Recent algorithmic advances for combinatorial optimization in graphical models

David Allouche, Simon de Givry, Georgios Katsirelos, Thomas Schiex, Matthias Zytnicki, Abdelkader Ouali, Samir Loudni

ISMP'18

Recent algorithmic advances for combinatorial optimization in graphical models

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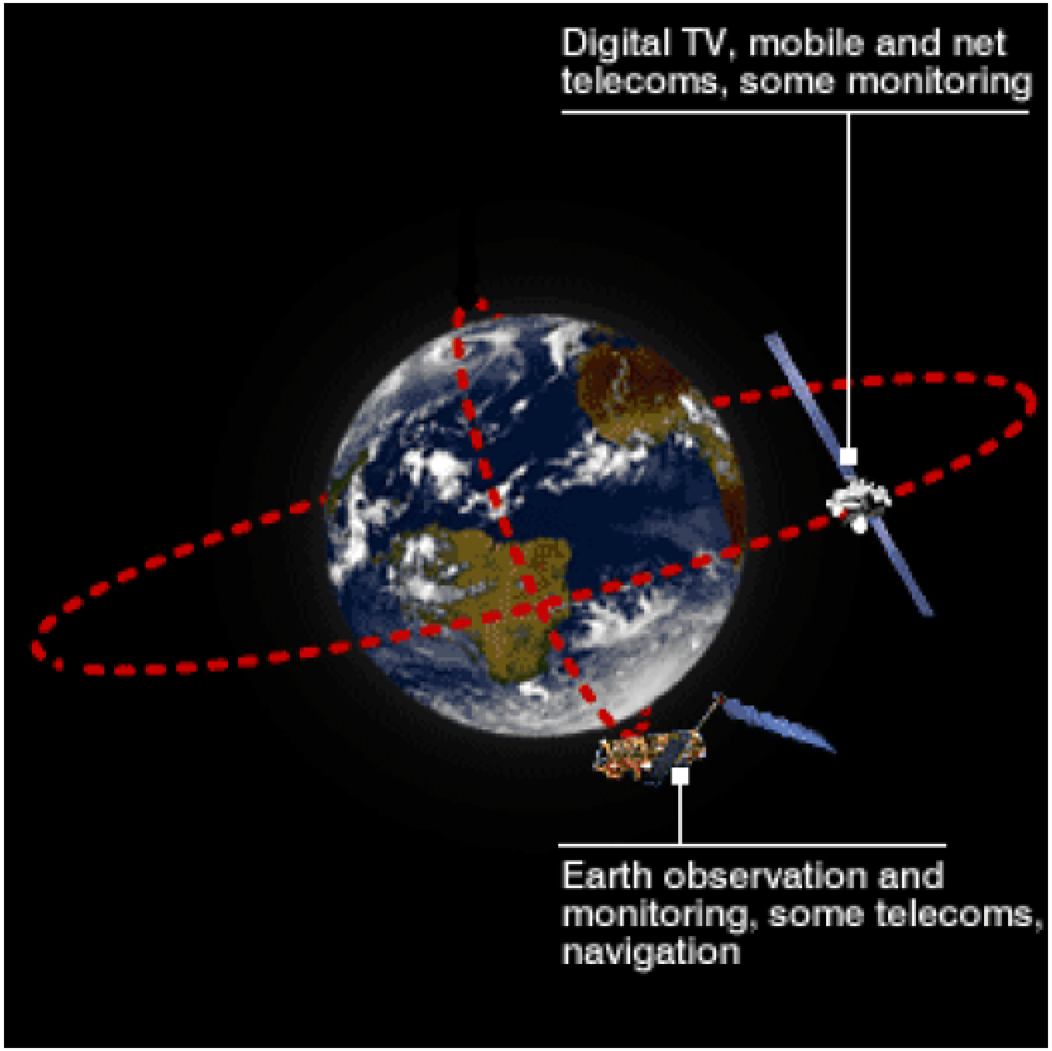
Plan

- 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

debian

Earth Observation Satellite Management (SPOT5)



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

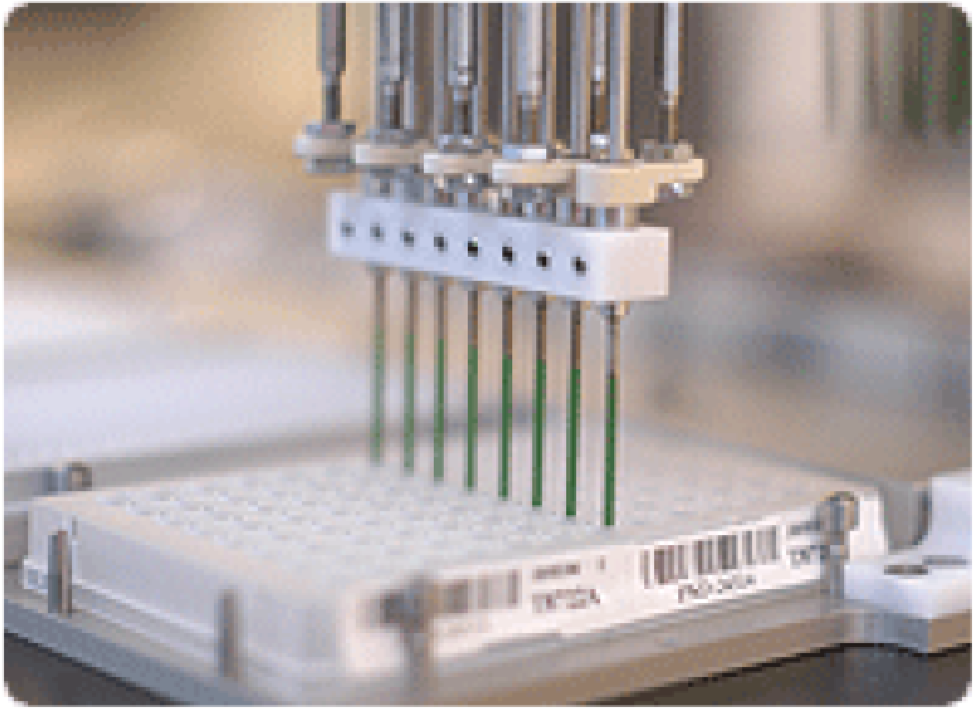
n ≤ 364, d=4, e(2-3) ≤ 10,108

Radio Link Frequency Assignment (CELAR)

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

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

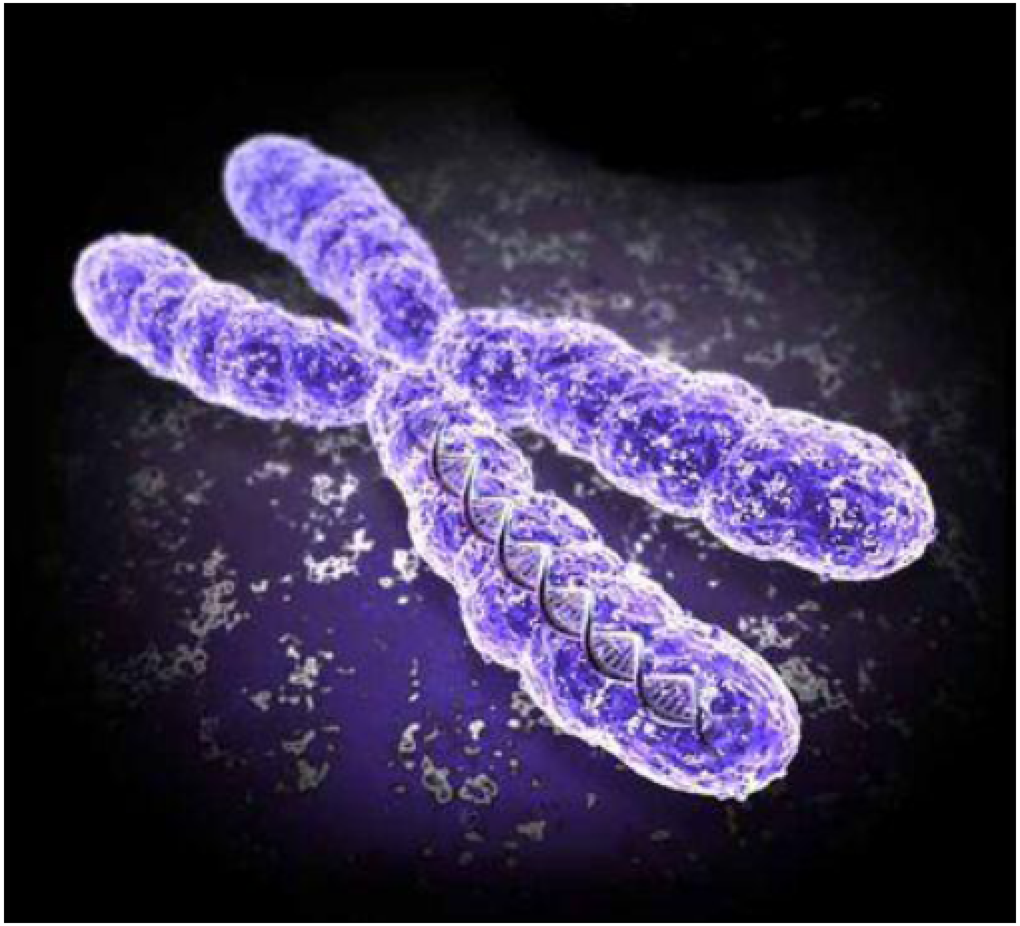
Mendelian error correction in complex pedigree (MendelSoft)



(Constraints08)

n≤20,000, d≤66, e(3)≤30,000

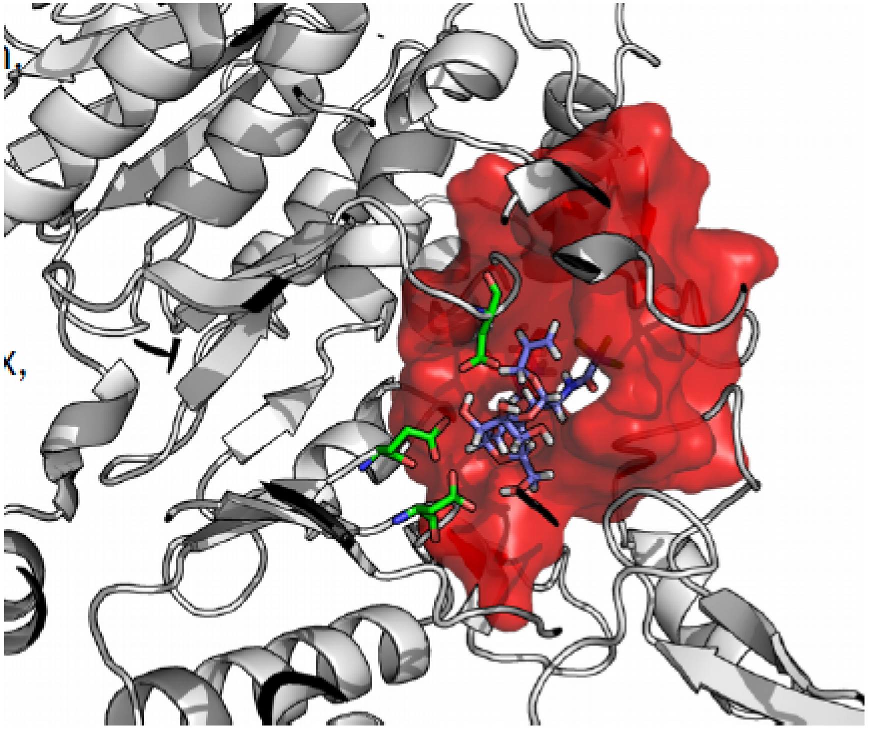
Genetic Linkage Analysis



(Marinescu & Dechter, AAAI 2006 ; IJCAI11)

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

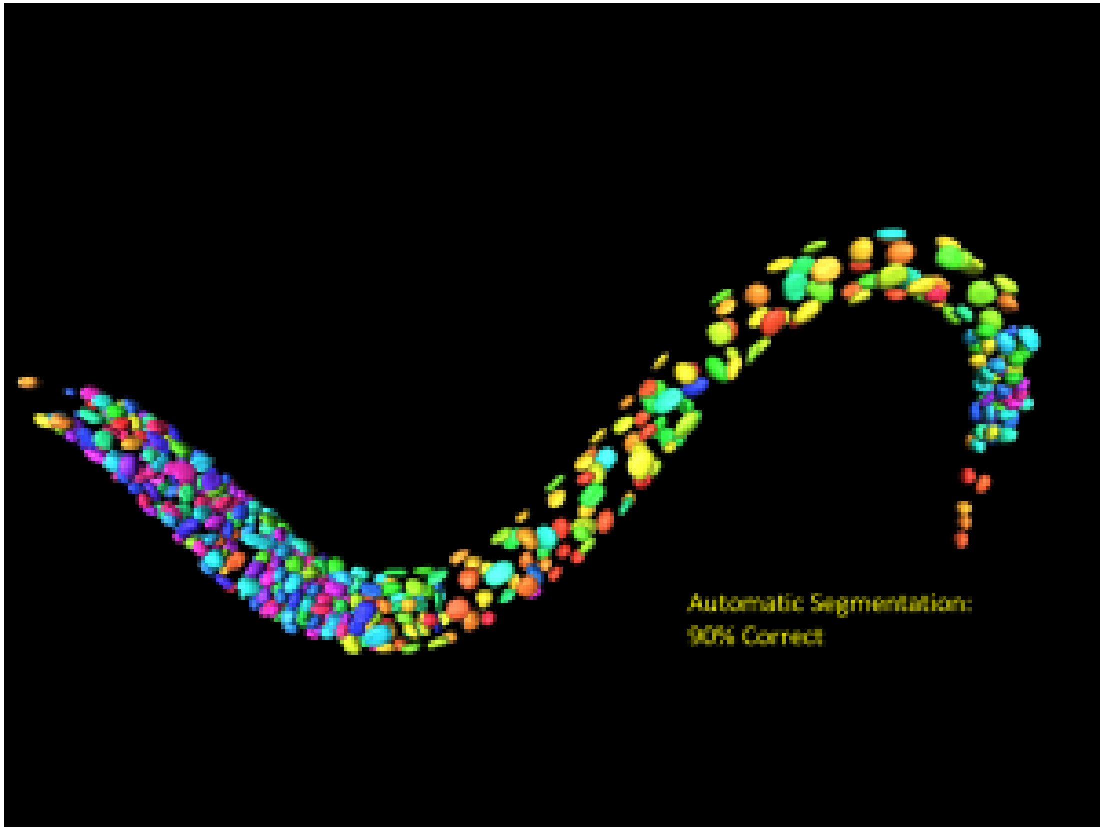
Protein Design



(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 $X = (X_1, \ldots, X_n)$ be a set of variables.
- X_i takes values in $\Lambda_i \subseteq \mathbb{R}$.
- A realization of X is denoted $x = (x_1, \ldots, x_n)$, with $x_i \in \Lambda_i$.
- A graphical model over X is a function $\psi : \prod_i \Lambda_i \to \mathbb{R}$, 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 $V = \{1, \ldots, n\}$, $\psi_B : \prod_{i \in B} \Lambda_i \to \mathbb{R}$ and $\odot \in \{\prod, \sum, \min, \max \ldots\}$ is a combination operator.

Slides from Sabbadin's invited talk at JFRB 2018

Probabilistic Graphical Models

Definition (Markov chain)

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

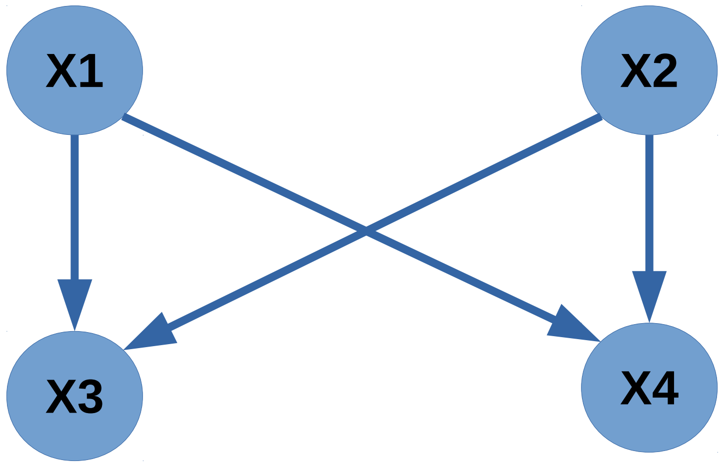
$$P(x_1, \ldots, x_n) = \underbrace{P(x_1)}_{\psi_1(x_1)} \times \underbrace{P(x_2|x_1)}_{\psi_{12}(x_1,x_2)} \times \ldots \times \underbrace{P(x_n|x_{n-1})}_{\psi_{(n-1)n}(x_{n-1},x_n)}$$

Probabilistic Graphical Models

Definition (Bayesian network)

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

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

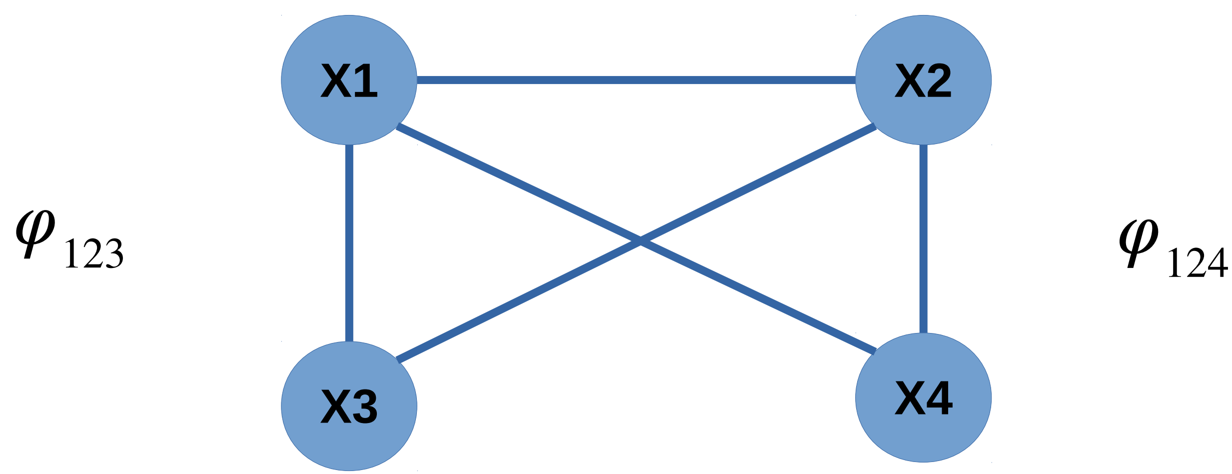


Probabilistic Graphical Models

Definition (Markov Random Field)

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

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

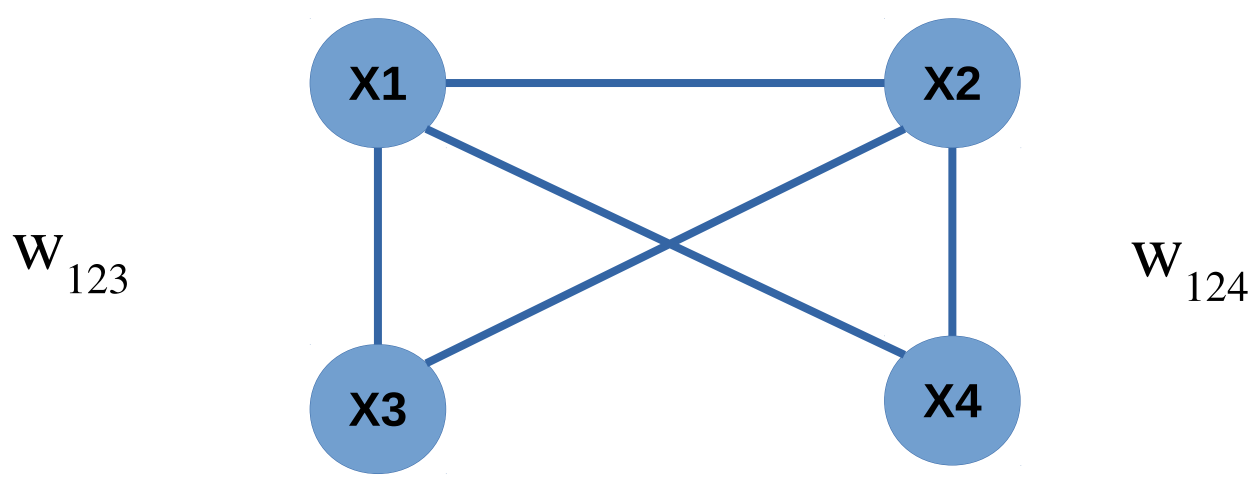


Deterministic Graphical Model

Definition (Cost Functions networks)

