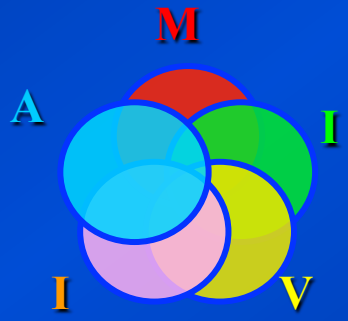


Graphs in Pattern Recognition
a one hour trip in the history

Prof. Mario Vento
University of Salerno

Outline

- Historical overview of GB methods in PR
  - The birth of graphs: promises and hopes
  - Pure Period: methods work in the graph space
    - Exact and inexact matching methods
    - Graph distance
  - Impure Period: fhe first steps toward vectors
  - Extreme Period: Graphs turn into vectors
- A brief survey of main methods and algorithms
- Conclusions and perspectives

The birth of graphs

Graphs vs Vectors

- SPR is based on a well founded mathematical framework: Vector Spaces
- Describing patterns by a vector of a set of measures has an immediate meaning
  - The pattern is a point in a Vector Space
  - (If the features are good) the distance of the points stands as a similarity measure between the corresponding patterns
  - Plenty of learning and classification methods

Are vectors really effective?

- The world is made of complex patterns
- Patterns generally contains subparts which are related each other
- Descriptions based on a set of features aren'effective: it is expected that the more complex an object is the more articulated its description be

Angela in a vector…
… and Silvio

How Similar are Silvio and Angela?

$d = 1.9$

F_W	F_H	M1
24.8	38.7	18.61

F_W	F_H	M1
25.2	39.5	20.33

From FV to Graphs

- … infact drawbacks pop up when the patterns have structural relationships
- … and statistical distribution of a feature set is not so effective to catch the differences
- CONS: Inadequacy to deal with the decomposition into parts

Graphs vs Vectors

- Graph-based representations decompose the object into parts
  - Single parts are individually described
  - Relations between the parts are represented
  - FV are added to edges and nodes
  - Different information for different nodes
- Object comparison exploits contextual knowledge (inside a single object)

Structural comparison

(Eye,black)

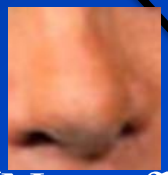
(Eye,black)

7.2

18.61

6.1

6.1



(Nose,flat)

3.1

(Lips,thin)

$d = 5.7$

(Eye,blue)

(Eye,blue)

8.9

7.3

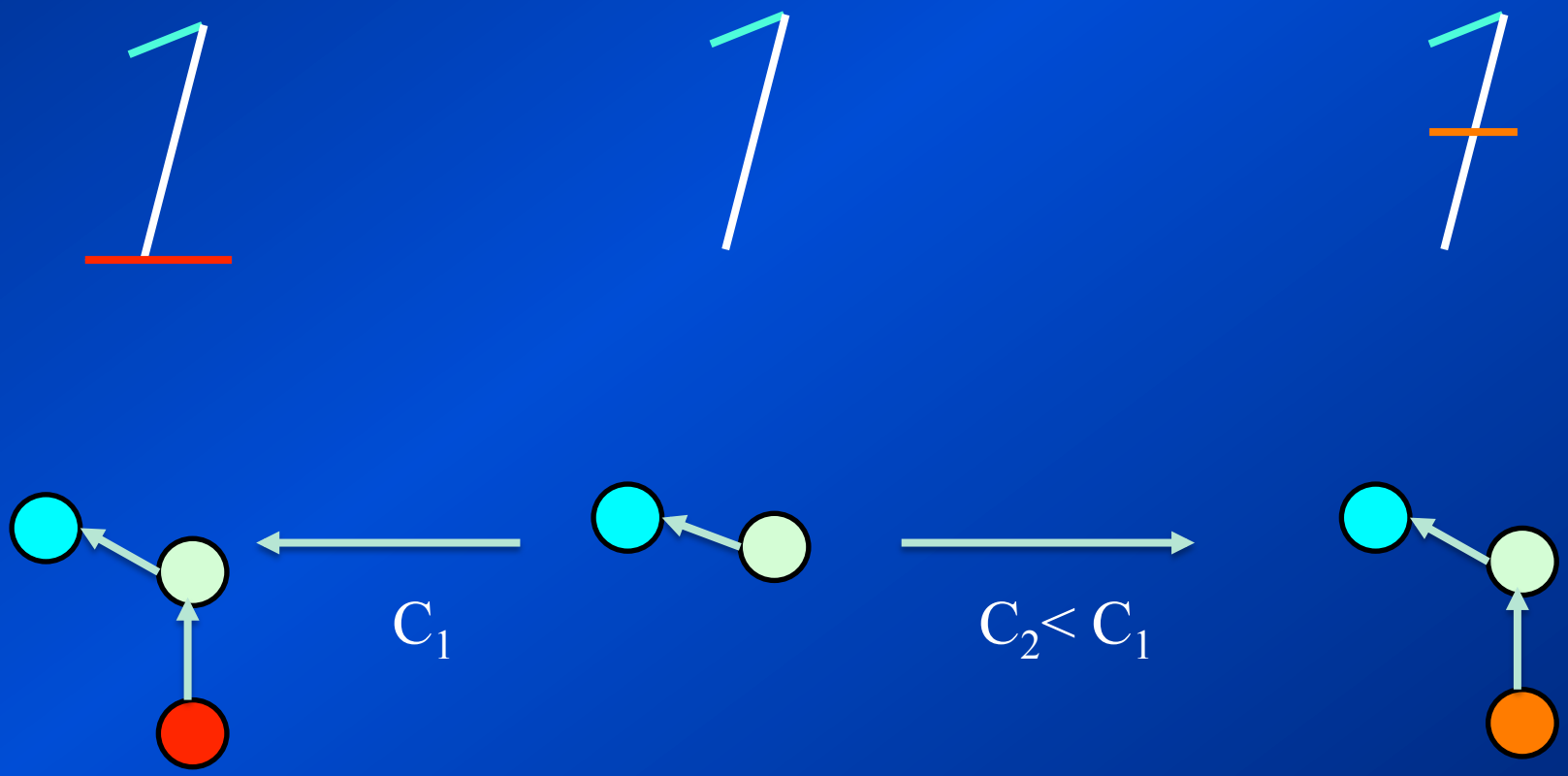
7.3

(Nose,flat)

3.8

(Lips,pulpy)

Preserving the semantic value of the context



Pure Methods

Working into “pure” graph domain

- Graph Comparison: compatibility between the structure of the input patterns
  - Morphism between graph structures
  - Node and Edge compatibilities
- Symbolic graph prototypes:
  - Manually
  - Learned automatically ??

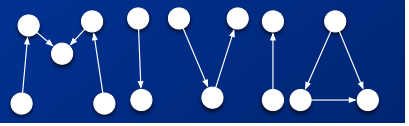
Exact Graph Matching

- Mapping between the nodes of two graphs:
  - edge-preserving: if two nodes in the first graph are linked by an edge, the corresponding nodes of the second graph must have an edge too
  - satisfying some general constraints:
    - Isomorphism
    - Sub graph isomorphism
    - Monomorphism
    - Homomorphism

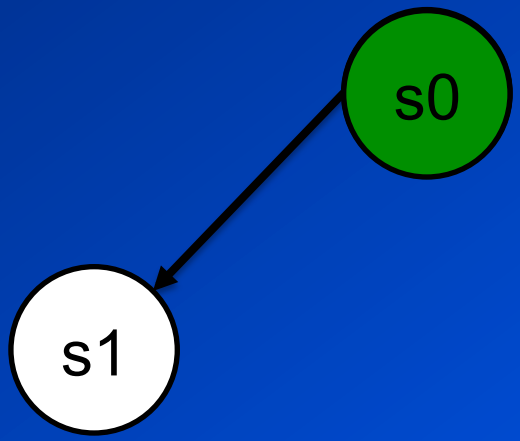
Exact Graph Matching
Optimal, Tree based Search

EGM: Tree Search

- Use of State Space Representation (SSR): Each state represents a Partial Match (consistent with the matching type)
- A partial match is iteratively expanded by adding to it new pairs of matched nodes.
- The candidate pair to add, is chosen using some necessary conditions ensuring its consistency with the matching type.
- Use some heuristic condition to prune as early as possible unfruitful search paths.

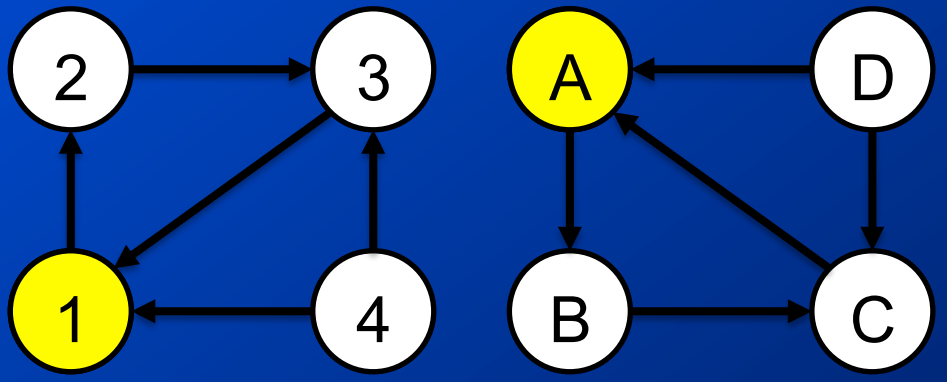


EGM: Tree Search Example

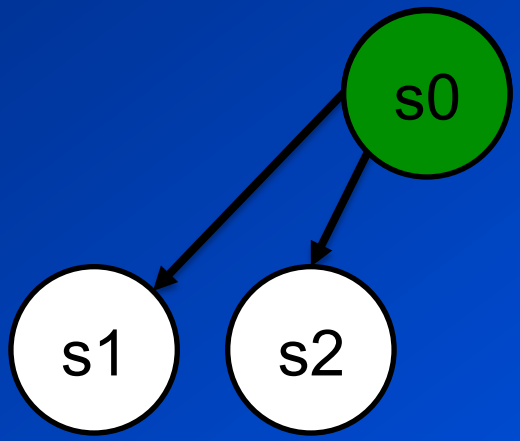


M(s0) = {}

M(s1) = {(1,A)}



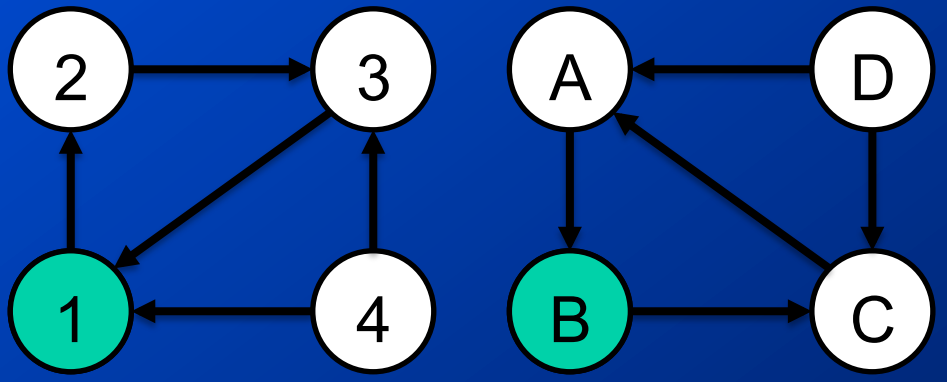
EGM: Tree Search Example



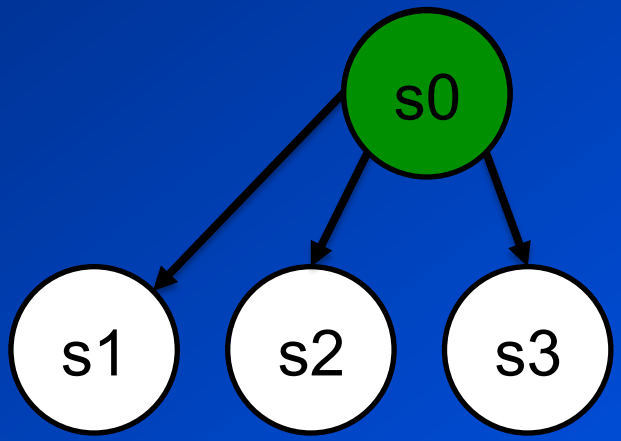
M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,B)}



EGM: Tree Search Example

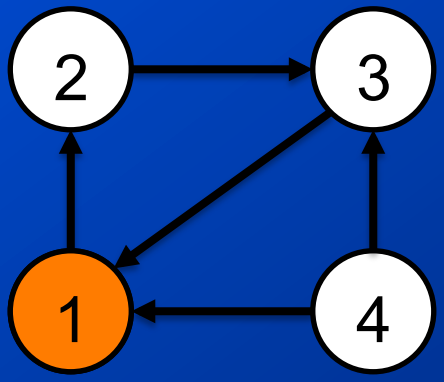


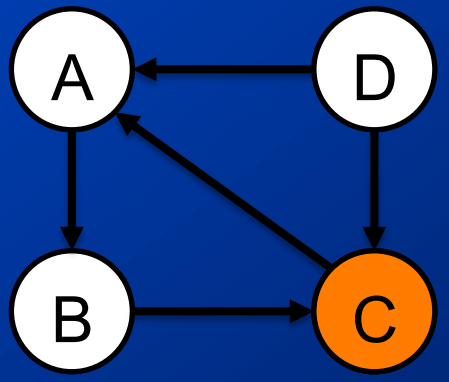
M(s0) = {0}

M(s1) = {(1,A)}

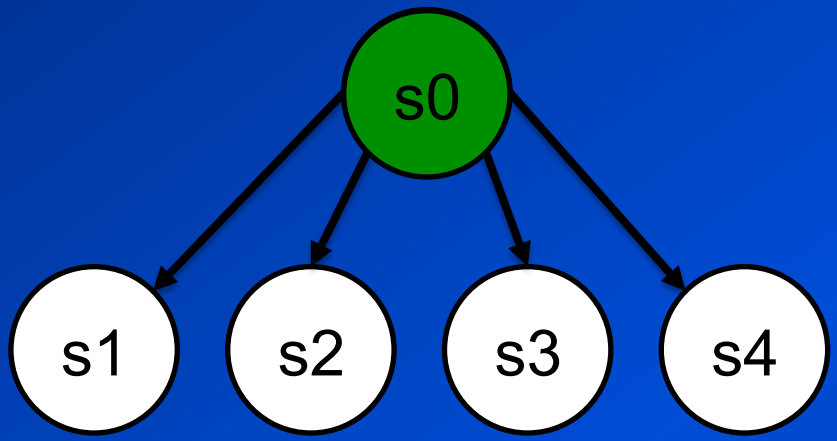
M(s2) = {(1,B)}

M(s3) = {(1,C)}





EGM: Tree Search Example



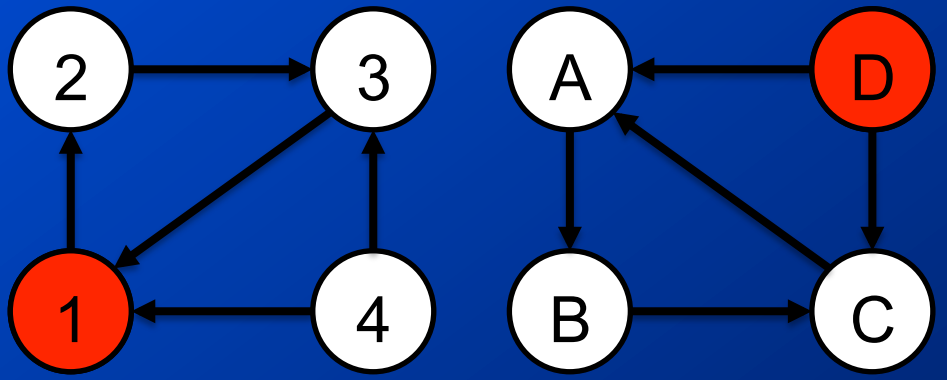
M(s0) = {0}

M(s1) = {(1,A)}

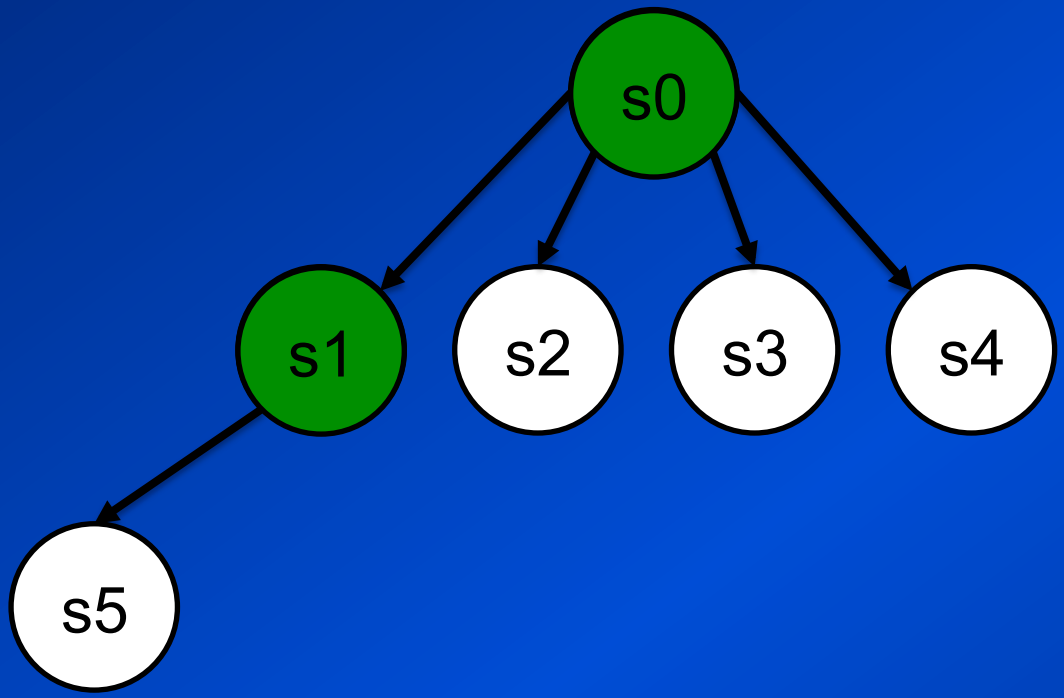
M(s2) = {(1,B)}

M(s3) = {(1,C)}

M(s4) = {(1,D)}



EGM: Tree Search Example



M(s0) = {0}

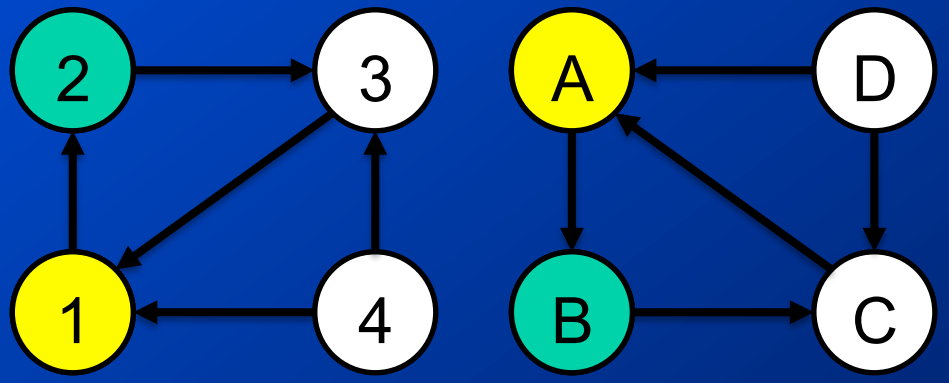
M(s1) = {(1,A)}

M(s2) = {(1,B)}

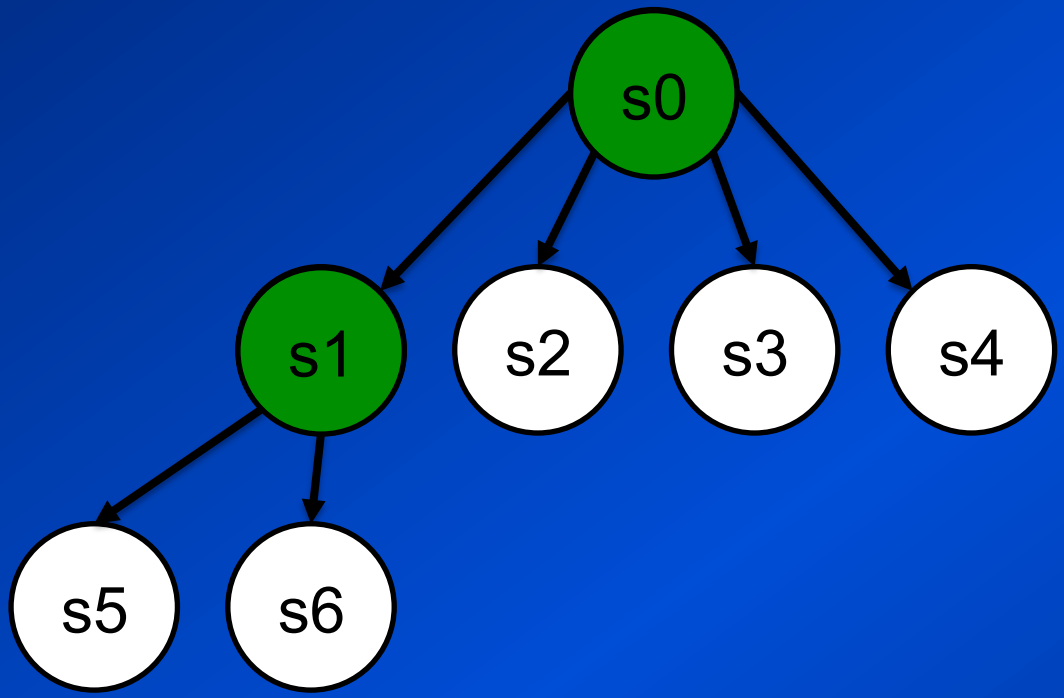
M(s3) = {(1,C)}

M(s4) = {(1,D)}

M(s5) = {(1,A) , (2,B)}



EGM: Tree Search Example



M(s0) = {0}

M(s1) = {(1,A)}

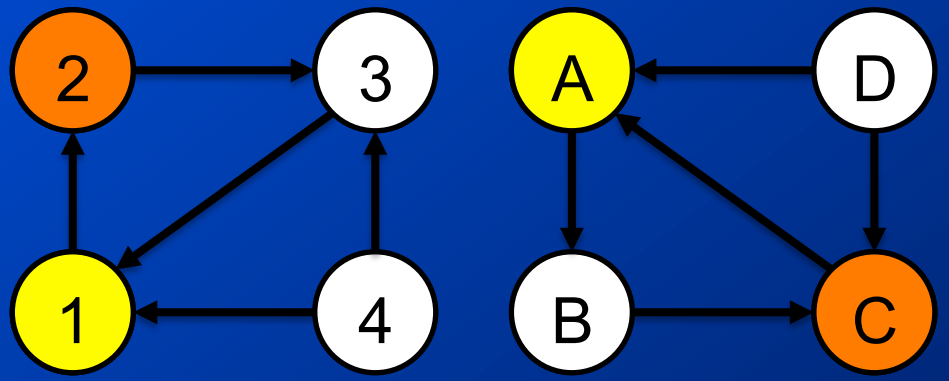
M(s2) = {(1,B)}

M(s3) = {(1,C)}

M(s4) = {(1,D)}

M(s5) = {(1,A) , (2,B)}

M(s6) = {(1,A) , (2,C)}



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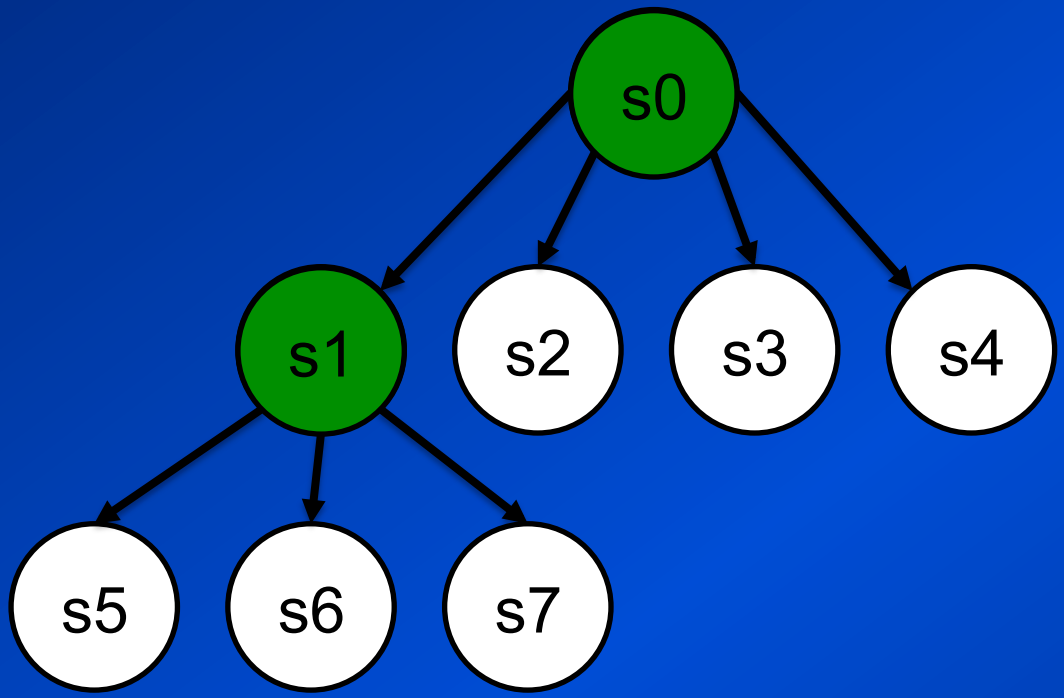


