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Recent algorithmic advances for combinatorial optimization in graphical models

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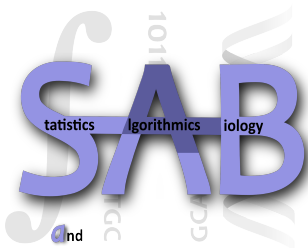
ISMP'18



Recent algorithmic advances for combinatorial optimization in graphical models

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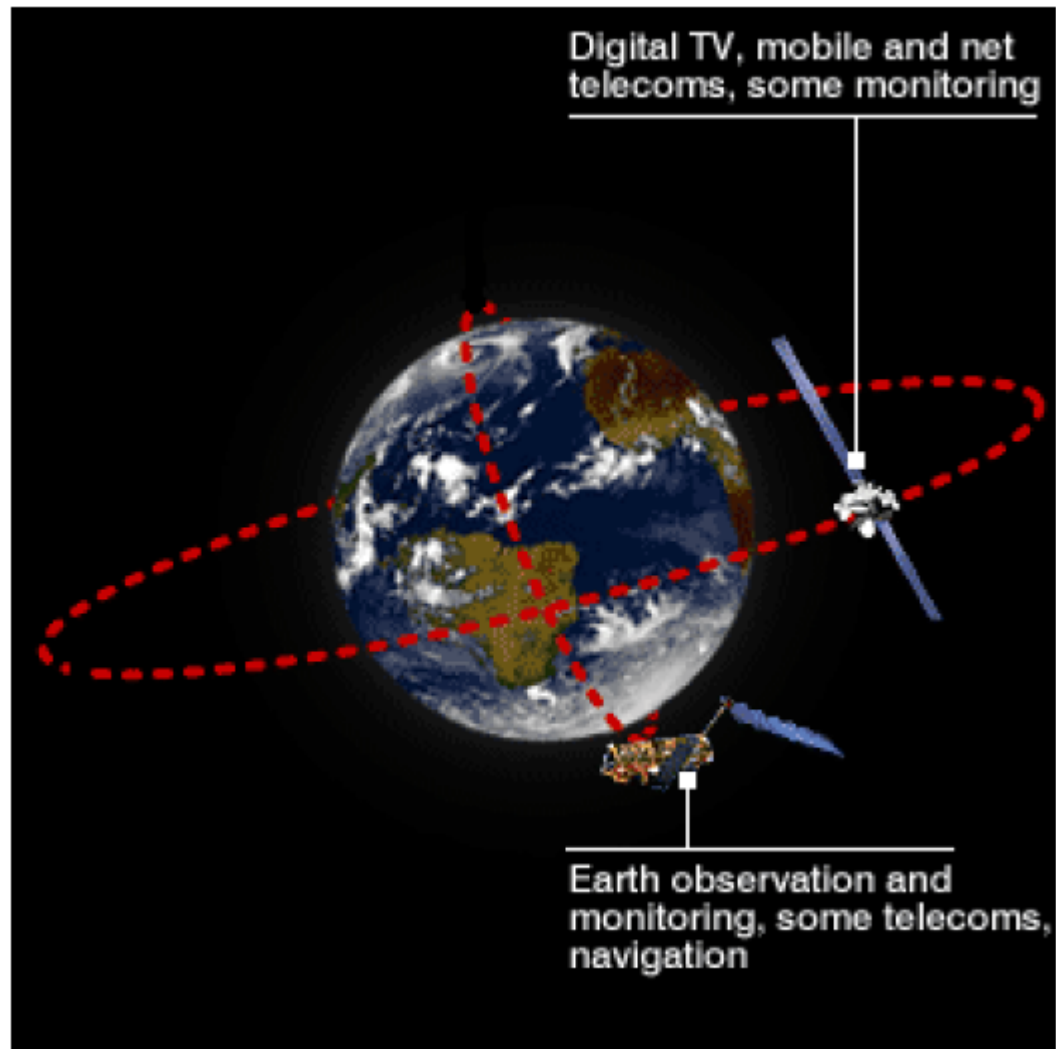
Plan

- Graphical models
 - Examples and definitions
- Local reasoning techniques
 - Bounding, clique cut, pruning
- Complete search methods
 - Hybrid search, iterative search, large neighborhood search
- Experimental results
 - Open-source C++ exact solver **toulbar2 v1.0.0**

<https://github.com/toulbar2/toulbar2>



Earth Observation Satellite Management (SPOT5)



(Bensana *et al*, Constraints 1999 ; IJCAI09)

$$n \leq 364, d=4, e(2-3) \leq 10,108$$

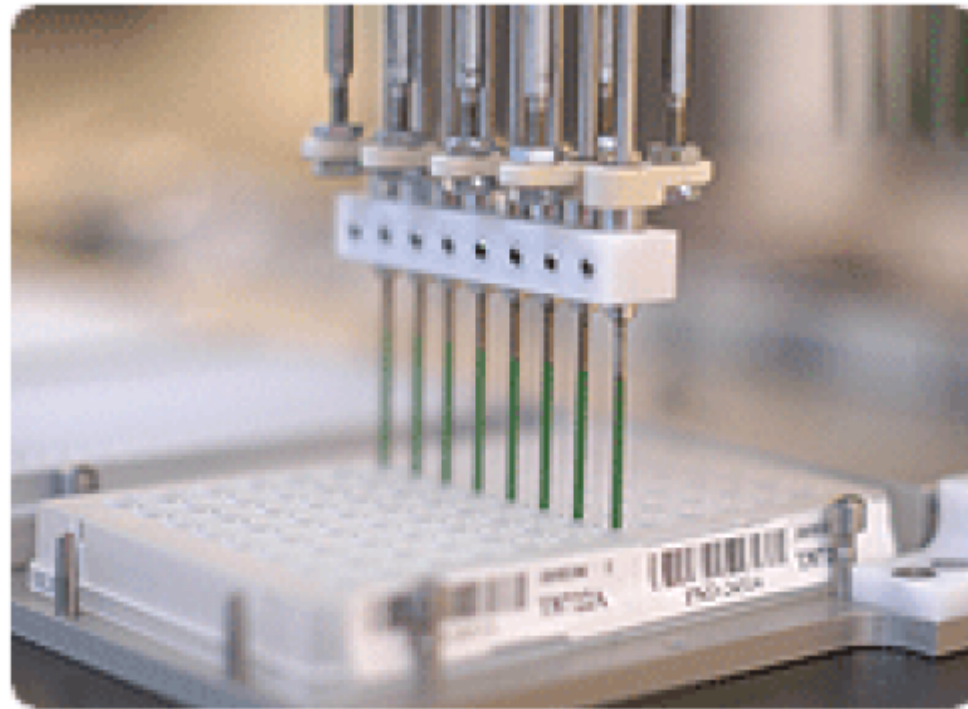
Radio Link Frequency Assignment (CELAR)



(Cabon *et al*, Constraints 1999 ; CP97 – AAAI06 – IJCAI07 – IJCAI09 – CP10)

$$n \leq 458, d=44, e(2) \leq 5,000$$

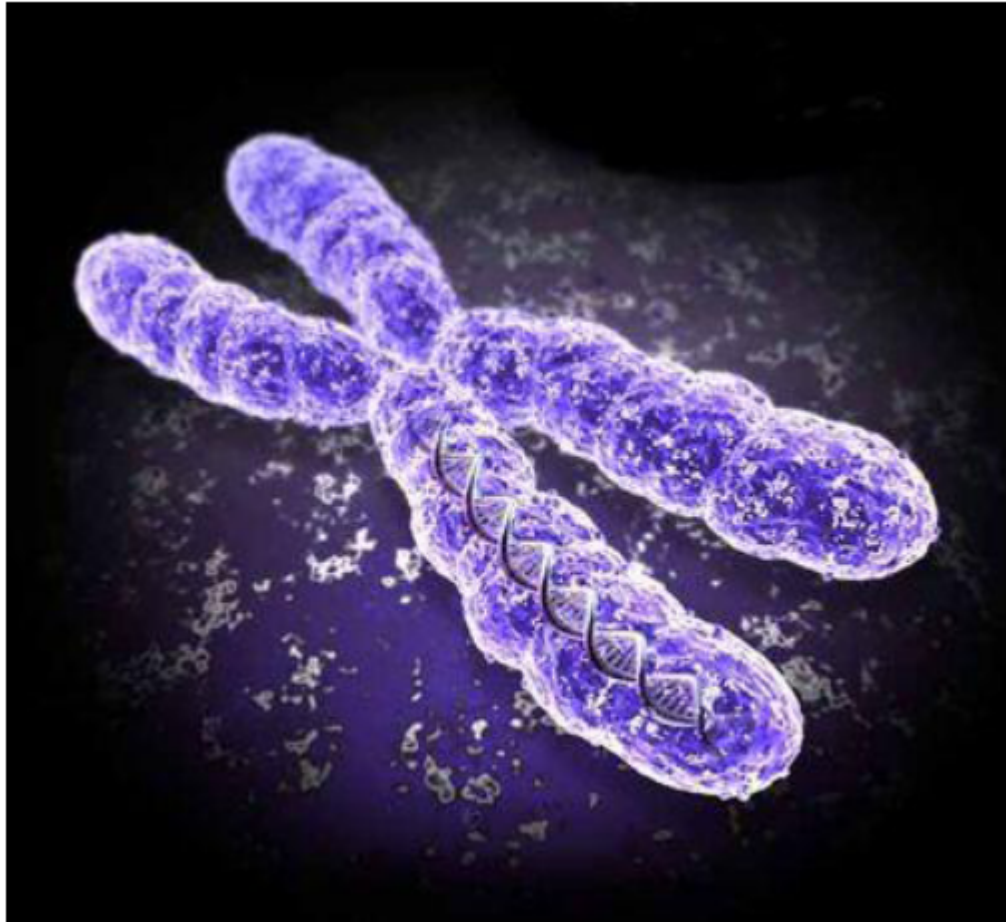
Mendelian error correction in complex pedigree (MendelSoft)



(Constraints08)

$n \leq 20,000$, $d \leq 66$, $e(3) \leq 30,000$

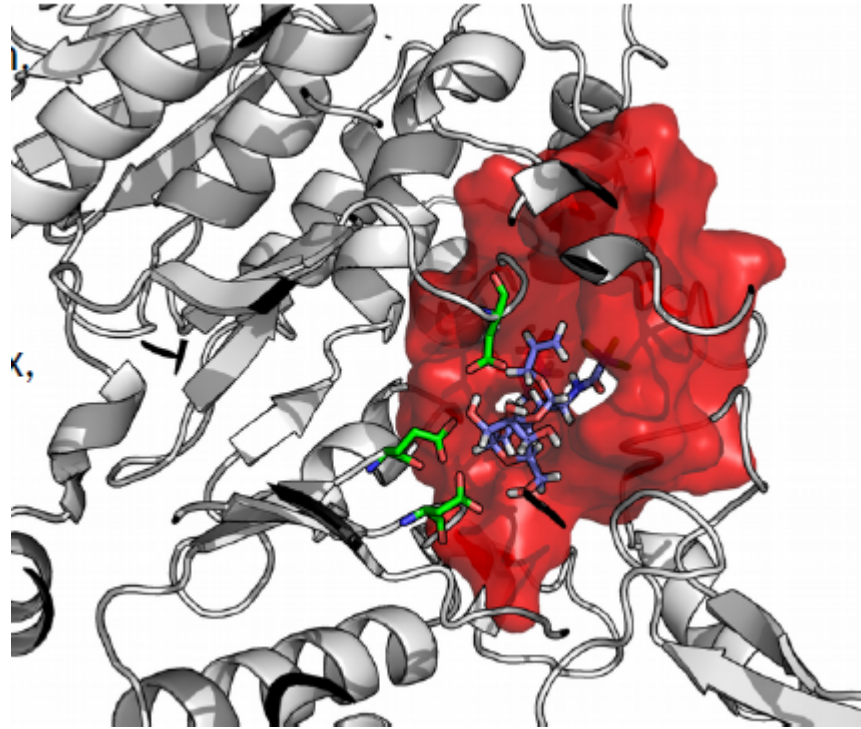
Genetic Linkage Analysis



(Marinescu & Dechter, AAAI 2006 ; IJCAI11)

$n \leq 1,200$, $d \leq 7$, $e(2-5) \leq 2,000$

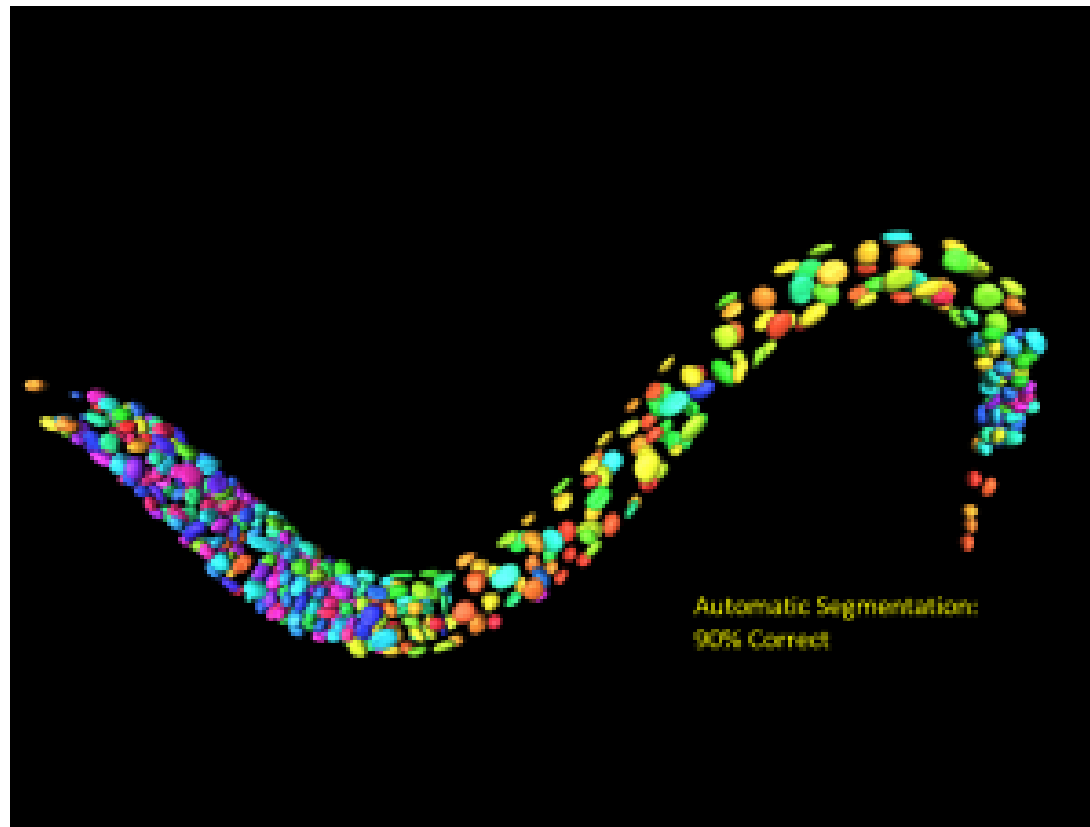
Protein Design



(CP12 – Bioinformatics13 - **AIJ14** – JCTC15 – ISMP18)

$n \leq 120$, $d \leq 190$, $e(2) \leq 7,260$

Graph Matching (worms segmentation)



(Kainmueller et al, Med Image Comput 2014 ; Haller et al, AAAI 2018)

$n \leq 558$, $d \leq 128$, $e(2) \leq 23,407$

Graphical Model

Definition (Graphical model)

- Let $X = (X_1, \dots, X_n)$ be a set of variables.
- X_i takes values in $\Lambda_i \subseteq \mathbb{R}$.
- A realization of X is denoted $x = (x_1, \dots, x_n)$, with $x_i \in \Lambda_i$.
- A graphical model over X is a function $\psi : \prod_i \Lambda_i \rightarrow \mathbb{R}$, which writes, $\forall x \in X$:

$$\psi(x) = \odot_{B \in \mathcal{B}} \psi_B(x_B),$$

where \mathcal{B} is a set of subsets of $V = \{1, \dots, n\}$, $\psi_B : \prod_{i \in B} \Lambda_i \rightarrow \mathbb{R}$ and $\odot \in \{\prod, \sum, \min, \max \dots\}$ is a combination operator.

Probabilistic Graphical Models

Definition (Markov chain)

- $X = (X_1, \dots, X_n)$ is a set of variables, with finite domains $\{\Lambda_i\}_{i=1, \dots, n}$.

$$P(x_1, \dots, x_n) = \underbrace{P(x_1)}_{\psi_1(x_1)} \times \underbrace{P(x_2|x_1)}_{\psi_{12}(x_1, x_2)} \times \dots \times \underbrace{P(x_n|x_{n-1})}_{\psi_{(n-1)n}(x_{n-1}, x_n)}$$

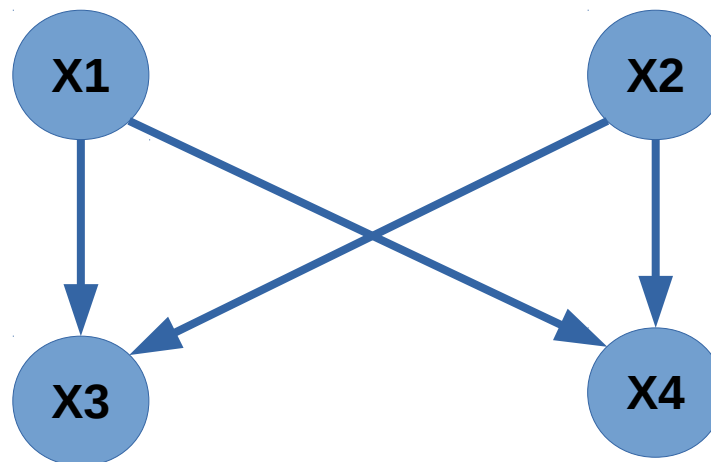


Probabilistic Graphical Models

Definition (Bayesian network)

- $X = (X_1, \dots, X_n)$ is a set of variables, with finite domains $\{\Lambda_i\}_{i=1, \dots, n}$.
- $Par(i) \subseteq \{1, \dots, i-1\}, \forall i = 2, \dots, n$.

$$P(x_1, \dots, x_n) = \underbrace{P(x_1)}_{\psi_1(x_1)} \times \prod_{i=2}^n \underbrace{P(x_i | X_{Par(i)})}_{\psi_{Par(i) \cup \{i\}}(x_i, X_{Par(i)})}$$

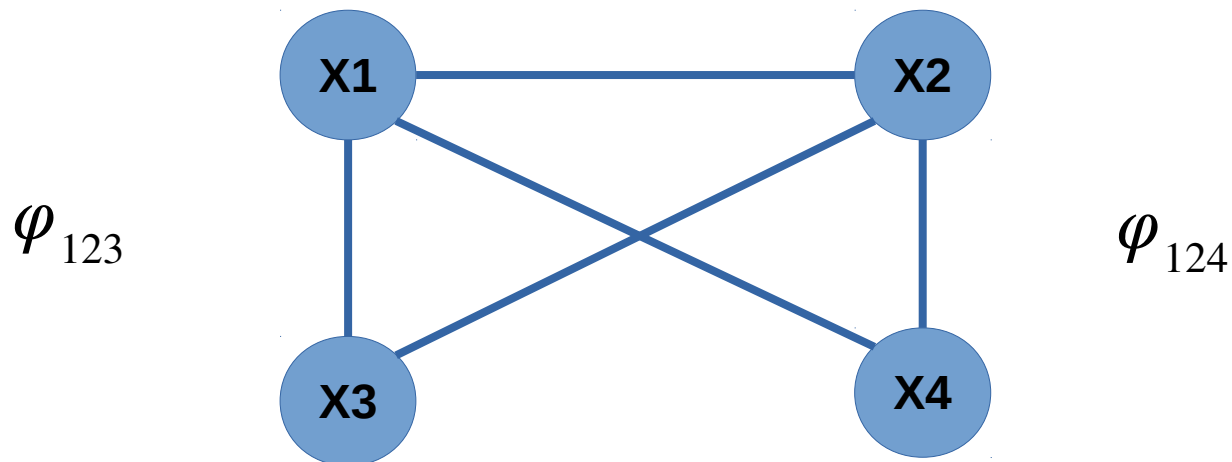


Probabilistic Graphical Models

Definition (Markov Random Field)

- $G = (V, E)$ is an undirected graph with vertices $V = \{1, \dots, n\}$, edges $E \in V \times V$ and \mathcal{C} is the set of *cliques* of G .
- $\{\psi_C : X_C \rightarrow \mathbb{R}^{+*}\}_{C \in \mathcal{C}}$ are strictly positive functions.

$$P(x_1, \dots, x_n) = \underbrace{\frac{1}{Z}}_{\psi_\emptyset, \text{ normalizing constant}} \times \prod_{C \in \mathcal{C}} \psi_C(x_C)$$

