Computer Vision

Lecture 7 – Learning in Graphical Models

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Agenda

7.1 Conditional Random Fields

7.2 Parameter Estimation

7.3 Deep Structured Models

7.1

Conditional Random Fields

Inference vs. Learning

Markov Random Field:

$$p(x_1, \dots, x_{100}) = \frac{1}{Z} \exp \left\{ \sum_i \psi_i(x_i) + \lambda \sum_{i \sim j} \psi_{ij}(x_i, x_j) \right\}$$

- ► So far: Inference
 - ightharpoonup Marginal distributions: $p(x_i) = \sum_{x \mid x_i} p(x_1, \dots x_{100})$
 - ► MAP solution: $x_1^*, \dots, x_{100}^* = \operatorname{argmax}_{x_1, \dots, x_{100}} p(x_1, \dots x_{100})$
- ► Now: **Learning**
 - ightharpoonup Estimate parameters (here regularization strength λ) from dataset
- ► Remark: In the literature, potentials are sometimes defined as the negative log factors, but here we will consider them as generic features and omit the sign

Conditional Random Fields

Markov Random Field:

$$p(\mathcal{X}) = \frac{1}{Z} \exp \left\{ \sum_{i} \psi_{i}(x_{i}) + \lambda \sum_{i \sim j} \psi_{ij}(x_{i}, x_{j}) \right\}$$

lacktriangleright Reason about output variables $\mathcal{X} \in \mathbb{X}$ given one particular model instantiation

Structured Output Learning:

$$f_{\mathbf{w}}: \mathbb{X} \to \mathbb{Y}$$

- ▶ Inputs $\mathcal{X} \in \mathbb{X}$ can be any kind of objects
- ▶ Outputs $\mathcal{Y} \in \mathbb{Y}$ are complex (structured) objects
 - ▶ images, text, parse trees, folds of a protein, computer programs, ...

Conditional Random Fields

Markov Random Field:

$$p(\mathcal{X}) = \frac{1}{Z} \exp \left\{ \sum_{i} \psi_{i}(x_{i}) + \lambda \sum_{i \sim j} \psi_{ij}(x_{i}, x_{j}) \right\}$$

lacktriangleright Reason about output variables $\mathcal{X} \in \mathbb{X}$ given one particular model instantiation

Conditional Random Field:

$$p(\mathcal{Y}|\mathcal{X}, \mathbf{w}) = \frac{1}{Z} \exp \left\{ \sum_{i} \psi_{i}(\mathcal{X}, y_{i}) + \lambda \sum_{i \sim j} \psi_{ij}(\mathcal{X}, y_{i}, y_{j}) \right\}$$

- lacktriangle Make conditioning of output ${\cal Y}$ on input ${\cal X}$ and parameters ${f w}$ explicit (here ${f w}=\lambda$)
- ▶ MRF notation: outputs $\mathcal{X} \in \mathbb{X} \Rightarrow$ CRF notation: inputs $\mathcal{X} \in \mathbb{X}$, outputs $\mathcal{Y} \in \mathbb{Y}$
- \blacktriangleright Learning: Estimate \mathbf{w} from dataset $\mathcal{D} = \{(\mathcal{X}^1,\mathcal{Y}^1),\dots,(\mathcal{X}^N,\mathcal{Y}^N)\}$

Conditional Random Fields

Conditional Random Field - General Form:

$$p(\mathcal{Y}|\mathcal{X}, \mathbf{w}) = \frac{1}{Z(\mathcal{X}, \mathbf{w})} \exp \{ \langle \mathbf{w}, \psi(\mathcal{X}, \mathcal{Y}) \rangle \}$$

Feature function: $\psi(\mathcal{X}, \mathcal{Y}) : \mathbb{X} \times \mathbb{R}^M \to \mathbb{R}^D$ (concatenates potentials/features) Graphical model specifies decomposition of ψ into potentials (=log factors) ψ_k :

$$\psi(\mathcal{X}, \mathcal{Y}) = (\psi_1(\mathcal{X}, \mathcal{Y}_1), \dots, \psi_K(\mathcal{X}, \mathcal{Y}_K))$$

- ▶ Parameter vector: $\mathbf{w} \in \mathbb{R}^D$ (M: num. output nodes, D: dim. of feature space) Note that this model is much more flexible than a model with a single λ
- ▶ Partition function: $Z(\mathcal{X}, \mathbf{w}) = \sum_{\mathcal{Y}} \exp \{ \langle \mathbf{w}, \psi(\mathcal{X}, \mathcal{Y}) \rangle \}$
- ▶ Learning: Estimate \mathbf{w} from dataset $\mathcal{D} = \{(\mathcal{X}^1, \mathcal{Y}^1), \dots, (\mathcal{X}^N, \mathcal{Y}^N)\}$