M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,B)}

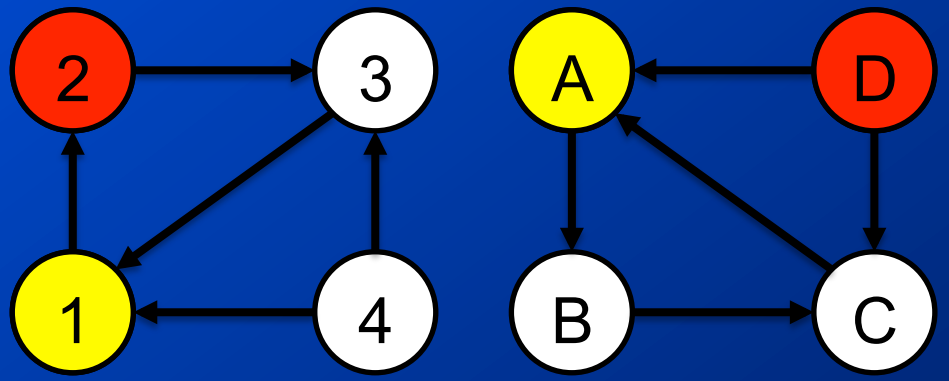
M(s3) = {(1,C)}

M(s4) = {(1,D)}

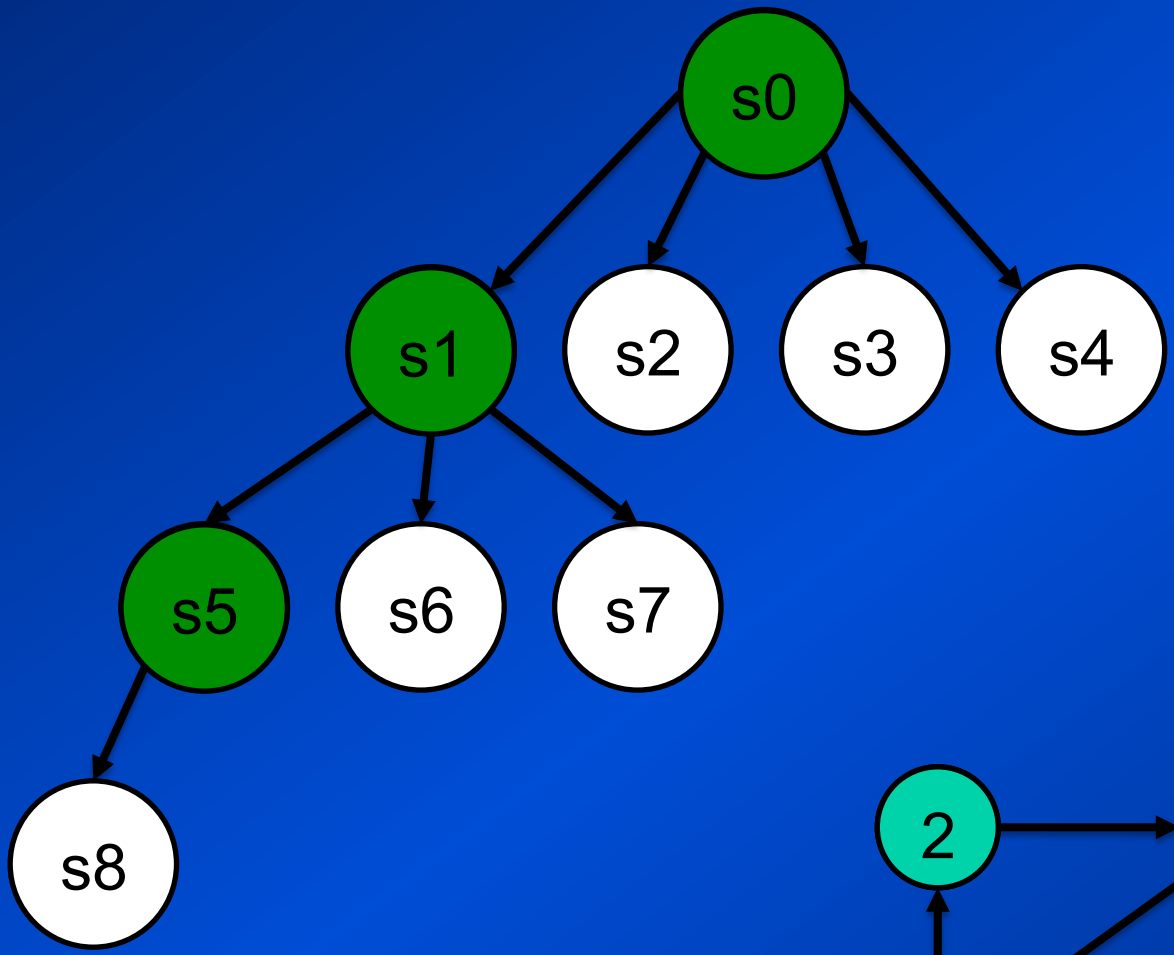
M(s5) = {(1,A) , (2,B)}

M(s6) = {(1,A) , (2,C)}

M(s7) = {(1,A) , (2,D)}



EGM: Tree Search Example



M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,B)}

M(s3) = {(1,C)}

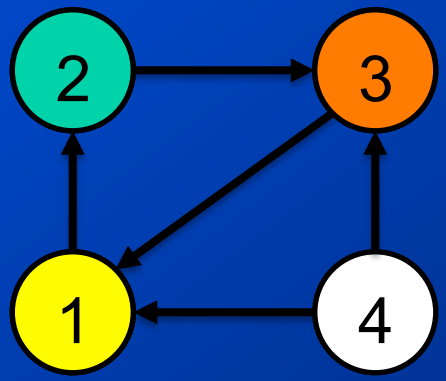
M(s4) = {(1,D)}

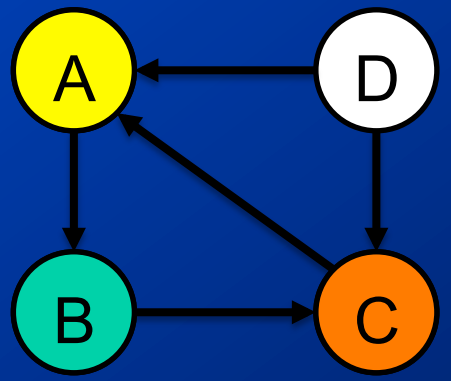
M(s5) = {(1,A) , (2,B)}

M(s6) = {(1,A) , (2,C)}

M(s7) = {(1,A) , (2,D)}

…





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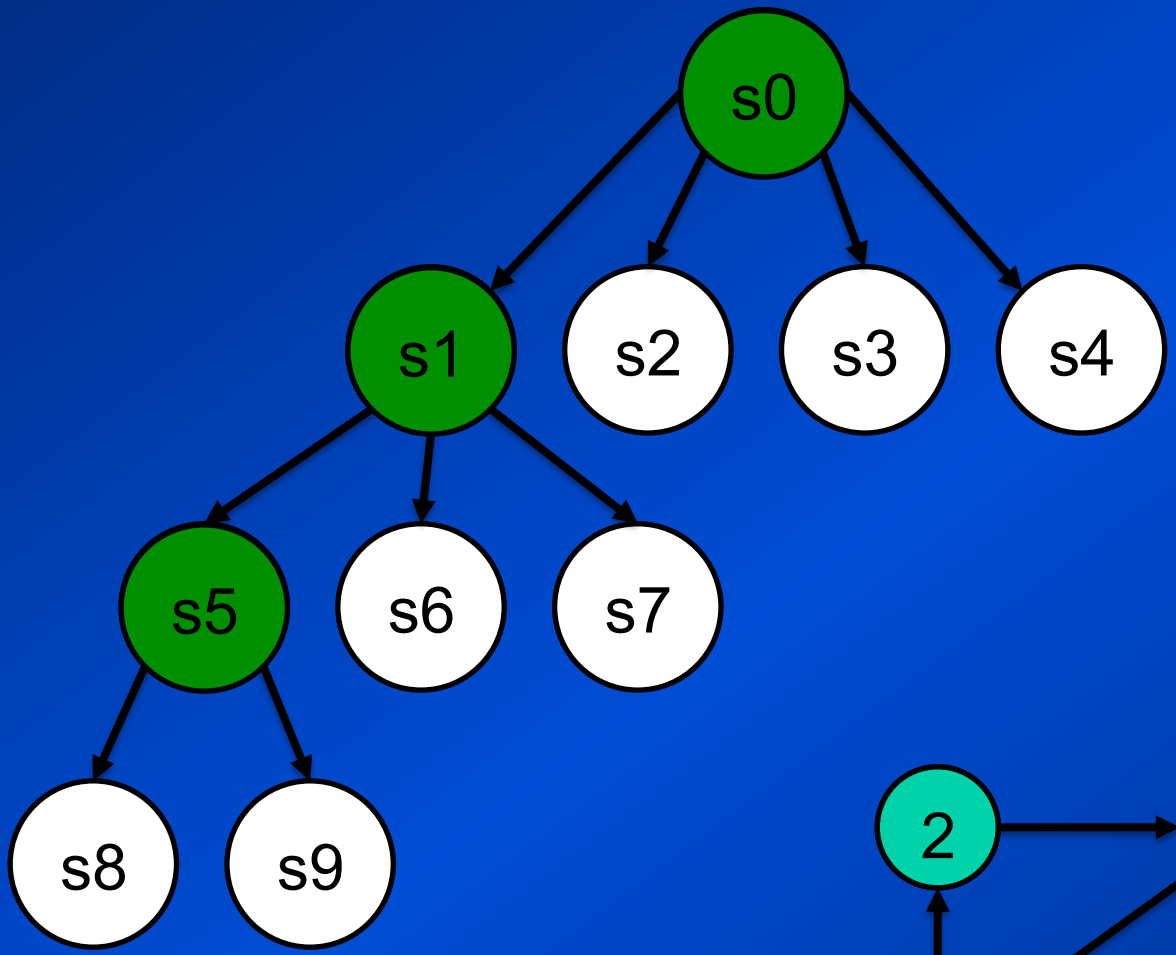


M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,B)}

M(s3) = {(1,C)}

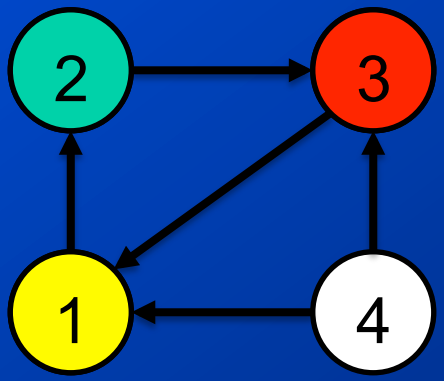
M(s4) = {(1,D)}

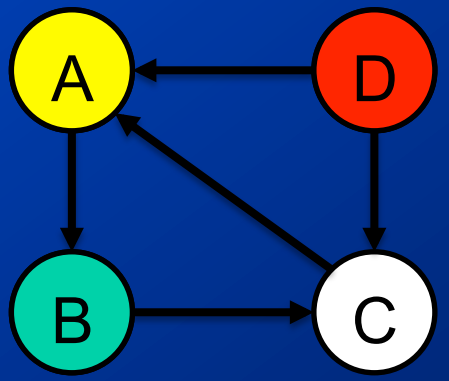
M(s5) = {(1,A) , (2,B)}

M(s6) = {(1,A) , (2,C)}

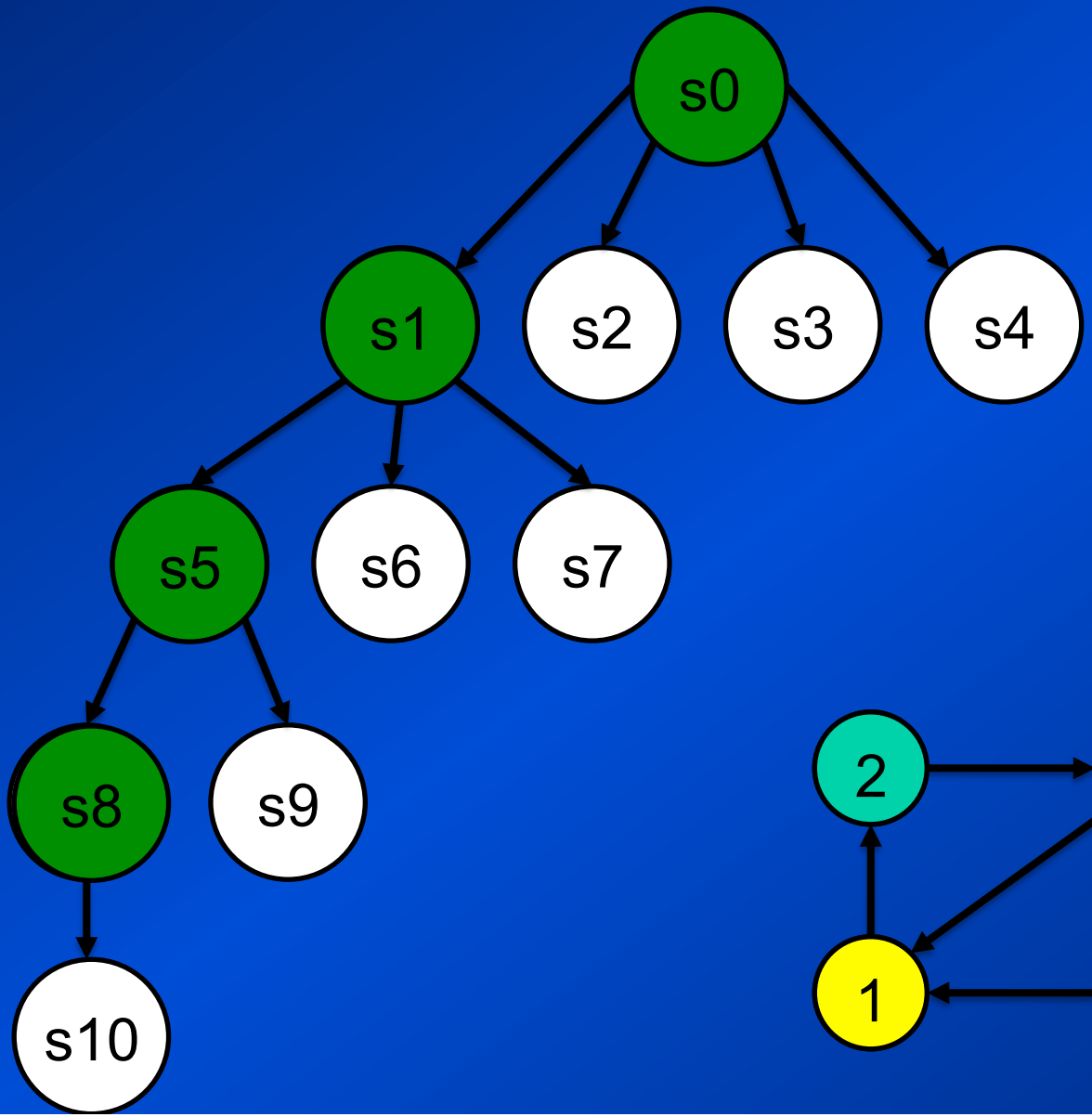
M(s7) = {(1,A) , (2,D)}

…





EGM: Tree Search Example



M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,B)}

M(s3) = {(1,C)}

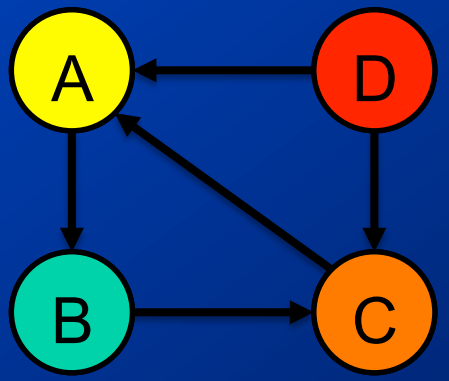
M(s4) = {(1,D)}

M(s5) = {(1,A) , (2,B)}

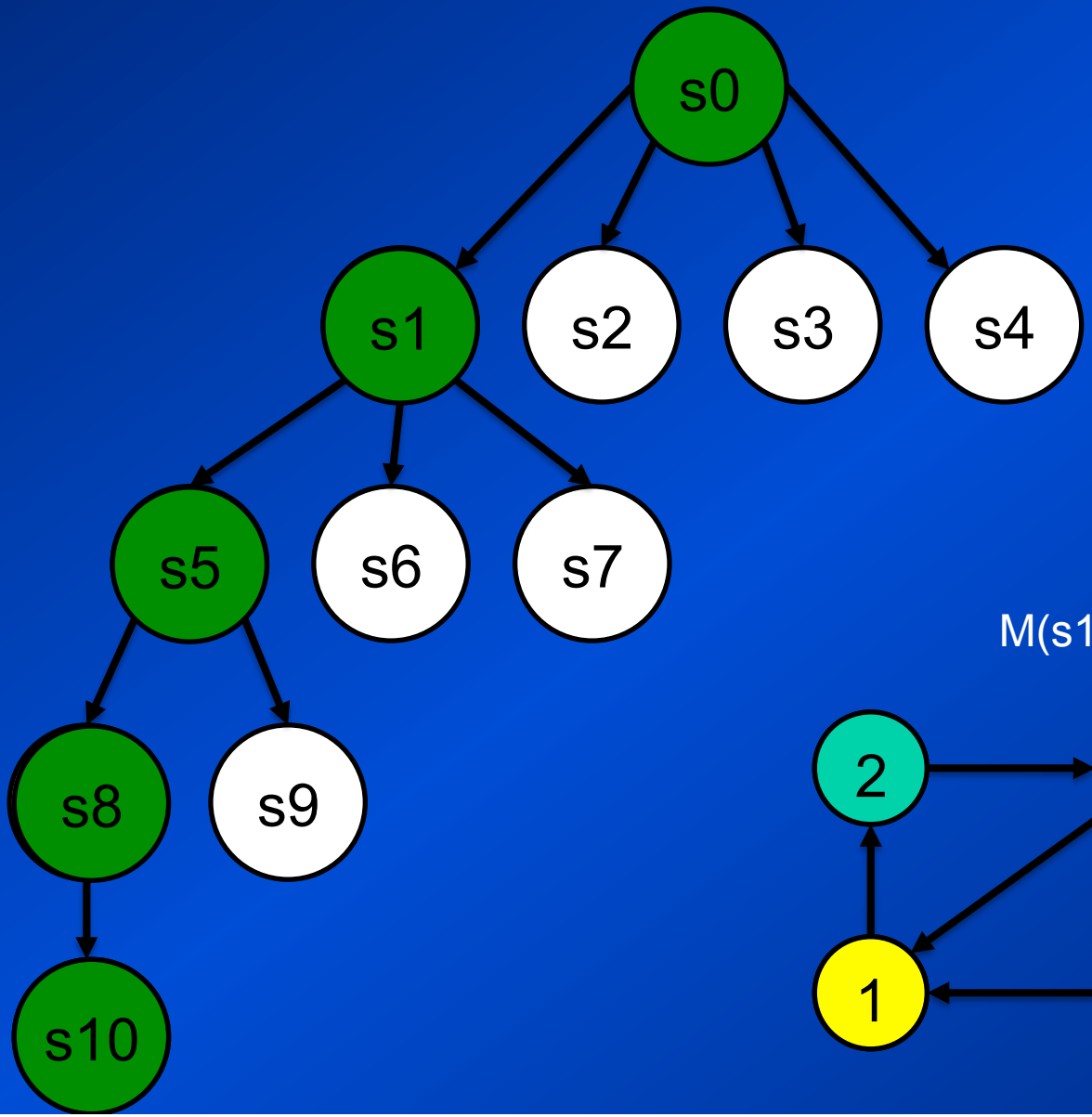
M(s6) = {(1,A) , (2,C)}

M(s7) = {(1,A) , (2,D)}

…



EGM: Tree Search Example



M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,B)}

M(s3) = {(1,C)}

M(s4) = {(1,D)}

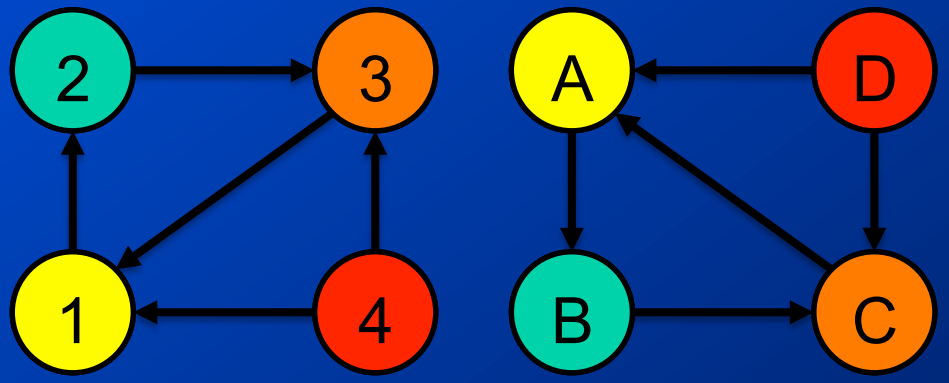
M(s5) = {(1,A) , (2,B)}

M(s6) = {(1,A) , (2,C)}

M(s7) = {(1,A) , (2,D)}

…

M(s10) = {(1,A) , (2,B) , (3,C) , (4,D)}



EGM: Tree Search

- For each couple of nodes requires additional time for feasibility
- But feasibility rules allow the pruning
- The more asymmetric is the graph the more is the reduction of the matching time

Ullmann's algorithm (1976)

- Based on tree search with backtracking
- Finds isomorphism and subgraph isomorphism
- Pruning by a bit matrix M for each state
- Mij=1 iff the matching of ni and nj is possible

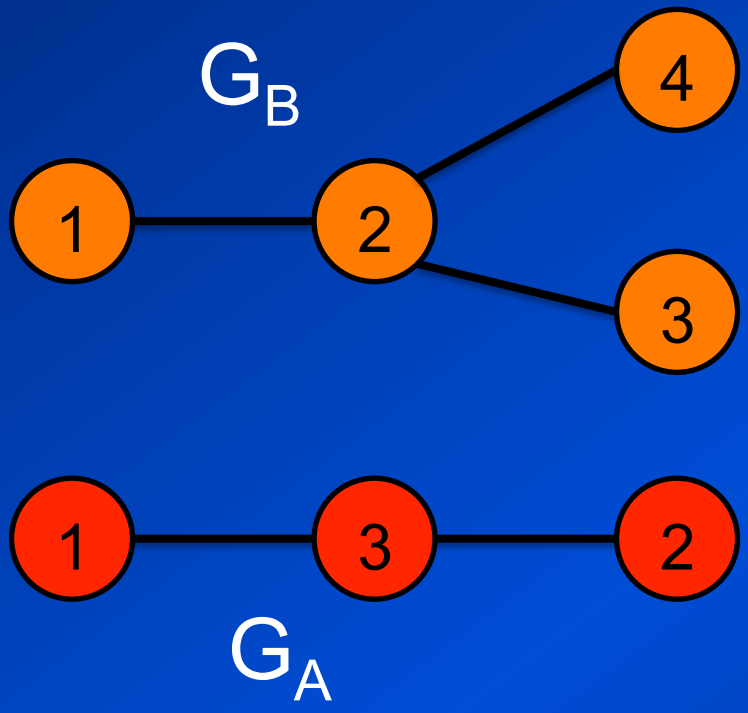
Refinement: delete 1's from M of the current state

Then, the state is extended using the node pairs corresponding to the remaining 1's

Ullmann's refinement procedure

1. For each (i,j) such as Mij = 1,
   - For each x such as (i, x) is an edge of G1,
   - if there is at least one y compatible with x (Mxy = 1) and with a corresponding edge, i.e. (j, y) is an edge of G2
     - THEN Mij remains unchanged
     - ELSE Mij is set to 0
2. Repeat until M remains unchanged

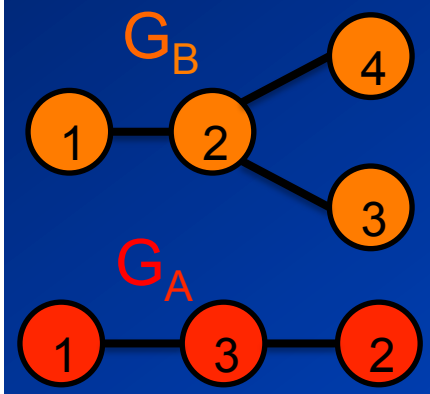
1. Ullmann (1976)



	1	2	3	4
1	1	0	0	0
2	0	0	1	0
3	0	1	0	0

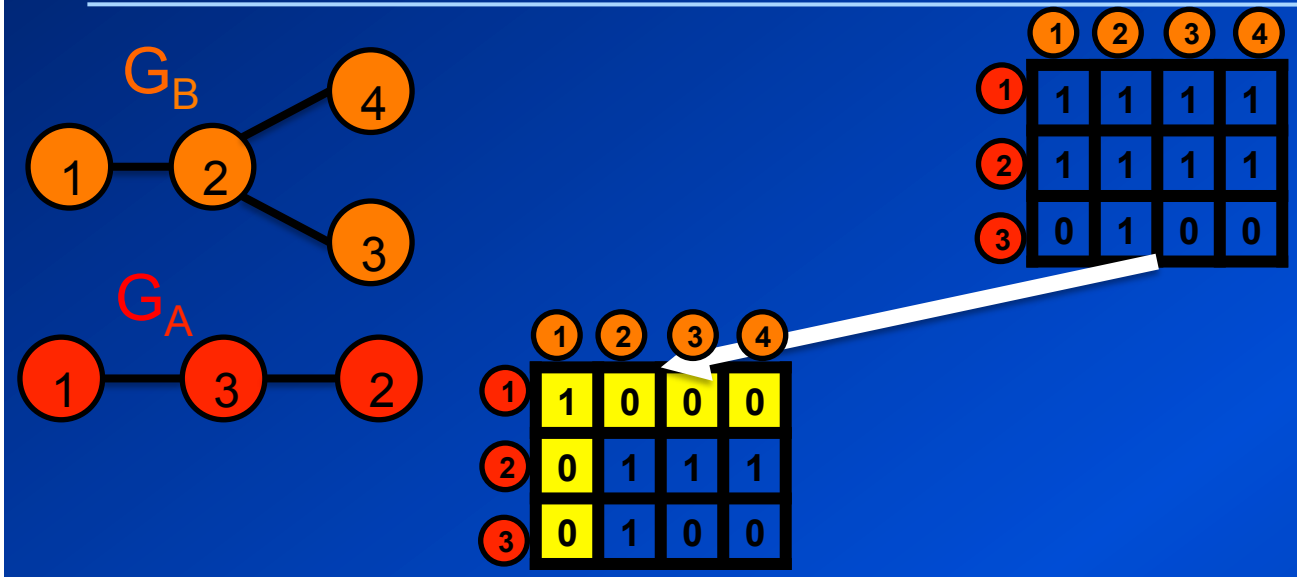
M=?

Is Ga isomorphic to a subgraph of Gb?



