edge is preceded by a vertex v_s s.t. $\exists u_s < v_s$ $(v_s - u_s \geq |s| \wedge \{u_s, v_s\} \in E_P)$

“Any path under the constant path”

Fixed parameter tractability

- We can also allow treewidth growth as long as it's logarithmic in n
- This yields a fixed-parameter tractable behaviour for BP (w.r.t. v_0)

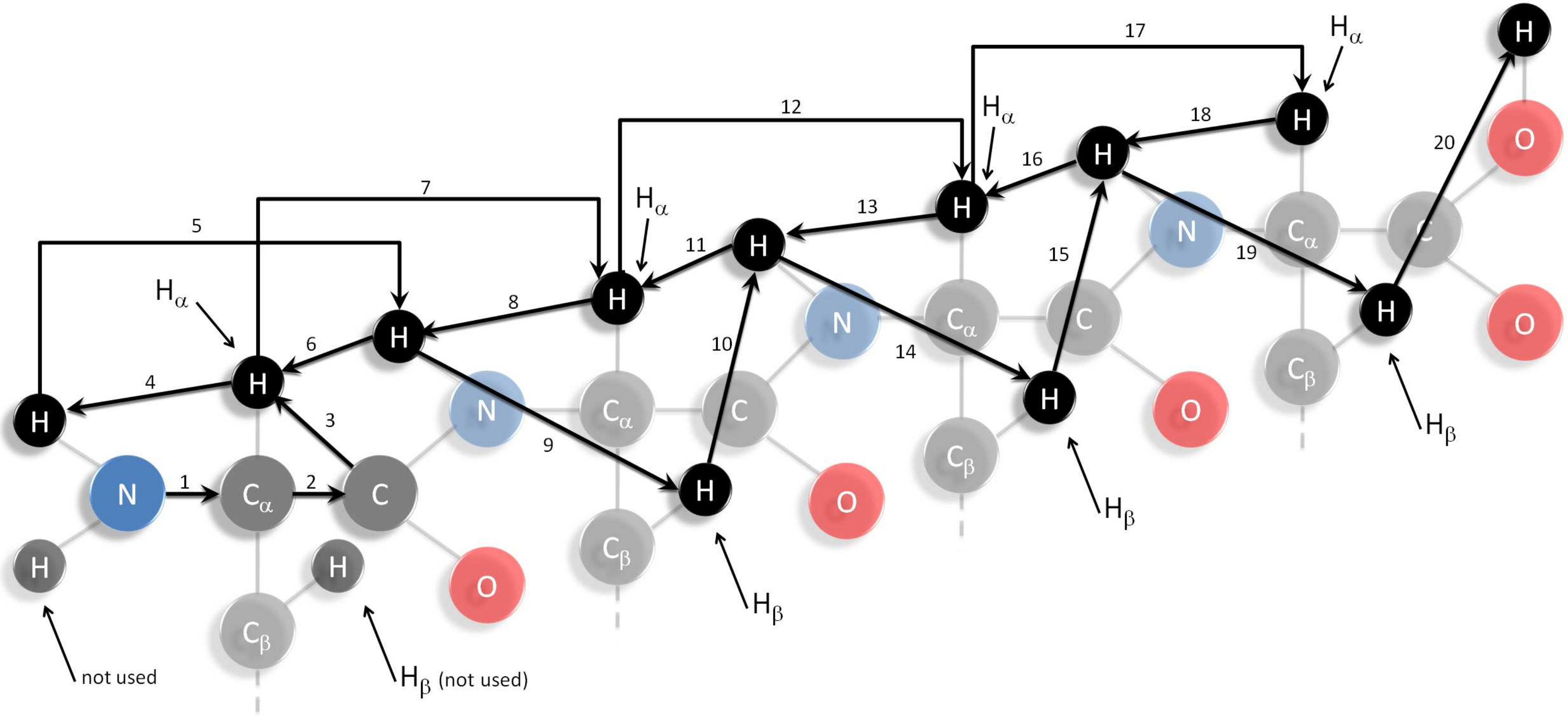
We tested all our protein instances: all display either constant or const-bounded treewidths **with very low** v_0 (i.e. $v_0 = 4$)

BP is polynomial on proteins (?)