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

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



Deterministic Graphical Model

Definition (Cost Functions networks)

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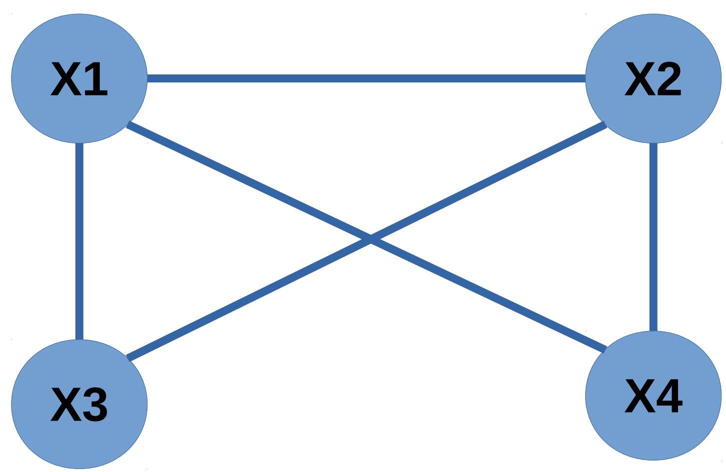
$$w(x_1, \ldots, x_n) = \sum_{c \in \mathcal{C}} w_C(x_C)$$

Minimization task: min $w(X_1,\ldots,X_n)$ NP-hard problem

$w_{123} = -\log \varphi_{123}$



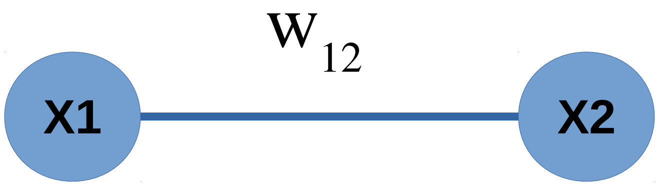
$w_{124} = -\log \varphi_{124}$

Energy minimization task is equivalent to finding the most probable explanation

Example

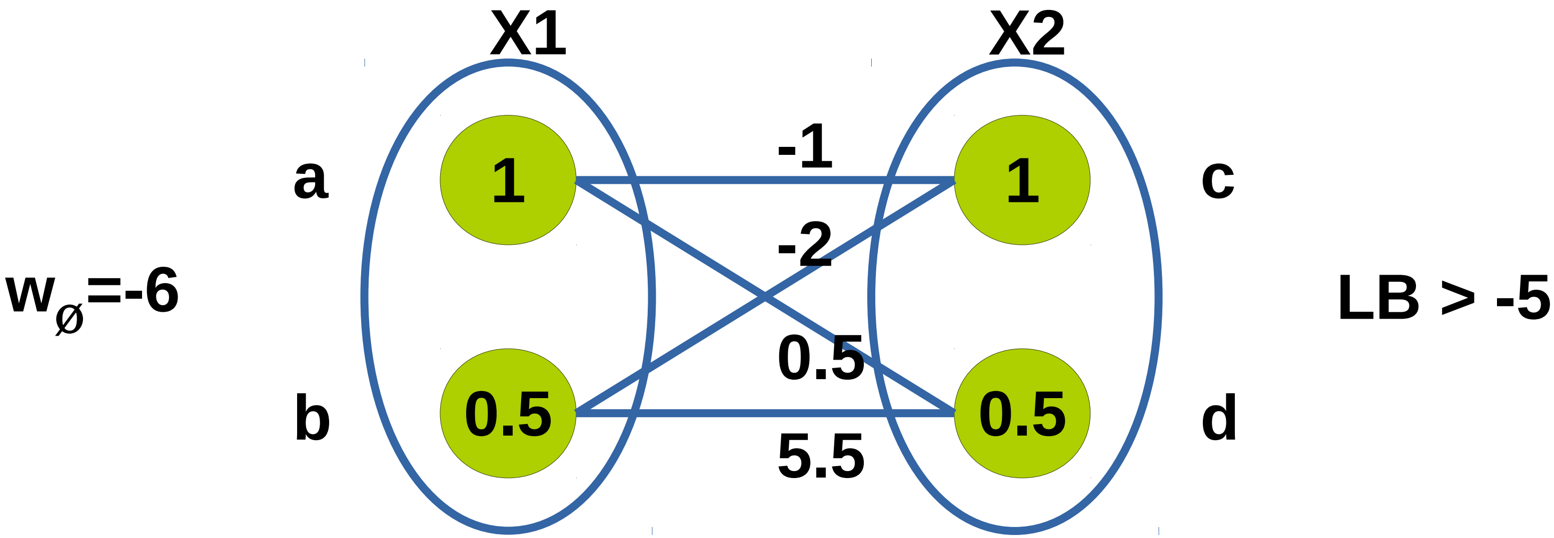
In JSON compatible toulbar2 *cfn* format

```
{
   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]}
   }
}
```



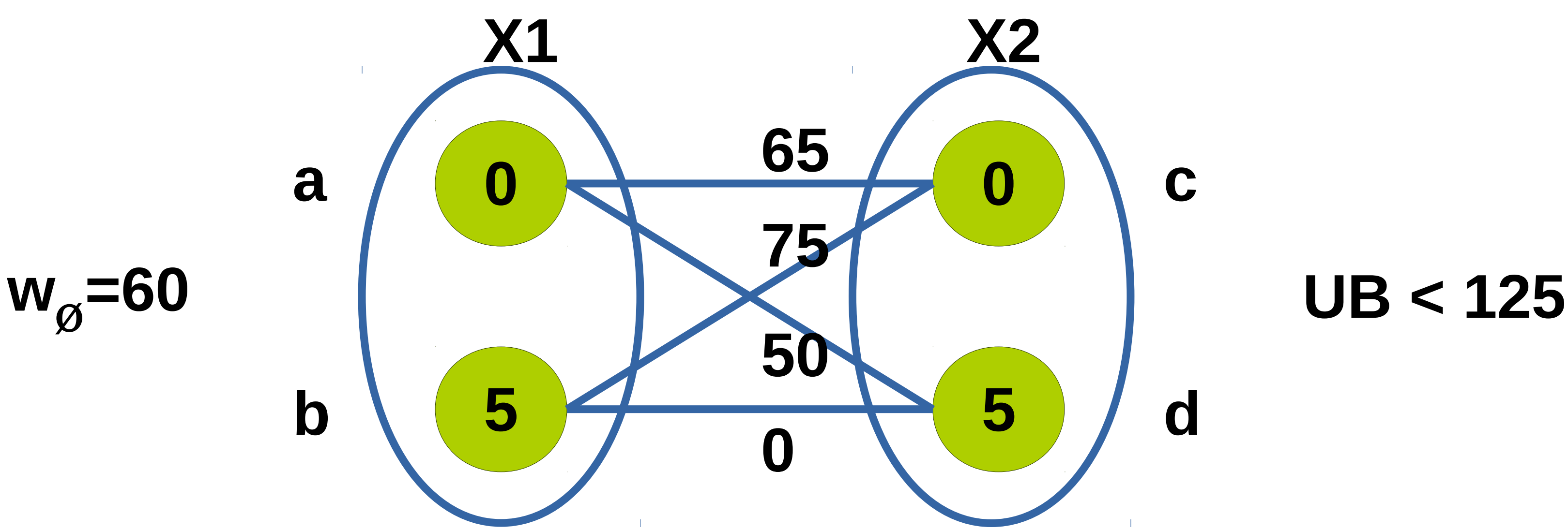
Micro-Structure

```
{
    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]}
    }
}
```



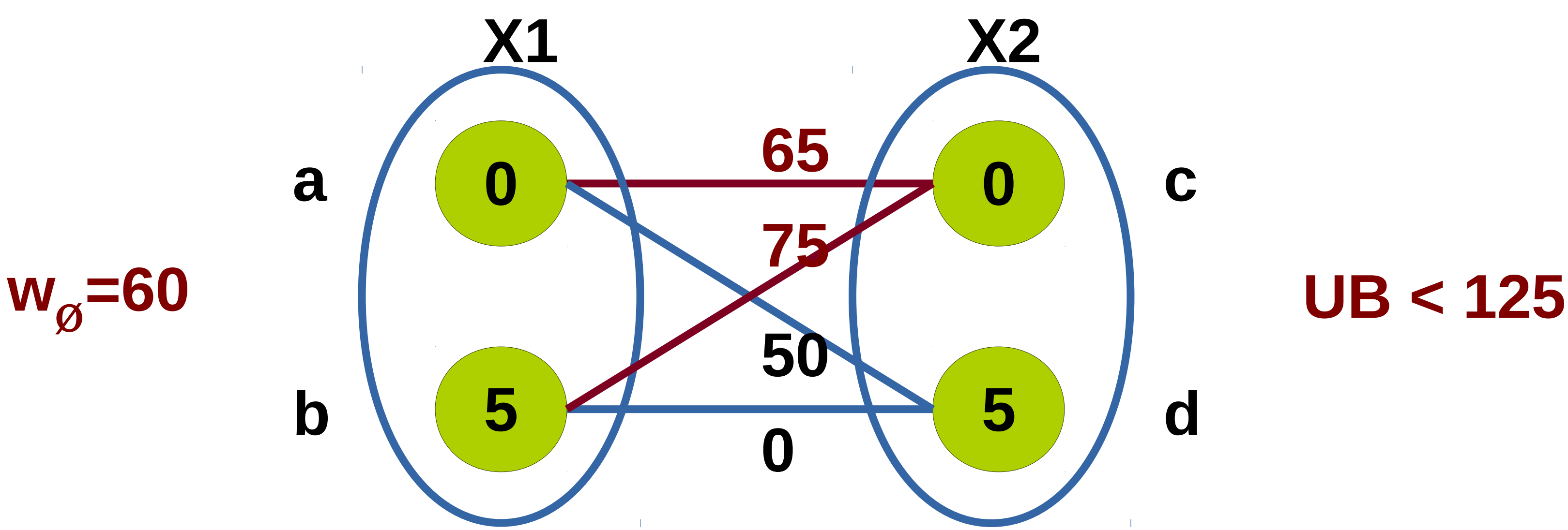
Minimization with non-negative integer costs

```
{
    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

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    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]},
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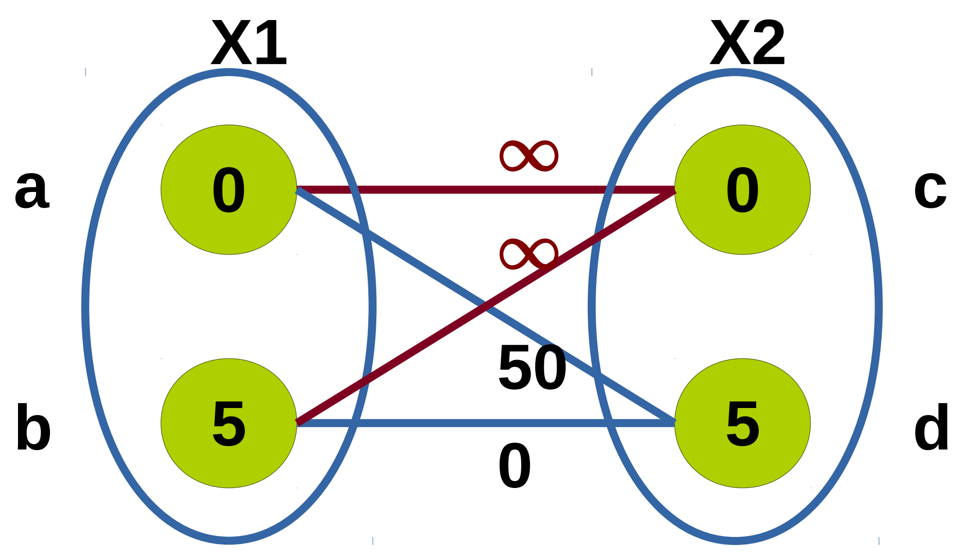
}
```



$w_{\varnothing}=60$

UB < 125

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

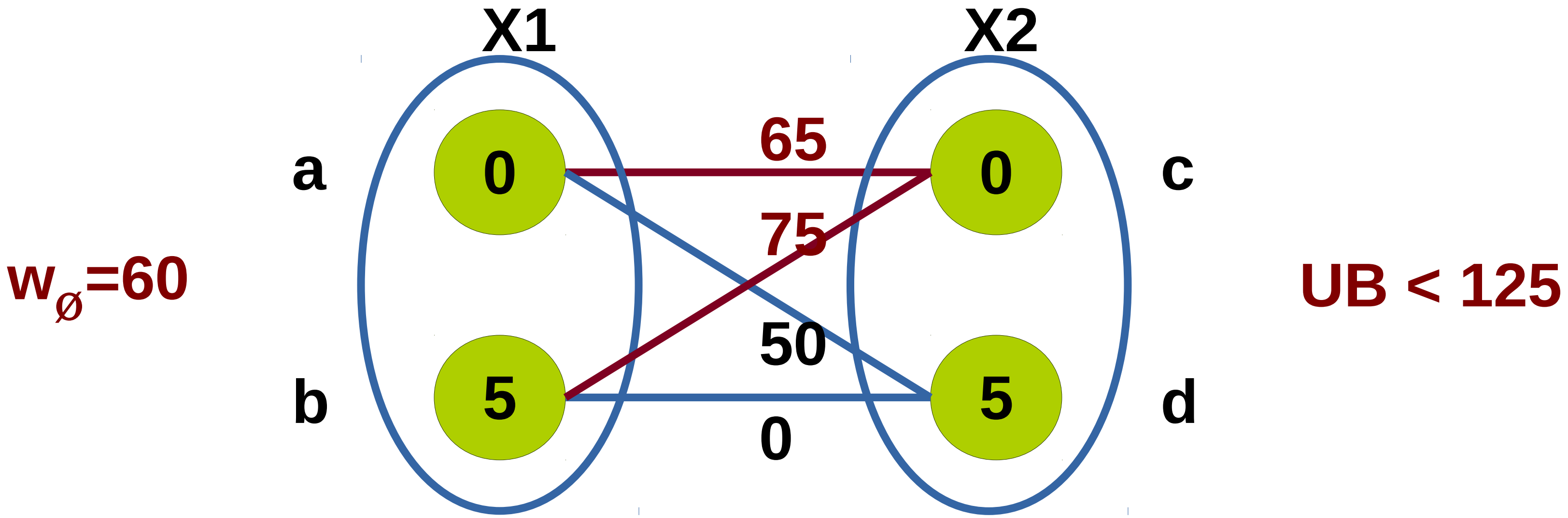
```
4 13
1 3 32.5
1 4 25
2 3 37.5
2 2 5
4 4 5
1 1 60
2 2 60
1 1 -1000
2 2 -1000
1 2 1000
3 3 -1000
4 4 -1000
3 4 1000
```

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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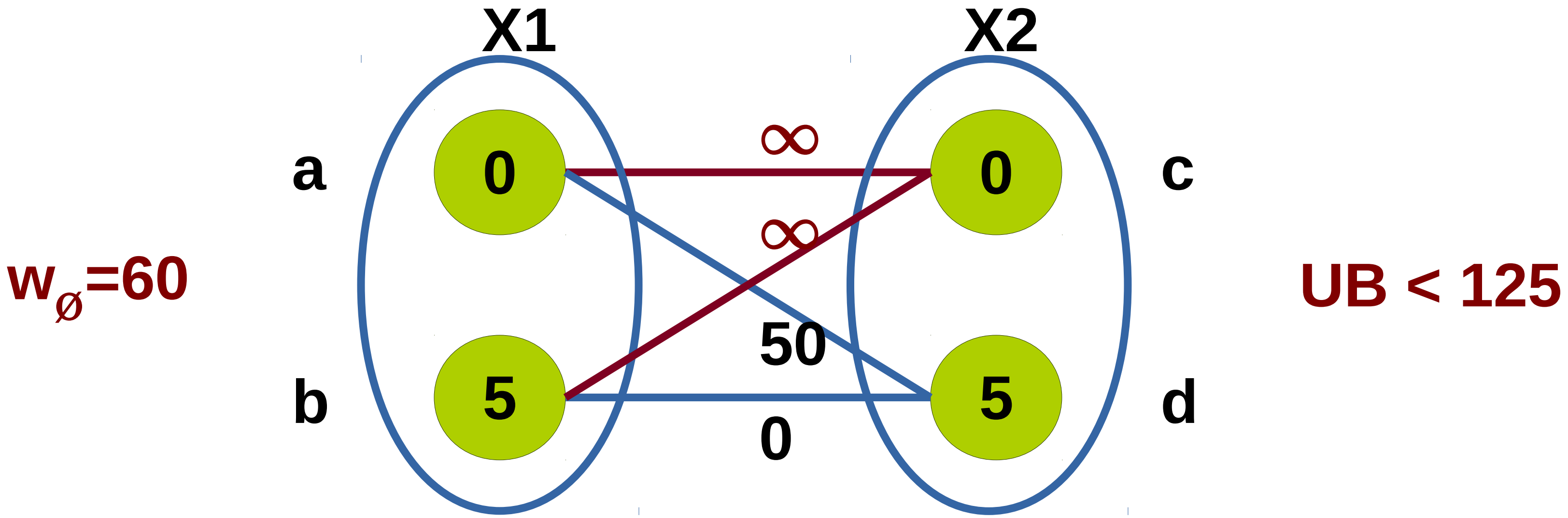