	1	2	3	4
1	1	1	1	1
2	1	1	1	1
3	0	1	0	0

$$M_{ij}^0 = \begin{cases} 1 & if \quad deg(B_j) \geq deg(A_i) \\ 0 & \text{otherwise} \end{cases} \quad , \forall i,j$$


G_B
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G_A
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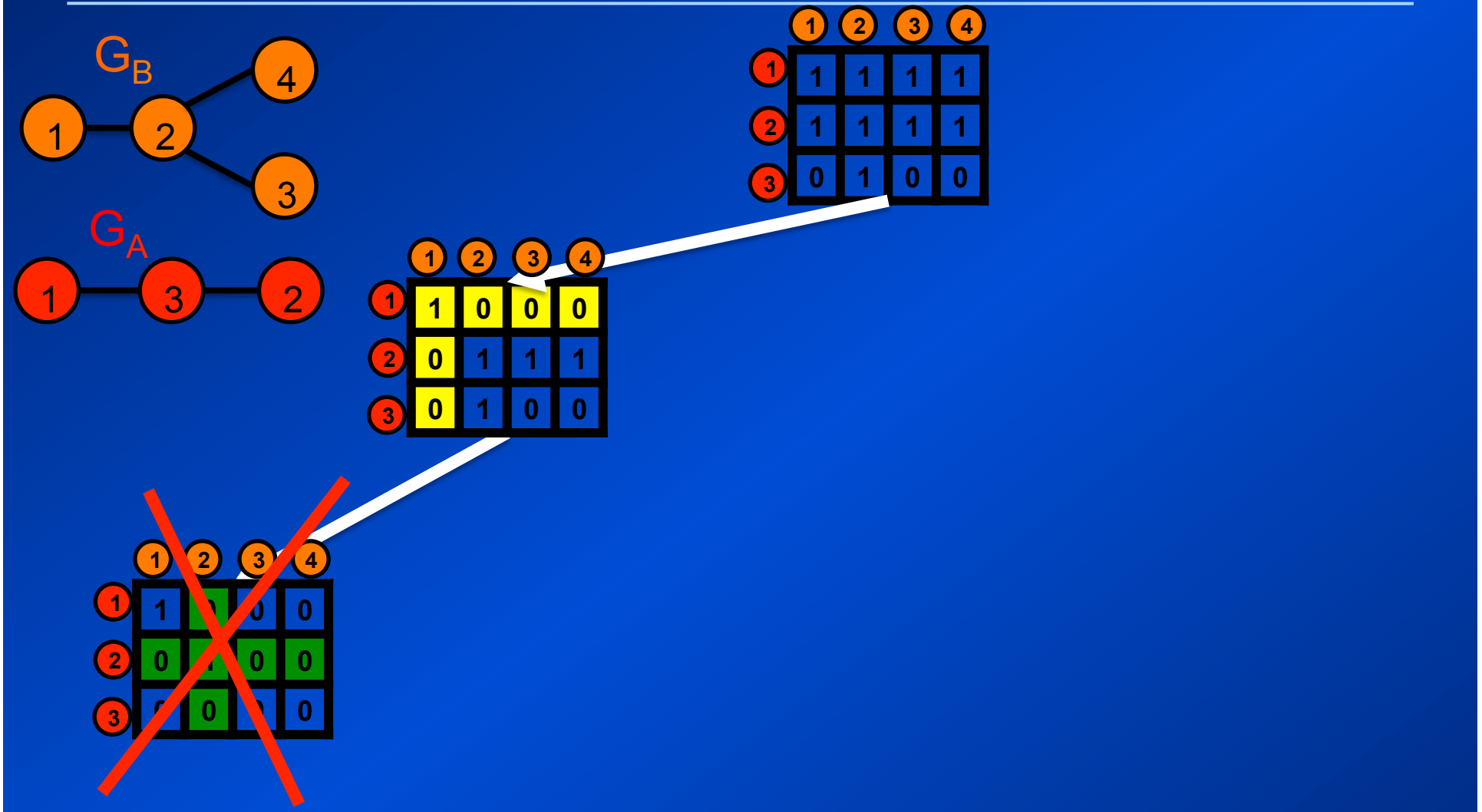
1 1 1 1
2 1 1 1 1
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 1 1 1
3 0 1 0 0


G_B
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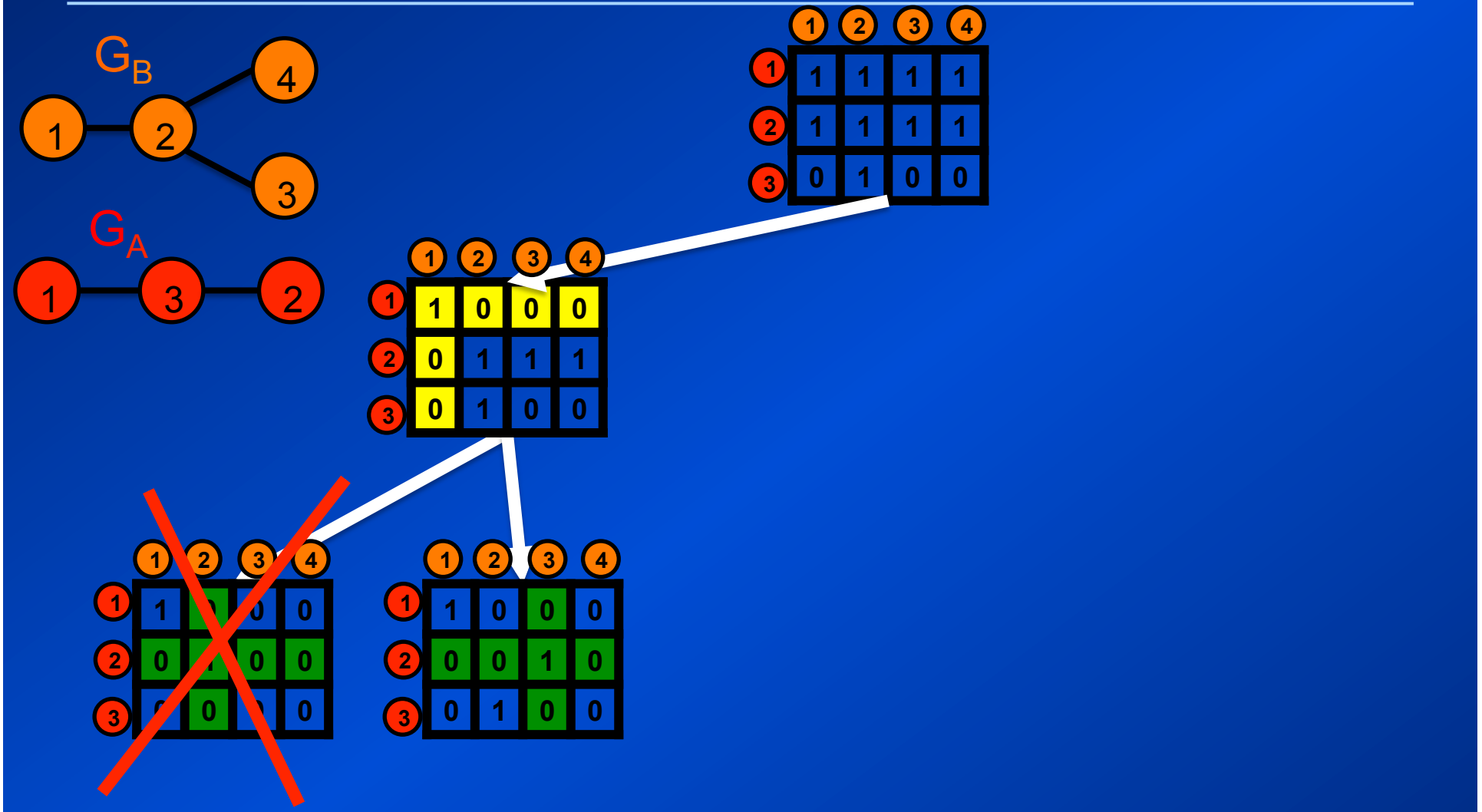
1 1 1 1 1
2 1 1 1 1
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 1 1 1
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 1 0 0
3 0 0 0


G_B
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G_A
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1 2 3 4
1 1 1 1 1
2 1 1 1 1
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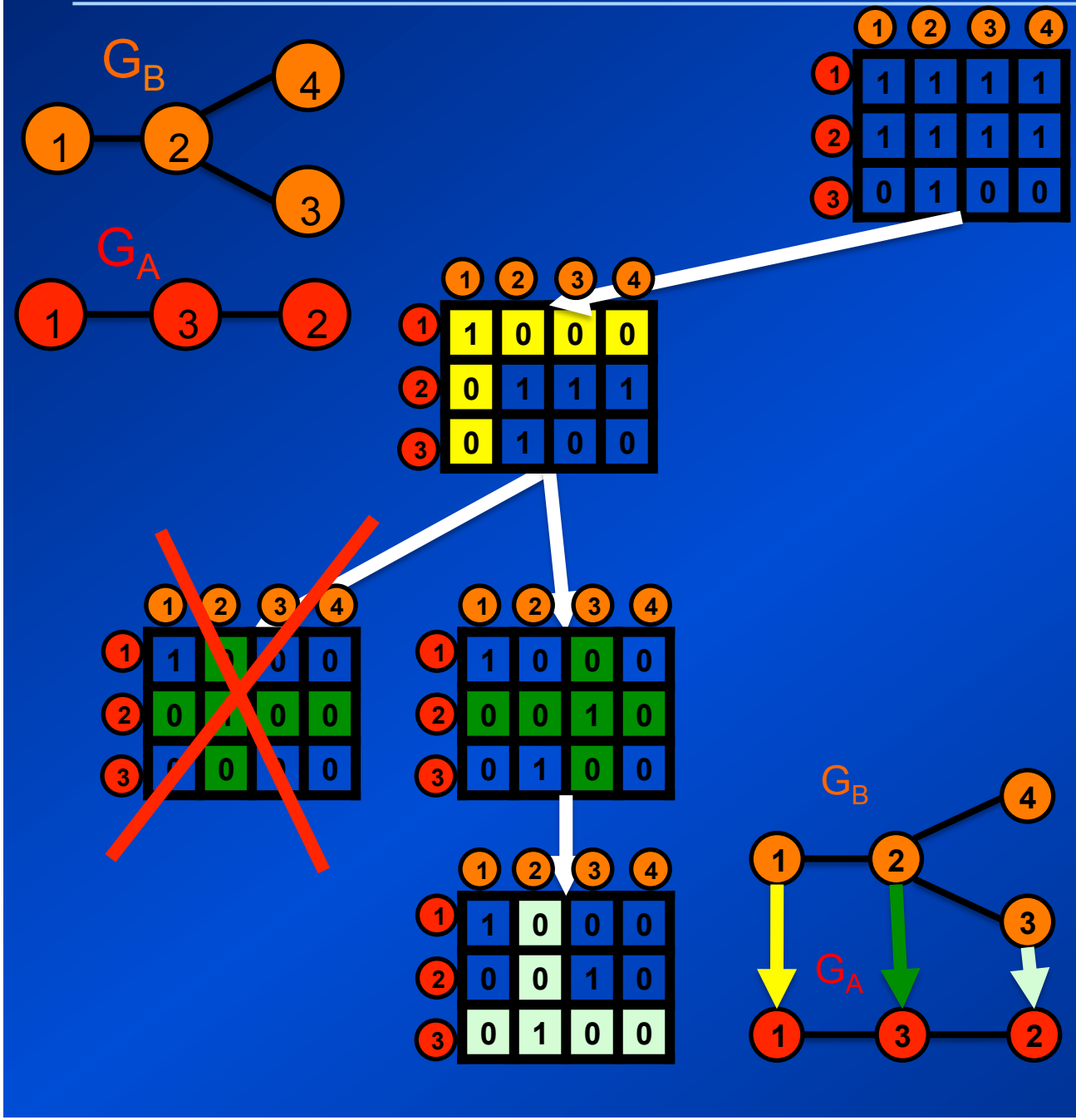
1 2 3 4
1 1 0 0 0
2 0 1 1 1
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 0 1 0
3 0 1 0 0


G_B
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G_A
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3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 1 1 1
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 0 1 0
3 0 1 0 0
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G_B
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G_A
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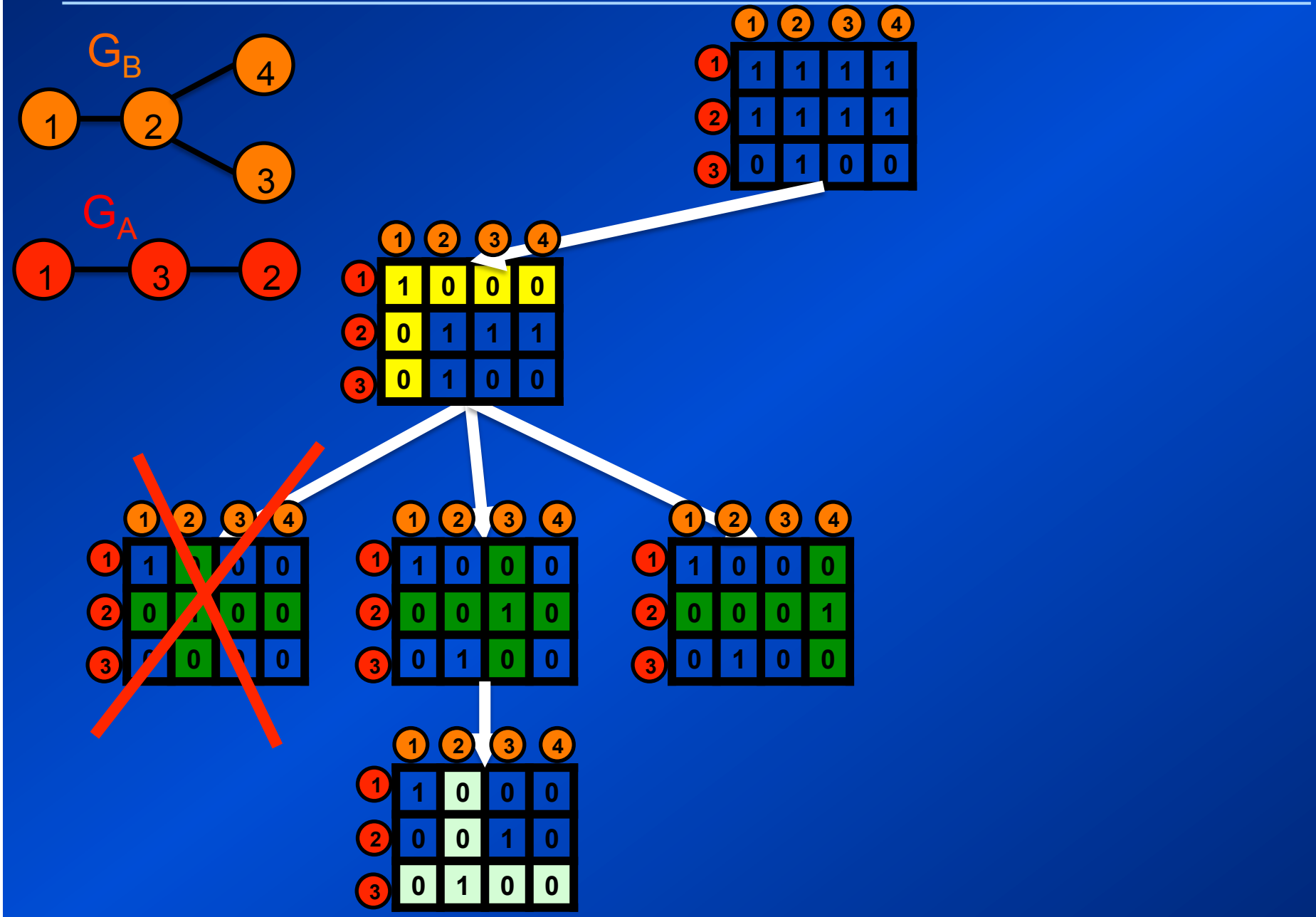
G_B
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G_A
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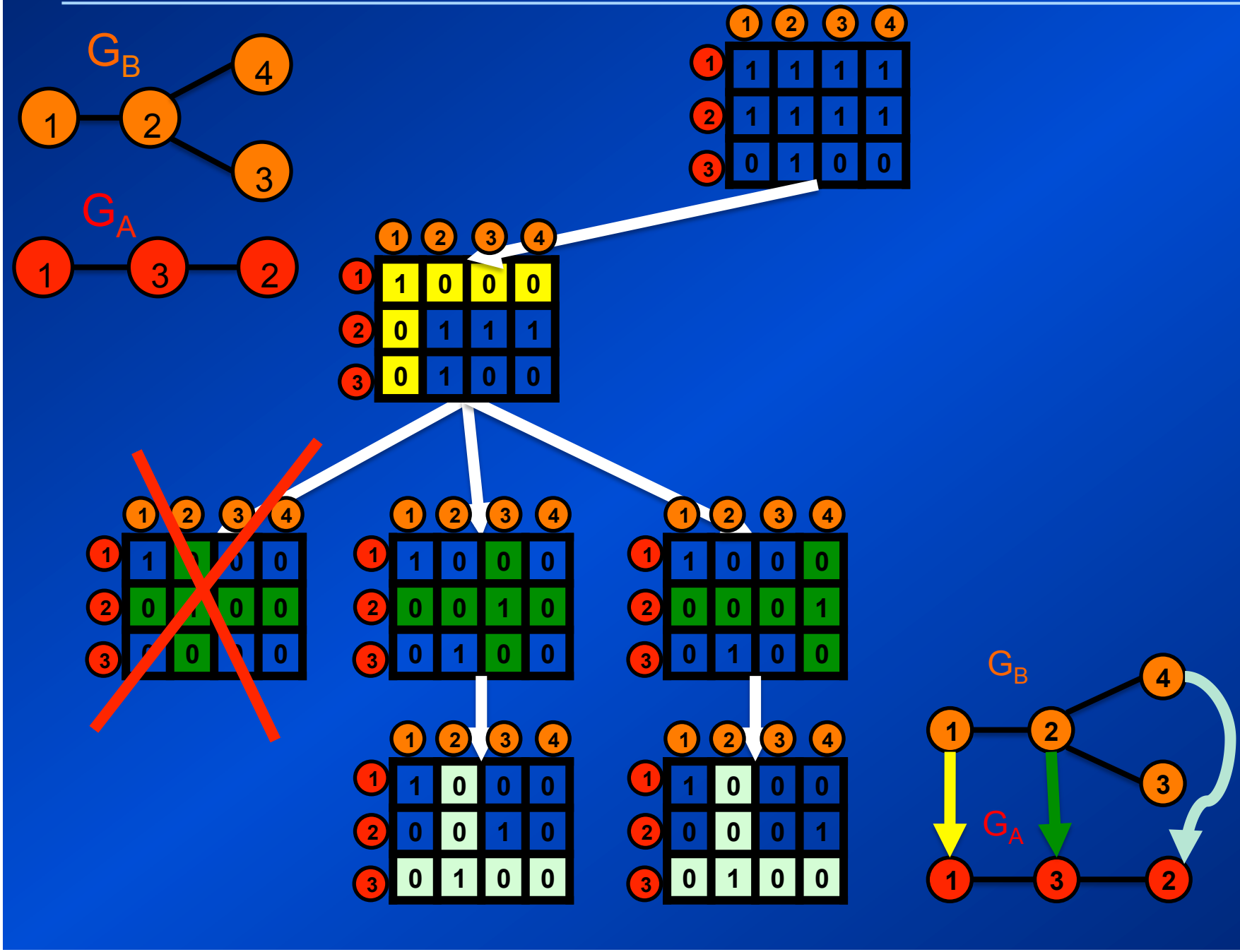
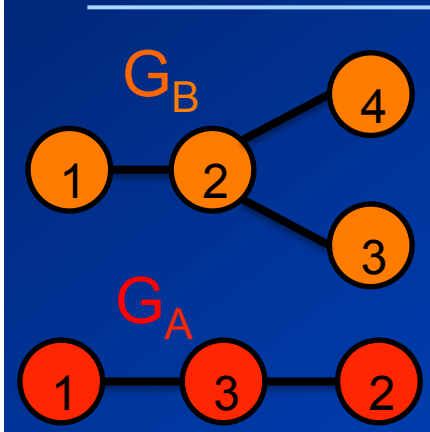
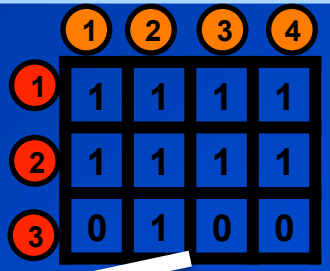
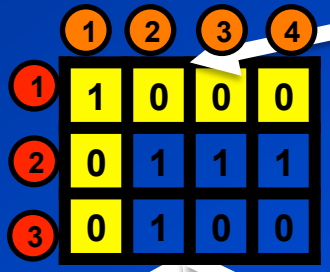
1 2 3 4
1 1 1 1 1
2 1 1 1 1
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 1 1 1
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 0 1 0
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 0 0 1
3 0 1 0 0
1 2 3 4
1 1 0 0 0
2 0 0 1 0
3 0 1 0 0


G_B
G_A
1 2 3 4
1 1 1 1 1
2 1 1 1 1
3 0 1 0 0
1 0 0 0
0 1 1 1
0 1 0 0
1 0 0 0
0 0 1 0
0 1 0 0
1 0 0 0
0 0 0 1
0 1 0 0
1 0 0 0
0 0 1 0
0 1 0 0
1 0 0 0
0 0 0 1
0 1 0 0
G_B
G_A

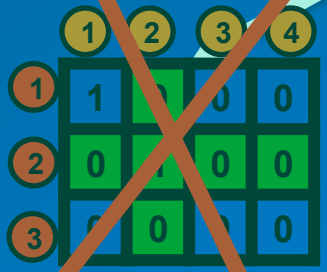


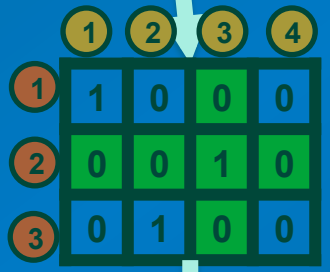


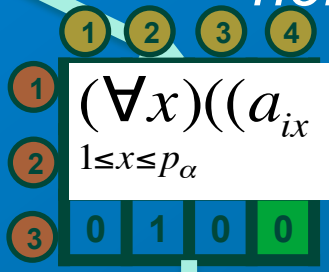


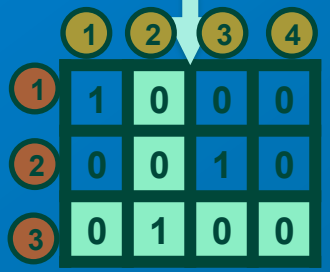
***ATTENTION**:*
the refinement procedure avoids to exploit all these states by evaluating "neighbour connections".

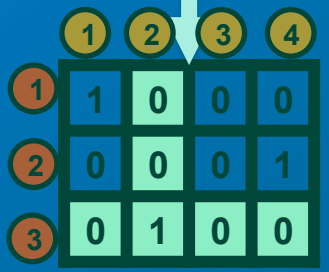
$$(\forall x)_{1\le x\le p_\alpha}((a_{ix}=1)\Rightarrow(\exists y)_{1\le y\le p_\beta}(m_{xy}\cdot b_{yj}=1))$$

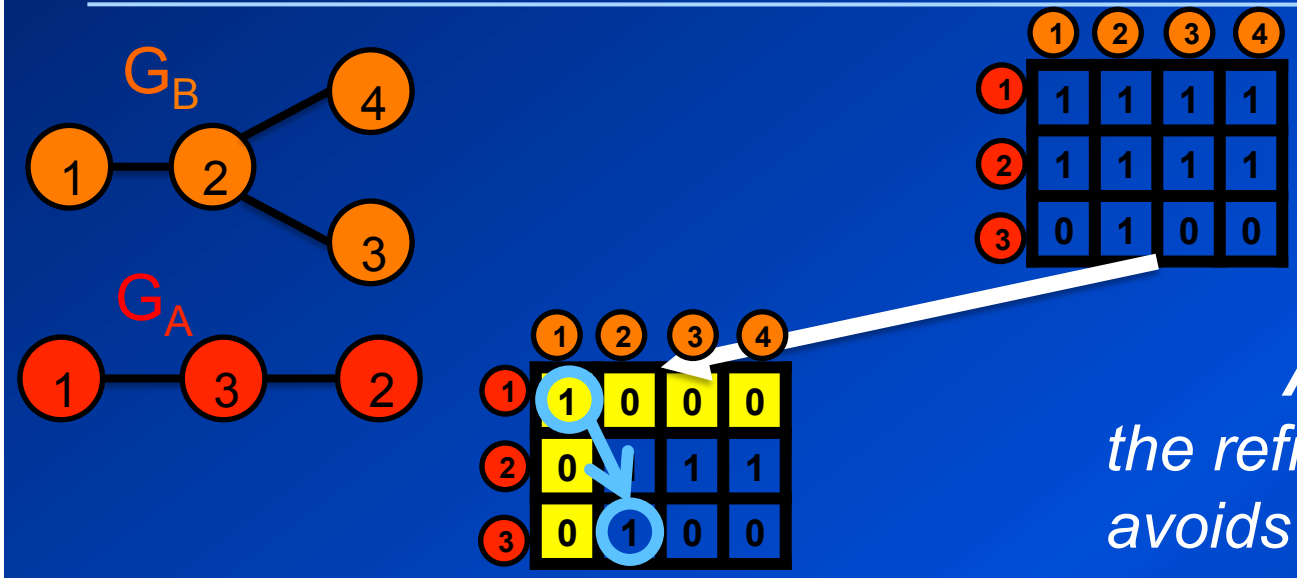




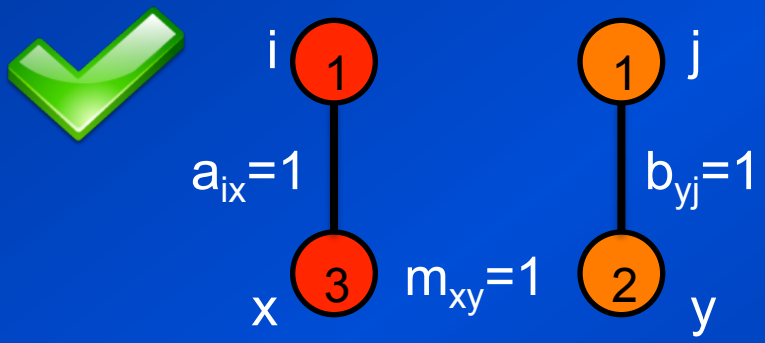




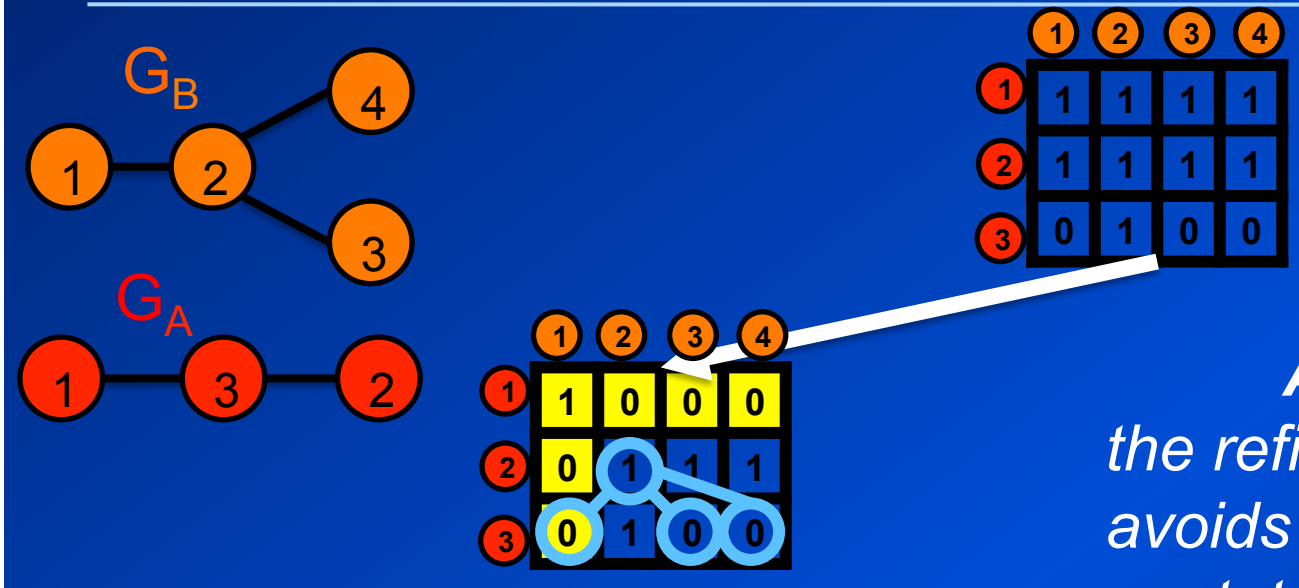




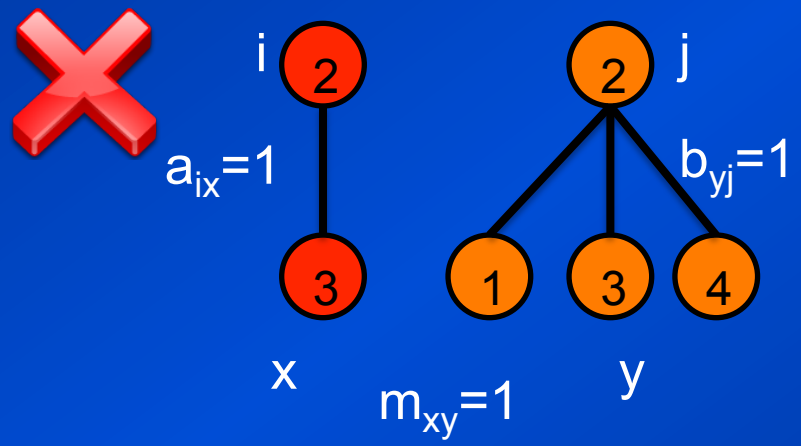
***ATTENTION**:*
the refinement procedure avoids to exploit all these states by evaluating "neighbour connections".



