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Introduction to Estimation of Distribution Algorithms

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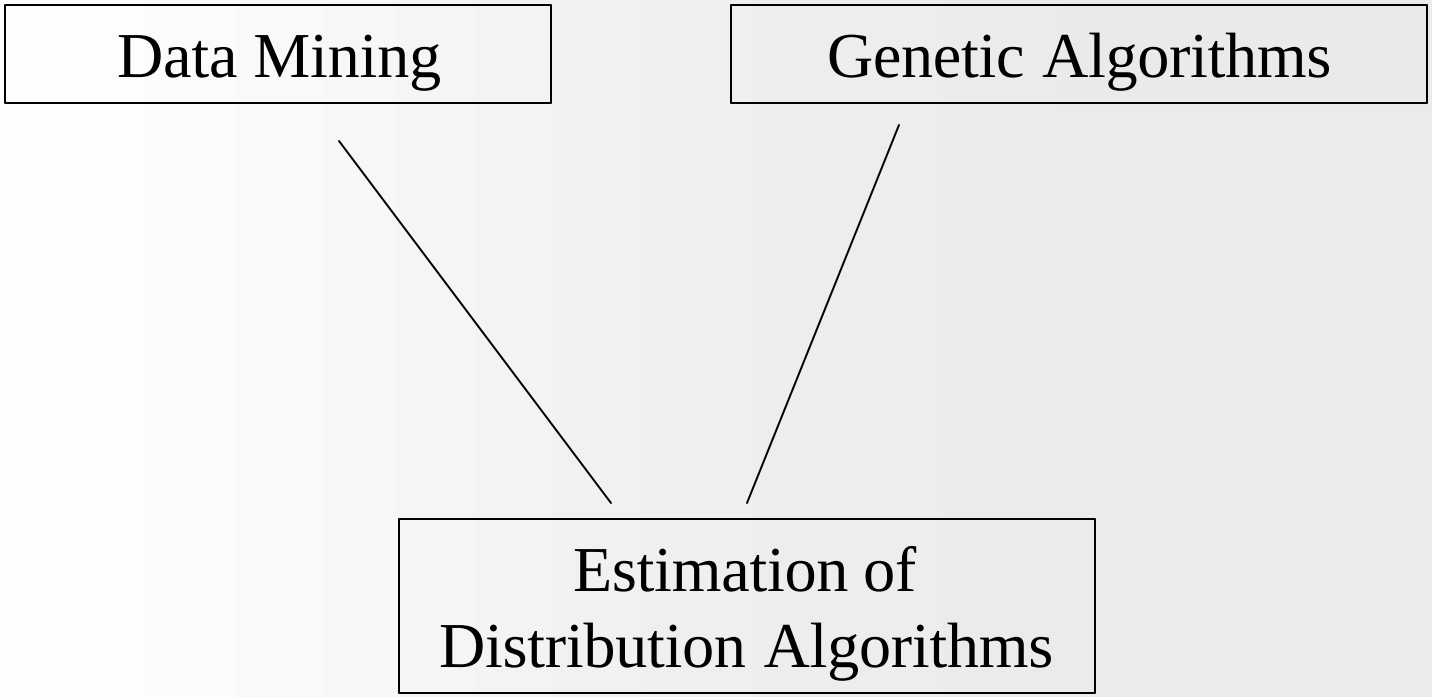
Context

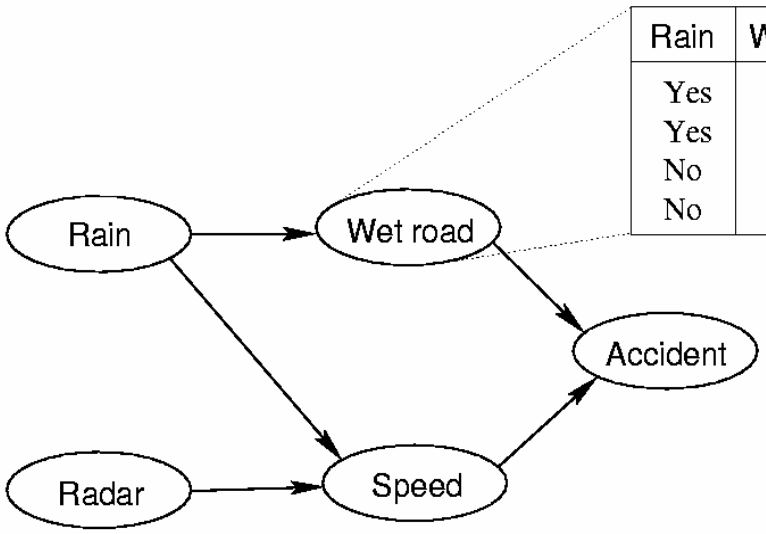

Data Mining
Genetic Algorithms
Estimation of
Distribution Algorithms

Data mining

- Knowledge extraction from databases
- Example: Customer’s cards in shops

Bayesian network

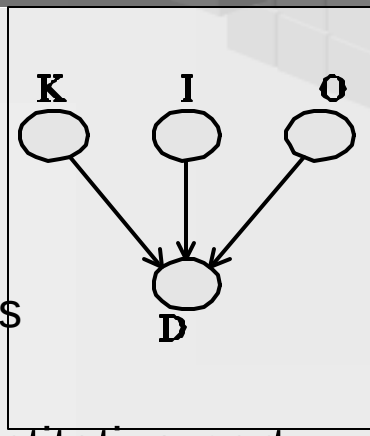
- An Example:



Rain	Wet Road	p(Wet Road | Rain)
Yes	Yes	0.995
Yes	No	0.005
No	Yes	0.060
No	No	0.940

- Another example:

Bayesian network – cont'd.



K I O	p(D|K,I,O)
1 1 1	0.00
1 1 0	0.00
1 0 1	0.95
1 0 0	0.95
0 1 1	0.00
0 1 0	0.00
0 0 1	0.40
0 0 0	0.05

- Formal definition: B = ($\mathcal{G}$, $\mathcal{L}$)

  $\mathcal{G}$ .. Dependency graph (DAG)

  - Vertices correspond to random variables
  - Edges capture dependencies

  $\mathcal{L}$ .. Conditional probabilities $p(X_i|P_i)$ - quantitative part

- Bayesian network encodes a joint probability distribution

$$p(X) = \prod_{i=0}^{n-1} p\left(X_i \mid \Pi_i\right)$$

  $\boldsymbol{X}=(X_0, X_1, \ldots, X_{n-1})$ is a vector of variables, P_i is the set of parents of X_i

- "Each variable X_i is independent of its nondescendants $\boldsymbol{X}\backslash P_i$, given its parents P_i in $\mathcal{G}$ "

Construction of Bayesian networks

- Dependency graph fixed
  - Only conditional probabilities are estimated

$$p(x_i \mid \boldsymbol{p_i}) \approx \frac{m(x_i, \boldsymbol{p_i})}{m(\boldsymbol{p_i})}$$

    - $m(p_i)$ … the number of individuals in the population having variables P_i set to concrete value $\mathrm{p_i}$
    - $m(x_i, p_i)$ … the number of individuals in the population having variables P_i set to concrete value p_i and X_i equal to concrete value x_i
- Dependency graph is not given
  - More complex task:
    - Search the space of possible dependency graphs (NP-hard problem)
    - Each hypothesis about the dependency graph has to be evaluated
    - For each evaluation the conditional probabilities have to be estimated

Incremental construction of a Bayesian network

```
Start with an empty network B;
while any edge can be added do
begin
  for each edge that can be added do
  begin
    compute the metrics of the network B' that
     can be constructed from B by adding this
     edge;
  end
  add the edge giving the highest improvement
     to the network B;
end
```

- Constraints
  - Acyclicity
  - Model complexity penalty

How to evaluate the quality of Bayesian networks?

