Introduction To Graphical Models

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Extended version in book form

Sebastian Nowozin and Christoph Lampert

Structured Learning and Prediction in Computer Vision

ca 200 pages

Available free online http://pub.ist.ac.at/~chl/



Slides mainly based on a tutorial version from Christoph - Thanks!

Literature Recommendation

David Barber

Bayesian Reasoning and Machine Learning

670 pages

Available free online http://web4.cs.ucl.ac.uk/ staff/D.Barber/pmwiki/pmwiki. php?n=Brml.Online



Standard Regression:

$$f: \mathcal{X} \to \mathbb{R}.$$

Structured Output Learning:

$$f: \mathcal{X} \to \mathcal{Y}.$$

Standard Regression:

$$f: \mathcal{X} \to \mathbb{R}.$$

- \blacktriangleright inputs ${\mathcal X}$ can be any kind of objects
- output y is a real number

Structured Output Learning:

$$f: \mathcal{X} \to \mathcal{Y}.$$

- \blacktriangleright inputs ${\mathcal X}$ can be any kind of objects
- outputs $y \in \mathcal{Y}$ are complex (structured) objects

What is structured output prediction?

Ad hoc definition: predicting structured outputs from input data (in contrast to predicting just a single number, like in classification or regression)

- Natural Language Processing:
 - Automatic Translation (output: sentences)
 - Sentence Parsing (output: parse trees)
- Bioinformatics:
 - Secondary Structure Prediction (output: bipartite graphs)
 - Enzyme Function Prediction (output: path in a tree)
- Speech Processing:
 - Automatic Transcription (output: sentences)
 - Text-to-Speech (output: audio signal)
- Robotics:
 - Planning (output: sequence of actions)

This tutorial: Applications and Examples from Computer Vision

Example: Human Pose Estimation



Given an image, where is a person and how is it articulated?

$$f: \mathcal{X} \to \mathcal{Y}$$

• Image x, but what is human pose $y \in \mathcal{Y}$ precisely?





Example y_{head}





Example y_{head}





Example y_{head}





Example y_{head}





Example y_{head}





Example y_{head}





Example y_{head}









Head detector

Idea: Have a head classifier (SVM, NN, ...)

 $\psi(y_{head}, x) \in \mathbb{R}_+$



 $\mathsf{Image}\ x \in \mathcal{X}$



0.8

Head detector

 Y_{head}

 $\psi(y_{head}, x)$

Idea: Have a head classifier (SVM, NN, ...)

 $\psi(y_{head}, x) \in \mathbb{R}_+$

Evaluate everywhere and record score



Image $x \in \mathcal{X}$



Example y_{head}



Head detector

Idea: Have a head classifier (SVM, NN, ...)

 $\psi(y_{head}, x) \in \mathbb{R}_+$

- Evaluate everywhere and record score
- Repeat for all body parts

Human Pose Estimation



 $\mathsf{Image}\ x \in \mathcal{X}$

Compute

$$y^* = (y^*_{head}, y^*_{torso}, \cdots) = \operatorname*{argmax}_{y_{head}, y_{torso}, \cdots} \psi(y_{head}, x) \psi(y_{torso}, x) \cdots$$

Human Pose Estimation



 $\mathsf{Image}\ x \in \mathcal{X}$

Compute

y

$$= (y_{head}^*, y_{torso}^*, \cdots) = \underset{\substack{y_{head}, y_{torso}, \cdots}}{\operatorname{argmax}} \psi(y_{head}, x) \psi(y_{torso}, x) \cdots$$
$$= (\underset{\substack{y_{head}}}{\operatorname{argmax}} \psi(y_{head}, x), \underset{\substack{y_{torso}}}{\operatorname{argmax}} \psi(y_{torso}, x), \cdots)$$

Human Pose Estimation





 $\mathsf{Image}\ x \in \mathcal{X}$

Prediction $y^* \in \mathcal{Y}$

Compute

 $y^* = (y^*_{head}, y^*_{torso}, \cdots) = \underset{\substack{y_{head}, y_{torso}, \cdots \\ y_{head}, y_{torso}, \cdots}}{\operatorname{argmax}} \psi(y_{head}, x) \psi(y_{torso}, x) \cdots$ $= (\underset{\substack{y_{head}}}{\operatorname{argmax}} \psi(y_{head}, x), \underset{\substack{y_{torso}}}{\operatorname{argmax}} \psi(y_{torso}, x), \cdots)$

• Great! Problem solved!?