Application to proteomics

Virtual hydrogen backbone

- The most accurate NMR distances are **between hydrogen atoms only**, but the actual backbone is a chain of N-C_α-C groups
- So find a *virtual* backbone composed of hydrogens only, and such that its order satisfies the DMDGP requirements



Certain hydrogens must be enumerated twice

[Lavor et al. JOGO]

Listing atoms twice

- If a hydrogen is listed twice, then there are $i \neq j \in V$ indexing the same atom
- Thus $x_i = x_j$ and $d_{ij} = 0$
- For all k such that $\{i,k\} \in E$, we have that $\{j,k\} \in E$ as $d_{jk} = d_{ik} + 0$, and

$$d_{ij} + d_{jk} = 0 + d_{jk} = d_{ik}$$

so STRICT TRIANGULAR INEQUALITIES do not hold for all atom triplets

- However, it only fails on *nonconsecutive* triplets

Hence, BP still applies

- Also, zero pruning distances help keeping floating point errors under control

Re-orders

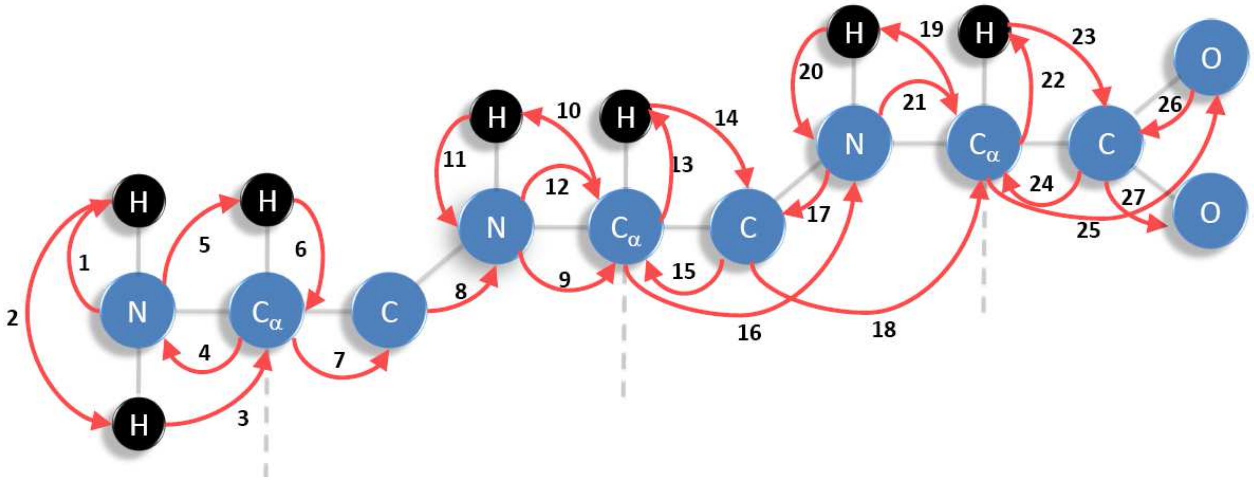
Defn.

A *repetition order* (re-order) is a finite sequence on V

- Re-orders generalize “counting vertices more than once”
- They add more flexibility to exploit certain distances as discretization distances
- Essentially, they provide a tool with which to hand-craft convenient vertex orders for interesting instance classes