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7.2

Parameter Estimation

Goal: Maximize likelihood of outputs $\mathcal Y$ conditioned on inputs $\mathcal X$ wrt. $\mathbf w$, assuming independent and identically distributed (IID) data (likelihood factorizes):

$$\hat{\mathbf{w}}_{ML} = \underset{\mathbf{w} \in \mathbb{R}^D}{\operatorname{argmax}} \ p(\mathcal{Y}|\mathcal{X}, \mathbf{w}) \quad \text{with} \quad p(\mathcal{Y}|\mathcal{X}, \mathbf{w}) = \prod_{n=1}^N p(\mathcal{Y}^n|\mathcal{X}^n, \mathbf{w})$$

In other words, find parameter vector $\hat{\mathbf{w}}_{ML}$ such that $p_{model}(\mathcal{Y}|\mathcal{X}, \hat{\mathbf{w}}_{ML}) \approx p_{data}(\mathcal{Y}|\mathcal{X})$.

This is equivalent to minimizing the **negative conditional log-likelihood:**

$$\hat{\mathbf{w}}_{ML} = \underset{\mathbf{w} \in \mathbb{R}^D}{\operatorname{argmin}} \ \mathcal{L}(\mathbf{w}) \quad \text{with} \quad \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^N \log p(\mathcal{Y}^n | \mathcal{X}^n, \mathbf{w})$$

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Parameter Estimation

Goal: Minimize negative conditional log-likelihood $\mathcal{L}(\mathbf{w})$

$$\hat{\mathbf{w}}_{ML} = \underset{\mathbf{w} \in \mathbb{R}^{D}}{\operatorname{argmin}} \ \mathcal{L}(\mathbf{w})$$

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \log p(\mathcal{Y}^{n} | \mathcal{X}^{n}, \mathbf{w})$$

$$= -\sum_{n=1}^{N} \left[\log \frac{1}{Z(\mathcal{X}^{n}, \mathbf{w})} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle \right\} \right]$$

$$= -\sum_{n=1}^{N} \left[-\log Z(\mathcal{X}^{n}, \mathbf{w}) + \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle \right]$$

$$= -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle - \log \sum_{\mathcal{Y} \in \mathbb{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \right]$$

Optimization

Gradient Descent:

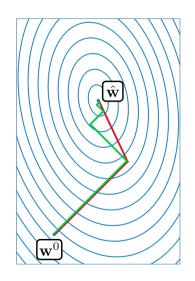
- ightharpoonup Pick step size η and tolerance ϵ
- ightharpoonup Initialize \mathbf{w}^0
- ▶ Repeat until $\|\mathbf{v}\| < \epsilon$

$$\mathbf{v} = \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = \sum_{i=1}^{N} \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w})$$

$$ightharpoonup \mathbf{w}^{t+1} = \mathbf{w}^t - \eta \mathbf{v}$$

Variants:

- ► Line search (green)
- ► Conjugate gradients (red)
- ► All require gradients, some (e.g., line search) require function evaluation



Gradient of Negative Conditional Log-Likelihood

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle - \log \sum_{\mathcal{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \frac{\sum_{\mathcal{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \psi(\mathcal{X}^{n}, \mathcal{Y})}{\sum_{\mathcal{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\}} \right]$$

$$= -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \sum_{\mathcal{Y}} \frac{\exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\}}{\sum_{\mathcal{Y}'} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\}} \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

$$= -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \sum_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

$$= -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \mathbb{E}_{\mathcal{Y} \sim p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w})} \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

Gradient of Negative Conditional Log-Likelihood

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \mathbb{E}_{\mathcal{Y} \sim p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w})} \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

When is $\mathcal{L}(\mathbf{w})$ minimal?

$$\mathbb{E}_{y \sim p(\mathcal{Y}|\mathcal{X}^n, \mathbf{w})} \psi(\mathcal{X}^n, \mathcal{Y}) = \psi(\mathcal{X}^n, \mathcal{Y}^n) \Rightarrow \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = 0$$

▶ Interpretation: we aim at **expectation matching**: $\mathbb{E}_{\mathcal{Y} \sim p(\cdot)} \psi(\mathcal{X}, \mathcal{Y}) = \psi(\mathcal{X}, \mathcal{Y}^{\text{obs}})$, but discriminatively: only for $\mathcal{X} \in \{\mathcal{X}^1, \dots, \mathcal{X}^N\}$

Note:

- $ightharpoonup \mathcal{L}(\mathbf{w})$ convex (Hessian positive semi-definite) $\Rightarrow \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = 0 \Rightarrow$ global optimum
- ▶ Only true as $p(\mathcal{Y}|\mathcal{X}, \mathbf{w})$ is log-linear in $\mathbf{w} \in \mathbb{R}^D$ (we will also see non-linear models)

LOG LINEAR!!

