



# *Introduction to Statistical Machine Learning*

Christfried Webers

Statistical Machine Learning Group

NICTA

and

College of Engineering and Computer Science

The Australian National University

Canberra

February – June 2015

(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")



*Markov Random Fields*

*Bayesian Networks vs.  
Markov Random Fields*

## Part XIV

# *Probabilistic Graphical Models 2*

# Markov Random Fields (MRFs)

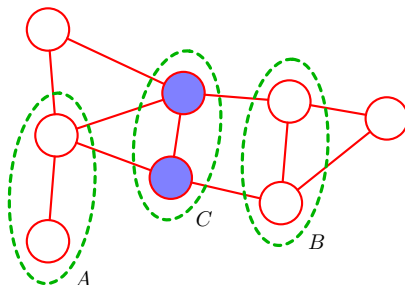


- Markov Random Fields (Markov network, undirected graphical model) are defined over a graph with undirected edges.
- MRFs allow for different conditional independence statements than Bayesian networks.
- In a Bayesian network, the definition of a blocked path was subtle for a HH-node because it did include that all descendants were unobservable.
- Is there an alternative graphical semantics for probability distributions such that conditional independence is determined by simple graph separation?
- Yes, removing the direction from the edges removes the asymmetry between parent and child nodes and subsequently the subtleties associated with the HH-node.



## Definition (Graph Separation)

In an undirected graph  $G$ , having  $A$ ,  $B$  and  $C$  disjoint subsets of nodes, if every path from  $A$  to  $B$  includes at least one node from  $C$ , then  $C$  is said to **separate**  $A$  from  $B$  in  $G$ .



# Conditional Independence in MRFs

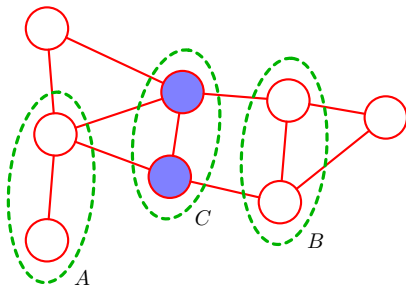


## Definition (Conditional Independence in Markov Random Field)

In an undirected graph  $G$ , having  $A$ ,  $B$  and  $C$  disjoint subsets of nodes,  $A$  is conditionally independent of  $B$  given  $C$

$$A \perp\!\!\!\perp B \mid C$$

iff  $C$  separates  $A$  from  $B$  in  $G$ .





## Definition (Markov Random Field)

A Markov Random Field is a set of probability distributions  $\{p(\mathbf{x}) \mid p(\mathbf{x}) > 0, \forall \mathbf{x}\}$  such that there exists an undirected graph  $G$  with disjoint subsets of nodes  $A$ ,  $B$  and  $C$ , in which whenever  $C$  separates  $A$  from  $B$  in  $G$ ,

$$A \perp\!\!\!\perp B \mid C.$$

- Although we sometimes say "the MRF is such an undirected graph", we mean "the MRF represents the set of all probability distributions whose conditional independency statements are precisely those given by graph separation in the graph".



- Assume two nodes  $x_i$  and  $x_j$  that are not connected by an edge.
- Given all other nodes in the graph,  $x_i$  and  $x_j$  must be conditionally independent as all paths between  $x_i$  and  $x_j$  are blocked by observed nodes.

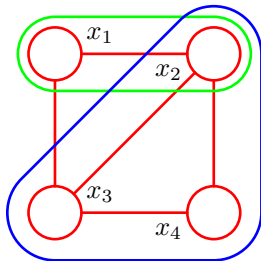
$$p(x_i, x_j \mid \mathbf{x}_{\setminus\{i,j\}}) = p(x_i \mid \mathbf{x}_{\setminus\{i,j\}}) p(x_j \mid \mathbf{x}_{\setminus\{i,j\}})$$

where  $\mathbf{x}_{\setminus\{i,j\}}$  denotes the set of all variables  $\mathbf{x}$  with  $x_i$  and  $x_j$  removed.

- Directly connected nodes are therefore not conditionally independent given all the others. Can we use this for the factorisation of the graph?

