CSC 2515: Structured Prediction

Raquel Urtasun & Rich Zemel

University of Toronto

March 16, 2015

Discriminant Functions for K > 2 classes

- Use K − 1 classifiers, each solving a two class problem of separating point in a class C_k from points not in the class.
- Known as 1 vs all or 1 vs the rest classifier



• PROBLEM: More than one good answer!

Urtasun & Zemel (UofT)

Discriminant Functions for K > 2 classes

- Introduce K(K-1)/2 two-way classifiers, one for each possible pair of classes
- Each point is classified according to majority vote amongst the disc. func.
- Known as the 1 vs 1 classifier



• PROBLEM: Two-way preferences need not be transitive

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k,0}$$

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k,0}$$

and then assigning a point \mathbf{x} to class C_k if

$$\forall j \neq k \qquad y_k(\mathbf{x}) > y_j(\mathbf{x})$$

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k,0}$$

and then assigning a point \mathbf{x} to class C_k if

$$\forall j \neq k \qquad y_k(\mathbf{x}) > y_j(\mathbf{x})$$

• Note that \mathbf{w}_k^T is now a vector, not the k-th coordinate

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k,0}$$

and then assigning a point \mathbf{x} to class C_k if

$$\forall j \neq k \qquad y_k(\mathbf{x}) > y_j(\mathbf{x})$$

- Note that \mathbf{w}_k^T is now a vector, not the k-th coordinate
- In this lecture we will look at generalizations of this idea.

- Introduction to Structured prediction
- Inference
- Learning

What is structured prediction?

• In "typical" machine learning

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

the input ${\cal X}$ can be anything, and the output is a real number (e.g., classification, regression)

• In "typical" machine learning

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

the input \mathcal{X} can be anything, and the output is a real number (e.g., classification, regression)

In Structured Prediction

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

the input \mathcal{X} can be anything, and the output is a **complex** object (e.g., image segmentation, parse tree)

• In "typical" machine learning

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

the input \mathcal{X} can be anything, and the output is a real number (e.g., classification, regression)

In Structured Prediction

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

the input \mathcal{X} can be anything, and the output is a **complex** object (e.g., image segmentation, parse tree)

 $\bullet\,$ In this lecture ${\cal Y}$ is a discrete space, ask me later if you are interested in continuous variables.

Structured Prediction and its Applications

We want to predict multiple random variables which are related

- Computer Vision:
 - Semantic Segmentation (output: pixel-wise labeling)
 - Object detection (output: 2D or 3D bounding boxes)
 - Stereo Reconstruction (output: 3D map)
 - Scene Understanding (output: 3D bounding box reprinting the layout)





Structured Prediction and its Applications

We want to predict multiple random variables which are related

- Natural Language processing
 - Machine Translation (output: sentence in another language)
 - Parsing (output: parse tree)



- Computational Biology
 - Protein Folding (output: 3D protein)

MRLLILALLGICSLTAYIVEGVGSEVSDKR TCVSLTTQRLPVSRIKTYTITEGSLRAVIF ITKRGLKVCADPQATWVRDVVRSMDRKSNT RNNMIQTKPTGTQQSTNTAVTLTG



• Independent prediction is good but...



• Independent prediction is good but...



• Neighboring pixels should have same labels (if they look similar).



A graphical model defines

- A family of probability distributions over a set of random variables
- This is expressed via a graph, which encodes the conditional independences of the distribution



• Two types of graphical models: Directed and undirected

Bayesian Networks (Directed Graphical Models)

- The graph $G = (V, \mathcal{E})$ is acyclic and directed
- Factorization over distributions by conditioning on parent nodes

$$p(\mathbf{y}) = \prod_{i \in V} p(y_i | y_{pa}(i))$$

• Example



$$p(\mathbf{y}) = p(y_i|y_k)p(y_k|y_i, y_j)p(y_i)p(y_j)$$

Undirected Graphical Model

- Also called Markov Random Field, or Markov Network
- Graph $G = (V, \mathcal{E})$ is undirected and has no self-edges
- Factorization over cliques

$$p(\mathbf{y}) = \frac{1}{Z} \prod_{r \in \mathcal{R}} \psi_r(\mathbf{y}_r)$$

with $Z = \sum_{\mathbf{y} \in \mathcal{Y}} \prod_{r \in \mathcal{R}} \psi_r(\mathbf{y}_r)$ the partition function

Example



$$p(\mathbf{y}) = \frac{1}{Z} \psi(y_i, y_j) \psi(y_j, y_k) \psi(y_i) \psi(y_j) \psi(y_k)$$

- Difficulty: Exponentially many configurations
- Undirected models will be the focus of this lecture

