New Local Move Operators for Learning the Structure of Bayesian Networks

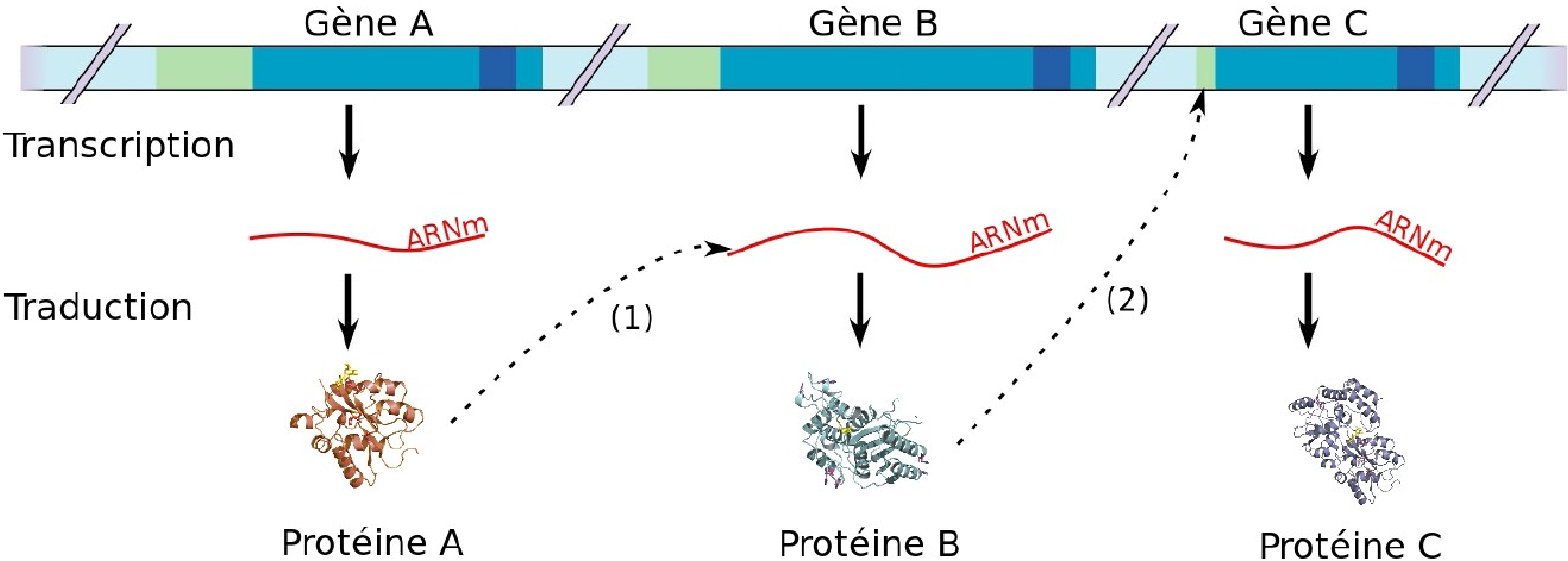
Jimmy Vandel, Brigitte Mangin & Simon de Givry

UR875 UBIA, INRA Toulouse

Plan

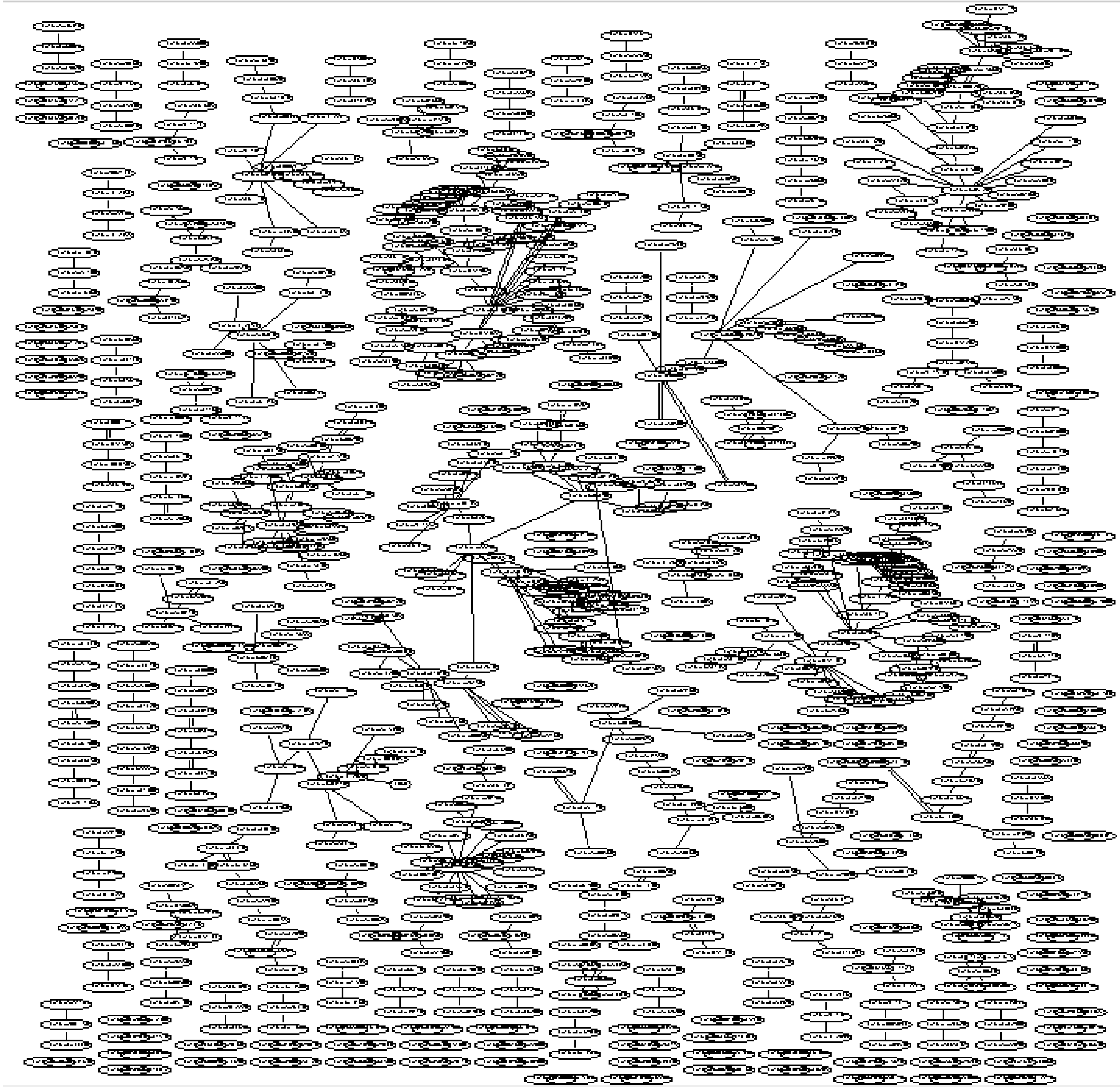
- Context
- Bayesian Network
- Stochastic Local Search (Greedy Search)
- New local move operators (*swap* and *swap**)
- Experiments on standard BN benchmarks
- Experiments in genetical genomics (DREAM 2012)
- Conclusion & perspectives

Different levels of regulation



Gene network of *trans regulations* for 2775 transcripts with high *eQTL* (LOD≥3) measured on 158 RIL Arabidopsis thaliana.

Bootstrap threshold = 0.3

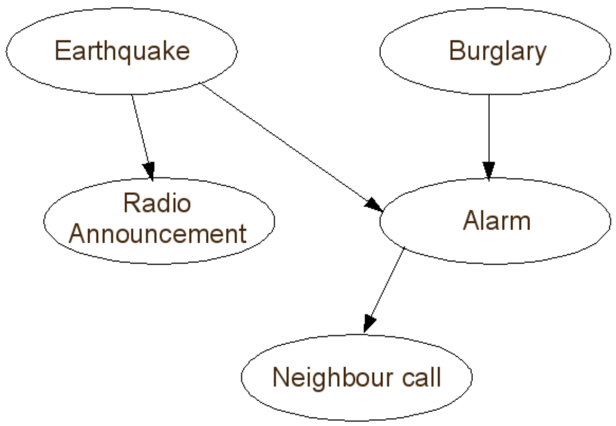


Discrete Bayesian network

Static Bayesian networks *(Friedman et al., Plos comput. bio., 2000)*

- Directed Acyclic Graph (DAG)
- Conditional probability distribution of X_i , given its parents Pa_i in G: $P_G(X_i / Pa_i^j) = \theta_i^j$

  (independence of these local probabilities)



Probability Distribution for the Alarm Node given the events of "Earthquakes" and "Burglaries"			
E	B	P(A | E,B)	P(!A | E,B)
E	B	0.90	0.10
E	! B	0.20	0.80
! E	B	0.90	0.10
! E	! B	0.01	0.99

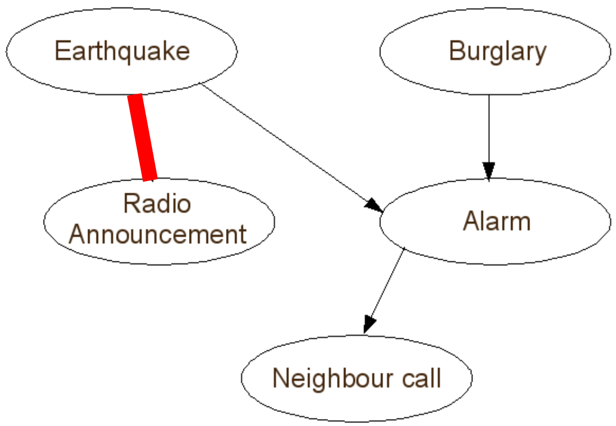
Graphic representation of a joint probability distribution:

$$P_G(X) = \prod_{i=1}^{n} P_G(X_i / Pa_i)$$

Discrete Bayesian network

$\{ Earthquake \perp Burglary , \ldots \}$

Partial DAG (PDAG)



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Structure Learning

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Alarm dataset (37 variables)

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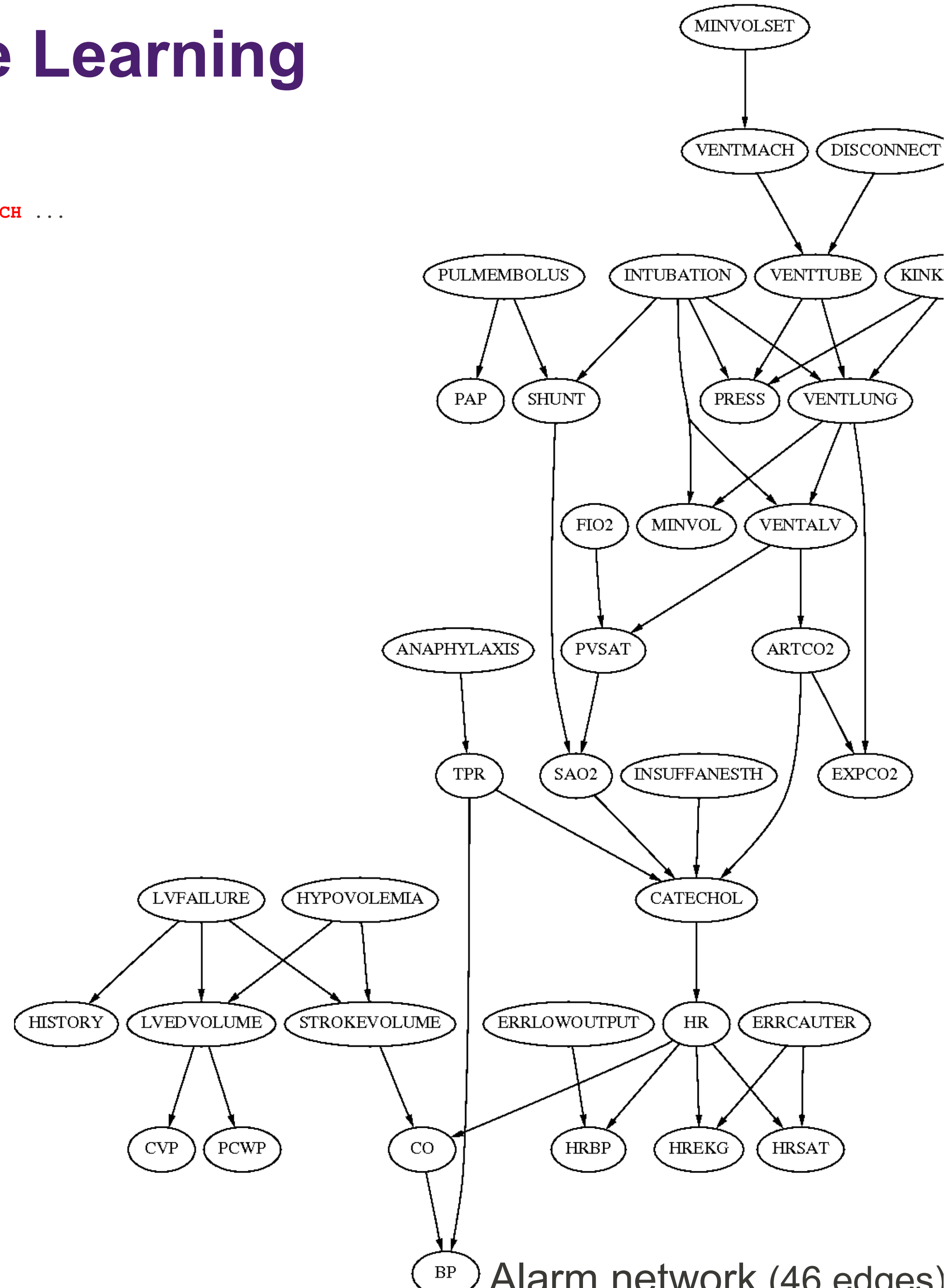