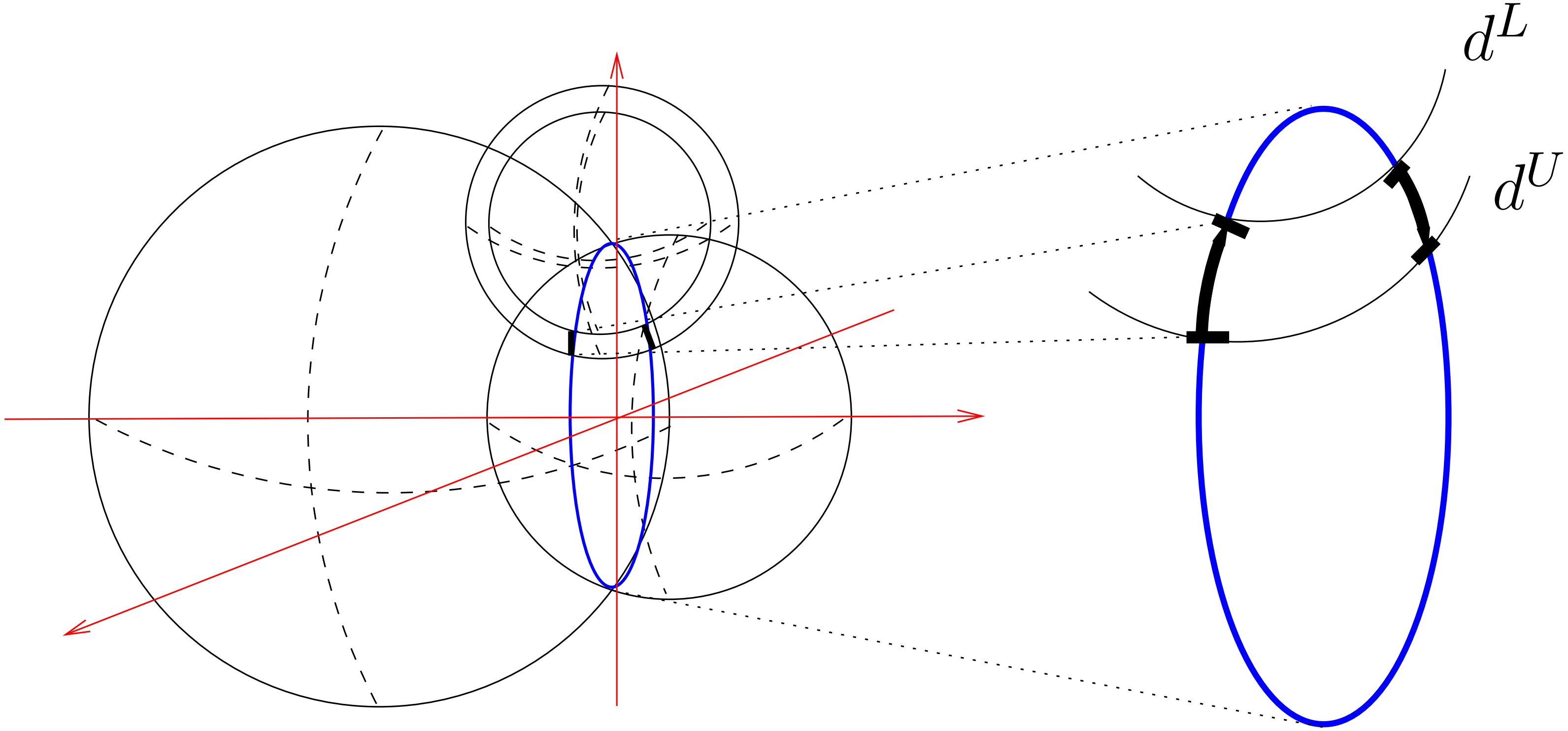
Not immediately evident how to best order proteins

Here’s a re-order applying to all backbones



Uncertain distances

- Typically, NMR provides uncertain distances, modelled by intervals $[d^L_{uv}, d^U_{uv}]$
- Cannot be used for discretization