Idea: Connect up the body



Ensure *head* is on top of *torso*

$$\psi(y_{head}, y_{torso}) \in \mathbb{R}_+$$

Compute

 $y^* = \operatorname*{argmax}_{y_{head}, y_{torso}, \cdots} \psi(y_{head}, x) \psi(y_{torso}, x) \psi(y_{head}, y_{torso}) \cdots$

but this does not decompose anymore!

left image from Ben Sapp

The recipe

Structured output function, $\mathcal{X} =$ anything, $\mathcal{Y} =$ anything

1) Define auxiliary function, $g: \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$,

$$e.g. \qquad g(x,y) = \prod_i \psi_i(y_i,x) \prod_{i \sim j} \psi_{ij}(y_i,y_j,x)$$

2) Obtain $f : \mathcal{X} \to \mathcal{Y}$ by maximimization:

 $f(x) = \operatorname*{argmax}_{y \in \mathcal{Y}} g(x, y)$

A Probabilistic View

▶ ...

Computer Vision problems usually deal with uncertain information

- Incomplete information (observe static images, projections, etc)
- Annotation is "noisy" (wrong or ambiguous cases)

Uncertainty is captured by (conditional) probability distributions: p(y|x)

• for input $x \in \mathcal{X}$, how *likely* is $y \in \mathcal{Y}$ the correct output?

We can also phrase this as

- what's the probability of observing y given x?
- how strong is our *belief* in y if we know x?

A Probabilistic View on $f : \mathcal{X} \to \mathcal{Y}$

Structured output function, $\mathcal{X} = anything$, $\mathcal{Y} = anything$

We need to define an auxiliary function, $g: \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$.

$$e.g. \qquad g(x,y) := p(y|x).$$

Then maximimization

$$f(x) = \operatorname*{argmax}_{y \in \mathcal{Y}} g(x, y) = \operatorname*{argmax}_{y \in \mathcal{Y}} p(y|x)$$

becomes maximum a posteriori (MAP) prediction.

Interpretation:

The MAP estimate $y \in \mathcal{Y}$, is the most probable value (there can be multiple).

Probability Distributions

$$\begin{aligned} \forall y \in \mathcal{Y} \quad p(y) \geq 0 \qquad \text{(positivity)} \\ \sum_{y \in \mathcal{Y}} p(y) = 1 \qquad \text{(normalization)} \end{aligned}$$

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Example: binary ("Bernoulli") variable $y \in \mathcal{Y} = \{0, 1\}$

- 2 values,
- ► 1 degree of freedom



Conditional Probability Distributions

$$\begin{aligned} \forall x \in \mathcal{X} \ \forall y \in \mathcal{Y} \quad p(y|x) \geq 0 \qquad \text{(positivity)} \\ \forall x \in \mathcal{X} \ \sum_{y \in \mathcal{Y}} p(y|x) = 1 \qquad \text{(normalization w.r.t. } y) \end{aligned}$$

For example: **binary** prediction $\mathcal{X} = \{\text{images}\}, y \in \mathcal{Y} = \{0, 1\}$

► each x: 2 values, 1 d.o.f. → one (or two) function



Multi-class prediction, $y \in \mathcal{Y} = \{1, \dots, K\}$

- ► each x: K values, K-1 d.o.f. $\rightarrow K-1$ functions
- ▶ or 1 vector-valued function with K-1 outputs



Typically: K functions, plus explicit normalization

Multi-class prediction, $y \in \mathcal{Y} = \{1, \dots, K\}$

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Typically: K functions, plus explicit normalization

Example: predicting the center point of an object

 $y \in \mathcal{Y} = \{(1, 1), \dots, (width, height)\}$ • for each x: $|\mathcal{Y}| = W \cdot H$ values,

$$\begin{split} y &= (y_1, y_2) \in \mathcal{Y}_1 \times \mathcal{Y}_2 \text{ with} \\ \mathcal{Y}_1 &= \{(1, \dots, \textit{width}\} \text{ and} \\ \mathcal{Y}_2 &= \{1, \dots, \textit{height}\}. \\ \bullet \text{ each } x: \ |\mathcal{Y}_1| \cdot |\mathcal{Y}_2| = W \cdot H \text{ values} \end{split}$$



Structured objects: predicting \boldsymbol{M} variables jointly

 $\mathcal{Y} = \{1, K\} \times \{1, K\} \cdots \times \{1, K\}$ For each x:

•
$$K^M$$
 values, $K^M - 1$ d.o.f.
 $\rightarrow K^M$ functions



Example: Object detection with variable size bounding box

$$\begin{split} \mathcal{Y} &\subset \{1, \dots, W\} \times \{1, \dots, H\} \\ &\times \{1, \dots, W\} \times \{1, \dots, H\} \\ y &= (\textit{left, top, right, bottom}) \end{split}$$

For each x:

• $\frac{1}{4}W(W-1)H(H-1)$ values (millions to billions...)