# Cliques in a graph

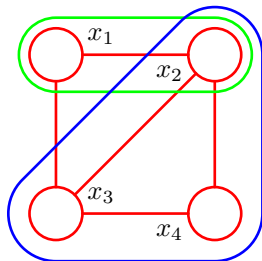
- A **clique** is a subset of nodes in a graph such that there exists an edge between all pairs of nodes in the subset. (The nodes in a clique are fully connected.)
- A **maximal clique** of a graph is a clique which is not a proper subset of another clique. (No other nodes of the graph can be added to a maximal clique without destroying the property of full connectedness.)





# Factorisation using Cliques

- We can express the factorisation with the help of the cliques.
- In fact, we only need the maximal cliques, as any function over the variables of a subset of a maximal clique can be expressed as a function of the members of the maximal clique.
- Denote by  $\mathcal{C}$  the set of maximal cliques of a graph.
- For a maximal clique  $C \in \mathcal{C}$ , denote by  $\mathbf{x}_C$  the subset of the variables  $\mathbf{x}$  which belong to  $C$ .





- A probability distribution  $p(\mathbf{x})$  **factorises** with respect to a given undirected graph  $G$  if it can be written as

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(\mathbf{x}_C)$$

where  $\mathcal{C}$  is the set of maximal cliques of  $G$ , and **potential functions**  $\psi_C(\mathbf{x}_C) \geq 0$ . The constant  $Z = \sum_{\mathbf{x}} p(\mathbf{x})$  ensures the correct normalisation of  $p(\mathbf{x})$ .

# Conditional Independence $\Leftrightarrow$ Factorisation



## Theorem (Factorisation $\Rightarrow$ Conditional Independence)

If a probability distribution factorises according to an undirected graph, and if  $A$ ,  $B$  and  $C$  are disjoint subsets of nodes such that  $C$  separates  $A$  from  $B$  in the graph, then the distribution satisfies  $A \perp\!\!\!\perp B \mid C$ .

## Theorem (Conditional Independence $\Rightarrow$ Factorisation (Hammersley-Clifford Theorem))

If a **strictly positive** probability distribution  $p(\mathbf{x}) > 0, \forall \mathbf{x}$ , satisfies the conditional independence statements implied by graph separation over a particular undirected graph, then it also factorises according to the graph.



# Factorisation with strictly positive potential functions

- As the potential functions  $\psi_C(\mathbf{x}_C)$  are strictly positive, one can express them as exponential

$$\psi_C(\mathbf{x}_C) = \exp\{-E(\mathbf{x}_C)\}$$

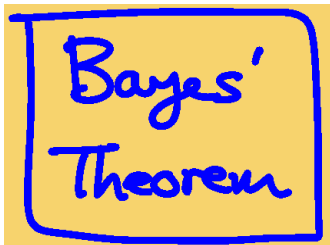
of an **energy function**  $E(\mathbf{x}_C)$ .

- The exponential distribution is called the **Boltzmann distribution**.
- The joint distribution is defined as the product of the potentials, and so the total energy is obtained by adding the energies of each of the maximal cliques.

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(\mathbf{x}_C) = \frac{1}{Z} \exp\left\{-\sum_{C \in \mathcal{C}} E(\mathbf{x}_C)\right\}$$

# Example of Image Denoising

- Given an unknown and noise-free image described by binary pixels  $x_i \in \{-1, +1\}$  for  $i = 1, \dots, D$ .
- Randomly flip the sign of some pixels with some small probability and denote the pixels of the noisy image by  $y_i$  for  $i = 1, \dots, D$ .
- Goal : Recover the original noise-free image.



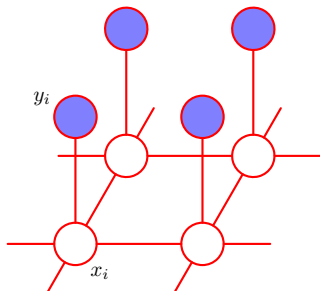
Original image.



After randomly changing  
10% of the pixels.