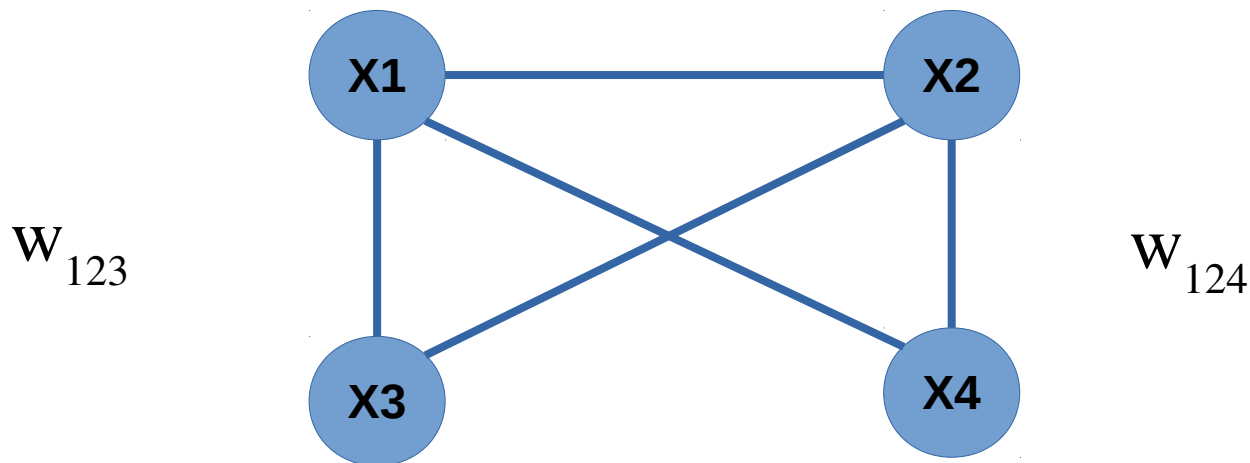


Deterministic Graphical Model

Definition (Cost Functions networks)

- $\{w_C : X_C \rightarrow \mathbb{R}^+\}_{C \in \mathcal{C}}$ are positive functions.

$$w(x_1, \dots, x_n) = \sum_{C \in \mathcal{C}} w_C(x_C)$$



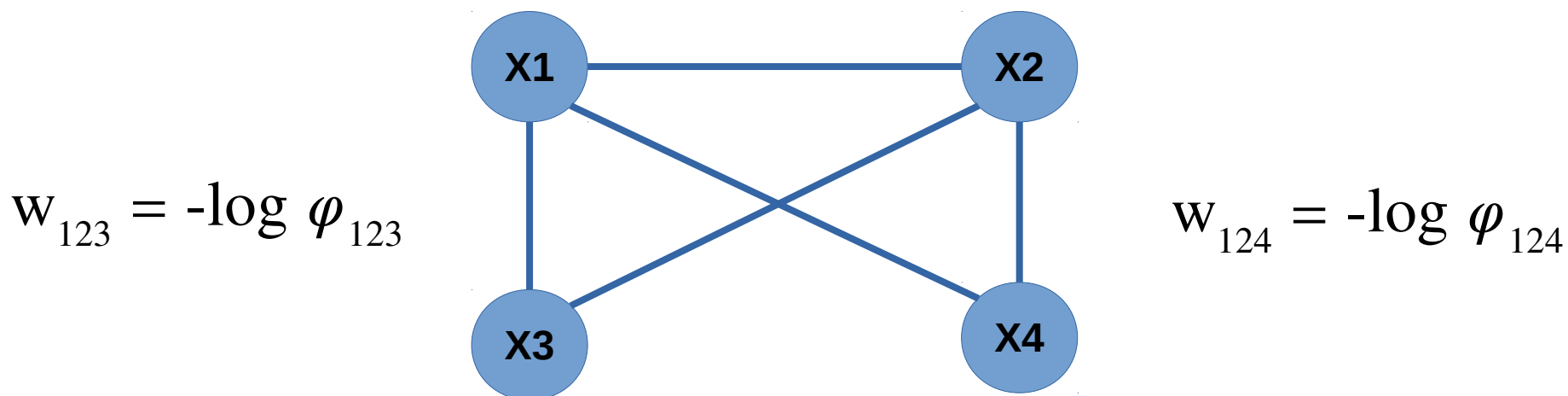
Deterministic Graphical Model

Definition (Cost Functions networks)

- $\{w_C : X_C \rightarrow \mathbb{R}^+\}_{C \in \mathcal{C}}$ are positive functions.

$$w(x_1, \dots, x_n) = \sum_{C \in \mathcal{C}} w_C(x_C)$$

Minimization task: $\min w(x_1, \dots, x_n)$ NP-hard problem



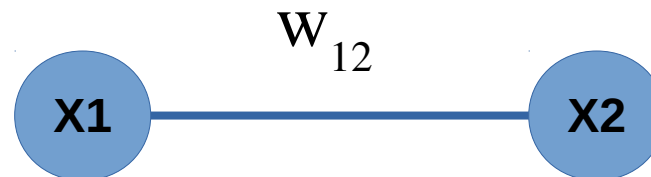
Energy minimization task is equivalent to finding the most probable explanation

Example

In JSON compatible toulbar2 *cfn* format



```
{
  problem: { name: "maximization", mustbe: ">-5.0"},
  variables: { "X1": ["a", "b"], "X2": ["c", "d"] },
  functions: {
    "w0": {scope: [], costs: [-6.0]},
    "w1": {scope: ["X1"], costs: [1.0, 0.5]},
    "w2": {scope: ["X2"], costs: [1.0, 0.5]},
    "w12": {scope: ["X1", "X2"], costs: [-1.0, 0.5, -2.0, 5.5]}
  }
}
```

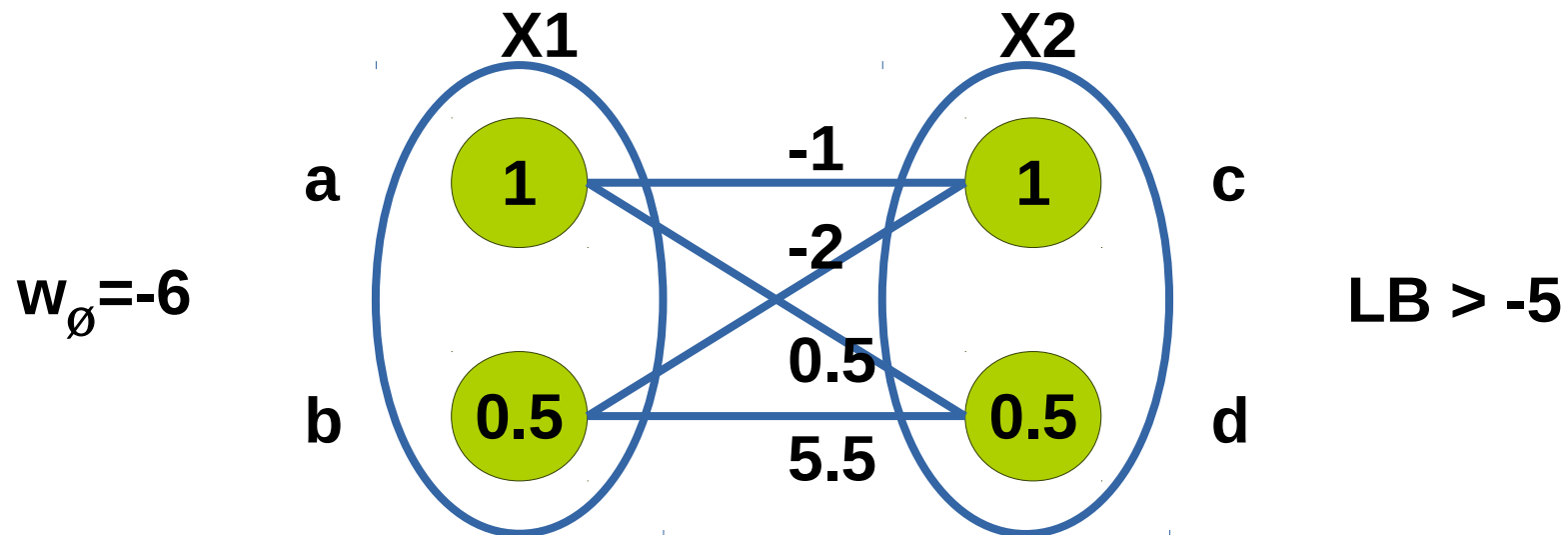


Micro-Structure

```

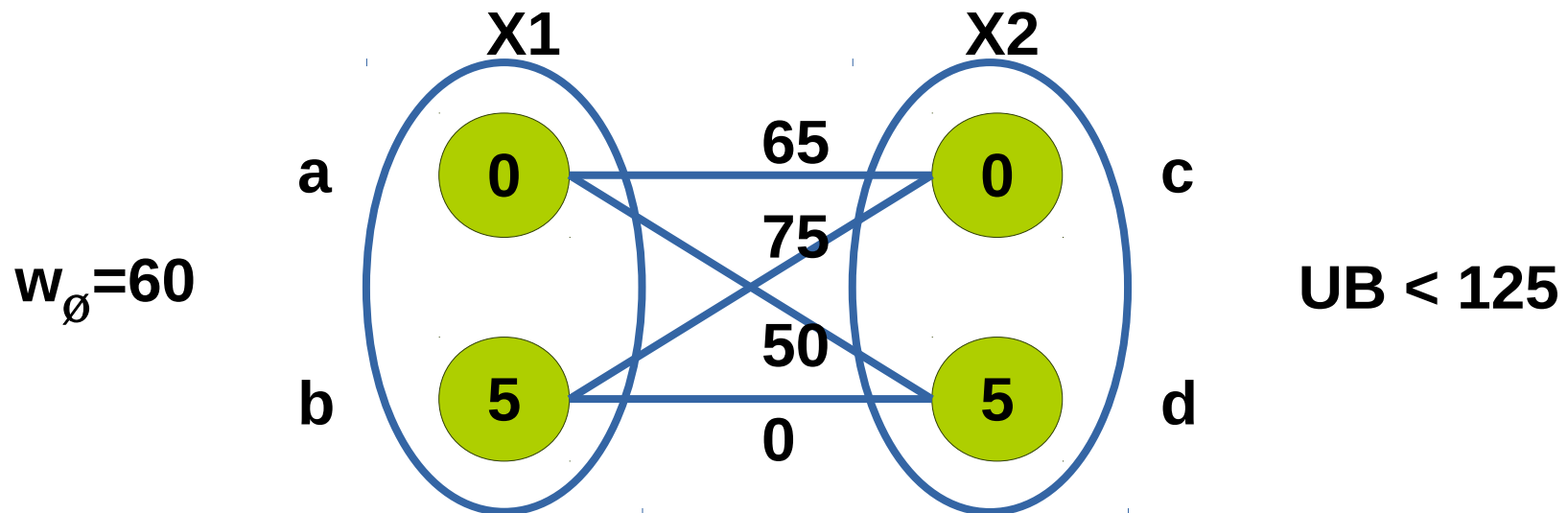
{
  problem: { name: "maximization", mustbe: ">-5.0"},
  variables: { "X1": ["a", "b"], "X2": ["c", "d"] },
  functions: {
    "w0": {scope: [], costs: [-6.0]},
    "w1": {scope: ["X1"], costs: [1.0, 0.5]},
    "w2": {scope: ["X2"], costs: [1.0, 0.5]},
    "w12": {scope: ["X1", "X2"], costs: [-1.0, 0.5, -2.0, 5.5]}
  }
}

```



Minimization with **non-negative integer** costs

```
{  
  problem: { name: "maximization", mustbe: ">-5.0"},  
  variables: { "X1": ["a", "b"], "X2": ["c", "d"] },  
  functions: {  
    "w0": {scope: [], costs: [-6.0]},  
    "w1": {scope: ["X1"], costs: [1.0, 0.5]},  
    "w2": {scope: ["X2"], costs: [1.0, 0.5]},  
    "w12": {scope: ["X1", "X2"], costs: [-1.0, 0.5, -2.0, 5.5]}  
  }  
}
```

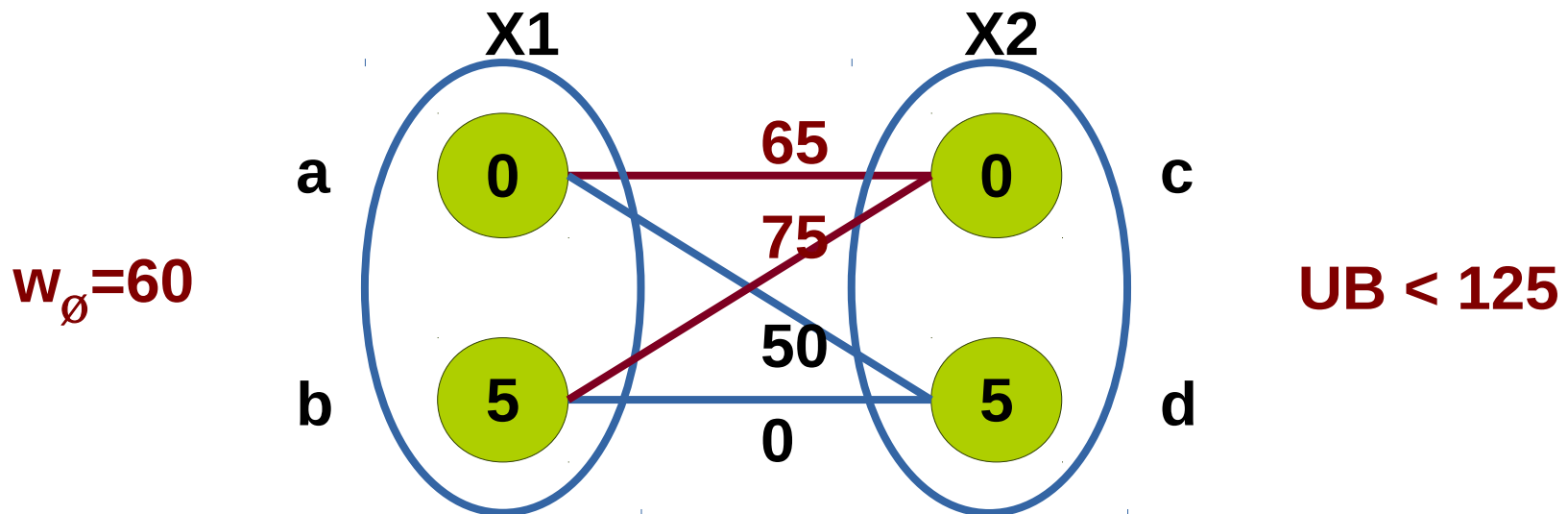


Constraints are Cost Functions

```

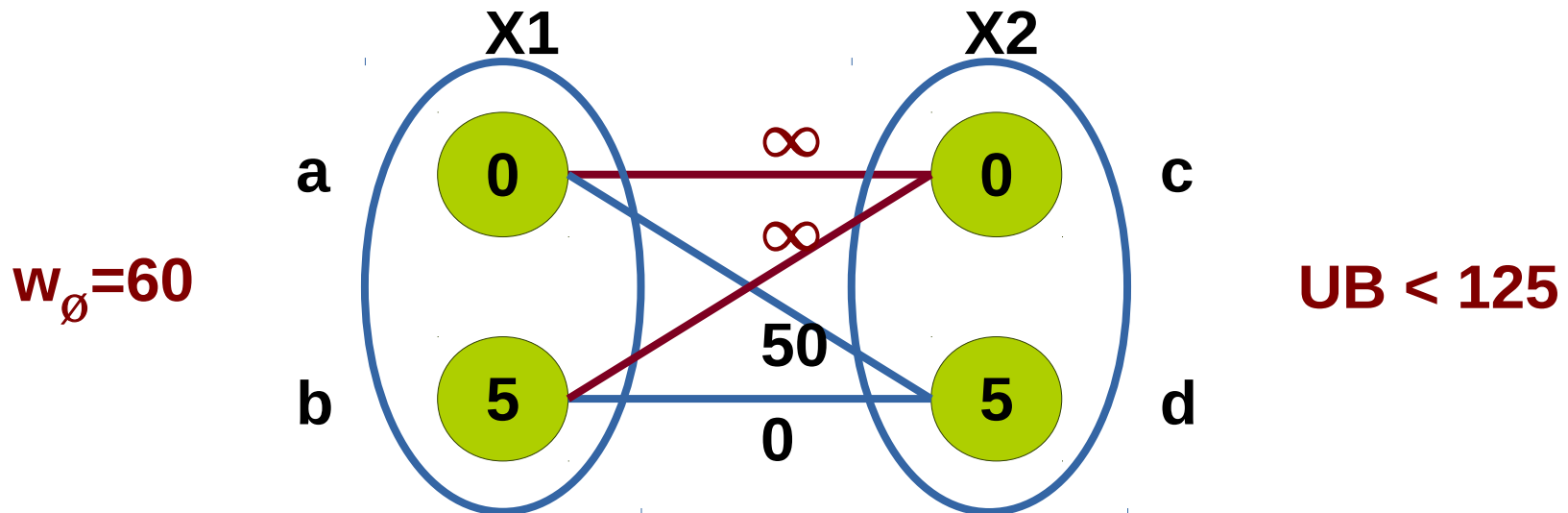
{
  problem: { name: "maximization", mustbe: ">-5.0"},
  variables: { "X1": ["a", "b"], "X2": ["c", "d"] },
  functions: {
    "w0": {scope: [], costs: [-6.0]},
    "w1": {scope: ["X1"], costs: [1.0, 0.5]},
    "w2": {scope: ["X2"], costs: [1.0, 0.5]},
    "w12": {scope: ["X1", "X2"], costs: [-1.0, 0.5, -2.0, 5.5]}
  }
}

```



Constraints are Cost Functions

```
{  
  problem: { name: "maximization", mustbe: ">-5.0"},  
  variables: { "X1": ["a", "b"], "X2": ["c", "d"] },  
  functions: {  
    "w0": {scope: [], costs: [-6.0]},  
    "w1": {scope: ["X1"], costs: [1.0, 0.5]},  
    "w2": {scope: ["X2"], costs: [1.0, 0.5]},  
    "w12": {scope: ["X1", "X2"], costs: [-1.0, 0.5, -2.0, 5.5]}  
  }  
}
```



Other equivalent formulations

In various toulbar2 input formats

- WCSP

```
wcsp 2 2 4 125
2 2
2 0 1 0 4
0 0 65
0 1 50
1 0 75
1 1 0
1 0 125 2
0 0
1 5
1 1 125 2
0 0
1 5
0 60 0
```

- MRF

```
MARKOV
2
2 2
4
2 0 1
1 0
1 1
1 0
4
0.000341454887383
0.00215443469003
0.0001
1.0
2
1.0
0.541169526546
2
1.0
0.541169526546
2
0.00063095734448
0.00063095734448
```

- Max-SAT

```
p wcnf 2 7 125
65 1 2 0
50 1 -2 0
75 -1 2 0
5 -1 0
5 -2 0
60 1 0
60 -1 0
```

- QPBO

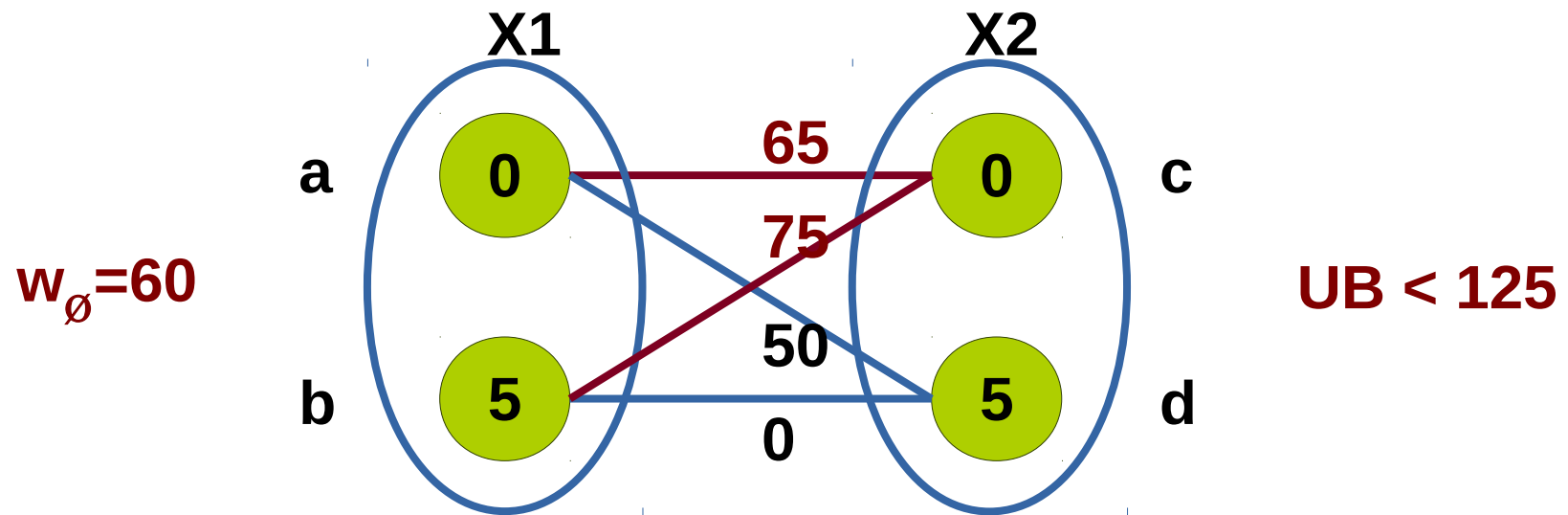
```
4 13
1 3 32.5
1 4 25
2 3 37.5
2 2 5
4 4 5
1 1 60
2 2 60
1 1 -1000
2 2 -1000
1 2 1000
3 3 -1000
4 4 -1000
3 4 1000
```