Urtasun & Zemel (UofT)

Factor Graph Representation

- Graph $G = (V, \mathcal{F}, \mathcal{E})$, with variable nodes \mathcal{V} , factor nodes \mathcal{F} and edges \mathcal{E}
- Scope of a factor $N(F) = \{i \in V : (i, F) \in \mathcal{E}\}$
- Factorization over factors

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



Factor Graph vs Graphical Model

• Factor graphs are explicit about the factorization



Figure : from [Nowozin et al]



• They define the family of distributions and thus the capacity



Figure : from [Nowozin et al]

Markov Random Fields vs Conditional Random Fields

• Markov Random Fields (MRFs) define

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

• Conditional Random Fields (CRFs) define

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

• x is not a random variable (i.e., not part of the probability distribution)



• The probability is completely determined by the energy

$$p(\mathbf{y}) = \frac{1}{Z} \prod_{F \in \mathcal{F}} \psi_F(\mathbf{y}_{N(F)})$$
$$= \frac{1}{Z} \exp\left(\log(\psi_F(\mathbf{y}_{N(F)}))\right)$$
$$= \frac{1}{Z} \exp\left(-\sum_{F \in \mathcal{F}} E_F(y_F)\right)$$

where $E_F(y_F) = -\log(\psi_F(\mathbf{y}_{N(F)}))$

Parameterization: log linear model

- Factor graphs define a family of distributions
- We are interestested in identifying individual members by parameters

$$E_F(\mathbf{y}_F) = -\mathbf{w}^T \phi_F(\mathbf{y}_F)$$



• Estimation of the parameters w

$$E_F(\mathbf{y}_F) = -\mathbf{w}^T \phi_F(\mathbf{y}_F)$$

- Learn the structure of the model
- Learn with hidden variables

Inference Tasks

Given an input $x \in \mathcal{X}$ we want to compute

• MAP estimate or minimum energy configuration

$$\underset{y \in \mathcal{Y}}{\operatorname{argmax}} p(\mathbf{y}|\mathbf{x}) = \operatorname{argmax}_{y \in \mathcal{Y}} \frac{1}{Z} \prod_{F \in \mathcal{F}} \psi_F(\mathbf{y}_{N(F)}; \mathbf{x}, \mathbf{w})$$

$$= \operatorname{argmax}_{y \in \mathcal{Y}} \exp(-\sum_{F \in \mathcal{F}} E_F(\mathbf{y}_F, \mathbf{x}, \mathbf{w}))$$

$$= \operatorname{argmin}_{y \in \mathcal{Y}} \sum_{F \in \mathcal{F}} E_F(\mathbf{y}_F, \mathbf{x}, \mathbf{w})$$

Inference Tasks

Given an input $x \in \mathcal{X}$ we want to compute

• MAP estimate or minimum energy configuration

$$\underset{y \in \mathcal{Y}}{\operatorname{argmax}} p(\mathbf{y}|\mathbf{x}) = \operatorname{argmax}_{y \in \mathcal{Y}} \frac{1}{Z} \prod_{F \in \mathcal{F}} \psi_F(\mathbf{y}_{N(F)}; \mathbf{x}, \mathbf{w})$$

$$= \operatorname{argmax}_{y \in \mathcal{Y}} \exp(-\sum_{F \in \mathcal{F}} E_F(\mathbf{y}_F, \mathbf{x}, \mathbf{w}))$$

$$= \operatorname{argmin}_{y \in \mathcal{Y}} \sum_{F \in \mathcal{F}} E_F(\mathbf{y}_F, \mathbf{x}, \mathbf{w})$$

 Marginals p(y_i) or max marginals max_{y_i∈y_i} p(y_i), which requires computing the partition function Z, i.e.,

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

Inference in Markov Random Fields

$$\max_{y \in \mathcal{Y}} p(\mathbf{y}|x) = \max_{y \in \mathcal{Y}} \sum_{r \in \mathcal{R}} \mathbf{w}^{T} \phi_{r}(\mathbf{y}_{r})$$

$$\max_{y \in \mathcal{Y}} p(\mathbf{y}|x) = \max_{y \in \mathcal{Y}} \sum_{r \in \mathcal{R}} \mathbf{w}^T \phi_r(\mathbf{y}_r)$$

Notable exceptions are:

• Belief propagation for tree-structure models

$$\max_{y \in \mathcal{Y}} p(\mathbf{y}|x) = \max_{y \in \mathcal{Y}} \sum_{r \in \mathcal{R}} \mathbf{w}^T \phi_r(\mathbf{y}_r)$$

Notable exceptions are:

- Belief propagation for tree-structure models
- Graph cuts for binary energies with sub modular potentials

$$\max_{y \in \mathcal{Y}} p(\mathbf{y}|x) = \max_{y \in \mathcal{Y}} \sum_{r \in \mathcal{R}} \mathbf{w}^T \phi_r(\mathbf{y}_r)$$

Notable exceptions are:

- Belief propagation for tree-structure models
- Graph cuts for binary energies with sub modular potentials
- Branch and bound: exponential in worst case, but works much faster in practice

$$\max_{y \in \mathcal{Y}} p(\mathbf{y}|x) = \max_{y \in \mathcal{Y}} \sum_{r \in \mathcal{R}} \mathbf{w}^T \phi_r(\mathbf{y}_r)$$

Notable exceptions are:

- Belief propagation for tree-structure models
- Graph cuts for binary energies with sub modular potentials
- Branch and bound: exponential in worst case, but works much faster in practice

Difficulties

• Deal with the exponentially many states in y

Belief Propagation

Compact notation

$$\theta_r(\mathbf{y}_r) = \mathbf{w}^T \phi_r(\mathbf{y}_r)$$

• Inference can be written as





• For the example

$$\max_{y_i, y_j, y_k, y_l} \{\theta_F(y_i, y_j) + \theta_G(y_j, y_k) + \theta_G(y_k, y_l)\}$$



$$\theta^*(\mathbf{y}) = \max_{y_i, y_j, y_k, y_l} \{\theta_F(y_i, y_j) + \theta_G(y_j, y_k) + \theta_H(y_k, y_l)\}$$

=


$$\theta^*(\mathbf{y}) = \max_{y_i, y_j, y_k, y_l} \{\theta_F(y_i, y_j) + \theta_G(y_j, y_k) + \theta_H(y_k, y_l)\}$$

$$= \max_{y_i,y_j} \theta_F(y_i,y_j) + \max_{y_k} \theta_G(y_j,y_k) + \max_{y_l} \theta_H(y_k,y_l)$$

Belief Propagation



$$\theta^*(\mathbf{y}) = \max_{y_i, y_j} \theta_F(y_i, y_j) + \max_{y_k} \theta_G(y_j, y_k) + \underbrace{\max_{y_l} \theta_H(y_k, y_l)}_{r_{H \to y_k}(y_k)}$$

Belief Propagation



$$\theta^*(\mathbf{y}) = \max_{y_i, y_j} \theta_F(y_i, y_j) + \max_{y_k} \theta_G(y_j, y_k) + \max_{y_l} \theta_H(y_k, y_l)$$

$$= \max_{y_i, y_j} \theta_F(y_i, y_j) + \max_{y_k} \theta_G(y_j, y_k) + r_{H \to y_k}(y_k)$$



$$\begin{aligned} \theta^*(\mathbf{y}) &= \max_{y_i, y_j} \theta_F(y_i, y_j) + \underbrace{\max_{y_k} \theta_G(y_j, y_k) + r_{H \to y_k}(y_k)}_{r_{G \to y_j}(y_j)} \\ &= \max_{y_i, y_j} \theta_F(y_i, y_j) + \end{aligned}$$

Belief Propagation



$$\theta^{*}(\mathbf{y}) = \max_{y_{i}, y_{j}} \theta_{F}(y_{i}, y_{j}) + \underbrace{\max_{y_{k}} \theta_{G}(y_{j}, y_{k}) + r_{H \to y_{k}}(y_{k})}_{r_{G \to y_{j}}(y_{j})}$$
$$= \max_{y_{i}, y_{j}} \theta_{F}(y_{i}, y_{j}) + r_{G \to y_{j}}(y_{j})$$



$\theta^*(\mathbf{y}) = \max_{y_i, y_k, y_k, y_l, y_m} \theta_F(y_i, y_j) + \theta_G(y_j, y_k) + \theta_I(y_m, y_k) + \theta_H(y_l, y_k)$



$$\begin{aligned} \theta^{*}(\mathbf{y}) &= \max_{y_{i}, y_{k}, y_{k}, y_{l}, y_{m}} \theta_{F}(y_{i}, y_{j}) + \theta_{G}(y_{j}, y_{k}) + \theta_{I}(y_{m}, y_{k}) + \theta_{H}(y_{I}, y_{k}) \\ &= \max_{y_{i}, y_{j}} \theta_{F}(y_{i}, y_{j}) + \max_{y_{k}} \theta_{G}(y_{j}, y_{k}) + \max_{y_{m}} \theta_{I}(y_{m}, y_{k}) + \max_{y_{l}} \theta_{H}(y_{l}, y_{k}) \end{aligned}$$