# Example of Image Denoising

- Prior knowledge 1 : We know the noise level is small.  
Therefore: Strong correlation between original pixels  $x_i$  and noisy pixels  $y_i$ .
- Prior knowledge 2 : Neighbouring pixels  $x_i$  and  $x_j$  in an image are strongly correlated (given a decent resolution).
- Prior knowledge can be captured in a Markov Random Field.



# Example of Image Denoising



- Cliques  $\{x_i, y_i\}$  : Choose an energy function of the form  $-\eta x_i y_i$  for  $\eta > 0$  resulting in a potential function  $\exp\{\eta x_i y_i\}$ . This favours equal signs for  $x_i$  and  $y_i$ .
- Cliques  $\{x_i, x_j\}$  where  $i$  and  $j$  are indices of neighbouring pixels : Choose an energy function of the form  $-\beta x_i x_j$  for  $\beta > 0$  again favouring equal signs for  $x_i$  and  $x_j$ .
- We need to accomodate for the fact that one kind of pixels might exist more often than the other kind. This can be done by adding a term  $h x_i$  for each pixel in the noise-free image. (Potential function is an arbitrary, nonnegative function over maximal cliques, so we are allowed to multiply it by any nonnegative function of subsets of the clique.)

# Example of Image Denoising

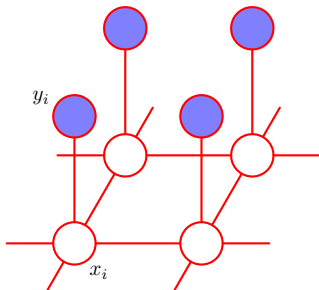


- Energy function

$$E(\mathbf{x}, \mathbf{y}) = h \sum_i x_i - \beta \sum_{i,j} x_i x_j - \eta \sum_i i x_i y_i$$

- which defines a joint distribution over  $\mathbf{x}$  and  $\mathbf{y}$

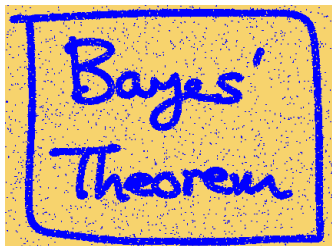
$$p(\mathbf{x}, \mathbf{y}) = \frac{1}{Z} \exp\{-E(\mathbf{x}, \mathbf{y})\}.$$



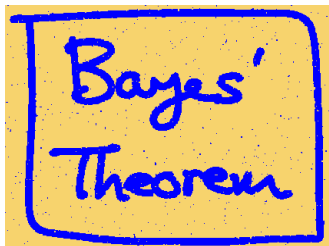


# Example - Iterated Conditional Modes (ICM)

- 1 Fix the elements for  $\mathbf{y}$  as we have them observed. (Implicitly defines  $p(\mathbf{x} | \mathbf{y})$ ).
- 2 Initialise  $x_i = y_i$  for  $i = 1, \dots, D$ .
- 3 Take one node  $x_j$  and evaluate the total energy for both possible states of  $x_j = \{-1, +1\}$  keeping all other variables fixed. Set  $x_j$  to the state having the lower energy.
- 4 Repeat for another node until stopping criterion is satisfied.



Local minimum (ICM).



Global minimum (graph-cut).



# Bayesian Networks vs. Markov Random Fields



- Two frameworks for graphical models, can we convert between them?
- Bayesian Network



$$p(\mathbf{x}) = p(x_1) p(x_2 | x_1) p(x_3 | x_2) \dots p(x_N | x_{N-1})$$

- Random Markov Field



$$p(\mathbf{x}) = \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \dots \psi_{N-1,N}(x_{N-1}, x_N)$$

# Bayesian Networks vs. Markov Random Fields



- Bayesian Network

$$p(\mathbf{x}) = p(x_1) p(x_2 | x_1) p(x_3 | x_2) \dots p(x_N | x_{N-1})$$

- Random Markov Field

$$p(\mathbf{x}) = \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \dots \psi_{N-1,N}(x_{N-1}, x_N)$$