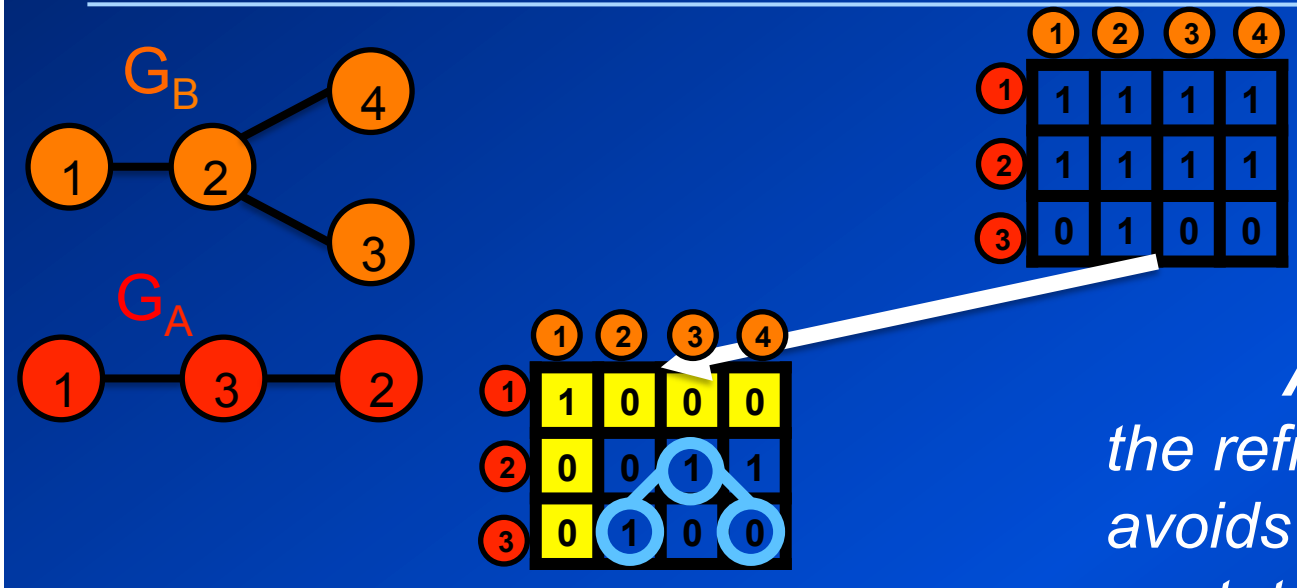
$$(\forall x)_{1\le x\le p_\alpha}((a_{ix}=1)\Rightarrow(\exists y)_{1\le y\le p_\beta}(m_{xy}\cdot b_{yj}=1))$$



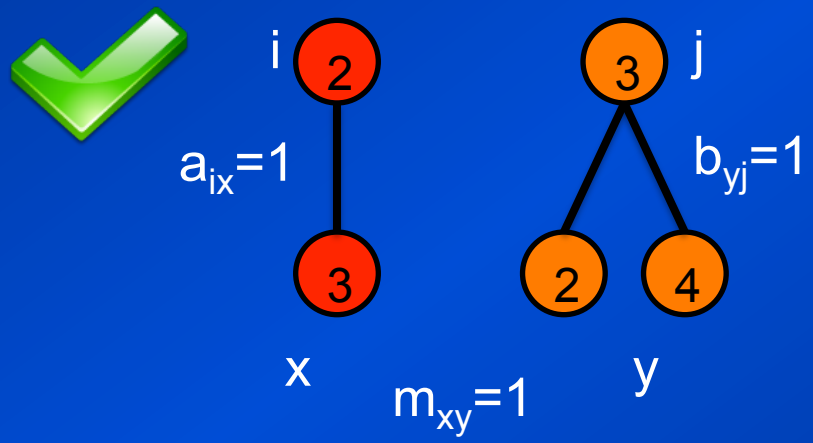
***ATTENTION**:*
the refinement procedure avoids to exploit all these states by evaluating "neighbour connections".



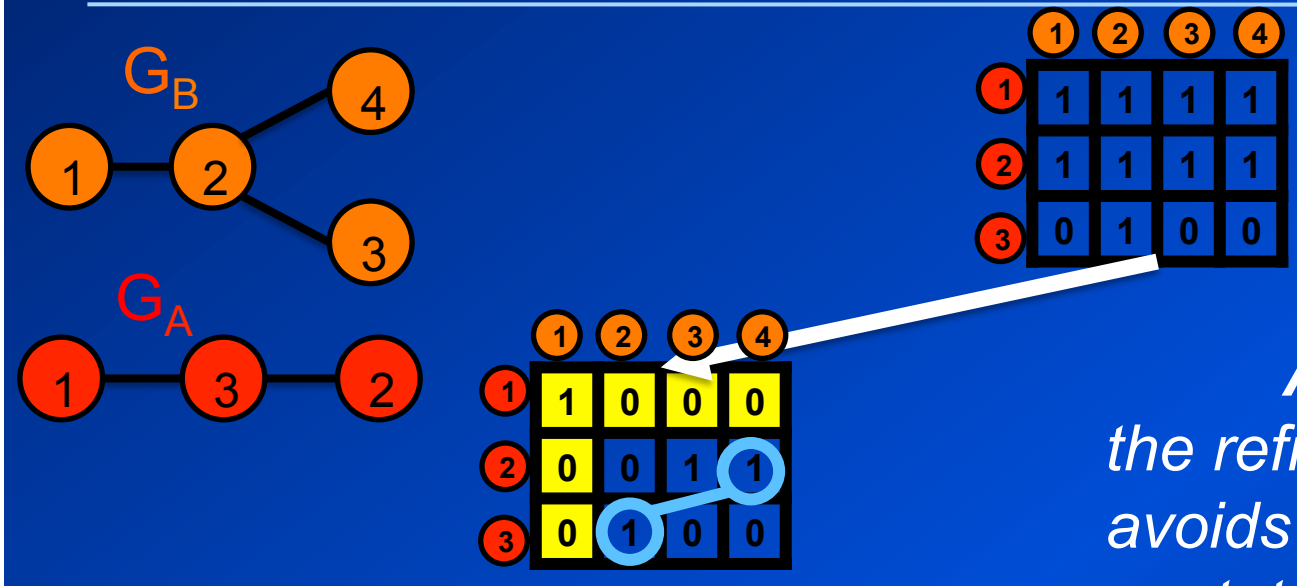
$$(\forall x)_{1\le x\le p_\alpha}((a_{ix}=1)\Rightarrow(\exists y)_{1\le y\le p_\beta}(m_{xy}\cdot b_{yj}=1))$$



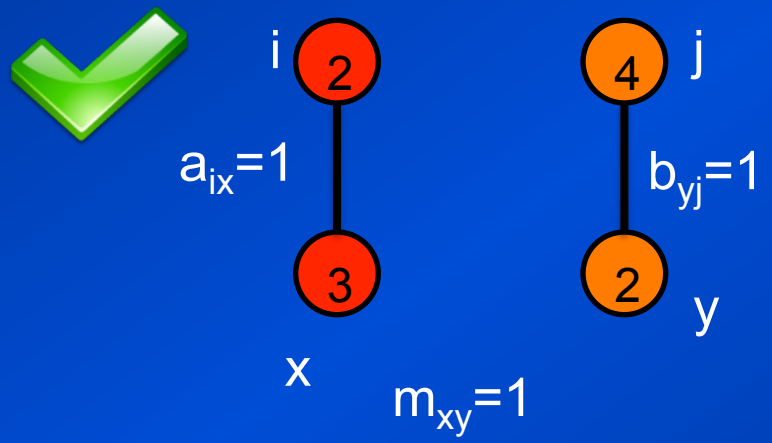
***ATTENTION**:*
the refinement procedure avoids to exploit all these states by evaluating "neighbour connections".



$$(\forall x)_{1\le x\le p_\alpha}((a_{ix}=1)\Rightarrow(\exists y)_{1\le y\le p_\beta}(m_{xy}\cdot b_{yj}=1))$$



***ATTENTION**:*
the refinement procedure avoids to exploit all these states by evaluating "neighbour connections".



$$(\forall x)_{1\le x\le p_\alpha}((a_{ix}=1)\Rightarrow(\exists y)_{1\le y\le p_\beta}(m_{xy}\cdot b_{yj}=1))$$

1. Ullmann (1976)

- PROS: the solution is found for each pair of graphs (the refinement procedures converges in a finite number of steps);
- CONS: exponential time; very high memory requirements;

3. VF2 (2004)

- The problem is formulated in terms of State Space Representation, where each state represents a partial mapping solution;
- A depth-first search is used;
- Five Feasibility rules are defined in order to prune the state space. These rules take into account:
  - the consistency of the current solution;
  - the consistency of the “future” solutions (1- and 2-look-ahead)

Outline of VF2

- *M*(*s*) is the partial mapping of state *s*, (current set of pairs of matched nodes)
- *P*(*s*) is the set of candidate pairs for extending the state *s*;
- *F*(*s*,*n*,*m*) is the *feasibility predicate*, which indicates whether the addition of pair (*n*,*m*) to state *s* can produce an inconsistent mapping

3. VF2 (2004)

- In more details, the feasibility rules are defined as follows:

$$F_{\text{syn}}(s,n,m) = R_{\text{pred}} \wedge R_{\text{succ}} \wedge R_{\text{in}} \wedge R_{\text{out}} \wedge R_{\text{new}}$$

$$\begin{aligned} R_{pred}(s,n,m) \iff & \\ & \forall n' \in \text{Pred}(G_1,n) \cap M_1(s) \\ & \exists m' \in \text{Pred}(G_2,m) \cap M_2(s) : (n',m') \in M(s) \\ \wedge \; & \forall m' \in \text{Pred}(G_2,m) \cap M_2(s) \\ & \exists n' \in \text{Pred}(G_1,n) \cap M_1(s) : (n',m') \in M(s) \end{aligned}$$

$$\begin{aligned} R_{succ}(s,n,m) \iff & \\ & \forall n' \in \text{Succ}(G_1,n) \cap M_1(s) \\ & \exists m' \in \text{Succ}(G_2,m) \cap M_2(s) : (n',m') \in M(s) \\ \wedge \; & \forall m' \in \text{Succ}(G_2,m) \cap M_2(s) \\ & \exists n' \in \text{Succ}(G_1,n) \cap M_1(s) : (n',m') \in M(s) \end{aligned}$$

$$\begin{aligned} & R_{\text{in}}(s,n,m) \Longleftrightarrow \\ & (\text{Card}(\text{Succ}(G_1,n) \cap T_1^{\text{in}}(s)) \geq \text{Card}(\text{Succ}(G_2,m) \cap T_2^{\text{in}}(s))) \wedge \\ & (\text{Card}(\text{Pred}(G_1,n) \cap T_1^{\text{in}}(s)) \geq \text{Card}(\text{Pred}(G_2,m) \cap T_2^{\text{in}}(s))), \end{aligned}$$

$$\begin{aligned} & R_{\text{out}}(s,n,m) \Longleftrightarrow \\ & (\text{Card}(\text{Succ}(G_1,n) \cap T_1^{\text{out}}(s)) \geq \text{Card}(\text{Succ}(G_2,m) \cap T_2^{\text{out}}(s))) \wedge \\ & (\text{Card}(\text{Pred}(G_1,n) \cap T_1^{\text{out}}(s)) \geq \text{Card}(\text{Pred}(G_2,m) \cap T_2^{\text{out}}(s))), \end{aligned}$$

$$\begin{aligned} & R_{\text{new}}(s,n,m) \Longleftrightarrow \\ & \text{Card}(\tilde{N}_1(s) \cap \text{Pred}(G_1,n)) \geq \text{Card}(\tilde{N}_2(s) \cap \text{Pred}(G_2,n)) \wedge \\ & \text{Card}(\tilde{N}_1(s) \cap \text{Succ}(G_1,n)) \geq \text{Card}(\tilde{N}_2(s) \cap \text{Succ}(G_2,n)). \end{aligned}$$

3. VF2 (2004)

M(s0) = {0}

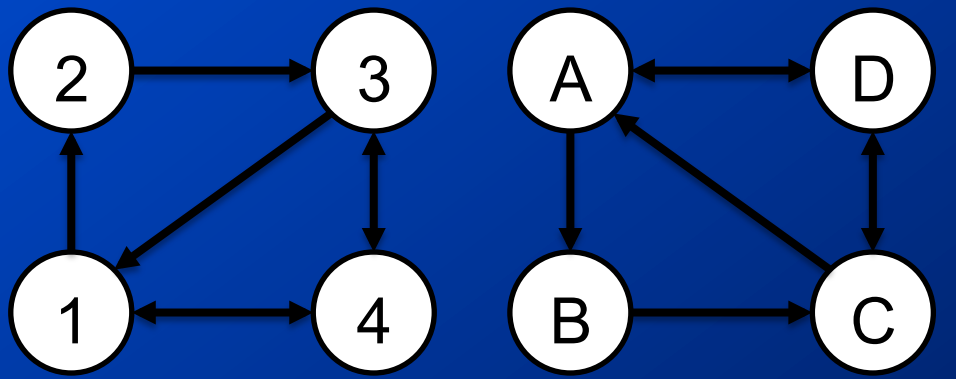
$T_1^{in}(s0) = \{\ \}$

$T_1^{out}(s0) = \{\ \}$ $\quad M_1(s0) = \{\ \}$

$T_2^{in}(s0) = \{\ \}$ $\quad M_2(s0) = \{\ \}$

$T_1^{out}(s0) = \{\ \}$

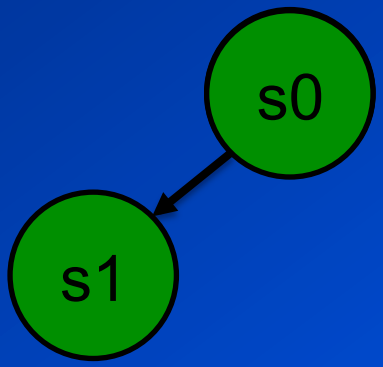
P(s0) = {**(1,A)**, (1,B), (1,C), (1,D),
…. (4,B), (4,C), (4,D)}



3. VF2 (2004)

M(s0) = {0}

M(s1) = {(1,A)}



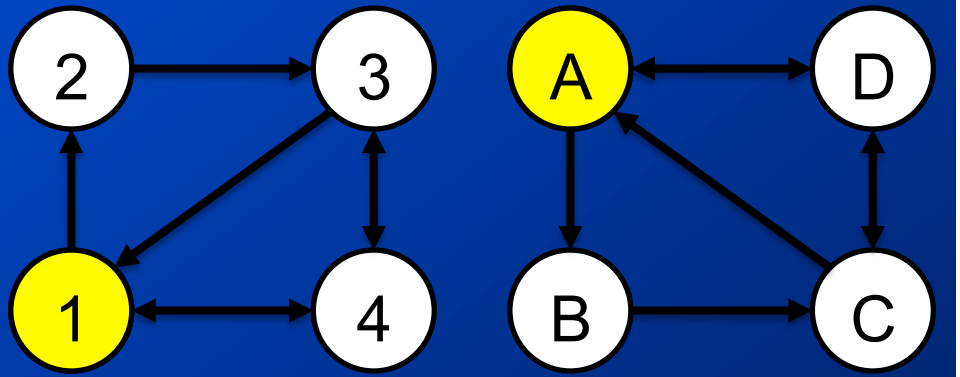
$T_1^{in}(s1) = \{3, 4\}$

$T_1^{out}(s1) = \{2, 4\}$ $M_1(s1) = \{1\}$

$T_2^{in}(s1) = \{C, D\}$ $M_2(s1) = \{A\}$

$T_2^{out}(s1) = \{B, D\}$

$P(s1) = \{(2,B), (2,D), (4,B), (4,D)\}$

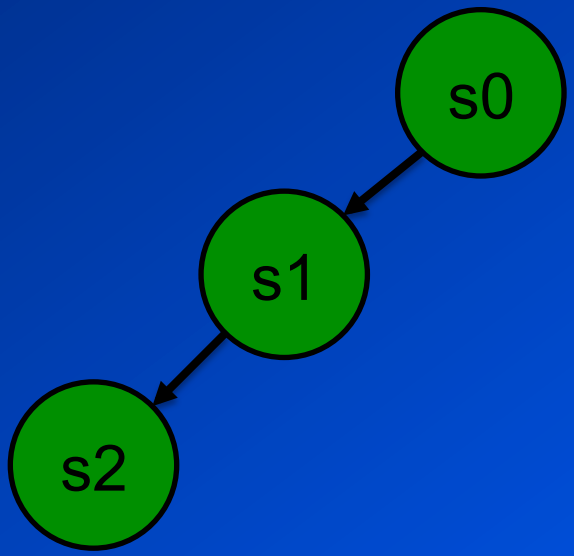


3. VF2 (2004)

M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}



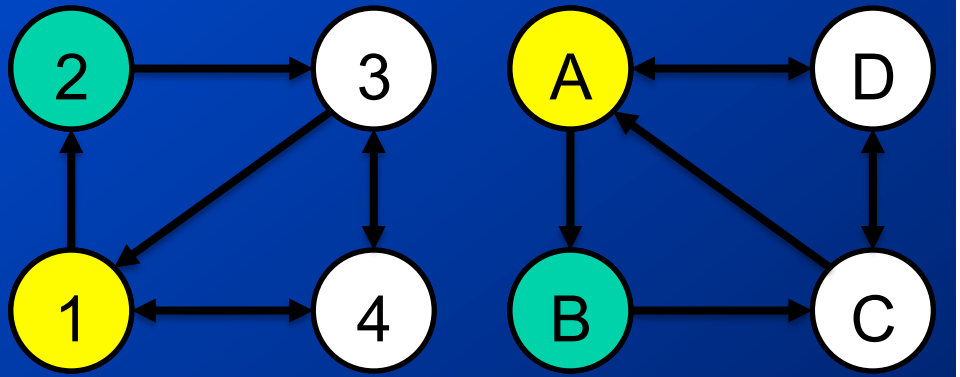
$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$ $M_1(s2) = \{1,2\}$

$T_2^{in}(s2) = \{C, D\}$ $M_2(s2) = \{A,B\}$

$T_2^{out}(s2) = \{C, D\}$

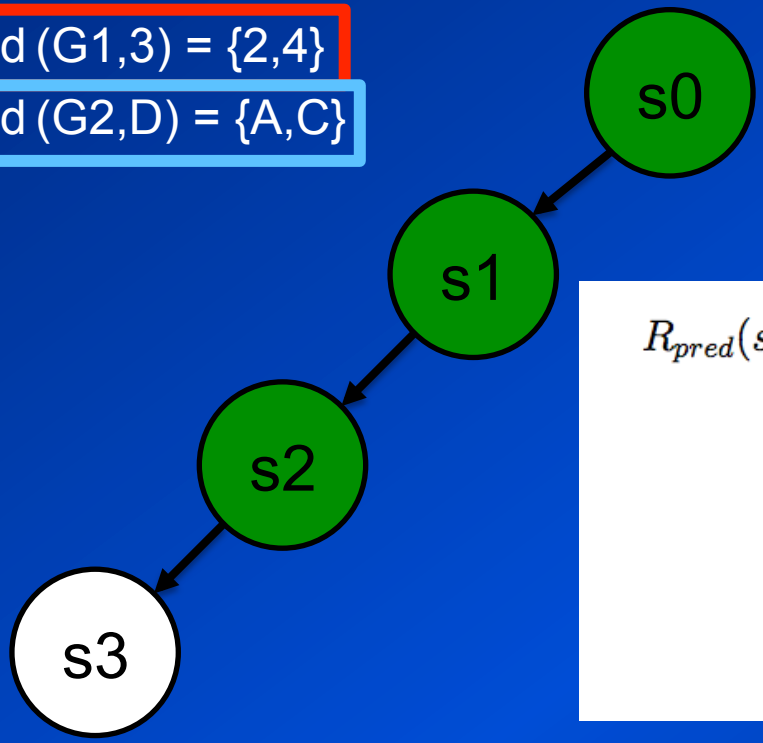
P(s2) = {**(3,D)**, (3,C), (4,D), (4,C)}



3. VF2 (2004)

Pred (G1,3) = {2,4}

Pred (G2,D) = {A,C}



M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

M(s3) = {(1,A), (2,B), (3,D)}

$$R_{pred}(s,n,m) \iff$$
$$\forall n' \in \mathrm{Pred}(G_1,n) \cap M_1(s) \; \exists m' \in \mathrm{Pred}(G_2,m) \cap M_2(s) : (n',m') \in M(s)$$
$$\wedge \; \forall m' \in \mathrm{Pred}(G_2,m) \cap M_2(s) \; \exists n' \in \mathrm{Pred}(G_1,n) \cap M_1(s) : (n',m') \in M(s)$$

2

A

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

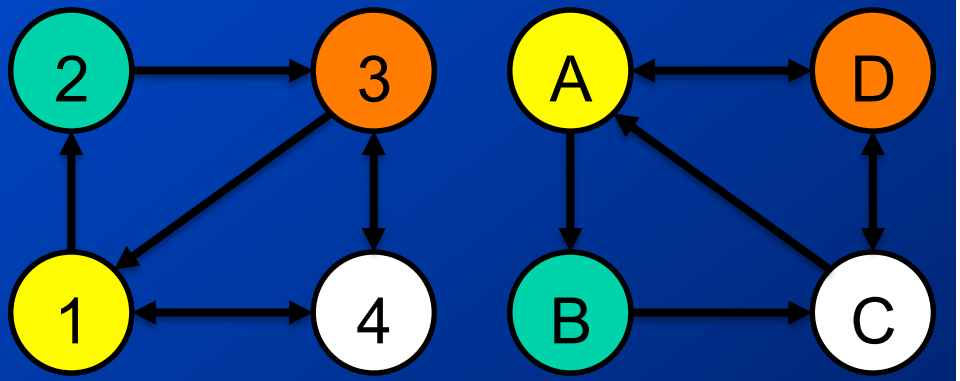
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$

$P(s2) = \{\mathbf{(3,D)}, (3,C), (4,D), (4,C)\}$



3. VF2 (2004)

M(s0) = {0}

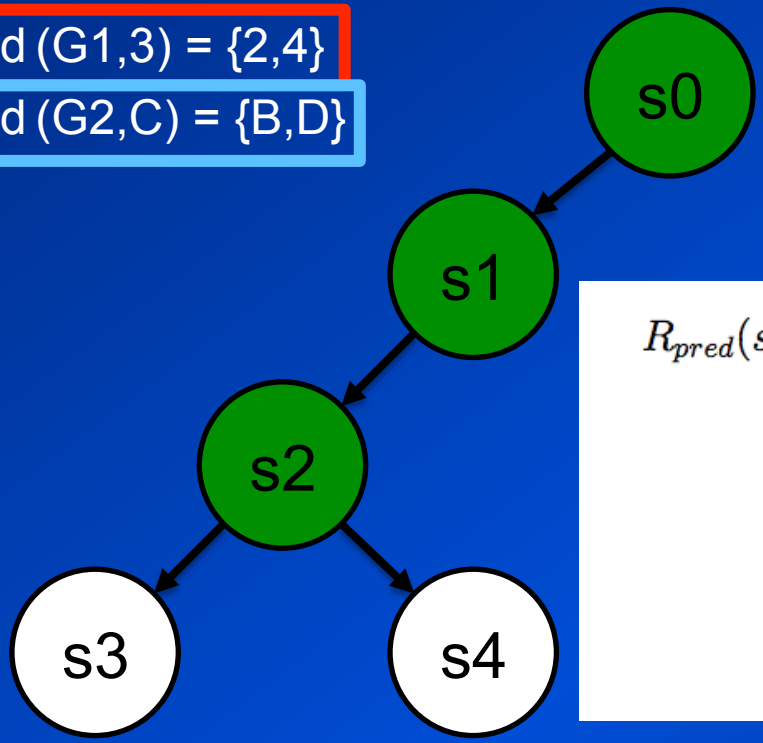
M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