Local reasoning techniques

Cost Function Propagation

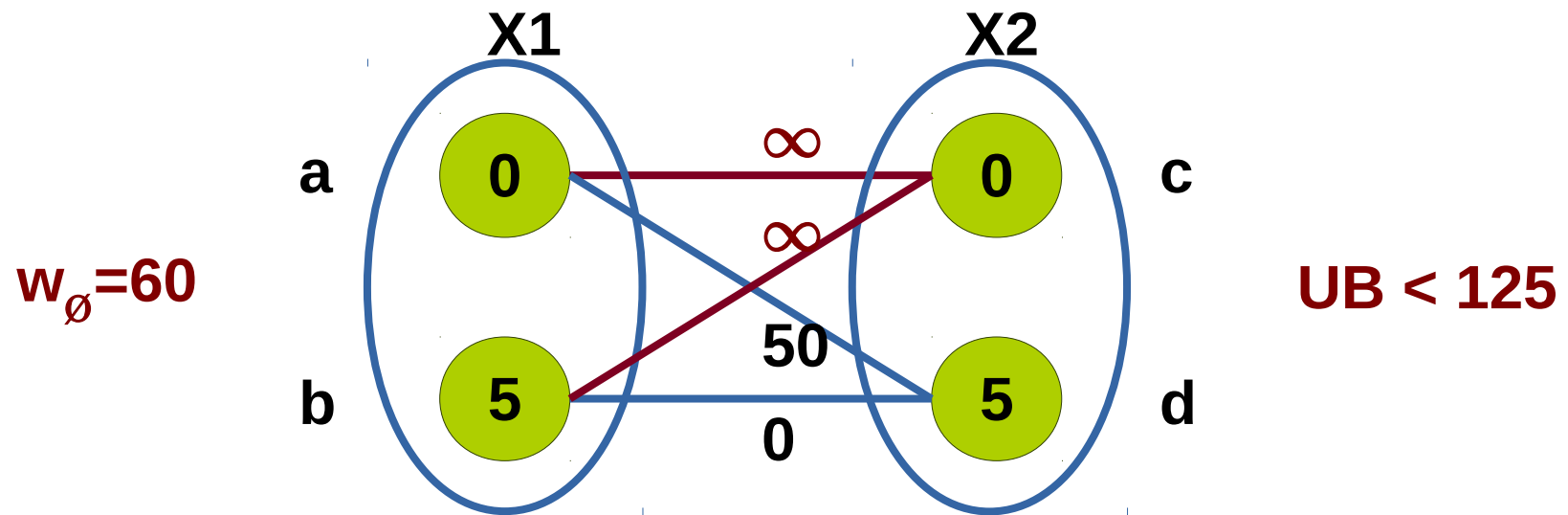
Reparameterization and pruning

(Schiex, CP 2000 ; Larrosa, AAAI 2002 ; Cooper, FSS 2003 ; IJCAI05 ; IJCAI07 ; AAAI08 ; AIJ10)



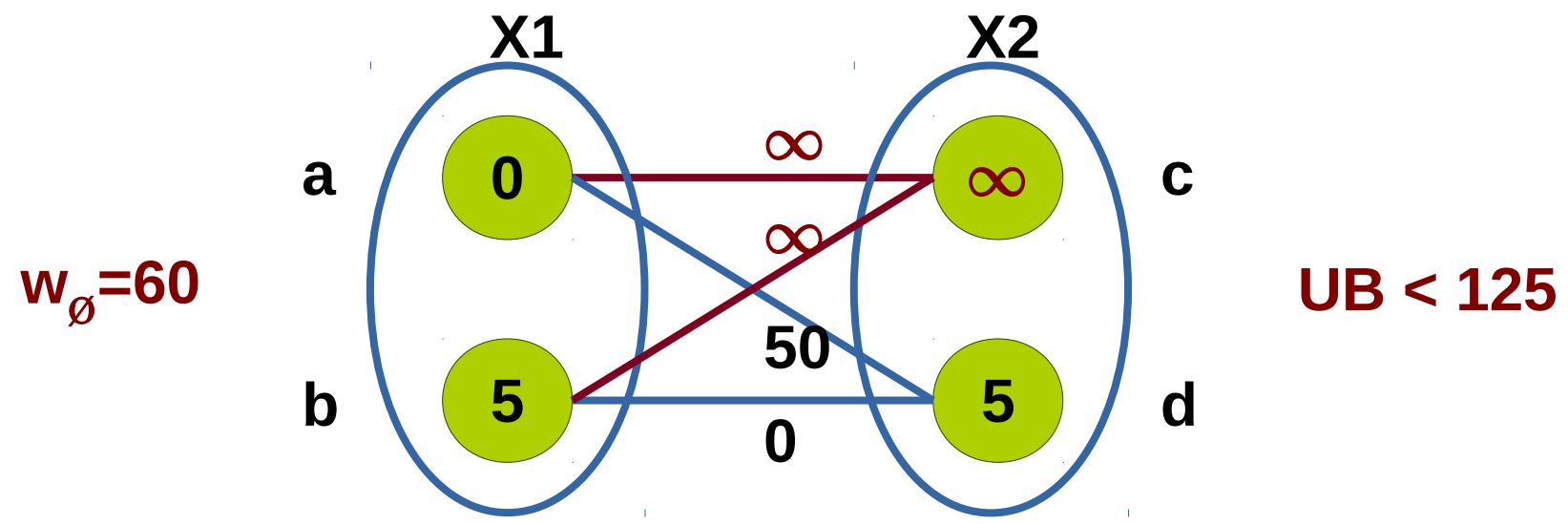
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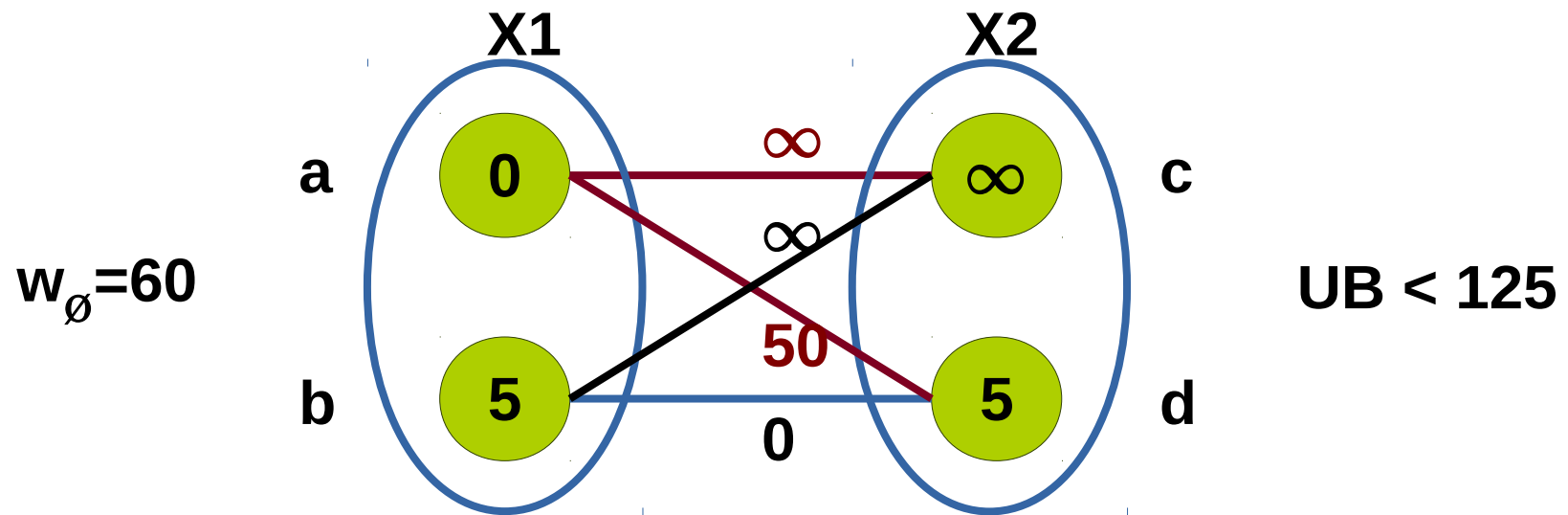
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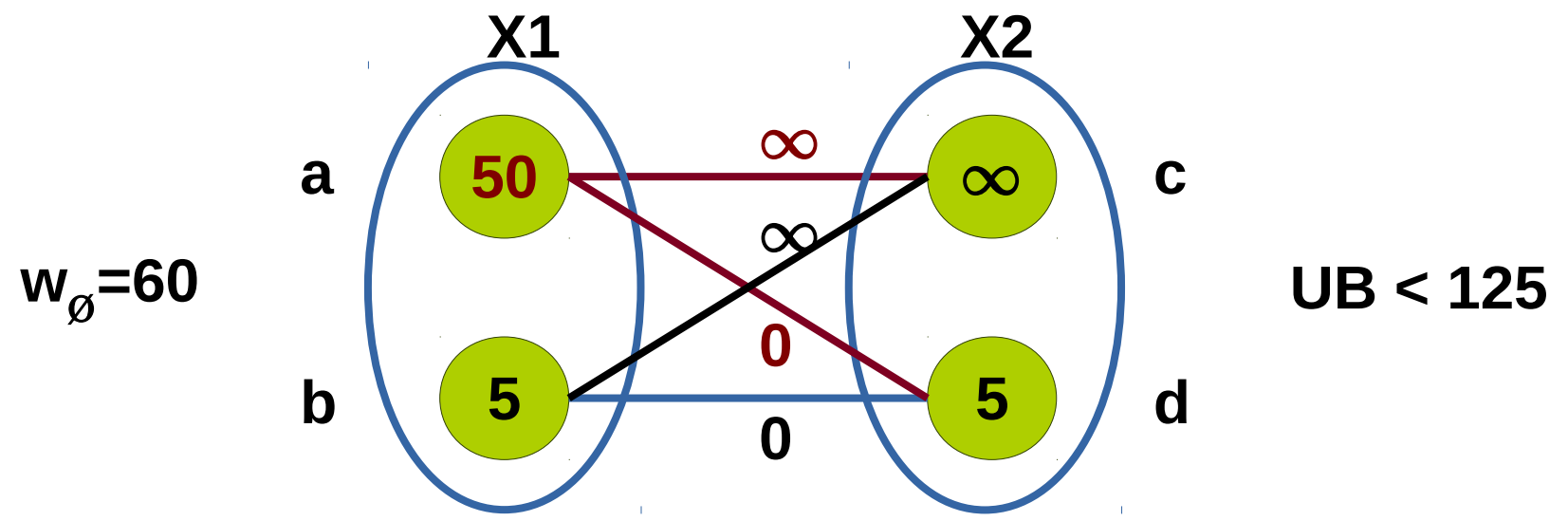
Reparameterization and pruning

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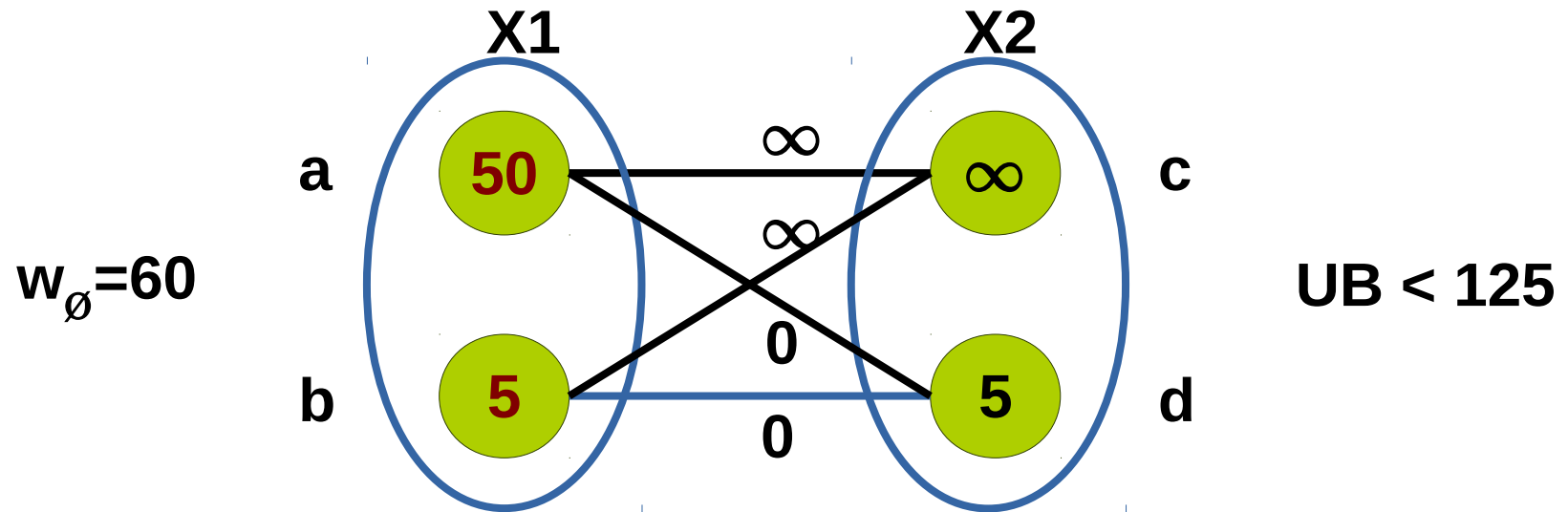
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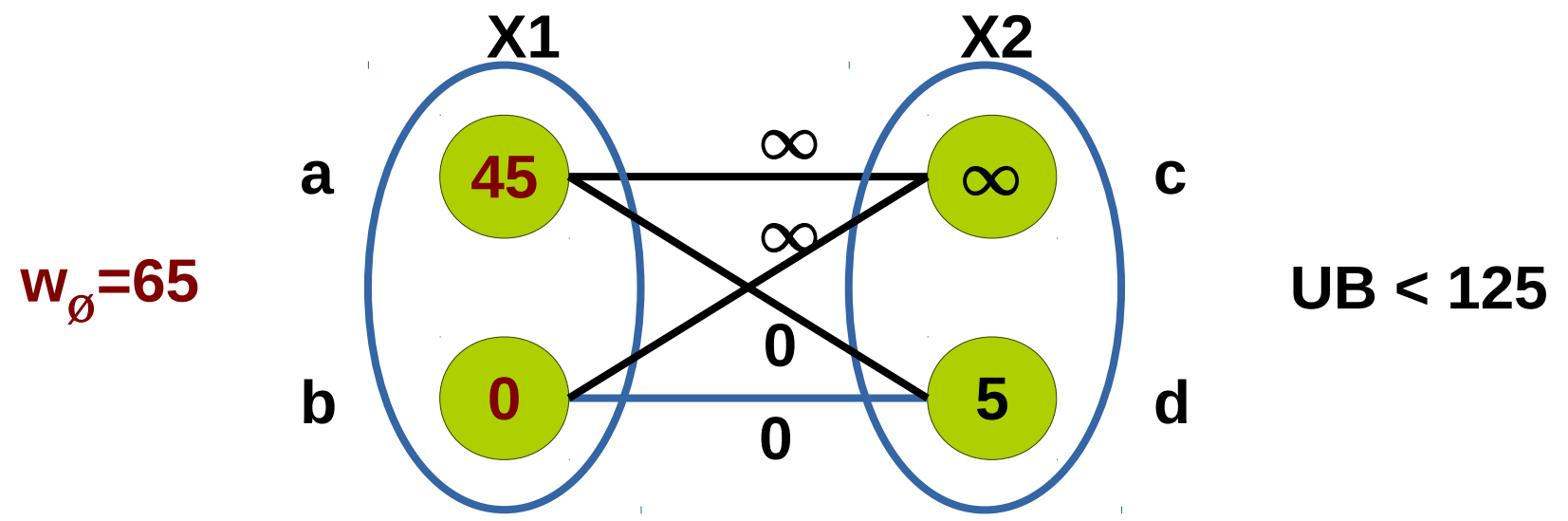
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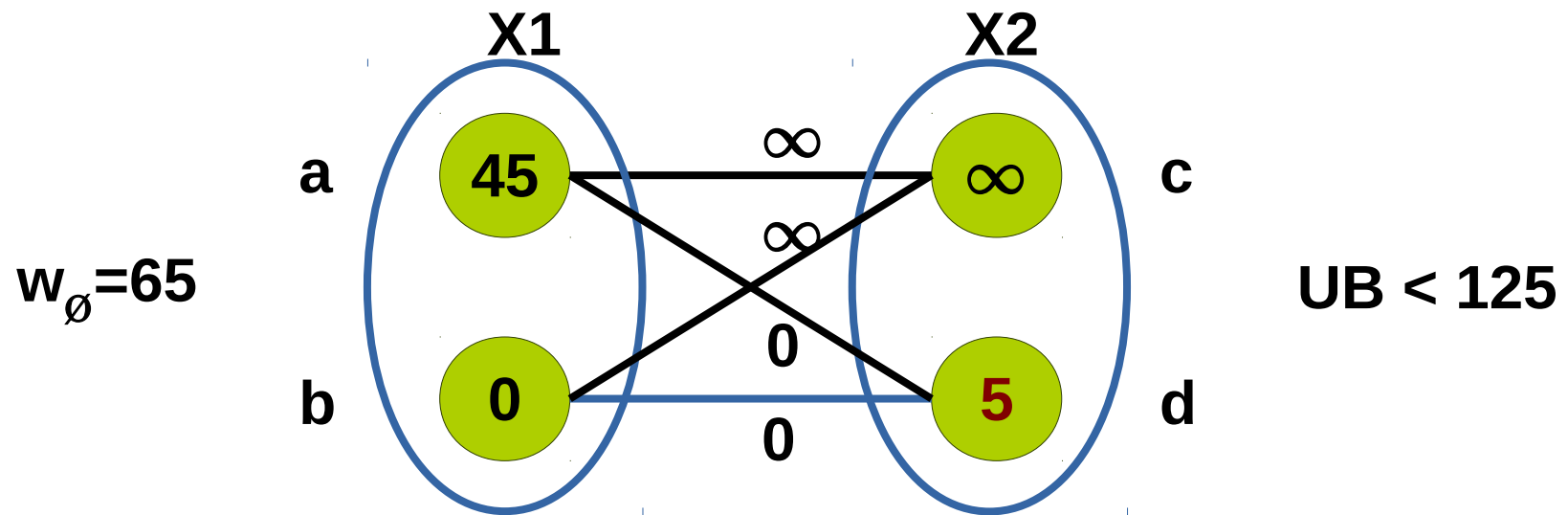
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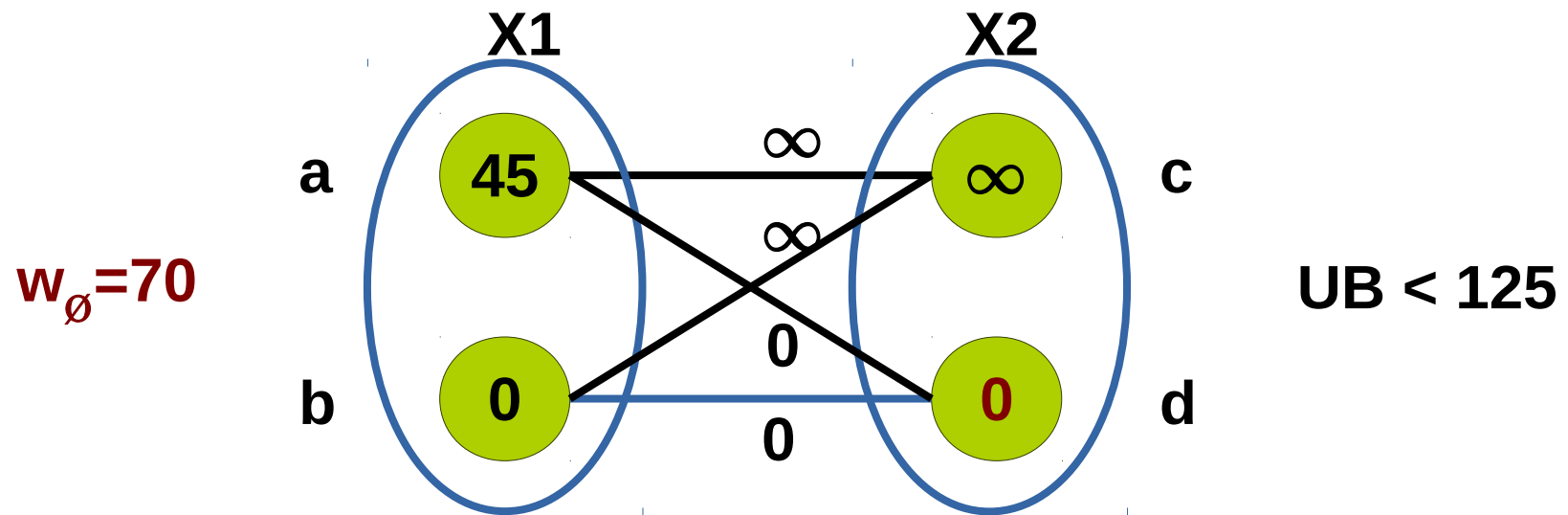
Reparameterization and pruning