Example: image denoising

```
\mathcal{Y} = \{640 \times 480 \text{ RGB images}\}
```

For each x:

- ▶ 16777216^{307200} values in p(y|x),
- $\blacktriangleright \geq 10^{2,000,000}$ functions

too much!

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For each x:

too much!

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- $> \ge 10^{2,000,000}$ functions

We cannot consider all possible distributions, we must impose structure.

A (probabilistic) graphical model defines

 a family of probability distributions over a set of random variables, by means of a graph.

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- Popular classes of graphical models,
 - ► Undirected graphical models (Markov random fields),
 - Directed graphical models (Bayesian networks),
 - Factor graphs,
 - Others: chain graphs, influence diagrams, etc.



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The graph encodes *conditional independence assumptions* between the variables:

• for N(i) are the neighbors of node i in the graph

$$p(y_i|y_{V\setminus\{i\}})=p(y_i|y_N(i))$$
 with $y_{V\setminus\{i\}}=(y_1,\ldots,y_{i-1},y_{i+1},y_n).$


Example: Pictorial Structures for Articulated Pose Estimation





- ► In principle, all parts depend on each other.
 - Knowing where the head is puts constraints on where the feet can be.
- But **conditional independences** as specified by the graph:
 - If we know where the left leg is, the left foot's position does not depend on the torso position anymore, etc.

$$p(y_{\mathsf{lfoot}}|y_{\mathsf{top}},\ldots,y_{\mathsf{torso}},\ldots,y_{\mathsf{rfoot}},x) = p(y_{\mathsf{lfoot}}|y_{\mathsf{lleg}},x)$$

• Decomposable output $y = (y_1, \dots, y_{|V|})$

• Graph:
$$G = (V, \mathcal{F}, \mathcal{E})$$
, $\mathcal{E} \subseteq V \times \mathcal{F}$

- ▶ variable nodes V (circles),
- ▶ factor nodes *F* (boxes),
- \blacktriangleright edges ${\cal E}$ between variable and factor nodes.
- each factor $F \in \mathcal{F}$ connects a subset of nodes,

• write
$$F = \{v_1, \dots, v_{|F|}\}$$
 and $y_F = (y_{v_1}, \dots, y_{v_{|F|}})$



```
Factor graph
```

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Factor graph

• Factorization into **potentials** ψ at **factors**:

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

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$$p(y) = \frac{1}{Z} \prod_{F \in \mathcal{F}} \psi_F(y_F) = \frac{1}{Z} \psi_1(Y_l) \psi_2(Y_j, Y_l) \psi_3(Y_i, Y_j) \psi_4(Y_i, Y_k, Y_l)$$

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► Z is a normalization constant, called **partition function**:

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

Conditional Distributions

How to model p(y|x)?

▶ Potentials become also functions of (part of) x: ψ_F(y_F; x_F) instead of just ψ_F(y_F)

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



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

 X_i X_j Y_i Y_j

Factor graph

▶ Note: *x* is treated just as an argument, not as a random variable.

Conditional random fields (CRFs)

Conventions: Potentials and Energy Functions

Assume $\psi_F(y_F) > 0$. Then

▶ instead of *potentials*, we can also work with *energies*:

$$\psi_F(y_F; x_F) = \exp(-E_F(y_F; x_F)),$$

or equivalently

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

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• p(y|x) can be written as $p(y|x) = \frac{1}{Z(x)} \prod_{F \in \mathcal{F}} \psi_F(y_F; x_F)$ $= \frac{1}{Z(x)} \exp(-\sum_{F \in \mathcal{F}} E_F(y_F; x_F)) = \frac{1}{Z(x)} \exp(-E(y; x))$ for $E(y; x) = \sum_{F \in \mathcal{F}} E_F(y_F; x_F)$

Conventions: Energy Minimization

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

MAP prediction can be performed by energy minimization.

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MAP prediction can be performed by energy minimization.

In practice, one typically models the energy function directly. \rightarrow the probability distribution is uniquely determined by it.