Alarm network (46 edges)

Score based learning

- We look for the graph maximizing an objective function
  - easy to evaluate, avoids over-fitting and Markov-equivalent
    - decomposable, penalized and equivalent scores
      - BDe score *(**D.Heckerman** Machine learning 1995)*
      - *BIC score (**G.Schwartz** Annals of statistics 1978)*

- Local score change from G to G' after operation OP_i modifying Pa_i

$$\Delta_{score} OP_i = f(G') - f(G) = f_{X_i}(G') - f_{X_i}(G)$$

(assuming G' is a DAG)

Local search components

1. Search space

   - Directed Acyclic Graph
   - Partial DAG (PDAG)

   - variable orders

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4. Meta-heuristics
   - greedy search (**GS**) (with restarts)
   - tabu search
   - simulated annealing
   - MCMC
   - genetic algorithms
   - ...

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PDAG	empty structure	addition & deletion	**GES**
		(*Greedy Equivalence Search*, Chickering 2002)	
DAG	empty structure	restricted 2 look-ahead	**LAGD**
		(*k Look-Ahead in l Good Directions*, Holland 2008)	

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   - **Directed Cyclic Graph**

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   - **swap of an edge ***
   - **Iterative operators ***

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   - **Stochastic Greedy Search**

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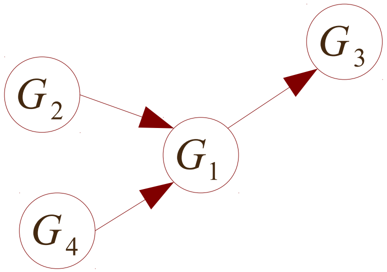
GS Algorithm

- **Greedy search**
  - *Start with an initial network (empty graph, a priori graph)*
  - *Score all possible local modifications (addition / deletion / reversal of one edge) and select the best of them (if it exist)*



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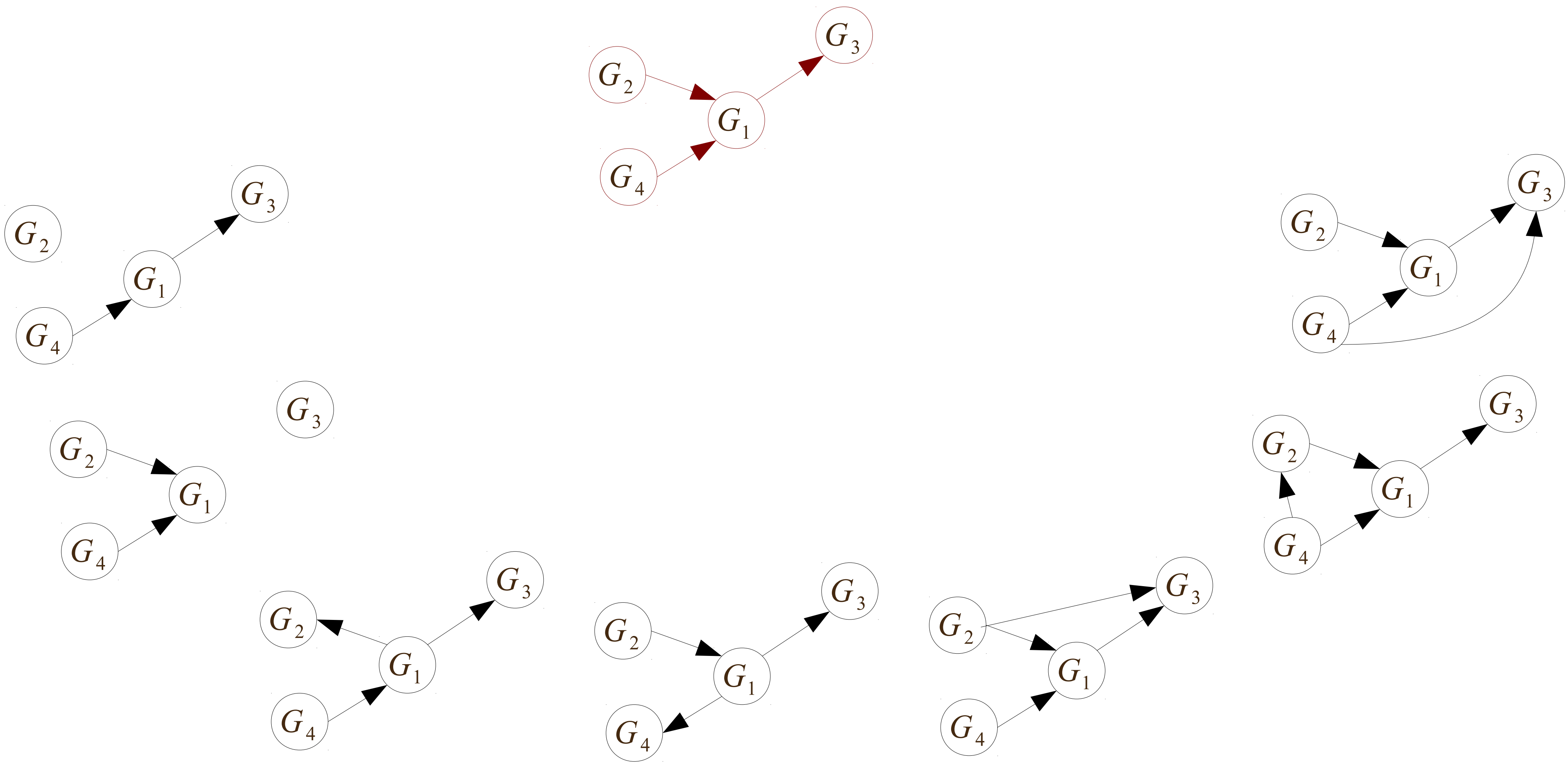

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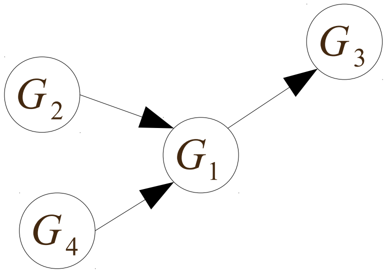

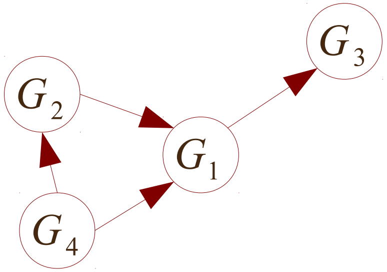

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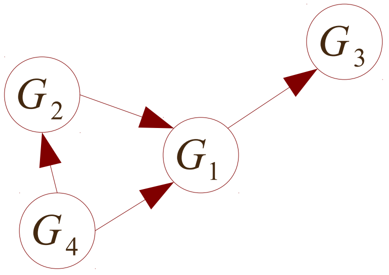

SGS Algorithm

- **Sochastic Greedy Search (SGS)**

classical Greedy Search (GS)
+
random edge orientation for Marvov-equivalent structures

- Markov-equivalent structures in Bayesian networks

G_1 G_2 G_3

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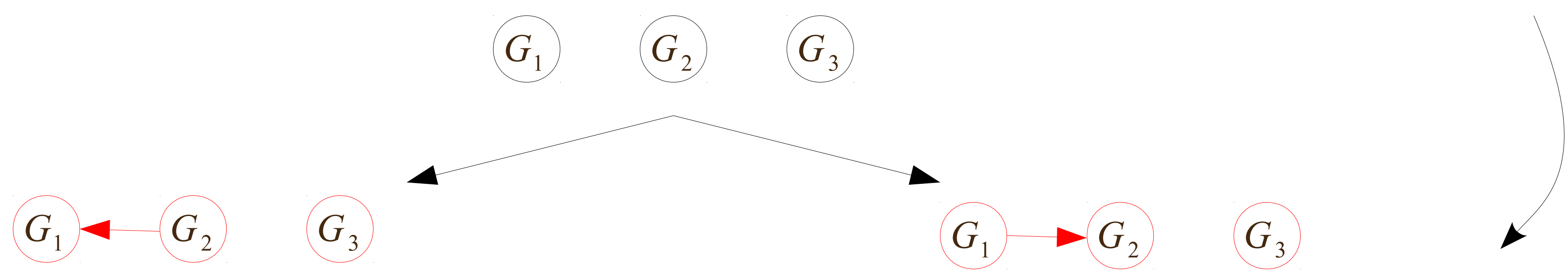
$G_1 \not\perp G_2$



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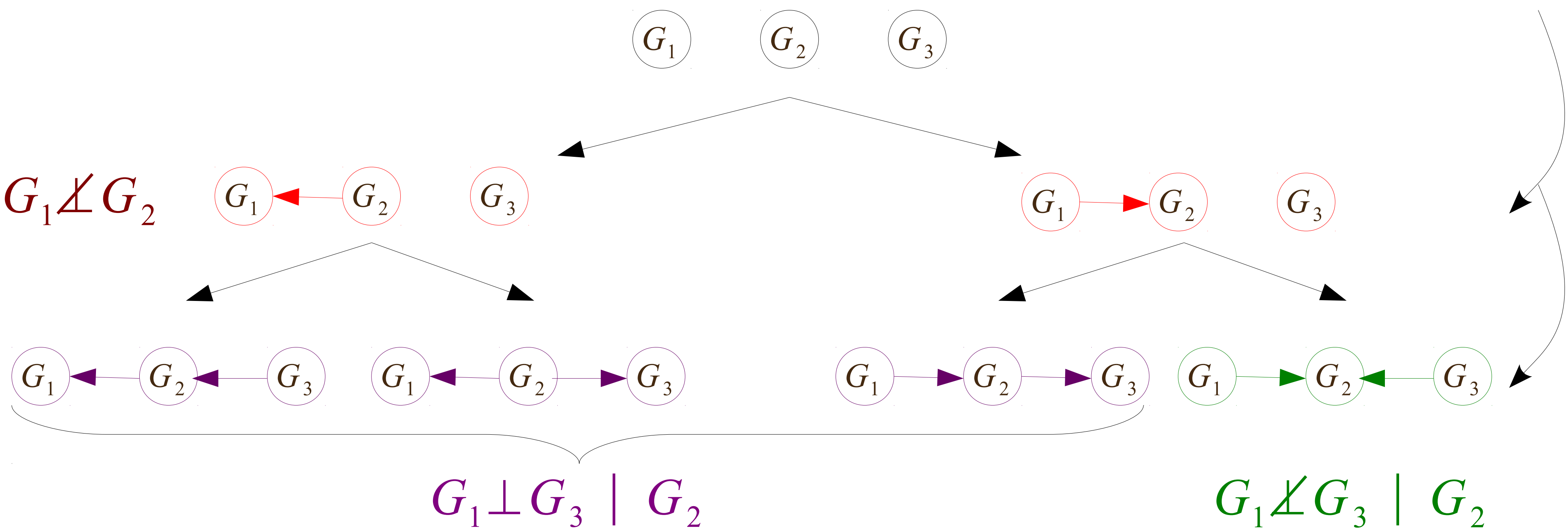