Two precise distances and an uncertain one

The actual situation

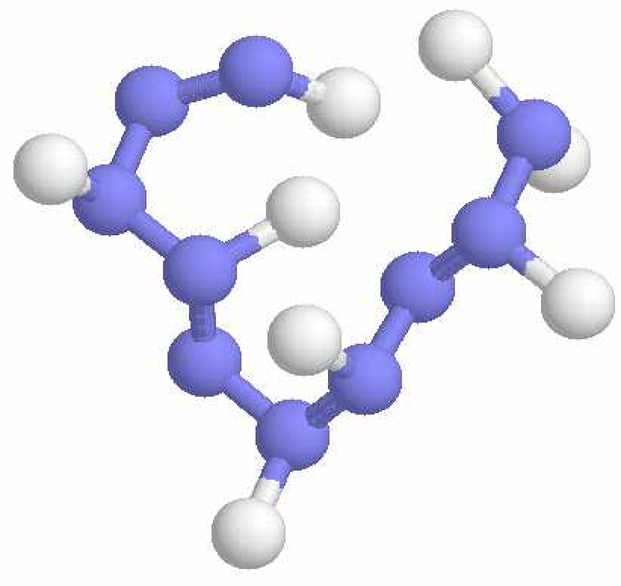
- We know several distances d_{uv} precisely because of chemical properties
- Some distances take values in a finite set D_{uv}
- The distribution of **precise/discrete/uncertain** distances on the protein backbone does not satisfy the DMDGP requirements

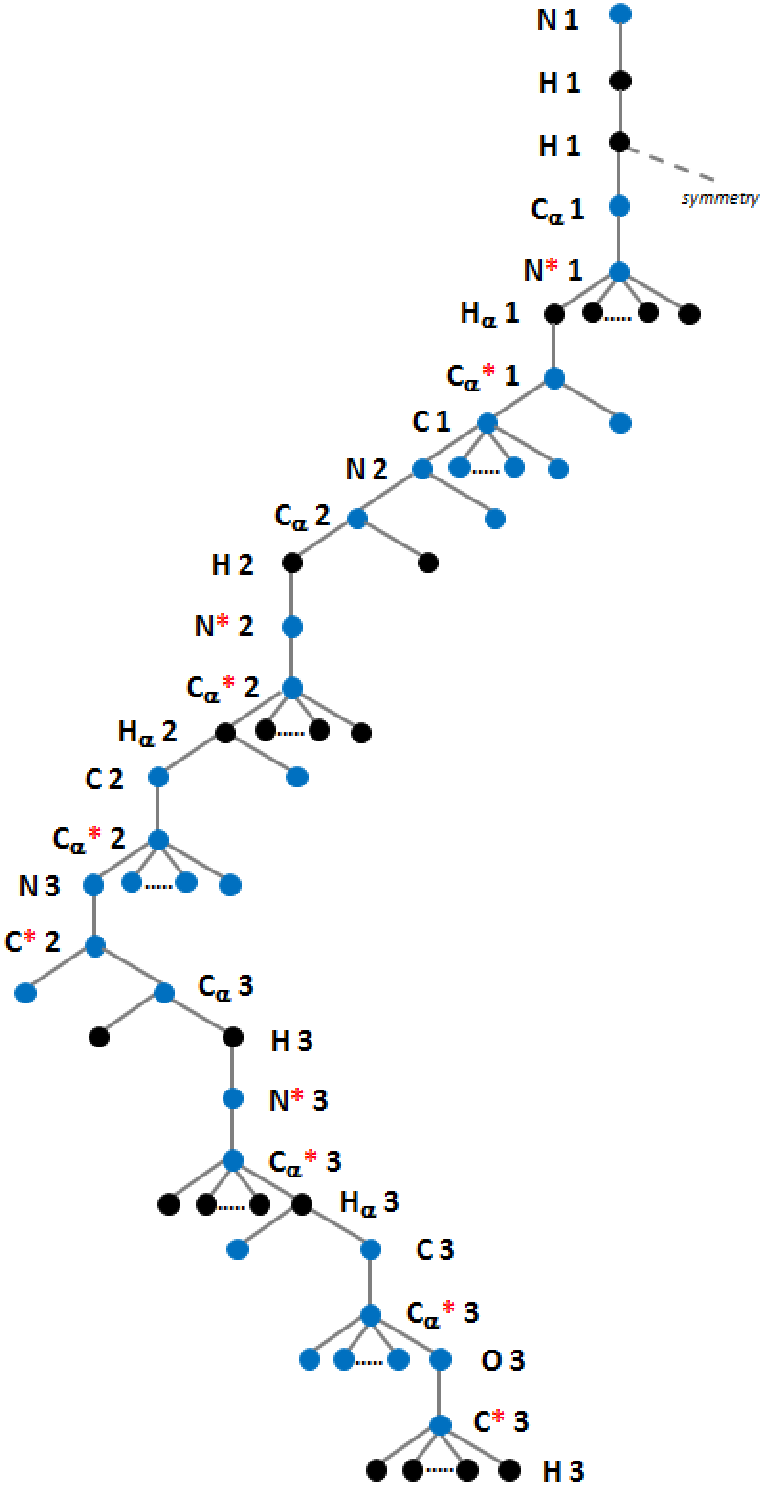
Re-orders provide a solution: use all **precise** distances for discretization, plus a few of the **discrete** whenever needed; **uncertain** distances are used for pruning

