

# HPDGClassifier

An R package for supervised classification using  
hybrid probabilistic decision graphs

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UNIÓN EUROPEA  
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# Contents

- 1 Motivation
- 2 Discrete PDGs
- 3 MoTBF-PDGs
- 4 The HPDGClassifier R package

## Using MoTBF-PDGs for supervised classification

- Take advantage of **context specific independencies**.
- **Inference** is carried out directly over the PDG structure in a **time linear** in the size.
- **No restrictions** on the model structure.
- No **normality** assumption.

# Motivation

## Using MoTBF-PDGs for supervised classification

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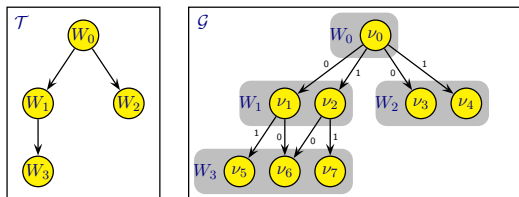
## Why an R package?

- Make it available to the data science community.
- Take advantage of the R framework.
- Facilitate experimentation and comparison.

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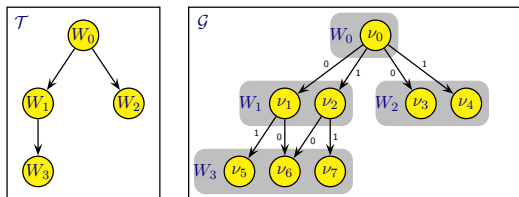
# The PDG model



## PDG structure

- Variables are organized in a **tree** structure  $\mathcal{T}$ .
- Each variable is represented by a set of **nodes** in  $\mathcal{G}$ .
- Every node  $\nu_j$  belongs to one unique variable  $W_i$ .
- Each node has an outgoing arc for every **state** of its variable.

# The PDG model



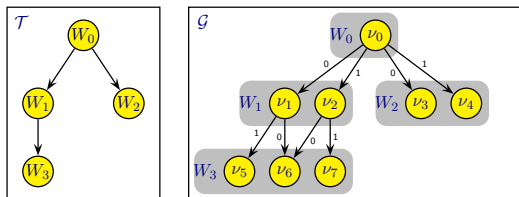
## Operation reach

Let  $\mathbf{w} = \{W_0 = 0, W_1 = 1, W_2 = 1, W_3 = 1\}$ . Then:

$$\text{reach}(W_0, \mathbf{w}) = \nu_0 ; \text{reach}(W_1, \mathbf{w}) = \nu_1$$

$$\text{reach}(W_2, \mathbf{w}) = \nu_3 ; \text{reach}(W_3, \mathbf{w}) = \nu_5$$

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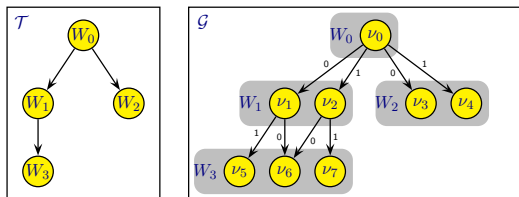
$$\text{reach}(W_2, \mathbf{w}) = \nu_3 ; \text{reach}(W_3, \mathbf{w}) = \nu_5$$

## Factorisation

$$f(\mathbf{w}) := \prod_{W_i \in \mathbf{w}} f^{\text{reach}(W_i, \mathbf{w})}(\mathbf{w}[W_i])$$



# The PDG model



- Every  $\nu_j$  contains a **local distribution**  $f^{\nu_j}$ :

$$f^{\nu_0} = P(W_0)$$

$$f^{\nu_1} = P(W_1|W_0 = 0)$$

$$f^{\nu_2} = P(W_1|W_0 = 1)$$

$$f^{\nu_3} = P(W_2|W_0 = 0)$$

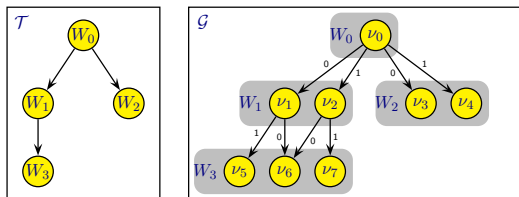
$$f^{\nu_4} = P(W_2|W_0 = 1)$$

$$f^{\nu_5} = P(W_3|W_0 = 0, W_1 = 1)$$

$$f^{\nu_6} = P(W_3|W_1 = 0, \{W_0 = 0 \vee W_0 = 1\})$$

$$f^{\nu_7} = P(W_3|W_0 = 1, W_1 = 1)$$

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Context-specific independencies:

$$I(W_3, W_0 | W_1 = 0) , \neg I(W_3, W_0 | W_1 = 1)$$

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# MoTBF model

## Univariate MoTBF potential

$$g_k(x) = \sum_{i=0}^k a_i \psi_i(x), \quad a_i \in \mathbb{R}.$$

## MoP example

$$\Psi = \{1, x, x^2, x^3\} : g(x) = 0.29 - 0.58x + 1.17x^2 + 0.44x^3$$

## MTE example

$$\Psi = \{1, e^{-x}, e^x, e^{-2x}, e^{2x}\} : g(x) = 0.14 + 0.29e^{-x} + 0.59e^x - 0.22e^{-2x} + 0.08e^{2x}$$

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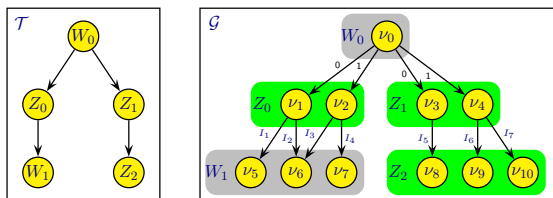
## MTE example

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## Conditional MoTBF potential

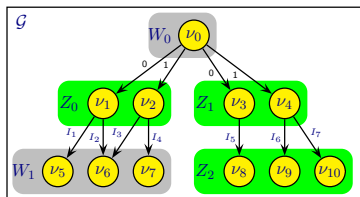
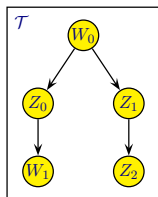
$$g_k^{(j)}(x \mid \mathbf{z} \in \Omega_Z^j) = \sum_{i=0}^k a_i^{(j)} \psi_i^{(j)}(x).$$

# MoTBF-PDG model



- **No restrictions** on the structure.
- A node  $\nu$  representing  $Z \in \mathbf{Z}$ :
  - ▶ can have **one or more** outgoing edges for each  $Z_i$  child of  $Z$  in  $\mathcal{T}$ .
  - ▶ each edge represents an interval of  $\Omega_Z$ .
- **Normality** assumption is not required.

# MoTBF-PDG model



$$\begin{array}{ccccccc}
 I_1 & I_2 & I_3 & I_4 & I_5 & I_6 & I_7 \\
 [0, 0.5) & [0.5, 1] & [0.5, 1] & [0, 0.5) & [0, 1] & [0, 0.3) & [0.3, 1]
 \end{array}$$

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$$\begin{array}{ll}
 f^{\nu_0} = P(W_0) & f^{\nu_5} = P(W_1|W_0 = 0, Z_0 \in [0, 0.5)) \\
 f^{\nu_1} = \rho(Z_0|W_0 = 0) & f^{\nu_6} = P(W_1|Z_0 \in [0.5, 1]) \\
 f^{\nu_2} = \rho(Z_0|W_0 = 1) & f^{\nu_7} = P(W_1|W_0 = 1, Z_0 \in [0, 0.5)) \\
 f^{\nu_3} = \rho(Z_1|W_0 = 0) & f^{\nu_8} = \rho(Z_2|W_0 = 0) \\
 f^{\nu_4} = \rho(Z_1|W_0 = 1) & f^{\nu_9} = \rho(Z_2|W_0 = 1, Z_1 \in [0, 0.3)) \\
 & f^{\nu_{10}} = \rho(Z_2|W_0 = 1, Z_1 \in [0.3, 1])
 \end{array}$$


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# MoTBF-PDG classifiers

## PDG classifier structure

- Contains a **single tree** over the variables  $\mathbf{C} = \{C\} \cup \mathbf{X}$
- Variable  $C$  must be the **root** of the tree.