- The posterior probability of a Bayesian network B given data D can be computed by applying Bayes theorem as :

$$p(B|D) = p(D|B)\, p(B) / p(D).$$

The higher the p(B|D), the more likely the network B is a correct model of the data. Therefore, the value of p(B|D) can be used to score different networks and measure their quality. Since we are interested in comparing different networks (hypotheses) for a fixed data set D, we can eliminate the denominator.

p(B) is a “prior” probability of B

p(D|B) is expressed e.g. by Bayes - Dirichlet metrics

Bayesian Dirichlet metrics

- A closed form of p(D|B) derived by Heckerman (under some additional assumptions about the parameters):

$$p(D \mid B) = \prod_{i=0}^{n-1} \prod_{\mathbf{p_i}} \frac{\Gamma(m'(\mathbf{p_i}))}{\Gamma(m(\mathbf{p_i}) + m'(\mathbf{p_i}))} \prod_{x_i} \frac{\Gamma(m(x_i, \mathbf{p_i}) + m'(x_i, \mathbf{p_i}))}{\Gamma(m'(x_i, \mathbf{p_i}))}$$

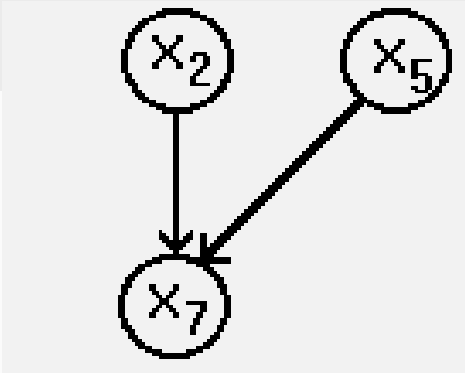
- In the variant K2:

=2

=1

An example of Bayesian Dirichlet metrics usage

- Part of BN:



$X_i \ldots X_7; \quad \Pi_I = \{X_2, X_5\}$

- Population:

X2		X5		X7		
. . .	1	. . .	0	. . .	1	. . .
. . .	0	. . .	0	. . .	0	. . .
. . .	1	. . .	0	. . .	1	. . .
. . .	1	. . .	1	. . .	1	. . .
. . .	0	. . .	0	. . .	0	. . .
. . .	0	. . .	1	. . .	0	. . .
. . .	0	. . .	0	. . .	1	. . .
. . .	1	. . .	1	. . .	0	. . .
. . .	0	. . .	0	. . .	0	. . .
. . .	0	. . .	1	. . .	0	. . .

p_i	x_i	$m(x_i, p_i)$	$m(p_i)$
00	0	3	} 4
	1	1	
01	0	2	} 2
	1	none	
10	0	none	} 2
	1	2	
11	0	1	} 2
	1	1	

..cont'd

$$p(D|B) = \underbrace{\ldots\ldots\ldots\ldots}_{X_0\ part} \cdot \ldots \cdot \underbrace{\underbrace{\frac{2!}{(2+m(X_2=0,X_5=0))!}\prod_{x_7=0}^{1}\frac{(1+m(X_7=x_7,X_2=0,X_5=0))\ !}{1\ !}}_{p_7:\ (X_2=0,X_5=0)} \cdot \underbrace{\frac{2!}{(2+m(X_2=0,X_5=1))!}\prod_{x_7=0}^{1}\frac{\ldots}{1!}}_{p_7:\ (X_2=0,X_5=1)}}_{X_7\ part} \cdot \ldots \cdot \ldots$$

$$p(D|B) = \underbrace{\ldots\ldots\ldots\ldots}_{X_0\ part} \cdot \ldots \cdot \underbrace{\underbrace{\frac{2!}{\left(2+\underbrace{1+3}_{X_2=0,X_5=0}\right)!}\ \underbrace{\frac{(1+1)\ !}{1\ !}}_{X_2=0,X_5=0,X_7=0}\ \underbrace{\frac{(1+3)\ !}{1\ !}}_{X_2=0,X_5=0,X_7=1}}_{p_7:\ (X_2=0,X_5=0)} \cdot \underbrace{\frac{2!}{\left(2+\underbrace{2+0}_{X_2=0,X_5=1}\right)!}\ \underbrace{\frac{(1+2)\ !}{1\ !}}_{X_2=0,X_5=1,X_7=0}\ \underbrace{\frac{(1+0)\ !}{1\ !}}_{X_2=0,X_5=1,X_7=1}}_{p_7:\ (X_2=0,X_5=1)}}_{X_7\ part} \cdot \ldots \cdot \ldots$$

- Incremental adding of edges – only part of the score has to be recomputed

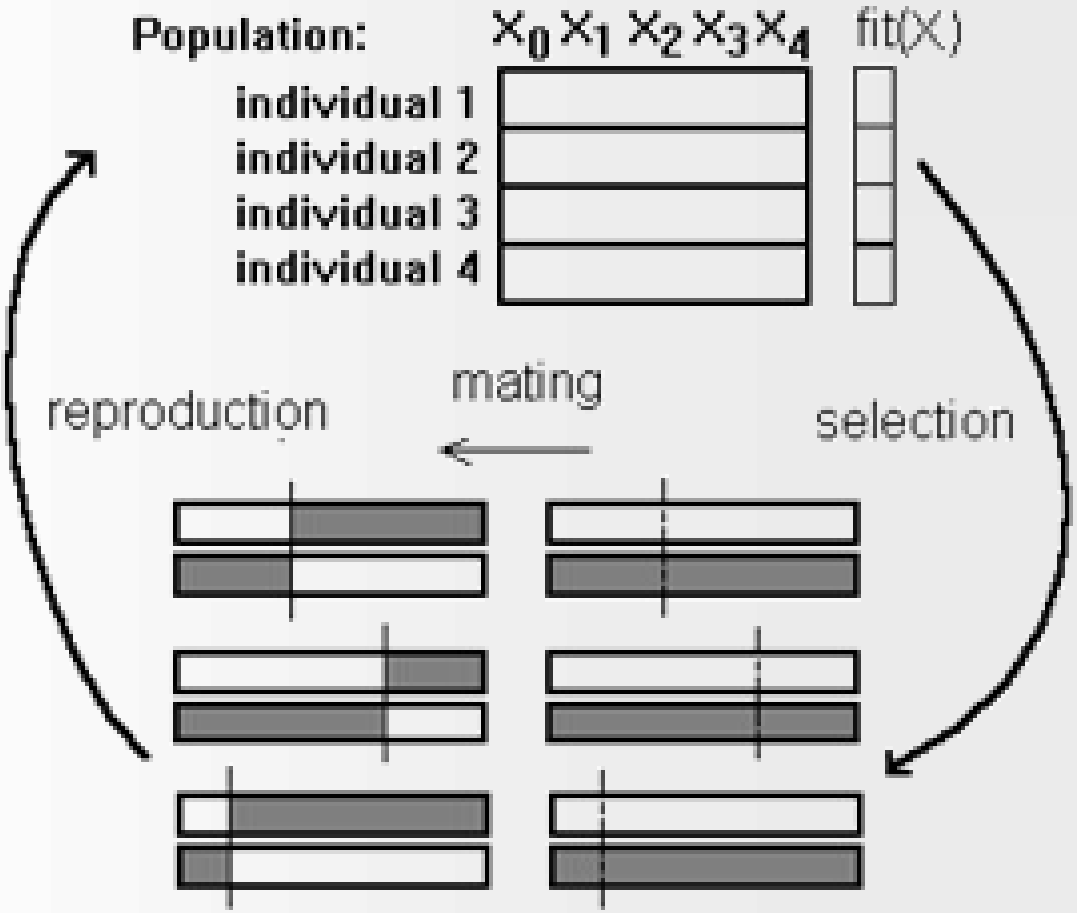
Another alternatives for scoring functions

- Minimum Description Length score (MDL):

$$DL(\mathcal{G}, D) = DL_{graph}(\mathcal{G}) + \sum_{i=0}^{n-1} DL_{tab}(X_i, \mathbf{?}_i) + \underbrace{N \sum_{i=0}^{n-1} H(X_i \mid \mathbf{?}_i)}_{DL_{data}}$$