- Pruning with intervals is easy: if the current point x_v is s.t. $\|x_v - x_u\| \in [d^L_{uv}, d^U_{uv}]$ for all $u \in \alpha(v)$ accept it, otherwise prune it
- Discrete distances D_{uv} simply give rise to BP nodes at level $v-1$ with potentially $2|D_{uv}|$ subnodes

*i*BP

[Mucherino et al. SEA11]





Implementations

Sequential code

Mucherino et al. LNCS 2010

- The code is available in open source
- Download:
  `http://www.antoniomucherino.it/en/mdjeep.php`
- Any doubt, ask the MASTER (Antonio)

Parallel code

Seconds of user CPU on Grid5000 (`www.grid5000.fr`)

$\lvert V\rvert$	CPUs 1	 2	 8	 64
5000	3.21	1.30	0.54	0.36
7500	4.73	3.15	1.25	0.93
10000	13.38	5.49	2.49	1.57

Embed subgraphs then glue embeddings (rigidity $\Rightarrow$ exact)

A selection of current work

- Work with biochemists/bioinformaticians at Institut Pasteur to access and treat real NMR data [Mucherino et al., LNCS 2011]
- Use $\mathcal{G}_P x = X$ result from symmetry to obtain all solutions from just one [Mucherino et al., IEEE 2011]
- Extend complexity study to actual problem with discrete/uncertain distances [Tech. rep. ready]
- Progress on “MDGP $\in$ **NP**?” question

See `http://www.lix.polytechnique.fr/~liberti/publications.html` for more papers

The end

- **Survey 1**: Liberti, Lavor, Mucherino, Maculan, *Molecular distance geometry methods: from continuous to discrete*, International Transactions in Operational Research, **18**:33-51, 2010
- **Survey 2**: Lavor, Liberti, Maculan, Mucherino, *Recent advances on the discretizable molecular distance geometry problem*, European Journal of Operational Research, **219**:698-706, 2012
- **Survey 3**: Liberti, Lavor, Maculan, Mucherino, *Euclidean distance geometry and applications*, SIAM Review, to appear (meanwhile: arXiv 1205.0349v1)

Appendix

Continuous formulation

- Solving the system

$$\forall \{i,j\} \in E \quad ||x_i - x_j|| = d_{ij}, \tag{6}$$

is numerically challenging

LHS involves $\sqrt{\text{arg}}$, floating point ops $\Rightarrow$ arg $< 0 \Rightarrow$ error and abort

$\Rightarrow$ square both sides

- Usually, cast as a penalty objective to be minimized

$$\min_x \sum_{\{i,j\} \in E} (||x_i - x_j||^2 - d_{ij}^2)^2. \tag{7}$$

- Unconstrained minimization of a polynomial of fourth degree

General-purpose methods

- sBB (exact) [L. et al. ’06]: OK on small and medium-sized instances

  because we know the optimal value of the objective (0), lower bound is tight at the initial tree levels