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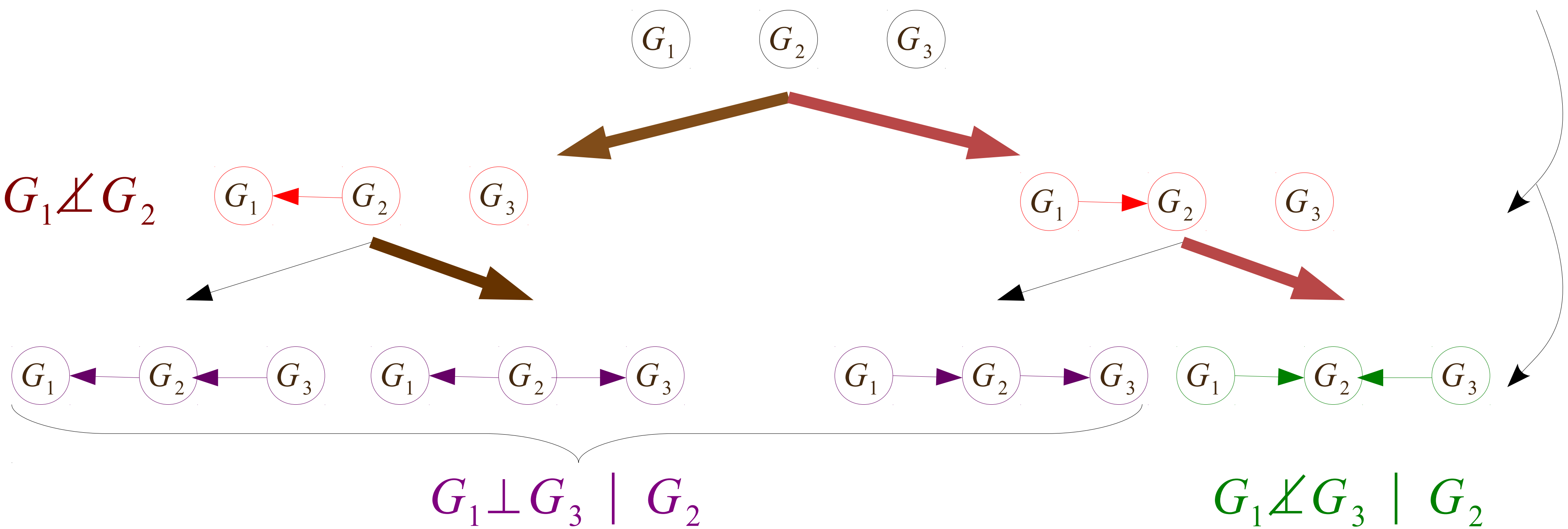

Swap Operator

- addition
- deletion
- reversal (deletion + addition on the same pair)
- **swap (deletion + addition including an extra node)**

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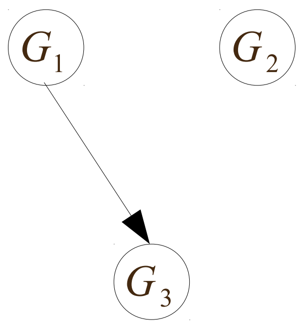
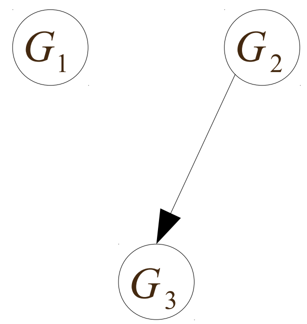
  <u>Example</u>:

Current situation



$$\Delta_{score} Add(G_{2,} G_3) > \Delta_{score} Add(G_{1,} G_3) > 0$$

Target situation



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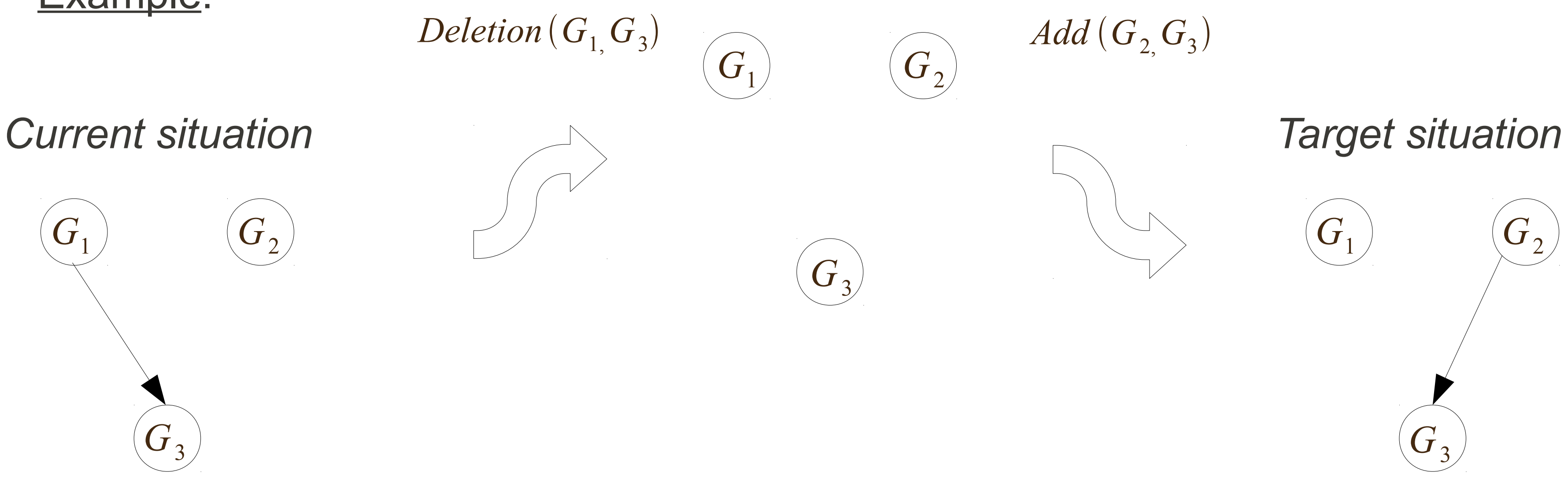

$$\Delta_{score} Add(G_2, G_3) > \Delta_{score} Add(G_1, G_3) > 0$$

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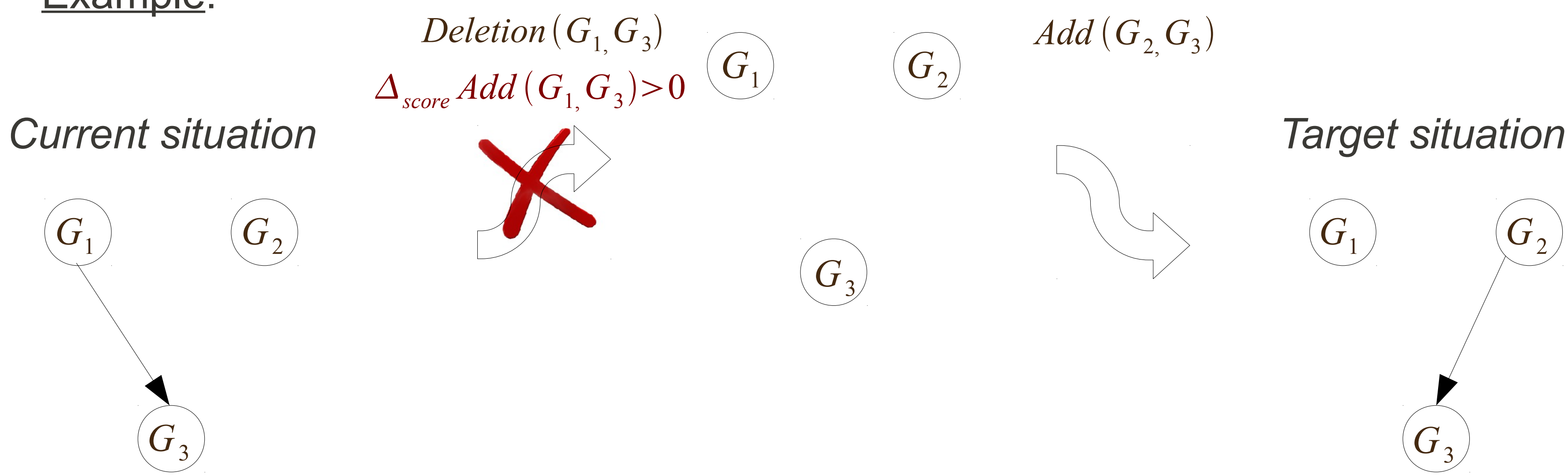

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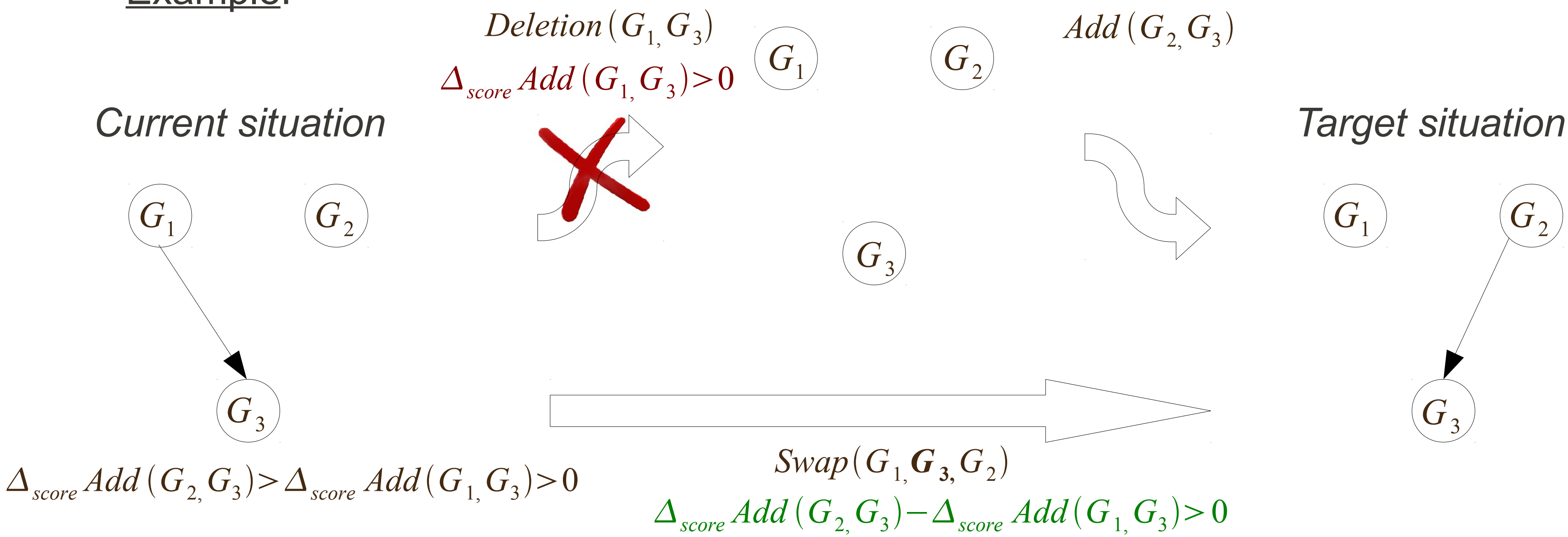