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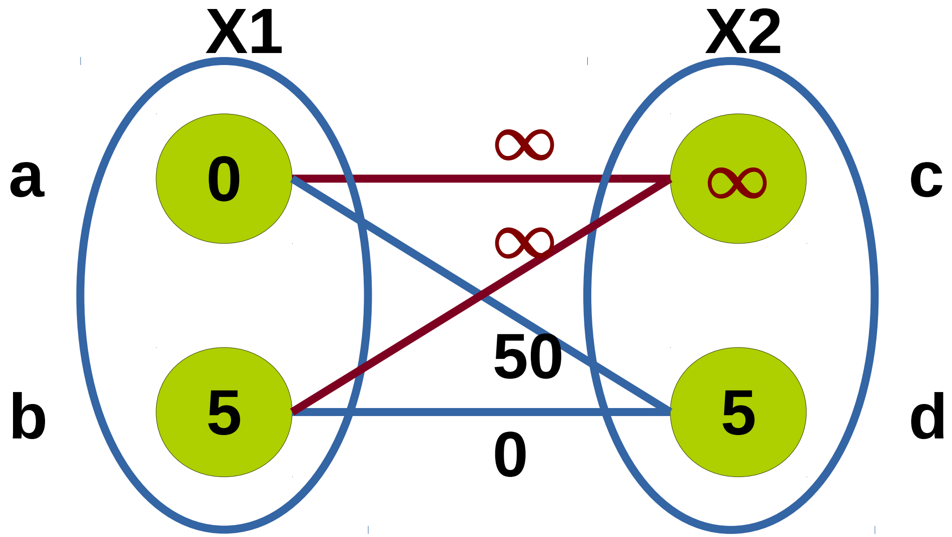
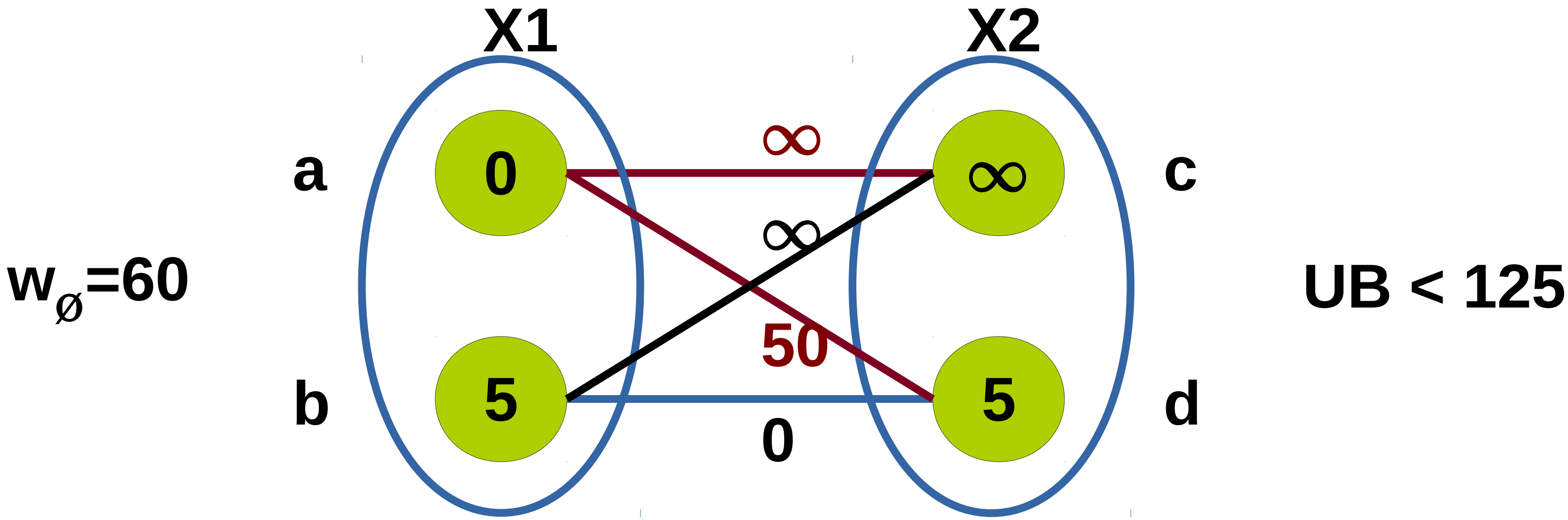


$w_\varnothing$=60

UB < 125

Reparameterization and pruning

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



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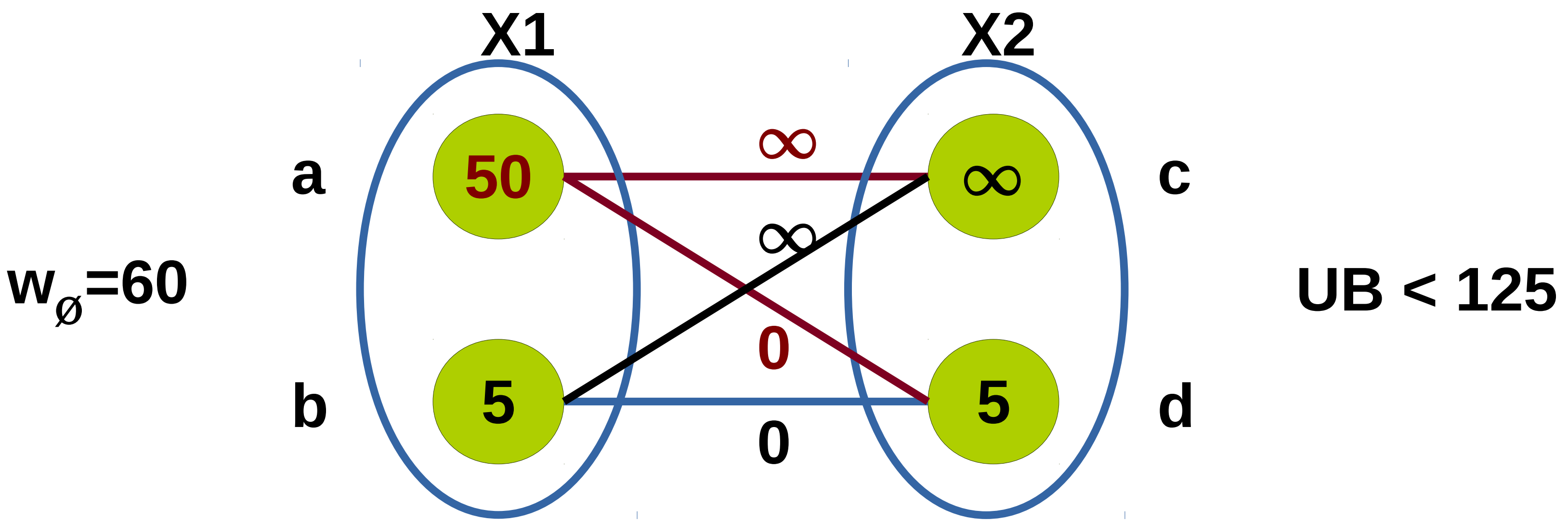

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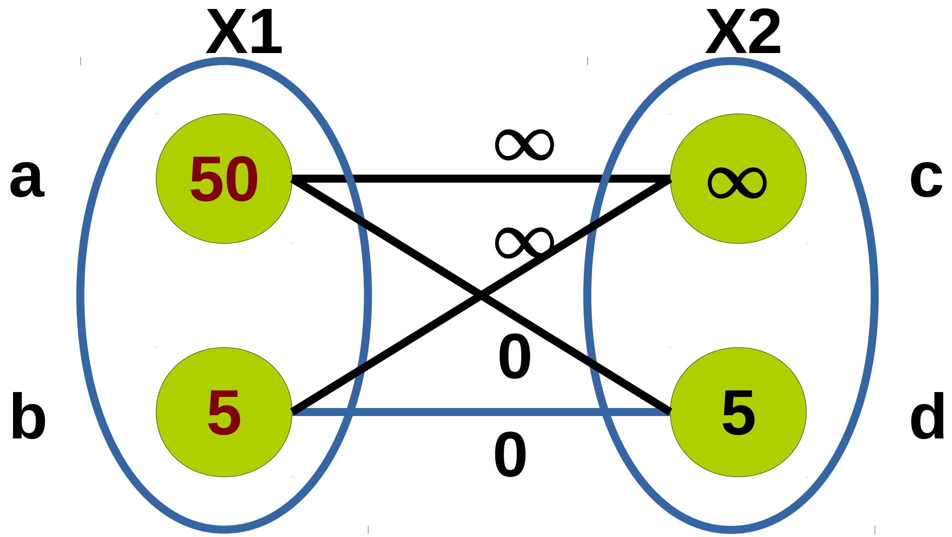
$w_{\varnothing}$=60



UB < 125

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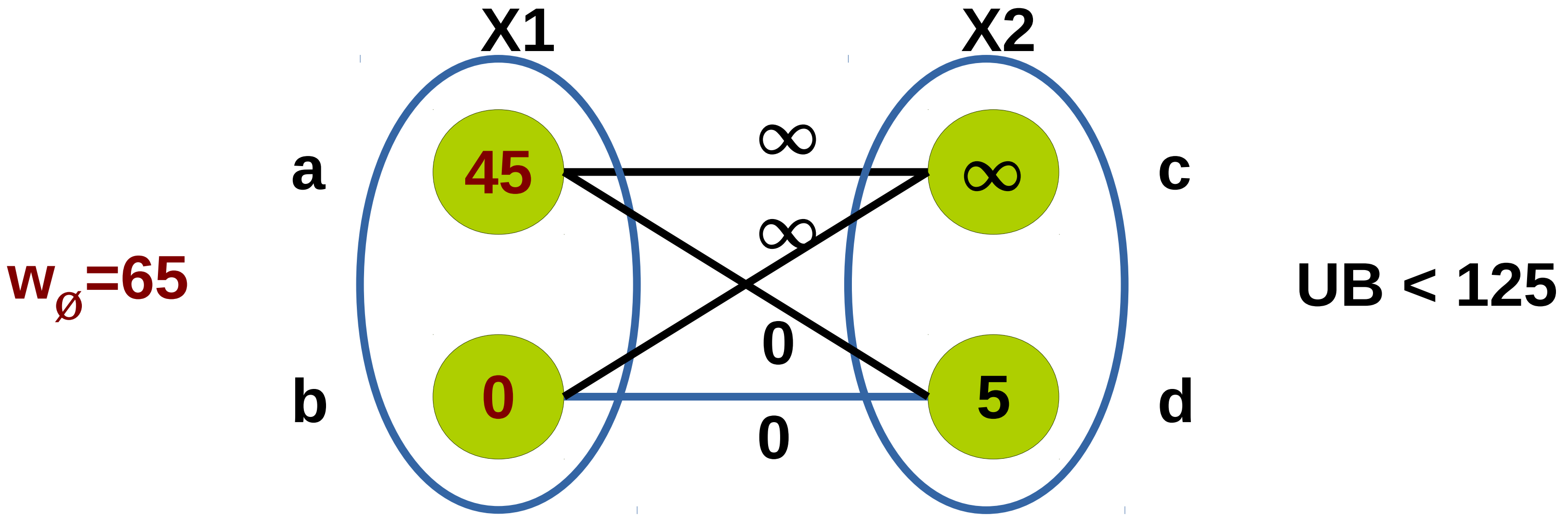

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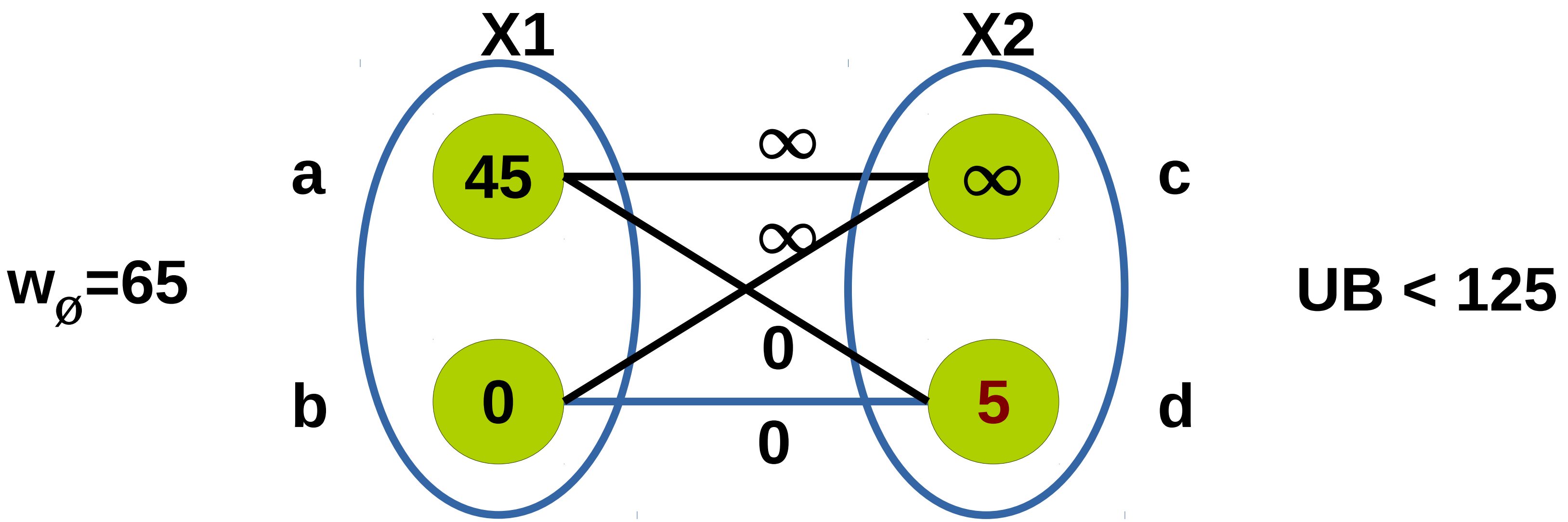

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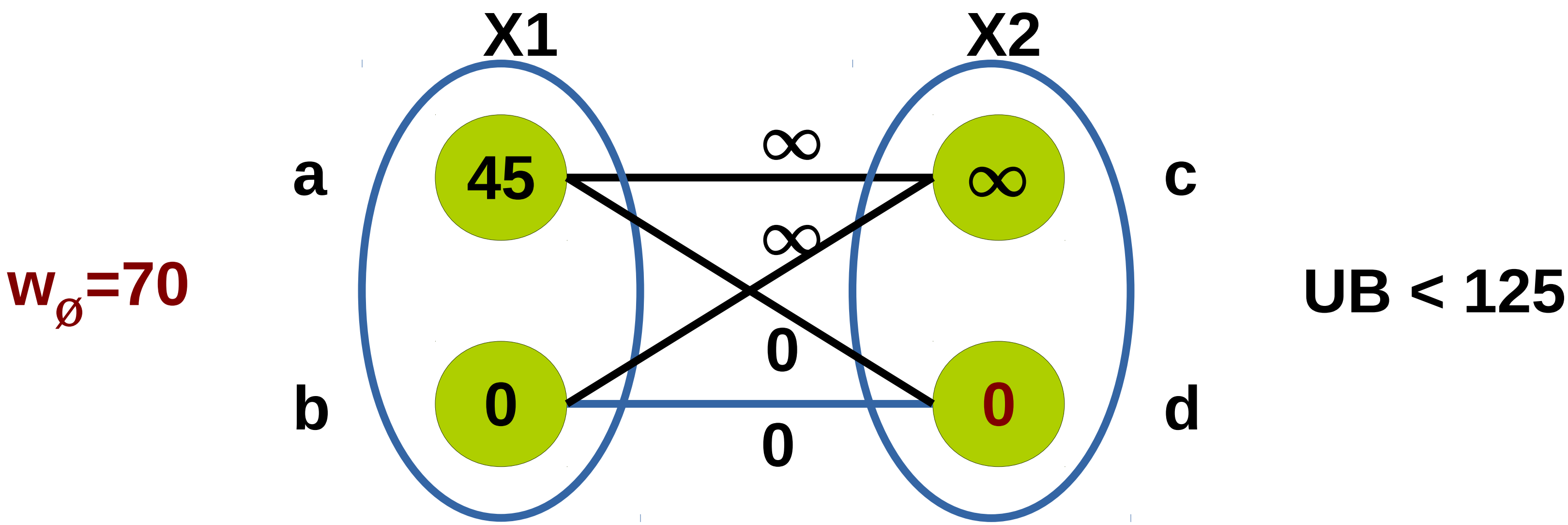


Reparameterization and pruning

(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

(Kratica 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

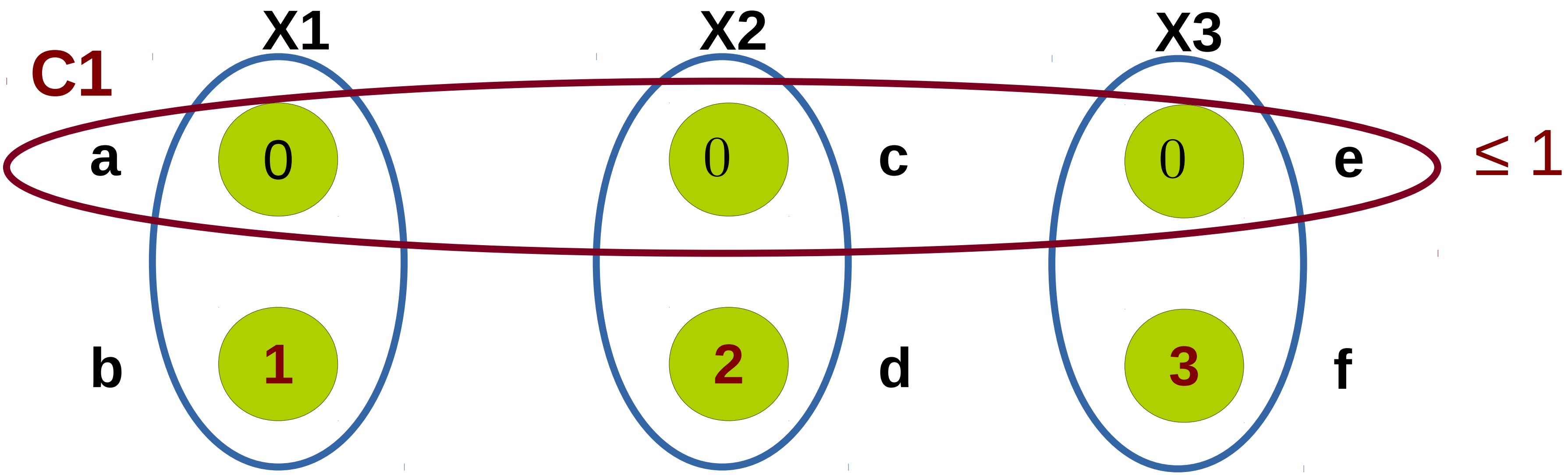
- $c_{ij}(v_i, v_j) = \infty$

Then derive

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

Reparameterization for clique

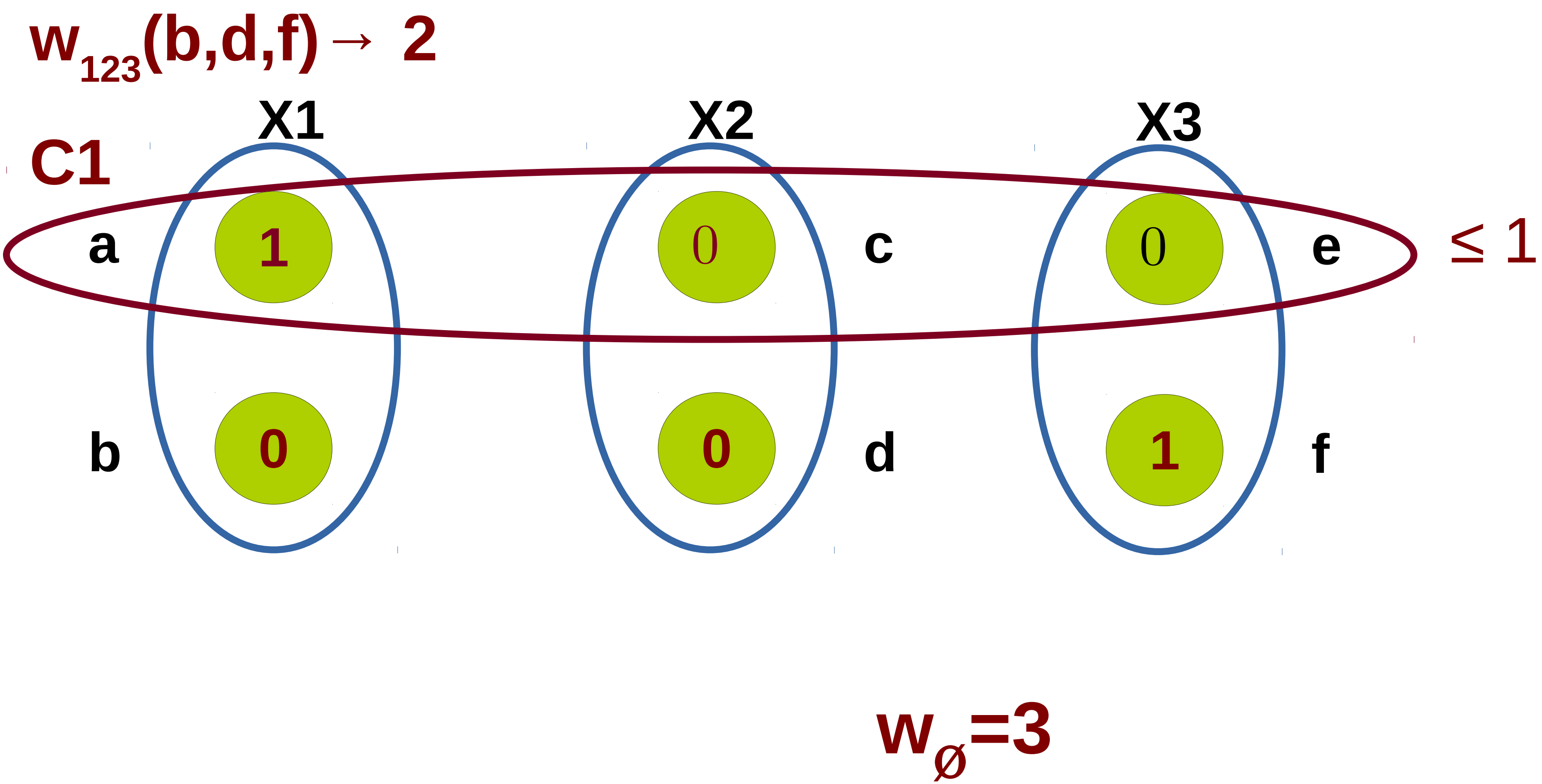
(CP17)