- VNS (heur) [L. et al. ’05, L. et al. ’06]: good for large(ish) instances
- MultiLevel Single Linkage (heur) [Kucherenko et al. ’06]: so-so

		sBB		VNS		MLSL	
Atoms	Variables	OF Value	Time	OF Value	Time	OF Value	Time
cube8	24	0	0.22	0	1.21	0	13.56
cube27	81	0	30.39	0	34.01	0	300.285
cube64	192	0	2237.73	0	398.875	0	2765.13
lavor5	15	0	0.02	0	0.48	0	0.57
lavor10	30	0	1.12	0	7.06	0	69.71
lavor20	60	0	2.25	0	49.99	0	411.152
lavor30	90	0	488.87	0	352.06	0	1634.09
lavor40	120	-	-	0.09	1258.13	0.547	2376.01
lavor50	150	-	-	0	673.48	0	3002.88

MDGP-specific methods

- Smoothing-based:
  - Continuation method (heur) [Moré, Wu '97]
  - Double VNS with smoothing (heur) [L. et al. '09]
  - DC optimization with smoothing (heur) [An et al. '03]
  - Hyperbolic smoothing (heur) [Xavier '08]
- Alternating projections algorithm (heur) [Glunt et al. 90]:

  iterative updating of a dissimilarity matrix
- Geometric build-up (exact/heur) [Dong, Wu '03 and '07]: *triangulation*
- GNOMAD (heur) [Williams et al. '01]

  iterative updating of atomic ordering minimizing error contribution
- Monotonic Basin Hopping (heur) [Grosso et al. '09]

  funnel-based population heuristic
- Self-organization heuristic (heur) [Xu et al. '03]

  pairwise atomic position modification heuristic
- SDP-based formulation *[Ye et al. '09]*

Geometric build-up

[Dong, Wu ’03], [Dong, Wu ’07]

Given $U = \{1,2,3,4\} \subseteq V$ and a partial embedding $x : U \to \mathbb{R}^3$

1. Consider $v \in V \smallsetminus U$ s.t. $U \subseteq \delta(v)$
2. Extend x to v by solving a linear system:

$$\boxed{\begin{array}{rcl} \|x_v - x_1\|^2 & = & d^2_{1v} \\ \|x_v - x_2\|^2 & = & d^2_{2v} \\ \|x_v - x_3\|^2 & = & d^2_{3v} \\ \|x_v - x_4\|^2 & = & d^2_{3v} \end{array}} \Rightarrow \boxed{\begin{array}{rcl} \|x_v\|^2 - 2x_v \cdot x_1 + \|x_1\|^2 & = & d^2_{1v} \text{ (8)} \\ \|x_v\|^2 - 2x_v \cdot x_2 + \|x_2\|^2 & = & d^2_{1v} \text{ (9)} \\ \|x_v\|^2 - 2x_v \cdot x_3 + \|x_3\|^2 & = & d^2_{1v} \text{ (10)} \\ \|x_v\|^2 - 2x_v \cdot x_4 + \|x_4\|^2 & = & d^2_{1v} \text{ (11)} \end{array}}$$

$$\boxed{\begin{array}{l} \text{(11)-(8)} \\ \text{(11)-(9)} \\ \text{(11)-} \\ \text{(10)} \end{array}} \Rightarrow \boxed{\begin{pmatrix} 2(x_1 - x_4) \\ 2(x_2 - x_4) \\ 2(x_3 - x_4) \end{pmatrix} x_v = \begin{pmatrix} (\|x_1\|^2 - \|x_4\|^2) - (d^2_{1v} - d^2_{4v}) \\ (\|x_2\|^2 - \|x_4\|^2) - (d^2_{2v} - d^2_{4v}) \\ (\|x_3\|^2 - \|x_4\|^2) - (d^2_{3v} - d^2_{4v}) \end{pmatrix}}$$

3. Let $U \leftarrow U \cup \{v\}$; if $U = V$ stop otherwise repeat from Step 1

Exact on complete and 3-trilateration graphs, heuristic otherwise