$$\begin{aligned} \theta^{*}(\mathbf{y}) &= \max_{\substack{y_{i}, y_{k}, y_{k}, y_{l}, y_{m}}} \theta_{F}(y_{i}, y_{j}) + \theta_{G}(y_{j}, y_{k}) + \theta_{I}(y_{m}, y_{k}) + \theta_{H}(y_{I}, y_{k}) \\ &= \max_{\substack{y_{i}, y_{j}}} \theta_{F}(y_{i}, y_{j}) + \max_{\substack{y_{k}}} \theta_{G}(y_{j}, y_{k}) + \max_{\substack{y_{m}}} \theta_{I}(y_{m}, y_{k}) + \max_{\substack{y_{l}}} \theta_{H}(y_{l}, y_{k}) \\ &= \max_{\substack{y_{i}, y_{j}}} \theta_{F}(y_{i}, y_{j}) + \max_{\substack{y_{k}}} \theta_{G}(y_{j}, y_{k}) + r_{H \rightarrow y_{k}}(y_{k}) + r_{I \rightarrow y_{k}}(y_{k}) \end{aligned}$$



$$\begin{aligned} \theta^{*}(\mathbf{y}) &= \max_{y_{i}, y_{k}, y_{k}, y_{l}, y_{m}} \theta_{F}(y_{i}, y_{j}) + \theta_{G}(y_{j}, y_{k}) + \theta_{I}(y_{m}, y_{k}) + \theta_{H}(y_{I}, y_{k}) \\ &= \max_{y_{i}, y_{j}} \theta_{F}(y_{i}, y_{j}) + \max_{y_{k}} \theta_{G}(y_{j}, y_{k}) + \max_{y_{m}} \theta_{I}(y_{m}, y_{k}) + \max_{y_{l}} \theta_{H}(y_{I}, y_{k}) \\ &= \max_{y_{i}, y_{j}} \theta_{F}(y_{i}, y_{j}) + \max_{y_{k}} \theta_{G}(y_{j}, y_{k}) + r_{H \to y_{k}}(y_{k}) + r_{I \to y_{k}}(y_{k}) \\ &= \max_{y_{i}, y_{j}} \theta_{F}(y_{i}, y_{j}) + \max_{y_{k}} \theta_{G}(y_{j}, y_{k}) + q_{y_{k} \to G}(y_{k}) \end{aligned}$$

Iteratively updates and passes messages:

- $r_{F \to y_i} \in \Re^{\mathcal{Y}_i}$: factor to variable message
- $q_{y_i \to F} \in \Re^{\mathcal{Y}_i}$: variable to factor message



Figure : from [Nowozin et al]

Variable to factor

- Let M(i) be the factors adjacent to variable i, $M(i) = \{F \in \mathcal{F} : (i, F) \in \mathcal{E}\}$
- Variable-to-factor message

$$q_{y_i \to F}(y_i) = \sum_{F' \in \mathcal{M}(i) \setminus \{F\}} r_{F' \to y_i}(y_i)$$



Figure : from [Nowozin et al]

Factor to variable

• Factor-to-variable message

$$r_{F \to y_i}(y_i) = \max_{y'_F \in \mathcal{Y}_F, y'_i = y_i} \left(\theta(y'_F) + \sum_{j \in \mathcal{N}(F) \setminus \{i\}} q_{y_j \to F}(y'_j) \right)$$



Figure : from [Nowozin et al]

Message Scheduling

- Select one variable as tree root
- Ompute leaf-to-root messages
- Ompute root-to-leaf messages



Figure : from [Nowozin et al]

Max Product v Sum Product

Max sum version of max-product

Compute leaf-to-root messages

$$q_{y_i \to F}(y_i) = \sum_{F' \in \mathcal{M}(i) \setminus \{F\}} r_{F' \to y_i}(y_i)$$

Ompute root-to-leaf messages

$$r_{F \to y_i}(y_i) = \max_{y'_F \in \mathcal{Y}_F, y'_i = y_i} \left(\theta(y'_F) + \sum_{j \in \mathcal{N}(F) \setminus \{i\}} q_{y_j \to F(y'_j)} \right)$$

,

`

Max Product v Sum Product

Max sum version of max-product

Compute leaf-to-root messages

$$q_{y_i \to F}(y_i) = \sum_{F' \in \mathcal{M}(i) \setminus \{F\}} r_{F' \to y_i}(y_i)$$

Ompute root-to-leaf messages

$$r_{F \to y_i}(y_i) = \max_{y'_F \in \mathcal{Y}_F, y'_i = y_i} \left(\theta(y'_F) + \sum_{j \in \mathcal{N}(F) \setminus \{i\}} q_{y_j \to F(y'_j)} \right)$$