(Schiex, CP 2000 ; Larrosa, AAI 2002 ; Cooper, FSS 2003 ; IJCAI05 ; IJCAI07 ; AAI08 ; AIJ10)



Reparameterization and pruning

(Schiex, CP 2000 ; Larrosa, AAI 2002 ; Cooper, FSS 2003 ; IJCAI05 ; IJCAI07 ; AAI08 ; AIJ10)



Reparameterization and pruning

(Schiex, CP 2000 ; Larrosa, AAAI 2002 ; Cooper, FSS 2003 ; IJCAI05 ; IJCAI07 ; AAAI08 ; AIJ10)

- Reparameterization produces a feasible solution of the **dual** of a strong LP relaxation
 - We use a **sequence** of reparameterizations
 - Faster than LP
 - Not optimal: weaker dual bounds than LP
 - Many fixpoints
- and domain value pruning

Same Example in 01LP

(CPAIOR16 – Constraints16)

• Direct LP formulation

Minimize

+50 t_0_0_1_1 +75 t_0_1_1_0 +65
t_0_0_1_0 -5 d0_0 -5 d1_0 +60 t +10 t

Subject to:

+1 d0_0 -1 d1_0 - t_0_0_1_1 <= 0

-1 d0_0 +1 d1_0 - t_0_1_1_0 <= 0

+1 d0_0 +1 d1_0 - t_0_0_1_0 <= 1

Bounds

t_0_0_1_0 <= 1

t_0_0_1_1 <= 1

t_0_1_1_0 <= 1

t = 1

Binary

d0_0 d1_0

End

• Stronger LP formulation

Minimize

+50 t_0_0_1_1 +75 t_0_1_1_0 +65 t_0_0_1_0 -5
d0_0 -5 d1_0 +60 t +10 t

Subject to:

+1 t_0_0_1_0 +1 t_0_0_1_1 -1 d0_0 = 0

+1 t_0_1_1_0 +1 t_0_1_1_1 +1 d0_0 = 1

+1 t_0_0_1_0 +1 t_0_1_1_0 -1 d1_0 = 0

+1 t_0_0_1_1 +1 t_0_1_1_1 +1 d1_0 = 1

Bounds

t_0_0_1_0 <= 1

t_0_0_1_1 <= 1

t_0_1_1_0 <= 1

t_0_1_1_1 <= 1

t = 1

Binary

d0_0 d1_0

End

Uncapacitated Warehouse Location Problem

(Kratika et al., RAIRO OR 2001)

Search nodes

Instance	cplex 12.7.1	toulbar2 1.0.0
Capmo1 100x100	155	7,581
Capmo2 100x100	25	2,024
Capmo3 100x100	93	5,439
Capmo4 100x100	23	4,055
Capmo5 100x100	28	2,664

CPU time (sec. on PC i7 3GHz)

Instance	cplex 12.7.1	toulbar2 1.0.0
Capmo1 100x100	13.01	20.13
Capmo2 100x100	3.06	3.02
Capmo3 100x100	13.32	11.40
Capmo4 100x100	3.26	7.45
Capmo5 100x100	2.68	4.62

Clique cuts

Given a set S

$$x_i + x_j \leq 1 \quad \forall x_i, x_j \in S$$

\Rightarrow Satisfied by $x_i = 0.5$

But we can get

$$\sum_{x_i \in S} x_i \leq 1$$

Clique cuts in CFN

(CP17)

Straightforward generalization

Given a set S of $\langle X_i, v_i \rangle$ with

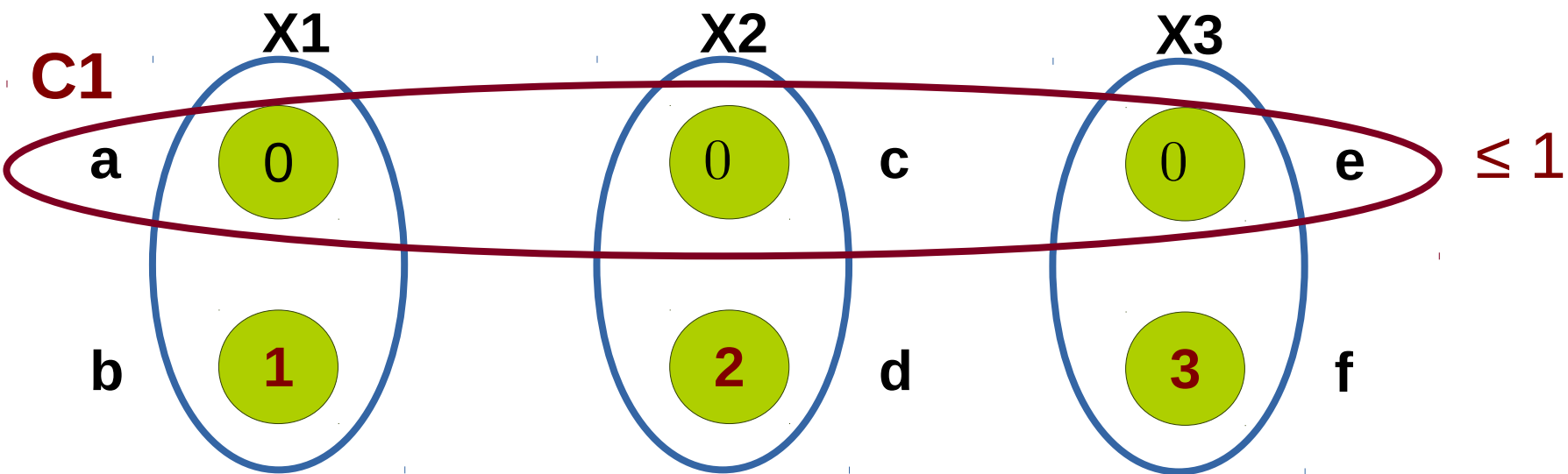
- $c_{ij}(v_i, v_j) = \infty$

Then derive

$$\sum_{ij \in S} x_{ij} \leq 1$$

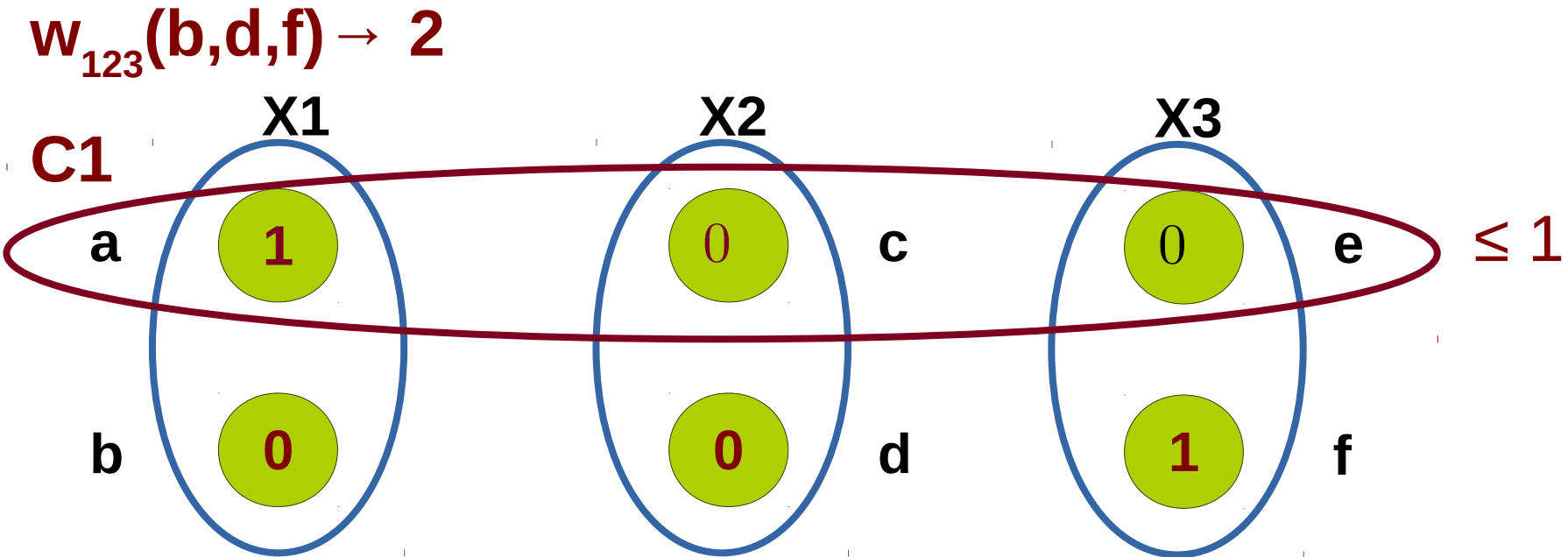
Reparameterization for clique

(CP17)



Reparameterization for clique

(CP17)

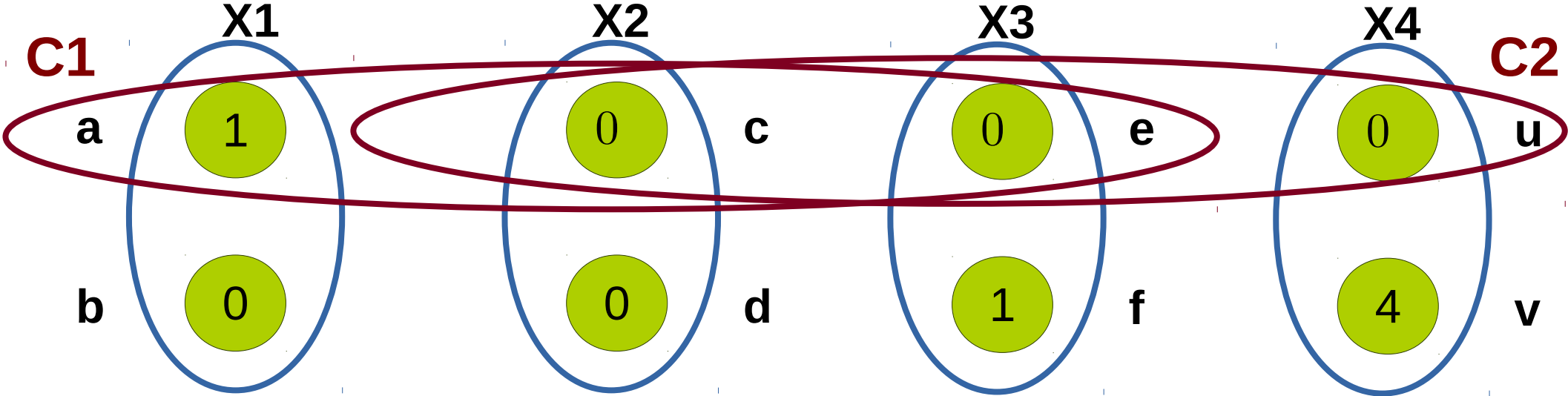


$$w_{\emptyset} = 3$$

Reparameterization for cliques

(CP17)

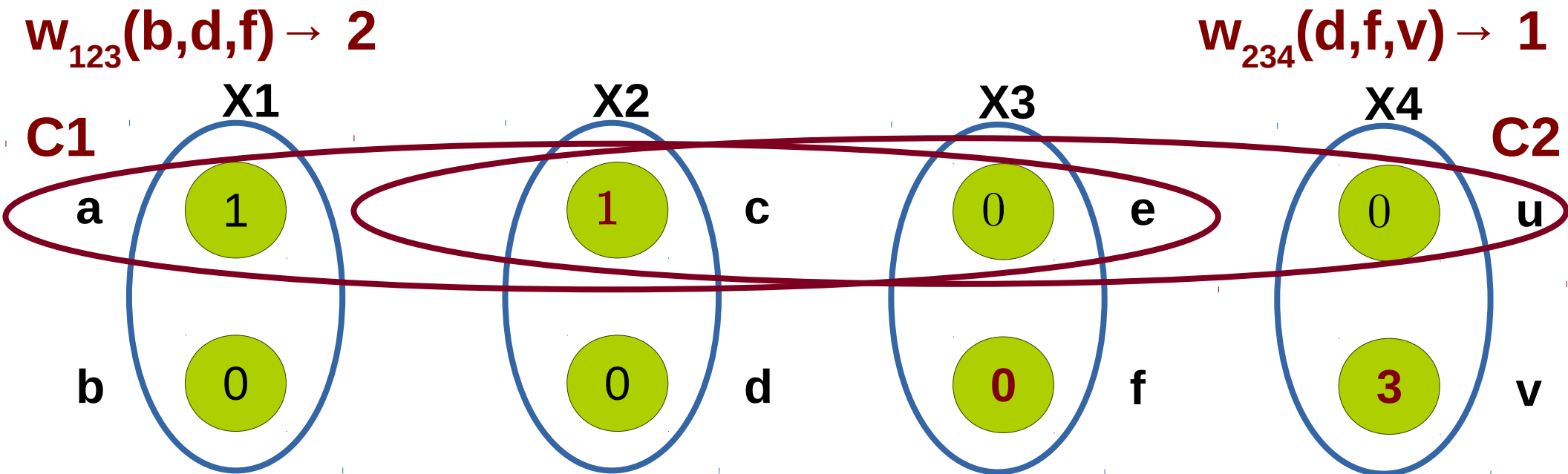
$$w_{123}(b,d,f) \rightarrow 2$$



$$w_{\emptyset} = 3$$

Reparameterization for cliques

(CP17)

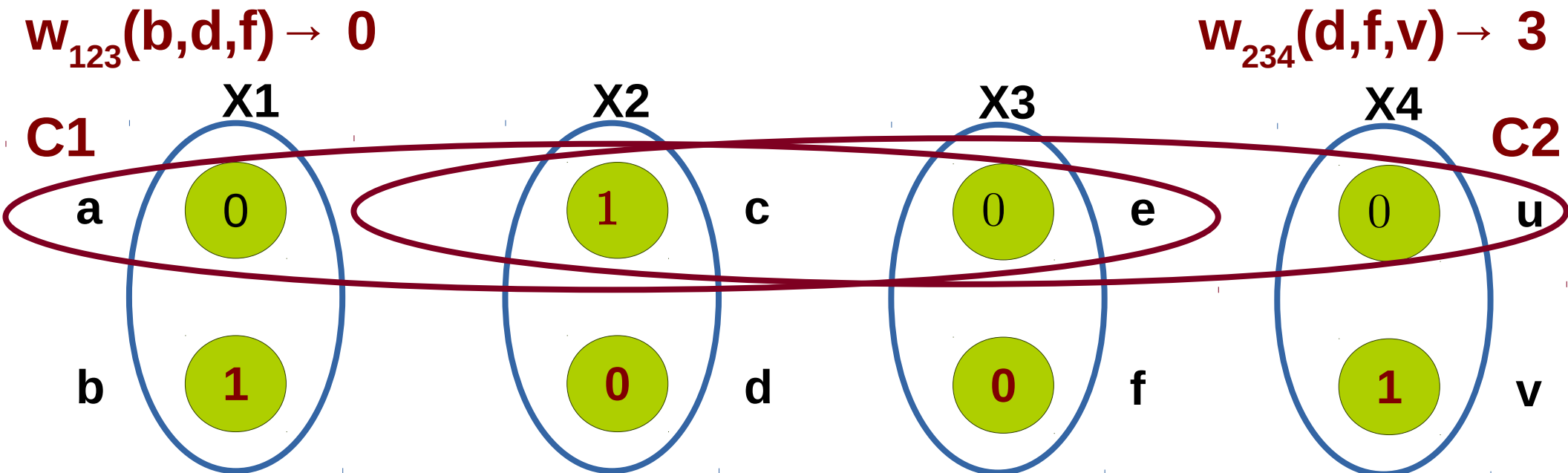


$$w_{\emptyset} = 4$$

Propagating C1 before C2

Reparameterization for cliques

(CP17)



$$w_{\emptyset} = 5$$

Propagating C2 before C1

Select the clique with the largest lower bound increase first

Experimental Results

(CP17)

problem	TOULBAR2		TOULBAR2 ^{clq}		CPLEX	
	solv.	time	solv.	time*	solv.	time
Auction/path	86	59	86	0.18	86	0.01
Auction/sched	84	110	84	0.23	84	0.04
MaxClique	31	1871	37	1508	38	1533
SPOT5	4	2884	6	2603	16	738

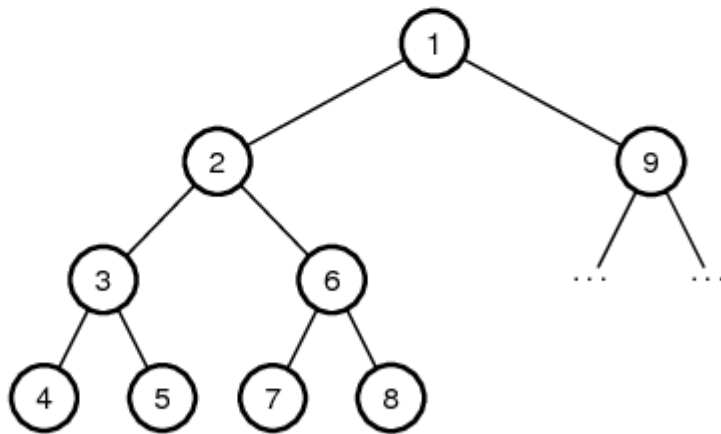
* Including bounded clique detection with Bron-Kerbosch algorithm in preprocessing

Complete tree search methods

Hybrid search

DFS

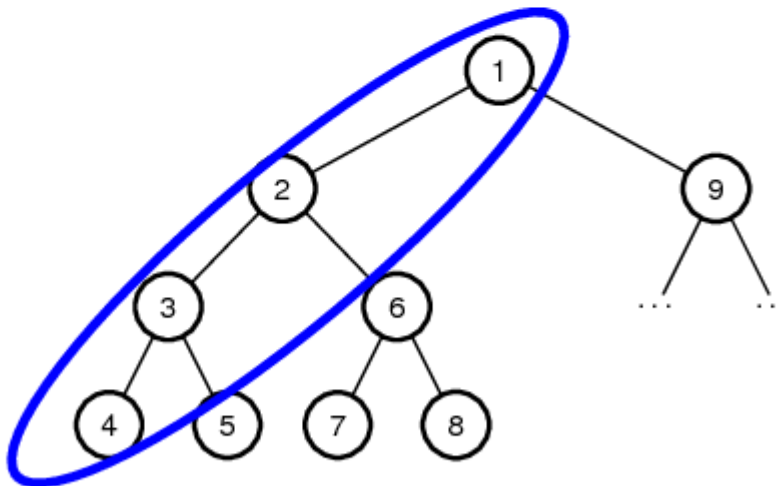
Depth First



DFS

Depth First Advantages

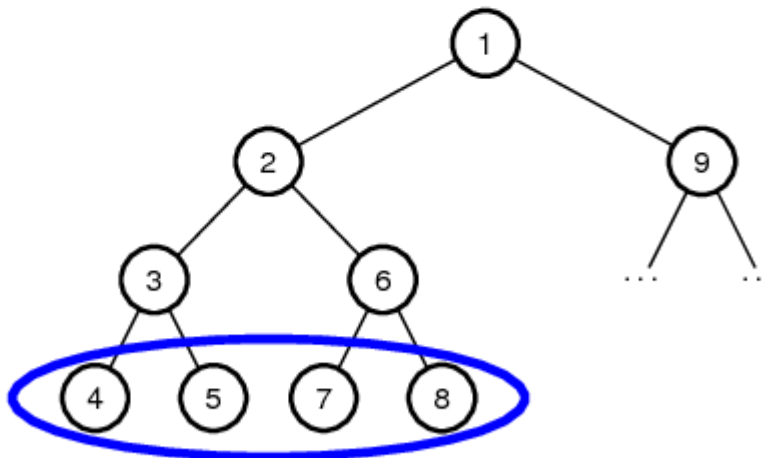
- Incrementality



DFS

Depth First Advantages

- Incrementality
- Anytime (sort of)