Example: An Energy Function for Image Segmentation

Foreground/background image segmentation

▶
$$\mathcal{X} = [0, 255]^{WH}$$
, $\mathcal{Y} = \{0, 1\}^{WH}$
foreground: $y_i = 1$, background: $y_i = 0$

- graph: 4-connected grid
- Each output pixel depends on
 - local grayvalue (inputs)
 - neighboring outputs



Energy function components ("Ising" model):

- ▶ $E_i(y_i = 1, x_i) = 1 \frac{1}{255}x_i$ $E_i(y_i = 0, x_i) = \frac{1}{255}x_i$ x_i bright $\rightarrow y_i$ rather foreground, x_i dark $\rightarrow y_i$ rather background
- ► $E_{ij}(0,0) = E_{ij}(1,1) = 0$, $E_{ij}(0,1) = E_{ij}(1,0) = \omega$ for $\omega > 0$ prefer that neighbors have the same label \rightarrow labeling *smooth*

$$E(y;x) = \sum_{i} \left((1 - \frac{1}{255}x_i) [\![y_i = 1]\!] + \frac{1}{255}x_i [\![y_i = 0]\!] \right) + \sum_{i \sim j} w [\![y_i \neq y_j]\!]$$



input image

segmentation from thresholding

segmentation from minimal energy

What to do with Structured Prediction Models?

Case 1) p(y|x) is known

MAP Prediction

Predict $f: \mathcal{X} \to \mathcal{Y}$ by solving

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

Probabilistic Inference

Compute marginal probabilities

 $p(y_F|x)$

for any factor F, in particular, $p(y_i|x)$ for all $i \in V$.

What to do with Structured Prediction Models?

Case 2) p(y|x) is unknown, but we have training data

Parameter Learning

Assume fixed graph structure, learn potentials/energies (ψ_F)

Among other tasks (learn the graph structure, variables, etc.)

 \Rightarrow Topic of Wednesdays' lecture

Example: Pictorial Structures



input image x

 $\operatorname{argmax}_y p(y|x)$

 $p(y_i|x)$

- MAP makes a single (structured) prediction (point estimate)
 - best overall pose
- Marginal probabilities $p(y_i|x)$ give us
 - potential positions
 - uncertainty

of the individual body parts.

Example: Man-made structure detection



- ▶ Task: Pixel depicts a man made structure or not? $y_i \in \{0, 1\}$
- Middle: MAP inference
- Right: variable marginals
- Attention: Max-Marginals \neq MAP

Probabilistic Inference

Compute $p(y_F|x)$ and Z(x).

Assume $y = (y_i, y_j, y_k, y_l)$, $\mathcal{Y} = \mathcal{Y}_i \times \mathcal{Y}_j \times \mathcal{Y}_k \times \mathcal{Y}_l$, and an energy function E(y; x) compatible with the following factor graph:

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Task 1: for any $y \in \mathcal{Y}$, compute p(y|x), using

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

Assume $y = (y_i, y_j, y_k, y_l)$, $\mathcal{Y} = \mathcal{Y}_i \times \mathcal{Y}_j \times \mathcal{Y}_k \times \mathcal{Y}_l$, and an energy function E(y; x) compatible with the following factor graph:

$$(Y_i) - (Y_j) - (Y_k) - (Y_k) - (Y_l)$$

Task 1: for any $y \in \mathcal{Y}$, compute p(y|x), using

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

Problem: We don't know Z(x), and computing it using

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

looks expensive (the sum has $|\mathcal{Y}_i| \cdot |\mathcal{Y}_j| \cdot |\mathcal{Y}_k| \cdot |\mathcal{Y}_l|$ terms).

A lot research has been done on how to efficiently compute Z(x).



For notational simplicity, we drop the dependence on (fixed) x:

$$Z = \sum_{y \in \mathcal{Y}} \exp(-E(y))$$



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$$Z = \sum_{y \in \mathcal{Y}} \exp(-E(y))$$
$$= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \sum_{y_k \in \mathcal{Y}_k} \sum_{y_l \in \mathcal{Y}_l} \exp(-E(y_i, y_j, y_k, y_l))$$



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= $\sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \sum_{y_k \in \mathcal{Y}_k} \sum_{y_l \in \mathcal{Y}_l} \exp(-(E_F(y_i, y_j) + E_G(y_j, y_k) + E_H(y_k, y_l)))$



 $Z = \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \sum_{y_k \in \mathcal{Y}_k} \sum_{y_l \in \mathcal{Y}_l} \exp(-(E_F(y_i, y_j) + E_G(y_j, y_k) + E_H(y_k, y_l)))$