Sum-product

$$q_{y_i \to F}(y_i) = \sum_{F' \in \mathcal{M}(i) \setminus \{F\}} r_{F' \to y_i}(y_i)$$

Ompute root-to-leaf messages

$$\mathsf{r}_{F o y_i}(y_i) = \log \sum_{y'_F \in \mathcal{Y}_F, y'_i = y_i} \exp \left(heta(y'_F) + \sum_{j \in \mathcal{N}(F) \setminus \{i\}} q_{y'_j o F}(y'_j)
ight)$$

Urtasun & Zemel (UofT)

Computing marginals

• Partition function can be evaluated at the root

$$\log Z = \log \sum_{y_r} \exp \left(\sum_{F \in M(r)} r_{F \to y_r}(y_r) \right)$$

• Marginal distributions, for each factor

$$\mu_F(y_F) = p(y_F) = \frac{1}{Z} \exp\left(\theta_F(y_F) + \sum_{i \in N(F)} q_{y_i \to F}(y_i)\right)$$



Urtasun & Zemel (UofT)

Computing marginals

• Partition function can be evaluated at the root

$$\log Z = \log \sum_{y_r} \exp \left(\sum_{F \in \mathcal{M}(r)} r_{F \to y_r}(y_r) \right)$$

Marginal distributions, for each factor

$$\mu_F(y_F) = p(y_F) = \frac{1}{Z} \exp\left(\theta_F(y_F) + \sum_{i \in N(F)} q_{y_i \to F}(y_i)\right)$$

Marginals at every node

$$\mu_{y_i}(y_i) = p(y_i) = \frac{1}{Z} \exp\left(\sum_{F \in \mathcal{M}(i)} r_{F \to y_i}(y_i)\right)$$

- It is call loopy belief propagation (Perl, 1988)
- No schedule that removes dependencies
- Different messaging schedules (synchronous/asynchronous, static/dynamic)
- Slight changes in the algorithm

Integer Linear Program (LP) equivalence [Werner 2007]:

$$\hat{\mathbf{y}} = \arg \max_{\mathbf{y}} \sum_{r} \theta_{r}(\mathbf{y}_{r})$$
• Variables $b_{r}(\mathbf{y}_{r})$:

$$\max_{b_{1},b_{2},b_{12}} \begin{bmatrix} b_{1}(0) \\ b_{1}(1) \\ b_{2}(0) \\ b_{2}(1) \\ b_{12}(0,0) \\ b_{12}(1,0) \\ b_{12}(0,1) \\ b_{12}(1,1) \end{bmatrix}^{\top} \begin{bmatrix} \theta_{1}(0) \\ \theta_{1}(1) \\ \theta_{2}(0) \\ \theta_{2}(1) \\ \theta_{12}(0,0) \\ \theta_{12}(1,0) \\ \theta_{12}(0,1) \\ \theta_{12}(1,1) \end{bmatrix}$$

Integer Linear Program (LP) equivalence [Werner 2007]:

$$\begin{split} \hat{\mathbf{y}} &= \arg \max_{\mathbf{y}} \sum_{r} \theta_{r}(\mathbf{y}_{r}) \\ \bullet \text{ Variables } b_{r}(\mathbf{y}_{r}): & & & & & \\ b_{1}(0) \\ b_{1}(1) \\ b_{2}(0) \\ b_{2}(1) \\ b_{12}(0,0) \\ b_{12}(1,0) \\ b_{12}(1,1) \\ b_{12}(1,1) \\ \end{bmatrix}^{\top} \begin{bmatrix} \theta_{1}(0) \\ \theta_{1}(1) \\ \theta_{2}(0) \\ \theta_{2}(1) \\ \theta_{2}(0) \\ \theta_{2}(1) \\ \theta_{12}(0,0) \\ \theta_{12}(1,0) \\ \theta_{12}(1,1) \\ \theta_{12}(1,1) \\ \end{bmatrix} & & & \\ \text{s.t.} & \\ b_{r}(\mathbf{y}_{r}) \in \{0,1\} \\ \text{s.t.} & \\ \end{split}$$