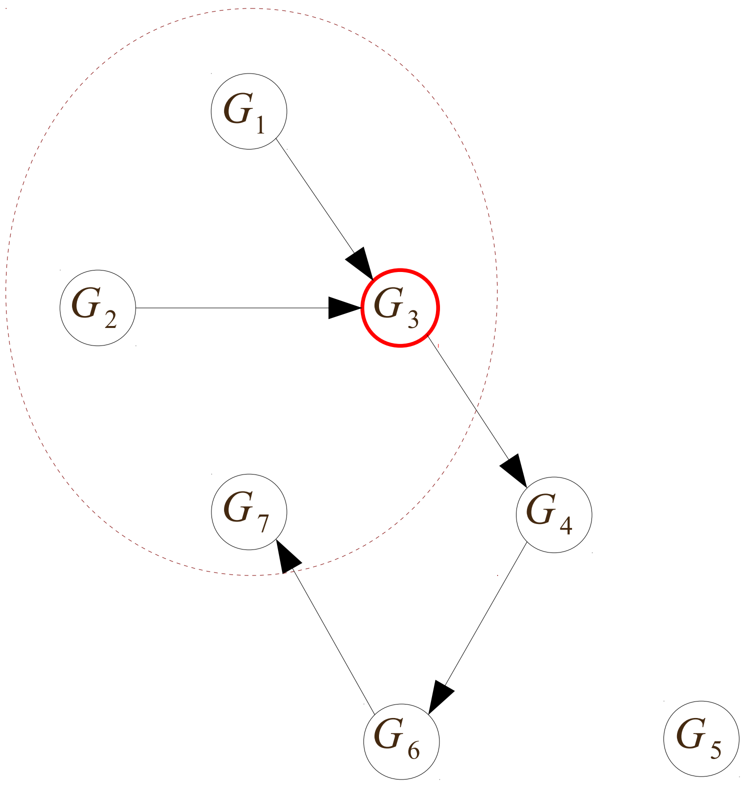
→ escape from some local maxima

Swap★ Operator

$Swap(G_{2,} \boldsymbol{G_{3,}} G_7)?$

Current situation

$\Delta_{score} Add(G_{7,} G_3|G_1) > \Delta_{score} Add(G_{2,} G_3|G_1) > 0$



Swap★ Operator

$$Swap(G_{2,} \mathbf{G_{3,}} G_7)? \longrightarrow Cycle\{G_{3,} G_{4,} G_{6,} G_7\}$$

Current situation

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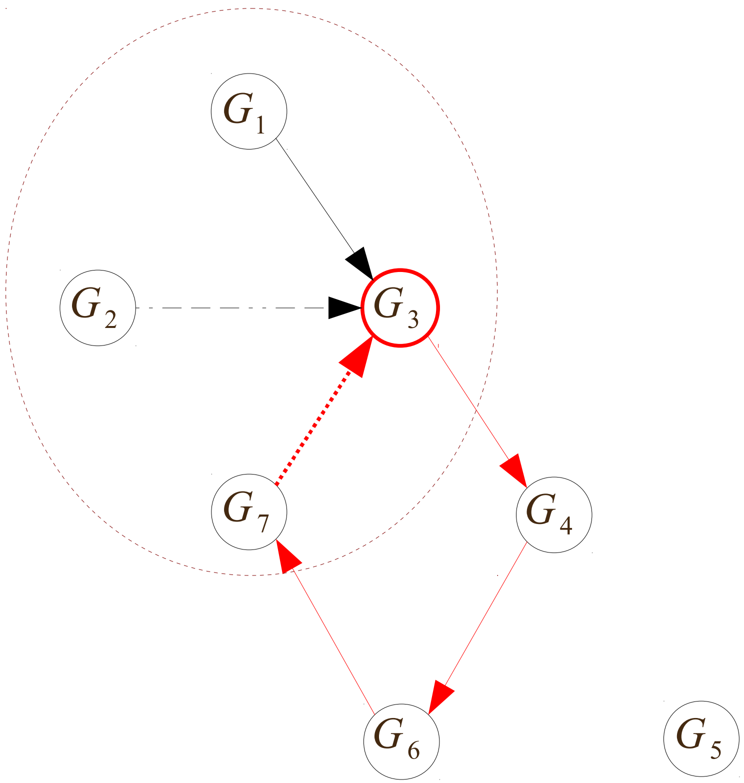
Objective : delete the cycles



Swap* Operator

$$Swap(G_2, \boldsymbol{G_3}, G_7)? \longrightarrow Cycle\{G_3, G_4, G_6, G_7\}$$

Current situation

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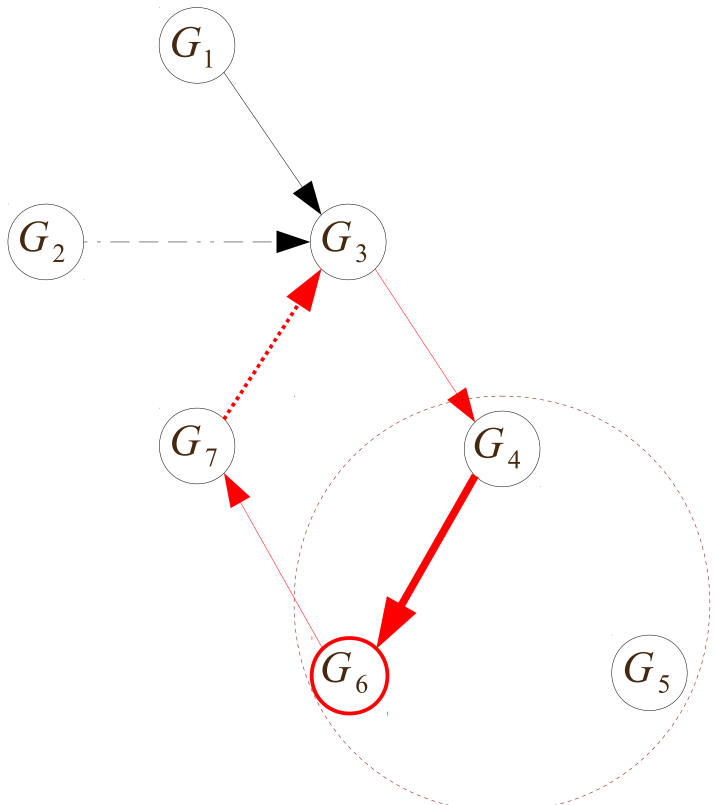


Objective : delete the cycles

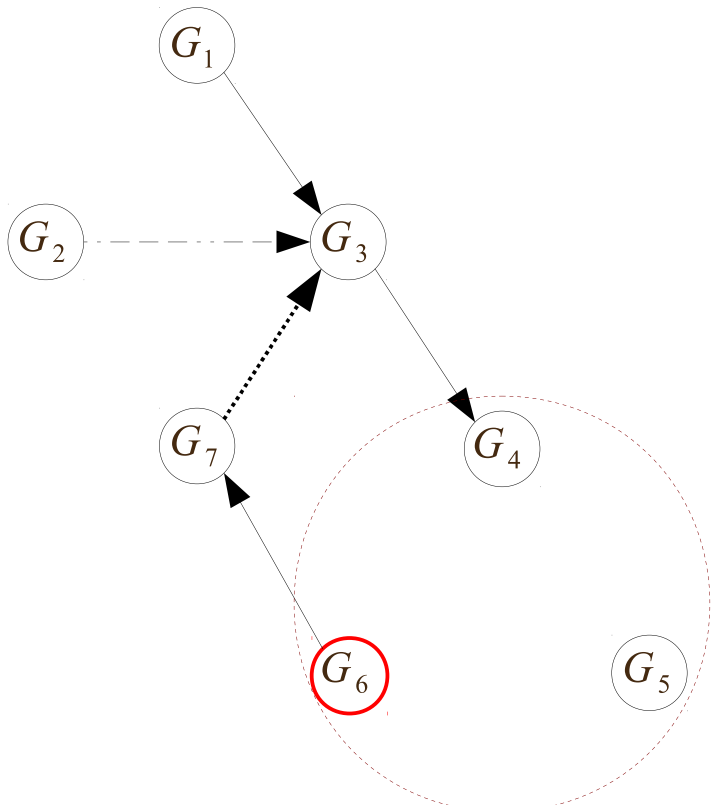
Step 1. Try to delete the edge minimizing $\Delta_{score} Add$

Swap* Operator

$Swap(G_2, \mathbf{G_3}, G_7)? \longrightarrow Cycle\{G_3, G_4, G_6, G_7\}$

Current situation

$\Delta_{score} Add(G_7, G_3 | G_1) > \Delta_{score} Add(G_2, G_3 | G_1) > 0$



Objective : delete the cycles

Step 1. Try to delete the edge minimizing $\Delta_{score} Add$

Improving score ?

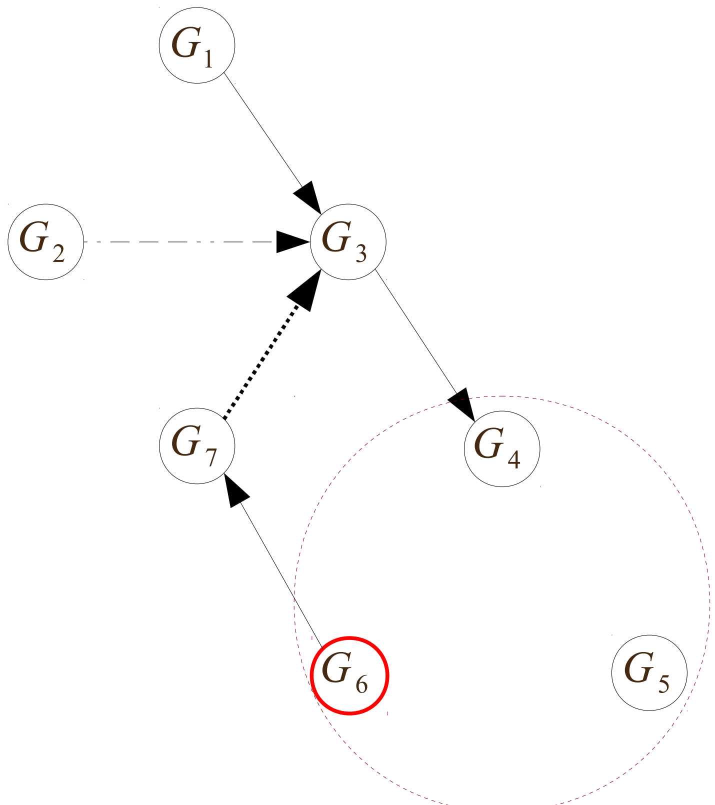
Yes

Swap★ Operator

$$Swap(G_2, \mathbf{G_3}, G_7)? \longrightarrow Cycle\{G_3, G_4, G_6, G_7\}$$

Current situation

$$\Delta_{score} Add(G_7, G_3|G_1) > \Delta_{score} Add(G_2, G_3|G_1) > 0$$



Objective : delete the cycles

Step 1. Try to delete the edge minimizing $\Delta_{score} Add$

Improving score ?

Yes → **Acyclic ?**

Yes → OK !

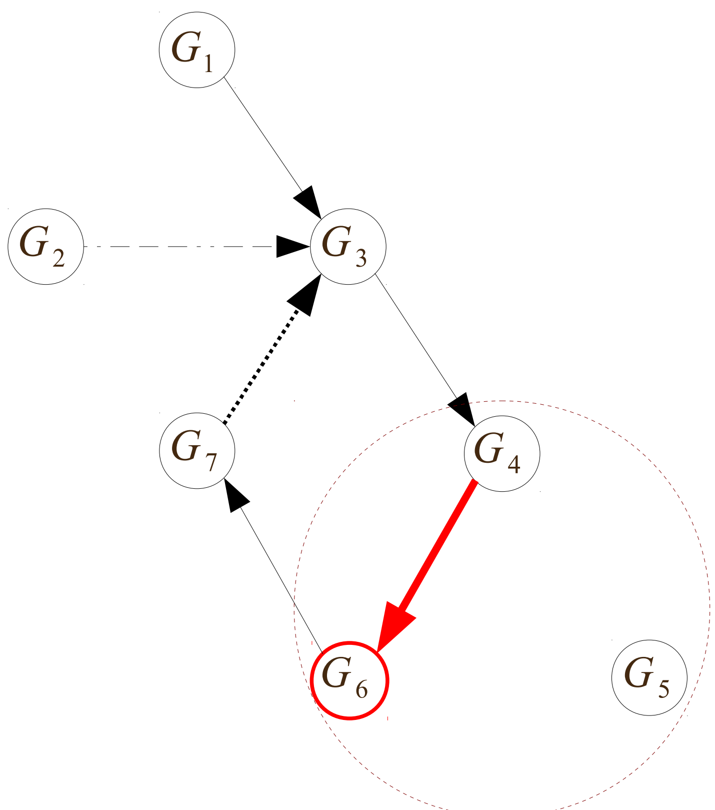
No → Return to Step 1

Swap* Operator

$Swap(G_2, \mathbf{G_3}, G_7)?$ $\longrightarrow$ $Cycle\{G_3, G_4, G_6, G_7\}$

Current situation

$\Delta_{score} Add(G_7, G_3 | G_1) > \Delta_{score} Add(G_2, G_3 | G_1) > 0$



Objective : delete the cycles

Step 1. Try to delete the edge minimizing $\Delta_{score} Add$

Improving score ?