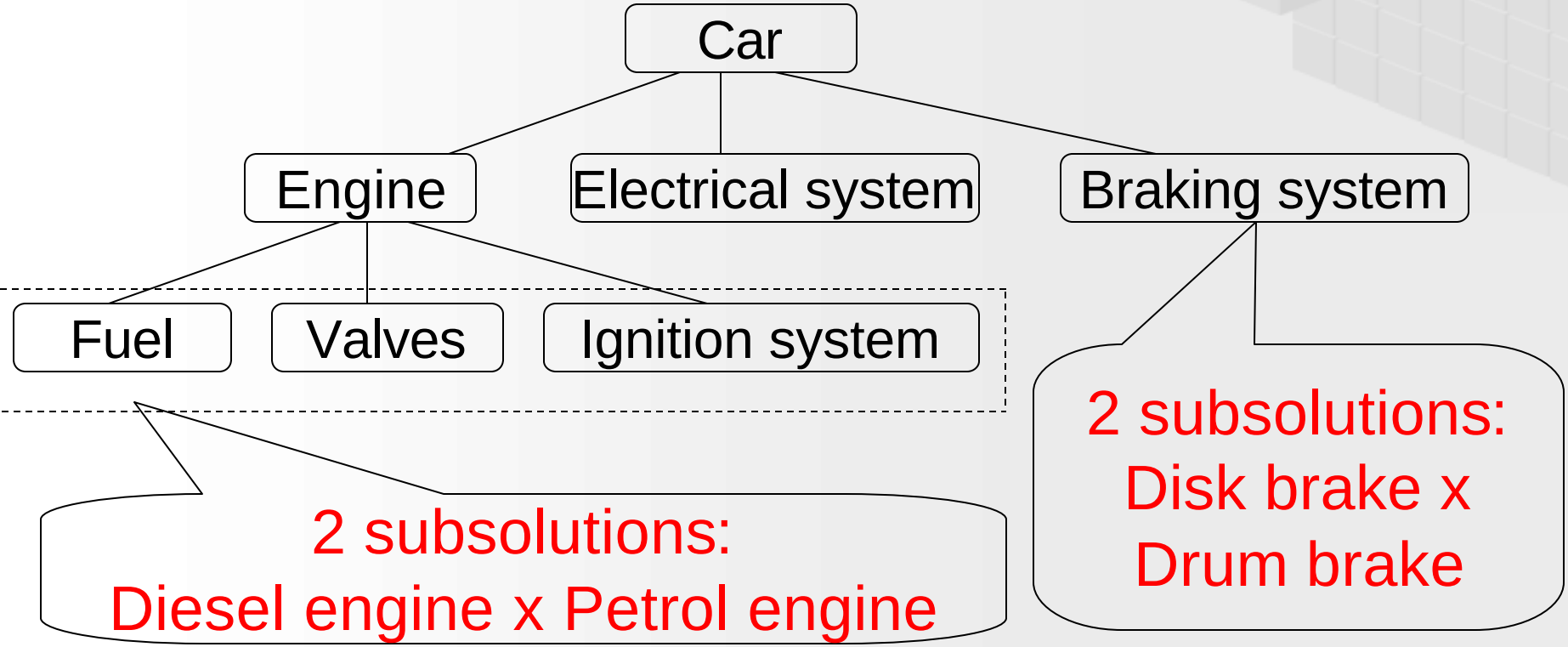
- Bayesian Information Criterion (BIC)
  - Equivalent to MDL when we ignore the description of dependency graph
- Information Gain
- Mutual Information
- …

Recall: Genetic Algorithms



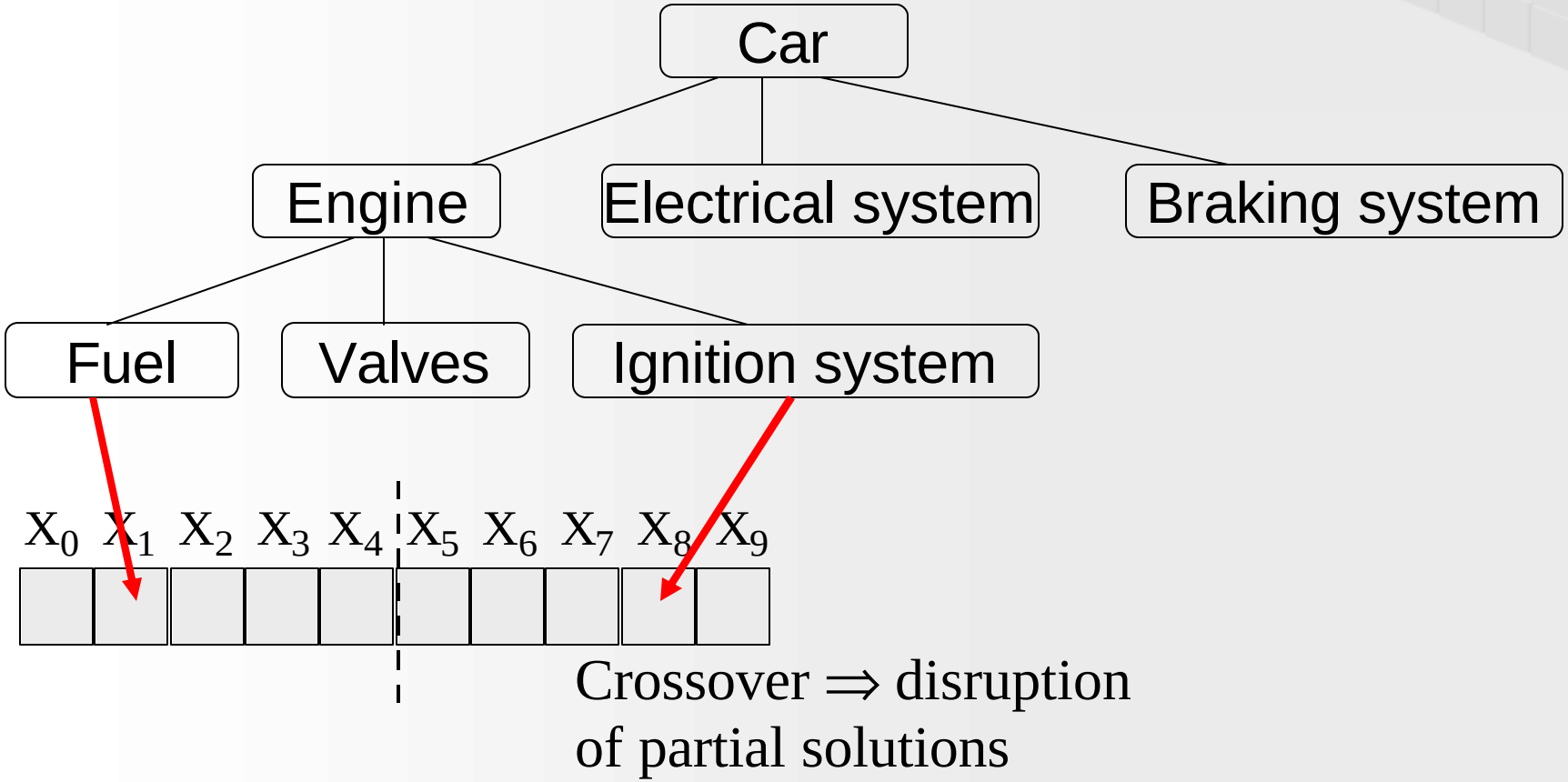
Problem decomposability

- An example: Automotive design



Motivation for Estimation of Distribution Algorithms

- Disruption of subsolutions:



Schema Theorem

- Schema example H: * * * 0 * 1 * * 0 *
  - Chromozome length n=10
  - Schema order o(H)=3
  - Schema defining length δ(H)=5
- Schema Theorem
  - Proportionate selection & one-point crossover with probability p_c and mutation with probability p_m:

$$\langle m(H,t+1)\rangle \geq m(H,t)\frac{f(H,t)}{\bar{f}(t)}\left[1-p_c\frac{d(H)}{n-1}-p_m o(H)\right]$$

