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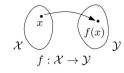
Winter Semester 2015/2016

Introduction

# 4. Introduction to Graphical Models

# THAT .

We often need to build a model of the real world that relates observed measurements  $x \in \mathcal{X}$  to quantities of interest  $y \in \mathcal{Y}$ .



### Running example:

Recognizing man-made structures in images (i.e. binary image segmentation)





Original image

Ground truth ( $24 \times 16$  blocks)

We have one binary variable per 16-by-16 block of pixels.

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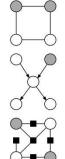
# Popular classes of graphical models



- Undirected graphical models (e.g., Markov random fields)
- Directed graphical models (e.g., Bayesian networks)
- Factor graphs

We will use the following notations

- $\blacksquare$  V denotes a set of output variables (e.g., for pixels) and the corresponding random variables are denoted by  $Y_i,\ i\in V$
- The output domain  $\mathcal{Y}$  is given by the product of individual variable domains  $\mathcal{Y}_i$  (e.g., a single label set  $\mathcal{L}$ ), so that  $\mathcal{Y} = \times_{i \in V} \mathcal{Y}_i$
- The input domain  $\mathcal X$  is application dependent (e.g.,  $\mathcal X$  is a set of images)
- $\blacksquare \quad \text{The } \mathbf{realization} \,\, Y = y \,\, \text{means that} \,\, Y_i = y_i \,\, \text{for all} \,\, i \in V$
- $\blacksquare$   $G=(V,\mathcal{E})$  is an (un)directed graph, where  $\mathcal{E}$  encodes the conditional independence assumption



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# Example: Man-made structure detection





Original image

Ground truth ( $24 \times 16$  blocks)

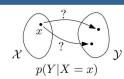
For each block we assign a random variable  $Y_i$ . Therefore, V consists of binary output variables corresponding to  $Y_i$ , for all  $i=1,\ldots,384$ .

For each random variable  $Y_i$  its output domain is  $\mathcal{Y}_i=\{0,1\}$ , therefore the output domain in this example is  $\mathcal{Y}=\{0,1\}^{384}$ 

 $\mathcal{X}$  is a set of images, and an input  $x \in \mathcal{X}$  is an image.

# Graphical models

# Probabilistic graphical models encode a joint p(x,y) or conditional $p(y\mid x)$ probability distribution such that given some observations we are provided with a full probability distribution over all feasible solutions.



The graphical models allow us to encode relationships between a set of random variables using a concise language, by means of a graph.

Suppose a graph such that for each node a random variable is assigned. The random variables satisfy **conditional independence assumptions** encoded in the graph.



For example: The variables  $Y_i$  and  $Y_l$  are conditionally independent given  $Y_j, Y_k$ :

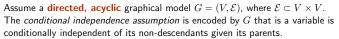
 $Y_i \perp \!\!\!\perp Y_l \mid Y_j, Y_k \Rightarrow p(Y_i, Y_l \mid Y_j, Y_k) = p(Y_i \mid Y_j, Y_k) p(Y_l \mid Y_j, Y_k) .$ 

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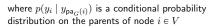
# •

# Bayesian networks



The factorization is given as

$$p(Y = y) = \prod_{i \in V} p(y_i \mid y_{\mathsf{pa}_G(i)}) ,$$





$$\begin{aligned} p(y) = & p(y_i, y_j, y_k, y_l) = p(y_l \mid y_i, y_j, y_k) \ p(y_i, y_j, y_k) \\ = & p(y_l \mid y_k) \ p(y_i, y_j, y_k) = p(y_l \mid y_k) \ p(y_k \mid y_i, y_j) \ p(y_i, y_j) \\ = & p(y_l \mid y_k) \ p(y_k \mid y_i, y_j) \ p(y_i) \ p(y_j) \ . \end{aligned}$$

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# THE

### **Example: Man-made structure detection**



Original image

Ground truth ( $24 \times 16$  blocks)

We consider a simple assumption: man-made structures are clustered locally together.

 $\ensuremath{\mathcal{E}}$  consists of edges between 4-connected blocks, which means that we model the relation between neighboring blocks only.