Yes $\rightarrow$ Acyclic ?

Yes $\rightarrow$ OK !

No $\rightarrow$ Return to Step 1

No $\rightarrow$ Continue to Step 2

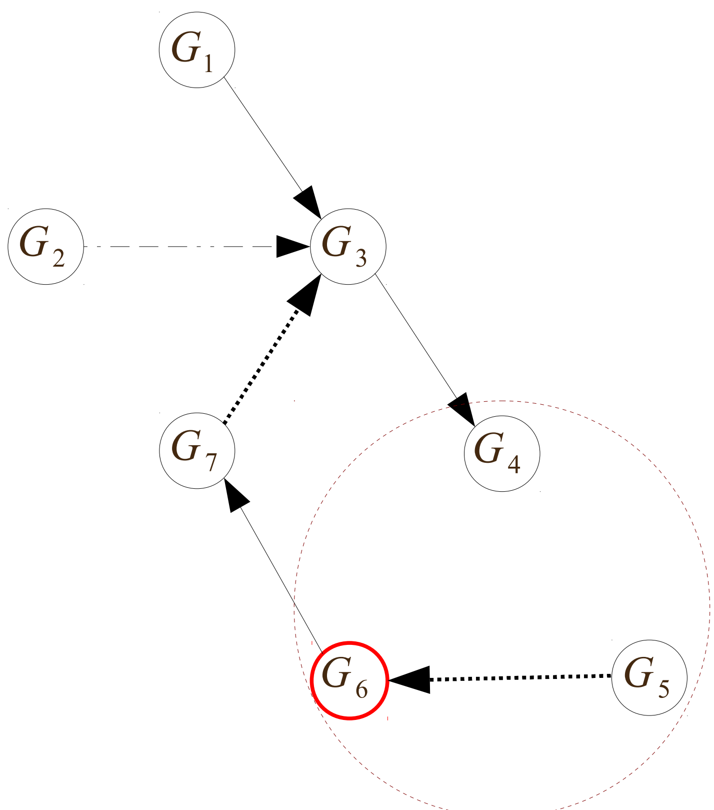
Step 2. Try to swap this edge

Swap* Operator

$Swap(G_2, \boldsymbol{G_3}, G_7)?$ $\longrightarrow$ $Cycle\{G_3, G_4, G_6, G_7\}$

Current situation

$\Delta_{score}Add(G_7, G_3|G_1) > \Delta_{score}Add(G_2, G_3|G_1) > 0$



Objective : delete the cycles

Step 1. Try to delete the edge minimizing $\Delta_{score}Add$

Improving score ?

Yes → Acyclic ?

Yes → OK !

No → Return to Step 1

No → Continue to Step 2

Step 2. Try to swap this edge

Improving score ?

Yes → Acyclic ?

Yes → OK !

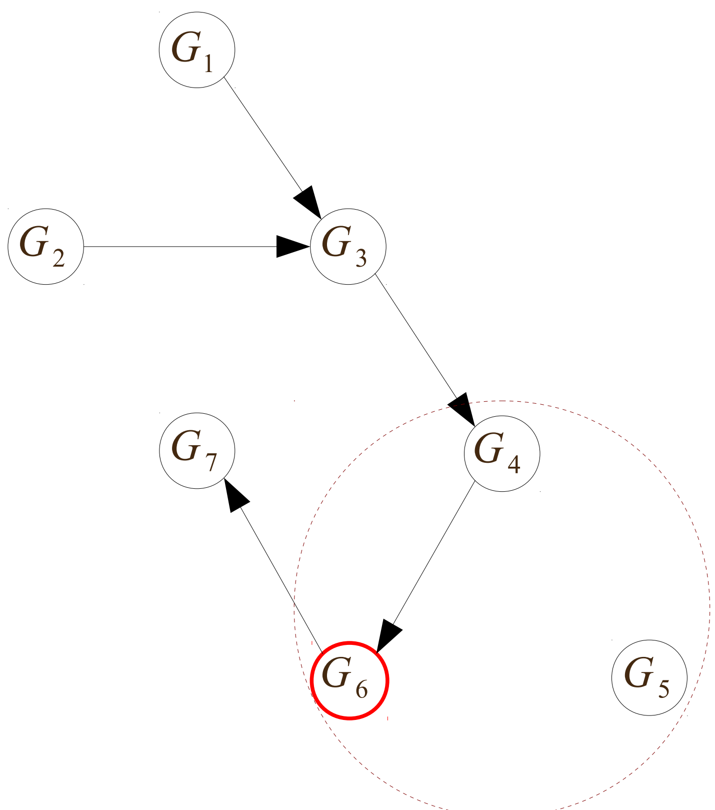
No → Return to Step 1

Swap* Operator

$Swap(G_2, \boldsymbol{G_3}, G_7)?$ $\longrightarrow$ $Cycle\{G_3, G_4, G_6, G_7\}$

Current situation

$\Delta_{score} Add(G_7, G_3|G_1) > \Delta_{score} Add(G_2, G_3|G_1) > 0$



Objective : delete the cycles

Step 1. Try to delete the edge minimizing $\Delta_{score} Add$

Improving score ?

- Yes → Acyclic ?
  - Yes → OK !
  - No → Return to Step 1
- No → Continue to Step 2

Step 2. Try to swap this edge

Improving score ?

- Yes → Acyclic ?
  - Yes → OK !
  - No → Return to Step 1
- **No → Game Over !**

SGS algorithms

- **SGS^1**: Addition + Deletion + Reversal
- **SGS^2**: Addition + Deletion + Reversal + Swap
- **SGS^3**: Addition* + Deletion + Reversal* + Swap*

- One parameter: number of restarts **r**

Experimental settings

- 4 benchmark networks:

	Alarm	*Insurance*	*Hailfinder*	*Pigs*
Nodes	37	27	56	441
Edges	46	52	66	592
In-degree	4	3	4	2

- Data generated from conditional probabilities:
  100 datasets with 500 and 5 000 sample sizes

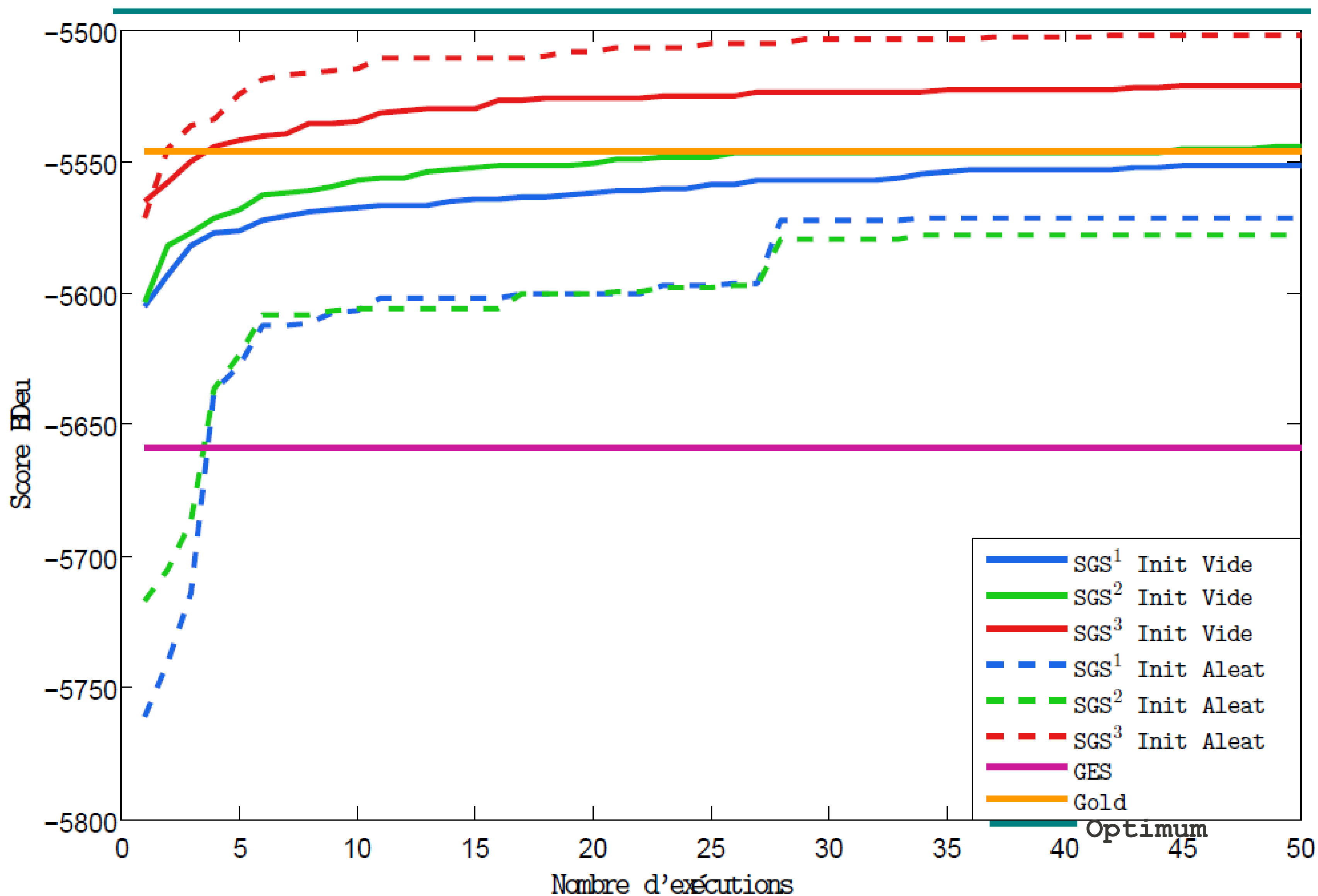
- **SGS** compared to: **LAGD** (2 look-ahead in 5 directions)
  GES

- Limit number of parents : 5

- Pre-filtering candidate parents under condition for Pigs network with SGS
  $$\Delta\, Add(Parent\,, Target) > 0$$

Results (1/4)