Some functions are deceptive for GAs

Additively decomposable functions:

$$f(\mathbf{X}) = \sum_{i=0}^{l-1} f_k(S_i)$$

An example: f_3 deceptive

Triplet	000	001	010	011	100	101	110	111
f_3	0,9	0,8	0,8	0	0,8	0	0	1

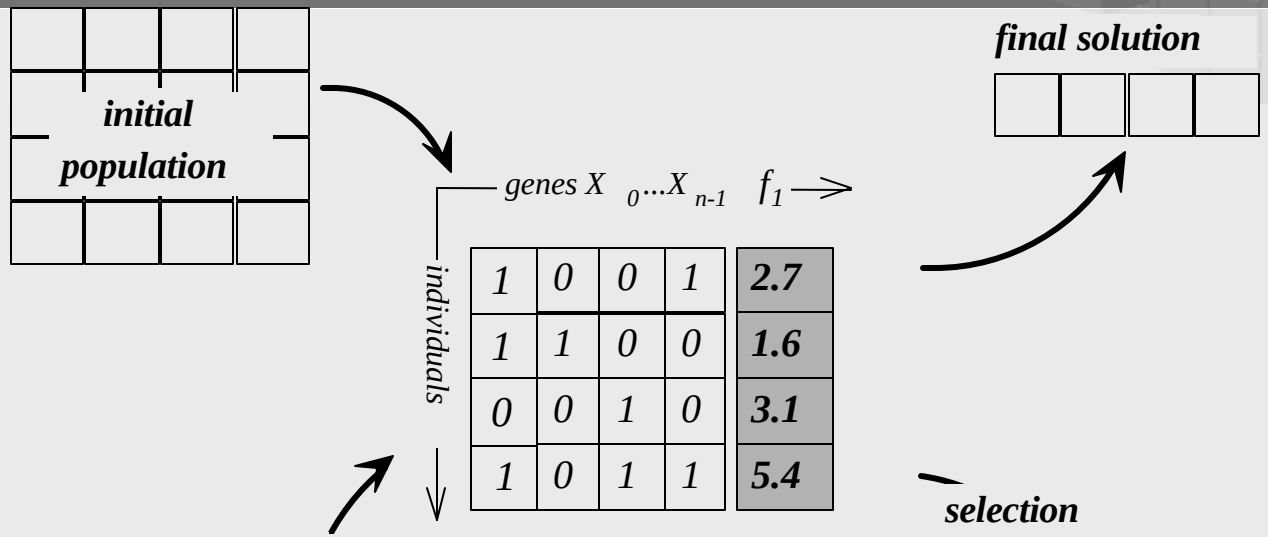
1**: $\frac{0{,}8+0+0+1}{4} = 0{,}45$

0**: $\frac{0{,}9+0{,}8+0{,}8+0}{4} = 0{,}625$

How datamining can help to improve GAs?

- Genes are treated as random variables
- The relationships between genes are captures in the form of probabilistic model

Classical GA Þ Bayesian Optimization Algorithm

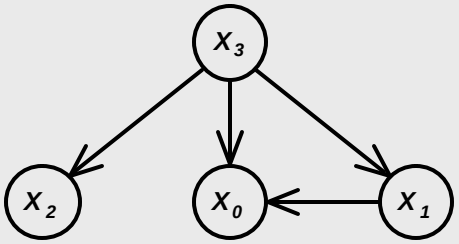


1	0	0	1	2.7
1	1	0	0	1.6
0	0	1	0	3.1
1	0	1	1	5.4

BOA EVOLUTIONARY CYCLE

model sampling (PLS - Probabilistic Logic Sampling)

data-mining techniques



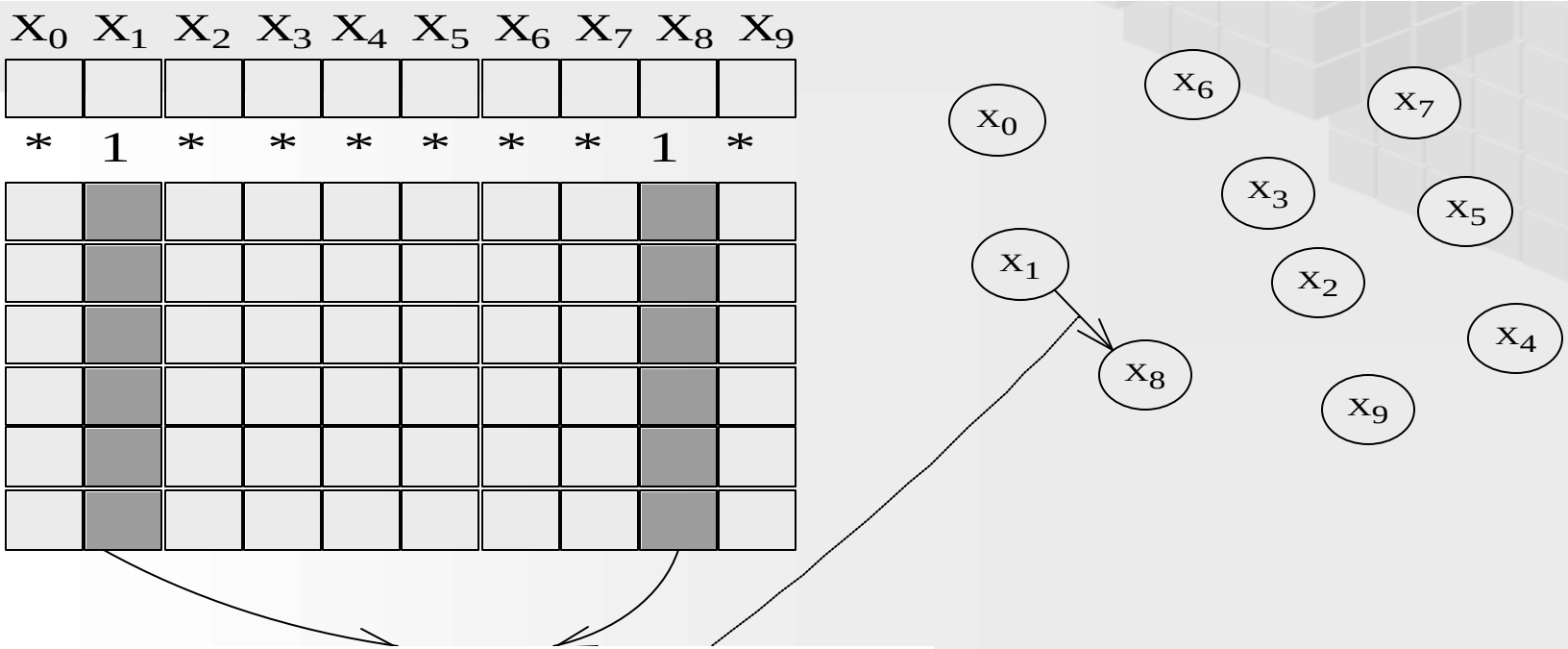
$$p(\mathbf{X})=p(X_3).p(X_1|X_3).p(X_2|X_3).p(X_0|X_1,X_3)$$

Conditional probability distributions (CPDs).