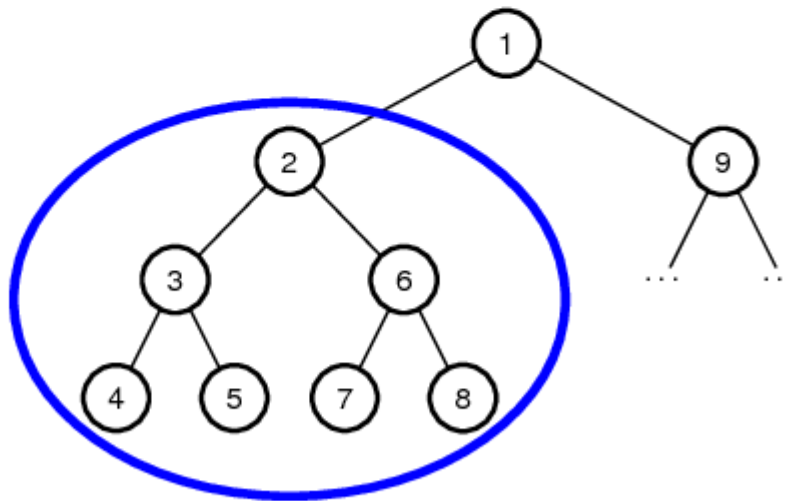
DFS

Depth First Advantages

- Incrementality
- Anytime (sort of)

But

- Thrashing



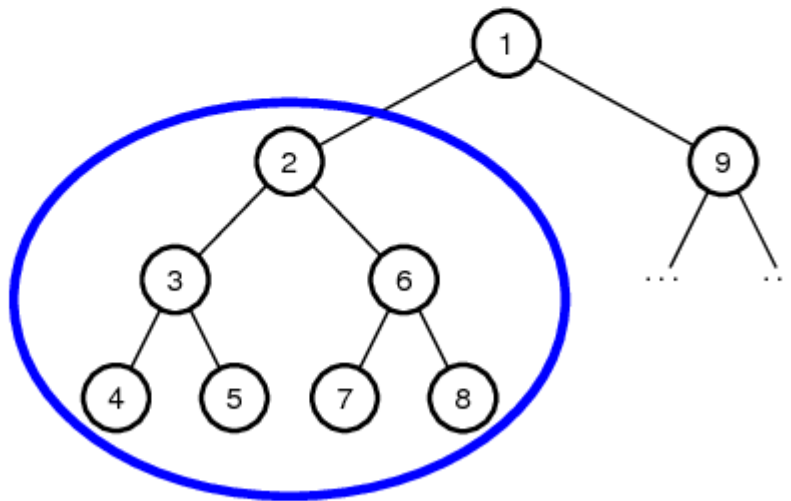
DFS

Depth First Advantages

- Incrementality
- Anytime (sort of)

But

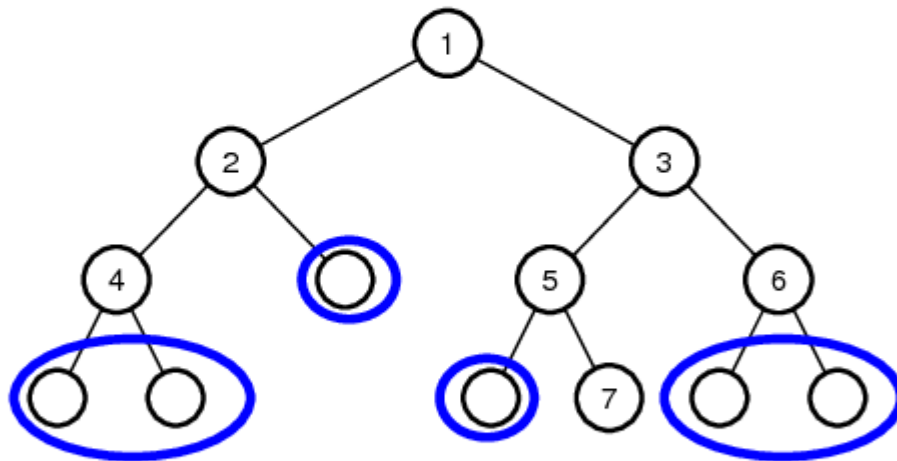
- Thrashing
- No global lower bounds



BFS

Best first

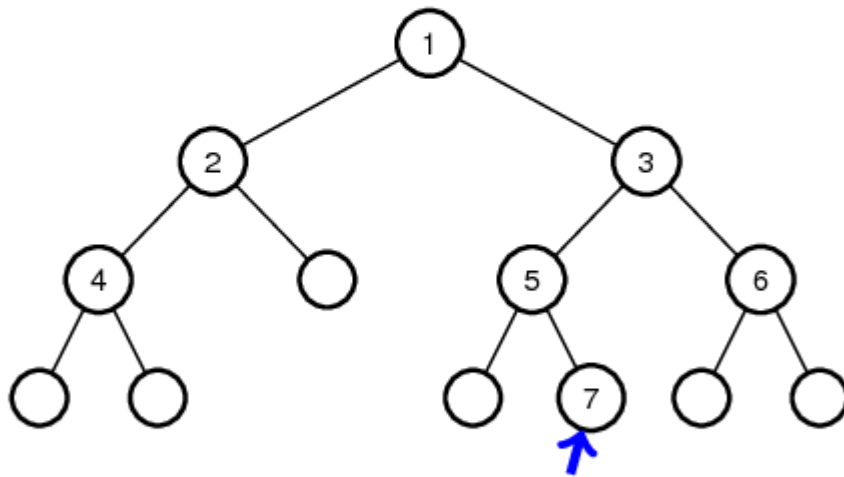
- Memory requirements



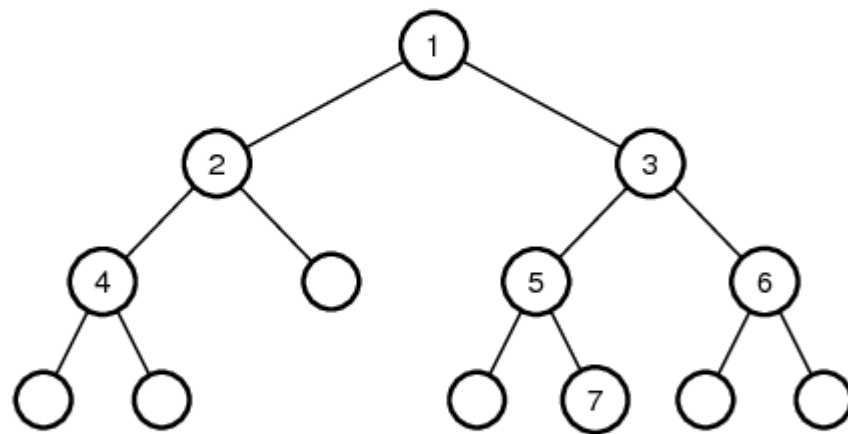
BFS

Best first

- Memory requirements
- No incrementality or even greater memory cost
- Not anytime



BFS



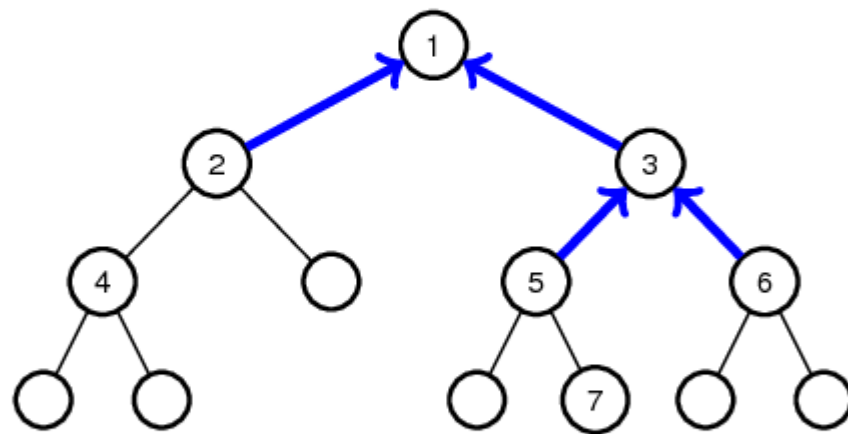
Best first

- Memory requirements
- No incrementality or even greater memory cost
- Not anytime

but

- Theoretical guarantees

BFS



Best first

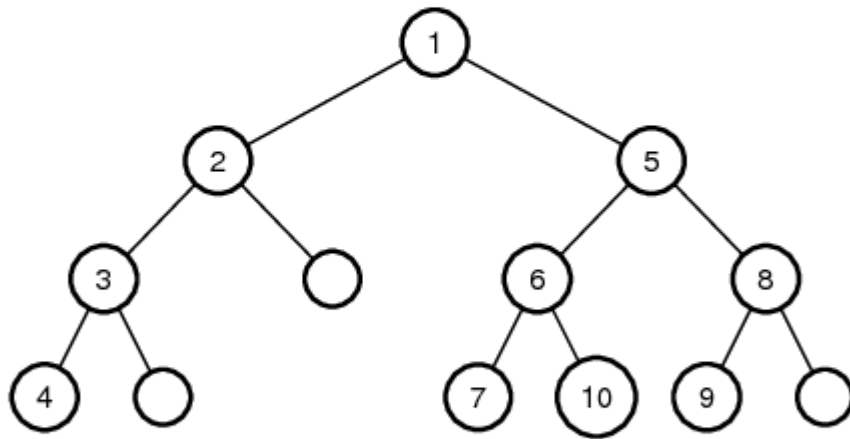
- Memory requirements
- No incrementality or even greater memory cost
- Not anytime

but

- Theoretical guarantees
- Global lower bounds

HBFS

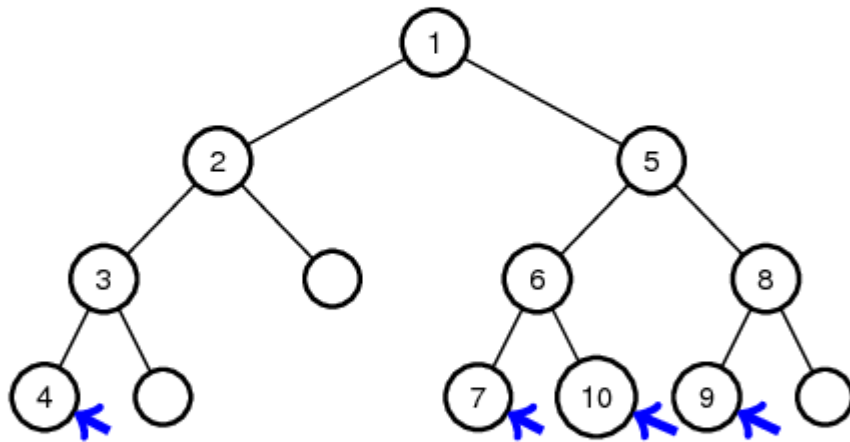
BFS with DFS probes*



HBFS

BFS with DFS probes*

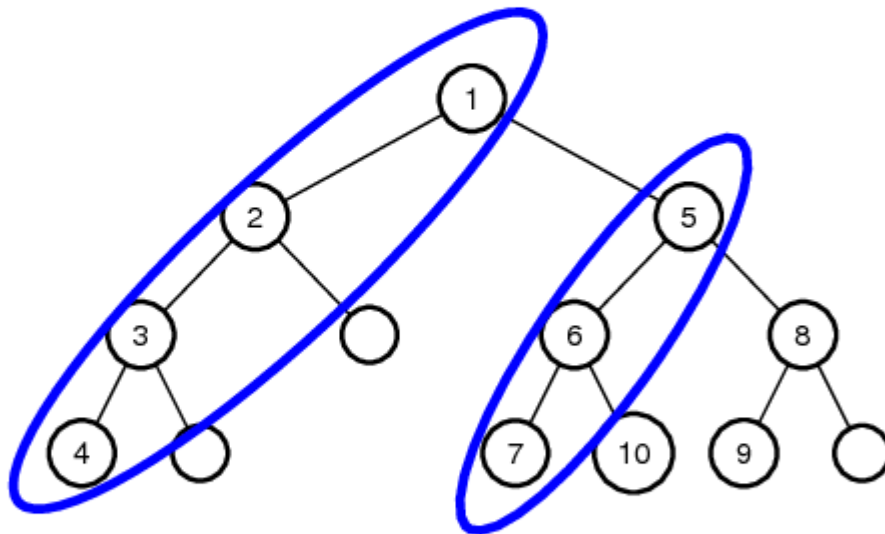
- Improved anytime behavior



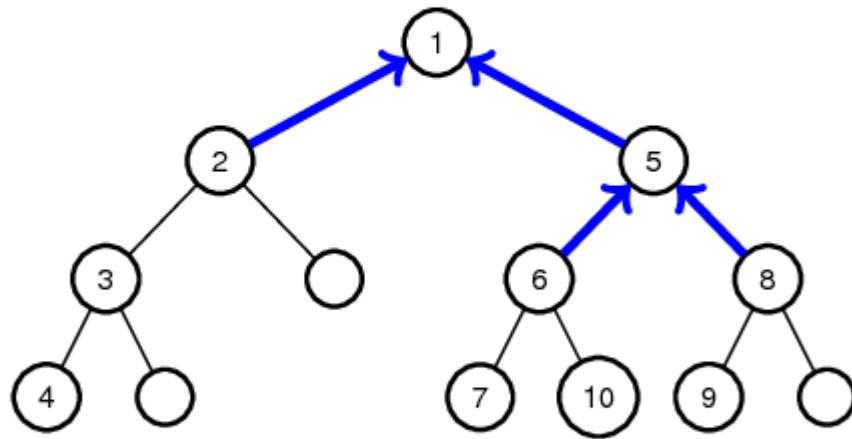
HBFS

BFS with DFS probes*

- Improved anytime behavior
- Incrementality without memory overhead



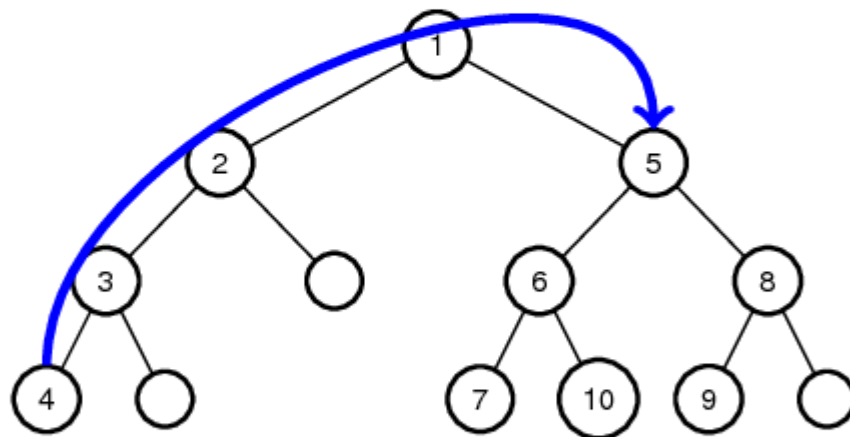
HBFS



BFS with DFS probes*

- Improved anytime behavior
- Incrementality without memory overhead
- Lower bounds

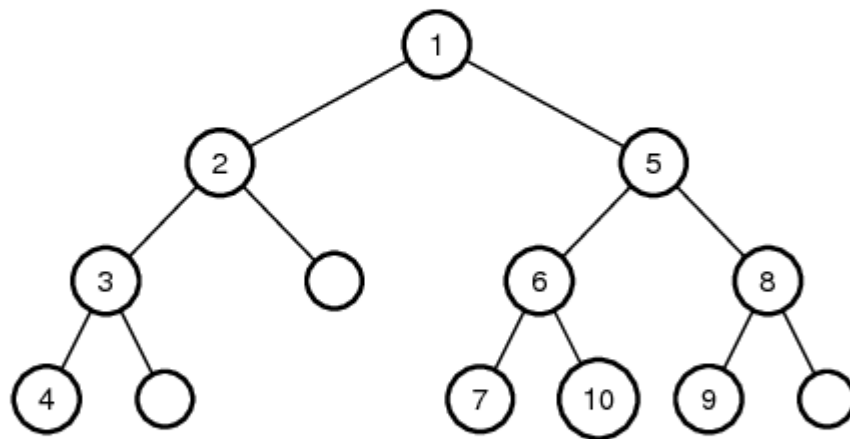
HBFS



BFS with DFS probes*

- Improved anytime behavior
- Incrementality without memory overhead
- Lower bounds
- Some of the advantages of restarting

HBFS



BFS with DFS probes*

- Improved anytime behavior
- Incrementality without memory overhead
- Lower bounds
- Some of the advantages of restarting

* With adaptive heuristic for probe size

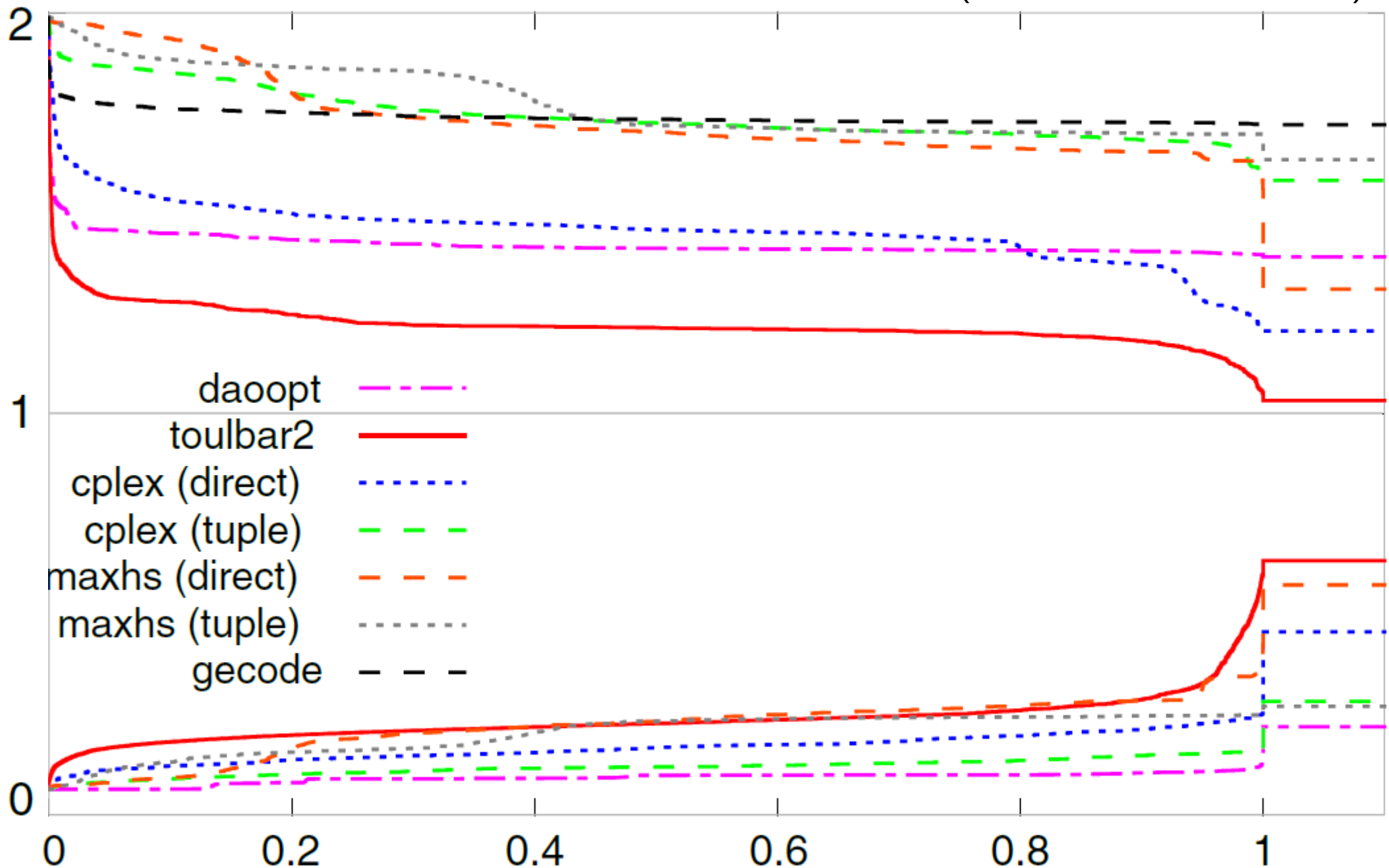
Benchmark

- MRF: Probabilistic Inference Challenge 2011 (uai format)
- CVPR: Computer Vision and Pattern Recognition OpenGM2 (uai)
- CFN: MaxCSP 2008 Competition and CFLib (wcsp format)
- WPMS: Weighted Partial MaxSAT Evaluation 2013 (wcnf format)
- CP: MiniZinc Challenge 2012 & 2013 (minizinc format)