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$$\begin{split} Z &= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \sum_{y_k \in \mathcal{Y}_k} \sum_{y_l \in \mathcal{Y}_l} \exp(-(E_F(y_i, y_j) + E_G(y_j, y_k) + E_H(y_k, y_l))) \\ &= \sum_{y_i} \sum_{y_j} \sum_{y_j} \sum_{y_k} \sum_{y_l} \exp(-E_F(y_i, y_j)) \exp(-E_G(y_j, y_k)) \exp(-E_H(y_k, y_l)) \\ &= \sum_{y_i} \sum_{y_j} \exp(-E_F(y_i, y_j)) \sum_{y_k} \exp(-E_G(y_j, y_k)) \sum_{y_l} \exp(-E_H(y_k, y_l)) \end{split}$$



$$\begin{split} & \underset{Y_i}{Y_i} \leftarrow \mathcal{R}^{\mathcal{Y}_k} \in \mathcal{R}^{\mathcal{Y}_k} \\ & \overbrace{F} & Y_j \leftarrow \mathcal{Y}_k \\ & \underset{G}{} \leftarrow \mathcal{Y}_k \leftarrow \mathcal{Y}_l \\ & \underset{H}{} \leftarrow \mathcal{Y}_l \\ &$$



$$r_{F \to Y_{i}} \in \mathcal{R}^{\mathcal{Y}_{i}}$$

$$Y_{i} \to Y_{j} \to Y_{j}$$

$$Z = \sum_{y_{i}} \sum_{y_{j}} \exp(-E_{F}(y_{i}, y_{j})) \sum_{y_{k}} \exp(-E_{G}(y_{j}, y_{k}))r_{H \to Y_{k}}(y_{k})$$

$$r_{G \to Y_{j}}(y_{j})$$

$$= \sum_{y_{i}} \sum_{y_{j}} \exp(-E_{F}(y_{i}, y_{j}))r_{G \to Y_{j}}(y_{j})$$

$$= \sum_{y_{i}} r_{F \to Y_{i}}(y_{i})$$



$$Z = \sum_{y \in \mathcal{Y}} \exp(-E(y))$$

=
$$\sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_i} \sum_{y_k \in \mathcal{Y}_i} \sum_{y_l \in \mathcal{Y}_i} \sum_{y_m \in \mathcal{Y}_m} \exp(-(E_F(y_i, y_j) + \dots + E_I(y_k, y_m)))$$

Example: Inference on Trees Y_i F Y_j G Y_k H Y_l I Y_m

$$Z = \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_F(y_i, y_j)) \sum_{y_k \in \mathcal{Y}_k} \exp(-E_G(y_j, y_k)) \cdot \left(\underbrace{\left(\sum_{y_l \in \mathcal{Y}_l} \exp(-E_H(y_k, y_l))\right)}_{r_H \to \mathbf{Y}_k} \cdot \underbrace{\left(\sum_{y_m \in \mathcal{Y}_m} \exp(-E_I(y_k, y_m))\right)}_{r_I \to \mathbf{Y}_k} \right)$$



$$Z = \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_F(y_i, y_j)) \sum_{y_k \in \mathcal{Y}_k} \exp(-E_G(y_j, y_k)) \cdot (r_{H \to Y_k}(y_k) \cdot r_{I \to Y_k}(y_k))$$



$$Z = \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_F(y_i, y_j)) \sum_{y_k \in \mathcal{Y}_k} \exp(-E_G(y_j, y_k)) \cdot \underbrace{(r_{H \to Y_k}(y_k) \cdot r_{I \to Y_k}(y_k))}_{q_{Y_k \to G}(y_k)}$$



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Factor Graph Sum-Product Algorithm

- "Message": pair of vectors at each factor graph edge $(i, F) \in \mathcal{E}$
 - 1. $r_{F \rightarrow Y_i} \in \mathbb{R}^{\mathcal{Y}_i}$: factor-to-variable message
 - 2. $q_{Y_i \to F} \in \mathbb{R}^{\mathcal{Y}_i}$: variable-to-factor message



Factor Graph Sum-Product Algorithm

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- Algorithm iteratively update messages
- After convergence: Z and $p(y_F)$ can be obtained from the messages.