$w_{\varnothing}=0$

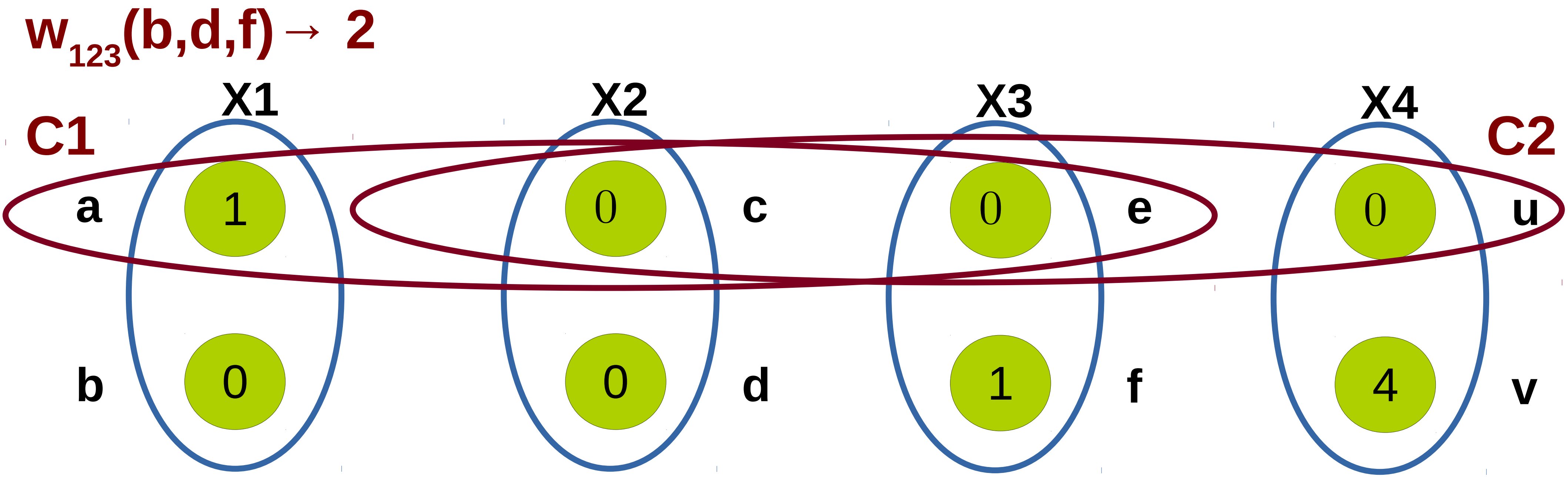
Reparameterization for clique

(CP17)



Reparameterization for cliques

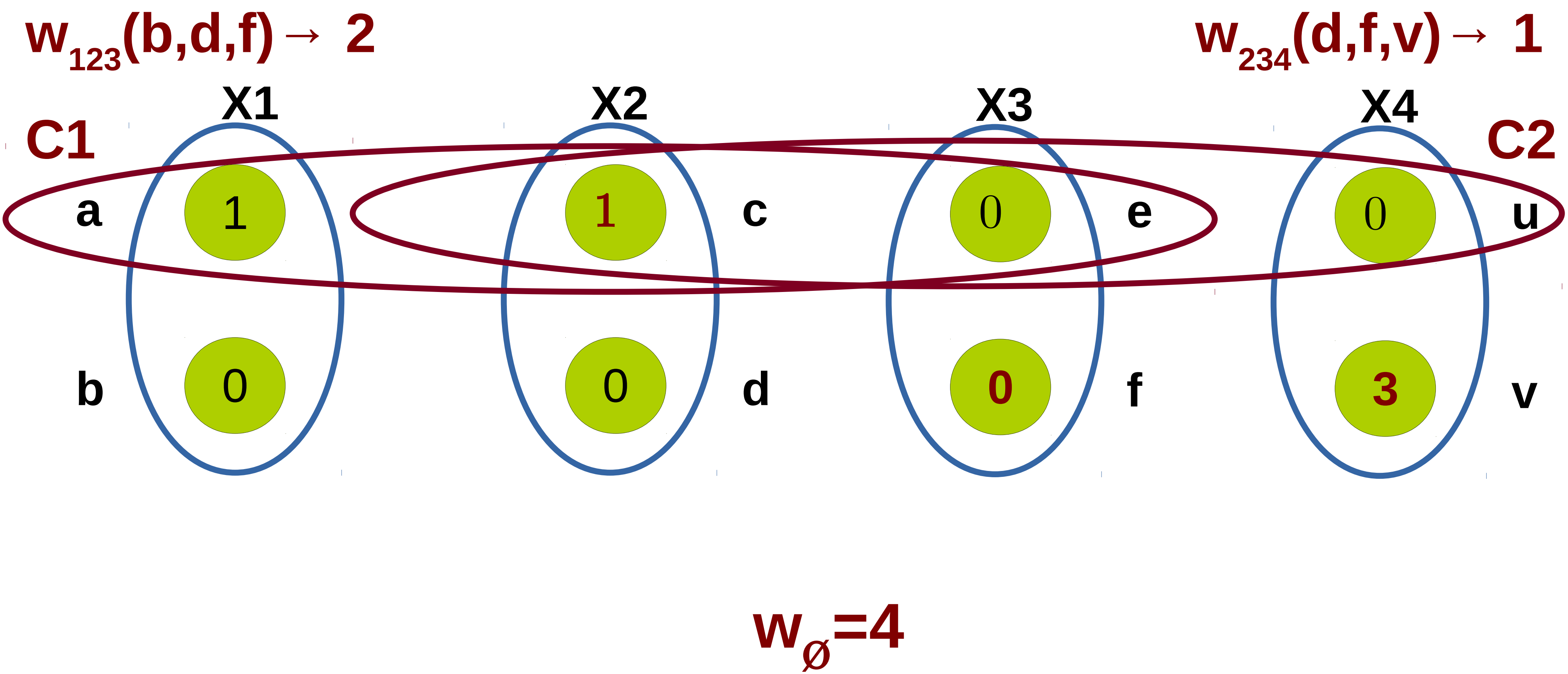
(CP17)



$w_{\varnothing}=3$

Reparameterization for cliques

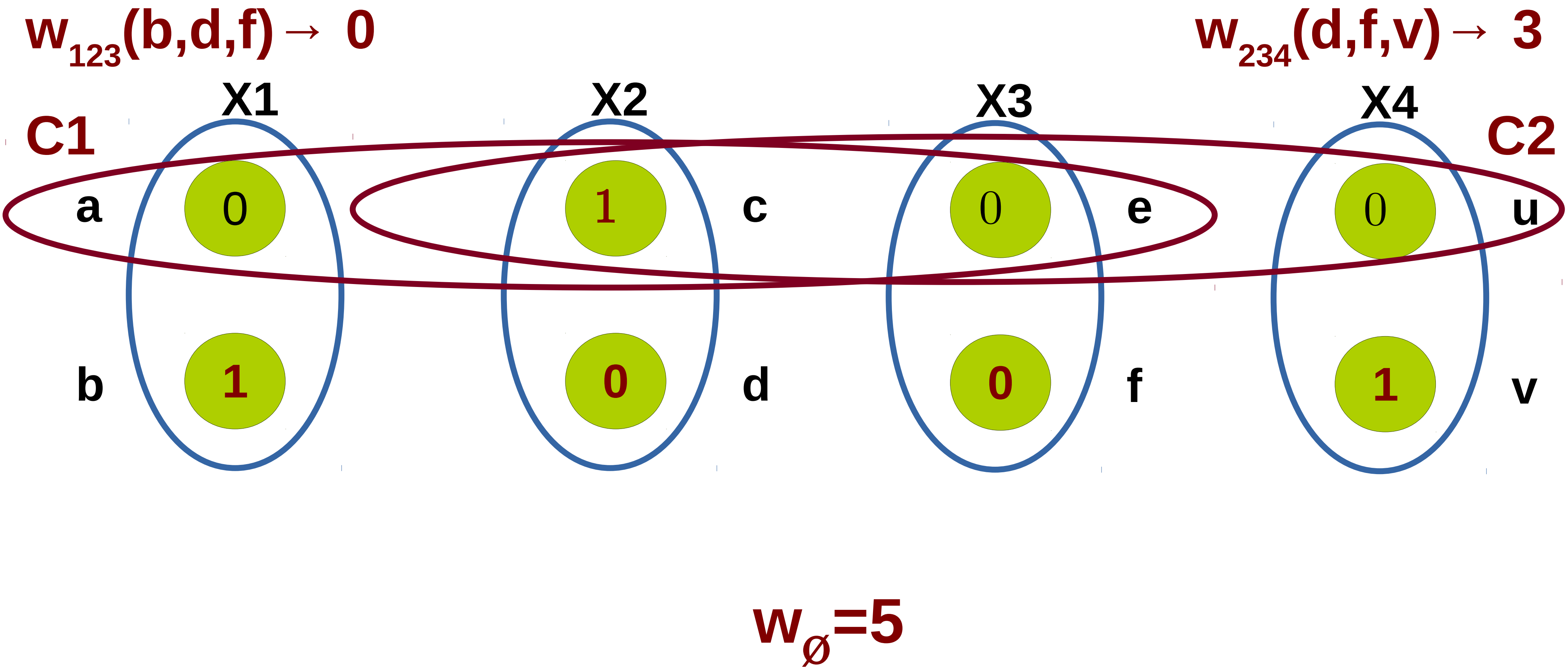
(CP17)



Propagating C1 before C2

Reparameterization for cliques

(CP17)



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

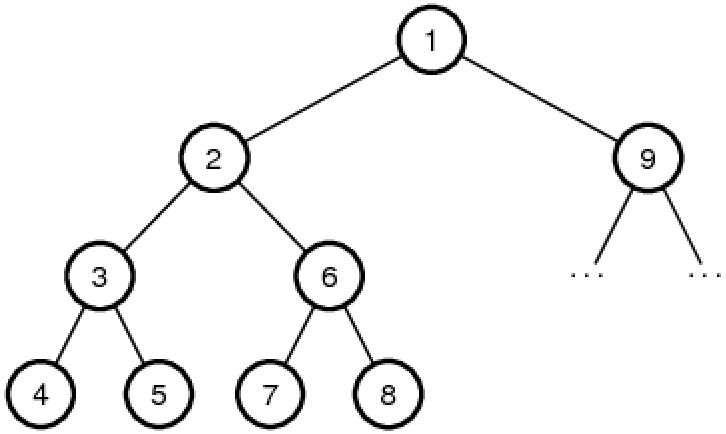
* Including bounded clique detection with Bron-Kerbosch algorithm in preprocessing

Complete tree search methods

Hybrid search

DFS

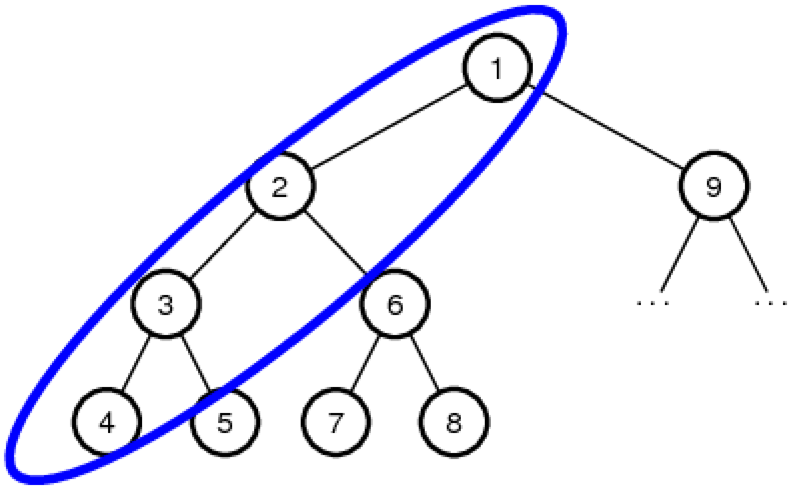
Depth First



DFS

Depth First
Advantages

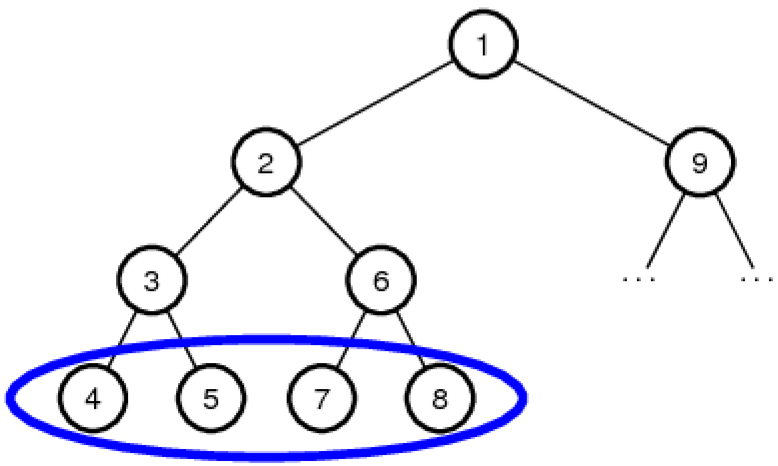
- Incrementality



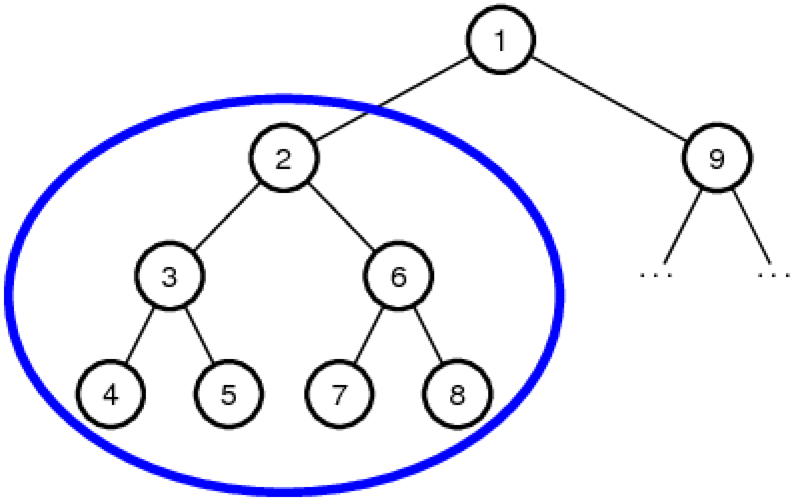
DFS

Depth First
Advantages

- Incrementality
- Anytime (sort of)



DFS



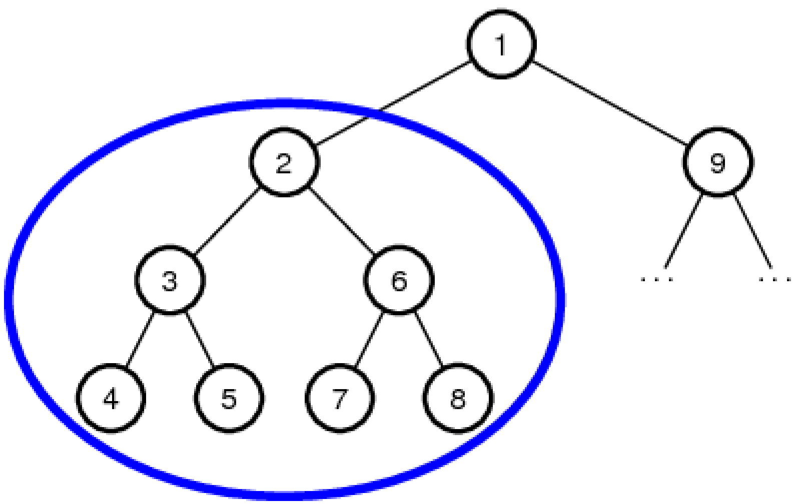
Depth First
Advantages

- Incrementality
- Anytime (sort of)

But

- Thrashing

DFS



Depth First

Advantages

- Incrementality
- Anytime (sort of)