Number of instances and their total compressed (gzipped) size:

Benchmark	Nb.	UAI	WCSP	LP(direct)	LP(tuple)	WCNF(direct)	WCNF(tuple)	MINIZINC
MRF	319	187MB	475MB	2.4G	2.0GB	518MB	2.9GB	473MB
CVPR	1461	430MB	557MB	9.8GB	11GB	3.0GB	15GB	N/A
CFN	281	43MB	122MB	300MB	3.5GB	389MB	5.7GB	69MB
MaxCSP	503	13MB	24MB	311MB	660MB	73MB	999MB	29MB
WPMS	427	N/A	387MB	433MB	N/A	717MB	N/A	631MB
CP	35	7.5MB	597MB	499MB	1.2GB	378MB	1.9GB	21KB
Total	3026	0.68G	2.2G	14G	18G	5G	27G	1.2G

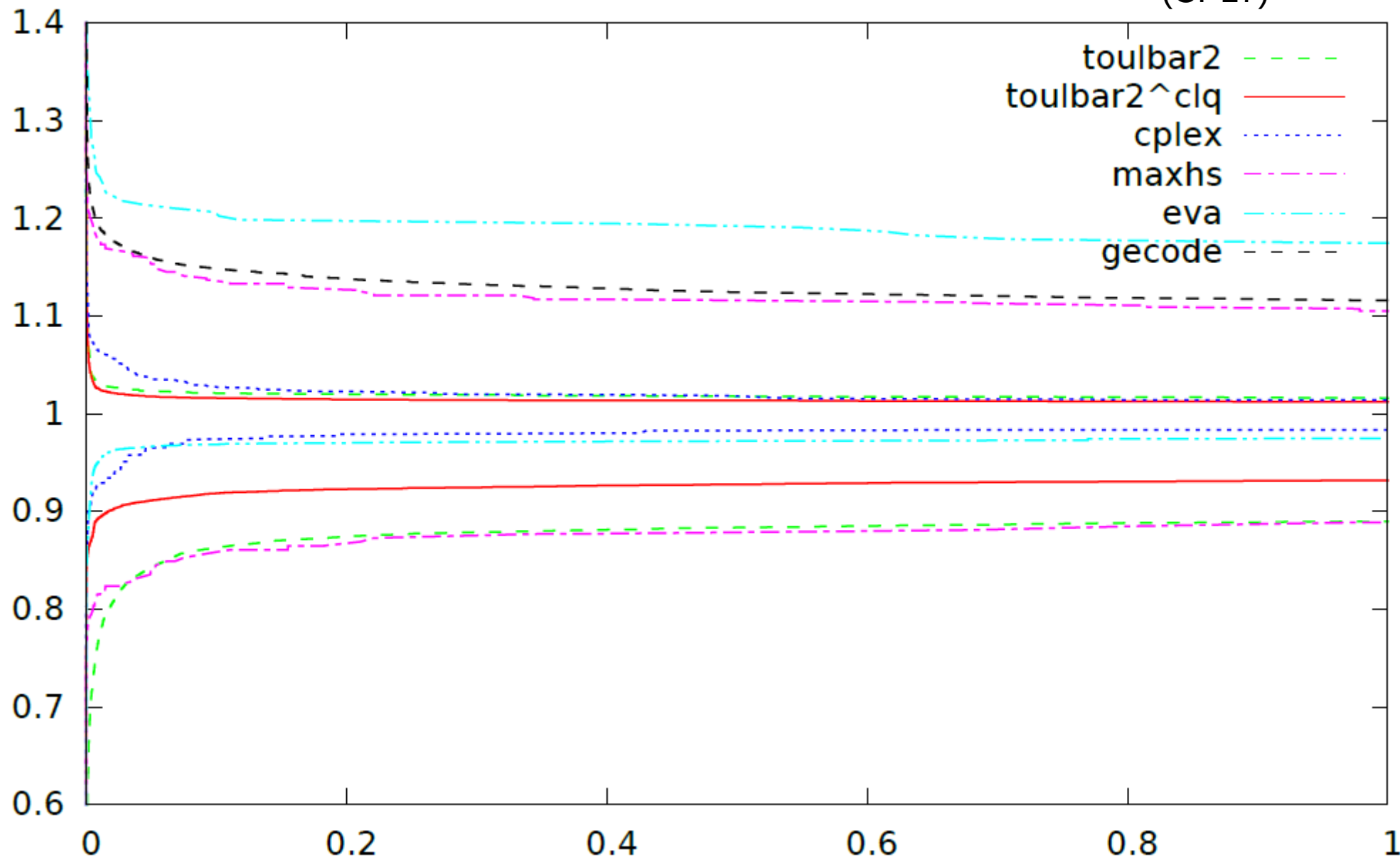
(CPAIOR16 – Constraints16)



Normalized lower and upper bounds on 1208 difficult instances as time passes

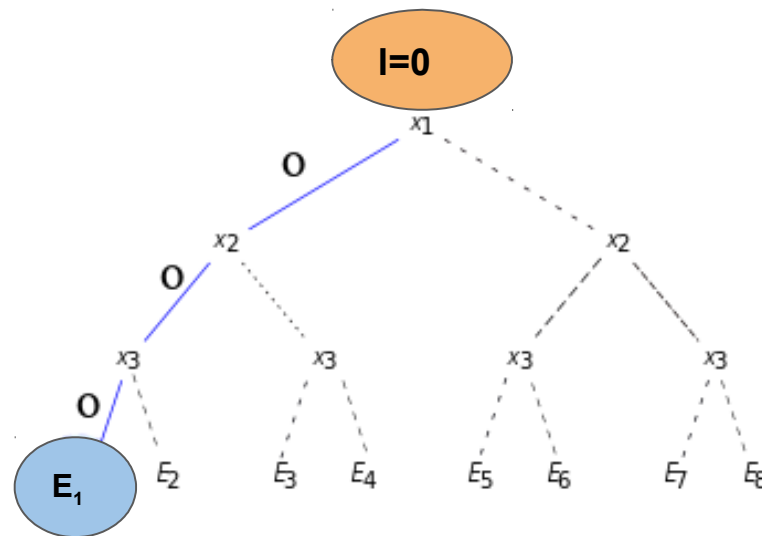
Results exploiting cliques

(CP17)



Normalized lower and upper bounds on 252 instances as time passes

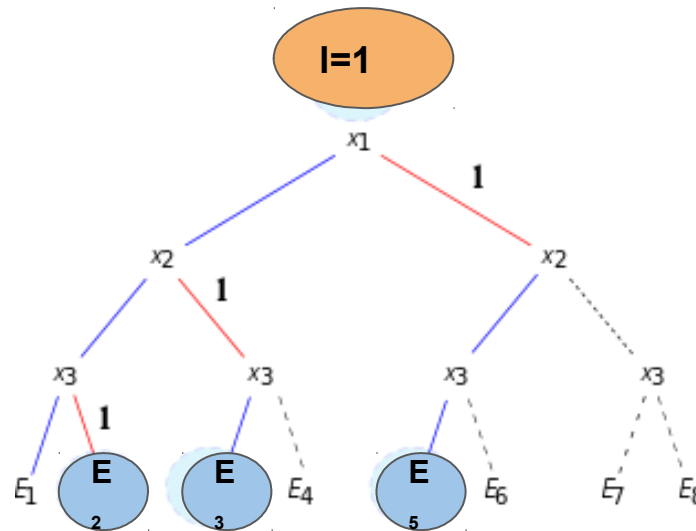
Limited Discrepancy Search *(Ginsberg 95)*



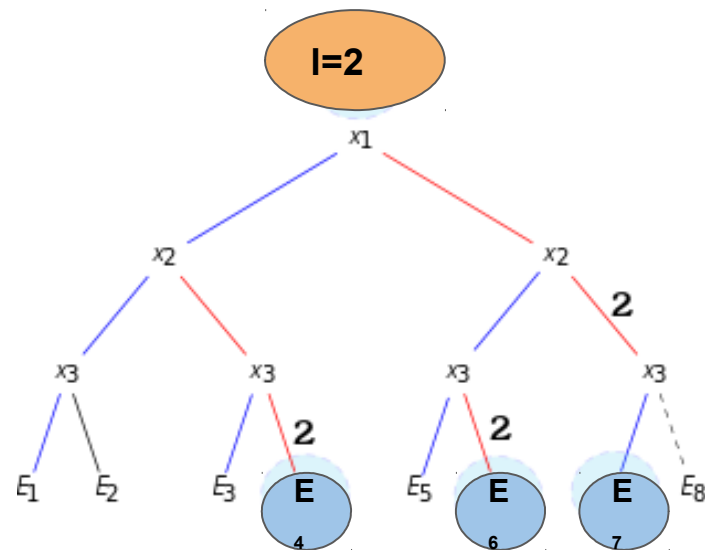
- **Small example with 3 variables and 2 values per domain**

Limited Discrepancy Search

- Small example with 3 variables and 2 values per domain



Limited Discrepancy Search *(Ginsberg 95)*

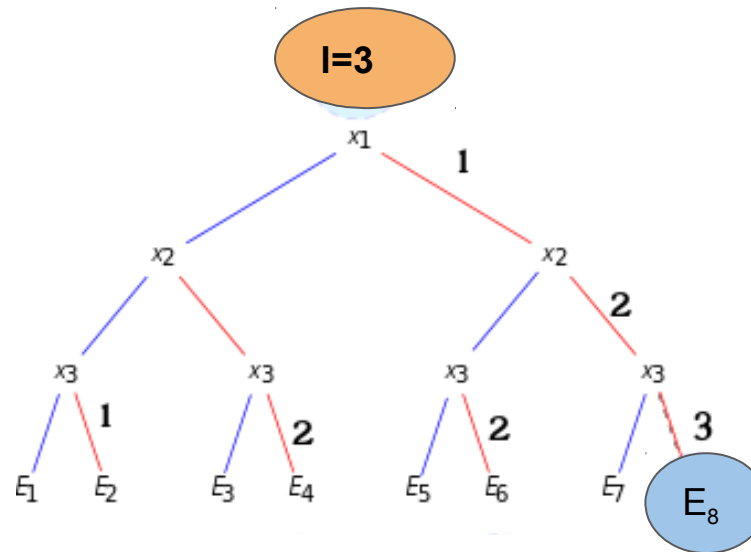


Limited Discrepancy Search *(Ginsberg 95)*

$$l_{\max} = n * (d - 1) \quad : \quad \text{in this case, } l_{\max} = 3 * (2 - 1) = 3$$



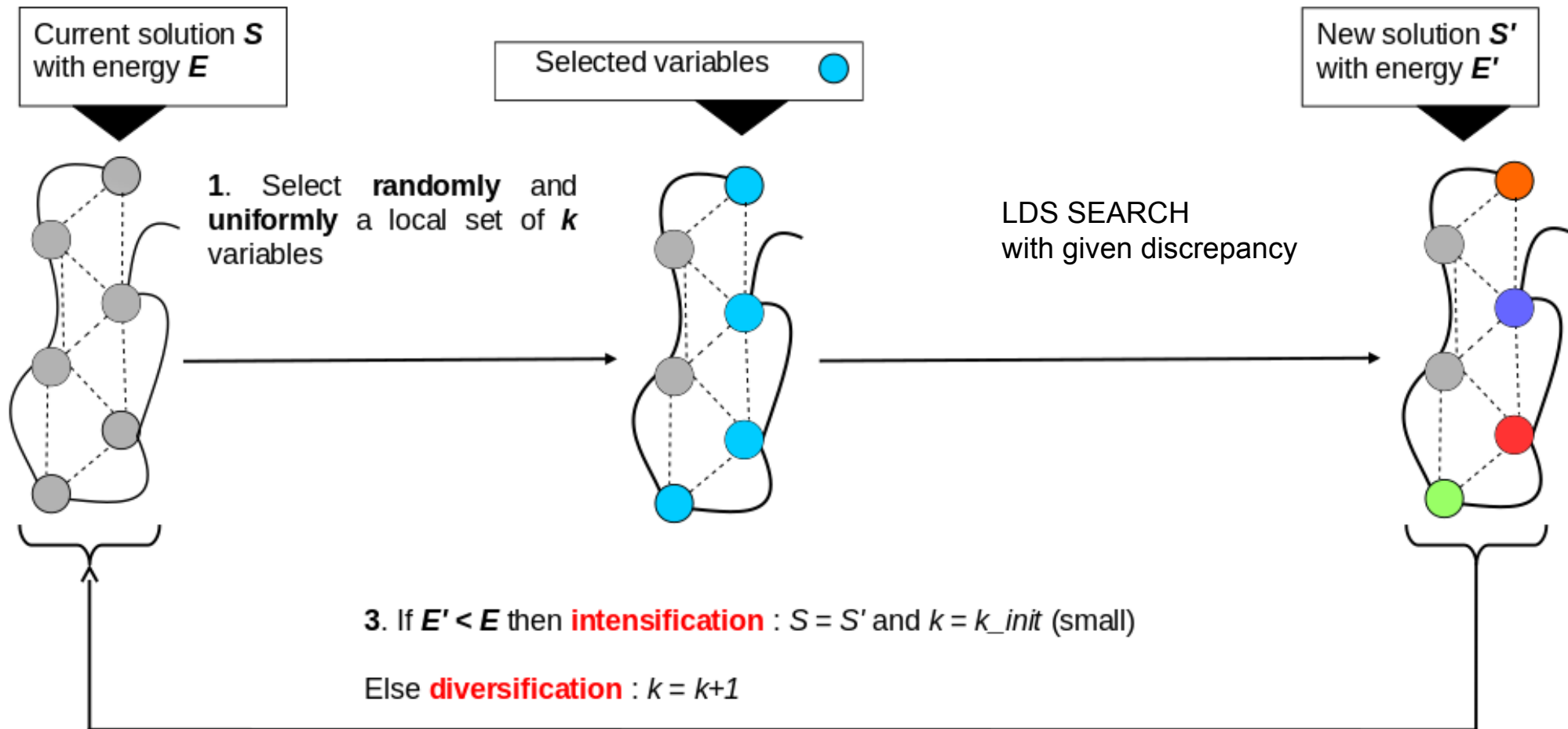
Full exploration



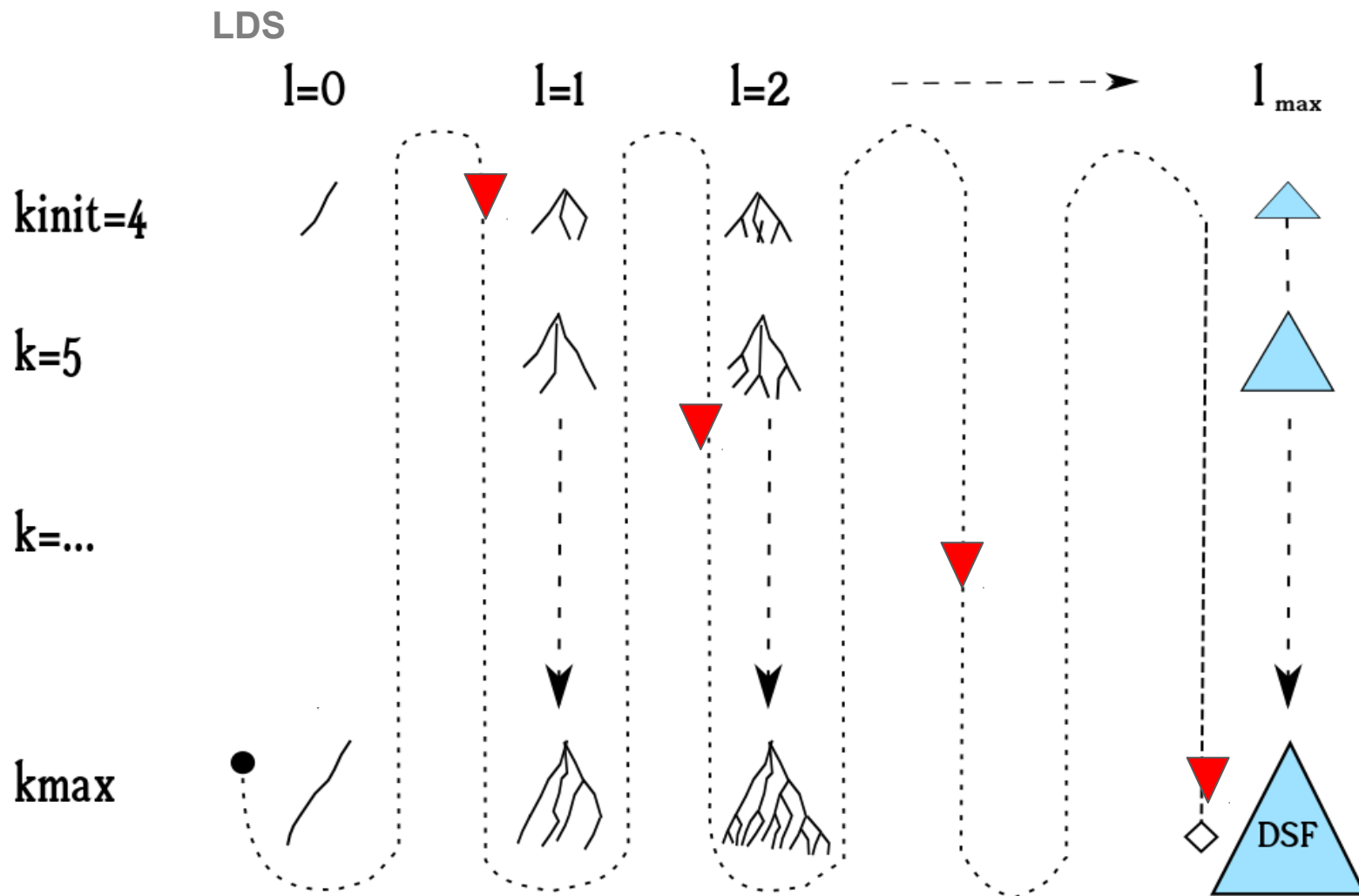
$l=3 \Rightarrow$ optimality proof

In practice, it occurs before l_{\max} thanks to bounding and pruning

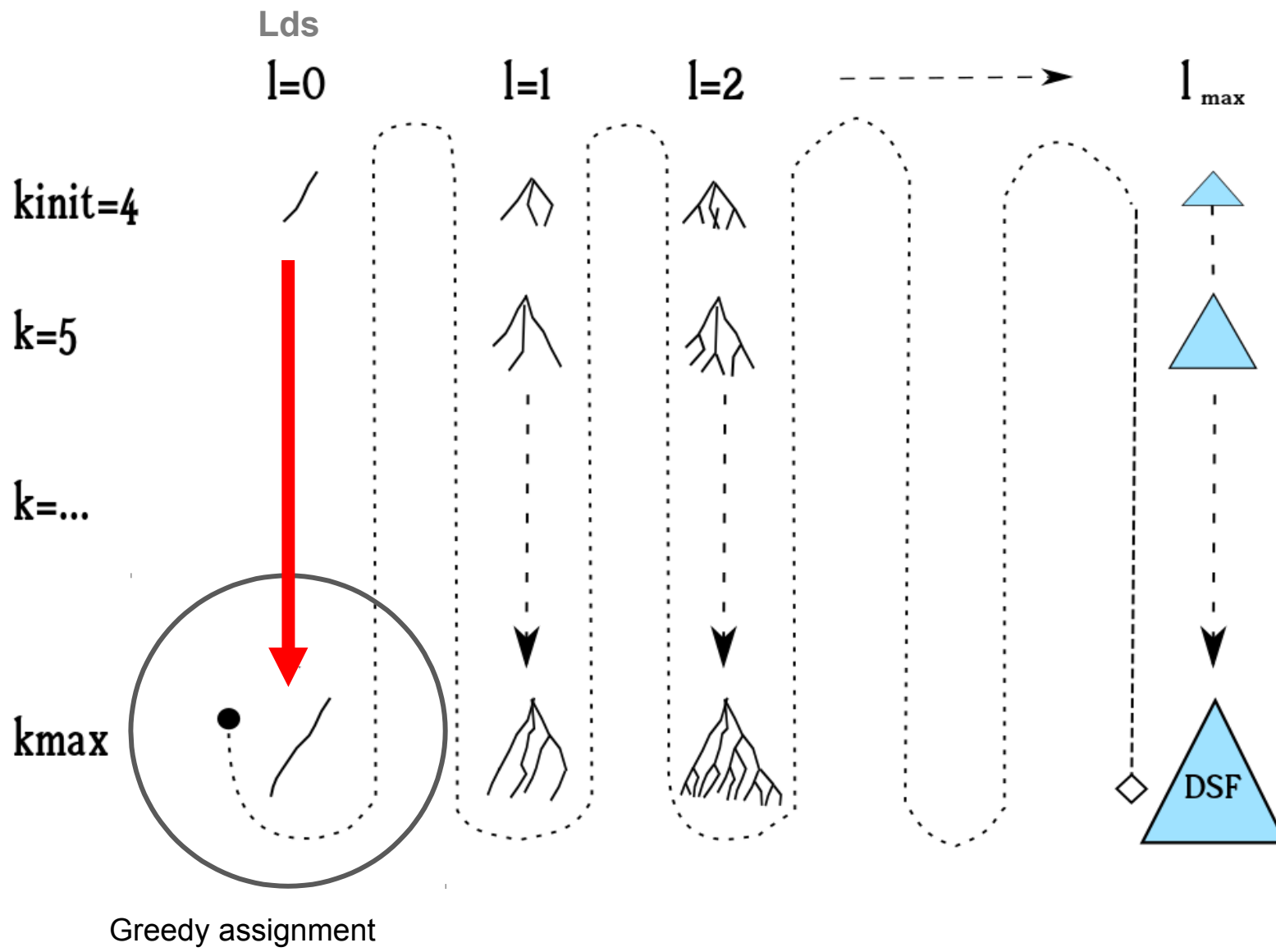
Variable Neighborhood Search *(Hansen 97)*