Belief Propagation

Example: Pictorial Structures





- Tree-structured model for articulated pose (Felzenszwalb and Huttenlocher, 2000), (Fischler and Elschlager, 1973)
- \blacktriangleright Body-part variables, states: discretized tuple (x,y,s,θ)
- (x,y) position, s scale, and θ rotation

Example: Pictorial Structures



Exact marginals although state space is huge and thus partition function is a huge sum.

$$Z(x) = \sum_{\text{all bodies } y} \exp\left(-E(y;x)\right)$$

Belief Propagation in Loopy Graphs

Can we do message passing also in graphs with loops?



Problem: There is no well-defined *leaf-to-root* order.

Suggested solution: Loopy Belief Propagation (LBP)

- initialize all messages as constant 1
- pass messages until convergence

Belief Propagation in Loopy Graphs



Loopy Belief Propagation is very popular, but has some problems:

- it might not converge (e.g. oscillate)
- ► even if it does, the computed probabilities are only *approximate*. Many improved message-passing schemes exist (see tutorial book).

Probabilistic Inference – Variational Inference / Mean Field

Task: Compute marginals $p(y_F|x)$ for general p(y|x)

Idea: Approximate p(y|x) by simpler q(y) and use marginals from that.

$$q^* = \operatorname*{argmin}_{q \in \mathcal{Q}} D_{KL}(q(y) \| p(y|x))$$

E.g. Naive Mean Field: Q all distributions of the form $q(y) = \prod_{i \in V} q_i(y_i)$.



Task: Compute marginals $p(y_F|x)$ for general p(y|x)

Idea: Rephrase as computing the expected value of a quantity:

$$\mathbb{E}_{y \sim p(y|x,w)}[h(x,y)],$$

for some (well-behaved) function $h : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$.

For probabilistic inference, this step is easy. Set

$$h_{F,z}(x,y) := [\![y_F = z]\!],$$

then

$$\begin{split} \mathbb{E}_{y \sim p(y|x,w)}[h_{F,z}(x,y)] &= \sum_{y \in \mathcal{Y}} p(y|x) \llbracket y_F = z \rrbracket \\ &= \sum_{y_F \in \mathcal{Y}_F} p(y_F|x) \llbracket y_F = z \rrbracket = \boxed{p(y_F = z|x)} \,. \end{split}$$

Expectations can be computed/approximated by sampling:

 \blacktriangleright For fixed x, let $y^{(1)},y^{(2)},\ldots$ be i.i.d. samples from p(y|x), then

$$\mathbb{E}_{y \sim p(y|x)}[h(x,y)] \approx \frac{1}{S} \sum_{s=1}^{S} h(x,y^{(s)}).$$

- The law of large numbers guarantees convergence for $S \to \infty$,
- For S independent samples, approximation error is $O(1/\sqrt{S})$, *independent* of the dimension of \mathcal{Y} .

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Problem:

• Producing i.i.d. samples, $y^{(s)}$, from p(y|x) is hard.

Solution:

► We can get away with a sequence of *dependent* samples → Monte-Carlo Markov Chain (MCMC) sampling

One example how to do MCMC sampling: Gibbs sampler

- Initialize $y^{(0)} = (y_1, \ldots, y_d)$ arbitrarily
- For $s = 1, \ldots, S$:
 - 1. Select a variable y_i ,
 - 2. Re-sample $y_i \sim p(y_i | y_{V \setminus \{i\}}^{(s-1)}, x)$.
 - 3. Output sample $y^{(s)} = (y_1^{(s-1)}, \dots, y_{i-1}^{(s-1)}, y_i, y_{i+1}^{(s-1)}, \dots, y_d^{(s-1)})$

$$\begin{split} p(y_i|y_{V\setminus\{i\}}^{(s)}, x) &= \frac{p(y_i, y_{V\setminus\{i\}}^{(t)}|x)}{\sum_{y_i \in \mathcal{Y}_i} p(y_i, y_{V\setminus\{i\}}^{(t)}|x)} \\ &= \frac{\exp(-E(y_i, y^{(t)}, x)}{\sum_{y_i \in \mathcal{Y}_i} \exp(-E(y_i, y^{(t)}, x))} \end{split}$$

MAP Prediction

Compute $y^* = \operatorname{argmax}_y p(y|x)$.

MAP Prediction – Belief Propagation / Message Passing



One can also derive message passing algorithms for MAP prediction.

- ► In trees: guaranteed to converge to optimal solution.
- ► In loopy graphs: convergence not guaranteed, approximate solution.