Impact of the number of restarts

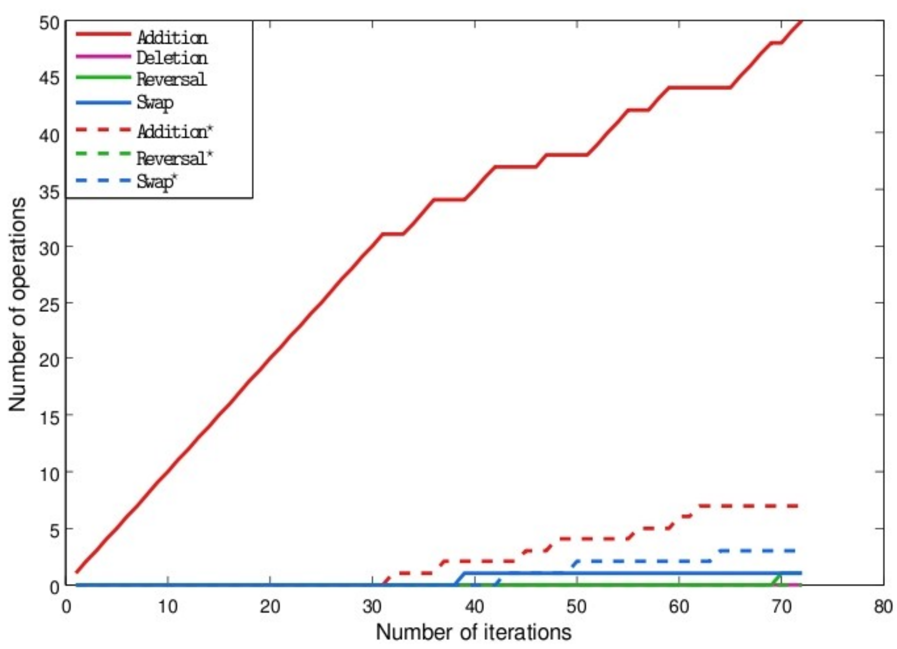


Alarm network (37 variables). Mean over 30 datasets with 500 samples

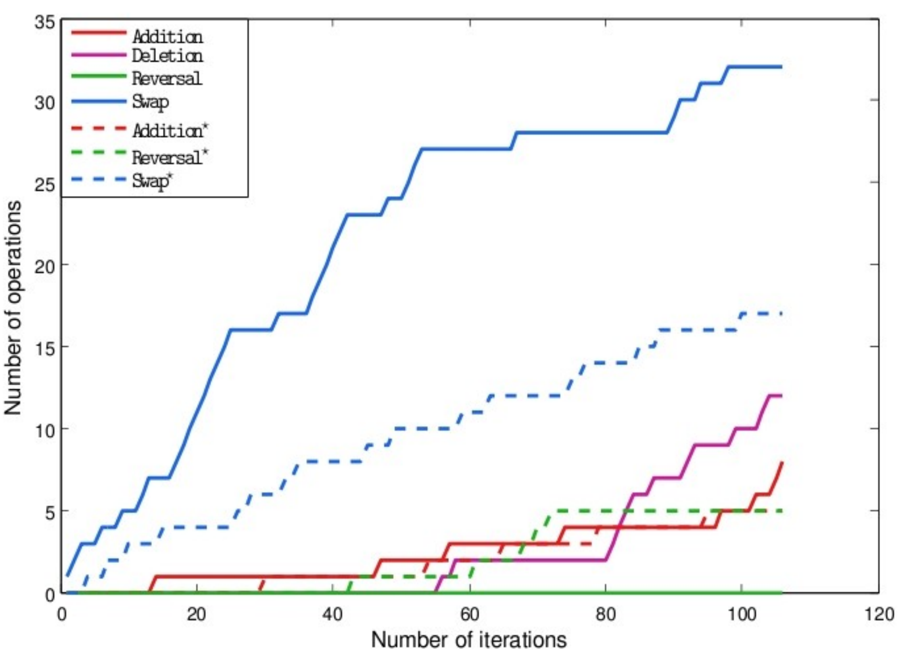
Results (2/4)

- Number of applied operators by type during the search
- *Alarm* network
- **1** run of **SGS³** (r=1) with 500 samples
- **SGS³** Initialized with **empty** and **random network** (2 parents max)

empty network



random network



Results (2/4)

- Comparison of BDeu scores reached by **SGS³**, **LAGD** and **GES**
- ***4*** benchmark networks, **500** and **5 000** samples
- Best of **10** runs for **SGS** and **LAGD** (r=10)
- **All methods** Initialized with a **empty network**

Wilcoxon test 5%	*Alarm*		*Insurance*		*Hailfinder*		*Pigs*	
	500	5 000	500	5 000	500	5 000	500	5 000
SGS³ vs **GES**	+	+	+	+	+	+	+	-
SGS³ vs **LAGD**	+	+	+	+	~	+	n/a	n/a
LAGD vs **GES**	+	~	+	+	+	+	n/a	n/a

Results (3/4)

- Comparison of **Hamming distances** for **SGS³**, **LAGD** and **GES**

Hamming distance = False Positive + False Negative

	Alarm		*Insurance*		*Hailfinder*		*Pigs*	
	500	5 000	500	5 000	500	5 000	500	5 000
SGS³	**11***	8	**24***	**10***	41	**29***	32	41
LAGD	15	10	**24***	16	47	39	n/a	n/a
GES	**11***	**6***	25	15	**39***	33	**9***	**0***

* best result

Results (4/4)

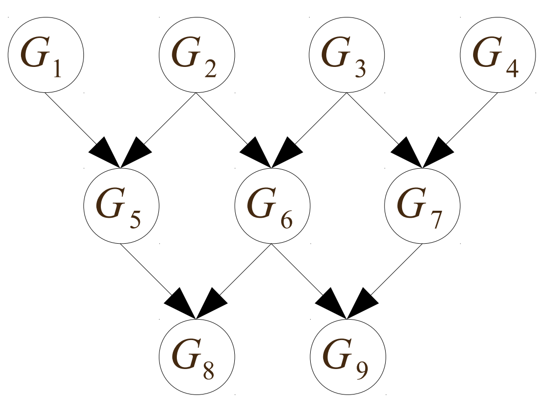
- Comparison of **Hamming distances** for **SGS³**, **LAGD** and **GES**

Hamming distance = False Positive + False Negative

	Alarm		*Insurance*		*Hailfinder*		*Pigs*	
	500	5 000	500	5 000	500	5 000	500	5 000
SGS³	**11***	8	**24***	**10***	41	**29***	32	41
LAGD	15	10	**24***	16	47	39	n/a	n/a
GES	**11***	**6***	25	15	**39***	33	**9***	**0***

* best result

Pigs network



Results (4/4)

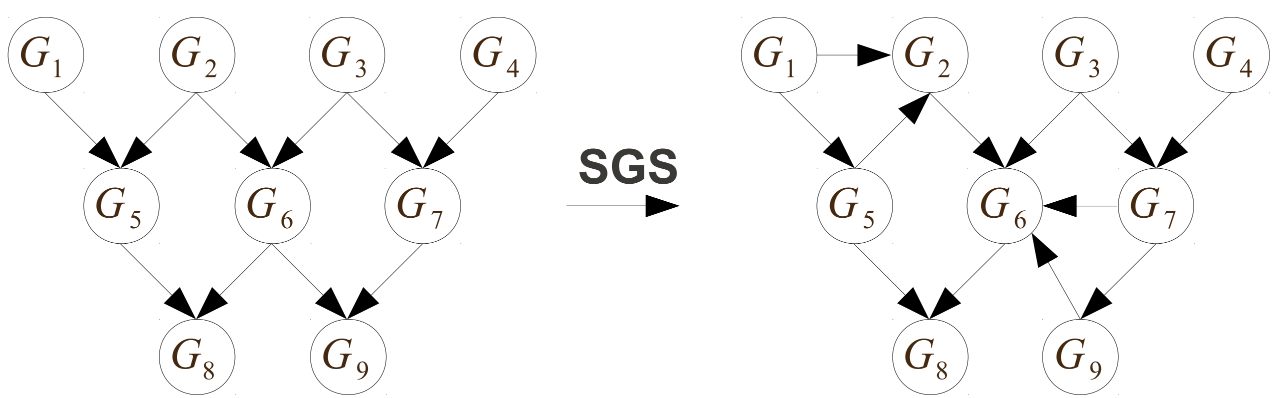
- Comparison of **Hamming distances** for **SGS**, **LAGD** and **GES**

Hamming distance = False Positive + False Negative

	Alarm		*Insurance*		*Hailfinder*		*Pigs*	
	500	5 000	500	5 000	500	5 000	500	5 000
SGS[3]	**11***	8	**24***	**10***	41	**29***	32	41
LAGD	15	10	**24***	16	47	39	n/a	n/a
GES	**11***	**6***	25	15	**39***	33	**9***	**0***

* best result

Pigs network



Results (4/4)

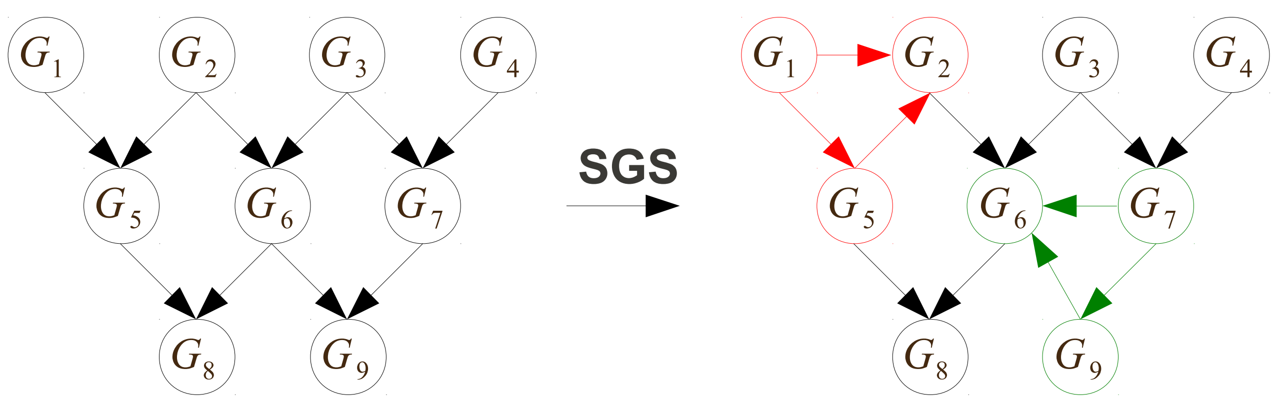
- Comparison of **Hamming distances** for **SGS**, **LAGD** and **GES**

Hamming distance = False Positive + False Negative

	Alarm		*Insurance*		*Hailfinder*		*Pigs*	
	500	5 000	500	5 000	500	5 000	500	5 000
SGS³	**11***	8	**24***	**10***	41	**29***	32	41
LAGD	15	10	**24***	16	47	39	n/a	n/a
GES	**11***	**6***	25	15	**39***	33	**9***	**0***

* best result

Pigs network



Results (4/4)

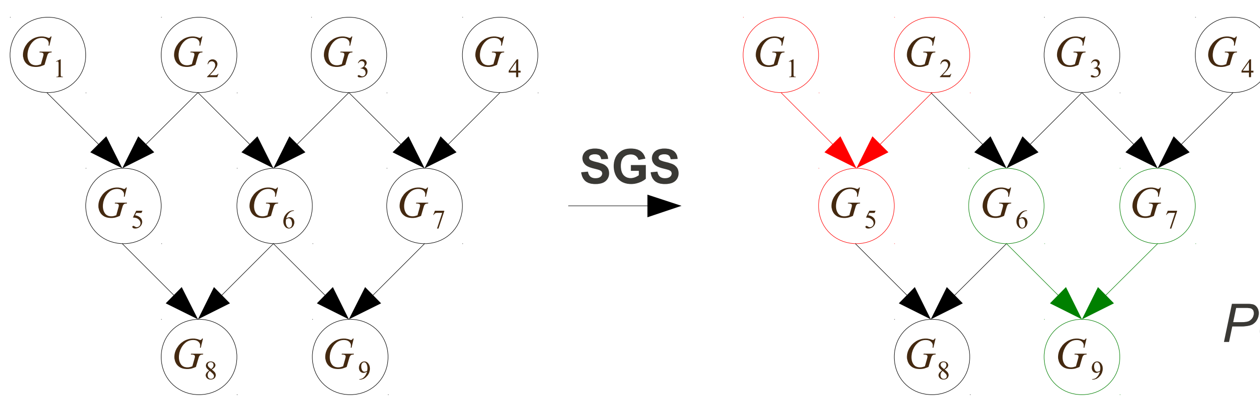
- Comparison of **Hamming distances** for **SGS**, **LAGD** and **GES**

Hamming distance = False Positive + False Negative

	Alarm		*Insurance*		*Hailfinder*		*Pigs*	
	500	5 000	500	5 000	500	5 000	500	5 000
SGS[3]	**9***	**4***	**24***	**9***	40	**26***	**1***	2
LAGD	15	10	**24***	16	47	39	n/a	n/a
GES	11	6	25	15	**39***	33	**9**	**0***