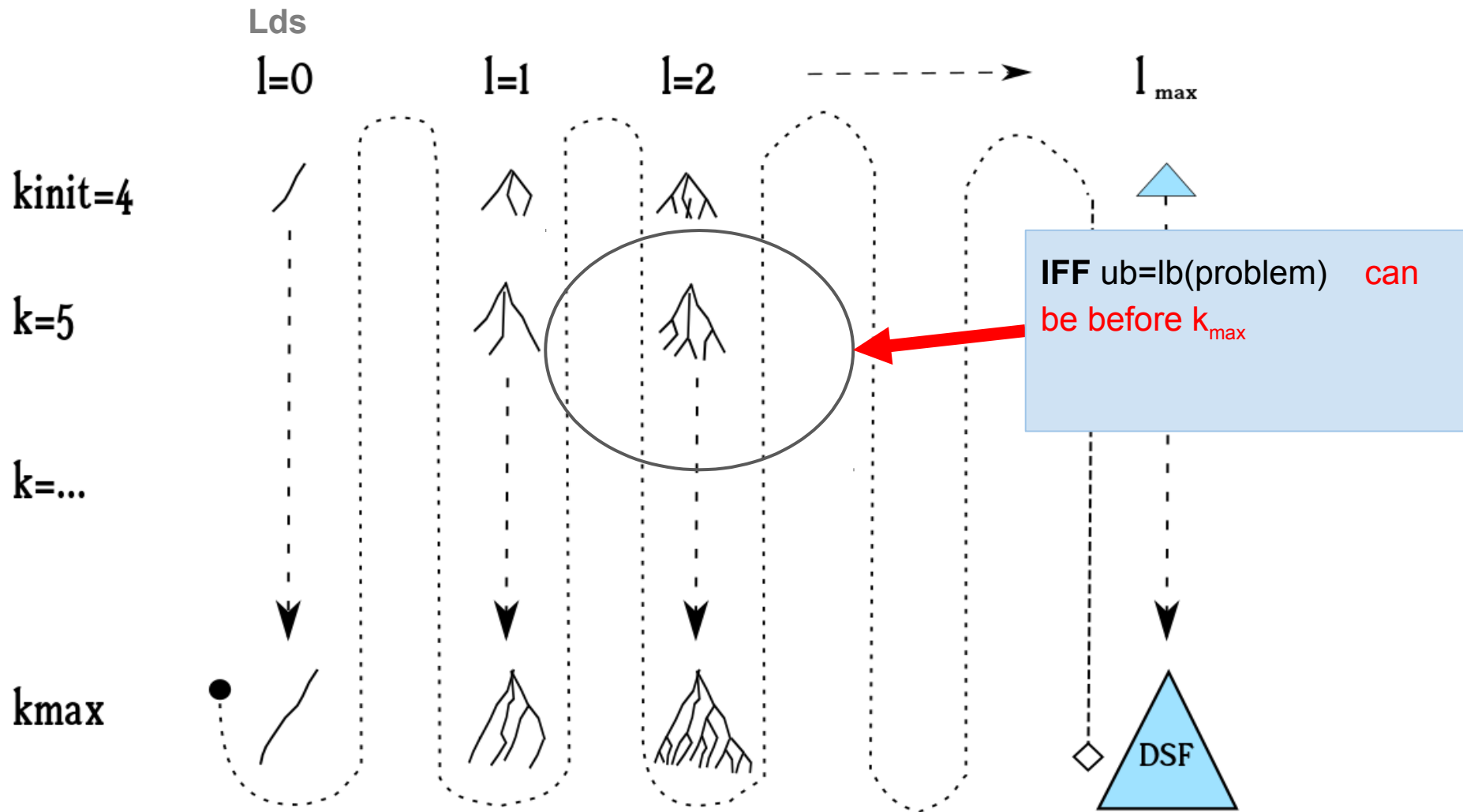
UDGVNS : Exploration of both k and l dimensions



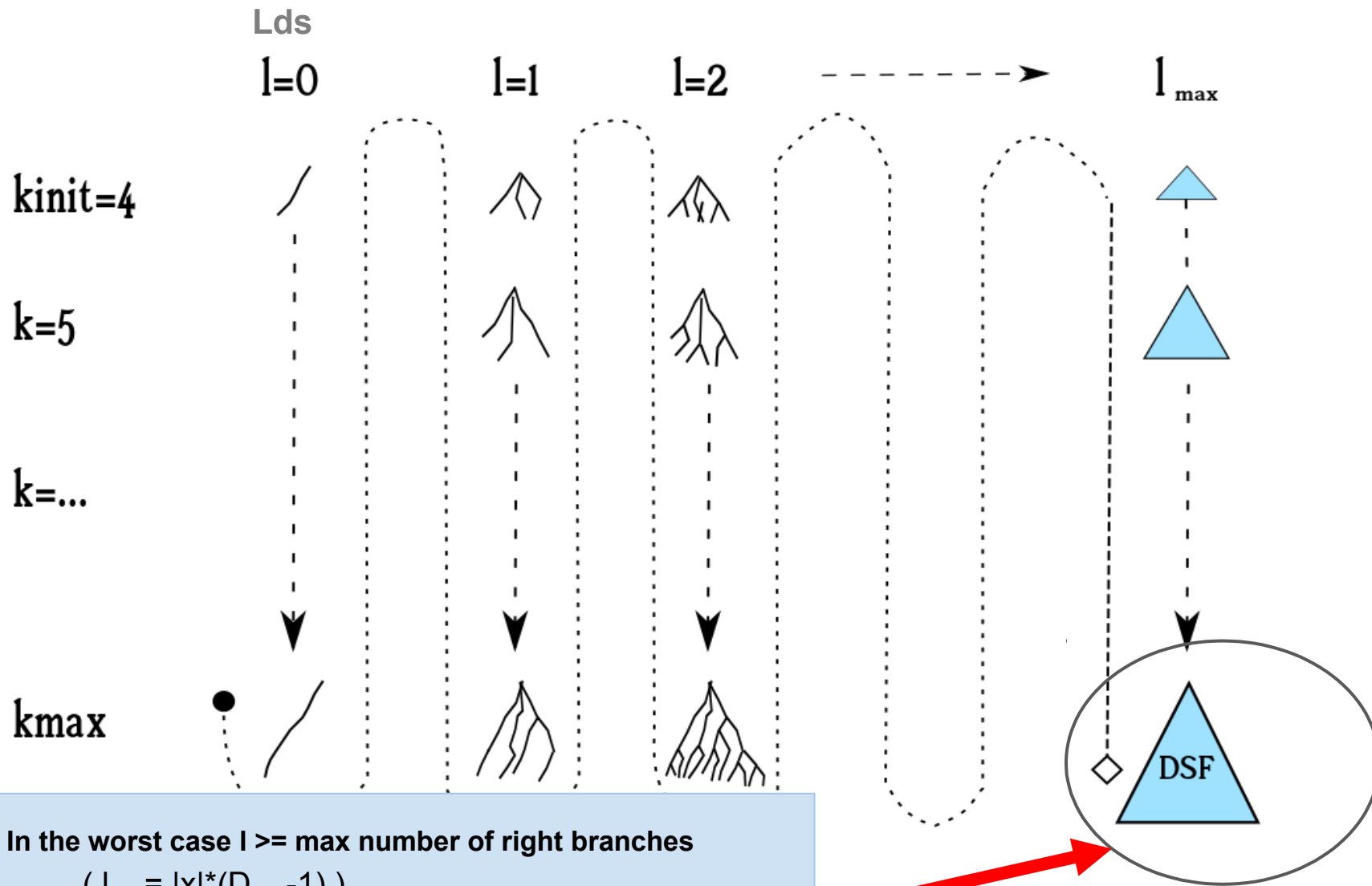
Step 1 : Initial solution



Proof of Optimality



Proof of Optimality

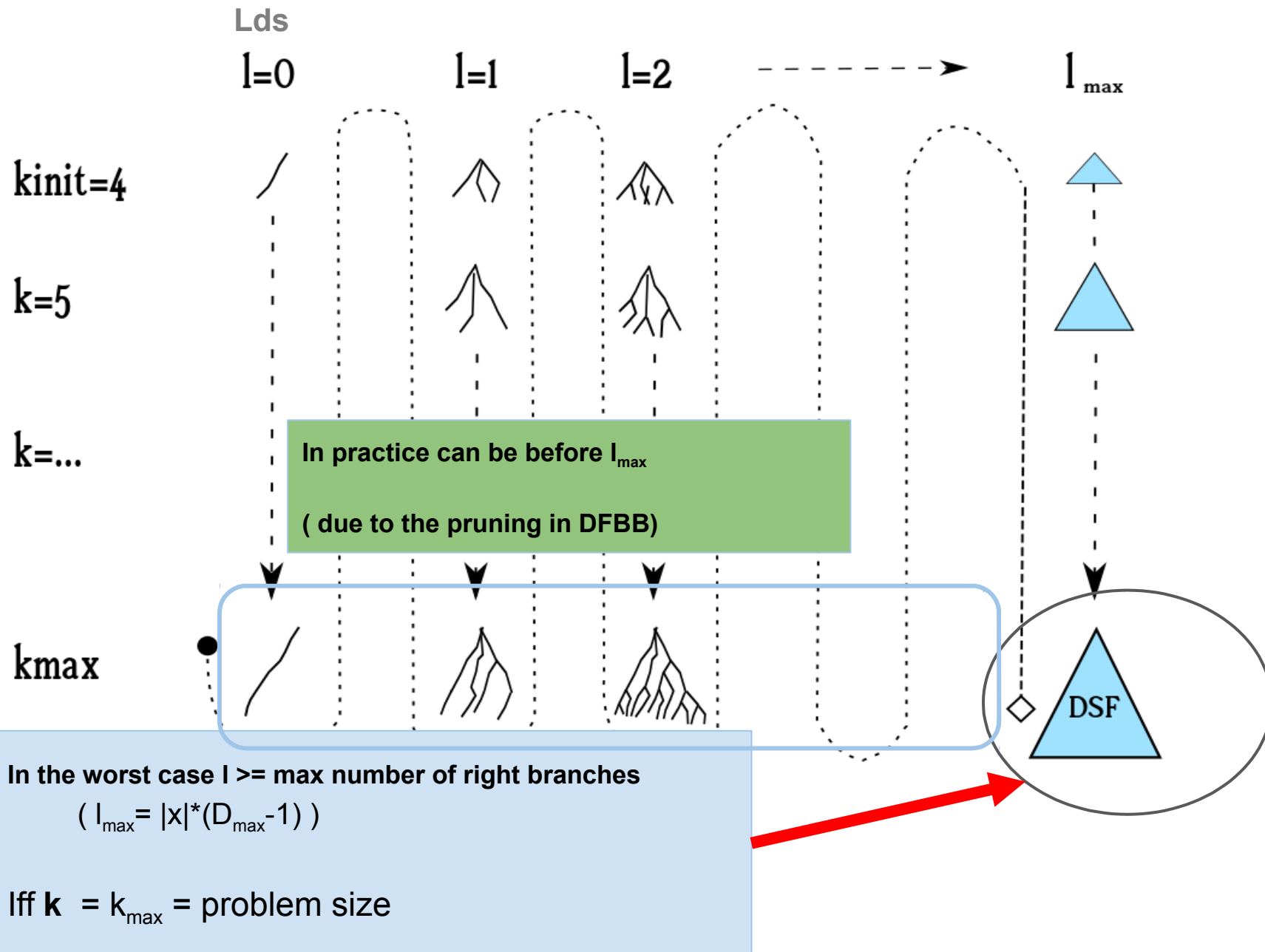


In the worst case $l \geq \text{max number of right branches}$

$$(l_{\max} = |x| * (D_{\max} - 1))$$

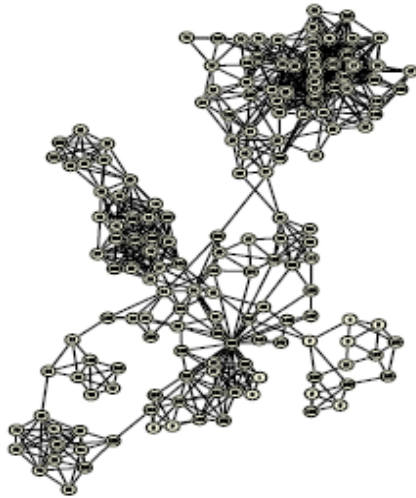
Iff $k = k_{\max} = \text{problem size}$

Proof of Optimality



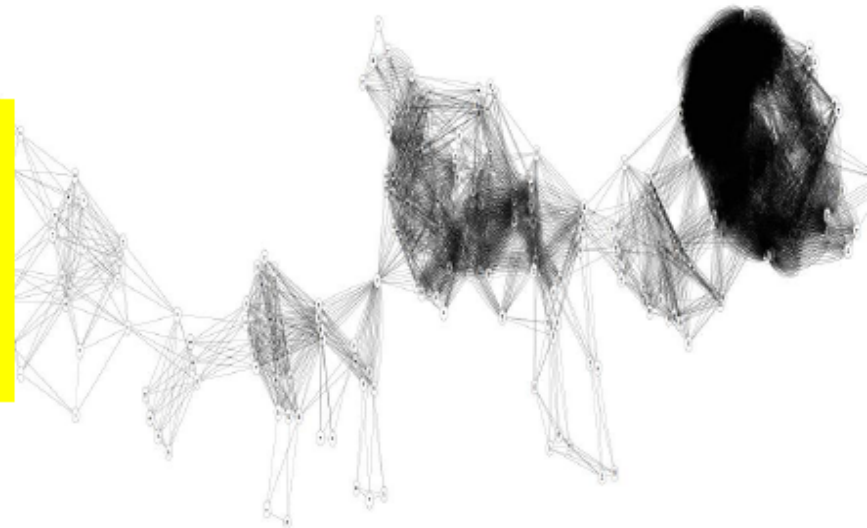
Neighborhoods using problem structure

Radio
Link
Frequency
Assignment



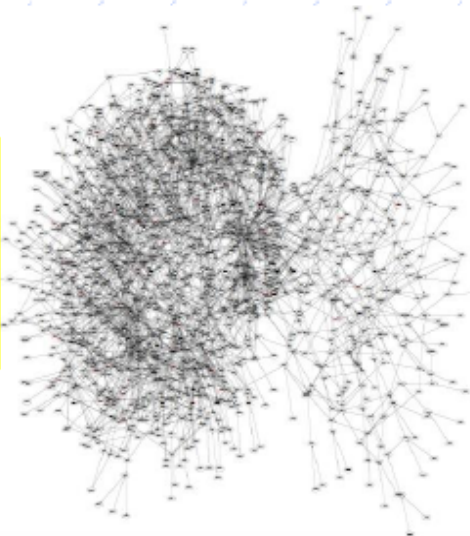
CELAR SCEN-07r
(Constraints 4(1), 1999)

Earth
Observation
Satellite
Management



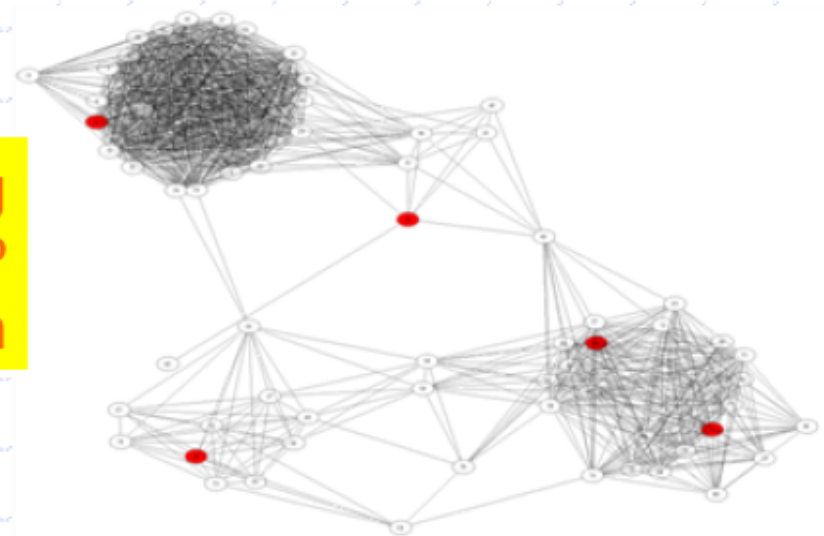
SPOT5 #509 (Constraints 4(3), 1999)

Mendelian
Error
Detection



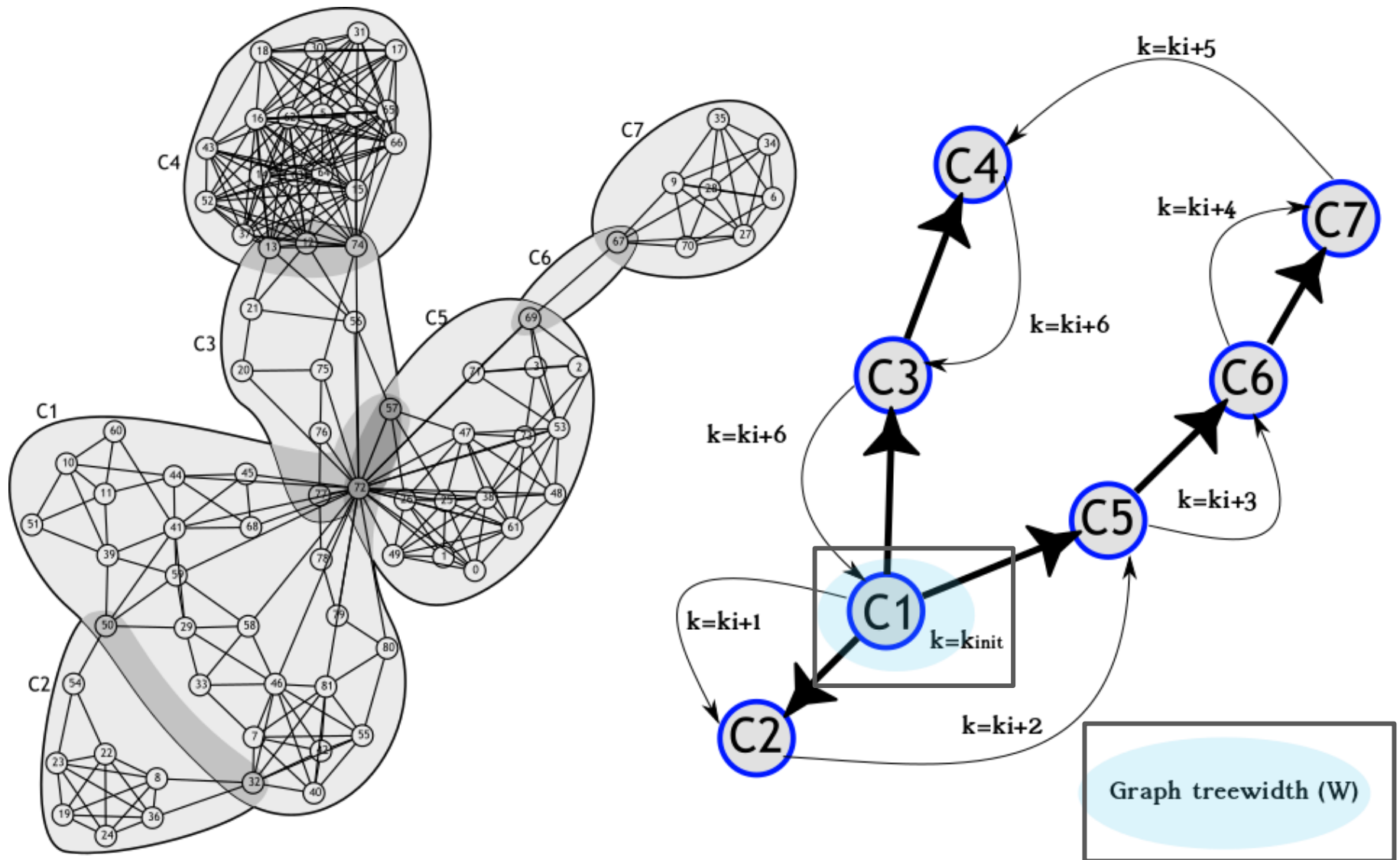
langladeM7 sheep pedigree
(Constraints 13(1), 2008)