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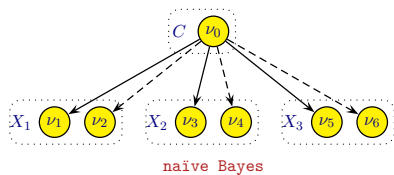
## Classification

Given an evidence  $\mathbf{x} = \{x_1, \dots, x_n\}$  the goal is to find  $c^*$  such that:

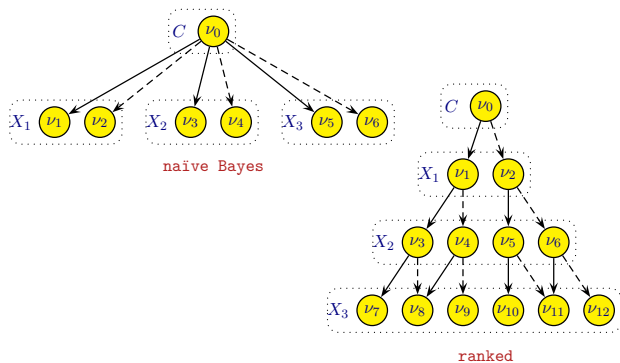
$$\begin{aligned}c^* &= \arg \max_{c \in R(C)} f(c \mid \mathbf{x}) = \arg \max_{c \in R(C)} \frac{f(c, \mathbf{x})}{\sum_{c \in R(C)} f(c, \mathbf{x})} \\ &\propto \arg \max_{c \in R(C)} f(c, \mathbf{x}) \\ &= \arg \max_{c \in R(C)} f(c) \times f(x_1 \mid c) \times \dots \times f(x_n \mid c, x_1, \dots, x_{n-1})\end{aligned}$$

Evaluate the conditional functions in the nodes **reached** by  $\mathbf{x}$  for each  $c \in R(C)$ .

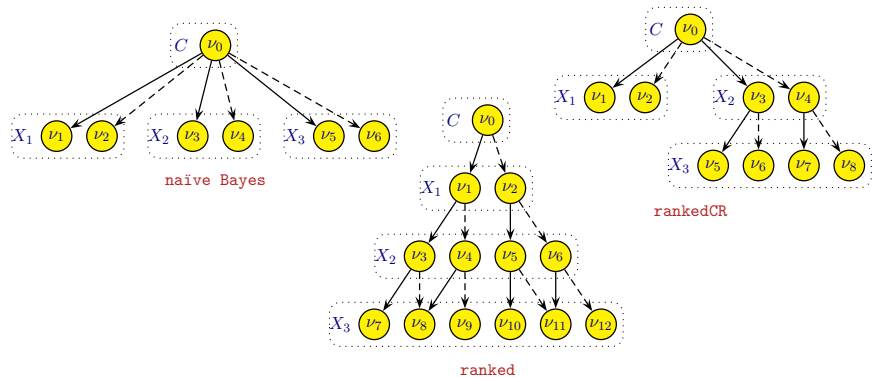
# Learning MoTBF-PDGs



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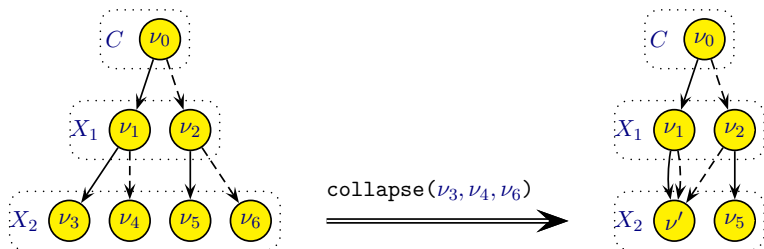
# Learning MoTBF-PDGs



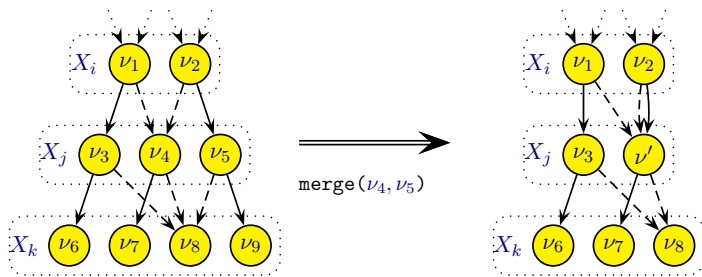
Other methods: CR, Chou-Liu

# Collapsing nodes

- PDG is **expanded** during learning: **reached data** goes down.
- **Collapse nodes** to avoid learning from tiny samples.
- Applied when a new variable is included.



# Merging nodes



- Merge operation is checked **bottom-up** once the model is learnt.
- Reduce **overfitting** and the model **size**.

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## Implementation

- Object oriented design.
- Uses packages:
  - ▶ polynom
  - ▶ quadprog
  - ▶ foreach
  - ▶ infotheo
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  - ▶ codetools



# The HPDGClassifier R package

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## Features

- Standard classification setting
- Parallelisation