Integer Linear Program (LP) equivalence [Werner 2007]:

$$\hat{\mathbf{y}} = \arg \max_{\mathbf{y}} \sum_{r} \theta_{r}(\mathbf{y}_{r})$$
• Variables $b_{r}(\mathbf{y}_{r})$:

$$\max_{b_{1},b_{2},b_{12}} \begin{bmatrix} b_{1}(0) \\ b_{1}(1) \\ b_{2}(0) \\ b_{2}(1) \\ b_{12}(0,0) \\ b_{12}(1,0) \\ b_{12}(1,1) \end{bmatrix}^{\top} \begin{bmatrix} \theta_{1}(0) \\ \theta_{1}(1) \\ \theta_{2}(0) \\ \theta_{2}(1) \\ \theta_{12}(0,0) \\ \theta_{12}(1,0) \\ \theta_{12}(1,0) \\ \theta_{12}(1,1) \end{bmatrix}$$
s.t. $\sum_{\mathbf{y}_{r}} b_{r}(\mathbf{y}_{r}) = 1$

Integer Linear Program (LP) equivalence [Werner 2007]:

$$\hat{\mathbf{y}} = \arg \max_{\mathbf{y}} \sum_{r} \theta_{r}(\mathbf{y}_{r})$$
• Variables $b_{r}(\mathbf{y}_{r})$:

$$max_{b_{1},b_{2},b_{12}} \begin{bmatrix} b_{1}(0) \\ b_{1}(1) \\ b_{2}(0) \\ b_{2}(1) \\ b_{12}(0,0) \\ b_{12}(1,0) \\ b_{12}(0,1) \\ b_{12}(1,1) \end{bmatrix}^{\top} \begin{bmatrix} \theta_{1}(0) \\ \theta_{1}(1) \\ \theta_{2}(0) \\ \theta_{2}(1) \\ \theta_{12}(0,0) \\ \theta_{12}(1,0) \\ \theta_{12}(1,0) \\ \theta_{12}(1,1) \end{bmatrix}$$
s.t.
$$b_{r}(\mathbf{y}_{r}) \in \{0,1\}$$
s.t.
$$\sum_{\mathbf{y}_{r}} b_{r}(\mathbf{y}_{r}) = 1$$

$$\sum_{\mathbf{y}_{p} \setminus \mathbf{y}_{r}} b_{p}(\mathbf{y}_{p}) = b_{r}(\mathbf{y}_{r})$$

$$\max_{b_1,b_2,b_{12}} \begin{bmatrix} b_1(1) \\ b_1(2) \\ b_2(1) \\ b_2(2) \\ b_{12}(1,1) \\ b_{12}(2,1) \\ b_{12}(1,2) \\ b_{12}(2,2) \end{bmatrix}^\top \begin{bmatrix} \theta_1(1) \\ \theta_1(2) \\ \theta_2(2) \\ \theta_2(1) \\ \theta_2(2) \\ \theta_{12}(1,1) \\ \theta_{12}(2,1) \\ \theta_{12}(1,2) \\ \theta_{12}(2,2) \end{bmatrix}$$

s.t.
$$egin{aligned} & b_r(\mathbf{y}_r) \in \{0,1\} \ & \sum_{y_r} b_r(\mathbf{y}_r) = 1 \ & \sum_{\mathbf{y}_p \setminus \mathbf{y}_r} b_p(\mathbf{y}_p) = b_r(\mathbf{y}_r) \end{aligned}$$

 $\max_{b_r} \sum_{r,\mathbf{y}_r} b_r(\mathbf{y}_r)\theta_r(\mathbf{y}_r)$

s.t. $egin{aligned} & b_r(\mathbf{y}_r) \in \{0,1\} \ & \sum_{y_r} b_r(\mathbf{y}_r) = 1 \ & \sum_{\mathbf{y}_p \setminus \mathbf{y}_r} b_p(\mathbf{y}_p) = b_r(\mathbf{y}_r) \end{aligned}$

 $\max_{b_r} \sum_{r,\mathbf{y}_r} b_r(\mathbf{y}_r)\theta_r(\mathbf{y}_r)$

$$egin{aligned} & b_r(\mathbf{y}_r) \in \{0,1\} \ & \sum_{y_r} b_r(\mathbf{y}_r) = 1 \end{aligned}$$
 s.t.

Marginalization

$$\max_{b_r} \sum_{r,\mathbf{y}_r} b_r(\mathbf{y}_r)\theta_r(\mathbf{y}_r)$$

 $b_r(\mathbf{y}_r) \in \{0,1\}$ Local probability b_r s.t.

Marginalization

LP relaxation:

 $\max_{b_r} \sum_{r,\mathbf{y}_r} b_r(\mathbf{y}_r) \theta_r(\mathbf{y}_r)$

 $\overline{b_r(\mathbf{y}_r)} \leftarrow \{0, \mathbf{I}\}$ Local probability b_r

Marginalization

s.t.