Tag
SNP
Selection



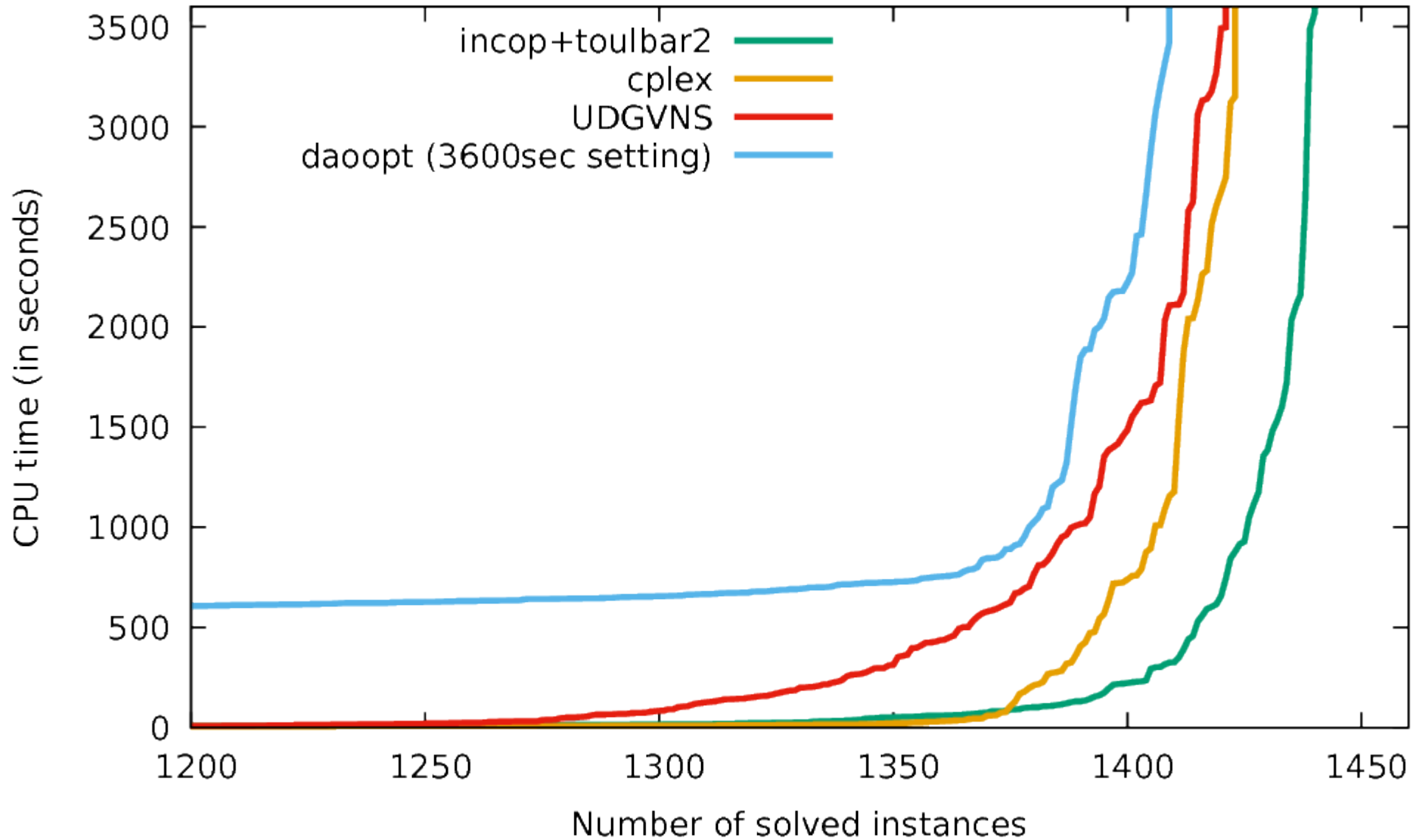
HapMap chr01 $r^2 \geq 0.8$ #14481
(Bioinformatics 22(2), 2006)

Cluster visit in a topological order :



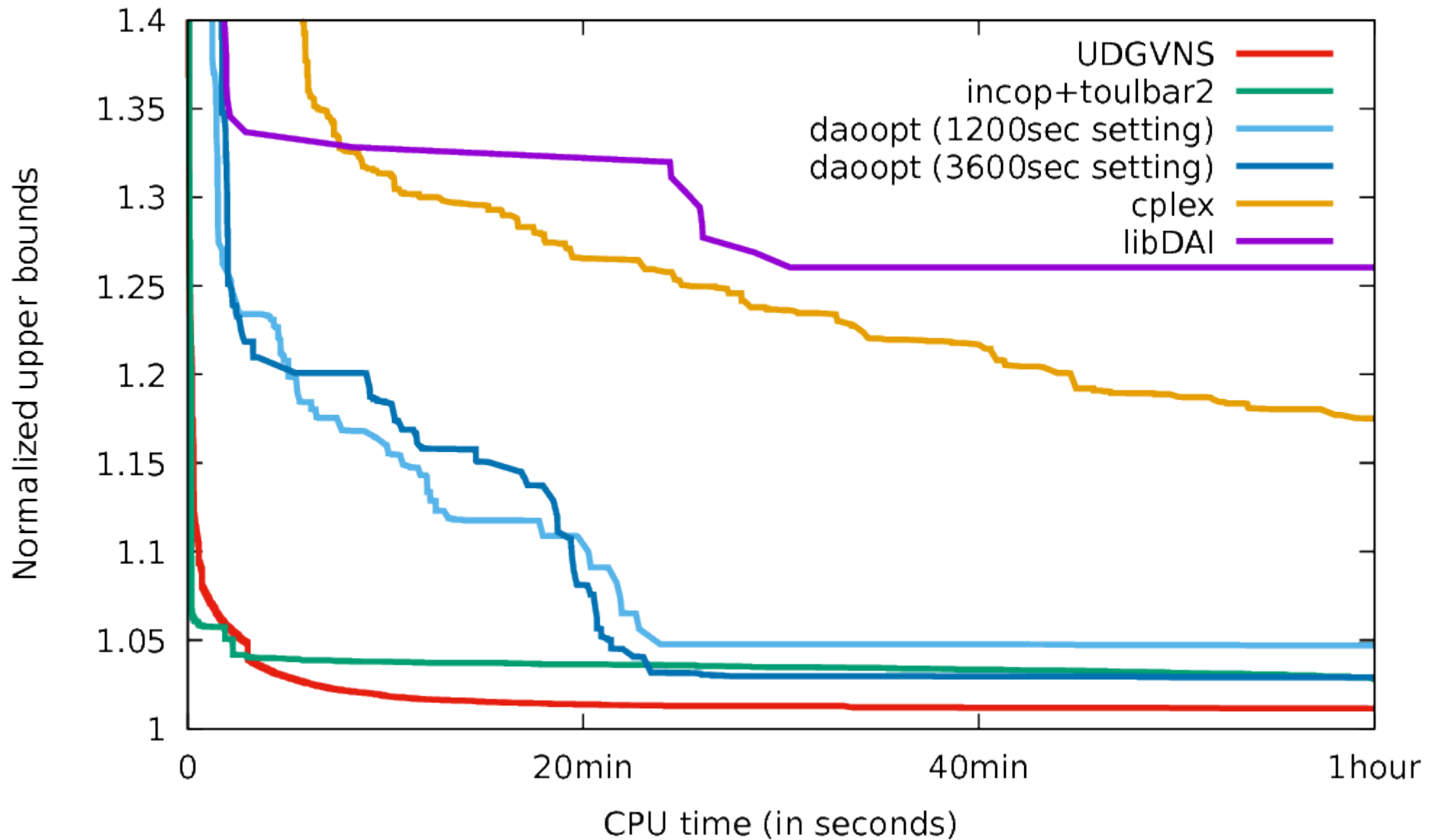
Results

(UAI17)



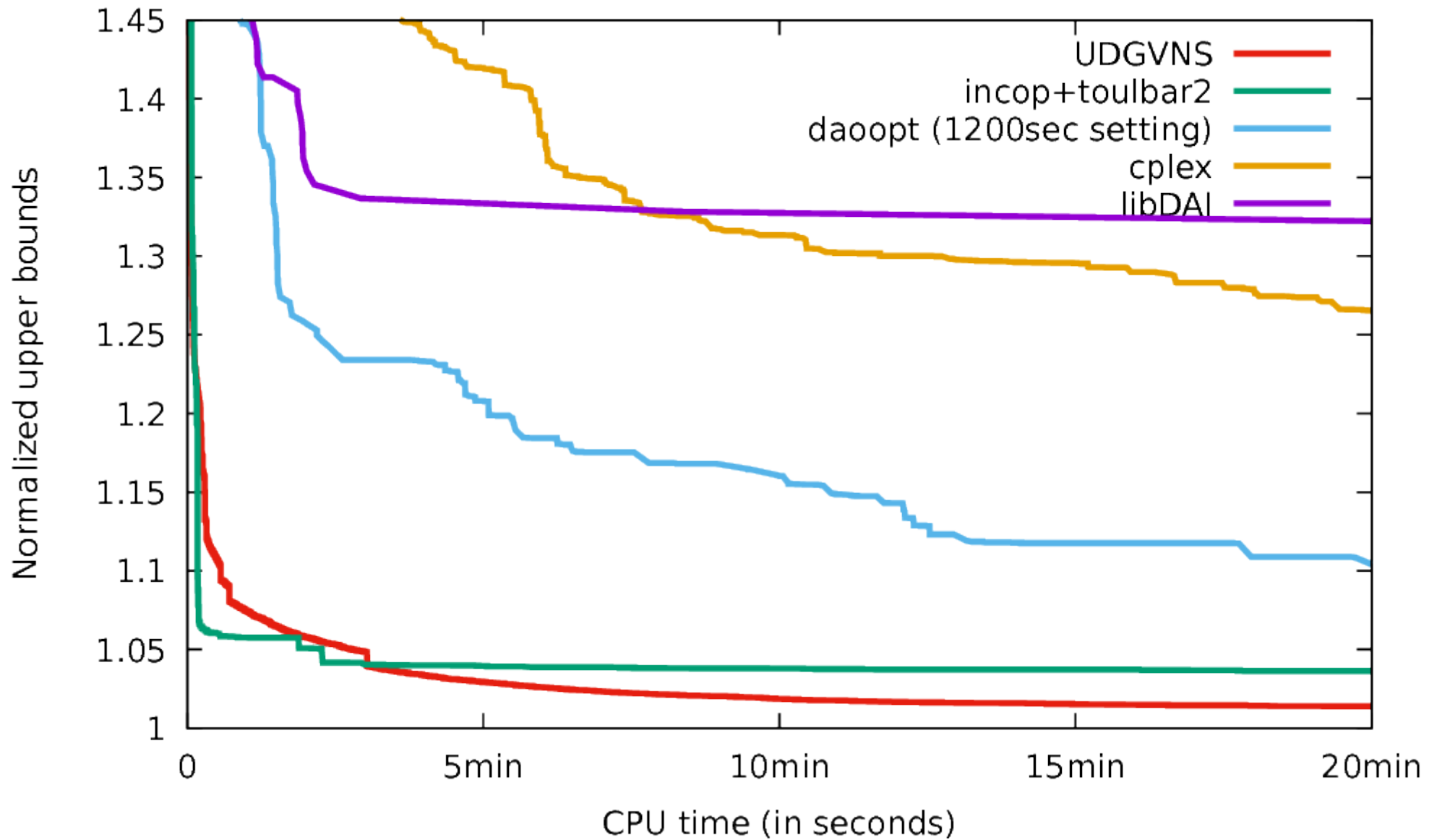
Results

(UAI17)

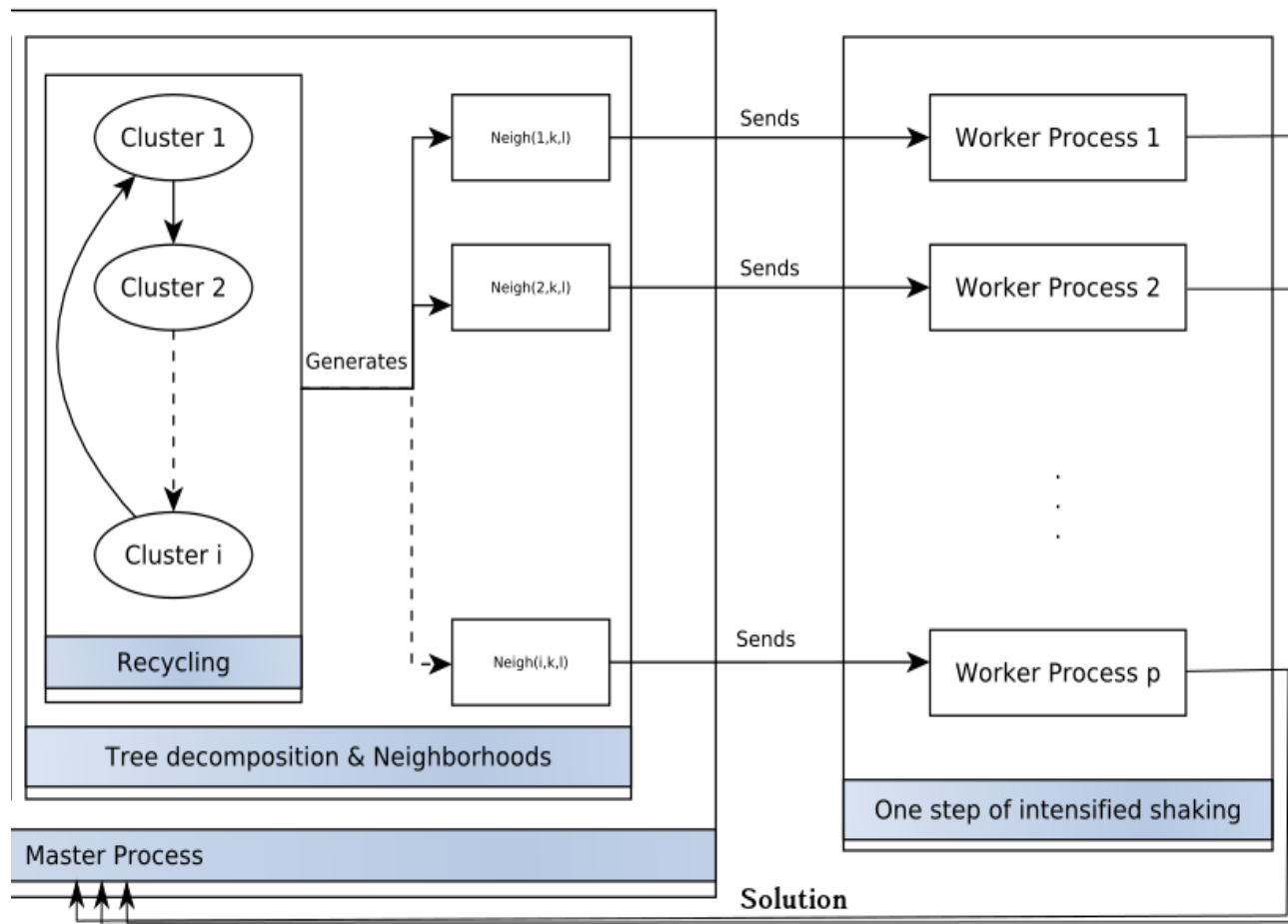


Results

(UAI17)



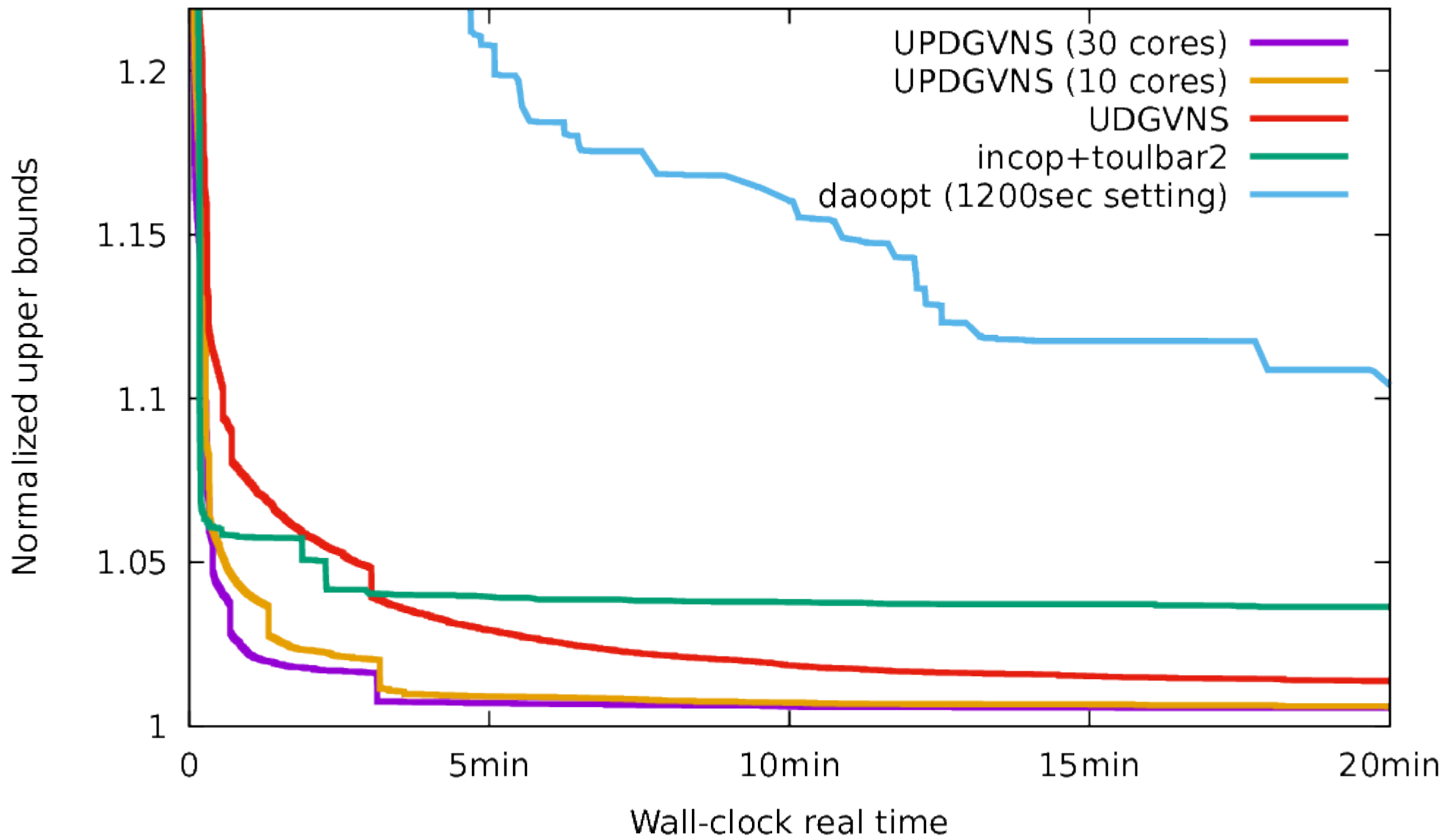
Parallel VNS



Unified Parallel Decomposition Guided VNS (UPDGVNS)

Results

(UAI17)



References

- Peyrard et al. *Exact and approximate inference in graphical models: variable elimination and beyond*, 2017.
<https://arxiv.org/pdf/1506.08544.pdf>
- Hurley et al. *Multi-Language Evaluation of Exact Solvers in Graphical Model Discrete Optimization*. Constraints, 2016.
<http://genoweb.toulouse.inra.fr/~degivry/evalgm>
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- Katsirelos et al. *Anytime Hybrid Best-First Search with Tree Decomposition for Weighted CSP*. In Proc. of CP-15, Cork, Ireland, 2015
- Ouali et al. *Iterative Decomposition Guided Variable Neighborhood Search for Graphical Model Energy Minimization*. In Proc. of UAI-17, Sydney, Australia, 2017

<https://github.com/toulbar2/toulbar2>