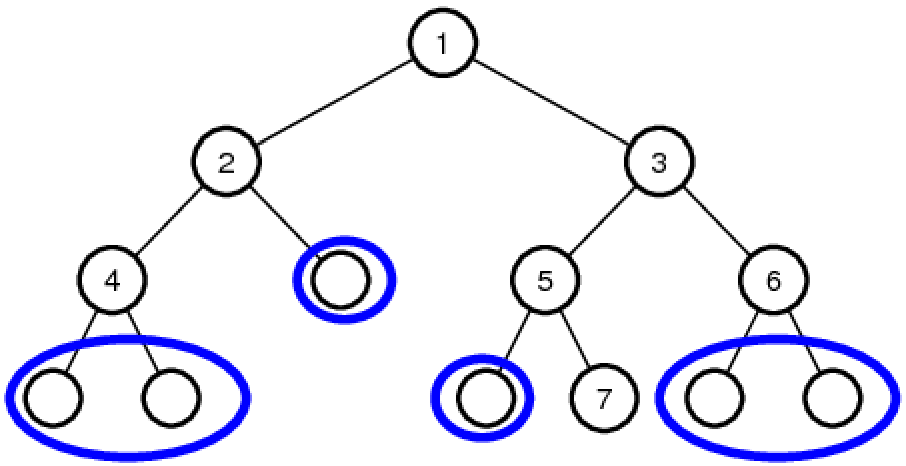
But

- Thrashing
- No global lower bounds

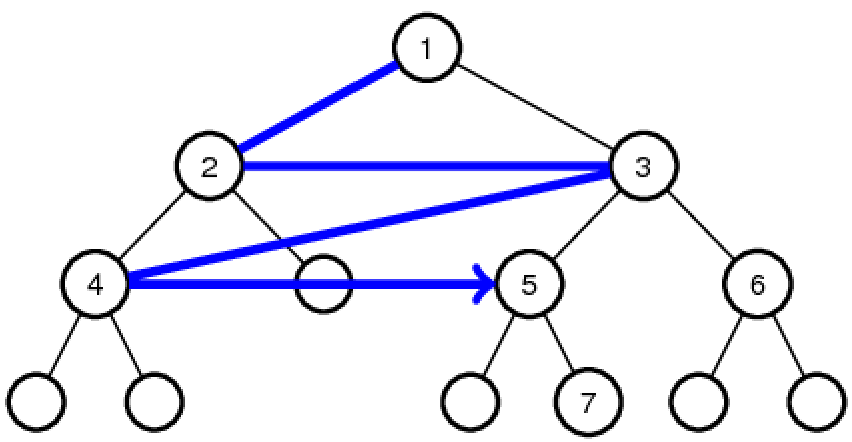
BFS

Best first

- Memory requirements



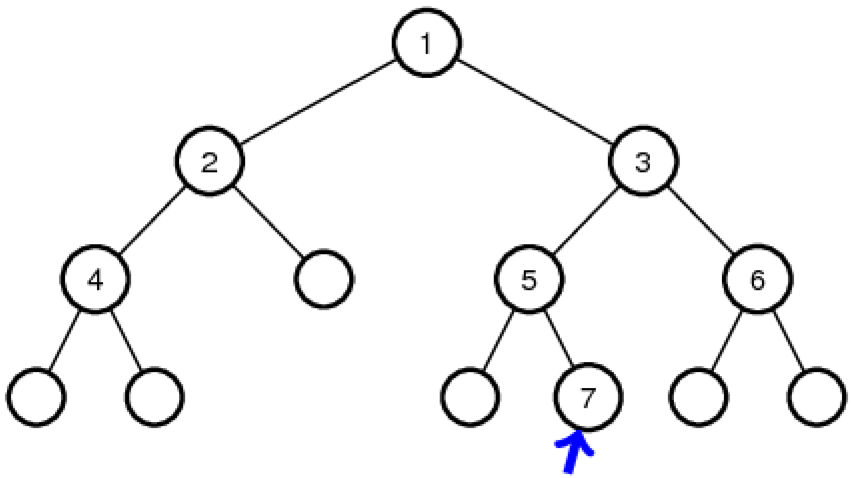
BFS



Best first

- Memory requirements
- No incrementality or even greater memory cost

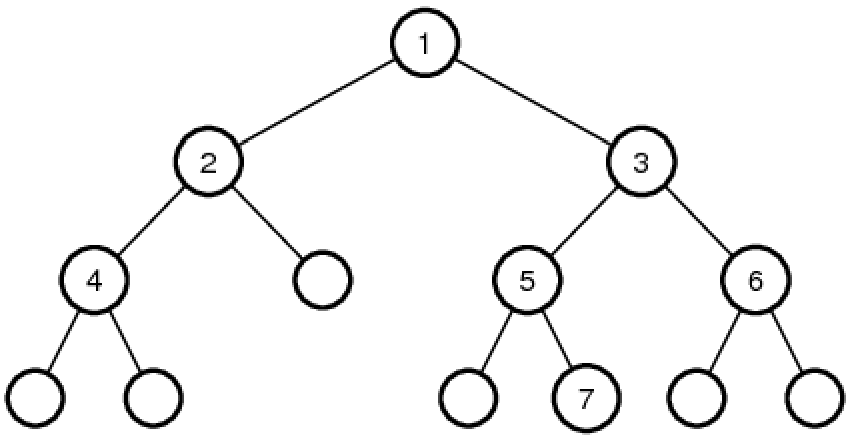
BFS



Best first

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

BFS



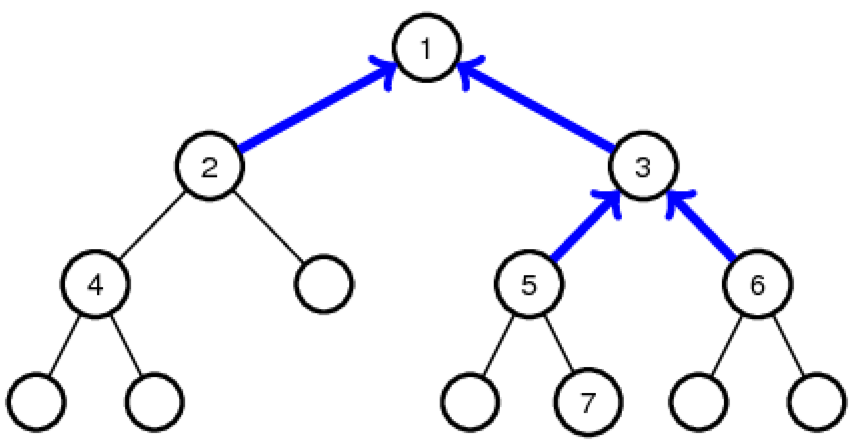
Best first

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

but

- Theoretical guarantees

BFS



Best first

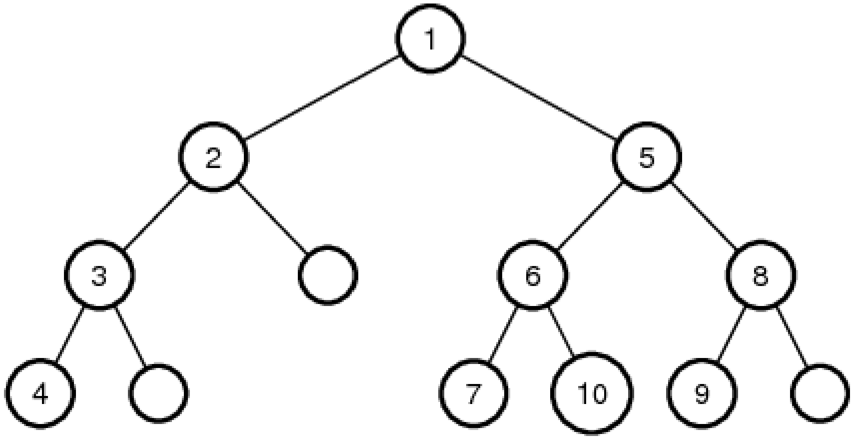
- Memory requirements
- No incrementality or even greater memory cost
- Not anytime

but

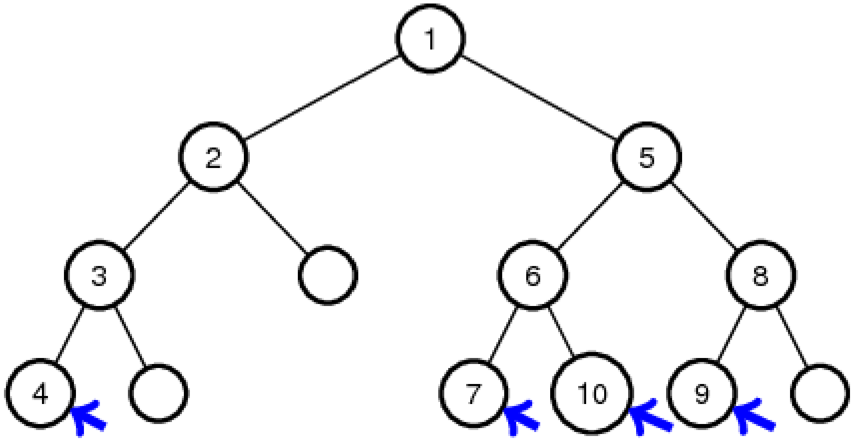
- Theoretical guarantees
- Global lower bounds

HBFS

BFS with DFS probes*



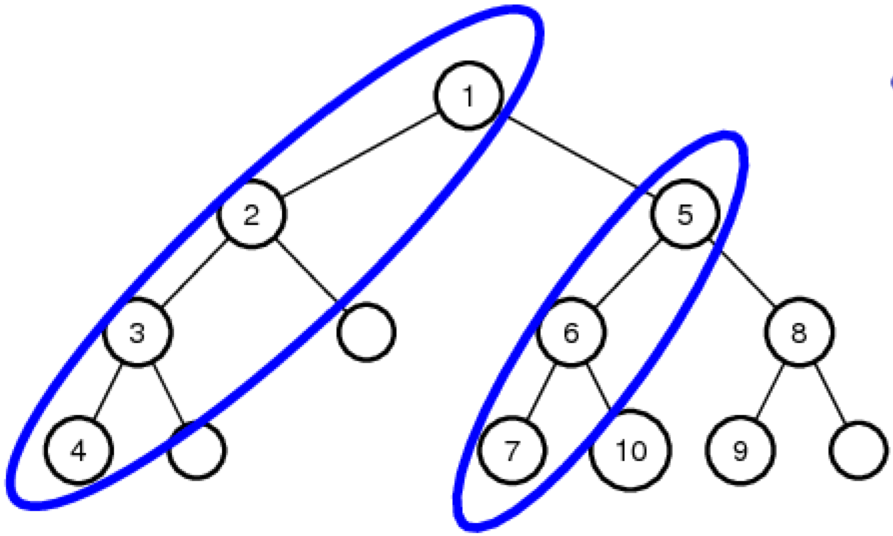
HBFS



BFS with DFS probes*

- Improved anytime behavior

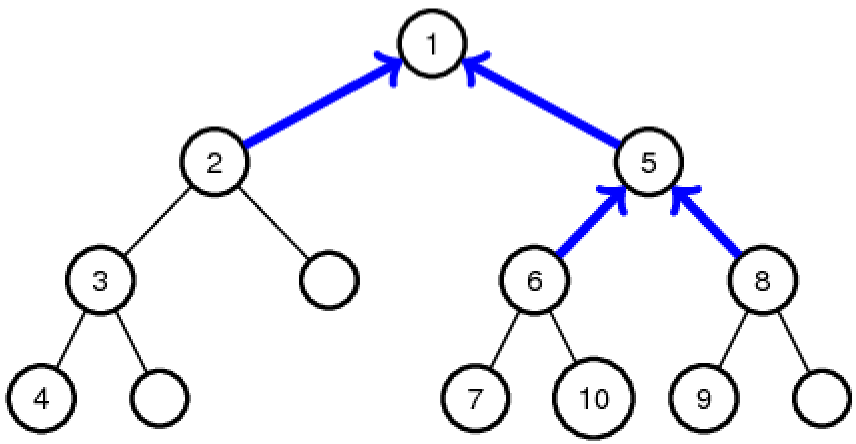
HBFS



BFS with DFS probes*

- Improved anytime behavior
- Incrementality
  without memory overhead

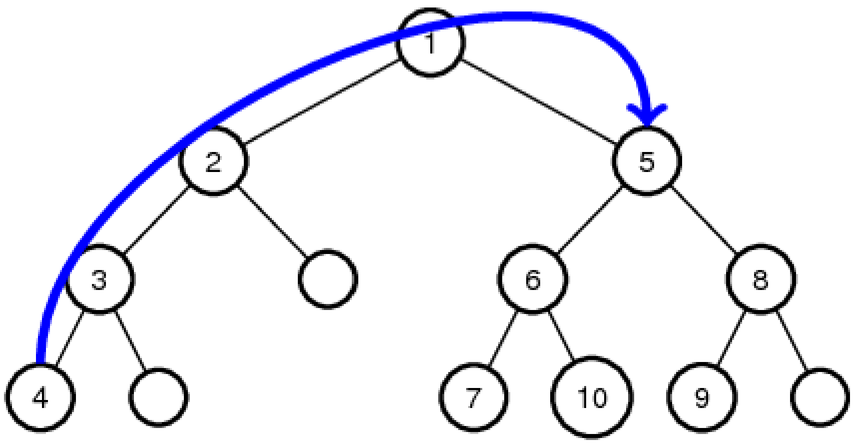
HBFS



BFS with DFS probes*

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

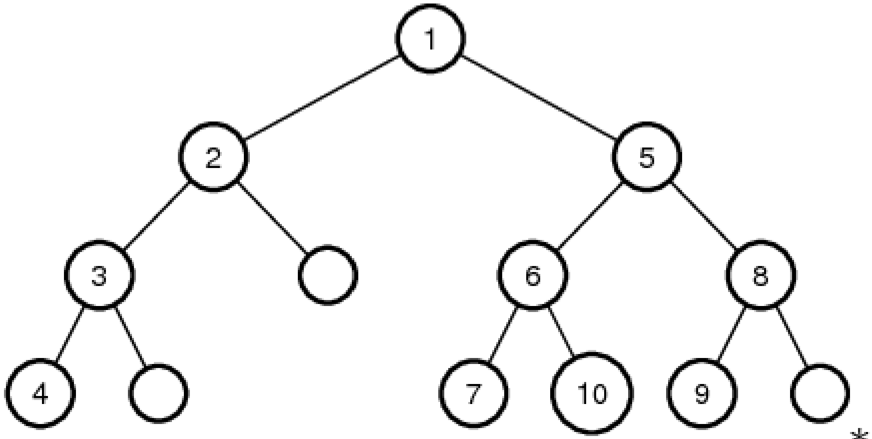
HBFS



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

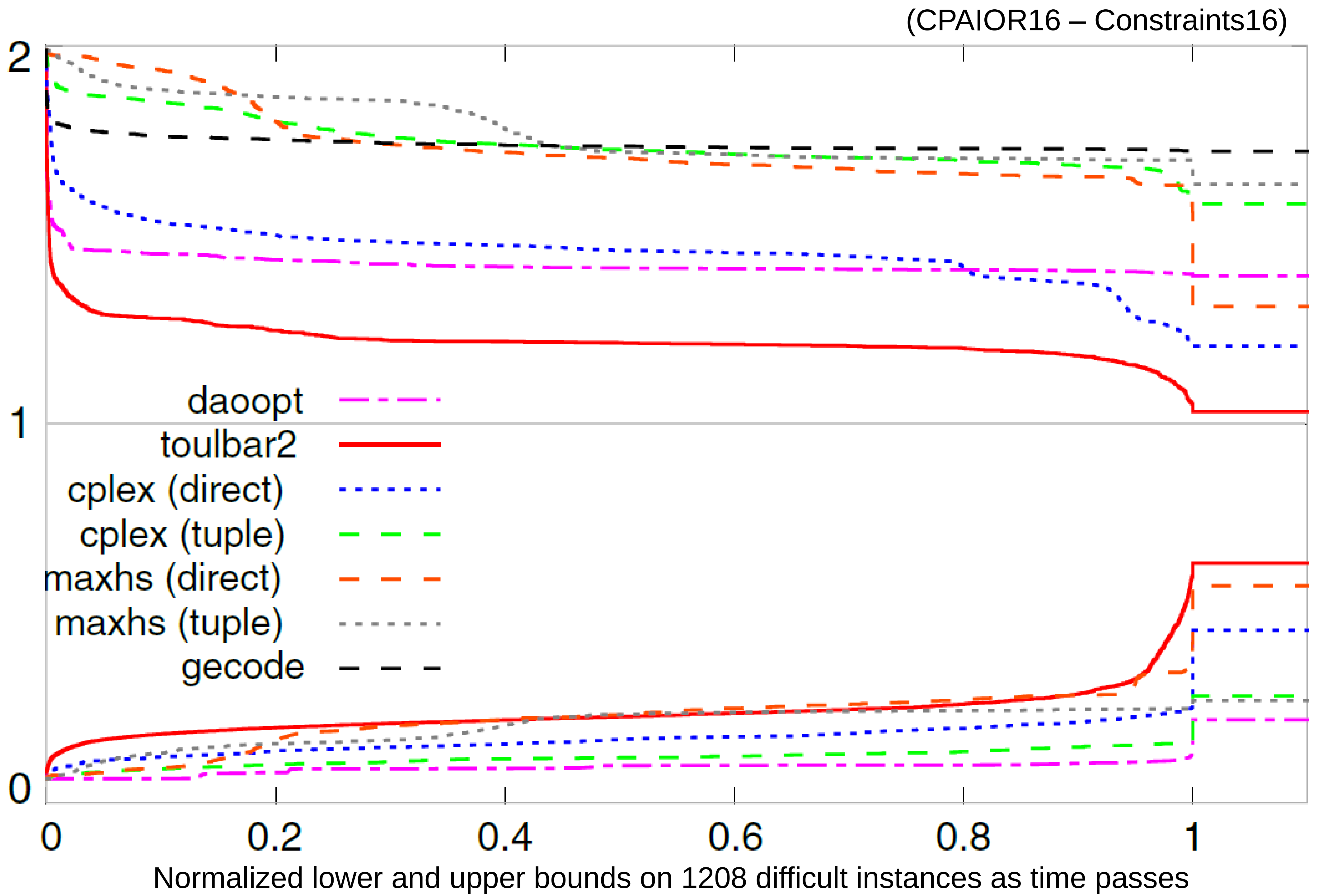
Benchmark

- 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)

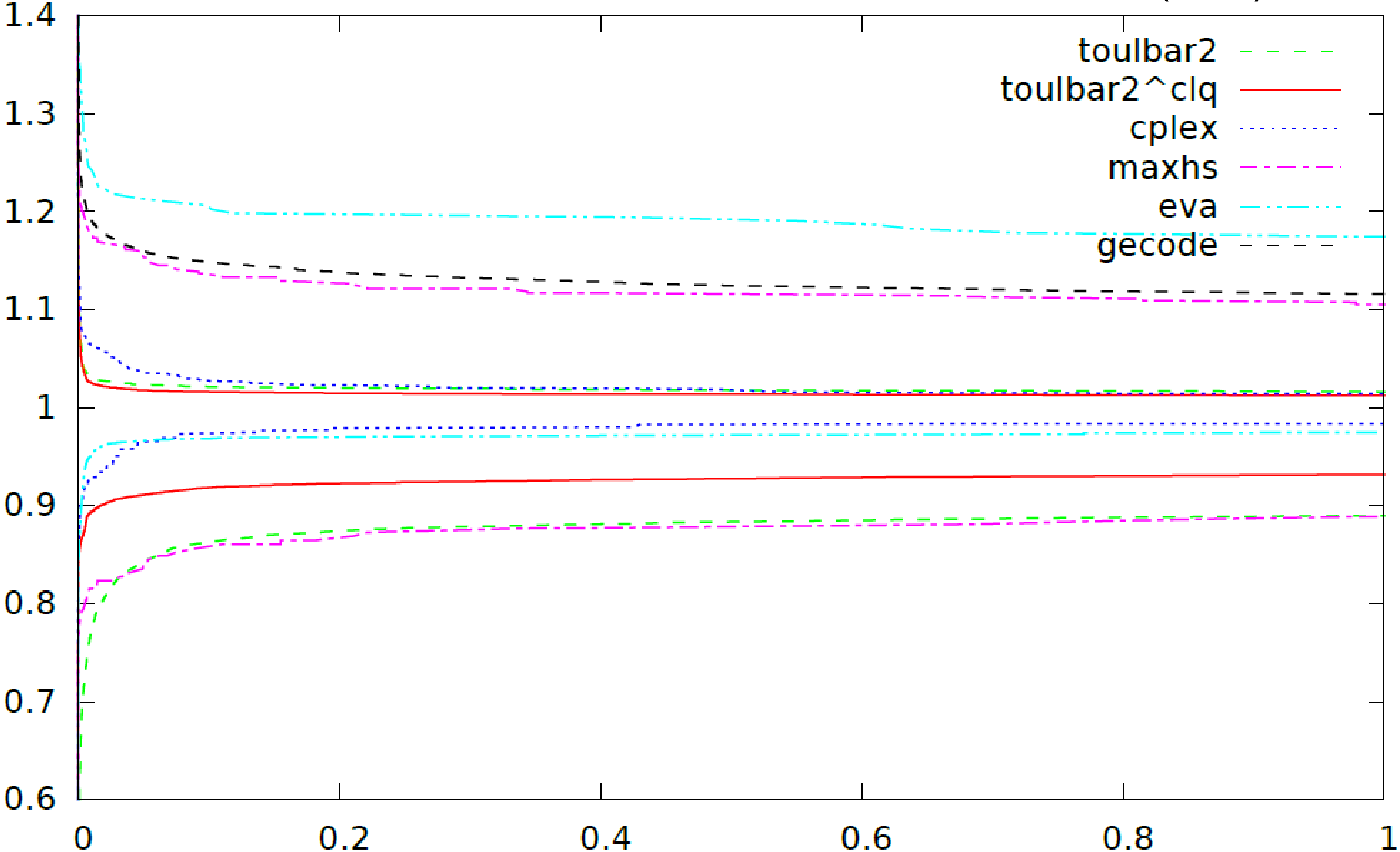
Number of instances and their total compressed (gzipped) size:

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

http://genoweb.toulouse.inra.fr/~degivry/evalgm

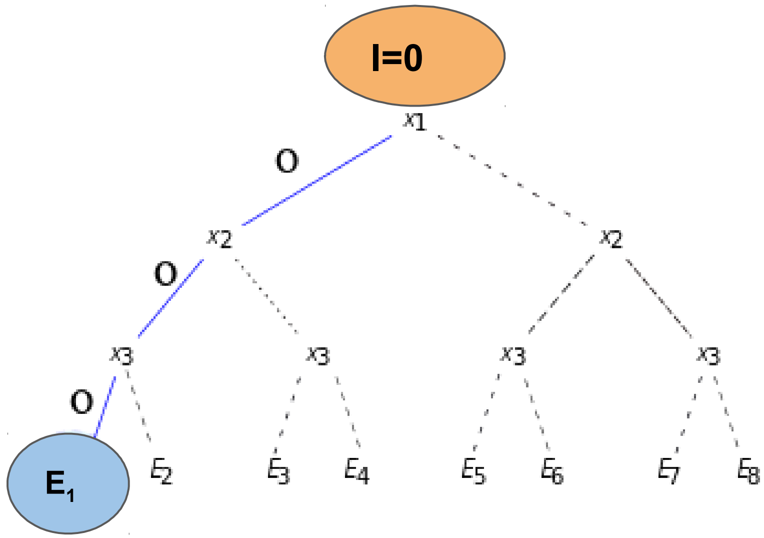

(CPAIOR16 – Constraints16)
2
1
0
daoopt
toulbar2
cplex (direct)
cplex (tuple)
maxhs (direct)
maxhs (tuple)
gecode
0
0.2
0.4
0.6
0.8
1
Normalized lower and upper bounds on 1208 difficult instances as time passes