Example of $p(X_0|X_1,X_3)$:

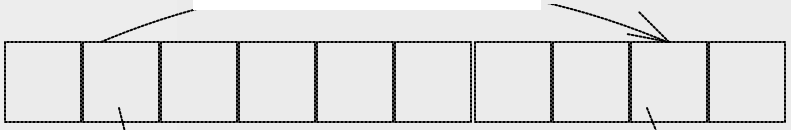
X_1	X_3	$p(X_0=1\|X_1,X_3)$
0	0	0.9
0	1	0.2
1	0	0.7
1	1	0.7

Building block detection & preservation



Bayes-Dirichet metrics

dependency



$p(X_1)=0.7$

$p(X_8| X_1)=0.9$

$p(X_8| \overline{X}_1)=0.3$

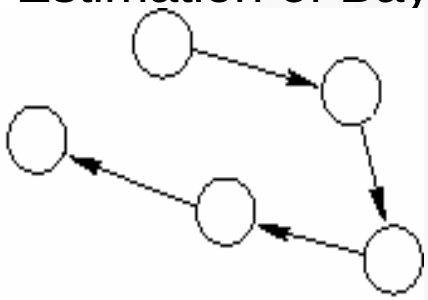
Main Idea

- Probabilistic model preserves significant combinations of parameters
  - Model complexity should be penalized to avoid overtraining (duplication of individuals)
- Selection is the source of progress
- Model complexity issues
  - Too complex model $\Rightarrow$ parent population is nearly reproduced
  - Too coarse model $\Rightarrow$ higher order dependencies are ignored (problem considered nearly separable)

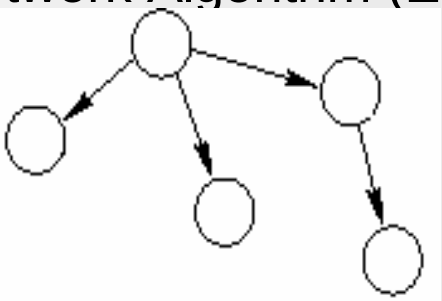
Predecessors of BOA

- The Univariate Marginal Distribution Algorithm (UMDA)
- The Mutual Information Maximization for Input Clustering (MIMIC)
- Combining Optimizers with Mutual Information Trees (COMIT)
- The Bivariate Marginal Distribution Algorithm (BMDA)
- The Learning Factorized Distribution Algorithm (LFDA)
- The Extended compact Genetic Algorithm (EcGA)
- The Estimation of Bayesian Network Algorithm (EBNA)

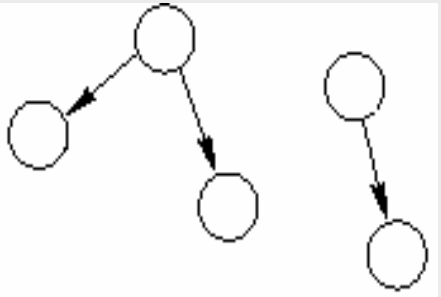
MIMIC



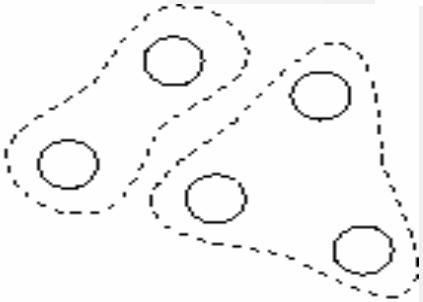
COMIT

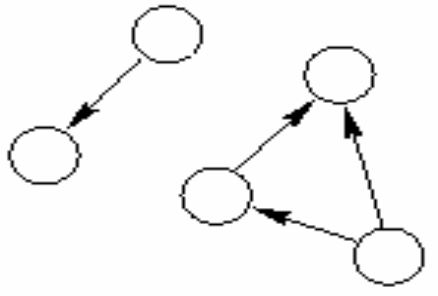


BMDA



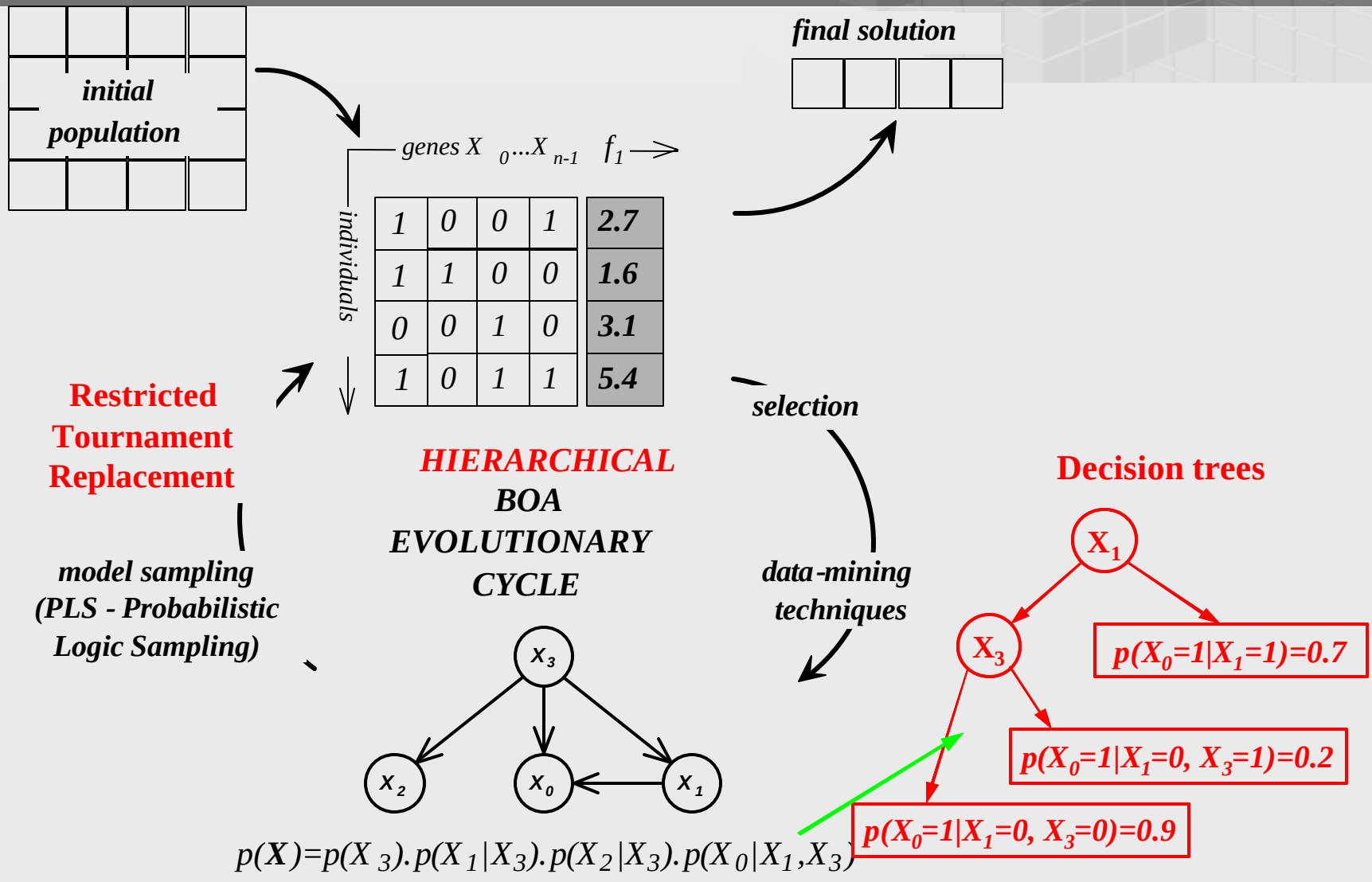
EcGA





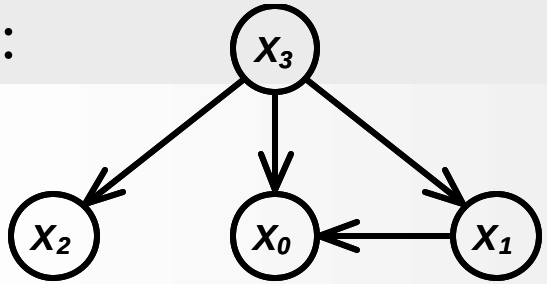
BOA/EBNA/LFDA

Recent advancements – hierarchical BOA



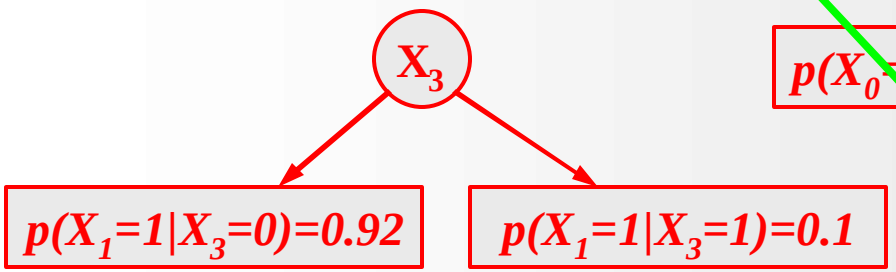
Example of Bayesian network with decision trees

