# Probabilistic Machine Learning: 6. Belief Networks: basic notation

Tomasz Kajdanowicz, Przemysław Kazienko (substitution)

Department of Computational Intelligence Wroclaw University of Technology





Wrocław University of Science and Technology

4 (0.0

The presentation was inspired by Chapter 2 and 3 of D. Barber book "Bayesian Reasoning and Machine Learning", 2012.

## Already covered

#### We have covered:

- inferring a distribution over a discrete variable drawn from a finite hypothesis space
- ▶ inferring the probability that a coin shows up heads and dice has given value
- given a series of discrete observations

Let's focus now on much more complex probabilities!

## Graphs

#### Graph

A graph G consists of nodes (also called vertices) and edges (also called links) between the nodes. Edges may be directed (they have an arrow in a single direction) or undirected. Edges can also have associated weights. A graph with all edges directed is called a directed graph, and one with all edges undirected is called an undirected graph

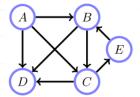


Figure: An directed graph G consists of directed edges between nodes

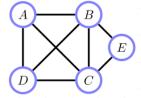


Figure: An undirected graph G consists of undirected edges between nodes

# What do we need graphs for?

- ▶ to form connection between directed graphs and probability
- two variables will be independent if they are not linked by a path on the graph

## Path, ancestors, descendants

#### Path

A path  $A \to B$  from node A to node B is a sequence of nodes that connects A to B. That is, a path is of the form  $A_0, A_1, \ldots, A_{n-1}, A_n$ , with  $A_0 = A$  and  $A_n = B$  and each edge  $(A_{k-1}, A_k)$ ,  $k = 1, \ldots, n$  being in the graph. A directed path is a sequence of nodes which when we follow the direction of the arrows leads us from A to B.

#### **Ancestor**

In directed graphs, the nodes A such that  $A \to B$  and  $B \not\to A$  are the *ancestors* of B.

#### Descendant

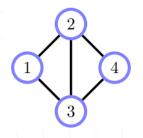
The nodes B such that A  $\rightarrow$  B and B  $\not\rightarrow$  A are the descendants of A.

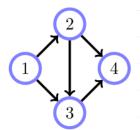


# Cycle

### Cycle

A cycle is a directed path that starts and returns to the same node  $a \to b \to \ldots \to z \to a$ 

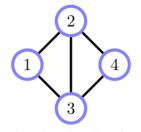


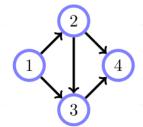


## Loop

#### Loop

A loop is a path containing more than two nodes, irrespective of edge direction, that starts and returns to the same node.

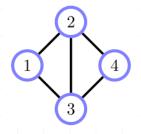


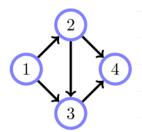


## Chord

#### Chord

A chord is an edge that connects two non-adjacent nodes in a loop.





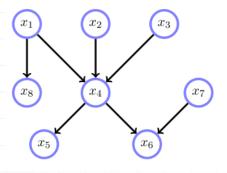
## Directed Acyclic Graph (DAG)

#### DAG

A DAG is a graph *G* with directed edges (arrows on each link) between the nodes such that by following a path of nodes from one node to another along the direction of each edge no path will revisit a node.

In a DAG the ancestors of B are those nodes who have a directed path ending at B. Conversely, the descendants of A are those nodes who have a directed path starting at A.

## Relationships in a DAG



#### parents, children, family

- the parents of  $x_4$  are  $pa(x_4) = \{x_1, x_2, x_3\}$
- the children of  $x_4$  are  $ch(x_4) = \{x_5, x_6\}$
- the family of a node is itself and its parents

#### Markov blanket

The Markov blanket of a node is its parents, children and the parents of its children, excluding itself. (Markov blanket of  $x_4$  is  $x_1, x_2, x_3, x_5, x_6, x_7$ 

## Neighbour, Clique

#### Neighbour

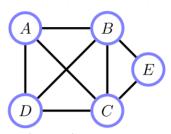
For an undirected graph G the neighbours of x, ne(x) are those nodes directly connected to x.

#### Clique

Given an undirected graph, a clique is a fully connected subset of nodes.

- all the members of the clique are neighbours
- ▶ for a maximal clique there is no larger clique that contains the clique

## Clique example



- ▶ the graph has two maximal cliques,  $C1 = \{A, B, C, D\} \text{ and } C2 = \{B, C, E\}$
- ► A, B, C are fully connected, but this is a non-maximal clique
- ▶ there is a larger fully connected set: A, B, C, D

#### Cliques play a role in:

- modelling describe variables that are all dependent on each other
- inference describe sets of variables with no simpler structure that makes the relationship between them and for which no simpler efficient inference procedure is likely to exist

## Connected graph

#### Connected graph

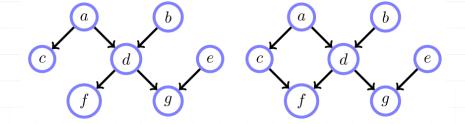
An undirected graph is connected if there is a path between every pair of nodes (i.e. there are no isolated islands). For a graph which is not connected, the connected components are those subgraphs which are connected.

#### Singly Connected Graph

A graph is *singly connected* if there is only one path from any node A to any other node B. Otherwise the graph is multiply connected (for directed and undirected graphs)

An alternative name for a singly connected graph is a tree. A multiply-connected graph is also called loopy.

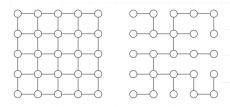
# Singly, multiply connected



## **Spanning Tree**

#### **Spanning Tree**

A spanning tree of an undirected graph *G* is a singly-connected subset of the existing edges such that the resulting singly-connected graph covers all nodes of *G* 



A maximum weight spanning tree is a spanning tree such that the sum of all weights on the edges of the tree is at least as large as any other spanning tree of G.

## **Spanning Tree**

Finding a maximal weight spanning tree

find a spanning tree with maximal weight()

- pick the next candidate edge which has the largest weight and add this to the edge set
- ▶ if this results in an edge set with cycles, then reject the candidate edge and propose the next largest edge weight
- pick the edge with the largest weight and add this to the edge set

There may be more than one maximal weight spanning tree.



# **Numerically Encoding Graphs**

- edge list
- adjacency matrix
- ▶ clique matrix
- graph2vec etc.



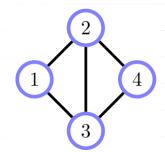
## Edge list

#### Edge list

Edge list simply lists which node-node pairs are in the graph.

$$L = \{(1, 2), (2, 1), (1, 3), (3, 1), (2, 3), (3, 2), (2, 4), (4, 2), (3, 4), (4, 3)\}$$

Undirected edges are listed twice, once for each direction

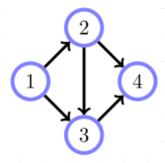


## Adjacency matrix

#### Adjacency matrix

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

where  $A_{ij} = 1$  if there is an edge from node i to node j in the graph, and 0 otherwise. An undirected graph has a symmetric adjacency matrix.



## Adjacency matrix

Adjacency matrices may seem wasteful since many of the entries are zero, but...

#### Adjacency matrix powers

For an  $N \times N$  adjacency matrix A, powers of the adjacency matrix  $[A^k]_{ij}$  specify how many paths there are from node i to node j in k edge hops.

## Clique matrix

For an undirected graph with N nodes and maximal cliques  $C_1, \ldots, C_K$  a clique matrix is an  $N \times K$  matrix in which each column  $c_k$  has zeros except for ones on entries describing the clique.

$$C = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