* best result

Pigs network



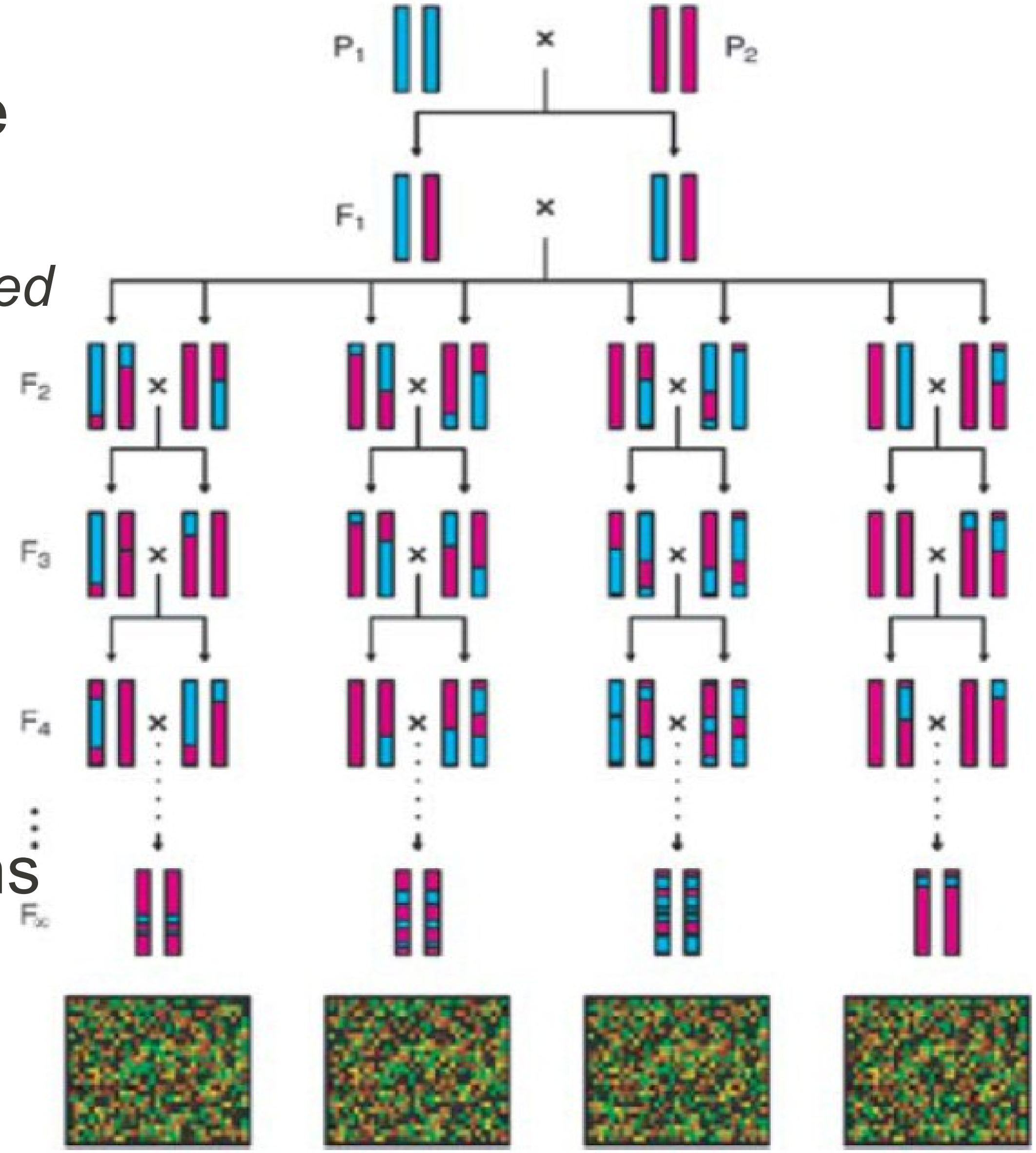
Post-processing

Genetical genomics

- Gene expressions vary due to polymorphisms

(stationary phenomenon in controlled environment)

- Data
  - expression levels
  - genotypes
  - marker/gene localisations on the genome



(Jansen & Nap, Trends in Gen. 2001)

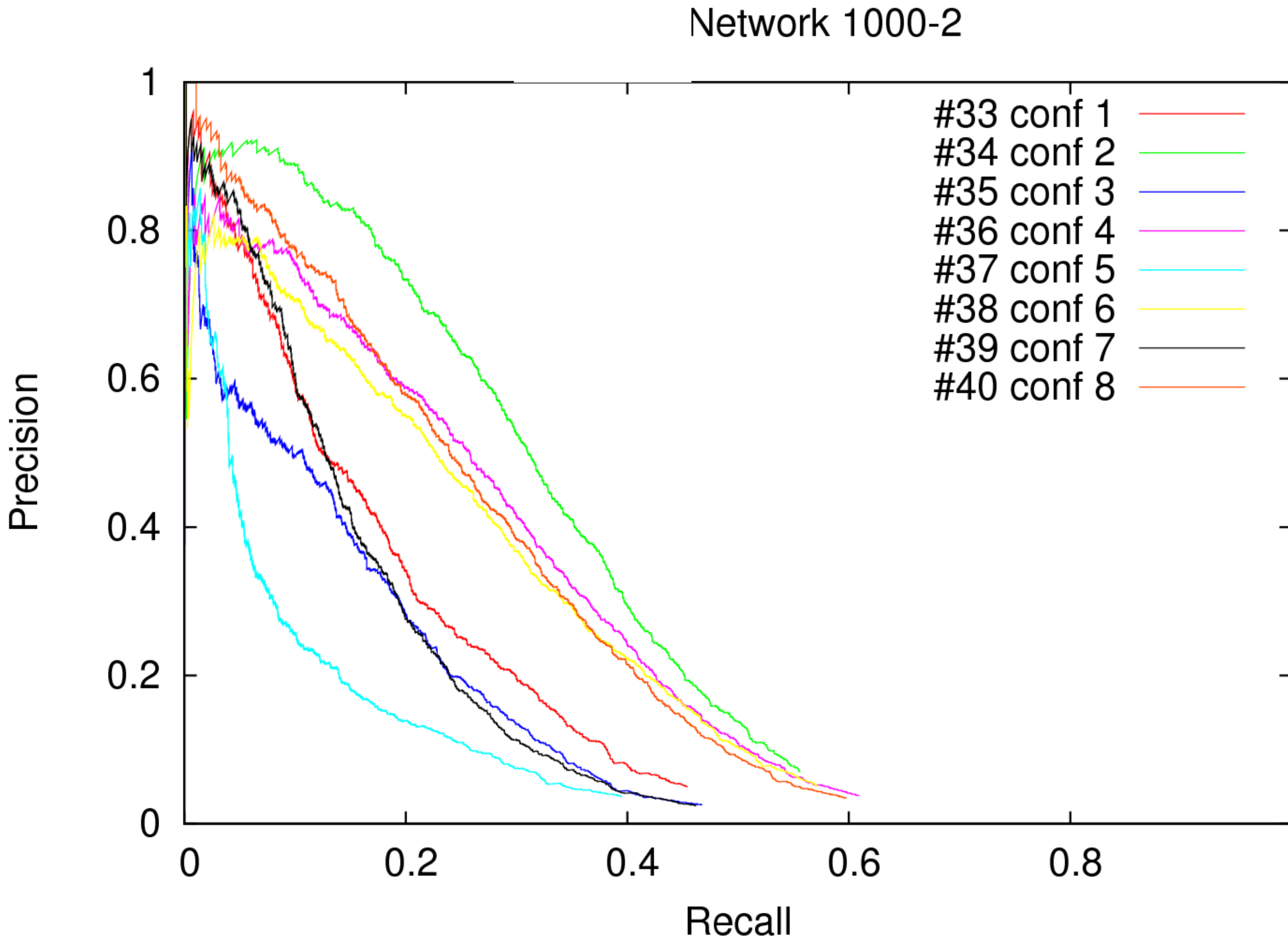
DREAM 2012
StatSeq Systems Genetics Benchmark

- 72 datasets: 9 gene networks (p=100,1000,5000, e~6p) x 8 configurations

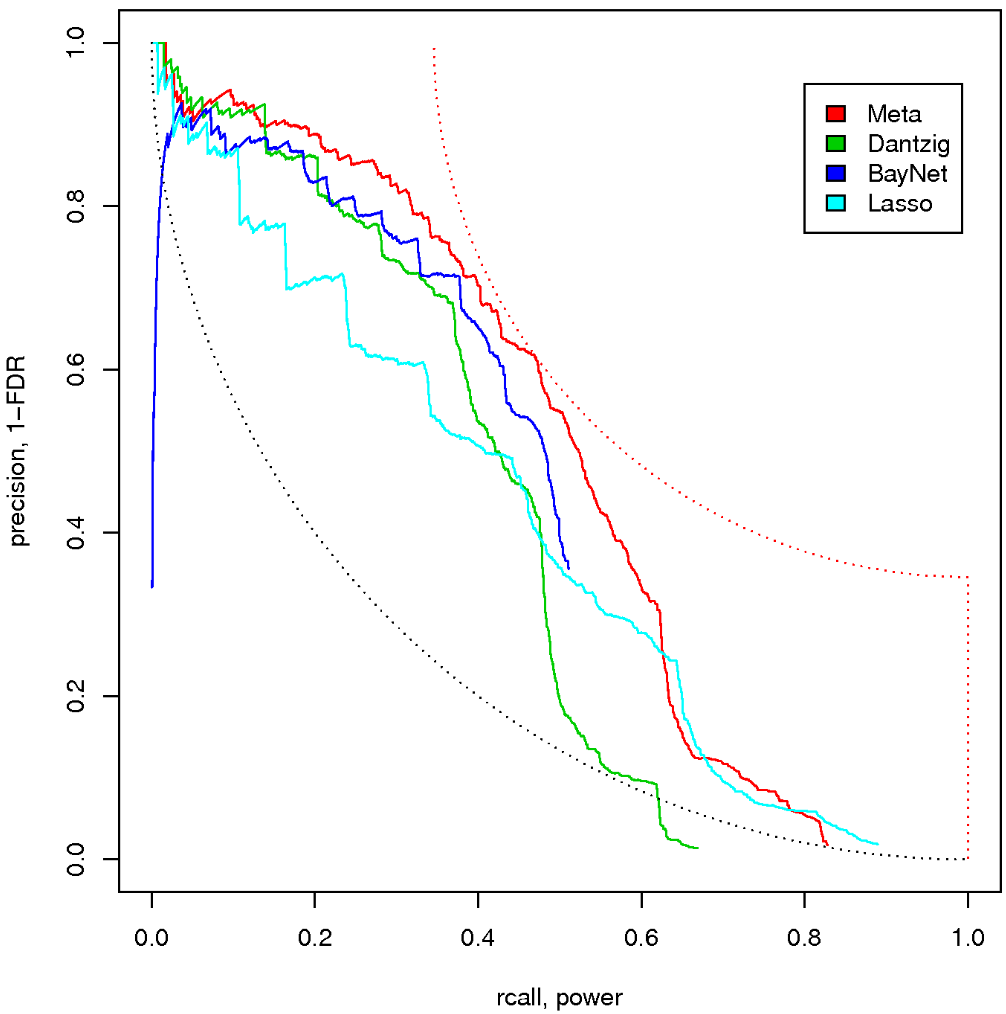
Configuration	Marker Distance	Biological Variance	Heritability	Population Size
1	N(5,1)	N(1,0.1)	High	300
2	N(5,1)	N(1,0.1)	High	900
3	N(5,1)	N(1,0.25)	Low	300
4	N(5,1)	N(1,0.25)	Low	900
5	N(1,0.1)	N(1,0.1)	High	300
6	N(1,0.1)	N(1,0.1)	High	900
7	N(1,0.1)	N(1,0.25)	Low	300
8	N(1,0.1)	N(1,0.25)	Low	900

SysGenSIM (de la Fuente et al, Bioinformatics 2011)