LP relaxation:

$$\max_{b_r} \sum_{r,\mathbf{y}_r} b_r(\mathbf{y}_r) \theta_r(\mathbf{y}_r) \qquad \text{s.t.}$$

 $\underline{b_r(y_r)} \leftarrow \{0, 1\}$ Local probability b_r Marginalization

Can be solved by any standard LP solver but **slow** because of typically many variables and constraints. Can we do better?

Observation: Graph structure in marginalization constraints.



Use dual to take advantage of structure in constraint set

- Set of parents of region r: P(r)
- Set of children of region r: C(r)

$$orall r, \mathbf{y}_r, p \in P(r)$$
 $\sum_{\mathbf{y}_p \setminus \mathbf{y}_r} b_p(\mathbf{y}_p) = b_r(\mathbf{y}_r)$

• Lagrange multipliers for every constraint:

$$\forall r, \mathbf{y}_r, p \in P(r) \qquad \lambda_{r \to p}(\mathbf{y}_r)$$

Re-parameterization of score $\theta_r(\mathbf{y}_r)$:

$$\hat{\theta}_r(\mathbf{y}_r) = \theta_r(\mathbf{y}_r) + \sum_{p \in P(r)} \lambda_{r \to p}(\mathbf{y}_r) - \sum_{c \in C(r)} \lambda_{c \to r}(\mathbf{y}_c)$$

Properties of dual program:

$$\min_{\lambda} q(\lambda) = \min_{\lambda} \sum_{r} \max_{\mathbf{y}_{r}} \hat{\theta}_{r}(\mathbf{y}_{r})$$

• Dual upper-bounds primal $\forall \lambda$

- Convex problem
- Unconstrained task
- Doing block coordinate descent in the dual results on message passing (Lagrange multipliers are your messages)

Block-coordinate descent solvers iterate the following steps:

- Take a block of Lagrange multipliers
- Optimize sub-problem of dual function w.r.t. this block while keeping all other variables fixed

Advantage: fast due to analytically computable sub-problems

Same type of algorithms also exist to compute approximate marginals

Theorem [Kolmogorov and Zabih, 2004]: If the energy function is a function of binary variables containing only unary and pairwise factors, the discrete energy minimization problem

$$\min_{\mathbf{y}} \sum_{r \in \mathcal{R}} E(\mathbf{y}_r, x)$$

can be formulated as a graph cut problem if an only off all pairwise energies are sub modular

$$E_{i,j}(0,0) + E_{i,j}(1,1) \le E_{i,j}(0,1) + E_{i,j}(1,0)$$

The ST-mincut problem

• The st-mincut is the st-cut with the minimum cost



Back to our energy minimization

Construct a graph such that

- 1 Any st-cut corresponds to an assignment of x
- 2 The cost of the cut is equal to the energy of x : E(x)





How are they equivalent?

 $A = \Theta_{ii}(0,0)$ $B = \Theta_{ii}(0,1)$ $C = \Theta_{ii}(1,0)$ $D = \Theta_{ii}(1,1)$



$$\begin{array}{l} \displaystyle \frac{\Theta_{ij}(x_{i},x_{j})}{+(\Theta_{ij}(1,0)-\Theta_{ij}(0,0)) \times_{i} + (\Theta_{ij}(1,0)-\Theta_{ij}(0,0)) \times_{j}} \\ \displaystyle + (\Theta_{ij}(1,0)+\Theta_{ij}(0,1) - \Theta_{ij}(0,0) - \Theta_{ij}(1,1)) (1-x_{i}) \times_{j} \end{array}$$

 $B+C-A-D \ge 0$ is true from the submodularity of θ_{ii}


[Source: P. Kohli]

Urtasun & Zemel (UofT)



[Source: P. Kohli]

Urtasun & Zemel (UofT)











[Source: P. Kohli] Urtasun & Zemel (UofT)







How to compute the St-mincut?



Solve the dual maximum flow problem

Compute the maximum flow between Source and Sink s.t.

Edges: Flow < Capacity

Nodes: Flow in = Flow out

Min-cut\Max-flow Theorem

In every network, the maximum flow equals the cost of the st-mincut

Assuming non-negative capacity

[Source: P. Kohli]

Urtasun & Zemel (UofT)







// is the label of pixel p (0 or 1)

[Source: P. Kohli]

Urtasun & Zemel (UofT)

Graph *g;

For all pixels p

/* Add a node to the graph */ nodeID(p) = g->add_node();

```
/* Set cost of terminal edges */
set_weights(nodeID(p), fgCost(p), bgCost(p));
```

end

```
g->compute_maxflow();
```

label_p = g->is_connected_to_source(nodeID(p));
// is the label of pixel p (0 or 1)



Example: Figure-Ground Segmentation

Binary labeling problem







(Indep. Prediction)

Example: Figure-Ground Segmentation

Markov Random Field

$$E(\mathbf{y}, \mathbf{x}, \mathbf{w}) = \sum_{i} \log p(y_i | x_i) + w \sum_{(i,j) \in \mathcal{E}} C(x_i, x_j) l(y_i \neq y_j)$$

with $C(x_i, x_j) = \exp(\gamma ||x_i - x_j||^2)$, and $w \ge 0$.