### Markov random fields

An undirected graphical model  $G = (V, \mathcal{E})$  is called Markov Random Field (MRF) if two nodes are conditionally independent whenever they are not connected. In other words, for any node  $Y_i$  in the graph, the local Markov property holds:

 $p(Y_i \mid Y_{V \setminus \{i\}}) = p(Y_i \mid Y_{N(i)})$ 

where N(i) are the neighbors of node i in the graph. Alternatively, one can use the following equivalent notation:



$$Y_i \perp \!\!\!\perp Y_{V \setminus \mathsf{cl}(i)} \mid Y_{N(i)}$$
,

where  $cl(i) = \{i\} \cup N(i)$  is the *closed neighborhood* of i.

For example:

$$Y_i \perp \!\!\! \perp Y_l \mid Y_j, Y_k \Rightarrow p(Y_i, Y_l \mid Y_j, Y_k) = p(Y_i \mid Y_j, Y_k) \ p(Y_l \mid Y_j, Y_k) \ .$$

and edges of G. That is,

# Hammersley-Clifford theorem



Let  $G=(V,\mathcal{E})$  be an undirected graphical model. The Hammersley-Clifford theorem tells us that the following are equivalent:

- G is an MRF model
- The joint probability distribution P(Y) on G has Gibbs-distribution.

An MRF defines a family of joint probability distributions by means of an undirected graph  $G=(V,\mathcal{E}),\ \mathcal{E}\subset V\times V$  (there are no self-edges), where the graph encodes conditional independence assumptions between the random variables corresponding to V.

Since, the potential functions  $\psi_C(y_c) > 0$ 

$$\psi_C(y_C) = \exp(-E_C(y_C)) \quad \Leftrightarrow \quad E_C(y_C) = -\log((\psi_C(y_C))) \; .$$

## **Examples**

Gibbs distribution

 $\psi_C(y_C)>0$  defined on cliques (i.e. fully connected subgraph) that cover all nodes

 $p(y) = \frac{1}{Z} \prod_{C \in \mathcal{C}(G)} \psi_C(y_C) ,$ 

 $Z = \sum_{y \in \mathcal{Y}} \prod_{C \in \mathcal{C}(G)} \psi_C(y_C) .$ 

is the normalization constant, Z is also known as partition function.

A probability distribution p(y) on an undirected graphical model  $G=(V,\mathcal{E})$ 

called Gibbs distribution if it can be factorized into potential functions

where  $\mathcal{C}(G)$  denotes the set of all (maximal) cliques and

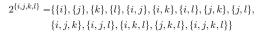


Cliques  $C(G_1)$ : set of nodes  $V' \subseteq V$  such that  $\mathcal{E} \cap (V' \times V') = V' \times V'$ Here  $\mathcal{C}(G_1) = \{\{i\}, \{j\}, \{k\}, \{i,j\}, \{j,k\}\}$ , hence

$$(Y_i)$$
  $(Y_j)$   $(Y_k)$   $G_1$ 

$$p(y) = \frac{1}{Z} \psi_i(y_i) \psi_j(y_j) \psi_k(y_k) \psi_{ij}(y_i, y_j) \psi_{jk}(y_j, y_k)$$
 Here  $\mathcal{C}(G_2) = 2^{\{i,j,k,l\}}$  (all subsets of  $V$ )

$$p(y) = \frac{1}{Z} \prod_{A \in 2^{\{i,j,k,l\}}} \psi_A(y_A)$$





# **Factor graphs**



Factor graphs are undirected graphical models that make explicit the factorization of the probability function.