Results exploiting cliques (CP17)



Normalized lower and upper bounds on 252 instances as time passes

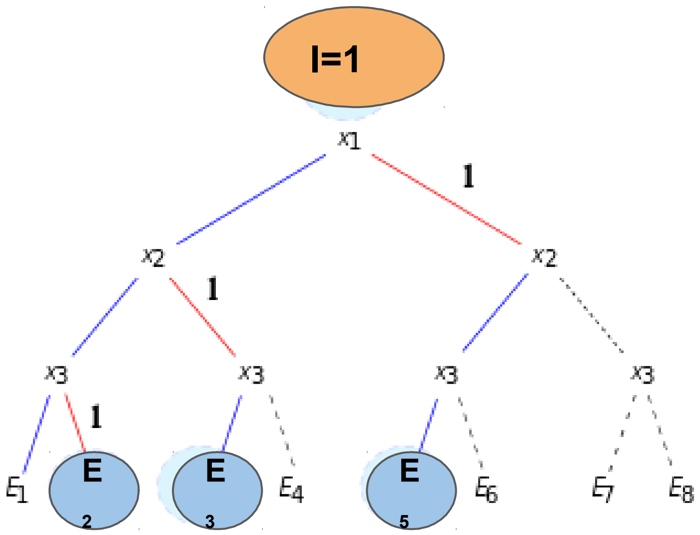
Limited Discrepancy Search *(Ginsberg 95)*



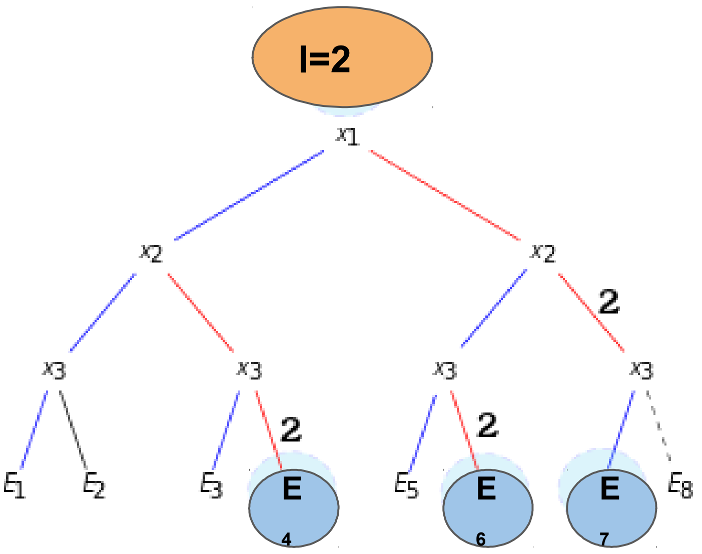
- Small example with 3 variables and 2 values per domain

Limited Discrepancy Search

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



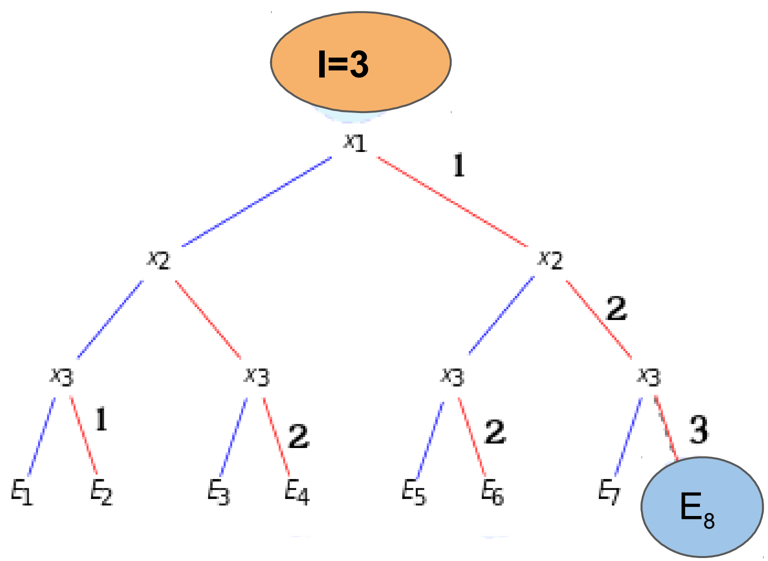
Limited Discrepancy Search *(Ginsberg 95)*



Limited Discrepancy Search *(Ginsberg 95)*

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

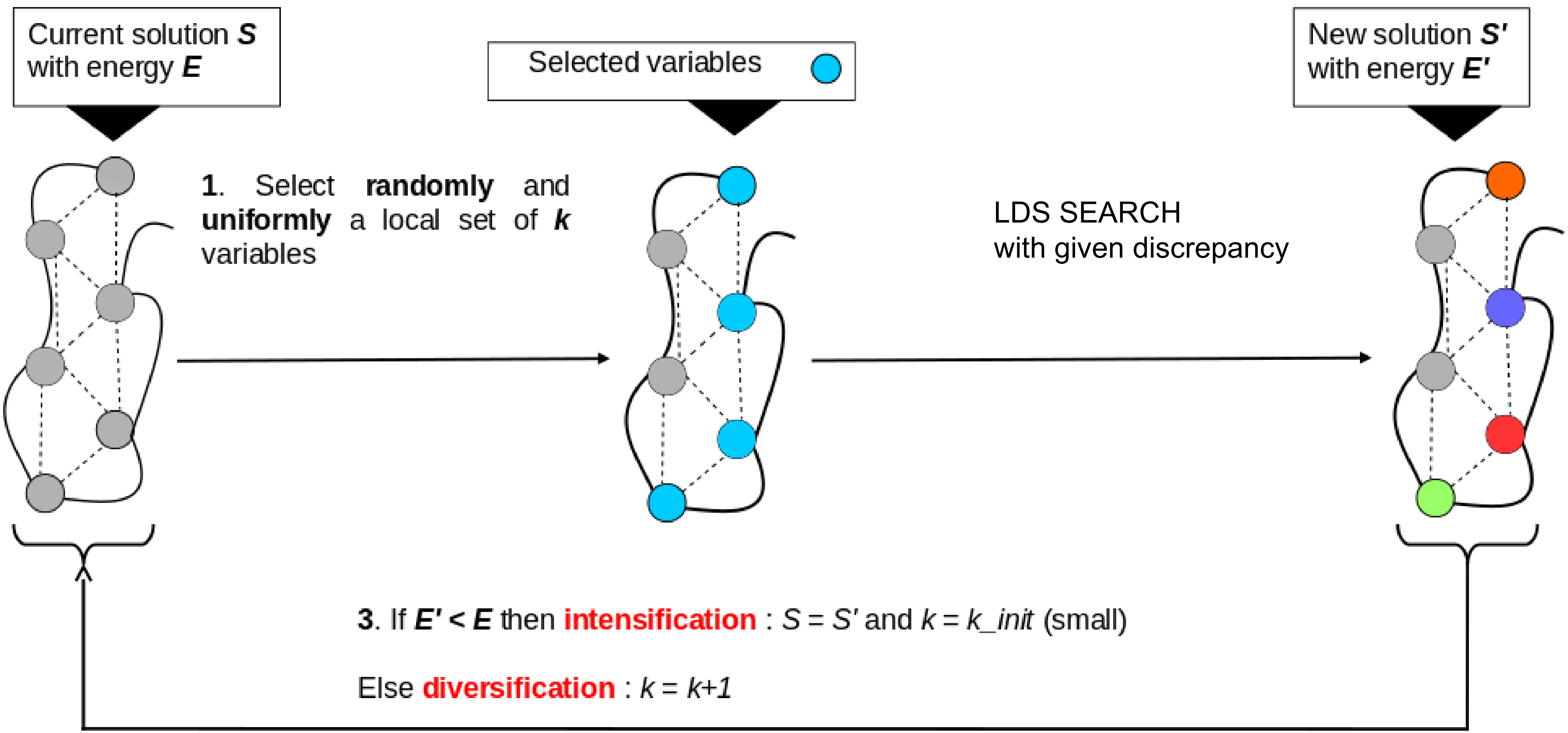
Full exploration



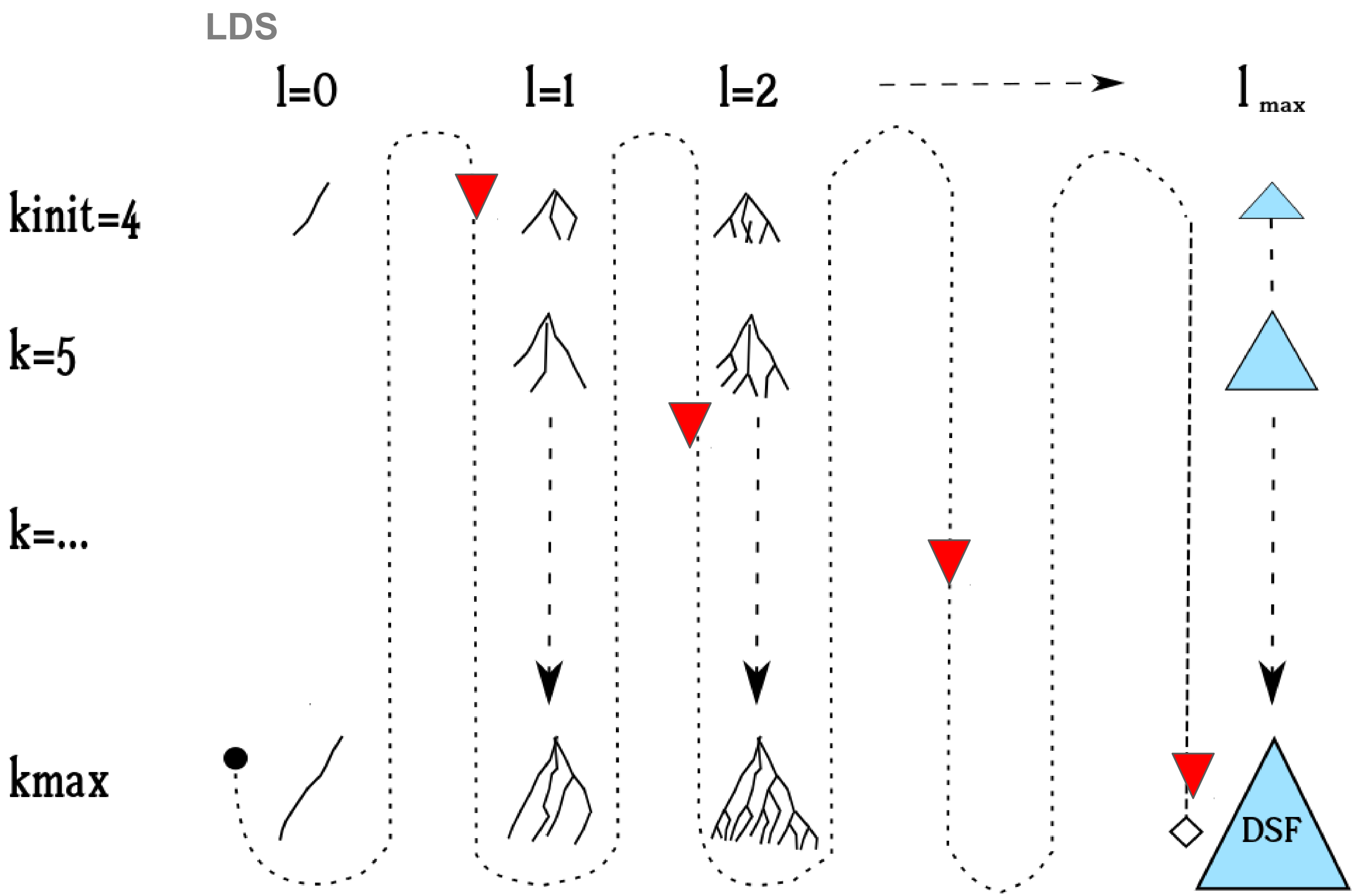
l=3 ⇒ optimality proof

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

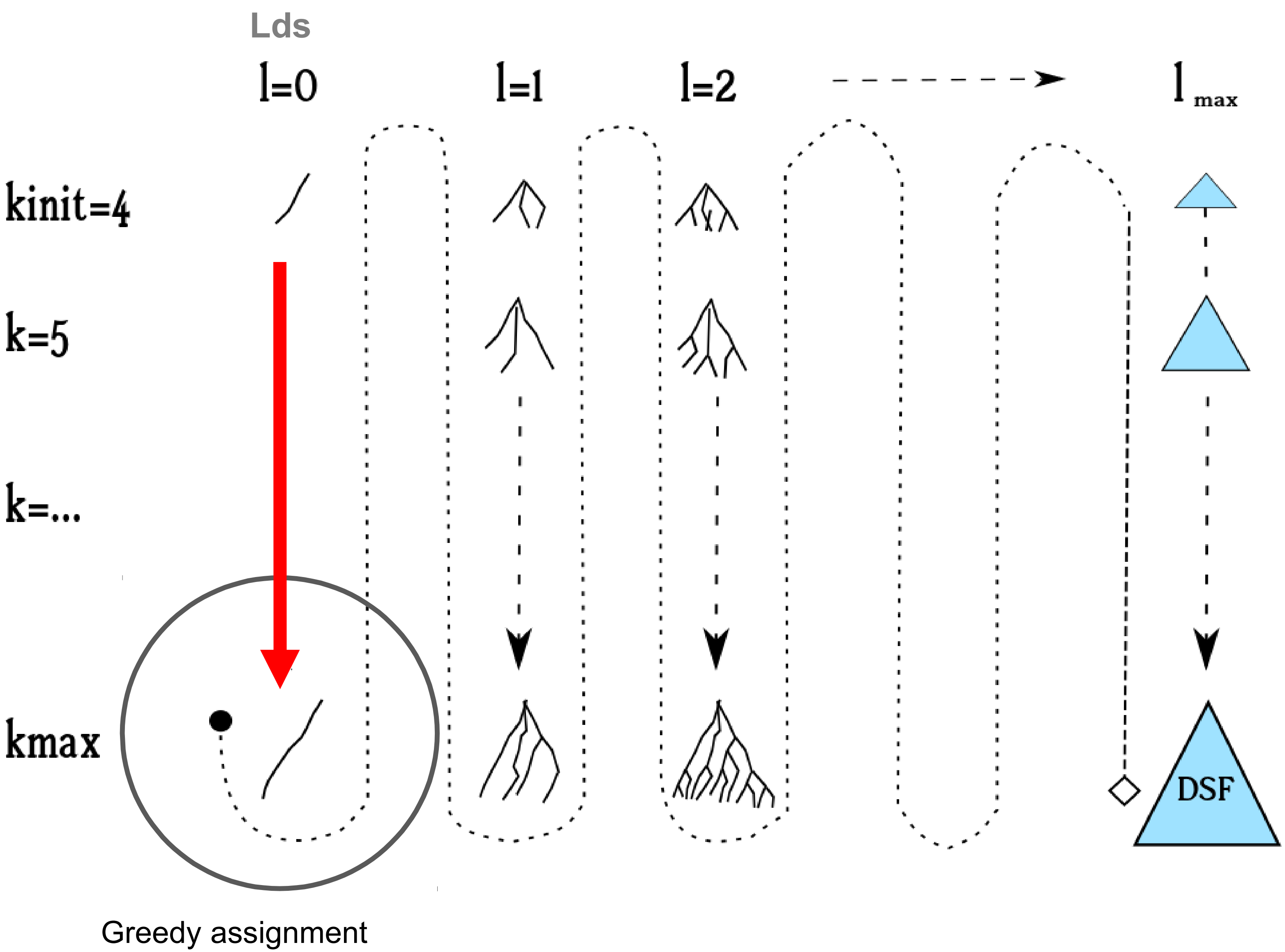
Variable Neighborhood Search *(Hansen 97)*



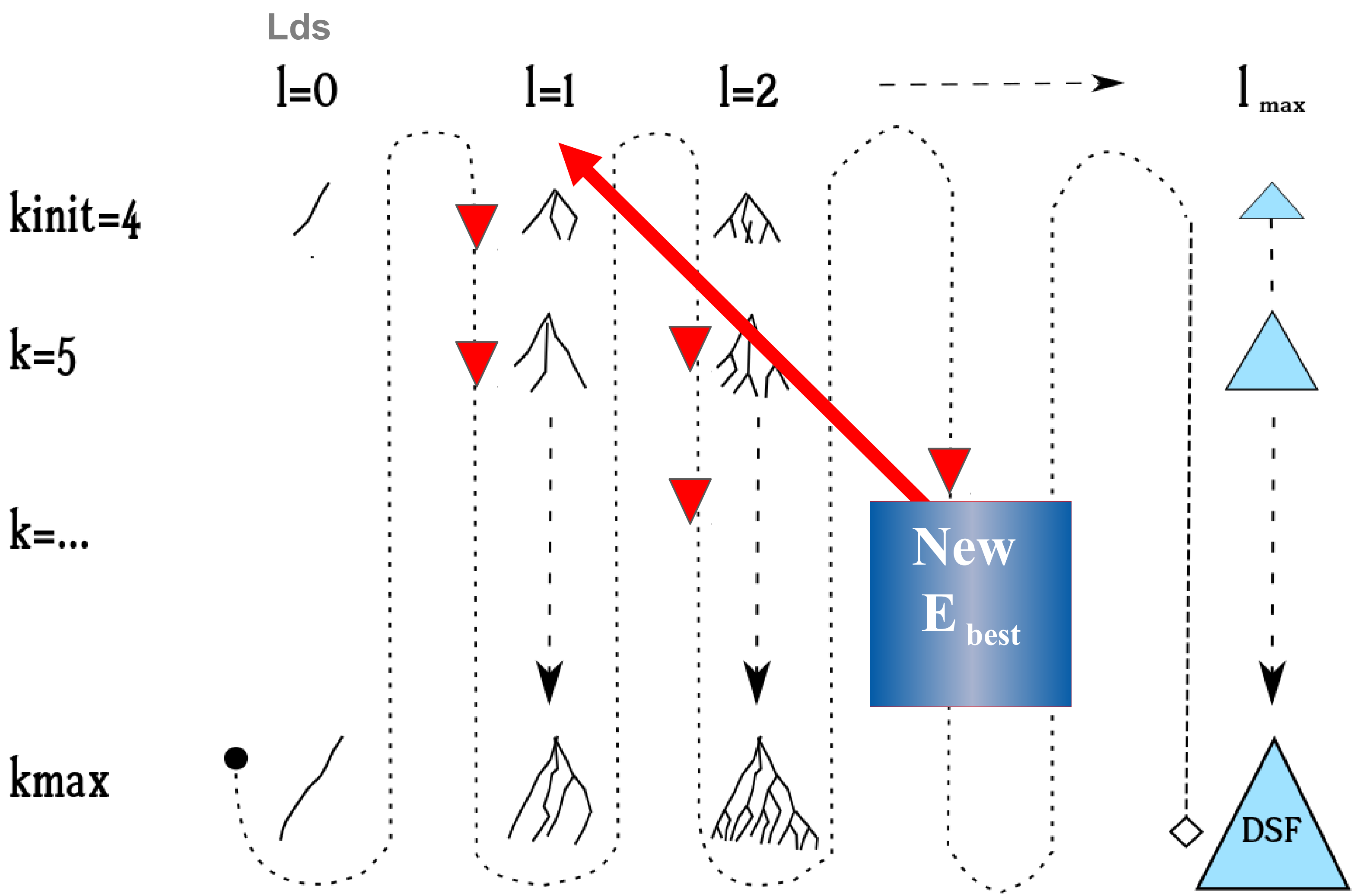
UDGVNS : Exploration of both k and l dimensions