- Find corresponding terms

$$\psi_{1,2}(x_1, x_2) = p(x_1) p(x_2 | x_1)$$

$$\psi_{2,3}(x_2, x_3) = p(x_3 | x_2)$$

$$\vdots$$

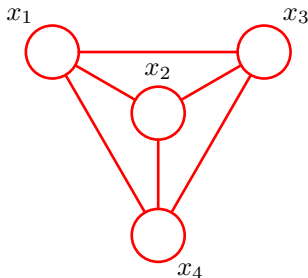
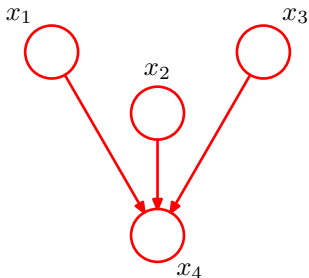
$$\psi_{N-1,N}(x_{N-1}, x_N) = p(x_N | x_{N-1})$$

and note that  $Z = 1$  in this case.

# Bayesian Networks vs. Markov Random Fields



- For other kind of Bayesian Networks (BNs), create the cliques of a MRF by adding undirected edges between all pairs of parents for each node in the graph.
- This process of 'marrying the parents' is called **moralisation**, and the result is a **moral graph**.
- BUT the resulting MRF may represent different conditional independence statements than the original BN.
- Example: The MRF is fully connected, and exhibits NO conditional independence properties, in contrast to the original directed graph.



# Bayesian Networks vs. Markov Random Fields



## Definition (D-map)

A graph is a **D-map** (dependency map) of a distribution if every conditional independence statement satisfied by the distribution is reflected in the graph.

## Definition (I-map)

A graph is an **I-map** (independence map) of a distribution if every conditional independence statement implied by the graph is satisfied in the distribution.

## Definition (P-map)

A graph is a **P-map** (perfect map) of a distribution if it is both a D-map and an I-map for the distribution.

# Bayesian Networks vs. Markov Random Fields

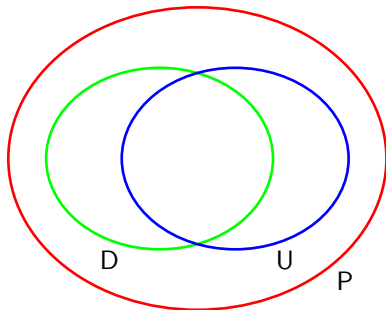


Consider probability distributions depending on  $N$  variables

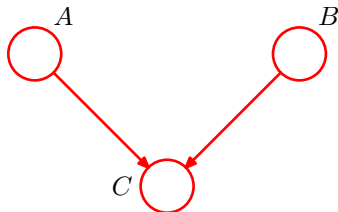
$P$  set of all probability distributions

$D$  set of all probability distributions that can be represented as a perfect map by an **directed** graph

$U$  set of all probability distributions that can be represented as a perfect map by an **undirected** graph

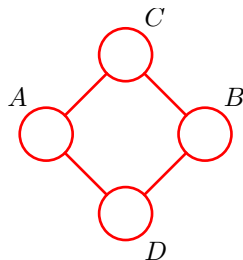


# Only as Bayesian Network



A directed graph whose conditional independence properties cannot be expressed using an undirected graph over the same three variables.

# Only as Random Markov Field



An undirected graph whose conditional independence properties cannot be expressed using a directed graph over the same four variables.





In both types of Graphical Models

- A relationship between the conditional independence statements satisfied by a distribution and the associated simplified algebraic structure of the distribution is made in term of graphical objects.
- The conditional independence statements are related to concepts of separation between variables in the graph.
- The simplified algebraic structure (factorisation of  $p(\mathbf{x})$ ) is related to 'local pieces' of the graph (child + its parents in BNs, cliques in MRFs).



## Differences

- The set of probability distributions that can be represented as MRFs is different from the set that can be represented as BNs.
- Although both MRFs and BNs are expressed as a factorisation of local functions on the graph, the MRF has a normalisation constant  $Z = \sum_{\mathbf{x}} \prod_{C \in \mathcal{C}} \psi_C(\mathbf{x}_C)$  that couples all factors, whereas the BN has not.
- The local 'pieces' of the BN are probability distributions themselves, whereas in MRFs they need only be non-negative functions (i.e. they may not have range  $[0, 1]$  as probabilities do).