M(s4) = {(1,A), (2,B), (3,C)}

Pred (G1,3) = {2,4}

Pred (G2,C) = {B,D}



$$R_{pred}(s,n,m) \iff$$

$$\forall n' \in \mathrm{Pred}(G_1,n) \cap M_1(s) \quad (2)$$

$$\exists m' \in \mathrm{Pred}(G_2,m) \cap M_2(s) : (n',m') \in M(s) \quad (B)$$

$$\wedge \quad \forall m' \in \mathrm{Pred}(G_2,m) \cap M_2(s)$$

$$\exists n' \in \mathrm{Pred}(G_1,n) \cap M_1(s) : (n',m') \in M(s)$$

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

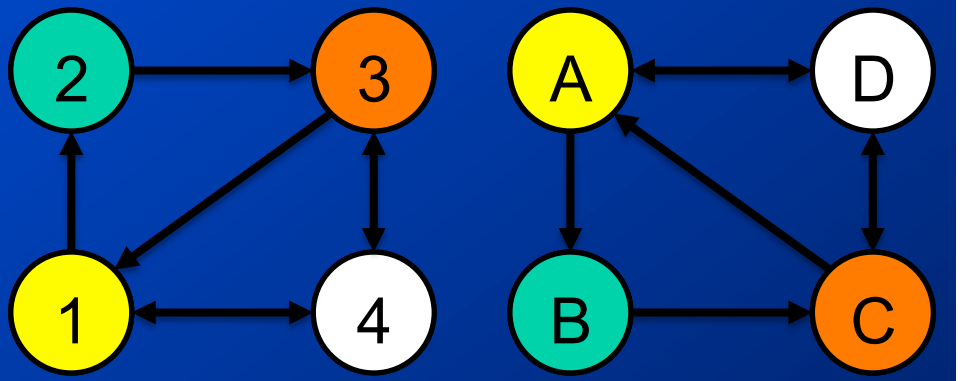
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$

P(s2) = {(3,D), **(3,C)**, (4,D), (4,C)}



3. VF2 (2004)

M(s0) = {0}

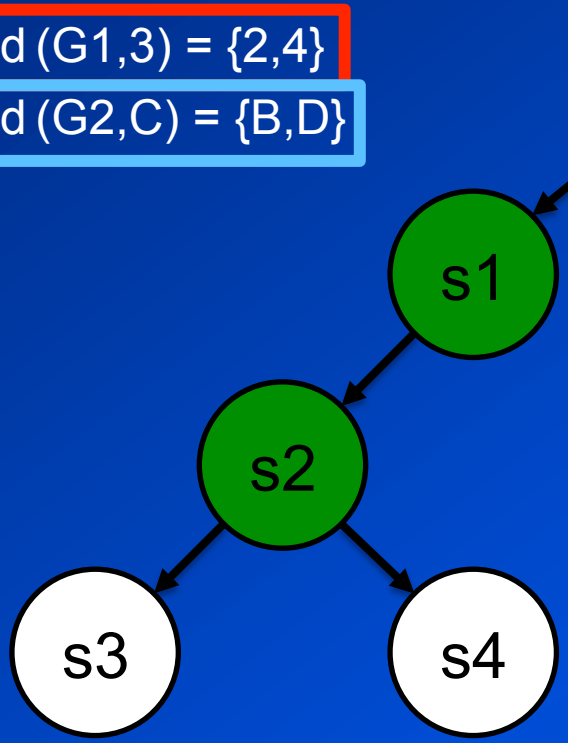
M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

M(s4) = {(1,A), (2,B), (3,C)}

Pred (G1,3) = {2,4}

Pred (G2,C) = {B,D}



$$R_{pred}(s,n,m) \iff$$

$$\forall n' \in \mathrm{Pred}(G_1,n) \cap M_1(s)$$

$$\exists m' \in \mathrm{Pred}(G_2,m) \cap M_2(s) : (n',m') \in M(s)$$

B

$$\wedge \quad \forall m' \in \mathrm{Pred}(G_2,m) \cap M_2(s)$$

$$\exists n' \in \mathrm{Pred}(G_1,n) \cap M_1(s) : (n',m') \in M(s)$$

2

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

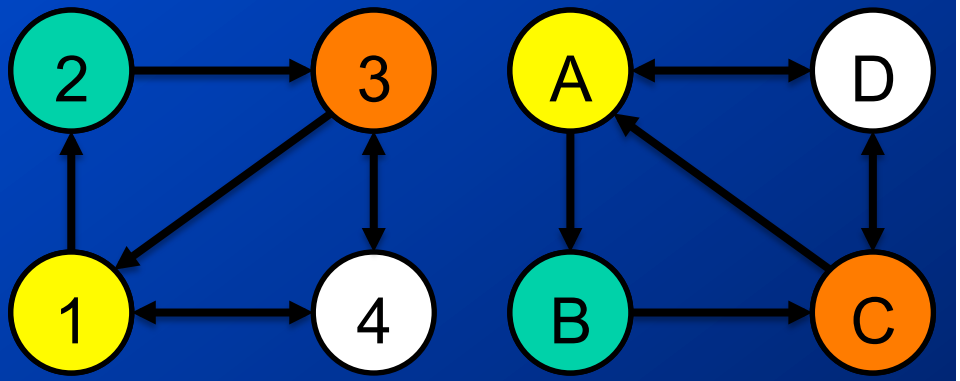
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

$P(s2) = \{(3,D), \mathbf{(3,C)}, (4,D), (4,C)\}$

$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$



3. VF2 (2004)

M(s0) = {0}

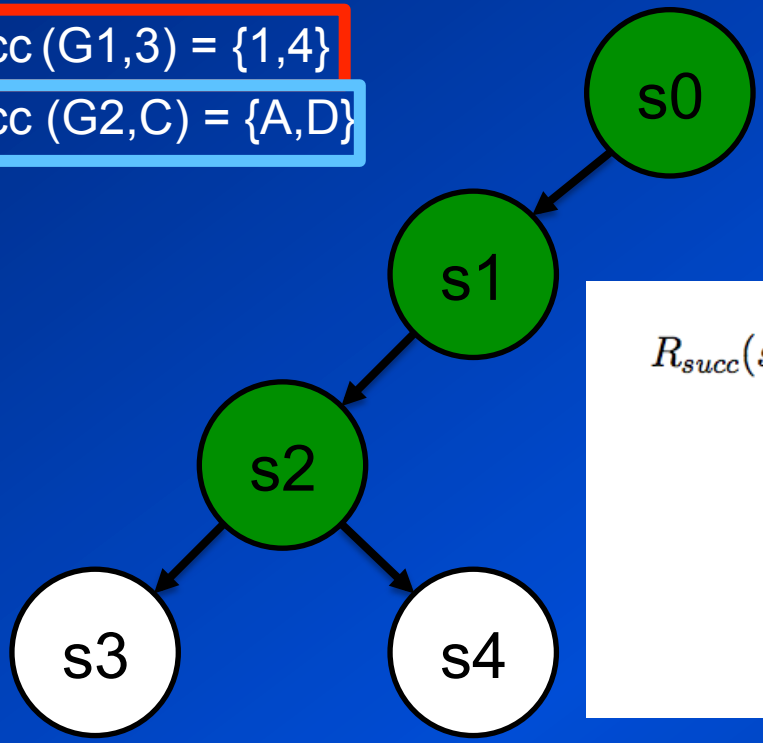
M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

M(s4) = {(1,A), (2,B), (3,C)}

Succ (G1,3) = {1,4}

Succ (G2,C) = {A,D}



$$R_{succ}(s,n,m) \iff$$

$$\forall n' \in \mathrm{Succ}(G_1,n) \cap M_1(s) \quad (1)$$

$$\exists m' \in \mathrm{Succ}(G_2,m) \cap M_2(s) : (n',m') \in M(s) \quad (A)$$

$$\wedge \quad \forall m' \in \mathrm{Succ}(G_2,m) \cap M_2(s)$$

$$\exists n' \in \mathrm{Succ}(G_1,n) \cap M_1(s) : (n',m') \in M(s)$$

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

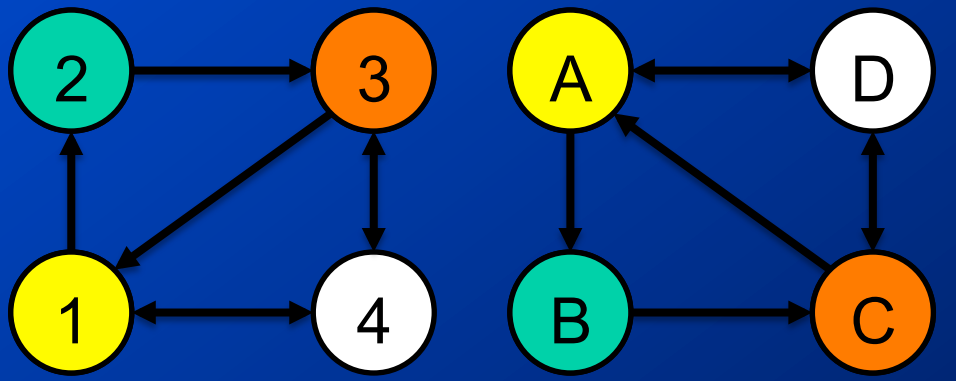
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

$P(s2) = \{(3,D), \mathbf{(3,C)}, (4,D), (4,C)\}$

$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$



3. VF2 (2004)

M(s0) = {0}

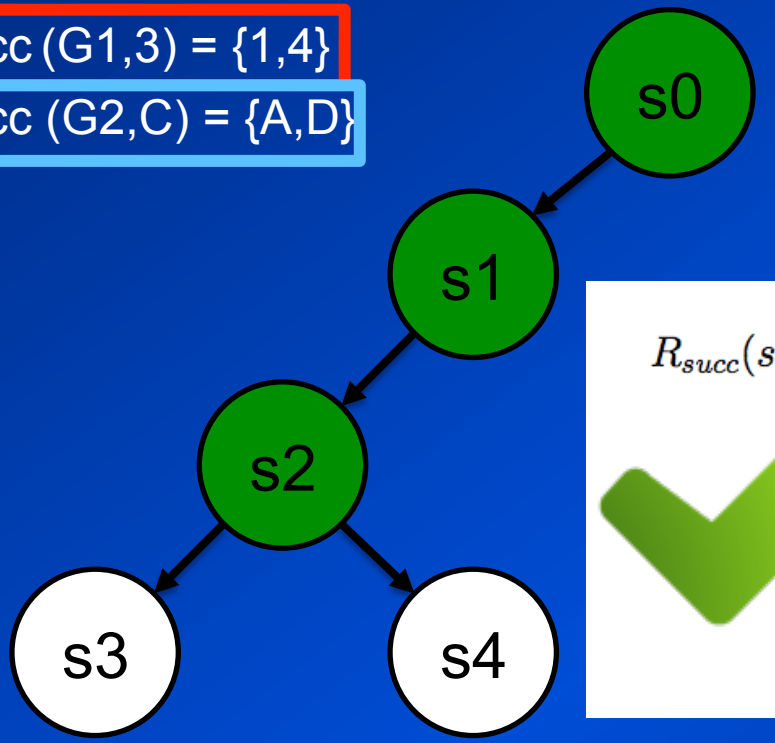
M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

M(s4) = {(1,A), (2,B), (3,C)}

Succ (G1,3) = {1,4}

Succ (G2,C) = {A,D}



$$R_{succ}(s,n,m) \iff$$

$$\forall n' \in \mathrm{Succ}(G_1,n) \cap M_1(s)$$

$$\exists m' \in \mathrm{Succ}(G_2,m) \cap M_2(s) : (n',m') \in M(s)$$

A

$$\wedge \quad \forall m' \in \mathrm{Succ}(G_2,m) \cap M_2(s)$$

$$\exists n' \in \mathrm{Succ}(G_1,n) \cap M_1(s) : (n',m') \in M(s)$$

1

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

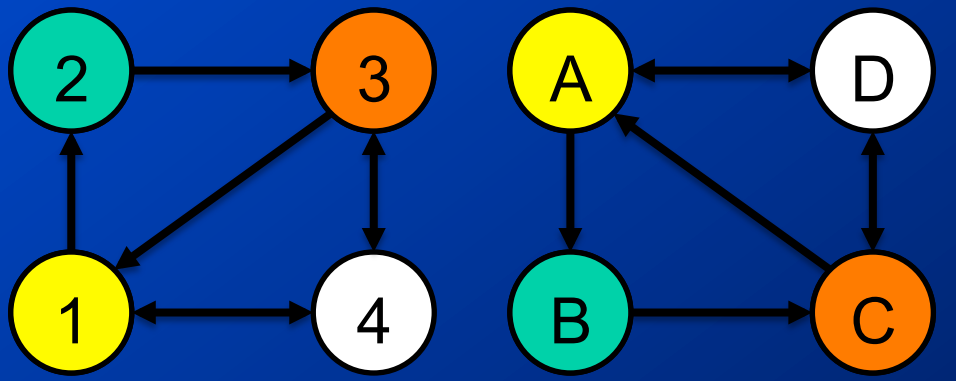
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$

P(s2) = {(3,D), **(3,C)**, (4,D), (4,C)}



3. VF2 (2004)

M(s0) = {0}

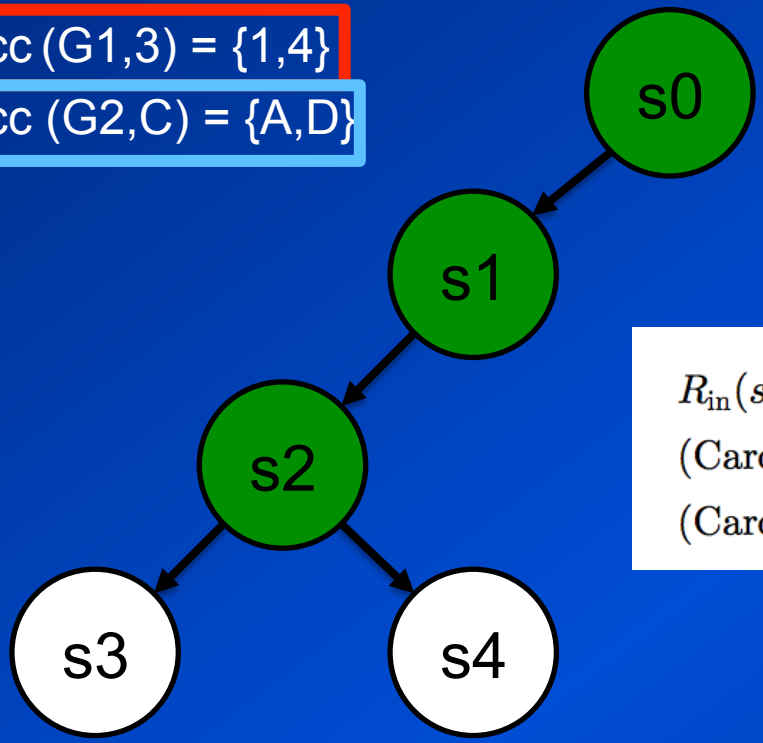
M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

M(s4) = {(1,A), (2,B), (3,C)}

Succ (G1,3) = {1,4}

Succ (G2,C) = {A,D}



$$R_{\text{in}}(s,n,m) \Longleftrightarrow$$
$$(\text{Card}(\text{Succ}(G_1,n) \cap T_1^{\text{in}}(s)) \geq \text{Card}(\text{Succ}(G_2,m) \cap T_2^{\text{in}}(s))) \wedge$$
$$(\text{Card}(\text{Pred}(G_1,n) \cap T_1^{\text{in}}(s)) \geq \text{Card}(\text{Pred}(G_2,m) \cap T_2^{\text{in}}(s))),$$

4

D

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

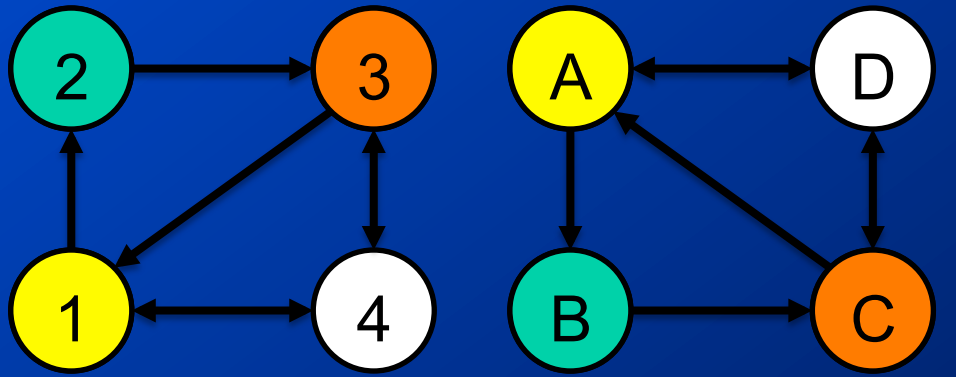
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$

P(s2) = {(3,D), **(3,C)**, (4,D), (4,C)}



3. VF2 (2004)

M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

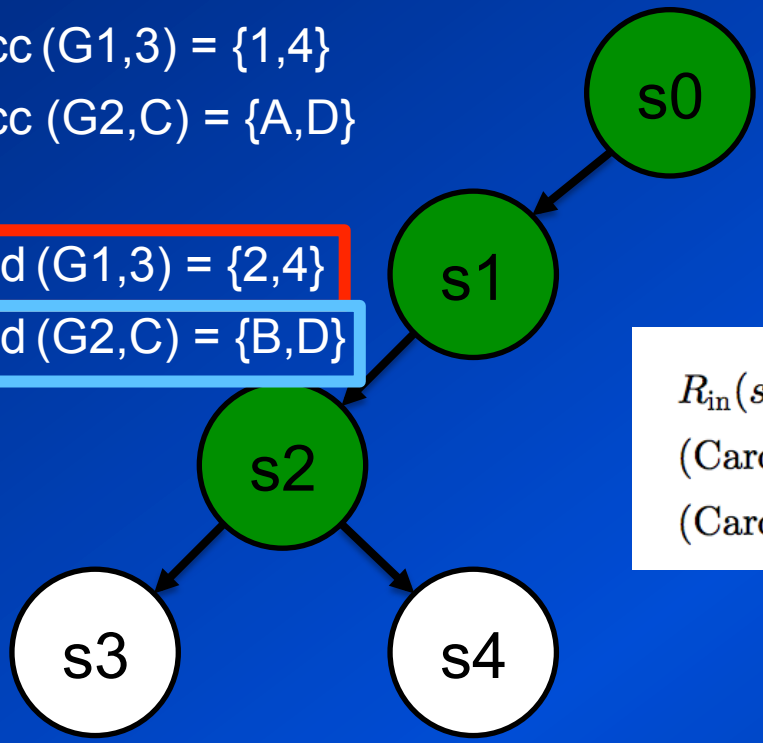
M(s4) = {(1,A), (2,B), (3,C)}

Succ (G1,3) = {1,4}

Succ (G2,C) = {A,D}

Pred (G1,3) = {2,4}

Pred (G2,C) = {B,D}



$$R_{\text{in}}(s,n,m) \Longleftrightarrow$$
$$(\text{Card}(\text{Succ}(G_1,n) \cap T_1^{\text{in}}(s)) \geq \text{Card}(\text{Succ}(G_2,m) \cap T_2^{\text{in}}(s))) \wedge$$
$$(\text{Card}(\text{Pred}(G_1,n) \cap T_1^{\text{in}}(s)) \geq \text{Card}(\text{Pred}(G_2,m) \cap T_2^{\text{in}}(s))),$$

4 D

1 ≥1 and 1 ≥1

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

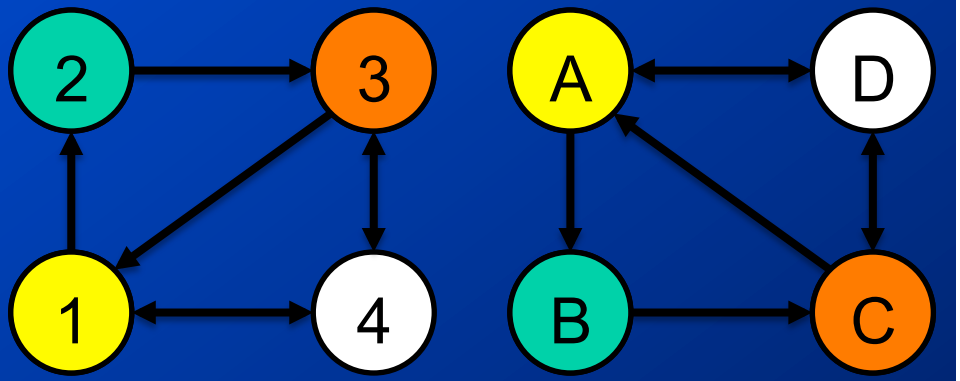
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$

P(s2) = {(3,D), **(3,C)**, (4,D), (4,C)}



3. VF2 (2004)

M(s0) = {0}

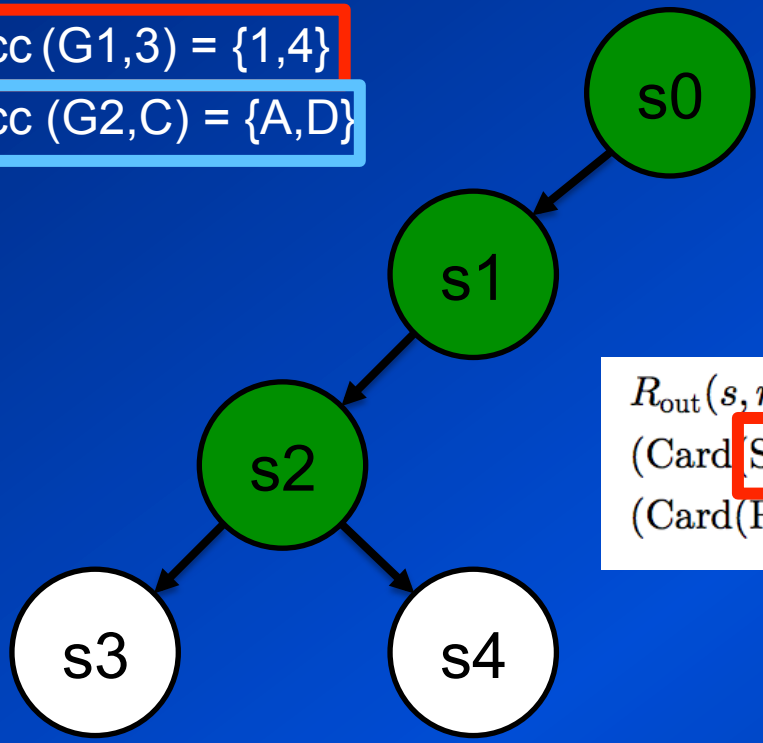
M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

M(s4) = {(1,A), (2,B), (3,C)}

Succ (G1,3) = {1,4}

Succ (G2,C) = {A,D}



$$R_{\text{out}}(s,n,m) \Longleftrightarrow$$
$$(\text{Card}(\text{Succ}(G_1,n) \cap T_1^{\text{out}}(s)) \geq \text{Card}(\text{Succ}(G_2,m) \cap T_2^{\text{out}}(s))) \wedge$$
$$(\text{Card}(\text{Pred}(G_1,n) \cap T_1^{\text{out}}(s)) \geq \text{Card}(\text{Pred}(G_2,m) \cap T_2^{\text{out}}(s))),$$

4

D

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

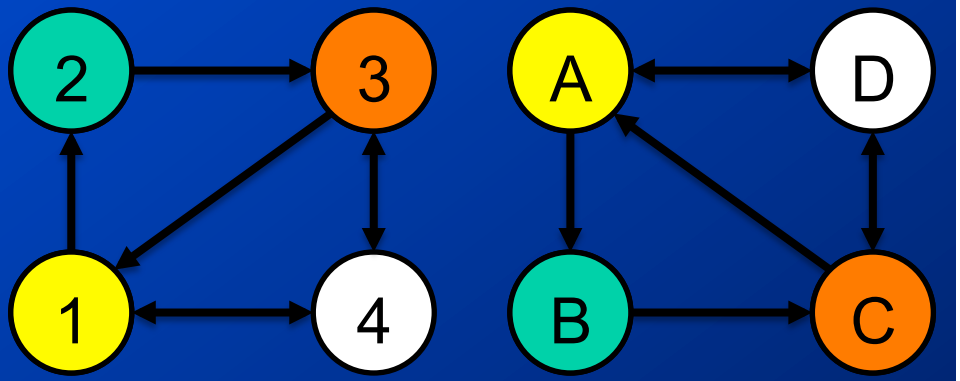
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$