MAP Prediction – Graph Cuts

For loopy graphs, we can find the global optimum only in **special cases**:

- Binary output variables: $\mathcal{Y}_i = \{0, 1\}$ for $i = 1, \dots, d$,
- Energy function with only unary and pairwise terms

$$E(y; x, w) = \sum_{i} E_i(y_i; x) + \sum_{i \sim j} E_{i,j}(y_i, y_j; x)$$

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$$E(y; x, w) = \sum_{i} E_i(y_i; x) + \sum_{i \sim j} E_{i,j}(y_i, y_j; x)$$

Restriction 1 (positive unary potentials):

 $E_F(y_i; x, w_{t_F}) \ge 0$ (always achievable by reparametrization)

Restriction 2 (regular/submodular/attractive pairwise potentials)

$$\begin{split} E_F(y_i, y_j; x, w_{t_F}) &= 0, \quad \text{if } y_i = y_j, \\ E_F(y_i, y_j; x, w_{t_F}) &= E_F(y_j, y_i; x, w_{t_F}) \geq 0, \quad \text{otherwise.} \end{split}$$

(not always achievable, depends on the task)

- Construct auxiliary undirected graph
- One node $\{i\}_{i \in V}$ per variable
- Two extra nodes: source s, sink t
- Edges

Edge Graph cut weight

$$\begin{array}{ll} \{i,j\} & E_F(y_i=0,y_j=1;x,w_{t_F}) \\ \{i,s\} & E_F(y_i=1;x,w_{t_F}) \\ \{i,t\} & E_F(y_i=0;x,w_{t_F}) \end{array}$$

- ► Find linear *s*-*t*-mincut
- Solution defines optimal binary labeling of the original energy minimization problem

GraphCuts algorithms

(Approximate) multi-class extensions exist, see tutorial book.



GraphCuts Example

Image segmentation energy:

$$E(y;x) = \sum_{i} \left((1 - \frac{1}{255}x_i) \llbracket y_i = 1 \rrbracket + \frac{1}{255}x_i \llbracket y_i = 0 \rrbracket \right) + \sum_{i \sim j} w \llbracket y_i \neq y_j \rrbracket$$

All conditions to apply GraphCuts are fulfilled.

•
$$E_i(y_i, x) \ge 0$$
,

•
$$E_{ij}(y_i, y_j) = 0$$
 for $y_i = y_j$,

•
$$E_{ij}(y_i, y_j) = w > 0$$
 for $y_i \neq y_j$.



input image



thresholding



GraphCuts

MAP Prediction – Linear Programming Relaxation

More general alternative, $\mathcal{Y}_i = \{1, \dots, K\}$:

$$E(y;x) = \sum_{i} \frac{E_i(y_i;x)}{E_{ij}} + \sum_{ij} \frac{E_{ij}(y_i,y_j;x)}{E_{ij}}$$

Linearize the energy using indicator functions:

$$E_{i}(y_{i};x) = \sum_{k=1}^{K} \underbrace{E_{i}(k;x)}_{=:a_{ik}} [\![y_{i} = k]\!] = \sum_{k=1}^{K} a_{i;k} \mu_{i;k}$$

for new variables $\mu_{i;k} \in \{0,1\}$ with $\sum_k \mu_{i;k} = 1$.

$$\underline{E_{ij}(y_i, y_j; x)} = \sum_{k=1}^{K} \sum_{l=1}^{K} \underbrace{E_{ij}(k, l; x)}_{=:a_{ij;kl}} [\![y_i = k \land y_j = l]\!] = \sum_{k=1}^{K} a_{ij;kl} \mu_{ij;kl}$$

for new variables $\mu_{ij;kl} \in \{0,1\}$ with $\sum_l \mu_{ij;kl} = \mu_{i;k}$ and $\sum_k \mu_{ij;kl} = \mu_{j;l}$.

MAP Prediction – Linear Programming Relaxation

Energy minimization becomes

$$y^* \leftarrow \mu^* := \underset{\mu}{\operatorname{argmin}} \sum_i a_{i;k} \mu_{i;k} + \sum_{ij} a_{ij;kl} \mu_{ij;kl} = \underset{\mu}{\operatorname{argmin}} \boldsymbol{A}\mu$$
 subject to

$$\mu_{i;k} \in \{0,1\} \qquad \mu_{ij;kl} \in \{0,1\} \\ \sum_{k} \mu_{i;k} = 1, \qquad \sum_{l} \mu_{ij;kl} = \mu_{i;k}, \qquad \sum_{k} \mu_{ij;kl} = \mu_{j;l}$$

Integer variables, linear objective function, linear constraints:

Integer linear program (ILP)

Unfortunately, ILPs are -in general- NP-hard.