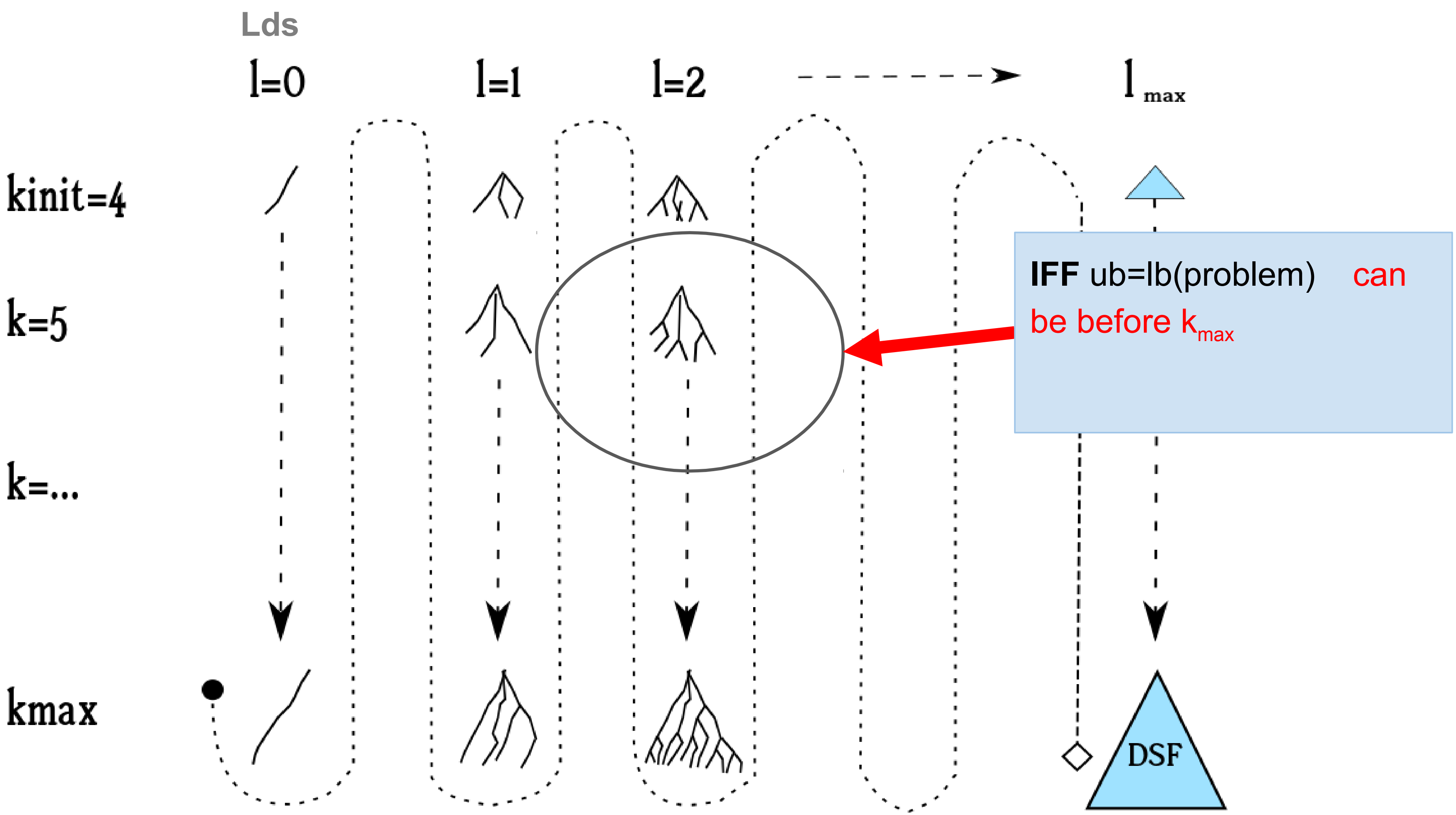
Step 1 : Initial solution



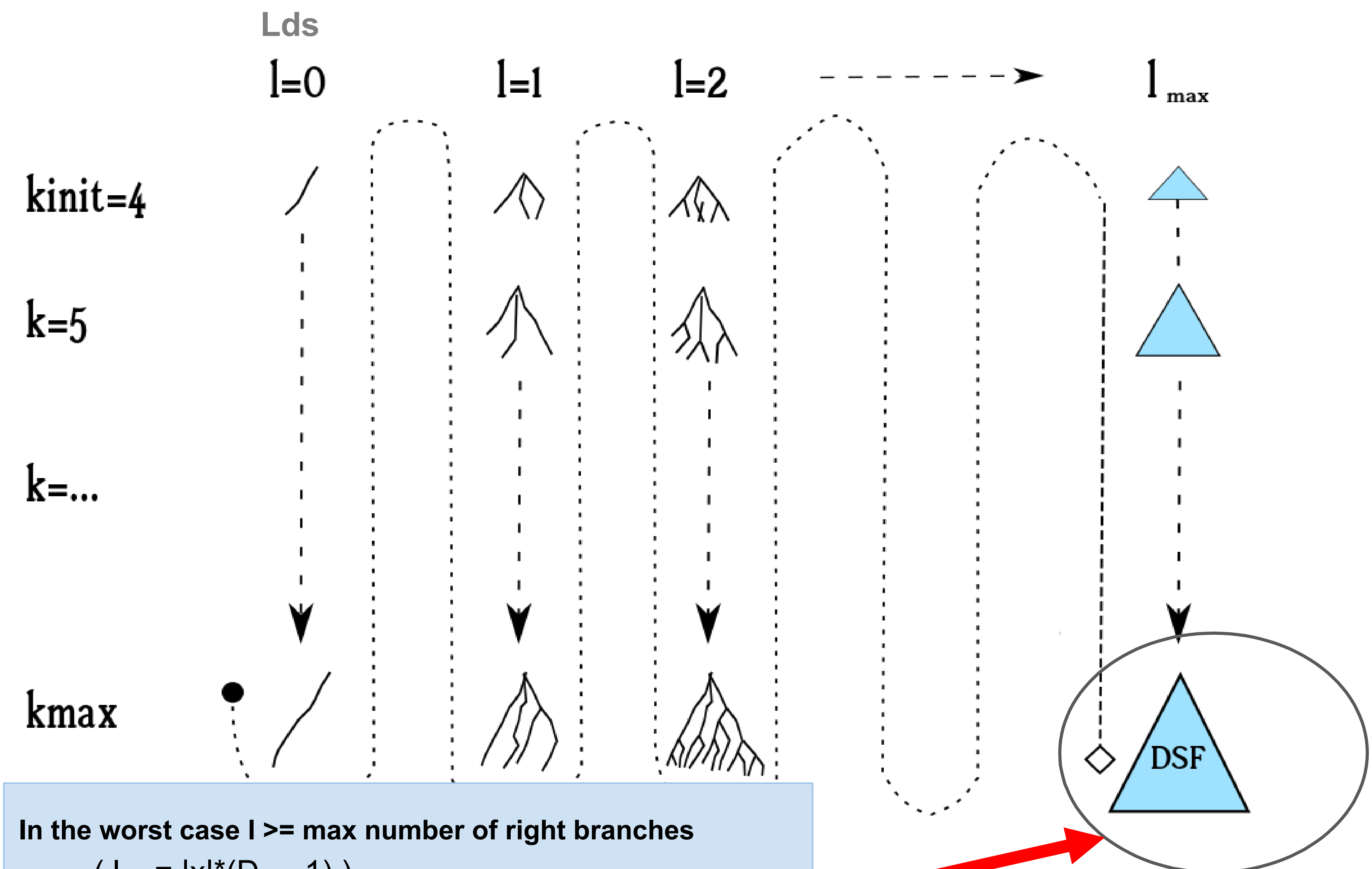
NEW SOLUTION WITH BETTER E → RESTART



Proof of Optimality



Proof of Optimality

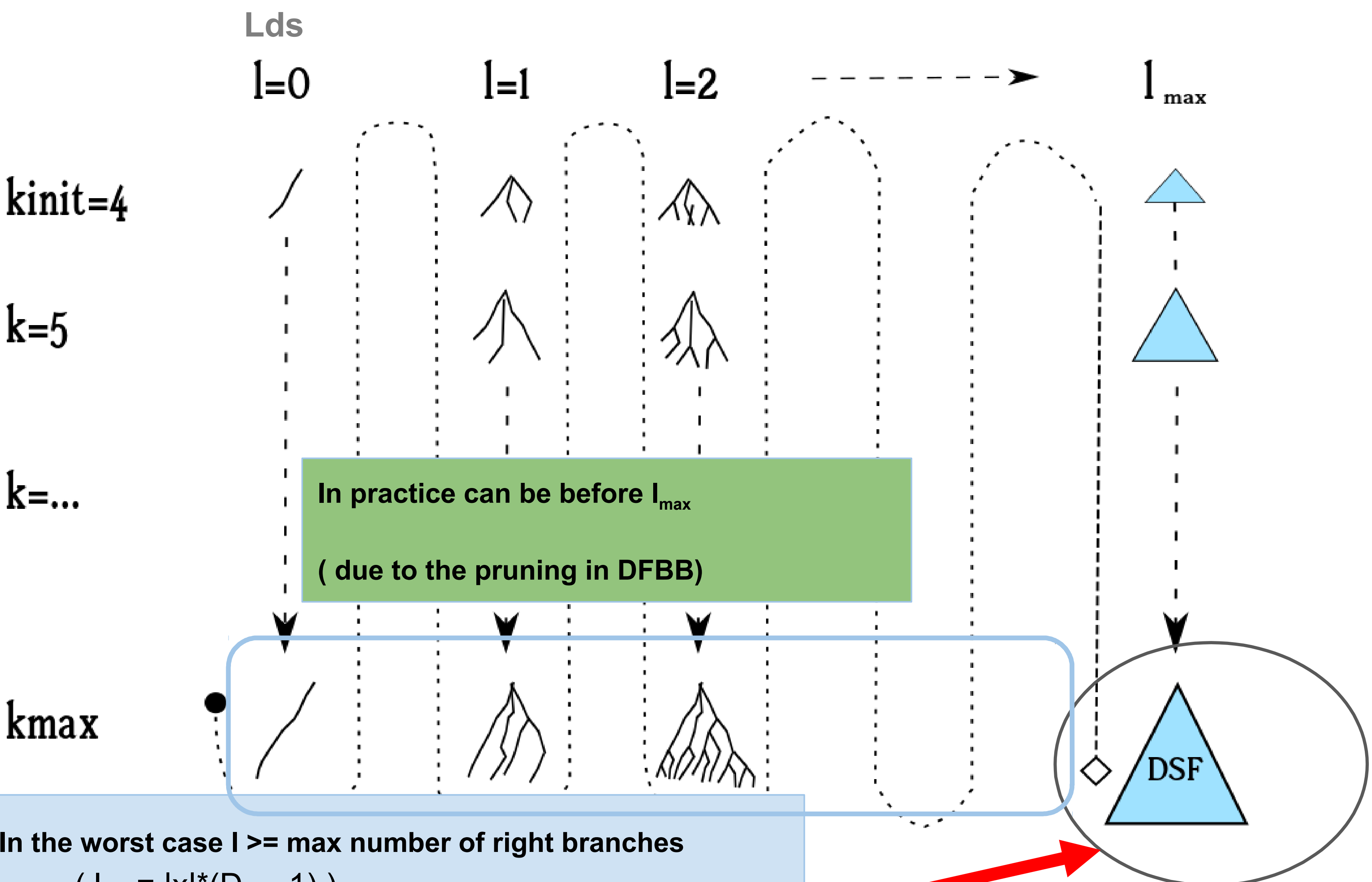


In the worst case l >= max number of right branches

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

Iff **k** $= k_{max}$ = problem size

Proof of Optimality



In practice can be before l_{max}

(due to the pruning in DFBB)

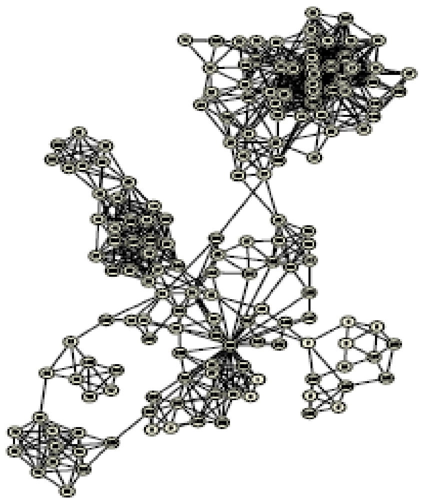
In the worst case l >= max number of right branches

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

Iff **k** = k_{max} = problem size

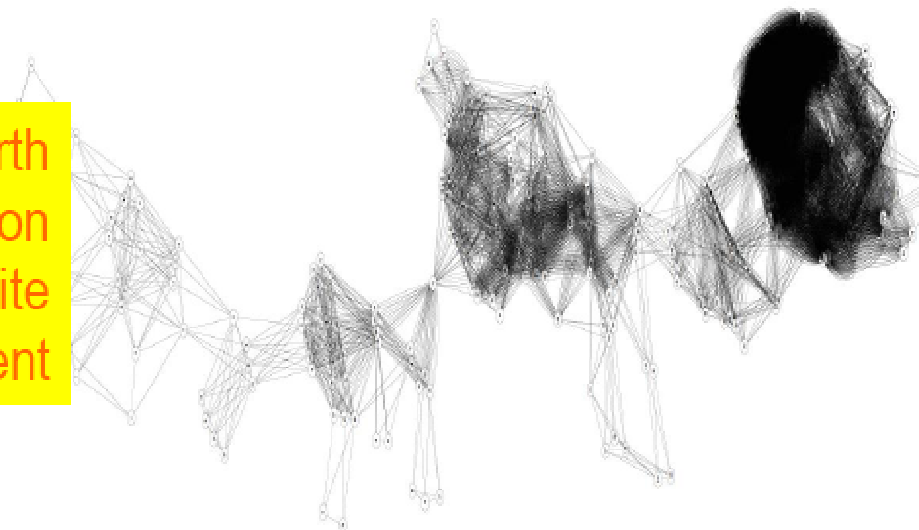
Neighborhoods using problem structure

Radio Link Frequency Assignment



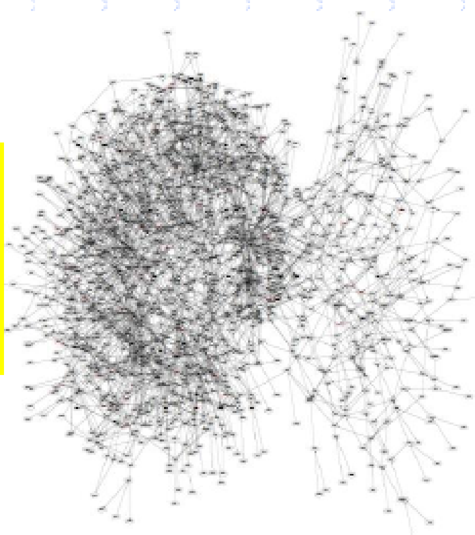
CELAR SCEN-07r
(*Constraints* 4(1), 1999)

Earth Observation Satellite Management



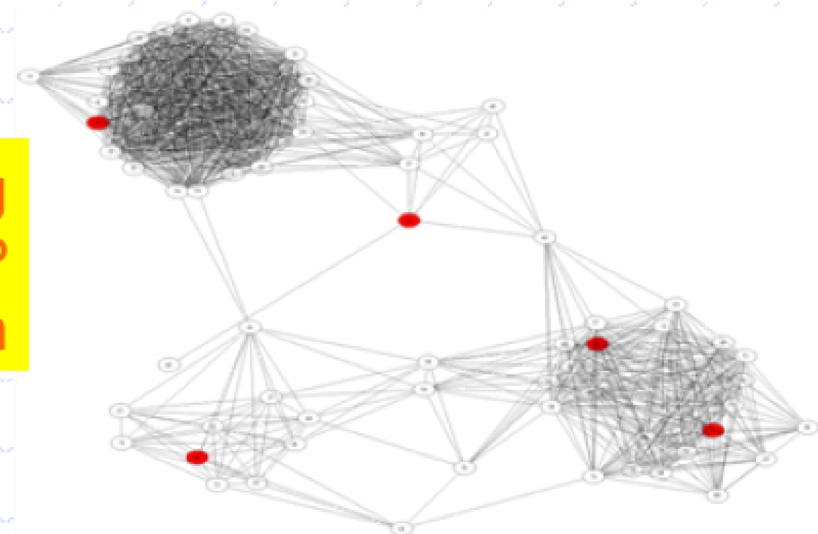
SPOT5 #509 (*Constraints* 4(3), 1999)

Mendelian Error Detection



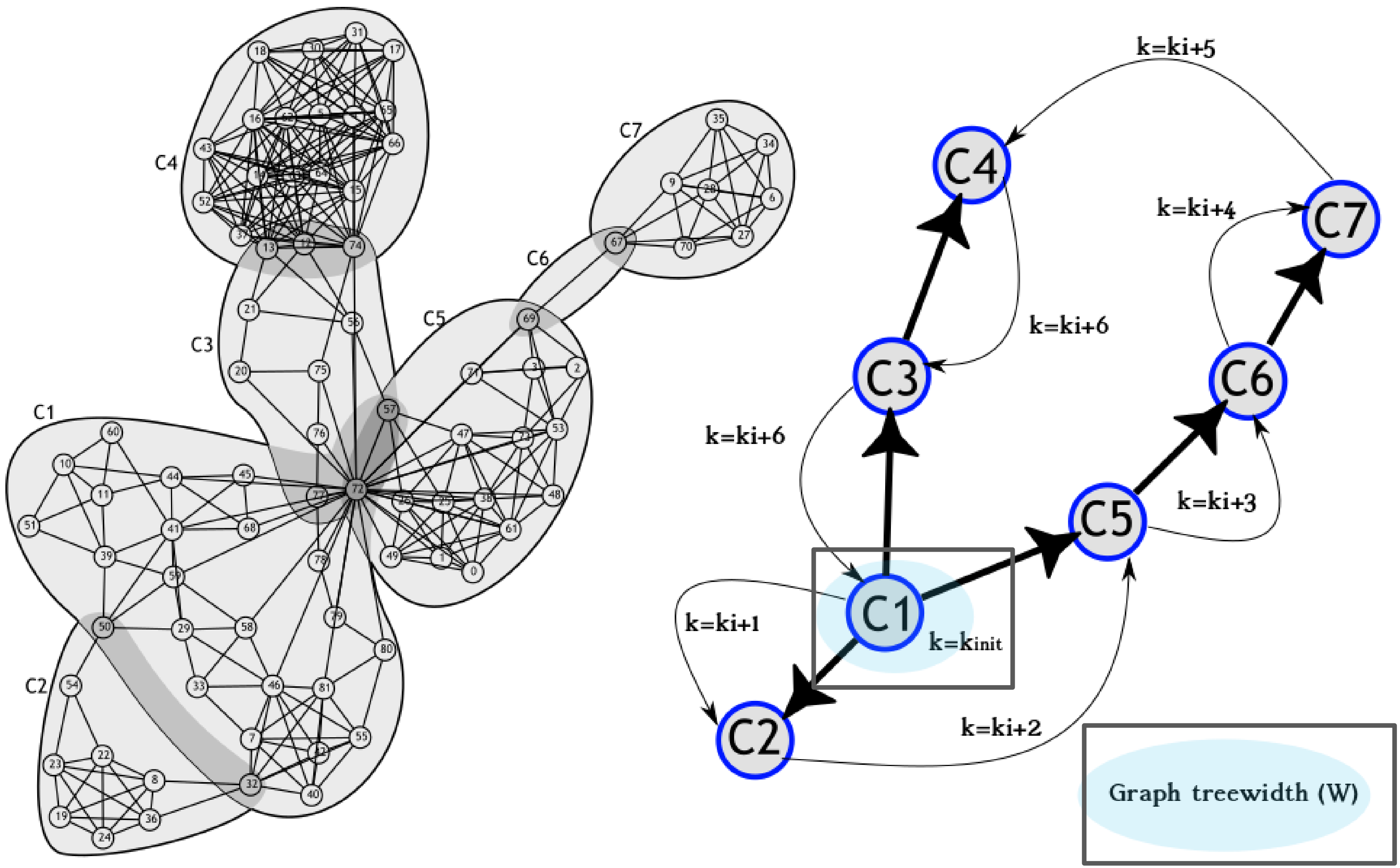
langladeM7 sheep pedigree
(*Constraints* 13(1), 2008)