A factor graph  $G=(V,\mathcal{F},\mathcal{E})$  consists of

- variable nodes  $V(\bigcirc)$  and factor nodes  $\mathcal{F}(\blacksquare)$ ,
- edges  $\mathcal{E} \subseteq V \times \mathcal{F}$  between variable and factor nodes
- $N:\mathcal{F} \to 2^V$  is the scope of a factor, defined as the set of neighboring variables, i.e.  $N(F) = \{i \in V : (i, F) \in \mathcal{E}\}.$



Factor graph

A family of distribution is defined that factorizes according to

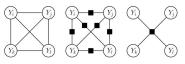
$$p(y) = \frac{1}{Z} \prod_{F \in \mathcal{F}} \psi_F(y_{N(F)}) \quad \text{with} \quad Z = \sum_{y \in \mathcal{Y}} \prod_{F \in \mathcal{F}} \psi_F(y_{N(F)}) \;.$$

Each factor  $F \in \mathcal{F}$  connects a subset of nodes, hence we write  $F = \{v_1, \dots, v_{|F|}\}$ and  $y_F = y_{N(F)} = (y_{v_1}, \dots, y_{v_{|F|}}).$ 

### **Examples**



Factor graphs are universal, explicit about the factorization, hence it is easier to work with them.



Examples:

Ulif.

$$\begin{aligned} p_1(y) &= \frac{1}{Z_1} \psi_{ij}(y_i, y_j) \psi_{ik}(y_i, y_k) \psi_{il}(y_i, y_l) \psi_{jk}(y_j, y_k) \psi_{jl}(y_j, y_l) \psi_{kl}(y_k, y_l) \\ p_2(y) &= \frac{1}{Z_2} \psi_{ijkl}(y_i, y_j, y_k, y_l) \end{aligned}$$



# **Conditional Random Fields**

# Conditional random fields



We have discussed the joint distribution

$$p(y) = \frac{1}{Z} \prod_{F \in \mathcal{F}} \psi_F(y_{N(F)}) \; ,$$

but we often have access to measurements  $\boldsymbol{X}=\boldsymbol{x}$ , hence the **conditional distribution**  $p(Y = y \mid X = x)$  can be directly modeled, too. This can be expressed compactly using conditional random fields (CRF) with the factorization  $p(y\mid x) = \frac{1}{Z(x)} \prod_{F \in \mathcal{F}} \psi_F(y_F; x_F)$ 

$$p(y \mid x) = \frac{1}{Z(x)} \prod_{F \in \mathcal{F}} \psi_F(y_F; x_F)$$

with the **partition function** depending on  $x_F$ 

$$Z(x) = \sum_{y \in \mathcal{Y}} \prod_{F \in \mathcal{F}} \psi_F(y_F; x_F) .$$



Shaded variables: The observations X = x.

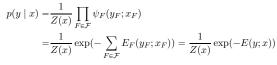


We typically would like to infer marginal probabilities  $p(Y_F = y_F \mid x)$  for some factors  $F \in \mathcal{F}$ .

Assuming  $\psi_F: \mathcal{Y}_F \to \mathbb{R}_+$ , where  $\mathcal{Y}_F = \times_{i \in N(F)} \mathcal{Y}_i$  is the product domain of the variables adjacent to F, instead of potentials, we can also work with energies.

We define an energy function  $E_F: \mathcal{Y}_{N(F)} \to \mathbb{R}$  for each factor  $F \in \mathcal{F}$ .

$$E_F(y_F; x_F) = -\log(\psi_F(y_F; x_F)) \quad \Leftrightarrow \quad \psi_F(y_F; x_F) = \exp(-E_F(y_F; x_F)) \; .$$



Potentials and energy functions (cont.)

for  $E(y;x) = \sum_{F \in \mathcal{F}} E_F(y_F;x_F)$ . Hence,  $p(y \mid x)$  is completely determined by E(y;x). This provides a natural way to quantify prediction uncertainty by means of marginal distributions  $p(y_F \mid x_F)$ .

Note that the potentials become also functions of (part of) x, i.e.  $\psi_F(y_F; x_F)$ instead of just  $\psi_F(y_F)$ . Nevertheless, x is **not** part of the probability model, i.e. it is not treated as random variable.