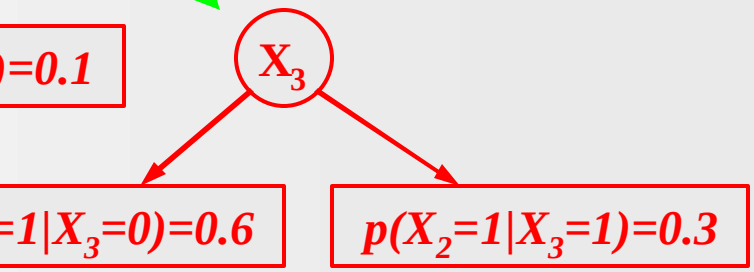
Example:

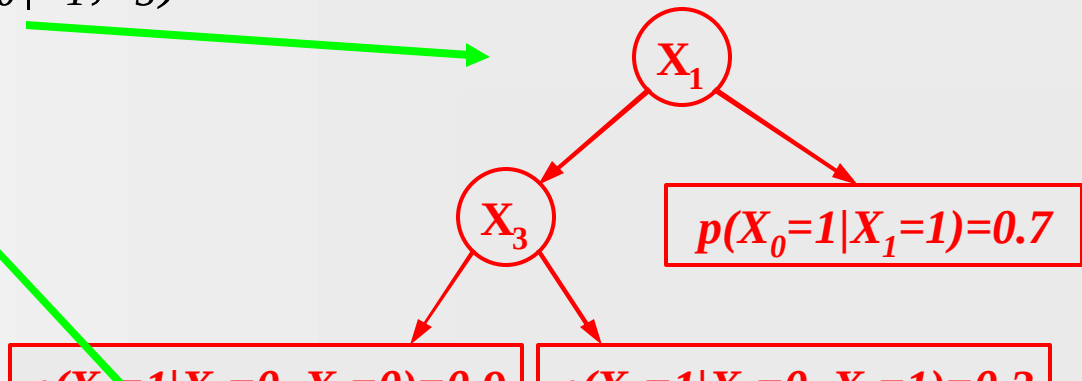


$$p(\mathbf{X})=p(X_3).p(X_1|X_3).p(X_2|X_3).p(X_0|X_1,X_3)$$

$p(X_3=1)=0.8$

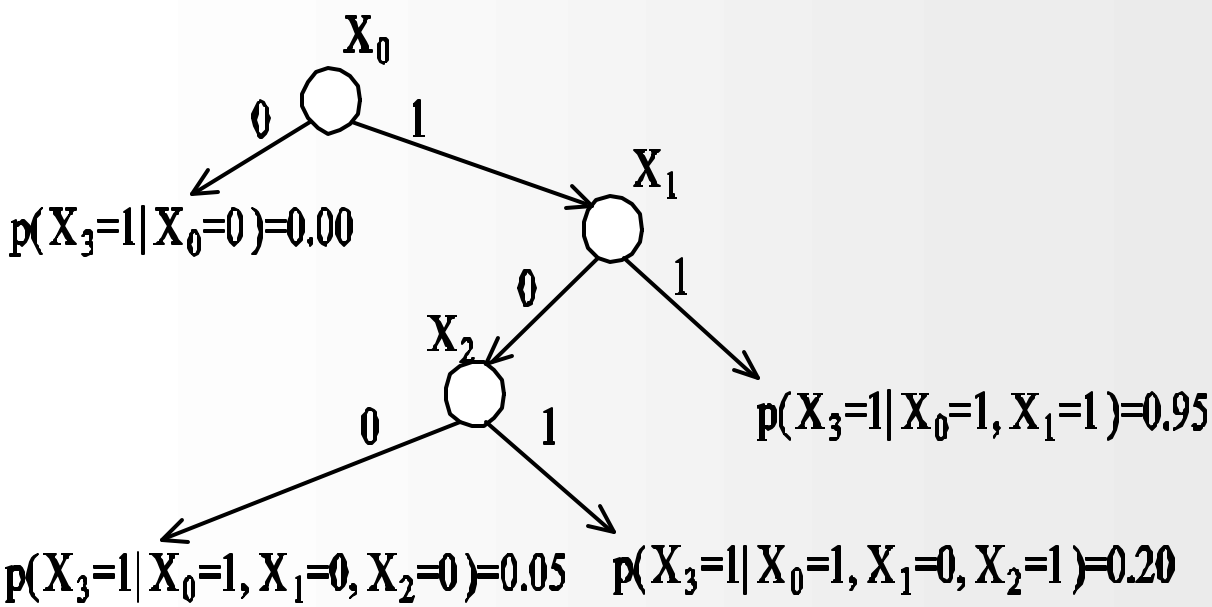






The advantages of decision trees

- Decision trees / graphs are more efficient:
  - Can capture longer building blocks
  - Are more robust



X_0	X_1	X_2	p(X3|X0,X1,X2)
0	0	0	0.00
0	0	1	0.00
0	1	0	0.00
0	1	1	0.00
1	0	0	0.05
1	0	1	0.20
1	1	0	0.95
1	1	1	0.95

Top-down building of decision trees

Population:

x_0	x_1	x_2	x_3
0	0	0	0
0	0	0	0
0	1	0	1
0	1	0	1
1	0	0	1
1	1	0	1
1	1	0	1
1	1	1	0

Split on x_0 :

	x_3=0	x_3=1
x_0 = 0	2	2
x_0 = 1	1	3

gain = 1.40

Split on x_1 :

	x_3=0	x_3=1
x_1 = 0	2	1
x_1 = 1	1	4

gain = 1.92

Split on x_2 :

	x_3=0	x_3=1
x_2 = 0	2	5
x_2 = 1	1	0

gain = 1.65

Sub-population x_1=0:

x_0	x_1	x_2	x_3
0	*	0	0
0	*	0	0
1	*	0	1

Sub-population x_1=1:

x_0	x_1	x_2	x_3
0	*	0	1
0	*	0	1
1	*	1	0
1	*	0	1
1	*	0	1

Split on x_0 :

	x_3=0	x_3=1
x_0 = 0	2	0
x_0 = 1	0	1

gain = 1.54

Split on x_2 :

	x_3=0	x_3=1
x_2 = 0	0	3
x_2 = 1	0	0

gain = 1.07

Split on x_0 :

	x_3=0	x_3=1
x_0 = 0	0	2
x_0 = 1	1	2

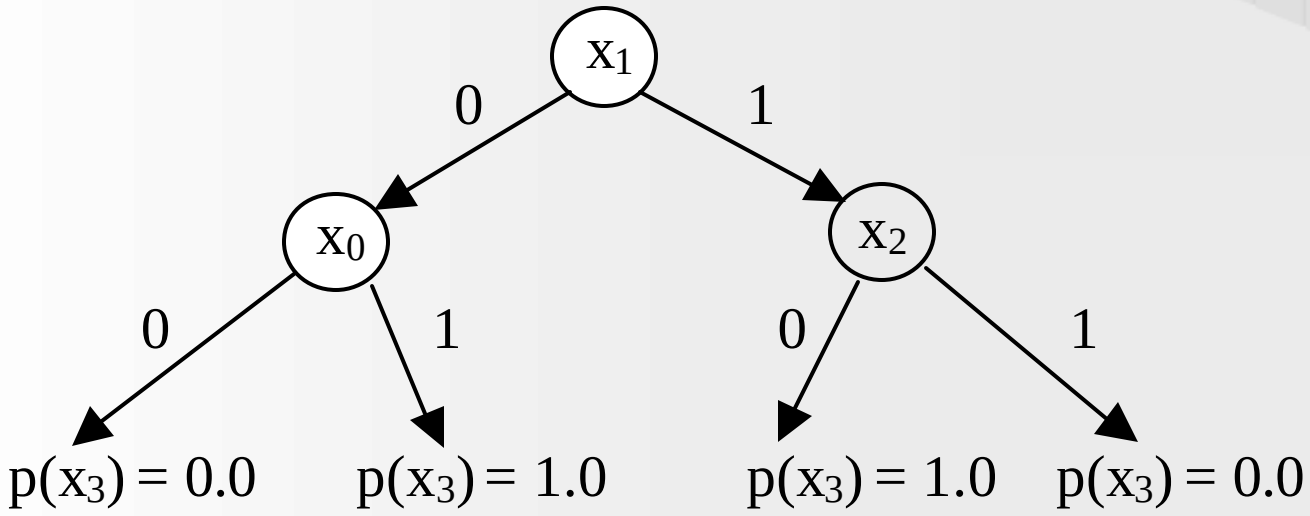
gain = 1.07

Split on x_2 :