SGS^3 (BDeu alpha=1) with 10 restarts and 100 bootstraps

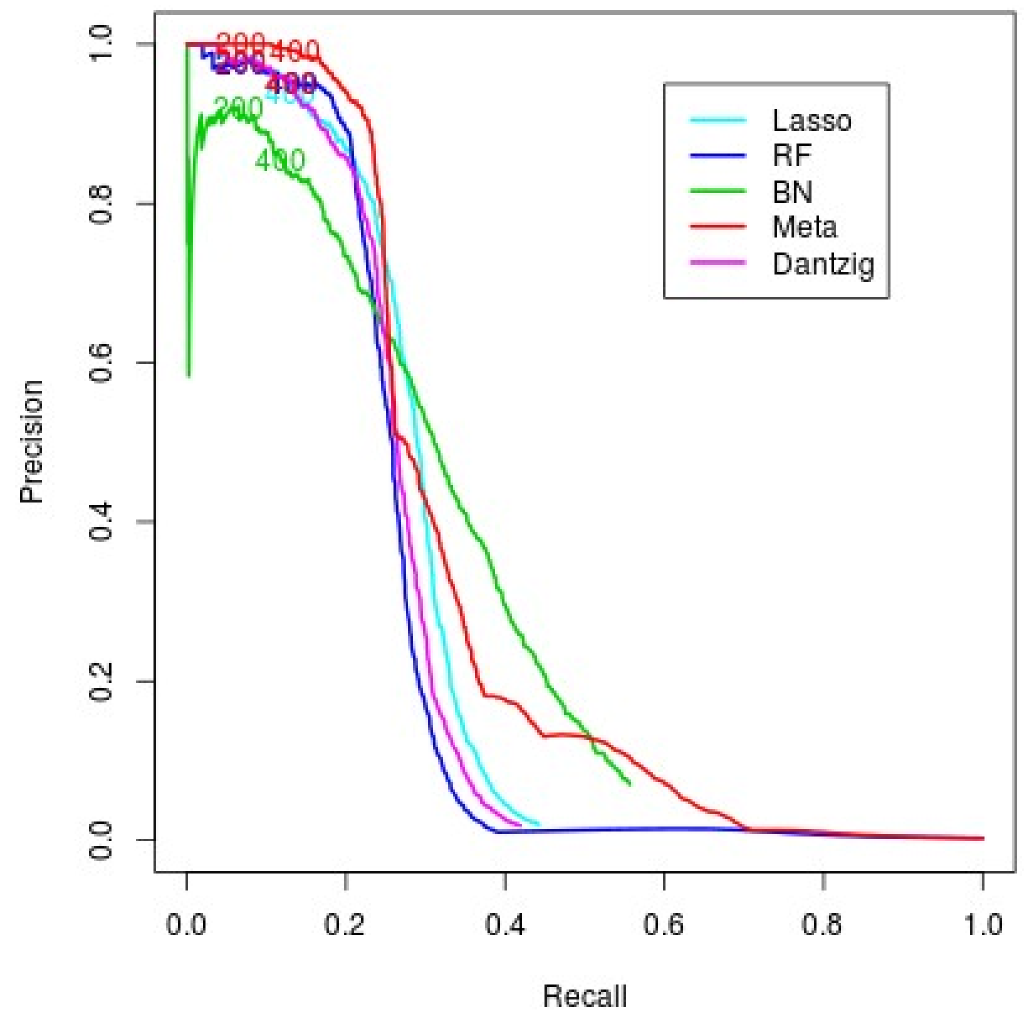


DREAM 2010 / 2012

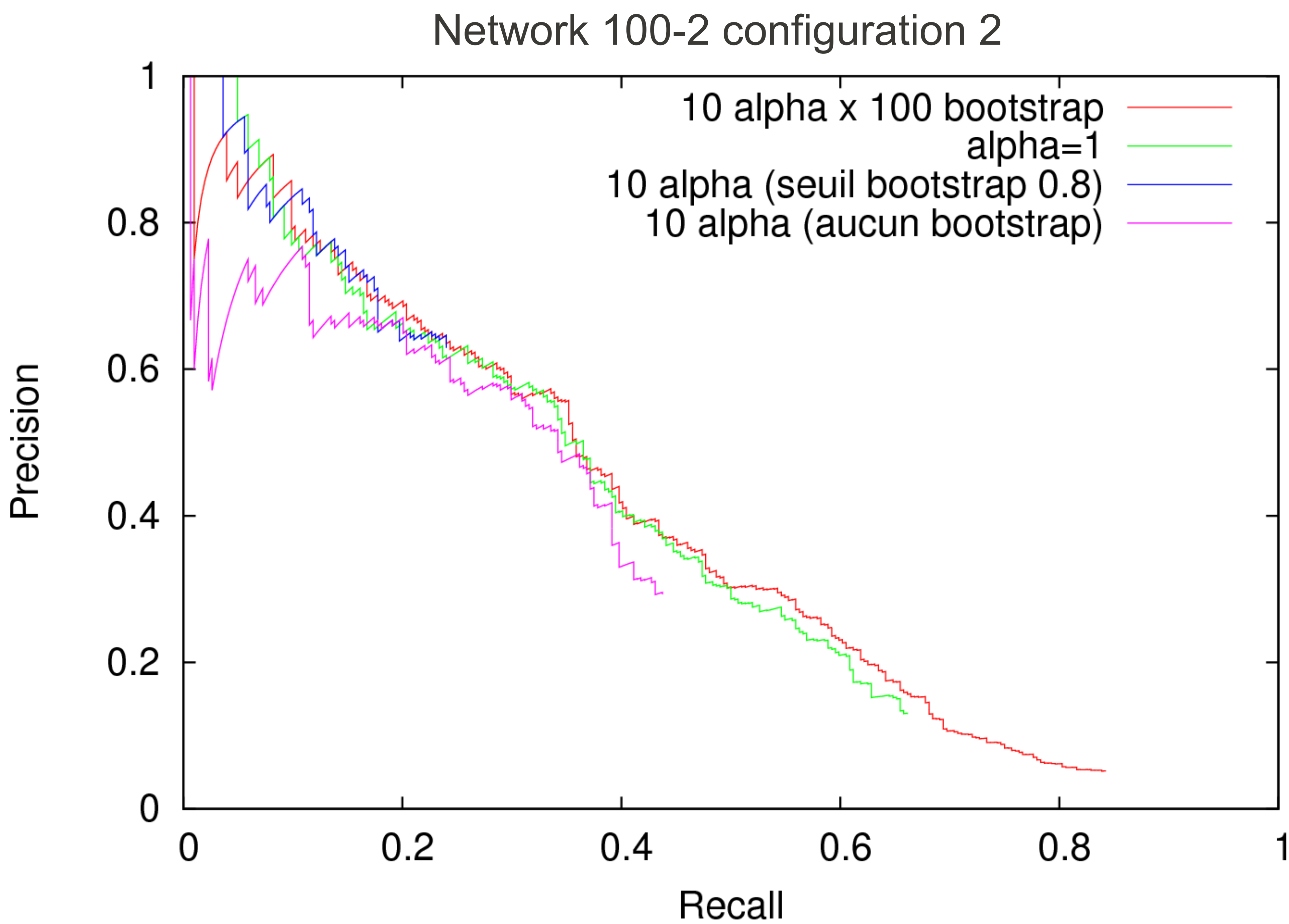


DREAM 2010 Net A1 (p=1000, 999 sample)

(Vignes et al., Plos One, 2011)

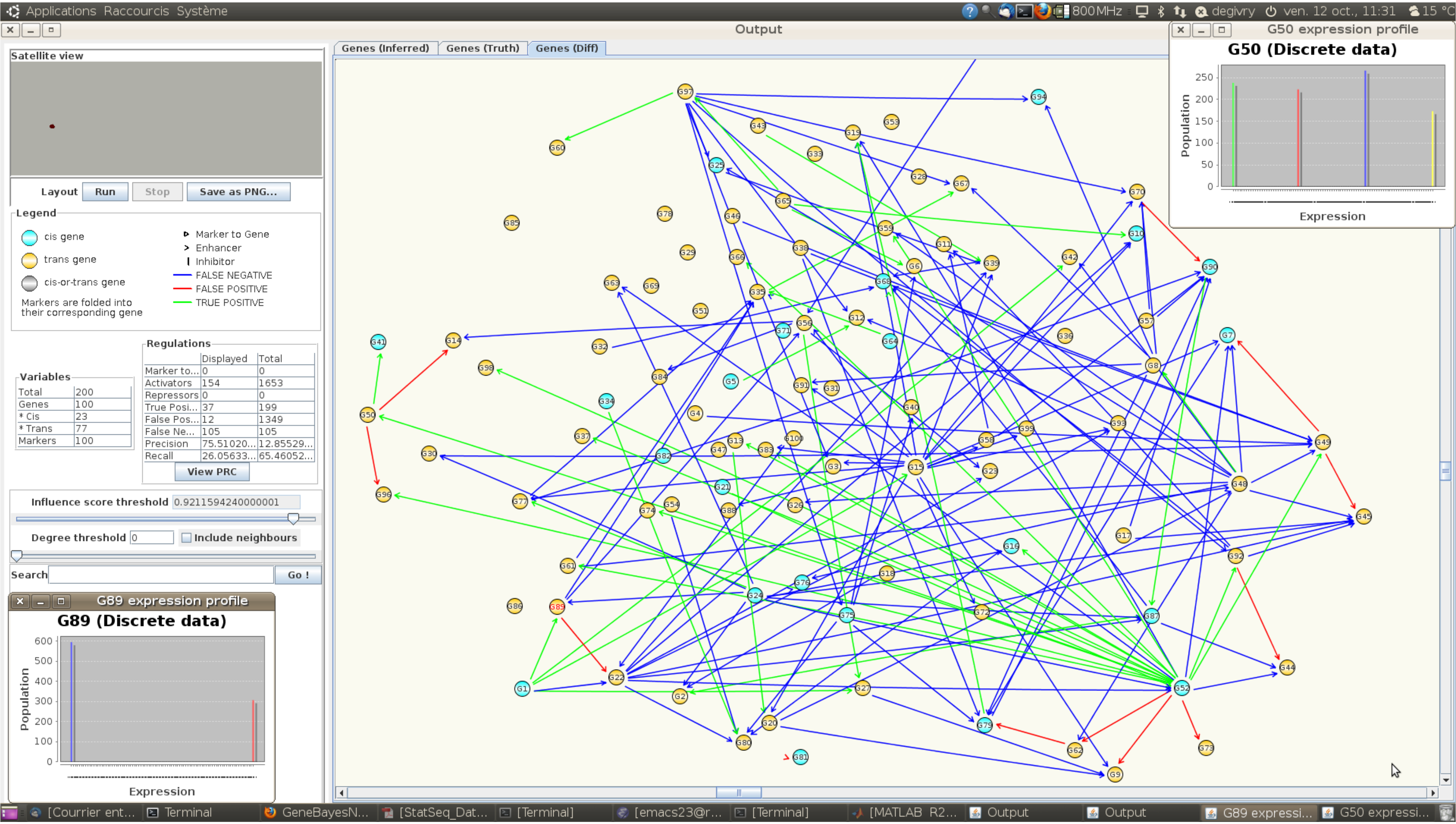


DREAM 2012 Net 1000-2-2 (p=1000, 900 s.)


Network 100-2 configuration 2
Precision
Recall
10 alpha x 100 bootstrap
alpha=1
10 alpha (seuil bootstrap 0.8)
10 alpha (aucun bootstrap)
0
0.2
0.4
0.6
0.8
1
0
0.2
0.4
0.6
0.8
1

GeneBayesNet

http://carlit.toulouse.inra.fr/genebayesnet/



Conclusion & Perspectives

We

- Propose a new algorithm SGS
- Propose a new local operator SWAP and iterative extensions for breaking cycles
- Improve BDeu scores of learned networks with these operators
- Compare with other methods on standard BN and genetical genomics benchs

TODO list:

- Reduce the number of restarts **r** required
- Try other meta-heuristics
- Try on real data (arabidopsis thaliana)
-
- Integrate other data sources (bibliome)