P(s2) = {(3,D), **(3,C)**, (4,D), (4,C)}



3. VF2 (2004)

M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,A), (2,B)}

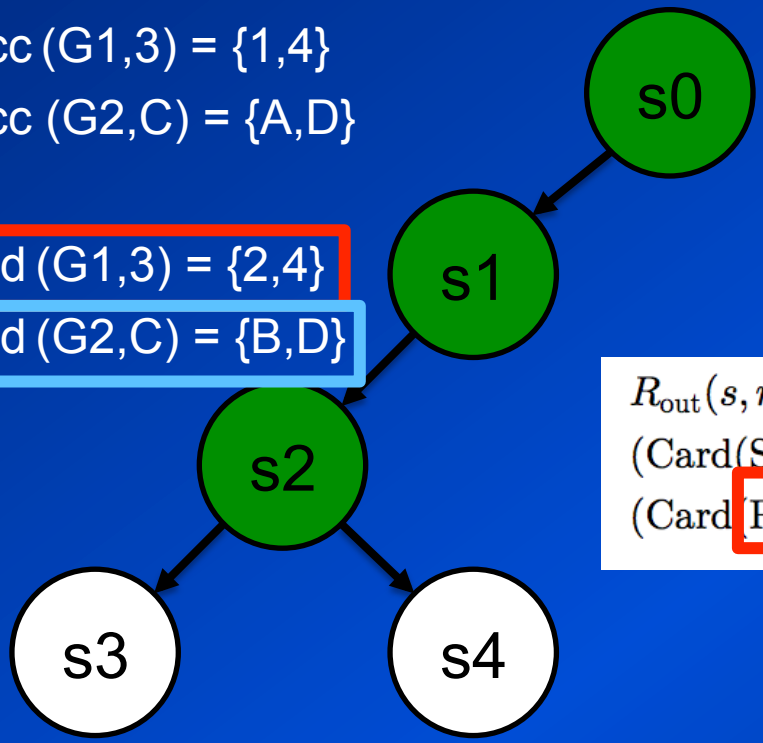
M(s4) = {(1,A), (2,B), (3,C)}

Succ (G1,3) = {1,4}

Succ (G2,C) = {A,D}

Pred (G1,3) = {2,4}

Pred (G2,C) = {B,D}



$$R_{\text{out}}(s,n,m) \Longleftrightarrow$$
$$(\text{Card}(\text{Succ}(G_1,n) \cap T_1^{\text{out}}(s)) \geq \text{Card}(\text{Succ}(G_2,m) \cap T_2^{\text{out}}(s))) \wedge$$
$$(\text{Card}(\text{Pred}(G_1,n) \cap T_1^{\text{out}}(s)) \geq \text{Card}(\text{Pred}(G_2,m) \cap T_2^{\text{out}}(s)))$$

4 D

1 ≥1 and 1 ≥1

$T_1^{in}(s2) = \{3, 4\}$

$T_1^{out}(s2) = \{3, 4\}$

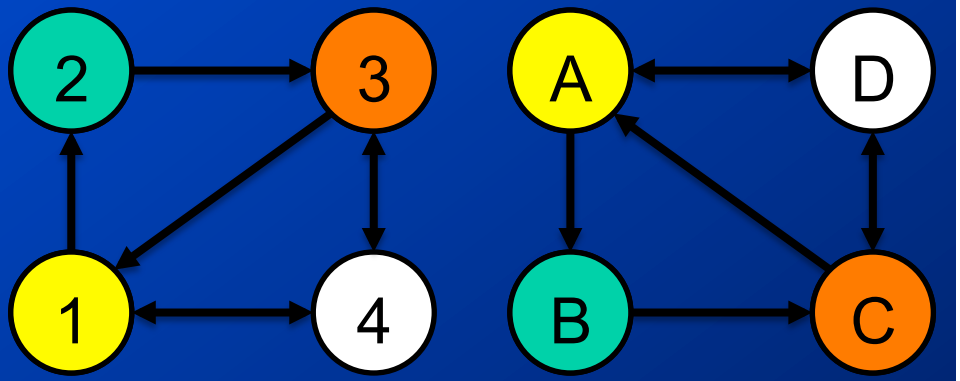
$T_2^{in}(s2) = \{C, D\}$

$T_2^{out}(s2) = \{C, D\}$

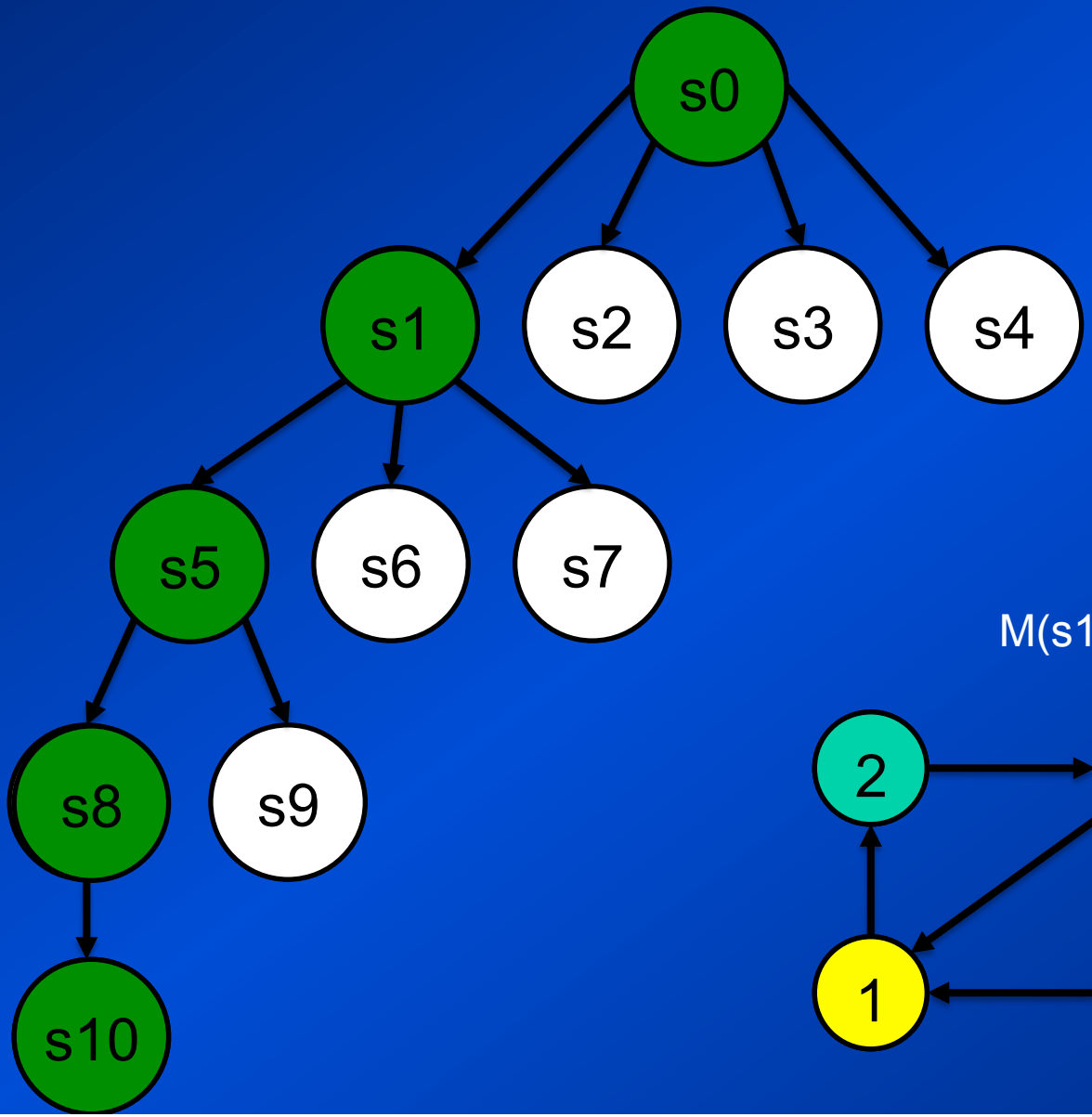
$M_1(s2) = \{1,2\}$

$M_2(s2) = \{A,B\}$

P(s2) = {(3,D), **(3,C)**, (4,D), (4,C)}



3. VF2 (2004)



M(s0) = {0}

M(s1) = {(1,A)}

M(s2) = {(1,B)}

M(s3) = {(1,C)}

M(s4) = {(1,D)}

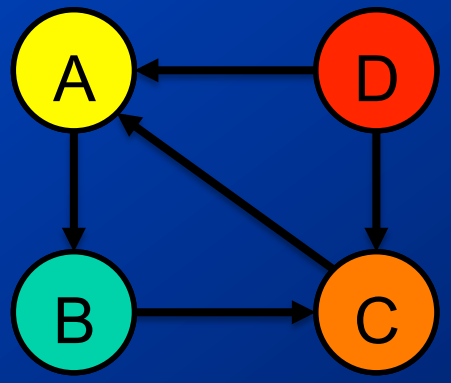
M(s5) = {(1,A) , (2,B)}

M(s6) = {(1,A) , (2,C)}

M(s7) = {(1,A) , (2,D)}

…

M(s10) = {(1,A) , (2,B) , (3,C) , (4,D)}



3. VF2 (2004)

- PROS:
  - It is applicable to any kind of graphs;
  - Linear Memory Complexity;
- CONS
  - Not yet found!

EGM: Other techniques

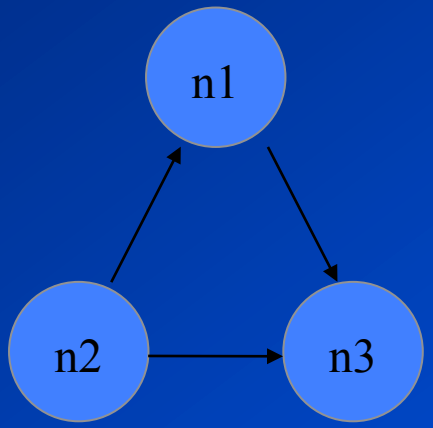
- The graph matching into a sort of vector-based matching
- From the input graphs a representation (not graph-based of course)
- We compare the two representations (in polinomial time)
- Generally give necessary but not sufficient solutions

Nauty (McKay 1981)

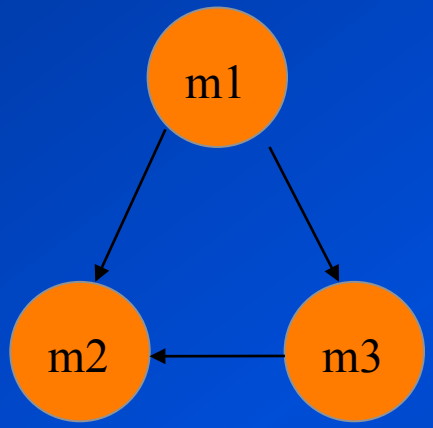
- based on permutation group theory
- only graph isomorphism
- first builds the group of automorphisms for each graph (automorphism = isomorphism of a graph with itself)
- then, the automorphisms groups are used to define a canonical ordering of the nodes
  - once the nodes are reordered, two graphs are isomorphic iff their adjacency matrices are equal

A simple Example (1/4)

G1



G2



Two graphs and their adjacency matrices

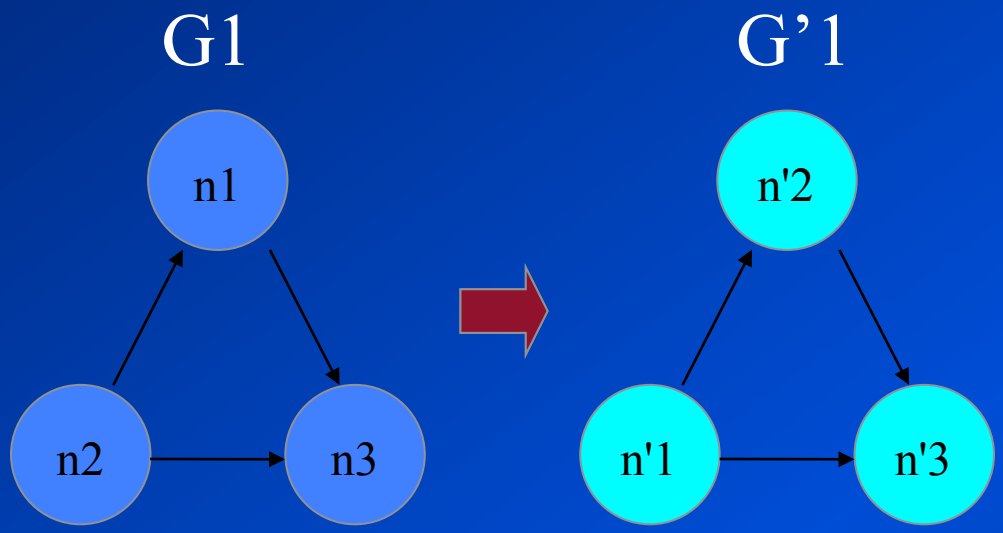
G1

0	0	1
1	0	1
0	0	0

G2

0	1	1
0	0	0
0	1	0

A simple Example (2/4)



Finds a a canonical labeling for G1 by the permutation groups:

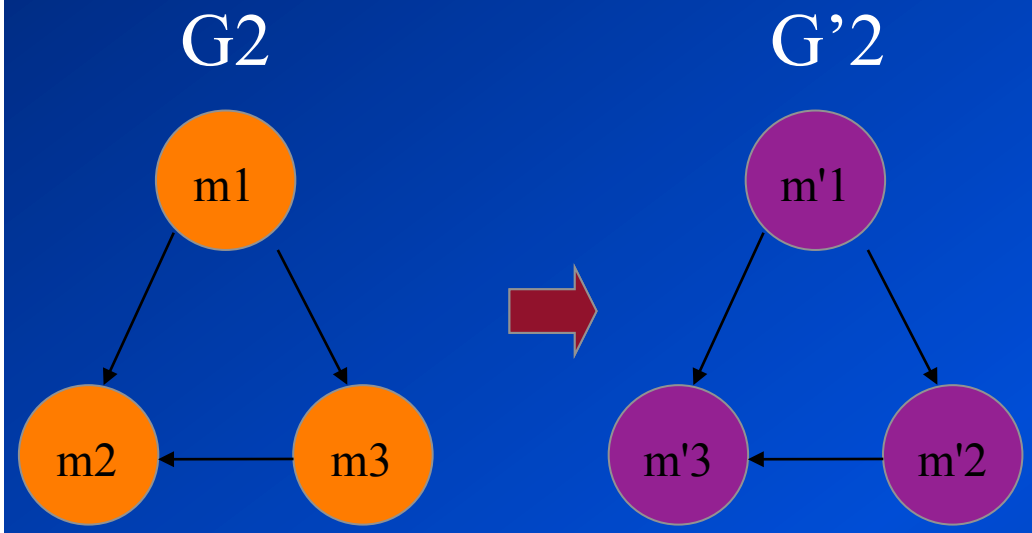
n1 => n'2
n2 => n'1
n3 => n'3

0	0	1
1	0	1
0	0	0

0	1	1
0	0	1
0	0	0

e.g. counting the output degree of the nodes

A simple Example (3/4)



The same is done for G2

m1 => m'1

m2 => m'3

m3 => m'2

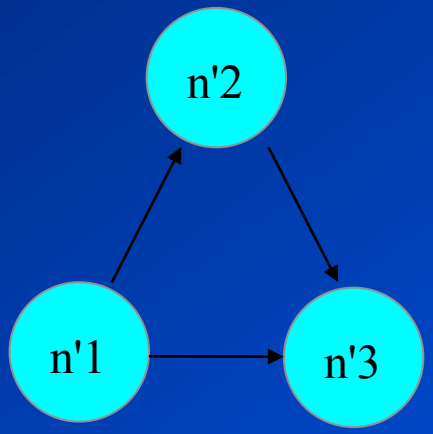
G2

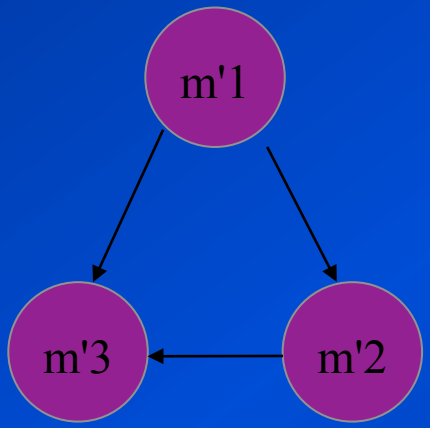
0	1	1
0	0	0
0	1	0

G'2

0	1	1
0	0	1
0	0	0

A simple Example (4/4)





The two canonically labeled graphs are compared directly using their adjacency matrices

G'1

0	1	1
0	0	1
0	0	0

=

G'2

0	1	1
0	0	1
0	0	0

5. Zampelli (2010)

- A new approach for solving the Subgraph isomorphism using constraint programming.
- The idea is to label every node by some invariant property (es. Node degrees), and iteratively extends labels by considering labels of adjacent nodes.
- Labeling is used to define a filtering algorithm for the subgraph isomorphism problem. (Iterative Labeling Filtering – ILF)

5. Zampelli (2010)

- Labeling process allows to filter, for every node in the graph G1, the set of target nodes in G2.
- The node compatibility is evaluated by a partial order, consistent with respect to the subgraph isomorphism function.
- A consistent labeling filters node domains, as strong as possible, without removing solutions to the subgraph isomorphism problem.

5. Zampelli (2010)

Label Assignment Function
α : Node set → Label Set

Partial Order

$$CC_l = \{(u, v) \in N_p \times N_t \mid \alpha(u) \preceq \alpha(v)\}$$

Set of compatible couples of nodes

- This compatibility relationship may be used to filter the node domain of the graph G1, removing from it every node in G2 not in CC_l
- A labelling is subgraph isomorphism consistent iff for any subgraph isomorphism function f, we have that for any node u in G1 (u, f(u)) is in CC_l

5. Zampelli (2010)

- Subgraph Isomorphism consistent labelling
  - Degree based
  - K-Distance based: nodes at distance k
  - K-Clique based

- Degree Based example:

deg(A) = deg(B) = deg(D) = deg(2) = deg(4) = 4

deg(C) = deg(E) = deg(F) = deg(G) = deg(1) = deg(3) = 3

deg(5) = deg(6) = 2

$$CC_{l_{deg}} = \{(u, v) \mid u \in \{2, 4\}, v \in \{A, B, D\}\} \cup \{(u, v) \mid u \in \{1, 3, 5, 6\}, v \in \{A, B, C, D, E, F, G\}\}$$

5. Zampelli (2010)

- The number of compatible nodes is reduced by an iterative labeling strengthening procedure using neighbor information.
- This procedure is terminated when the compatible couple set cannot be further reduced, or when a user defined threshold is reached.

5. Zampelli (2010)

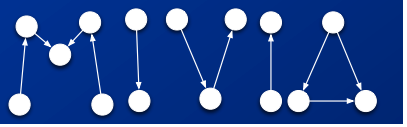
- PROS:
  - Different approach in respect to the to the classical CSP based on Forward Checking or Arc Consistency.
  - Time Efficient.
- CONS:
  - The precision and the time of convergence depend on the chosen threshold.
  - Only for subgraph isomorphism.

Pure Methods
Inexact Graph Matching

IGM: Tree Search Main algorithms

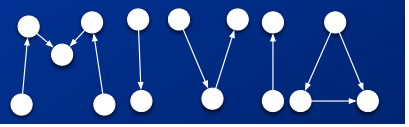
- Tsai–Fu,1979
- Shapiro–Haralick,1981
- Wong,1990
- Sasha,1994
- Allen,1997
- Berretti,2000

Gharaman,1980
Eshera – Fu,1984
Dumay,1992
Cordella,1996
Serratosa,1999
Gregory – Kittler,2002



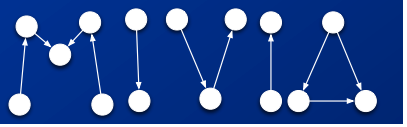
IGM: Continuous Optimization

- Casting graph matching into a *continuous, non linear optimization problem* by removing some constraints.
- The solution is built by successive improvements of a continuous goal function.
- The solution needs to be converted back from continuous domain: this may introduce further approximation.

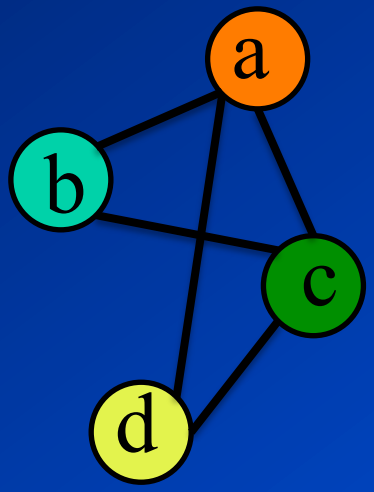


IGM: Error-correcting

- **Error Correcting Cost**: the matching cost is based on an explicit model of the errors
- **Graph Edit Cost**: based on a set of graph-edit operation (node insertion, edge insertion, edge deletion, etc..); is the cost of the operations sequence to transform one of the graphs into the other.
- **Graph Edit Distance**: the edit cost is used as a measure of dissimilarity of the graphs.

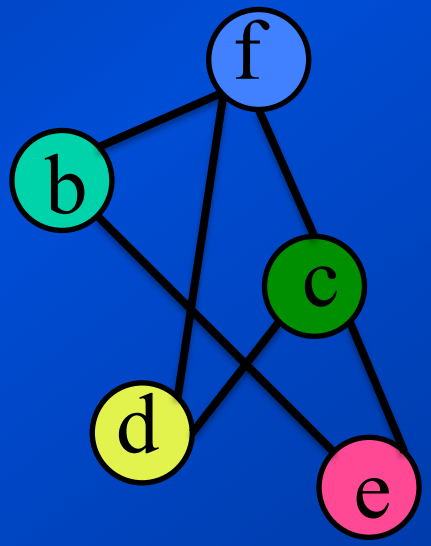


Examples:

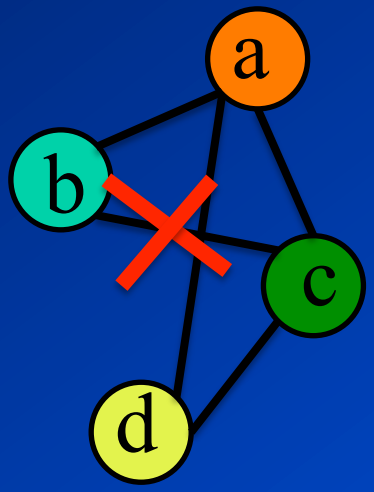


G1

G2

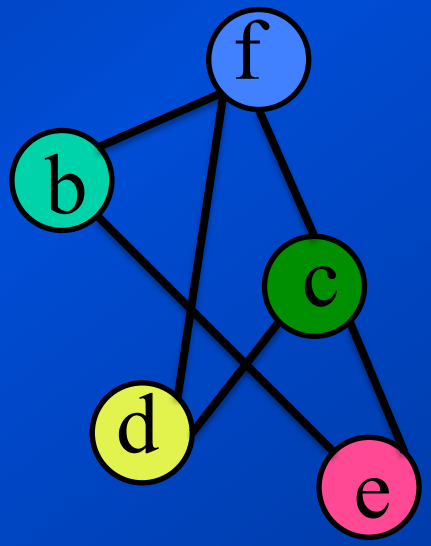


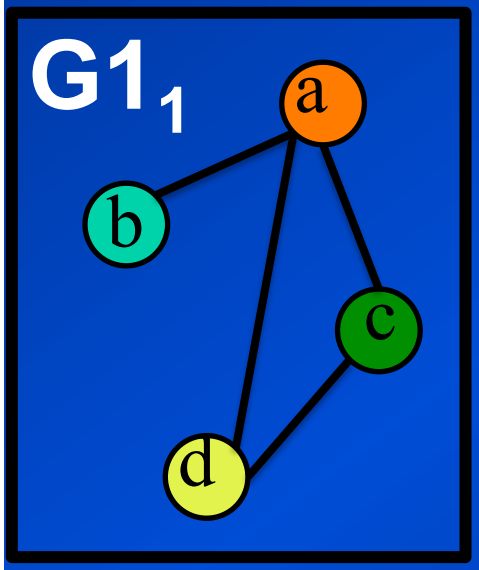
Examples:



G1

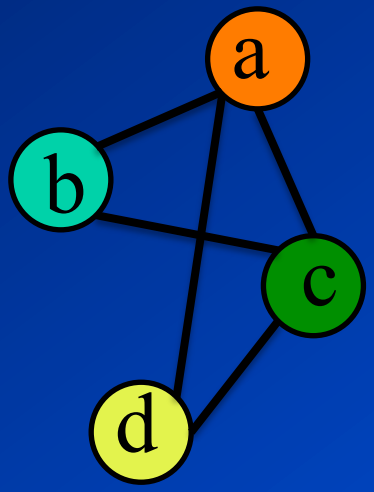
G2





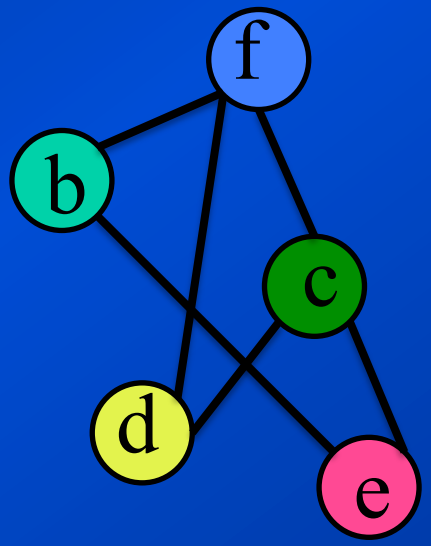
edge-removal(b,c)

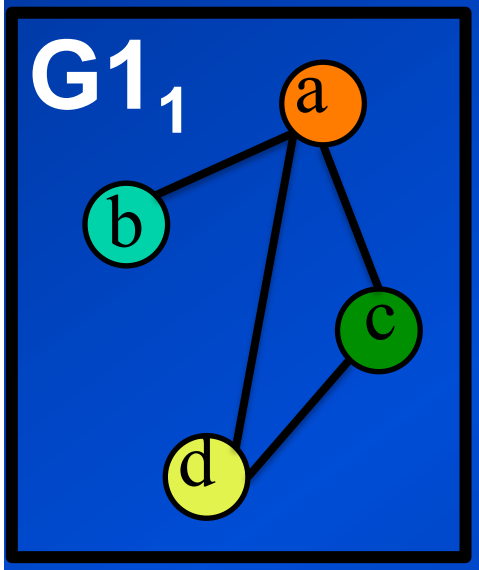
Examples:

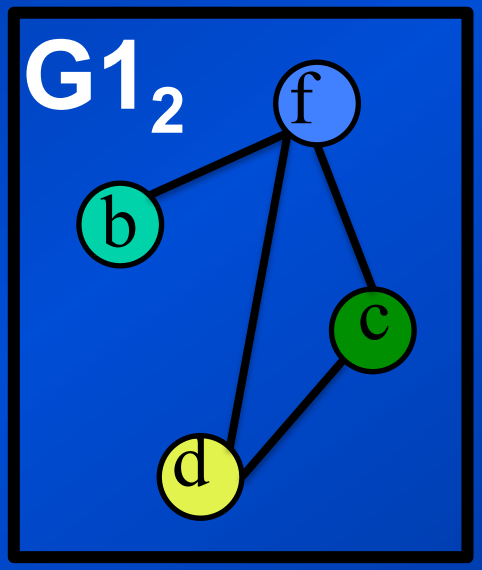


G1

G2

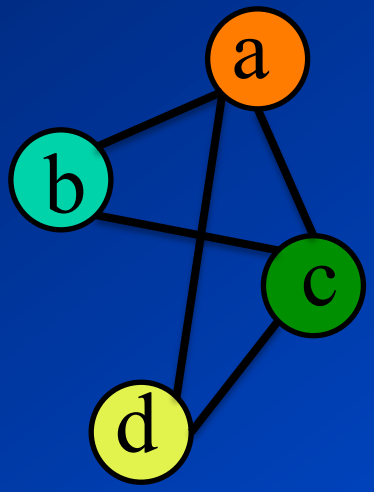






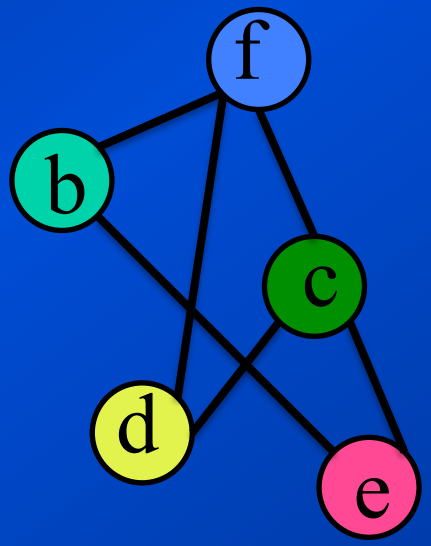
attribute-changing(a,f): attributes *a* of G1 and *f* of G2 are compatible

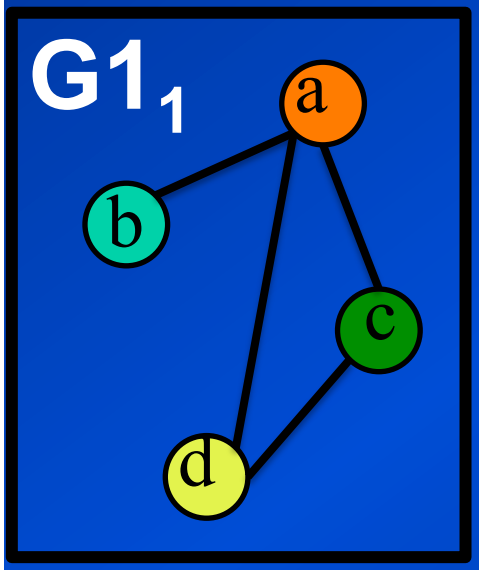
Examples:

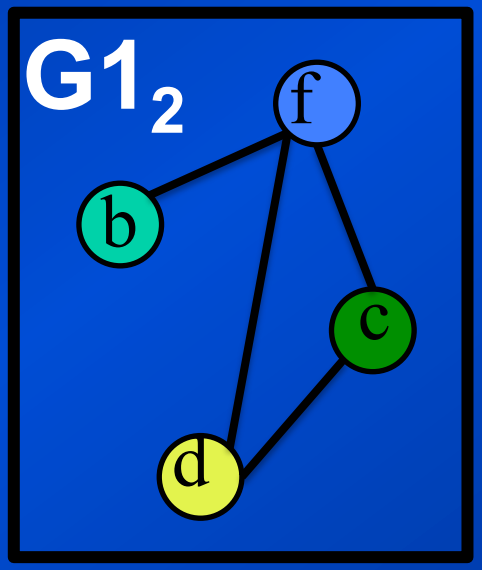


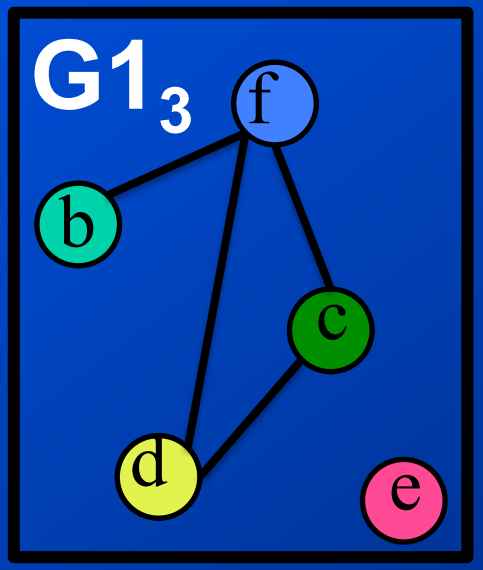
G1

G2



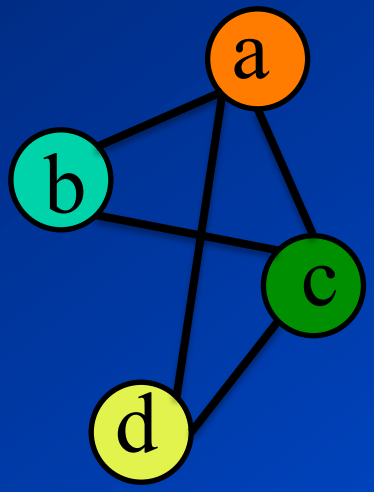






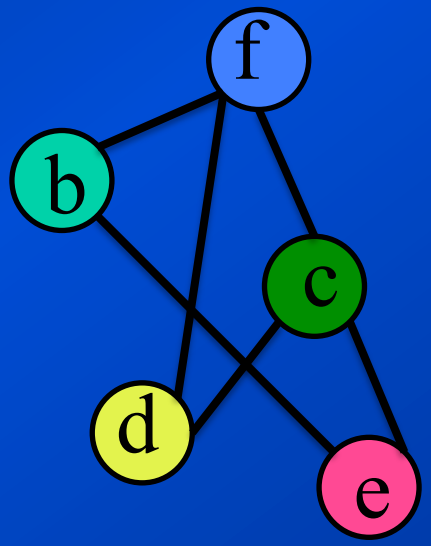
node-addition(e)

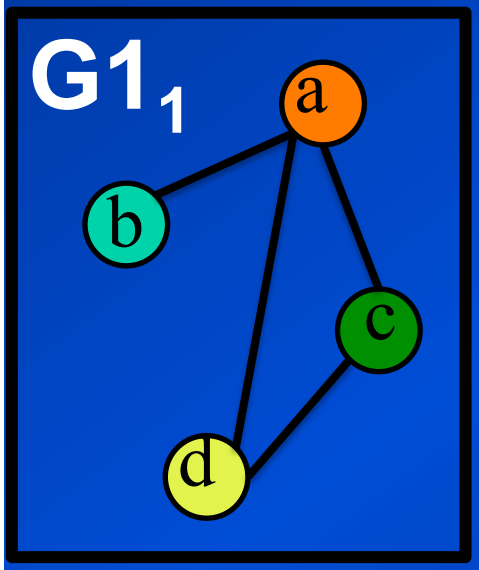
Examples:

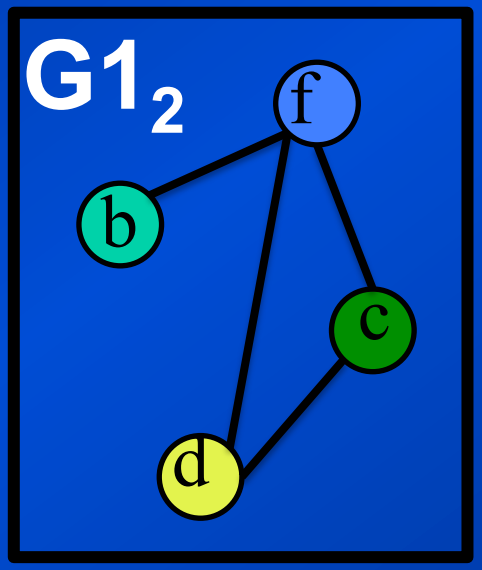


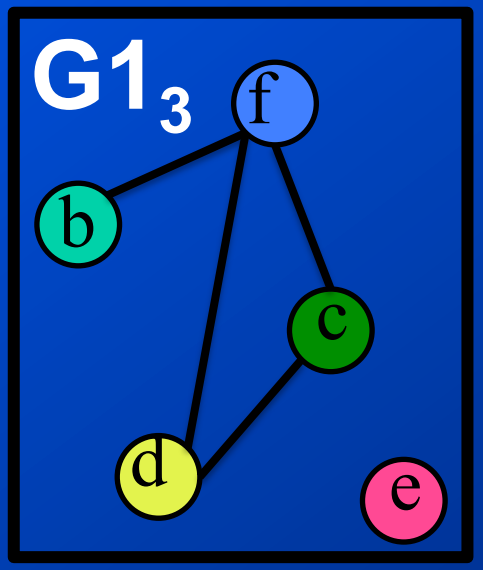
G1

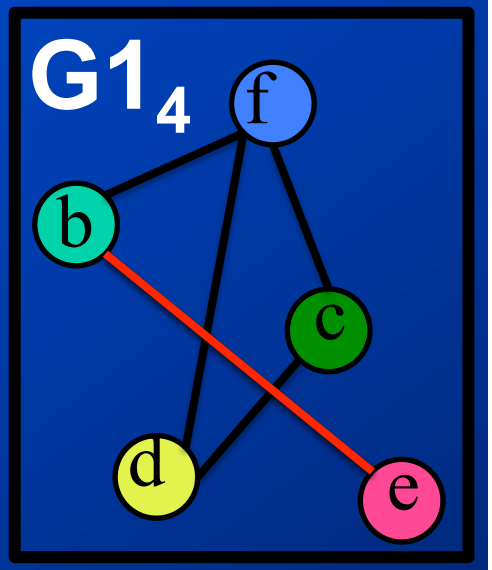
G2





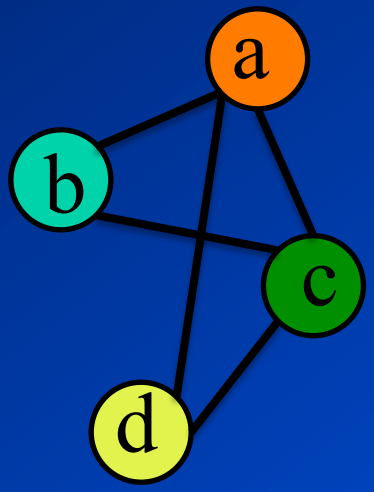






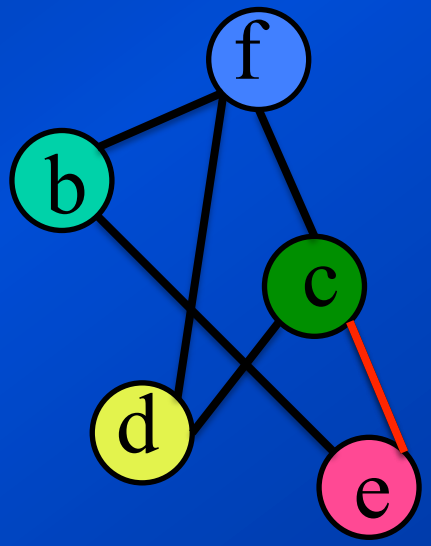
edge-addition(b,e)

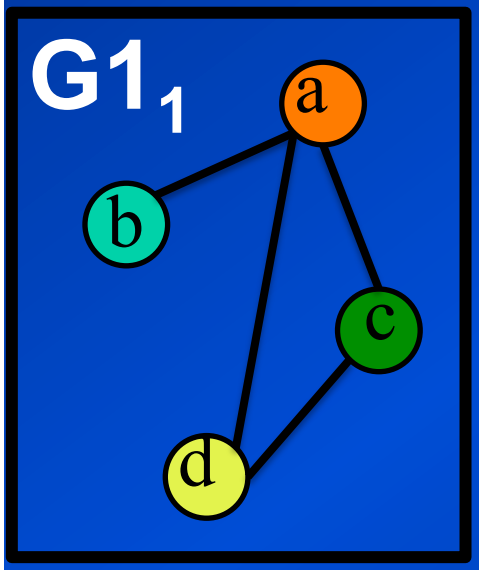
Examples:

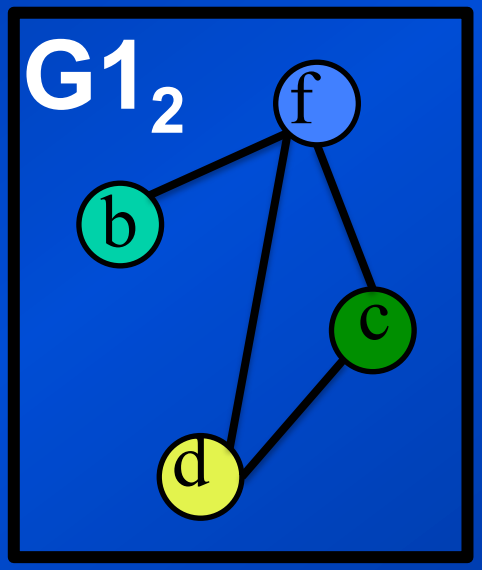


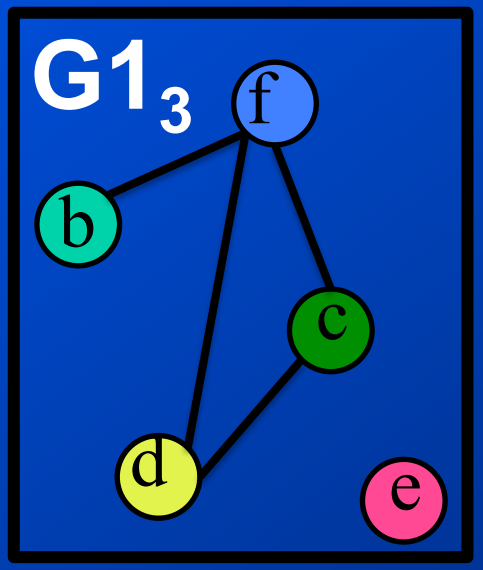
G1

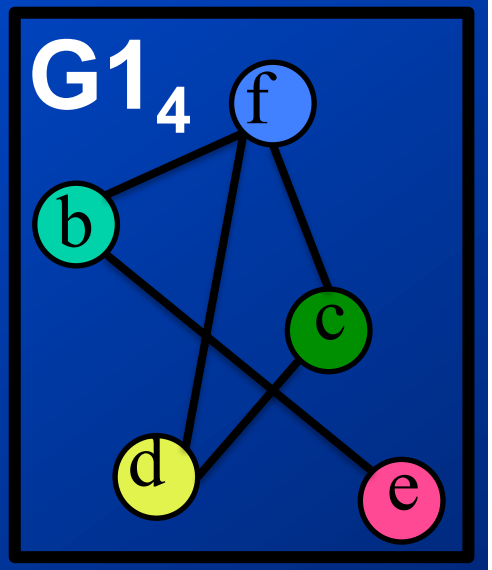
G2





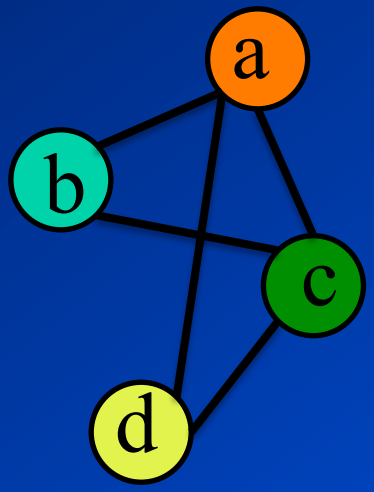






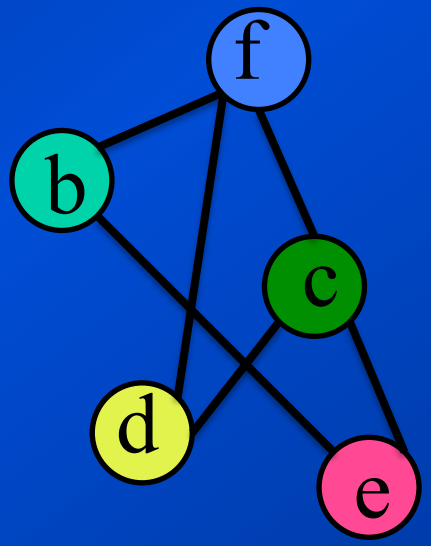
edge-addition(c,e)

Examples:

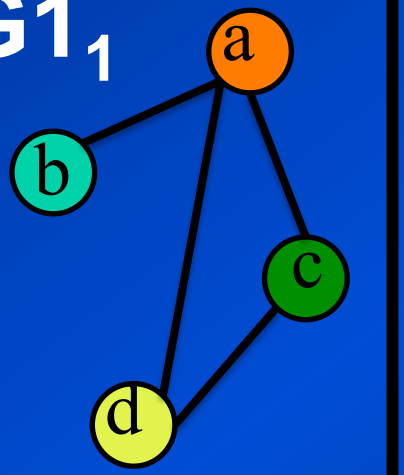


G1

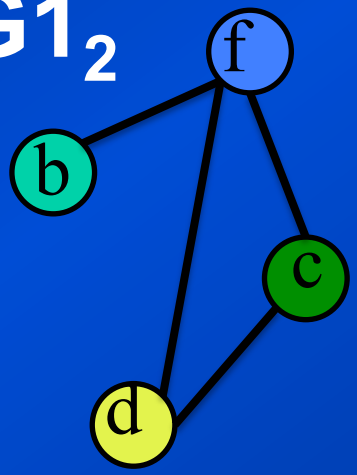
G2



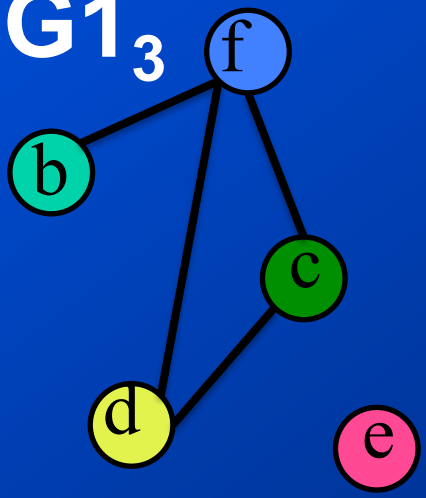
$G1_1$



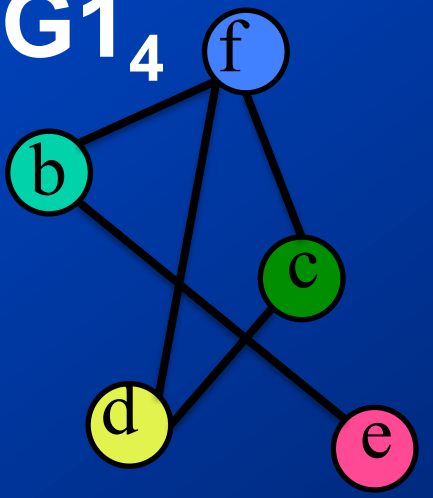
$G1_2$



$G1_3$



$G1_4$

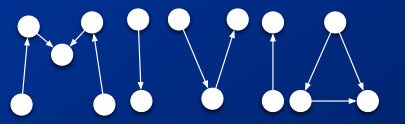


Error-correcting Edit distance

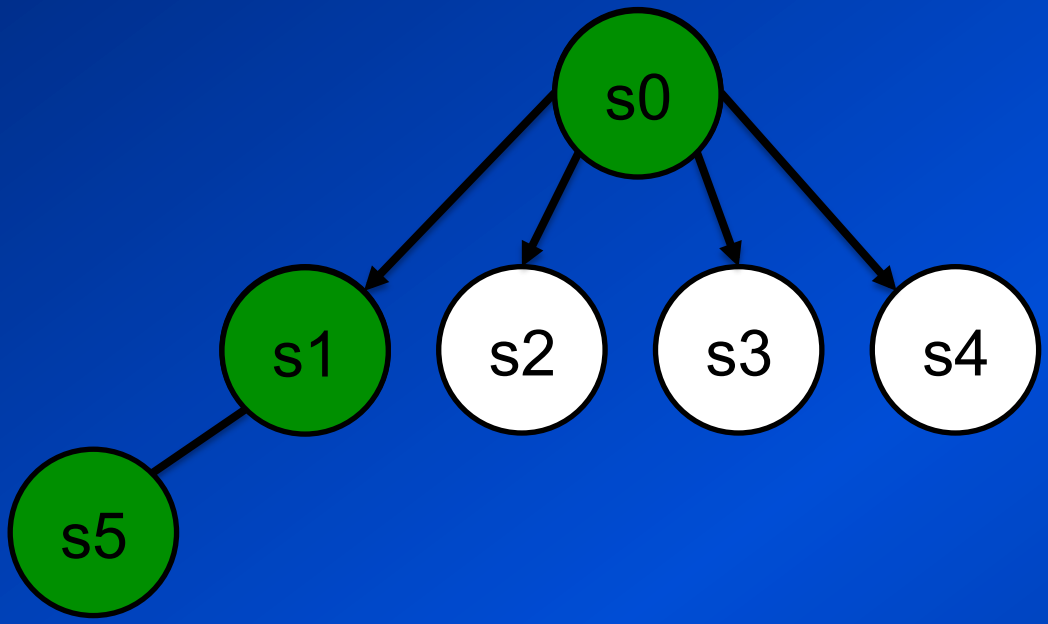
- Uses a tree based search for finding the edit paths which can tranform G1 into G2 having the minimum cost
- The algorithm works into SSR: a path in the tree represents an edit path among the graphs
- A current edit-path is closed if it allows to reach a same intermediate state with an higher edit-cost

IGM: Tree Search

- Use tree search with backtracking.
- Direct the search by the cost of the Partial Matching.
- Use, as heuristic, estimate of the matching cost for the remaining nodes.
- Use A* like algorithm to prune unfruitful paths.



IGM: Tree Based Edit-Paths



M(s0) = {0}

M(s1) = {(1,A)}

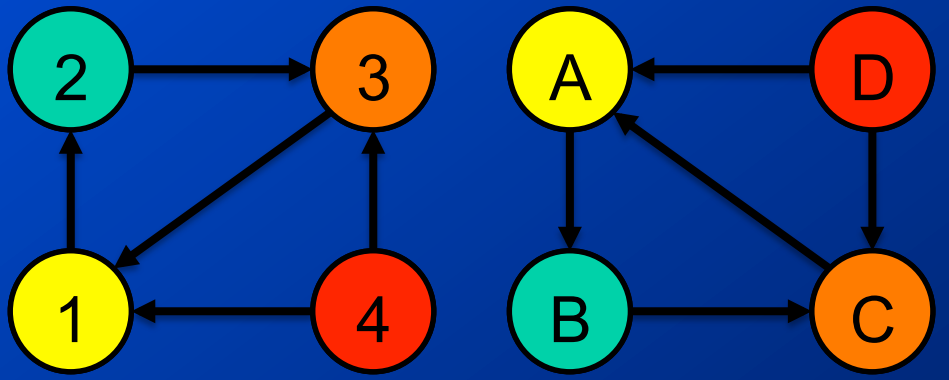
M(s2) = {(1,B)}

M(s3) = {(1,C)}

M(s4) = {(1,D)}

M(s5) = {(1,A) , (2,B)}

Each state represents a possible partial matching by considering the needed edit operations and a cost is associated to.



Impure Methods

Basic operations in a vector space

- Impure methods report in the graph space the main operations defined in a vector space
- The idea is to reuse on graphs the basic methods in SPR:
  - The first important achievement is the concept of distance between graphs

Impure Graph Matching and Learning

- Once the graph distance has been defined we can reuse effective SPR methods for learning and classifying graphs, as:
  - NN, K-NN, (K-K')-NN
- The latter allows to solve a supervised classification problem given a set of labelled graphs, only using the distance

Are we ready?

- We have a graph distance (edit cost dist.)
- … not all the properties are always valid:
  - $D(G_1,G_2) \geq 0$
  - **$D(G_1,G_2) = D(G_2,G_1)$ Doesn't hold**
  - **$D(G_1,G_x) \leq D(G_2,G_x) + D(G_x,G_2)$ Triang disequality holds only using exhaustive A* search of edit-cost searching algorithm**
- It's a similarity measure not a distance

NN Classifier

- Given a set S of labeled graphs (reference set)
- An input graph G (to classify)
- The graph G_x of S having the minimum edit distance from G is determined
- G is assigned the class of G_x
- With simple variants we obtain K-NN and (K-K')-NN

Other achievements with graph distance

- Many learning procedures in a vector space use the centroid of points as a prototype (K-means clustering)
- Points are graphs and centroids prototypes.
- We are required to define graph centroids:
  - Median graphs
  - Generalized Median Graph

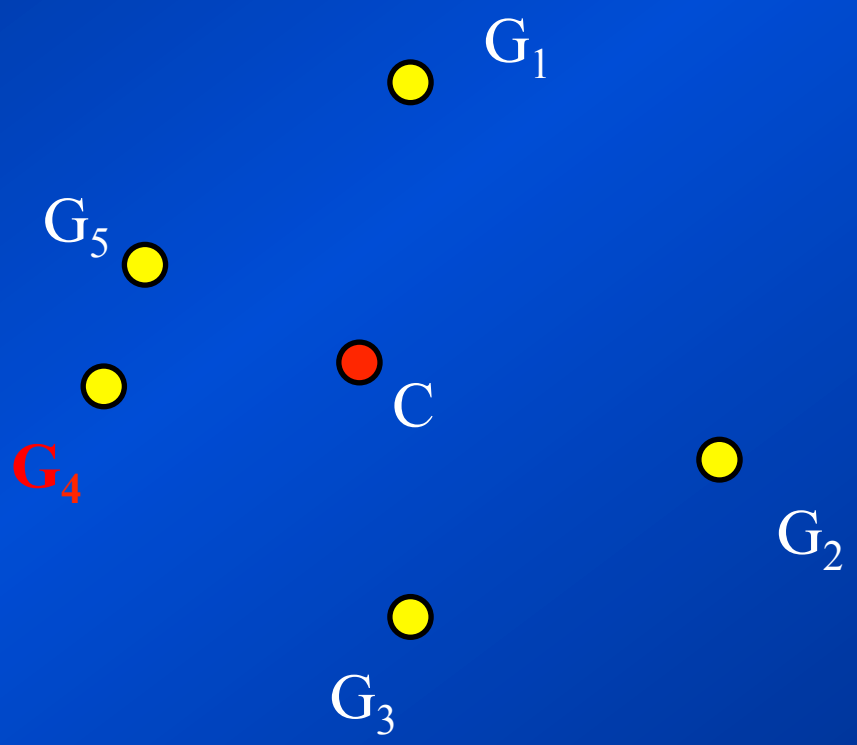
Graph prototype as the median graph

- Given a set S of graphs of a same class, a prototype C of S is the graph which minimizes the sum of its distances from the graph in S (Median Graph)

$$\hat{S} = \underset{g_1 \in S}{\operatorname{argmin}} \sum_{g_2 \in S} d(g_1, g_2)$$

Differences with a space vector: the space is discrete and the median graph belonging to S!