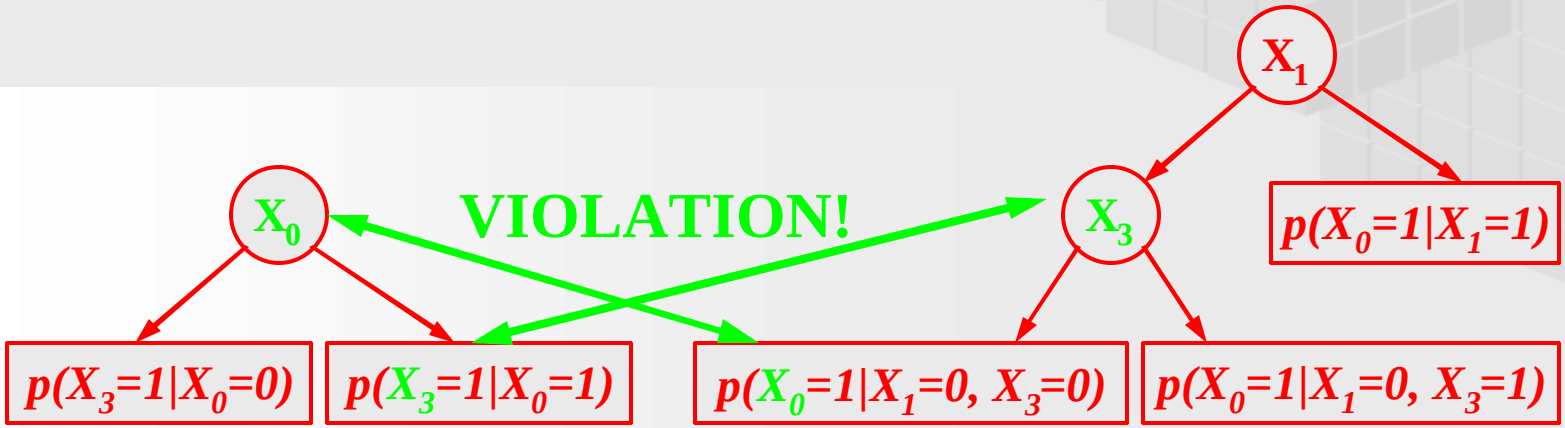
	x_3=0	x_3=1
x_2 = 0	4	0
x_2 = 1	0	1

gain = 2.22

Top-down building of decision trees - cont'd: The resulting decision tree



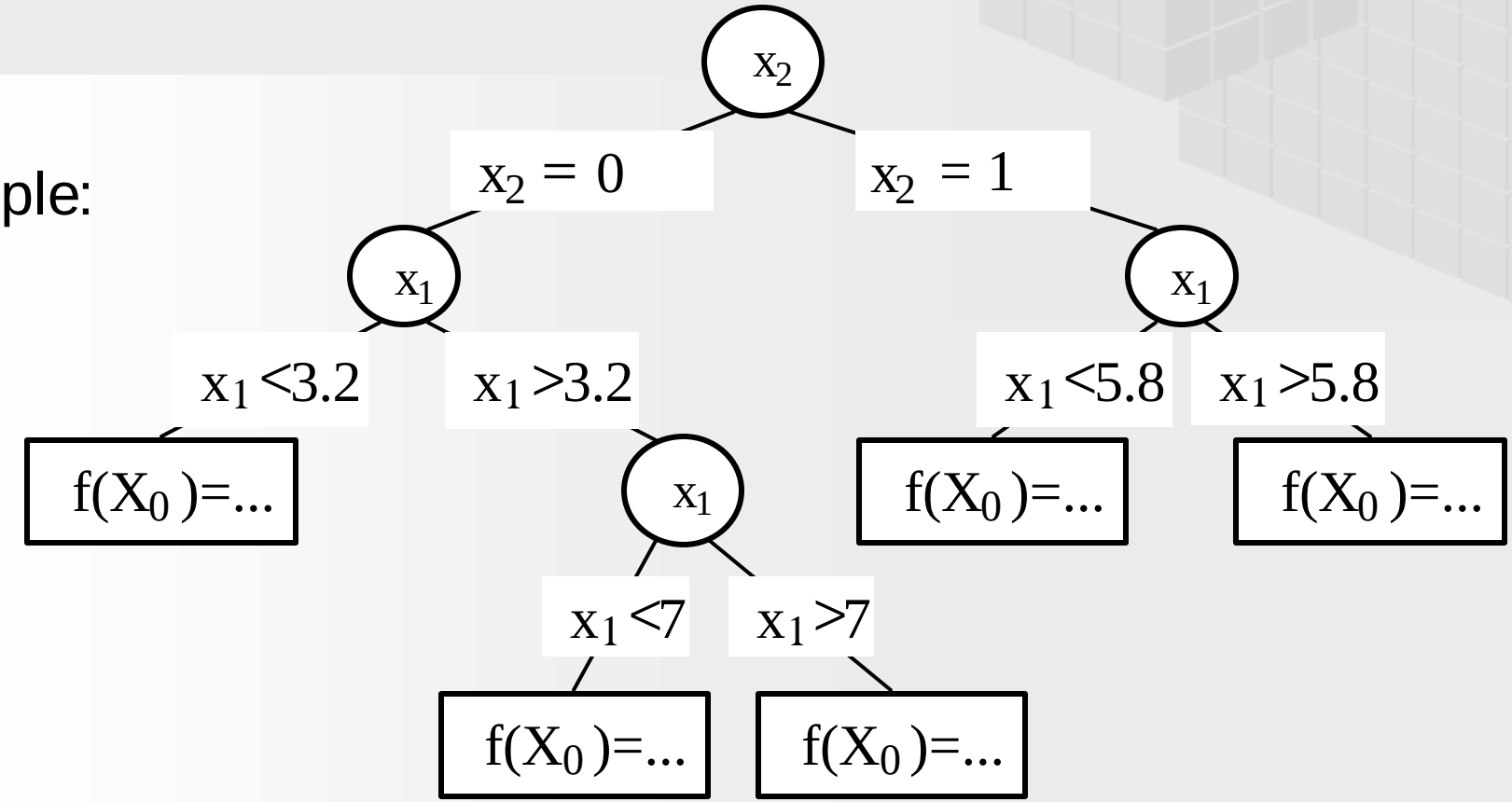
Avoiding cycles



- While constructing all the trees simultaneously, cycles have to be avoided

Mixed decision trees

- Example:



- **Compatible with discrete and continuous domains**

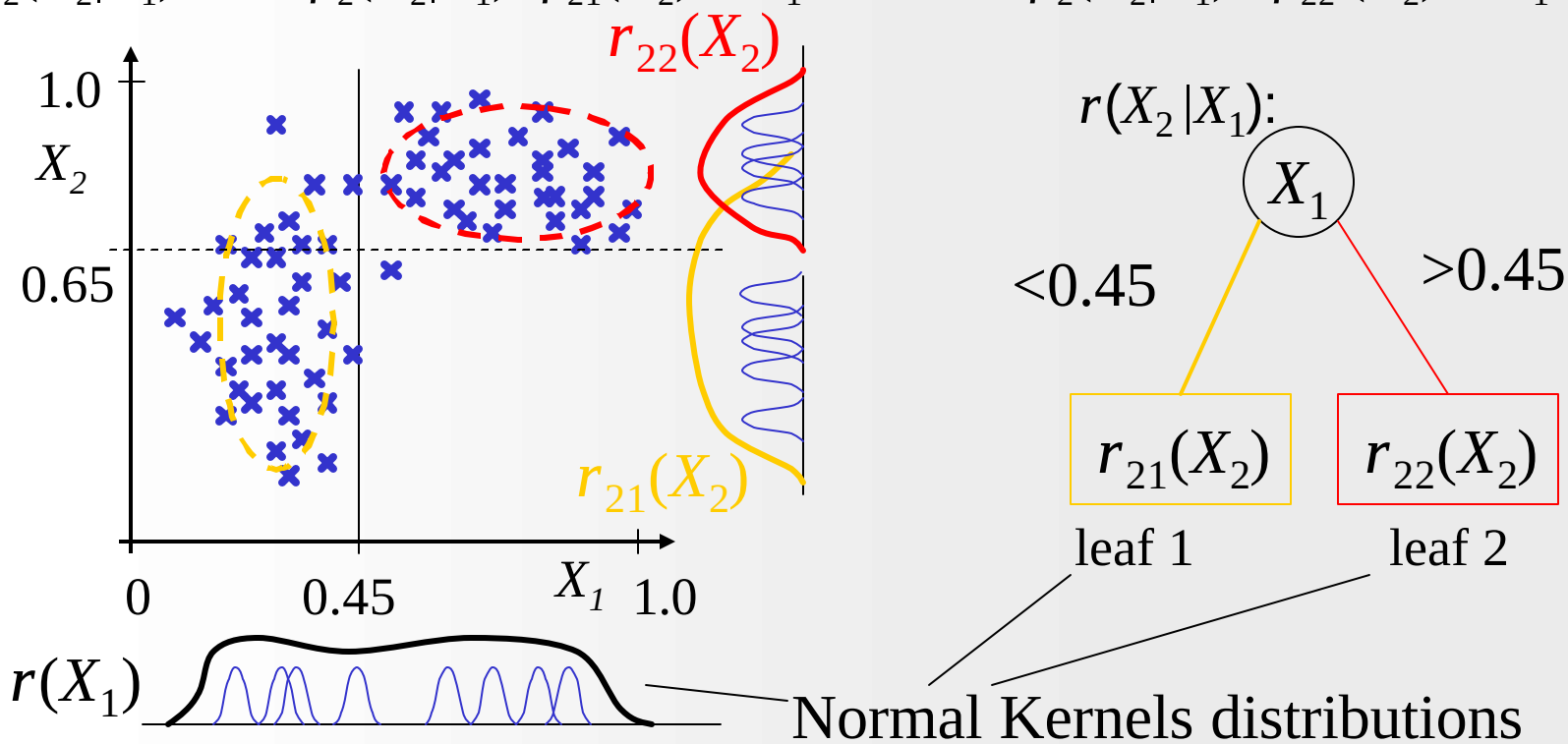
Mixed Bayesian Optimization Algorithm

- Discretization of continuous parameters is an integral part of the learning process.
- 2-level approach:
  - The dependencies are detected using the discretized variables and they are used to partition the search space into subspaces where no correlation appears
  - The Gaussian kernel distribution is used in each subspace to approximate the underlying distribution

Example of probabilistic model in continuous domain (Mixed BOA)

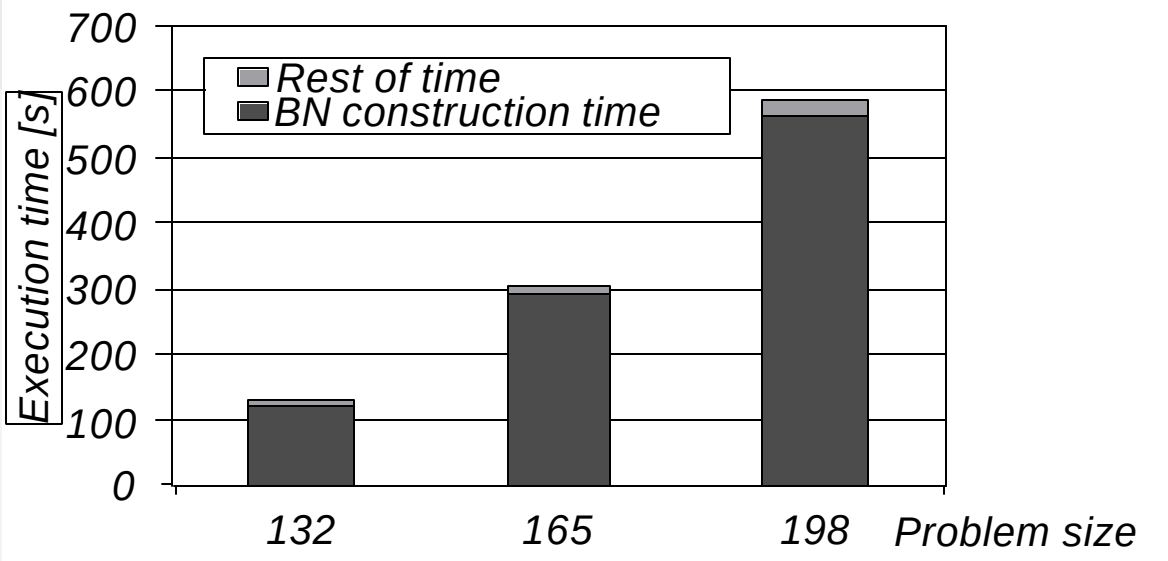
- Decision trees imply conditional factorization
- Example – 2 continuous genes:

$P(X_1,X_2)$ is factorized as $P(X_1,X_2)=P(X_1).P(X_2|X_1)$.
$P(X_1)$ is described by the density function $\rho_1(X_1)$ and $P(X_2|X_1)$ by the density function $\rho_2(X_2|X_1)$, with $\rho_2(X_2|X_1)=\rho_{21}(X_2)$ if $X_1<0.45$ and $\rho_2(X_2|X_1)= \rho_{22}(X_2)$ if $X_1\geq 0.45$

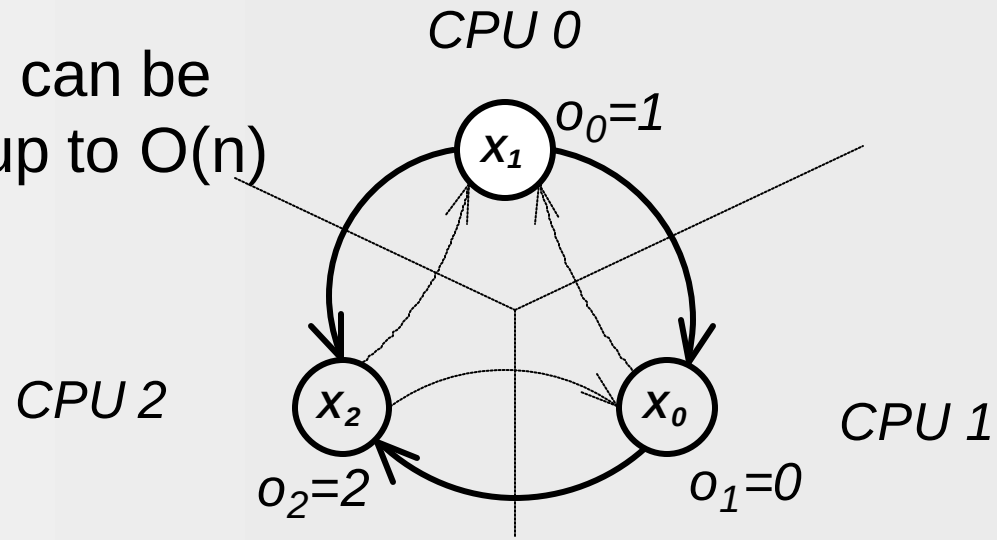


Disadvantages of Model building

- Time profile:



- Solution: model building can be performed in parallel – up to O(n) speedup



GA versus EDA

- Uses the information from individuals in a pairwise manner
- Sensitive to the ordering of parameters
- Recombination is fast

- In EDA the information from all individuals is aggregated in the model
- Not sensitive to the ordering of parameters
- Model building takes time (but can be parallelized)

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