• Why do we need the condition $w \ge 0$?

- Optimal solution is not possible anymore
- Solve to optimality subproblems that include current iterate
- This guarantees decrease in the objective



- Optimal solution is not possible anymore
- Solve to optimality subproblems that include current iterate
- This guarantees decrease in the objective



- Optimal solution is not possible anymore
- Solve to optimality subproblems that include current iterate
- This guarantees decrease in the objective



- Optimal solution is not possible anymore
- Solve to optimality subproblems that include current iterate
- This guarantees decrease in the objective



Two general classes of pairwise interactions

• Metric if it satisfies for any set of labels α, β, γ

۱

$$egin{array}{lll} V(lpha,eta)=0 & \leftrightarrow & lpha=eta \ V(lpha,eta) & = & V(eta,lpha)\geq 0 \ V(lpha,eta) & \leq & V(lpha,\gamma)+V(\gamma,eta) \end{array}$$

Two general classes of pairwise interactions

• Metric if it satisfies for any set of labels α,β,γ

$$egin{array}{rcl} V(lpha,eta)=0&\leftrightarrow&lpha=eta\ V(lpha,eta)&=&V(eta,lpha)\geq 0\ V(lpha,eta)&\leq&V(lpha,\gamma)+V(\gamma,eta) \end{array}$$

• Semi-metric if it satisfies for any set of labels α, β, γ

$$egin{array}{rcl} V(lpha,eta)=0&\leftrightarrow&lpha=eta\ V(lpha,eta)&=&V(eta,lpha)\geq 0 \end{array}$$

Examples for 1D label set

• Truncated quadratic is a semi-metric

$$V(\alpha, \beta) = \min(K, |\alpha - \beta|^2)$$

with K a constant.

Examples for 1D label set

• Truncated quadratic is a semi-metric

$$V(\alpha,\beta) = \min(K, |\alpha - \beta|^2)$$

with K a constant.

• Truncated absolute distance is a metric

$$V(\alpha,\beta) = \min(K, |\alpha - \beta|)$$

with K a constant.

Examples for 1D label set

• Truncated quadratic is a semi-metric

$$V(\alpha,\beta) = \min(K, |\alpha - \beta|^2)$$

with K a constant.

• Truncated absolute distance is a metric

$$V(\alpha,\beta) = \min(K, |\alpha - \beta|)$$

with K a constant.

• Potts model is a metric

$$V(\alpha,\beta) = K \cdot T(\alpha \neq \beta)$$

with $T(\cdot) = 1$ if the argument is true and 0 otherwise.

- Alpha Expansion: Checks if current nodes want to switch to label α
- Alpha Beta Swaps: Checks if a node with class α wants to switch to β .
- Binary problems that can be solve exactly for certain type of potentials



- Alpha Expansion: Checks if current nodes want to switch to label α
- Alpha Beta Swaps: Checks if a node with class α wants to switch to β .
- Binary problems that can be solve exactly for certain type of potentials



- Alpha Expansion: Checks if current nodes want to switch to label α
- Alpha Beta Swaps: Checks if a node with class α wants to switch to β .
- Binary problems that can be solve exactly for certain type of potentials



- Alpha Expansion: Checks if current nodes want to switch to label α
- Alpha Beta Swaps: Checks if a node with class α wants to switch to β .
- Binary problems that can be solve exactly for certain type of potentials



- Alpha Expansion: Checks if current nodes want to switch to label α
- Alpha Beta Swaps: Checks if a node with class α wants to switch to β .
- Binary problems that can be solve exactly for certain type of potentials



Binary Moves

- $\alpha \beta$ moves works for semi-metrics
- α expansion works for V being a metric



Figure : from P. Kohli tutorial on graph-cuts

• For certain x^1 and x^2 , the move energy is sub-modular

Urtasun & Zemel (UofT)

- The set of vertices includes the two terminals α and β, as well as image pixels p in the sets P_α and P_β (i.e., f_p ∈ {α, β}).
- Each pixel $p \in \mathcal{P}_{\alpha\beta}$ is connected to the terminals α and β , called *t*-links.
- Each set of pixels $p,q\in \mathcal{P}_{lphaeta}$ which are neighbors is connected by an edge $e_{p,q}$