From Median to Generalized Median Graph

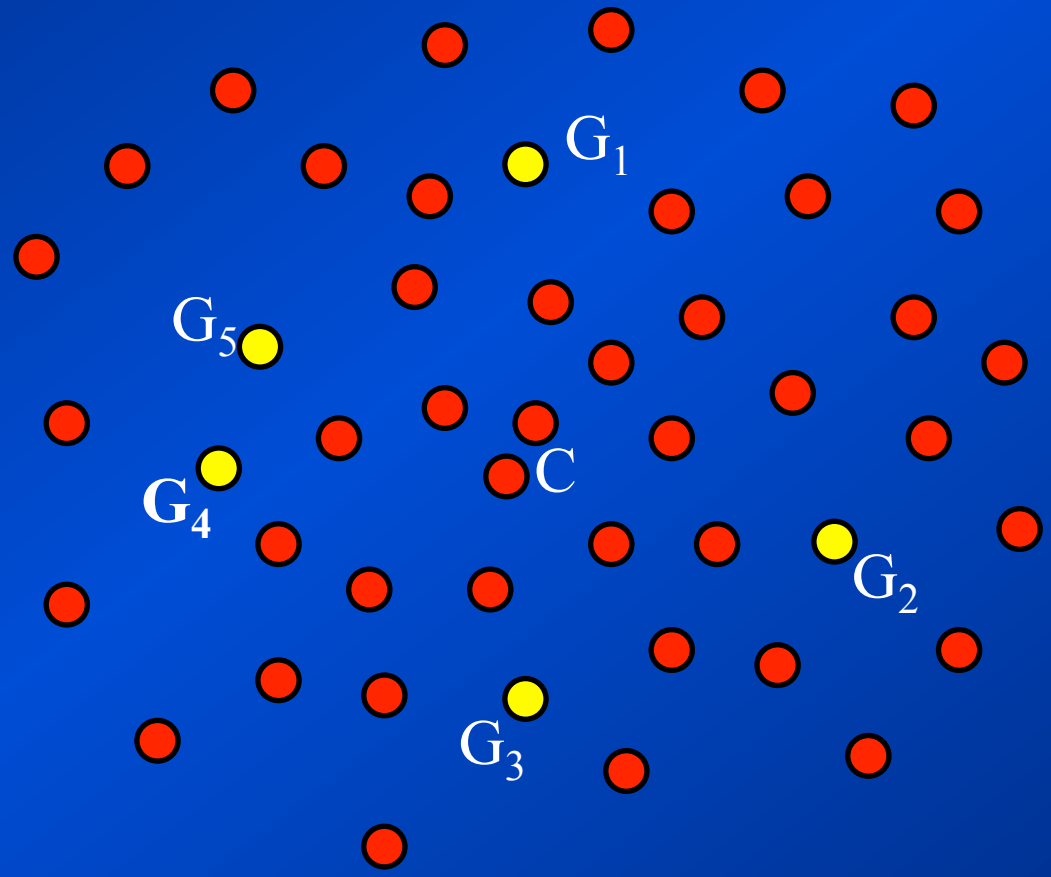


Improving graph prototypes

- The graph Generalized Median of a set S of graphs graph is obtained by preliminarily buiding S'
- S' is a very wide set of graphs obtained by the graphs in S changing in any possible mode all the (edge and node) labels to any of the graphs in S

$$\hat{S} = \underset{g_1 \in S}{\operatorname{argmin}} \sum_{g_2 \in S'} d(g_1, g_2)$$

From Median to Generalized Median Graph



Another achievement

- Up to now:
  - NN Classifiers
  - Supervised Clustering
- Going ahead:
  - Weightd Sum of Graphs: the graph obtained as cG1 + aG2

We can reuse LVQ

- A simple LVQ algorithm determining the vector centroids of n classes C_1, C_n, is:
- 1) Pick a graph G_{in} randomly from TS and calculate the nearest quantization graph C_w
- 2) Move C_w (median graph) towards G_{in} by a fraction of the distance, if the class of Cw is correct, otherwise move in the opposite
- Repeat until the total error on the training becomes stable

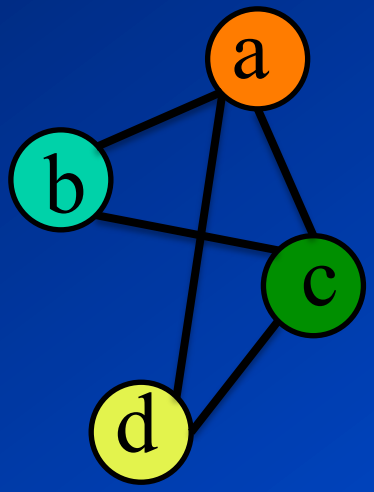
Extending LVQ to Graphs

- Given two graphs G_1 and G_2 we need to tranform G_1 into another graph G' so as to reduce the distance between G' and G_2

Graph LVQ: What we need? 2/2

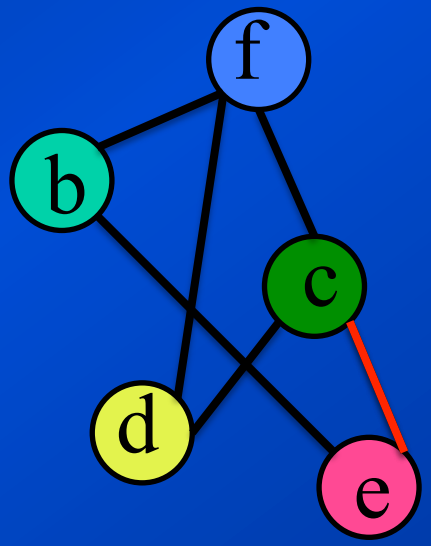
- The distance between graphs gives the edit operations $e_1, e_2, \ldots, e_k$ that transform G_1 into G_2 with minimum cost
- Dropping the k first edit operations, we have a new sequence that transforms G' into another graph G_2
- It derives that G' is more similar than G_1 to G_2 by the amount given by the sum of the edit cost dropped

Example:



G_1

G_2



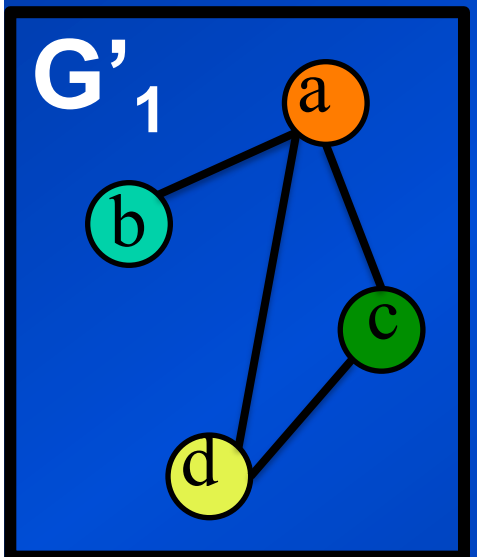
C1

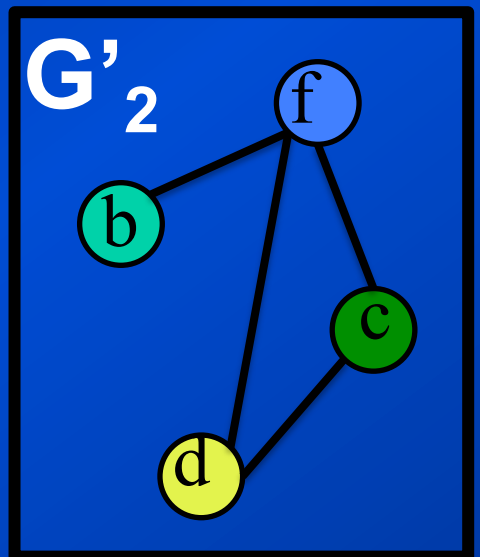
C2

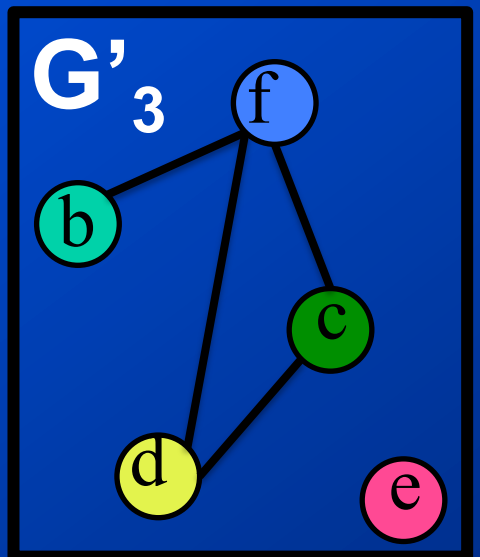
C3

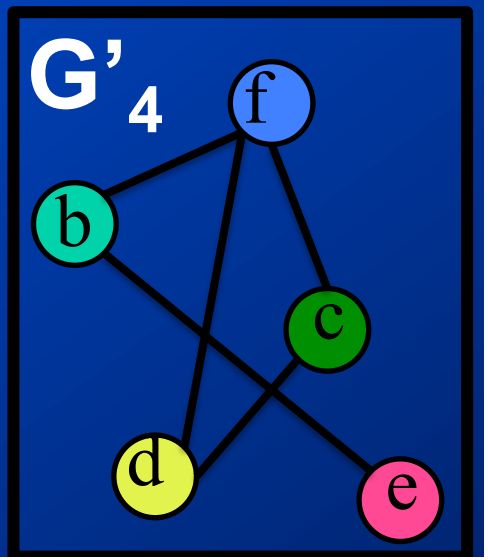
C4

C5









Further acquisitions

- Any other learning algorithm based on distance can be used:
  - Unsupervised Self Organizing Maps

Considerations

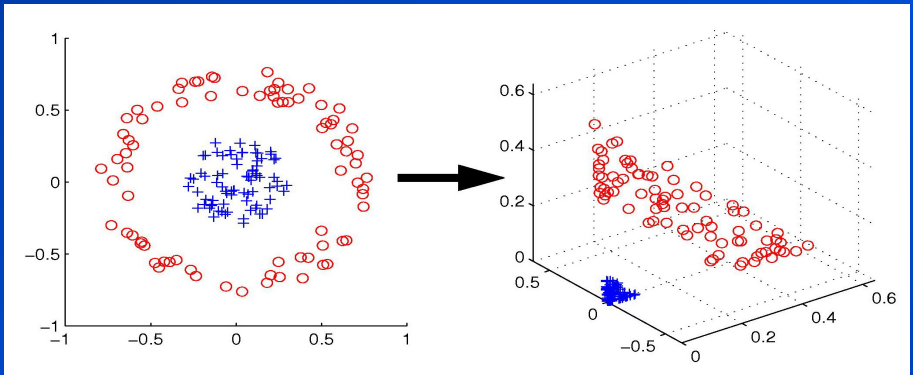
- The extension to graphs of vector space operations has a practical huge impact:
  - Standard learning and classification methods
- The theoretical framework isn't robust:
  - the graph distance is discrete, as related to edit operations!
  - This distance is affected by uncontrollable errors as the edit distance depends on domain-based edit cost assignment

Graph Kernels

Kernels in PR

- They allow to extend basic linear algorithms to complex non-linear ones
- Non-linear regularities in the data is inherently treated
- Under some conditions kernel methods give better results in difficult PR tasks than traditional methods (Svm Vapnik)

Kernel trick: Mercer's theorem



Given a vector space V_1 with a Kernel function K, there is at least another vector space V_2, usually having a higher dimensionality and a function F mapping V_1 to V_2, such as:

- For every a,b in V_1:
- $K(a,b) = F(a) \bullet F(b)$

Implications

- If the problem is not linearly separable it may became linear in the transformed space using a suited (unknown) kernel
- There is no guarantee that this happens even considering thousands of kernels
- Given a kernel there are no criteria to check whether it linearizes the problem

Graph Kernel: meaning

- Informally, a graph kernel can be considered as a measure of the similarity between two graphs;
- however its formal properties allow a kernel to replace the dot product in several vector-based algorithms using it (and other functions related to dot product, such as the Euclidean norm).

Implications

- The Kernel stands as dot product between the considered points in V_1
- With this assumption it's possible to reuse the Kernel machines:
  - SVM
  - PCA
  - Perceptron

Kernels on Graph

- A graph kernel is a function that maps a couple of graphs onto a real number

$$k : G \times G \rightarrow R$$

$$k(G_1, G_2) = k(G_2, G_1) \qquad \forall \; G_1, G_2 \in G$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i \cdot c_j \cdot k(G_1, G_2) \geq 0$$

Examples of graph Kernels

- $K(G_1,G_2) = 1$
- $K(G_1,G_2) = n_1\, n_2$
- $K(G_1,G_2) = (n_1+e_1)\,(n_2+e_2)$
- $K(G_1,G_2) = \mathrm{Diam}(G_1)\,\mathrm{Diam}(G_2)$

- Are these examples good?

Basic criteria for building (hopely) a good graph kernel

- A Kernel should catch the similarity between graphs (the one good for the application at hand). For any graph:

  If $K(G_1,G_2) > K(G_3,G_4)$, it is worth that:

  $Similarity(G_1,G_2) < Similarity(G_3,G_4)$

Note that the latter is not trivial; semantic cannot be simply included

Diffusion Kernels

- Applicable when we are dealing with a known finite set T of n graphs
- Defined on the basis of a similarity measure s (any kind on the graph space)
- From s a pairwise similarity matrix S is obtained:
  - $S=S_{ij}=s(G_i,G_j)\ i,j=1,n$

Diffusion Kernels

- Exponential diffusion Kernel (λ< 1)

$$\boldsymbol{K} = \sum_{k=0}^{\infty} \frac{1}{k!} \lambda^k \boldsymbol{S}^k = \exp(\lambda \boldsymbol{S})$$

- Neumann diffusion Kernel

$$\boldsymbol{K} = \sum_{k=0}^{\infty} \lambda^k \boldsymbol{S}^k.$$

Diffusion Kernels

- The sum is cut for practical issues
- Given G_i and G_j of the set T, their Kernel is the element (i,j) of the matrix
- Note that in the evaluation of K also other graphs will contribute (power of K)
- Heavy limitations for PR: closed sets of graphs

Convolution Kernel

- Convolution kernels infer the similarity of composite objects from the similarity of their parts:
  - Similarity between the parts are simpler to define
  - Given the similarities between the simpler parts a convolution operation is applied in order to turn them into a kernel function

Convolution Kernels

- From G we obtain the set D of all its decompositions (e.g. the simplest is its decomposition into the set of its nodes)
- A kernel K_{ji} is required for each element of D (e.g. the distance between nodes)

$$\kappa(g,g') = \sum_{(g'_1,\ldots,g'_d)\in R^{-1}(g')} \sum_{(g_1,\ldots,g_d)\in R^{-1}(g)} \prod_{i=1}^{d} \kappa_i(g_i,g'_i).$$

Pros and Cons

- Well established theoretical assumption
- Usually they have a high computational complexity (it mainly depends on how the graph is decomposed)
- An example: decomposing the graph in its walks

Random walk kernel

- They measure the similarity of two graphs by evaluating the number of random walks in both graphs sharing some properties
- Note: The number of matching walks in G_1 and G_2 can be computed by means of the direct product of the two graphs, without explicitly enumerate the walks.

Other Recents

- Laplacian Kernel: an evolution of the diffusion kernels
- Treetlet Kernel: a particular case of the convolution kernels; the graphs are decomposed in terms of treelet (a node with its neighborhood)

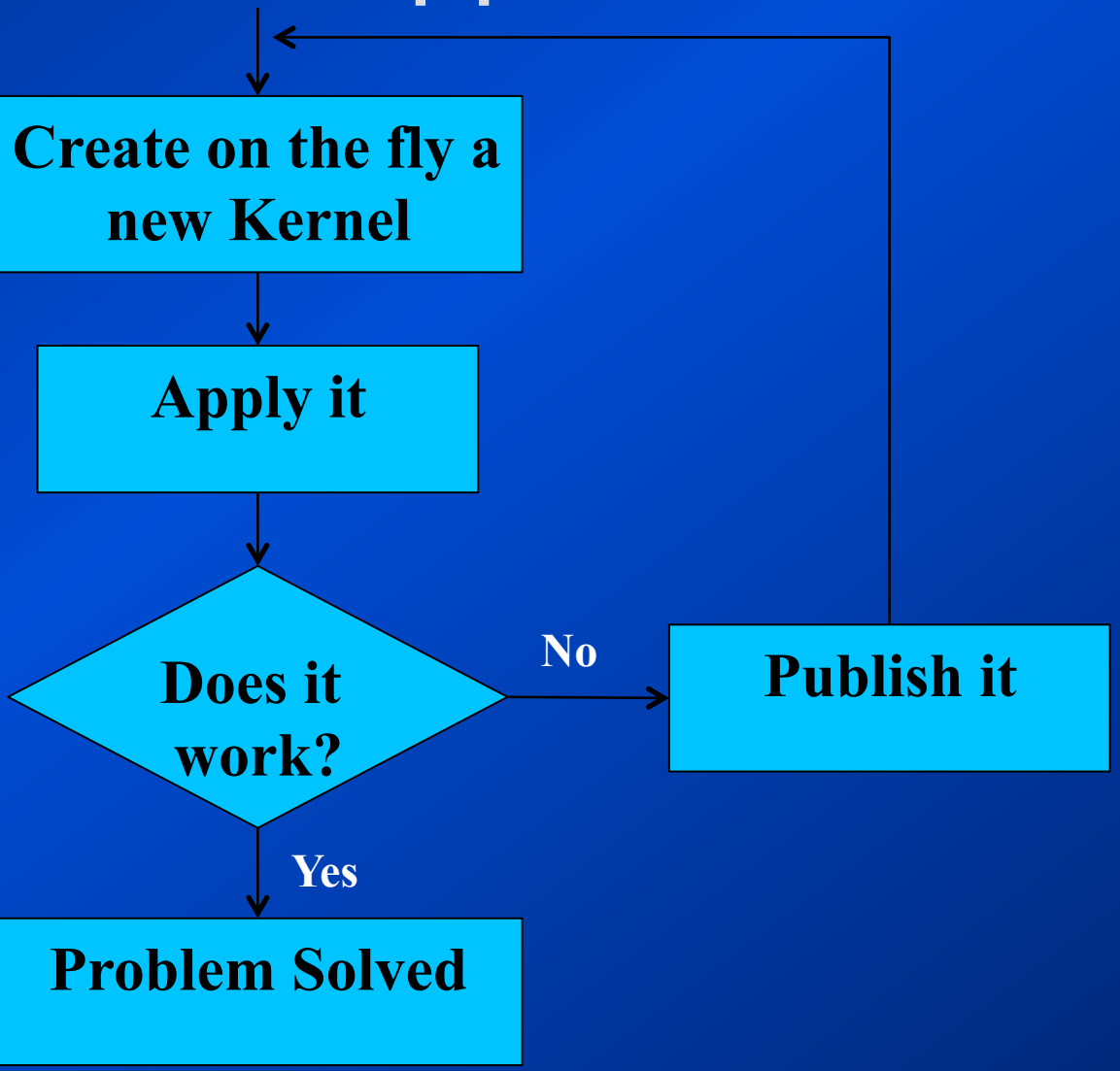
Kernel on Graph Distance

- By Bunke: Graph distance as kernel; requires a 0-pattern (difficult to define)
- Other kernels: sum and the product of the previous over a set of 0-patterns
- Same theoretical properties, but more robust with respect to the choice of 0-pattern

Kernels: Conclusions?

- Mercer's theorem doesn't hold for graph kernels! Even the (few) guarantees of this theorem are lost
- The actual performance strongly depend on how appropriate is for task at hand the used similarity measure included in the graph kernel

The Kernel approach

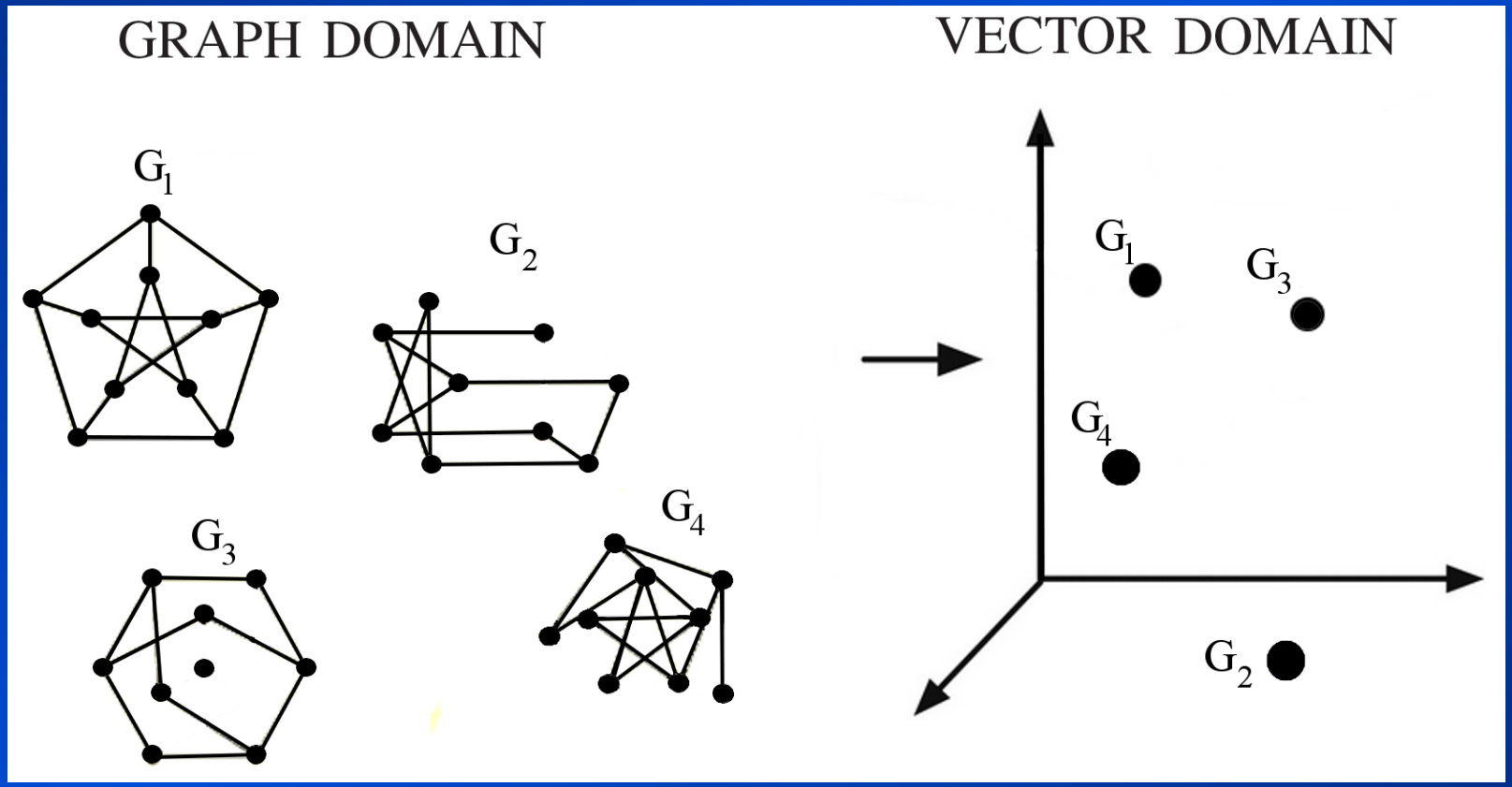


Extreme methods: Graph embedding

Graph embedding

- Graph embedding is used with two slightly different meanings:
- maps the nodes of a graph onto points in a vector space; nodes having similar structural properties will be mapped onto points which are close in this space;
- maps whole graphs onto points in a vector space, in such a way that similar graphs are mapped onto close points.

Graph Embedding



Graph embeddings

- It is easy to define a graph embedding...
  - any function from a graph g to a vector can be considered an embedding!
- ... But how effective is it?

Graph embeddings

- … the embedding should be invariant wrt node permutation...
  - ... so the adjacency matrix viewed as a vector is definitely NOT a good embedding
- ... but this is not enough!
  - for instance, the vector (Nn, Ne) with number of nodes and edges is invariant wrt permutations, but it is hardly an effective embedding in most applications

Graph embeddings: better properties

- Graphs that are similar should be mapped to vectors that are close according to a simple metric
- graphs that are different should be mapped to vectors that are distant
- ... but of course, “similar” and “different” depends on what one wants to use the graphs for...

Graph embeddings

- Representation by the eigenvalues of the adjacency matrix in decreasing order
  - the eigenvalues are invariant wrt permutation
  - a slight alteration of a graph does not change very much its eigenvalues
- ... this is the basis for several spectral embedding techniques.

Graph embeddings

- BUT....
  - unfortunately, there are very different graphs with the same eigenvalues...

Graph embeddings

- Currently the theoretical characterization of the embedding properties is still in its infancy...
  - ... no guarantees of suitability for any specific application: you have to try and cross your fingers...

Conclusions

- Pure methods: operations directly in the graph domain
- Impure methods: operations on vectors are turned into operations on graphs
- Extreme methods: graphs are entirely and directly reconducted to vectors

Pure Methods: Conclusions

- Pros: Management of contextual semantic information. Solid theoretical framework
- Cons: Few learning and classification algorithms available.
- Open issues: Reduction of computational complexity, Lack of efficient algorithms for MCS, Need of good symbolic graph learning methods, Theoretical models for evaluating upper-bound of the error for IGM, Exploiting applications in the Bio-informatics

Impure Methods: Conclusions

- Pros: Use of well known learning and classification algorithms derived from SPR.
- Cons: Lack of a theoretical framework for properly assigning edit cost in a general way. Discrete nature of the graph space. Contextual semantic cannot be directly handled.
- Open issues: Improving the edit graph distance. Improvements of weighted sum of graphs (too discrete). Improvements in theoretical assignment of edit cost on a domain.

Kernel Methods: Conclusions

- Pros: Kernel machines available
- Cons: No theoretical guarantee about the goodness of used Kernel. Contextual semantic cannot be directly handled.
- Open issues: Definition of a theoretical framework for evaluating the goodness of a graph kernels. Improvement of graph-based similarity Kernel.

Embedding Methods: Conclusions

- Pros: Potentially all SPR methods
- Cons: Very young theoretical framework
- Open issues: A lot of work to do…
- A bit of philosophy….
- Is it more convenient to start from patterns, obtaining graphs and then embed them, OR
- to try directly good representations of object into vecotors?