Tag SNP Selection



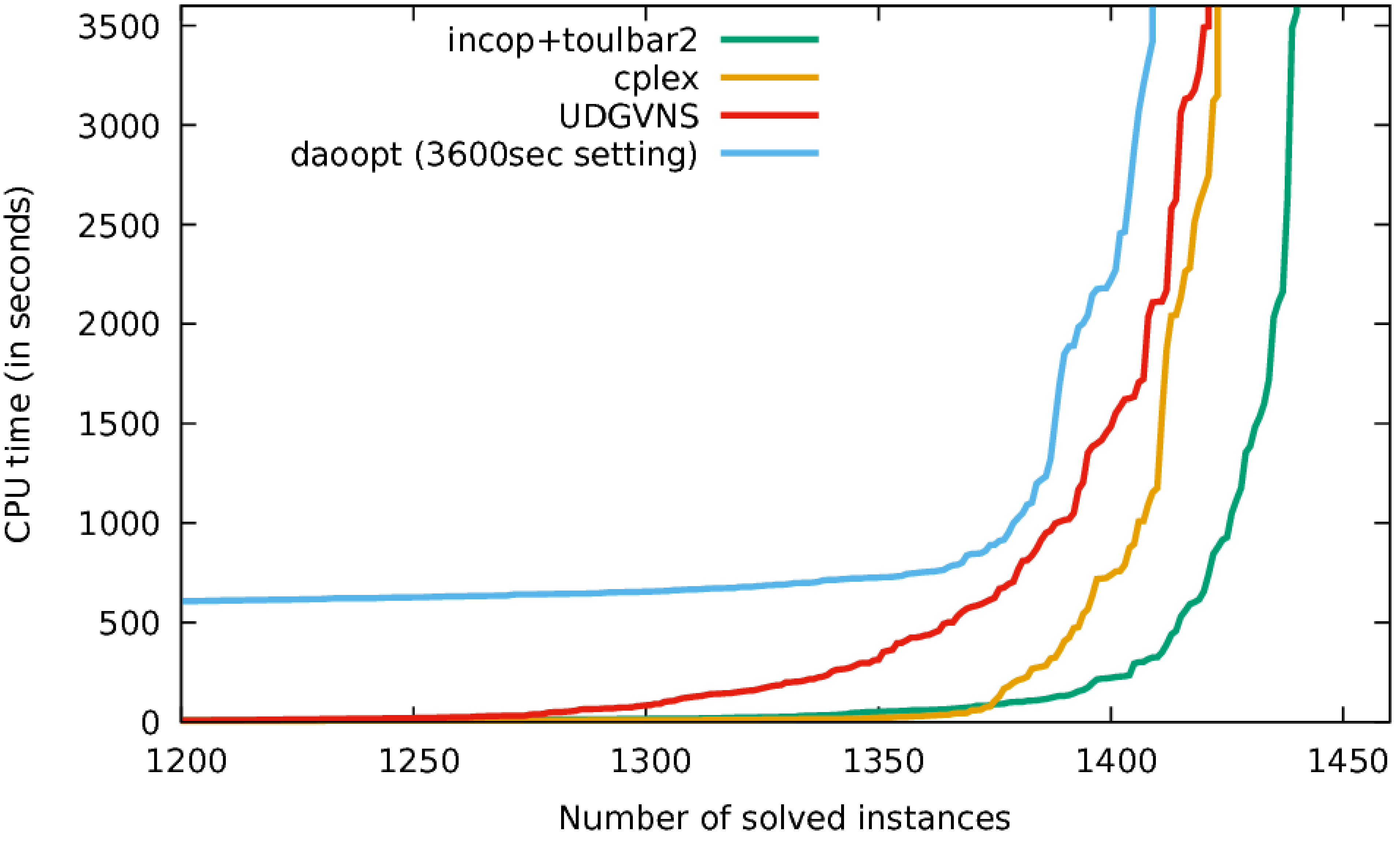
HapMap chr01 $r^2 \geq 0.8$ #14481
(*Bioinformatics* 22(2), 2006)

Cluster visit in a topological order :



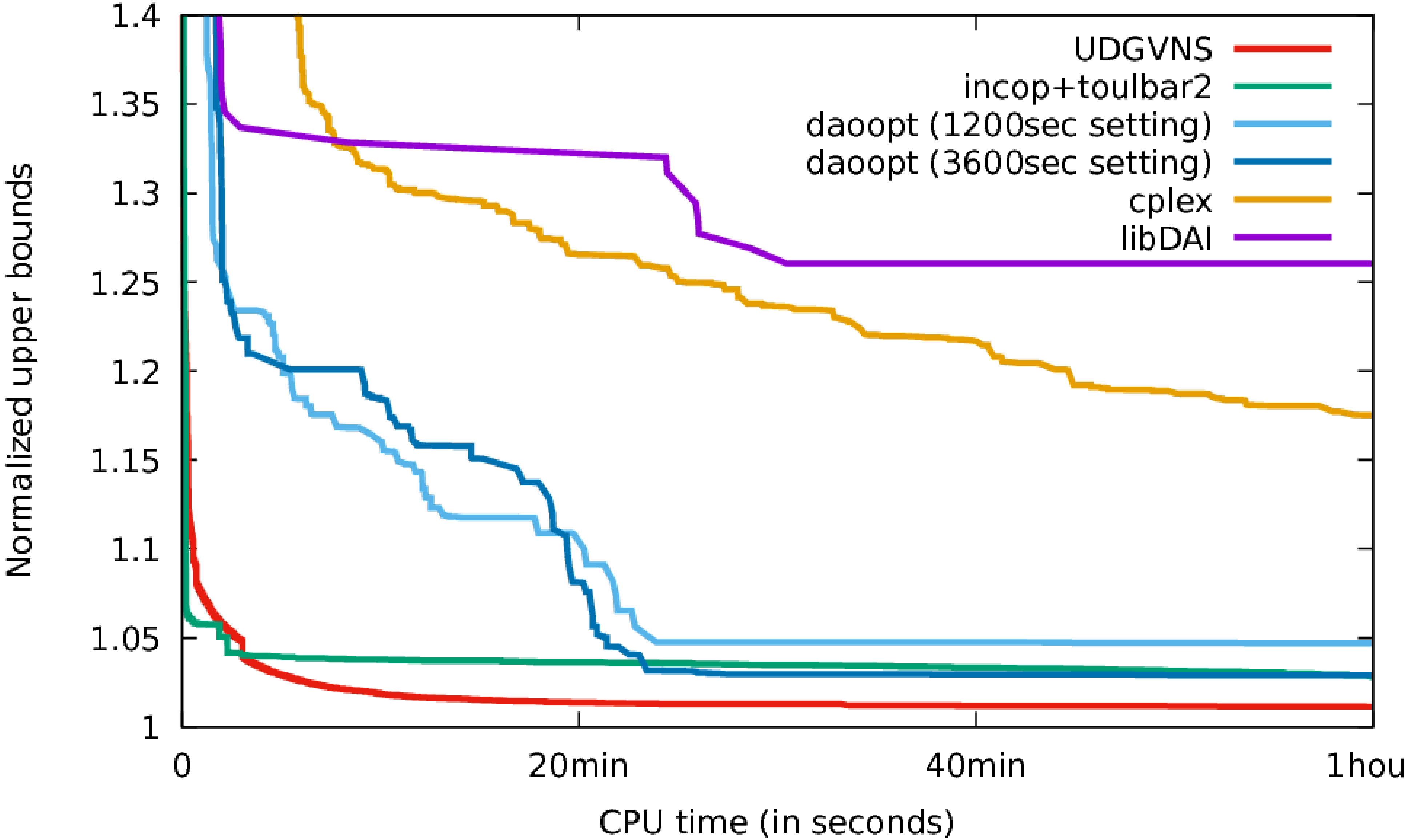
Results

(UAI17)



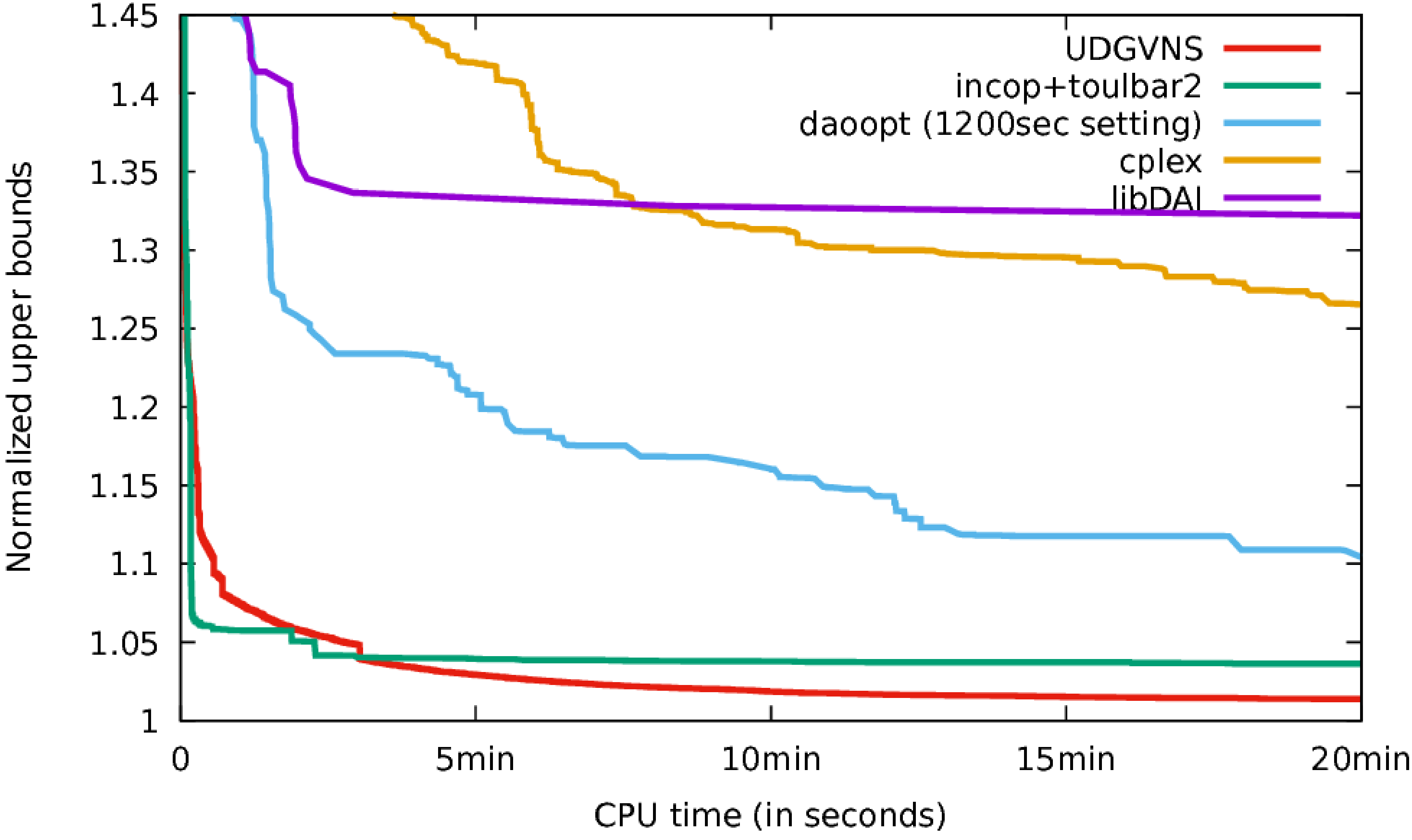
Results

(UAI17)

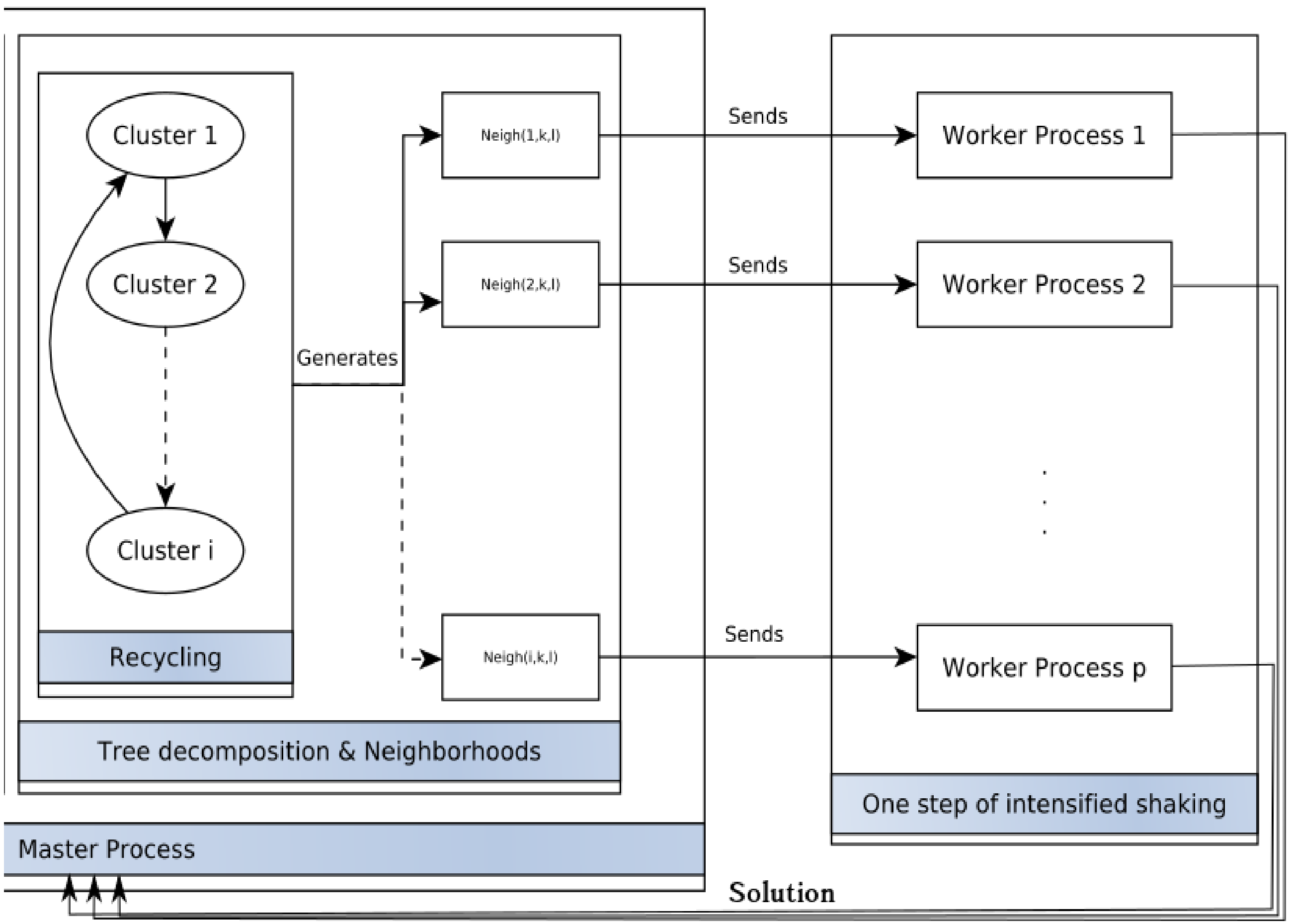


Results

(UAI17)



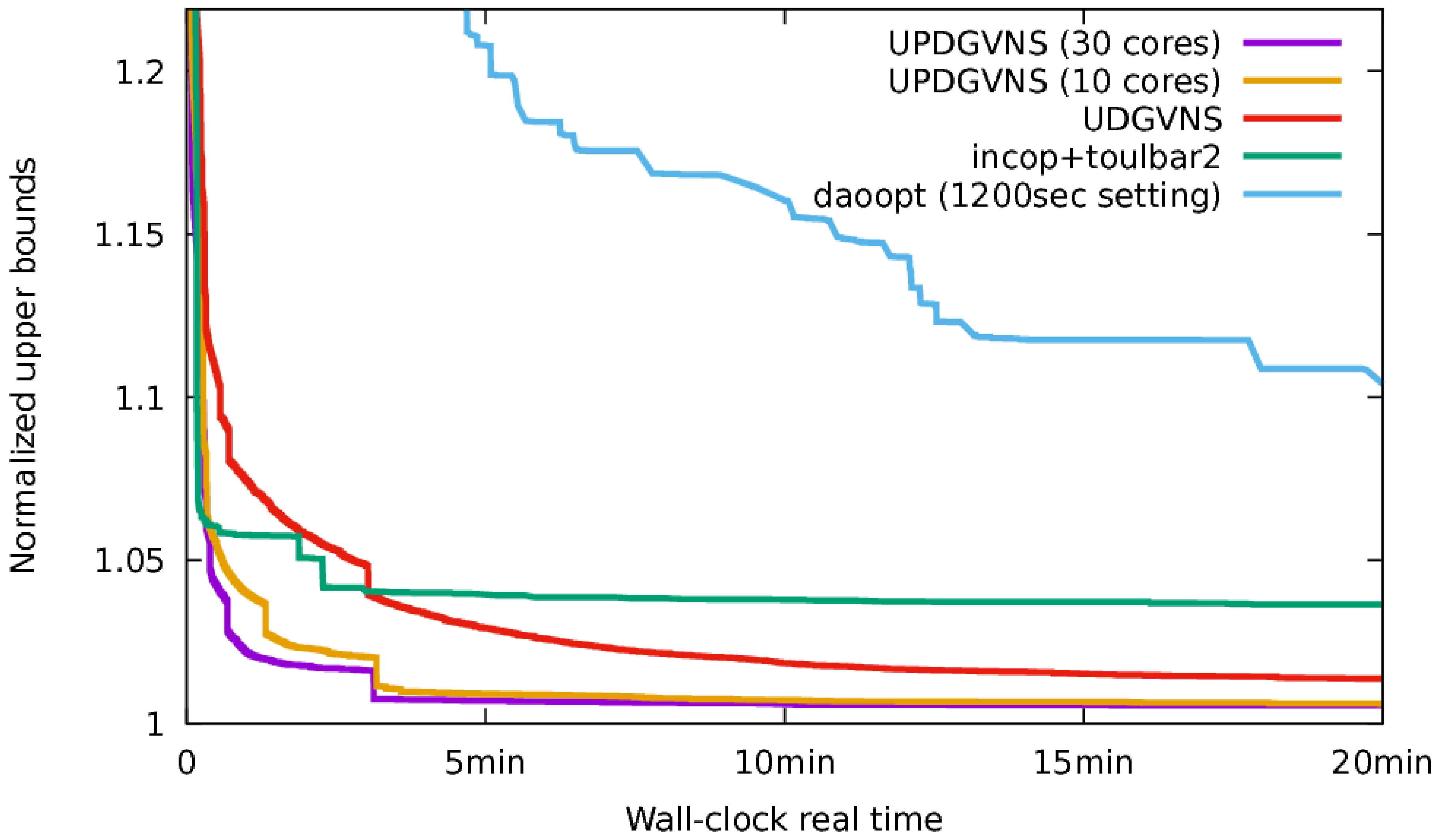
Parallel VNS



Unified Parallel Decomposition Guided VNS (UPDGVNS)

Results

(UAI17)



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https://github.com/toulbar2/toulbar2

debian