MAP Prediction – Linear Programming Relaxation

Energy minimization becomes

$$y^* \leftarrow \mu^* := \underset{\mu}{\operatorname{argmin}} \sum_i a_{i;k} \mu_{i;k} + \sum_{ij} a_{ij;kl} \mu_{ij;kl} = \underset{\mu}{\operatorname{argmin}} \boldsymbol{A} \mu$$
 subject to

$$\begin{array}{l} \mu_{i;k} \in [0,1] \\ \sum_{k} \mu_{i;k} = 1, \\ k \end{array} \begin{array}{l} \mu_{ij;kl} \in [0,1] \\ \sum_{l} \mu_{ij;kl} = \mu_{i;k}, \\ k \end{array} \begin{array}{l} \sum_{k} \mu_{ij;kl} = \mu_{j;l} \end{array}$$

Integer real-values variables, linear objective function, linear constraints:

Linear program (LP) relaxation

LPs can be solved very efficiently, μ^* yields approximate solution for y^* .

Note: we just try to solve an optimization problem

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

We can use any optimization technique that fits the problem.

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Optimal Prediction

Predict with loss function $\Delta(\bar{y}, y)$.

Optimal Prediction

 Optimal prediction is minimum expected risk – an expectation

$$y^* = \operatorname{argmin}_{\bar{y} \in \mathcal{Y}} \sum_{y \in \mathcal{Y}} \Delta(\bar{y}, y) p(y|x)$$



Optimal Prediction

 Optimal prediction is minimum expected risk – an expectation

$$y^* = \operatorname{argmin}_{\bar{y} \in \mathcal{Y}} \sum_{y \in \mathcal{Y}} \Delta(\bar{y}, y) p(y|x)$$

$$= \operatorname{argmin}_{\bar{y} \in \mathcal{Y}} \sum_{y \in \mathcal{Y}} \Delta(\bar{y}, y) \prod_F \psi_F(y_F; x)$$

- \blacktriangleright Can think of Δ as another CRF factor
- Reuse inference techniques



Example: Hamming loss

Count the number of mislabeled variables:

$$\Delta_H(y',y) = \frac{1}{|V|} \sum_{i \in V} I(y'_i \neq y_i)$$



- Makes more sense than 0/1 loss for image segmentation
- Optimal: predict maximum marginals (exercise)

$$y^* = (\operatorname*{argmax}_{y_1} p(y_1|x), \operatorname*{argmax}_{y_2} p(y_2|x), \ldots)$$

Example: Pixel error

If we can add elements in \mathcal{Y}_i (pixel intensities, optical flow vectors, etc.).

Sum of squared errors

$$\Delta_Q(y', y) = \frac{1}{|V|} \sum_{i \in V} ||y'_i - y_i||^2.$$



Used, e.g., in stereo reconstruction, part-based object detection.

Optimal: predict marginal mean (exercise)

$$y^* = (\mathbb{E}_{p(y|x)}[y_1], \mathbb{E}_{p(y|x)}[y_2], \ldots)$$

Example: Task specific losses

- Object detection
 - bounding boxes, or
 - arbitrary regions

detection ground truth image

Area overlap loss:

$$\Delta_{AO}(y',y) = 1 - \frac{\operatorname{area}(y' \cap y)}{\operatorname{area}(y' \cup y)} = 1 - \frac{1}{1 - \frac{1$$

Used, e.g., in PASCAL VOC challenges for object detection, because it scale-invariants (no bias for or against big objects).

Summary: Inference and Prediction

Two main tasks for a given probability distribution p(y|x):

Probabilistic Inference

Compute $p(y_I|x)$ for a subset I of variables, in particular $p(y_i|x)$

▶ (Loopy) Belief Propagation, Variation Inference, Sampling, ...

MAP Prediction

Identify $y^* \in \mathcal{Y}$ that maximizes p(y|x) (minimizes energy)

▶ (Loopy) Belief Propagation, GraphCuts, LP-relaxation, custom, ...

Structured prediction comes with structured loss functions, $\Delta: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}.$

Loss Function

 $\Delta(y',y) \text{ is loss (or cost) for predicting } y \in \mathcal{Y} \text{ if } y' \in \mathcal{Y} \text{ is correct.}$

► Task specific: use 0/1-loss, Hamming loss, area overlap, ...
Max Planck Institute for Intelligent Systems



Other groups on Campus

- Empirical Inference (Machine Learning)
- Perceiving Systems (Computer Vision)
- Autonomous Motion (Robotics)

More information: http://ps.is.tue.mpg.de/