# **Energy Minimization**



Assuming a finite  $\mathcal{X}$ , the goal is to predict  $f: \mathcal{X} \to \mathcal{Y}$  by solving  $y^* = \operatorname{argmax}_{y \in \mathcal{Y}} p(y|x)$ 

$$\begin{aligned} \underset{y \in \mathcal{Y}}{\operatorname{argmax}} \ p(y|x) &= \underset{y \in \mathcal{Y}}{\operatorname{argmax}} \ \frac{1}{Z(x)} \exp(-E(y;x)) \\ &= \underset{y \in \mathcal{Y}}{\operatorname{argmax}} \ \exp(-E(y;x)) \\ &= \underset{y \in \mathcal{Y}}{\operatorname{argmax}} \ -E(y;x) \\ &= \underset{y \in \mathcal{Y}}{\operatorname{argmin}} \ E(y;x) \ . \end{aligned}$$

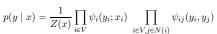
Energy minimization can be interpreted as solving for the most likely state of factor graph.

In practice, one typically models the energy function directly.

# Example: Man-made structure detection



Conditional independences are specified by the factor graph, i.e. all blocks only depend on the neighboring ones. The conditional distribution factorizes (up to pairwise



$$Z(x) = \sum_{y \in \{0,1\}^{384}} \prod_{i \in V} \psi_i(y_i; x_i) \prod_{i \in V, j \in N(i)} \psi_{ij}(y_i, y_j)$$

$$E(y;x) = \sum_{i \in V} E_i(y_i;x_i) + \sum_{i \in \mathcal{V}, j \in N_i} E_{ij}(y_i,y_j) \;. \label{eq:energy}$$

# Example: Man-made structure detection



In order to define energy functions for unary factors, one can consider a set of functions  $\phi_i: \mathcal{Y}_i \times \mathcal{X}_i \to [0; 1]$ :

$$E_i(y_i; x_i) = -\log \phi_i(y_i; x_i)$$
 for all  $i \in V$ .

For pairwise factor energies here we use the Potts model, that is

$$E_{ij}(y_i, y_j) = \llbracket y_i \neq y_j \rrbracket = \begin{cases} 0, & \text{if } y_i = y_j \\ 1, & \text{otherwise.} \end{cases}$$

The resulting energy function given as

$$\begin{split} E(y;x) &= \sum_{i \in V} E_i(y_i;x_i) + \sum_{i \in V, j \in N(i)} E_{ij}(y_i,y_j) \\ &= \sum_{i \in V} -\log \phi_i(y_i;x_i) + \sum_{i \in V, i \in N(i)} \llbracket y_i \neq y_j \rrbracket \;. \end{split}$$

## Inference



The goal is to make predictions  $y \in \mathcal{Y}$ , as good as possible, about unobserved properties for a given data instance  $x \in \mathcal{X}$ 

Suppose we are given a graphical model (e.g., a factor graph). Inference means the procedure to estimate the probability distribution, encoded by the graphical model, for a given data (or observation).

Maximum A Posteriori (MAP) inference: Given a factor graph and the observation x, find the state  $y^* \in \mathcal{Y}$  of maximum probability,

$$y^* = \operatorname*{argmax}_{y \in \mathcal{Y}} p(Y = y \mid x) = \operatorname*{argmin}_{y \in \mathcal{Y}} E(y; x) \; .$$

### Inference (cont.)



Probabilistic inference: Given a factor graph and the observation x, find the value of the log partition function and the marginal distributions for each factor,

$$\log Z(x) = \log \sum_{y \in \mathcal{Y}} \exp(-E(y; x)) ,$$
  
$$\mu_F(y_F) = p(Y_F = y_F \mid x) \quad \forall F \in \mathcal{F}, \forall y_F \in \mathcal{Y}_F .$$

This typically includes variable marginals, i.e.  $\mu_i = p(y_i \mid x)$ , to make a single joint

Both inference problems are known to be NP-hard for general graphs and factors, but can be tractable if suitably restricted (see for example pseudo boolean optimization).

### **Example: Man-made structure detection**



Input image



MAP inference



Ground truth

Probabilistic inference



Sebastian Nowozin and Christoph H. Lampert.

Structured Prediction and Learning in Computer Vision.

In Foundations and Trends in Computer Graphics and Vision, Volume 6, Number 3-4. Note: Chapter 2.

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