Combinatorial Optimization in Computer Vision (IN2245)

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Winter Semester 2015/2016

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4. Introduction to Graphical Models

Introduction

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 (24×16 blocks)

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

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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. x0 X V p(Y|X = x)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** Y_i Y_i independence assumptions encoded in the graph. For example: The variables Y_i and Y_l are conditionally independent given Y_i, Y_k : Y_l Y_k $Y_i \perp Y_l \mid Y_i, Y_k \Rightarrow p(Y_i, Y_l \mid Y_i, Y_k) = p(Y_i \mid Y_i, Y_k)p(Y_l \mid Y_i, Y_k).$

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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

- 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
 - $\mathcal{Y} = imes_{i \in V} \mathcal{Y}_i$
- The **input domain** \mathcal{X} is application dependent (e.g., \mathcal{X} is a set of images)
- **The realization** Y = y means that $Y_i = y_i$ 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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Bayesian networks

Assume a **directed**, acyclic graphical model $G = (V, \mathcal{E})$, where $\mathcal{E} \subset V \times V$. The conditional independence assumption is encoded by G that is two variables are conditionally independent given any other one, if they are not connected. The factorization is given as $p(Y = y) = \prod_{i \in V} p(y_i \mid y_{\mathsf{pa}_G(i)}) ,$ where $p(y_i \mid y_{\mathsf{pa}_G(i)})$ is a conditional probability distribution on the parents of node $i \in V$ YL For example: $p(Y) = p(y_i, y_j, y_k, y_l) = p(y_l \mid y_i, y_j, y_k) \ p(y_i, y_j, y_k)$ $=p(y_{l} | y_{k}) p(y_{i}, y_{j}, y_{k}) = p(y_{l} | y_{k}) p(y_{k} | y_{i}, y_{j}) p(y_{i}, y_{j})$ $=p(y_l | y_k) p(y_k | y_i, y_j) p(y_i) p(y_j).$

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Example: Man-made structure detection



Original image Ground

Ground truth (24 imes 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, ..., 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.

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Example: Man-made structure detectionImage: Driginal imageImage: Driginal imageOriginal image: Driginal imageGround truth $(24 \times 16 \text{ blocks})$ We consider a simple assumption:
man-made structures are clustered locally together.
 \mathcal{E} consists of edges between 4-connected blocks, which means that we model the relation between
neighboring blocks only.Image: Driginal image \mathcal{E} consists of edges between 4-connected blocks, which means that we model the relation between
neighboring blocks only.Image: Driginal image

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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:

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

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

For example:

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

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Gibbs distribution

A probability distribution p(Y) on an undirected graphical model $G = (V, \mathcal{E})$ is called **Gibbs distribution** if it can be factorized into potential functions $\psi_C(y_C) > 0$ defined on cliques (i.e. fully connected subgraph) that cover all nodes and edges of G. That is,

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

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

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

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

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 Y_l Y_{k}

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Hammersley-Clifford theorem

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

- $\blacksquare \quad G \text{ is an MRF model}$
- $\blacksquare \quad \text{The joint probability distribution } P(Y) \text{ on } G \text{ has Gibbs-distribution.}$

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 $\psi_C(y_c) > 0$

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

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Examples

Cliques $\mathcal{C}(G_1)$: 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

$$p(y) = \frac{1}{Z} \psi_i(y_i) \psi_j(y_j) \psi_k(y_k) \psi_{ij}(y_i, y_j) \psi_{jk}(y_j, y_k)$$

Here $C(G_2) = 2^{\{i,j,k,l\}}$ (all subsets of V)

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

$$\begin{split} 2^{\{i,j,k,l\}} =& \{\{i\},\{j\},\{k\},\{l\},\{i,j\},\{i,k\},\{i,l\},\{j,k\},\{j,l\},\\ & \{i,j,k\},\{i,j,l\},\{i,k,l\},\{j,k,l\},\{i,j,k,l\}\} \end{split}$$



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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. $N(F) = \{i \in V : (i, F) \in \mathcal{E}\}$. A family of distribution is defined that factorizes according to $p(y) = \frac{1}{Z} \prod_{F \in \mathcal{F}} \psi_F(y_{N(F)})$ with $Z = \sum_{y \in \mathcal{Y}} \prod_{F \in \mathcal{F}} \psi_F(y_{N(F)})$. Each factor $F \in \mathcal{F}$ connects a subset of nodes, hence we write $F = \{v_1, \dots, v_{|F|}\}$ and $y_F = y_{N(F)} = (y_{v_1}, \dots, y_{v_{|F|}})$.

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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 X = x, hence the **conditional distribution** p(Y = y | X = x) can be directly modeled, too. This can be expressed compactly using **conditional random fields** (CRF) with the factorization

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

with the partition function depending on x_F

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



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Potentials and energy functions

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 $F \in \mathcal{F}$.

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

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Potentials and energy functions (cont.)

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

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.

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Energy Minimization

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

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

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

In practice, one typically models the energy function directly.

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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 factors) as

$$p(y \mid x) = \frac{1}{Z(x)} \prod_{i \in V} \psi_i(y_i; x_i) \prod_{i \in V, j \in N(i)} \psi_{ij}(y_i, y_j)$$

with

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

The corresponding energy function:

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



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Example: Man-made structure detection

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

$$E_i(y_i; x_i) = -\log \phi_i(y_i; x_i)$$
 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

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

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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, parameterization and weight vector w, and given the observation x, find the state $y^* \in \mathcal{Y}$ of maximum probability,

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

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Inference (cont.)

Probabilistic inference: Given a factor graph, parameterization and weight vector w, and given the observation x, find the value of the *log partition* function and the marginal distributions for each factor,

$$\log Z(x, w) = \log \sum_{y \in \mathcal{Y}} \exp(-E(y; x, w)) ,$$

$$\mu_F(y_F) = p(Y_F = y_F \mid x, w) \quad \forall F \in \mathcal{F}, \forall y_F \in \mathcal{Y}_F .$$

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

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).

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Literature

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