Task: For gradient descent with line search we must evaluate $\mathcal{L}(\mathbf{w})$ and $\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w})$:

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle - \log \sum_{\mathcal{Y} \in \mathbb{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \sum_{\mathcal{Y} \in \mathbb{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

Problem: Y is typically very (exponentially) large!

- ▶ Binary image segmentation: $|\mathbb{Y}| = 2^{640 \times 480} \approx 10^{92475}$
- ightharpoonup We must use the structure in \mathbb{Y} , or we are lost!

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle - \log \sum_{\mathcal{Y} \in \mathbb{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \sum_{\mathcal{Y} \in \mathbb{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

Computational complexity: $O(NC^MD)$

- ▶ N: number of samples in dataset (\approx 100 to 1,000,000)
- ► M: number of output nodes (\approx 100 to 1,000,000)
- ► C: maximal number of labels per output node (\approx 2 to 100)
- lacktriangleright D: dimensionality of feature space ψ

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle - \log \sum_{\mathcal{Y} \in \mathbb{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \sum_{\mathcal{Y} \in \mathbb{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

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- ► C: maximal number of labels per output node (\approx 2 to 100)
- ► D: dimensionality of feature space

Probabilistic Inference to the Rescue

Remember: in a graphical model, features and weights decompose as follows

$$\psi(\mathcal{X}, \mathcal{Y}) = (\psi_1(\mathcal{X}, \mathcal{Y}_1), \dots, \psi_K(\mathcal{X}, \mathcal{Y}_K))$$
 $\mathbf{w} = (\mathbf{w}_1, \dots, \mathbf{w}_K)$

Thus, the partition function simplifies as:

$$\sum_{\mathcal{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^n, \mathcal{Y}) \rangle \right\} = \sum_{\mathcal{Y}} \exp \left\{ \sum_{k} \langle \mathbf{w}_k, \psi_k(\mathcal{X}^n, \mathcal{Y}_k) \rangle \right\}$$
$$= \sum_{\mathcal{Y}} \prod_{k} \exp \left\{ \langle \mathbf{w}_k, \psi_k(\mathcal{X}^n, \mathcal{Y}_k) \rangle \right\}$$

我的理解:把一张大图Y做了分割,yk = $\sum_{\mathcal{V}} \prod_{k} \underbrace{\exp\left\{\langle \mathbf{w}_k, \psi_k(\mathcal{X}^n, \mathcal{Y}_k) \rangle\right\}}_{\text{K'th factor}}$ 这样去简化对整个图片的计算

► Can be efficiently calculated/approximated using **message passing** (run sum-product belief propagation, sum over any of the unnorm. marginals)

Probabilistic Inference to the Rescue

Similarly, the **feature expectation simplifies** as:

$$\sum_{\mathbf{y}} p(\mathbf{y}|\mathbf{x}^{n}, \mathbf{w}) \psi(\mathbf{x}^{n}, \mathbf{y}) = \mathbb{E}_{\mathbf{y} \sim p(\mathbf{y}|\mathbf{x}^{n}, \mathbf{w})} \psi(\mathbf{x}^{n}, \mathbf{y})$$

$$= \left(\mathbb{E}_{\mathbf{y} \sim p(\mathbf{y}|\mathbf{x}^{n}, \mathbf{w})} \psi_{k}(\mathbf{x}^{n}, \mathbf{y}_{k}) \right)_{k \in 1, \dots, K}$$

$$= \left(\mathbb{E}_{\mathbf{y}_{k} \sim p(\mathbf{y}_{k}|\mathbf{x}^{n}, \mathbf{w})} \psi_{k}(\mathbf{x}^{n}, \mathbf{y}_{k}) \right)_{k \in 1, \dots, K}$$

$$= \left(\sum_{\mathbf{y}_{k}} p(\mathbf{y}_{k}|\mathbf{x}^{n}, \mathbf{w}) \psi_{k}(\mathbf{x}^{n}, \mathbf{y}_{k}) \right)_{k \in 1, \dots, K}$$

- Now only C^F terms in sum over \mathcal{Y}_k (C: max. number of labels, F: largest order)
- ▶ Marginals $p(\mathcal{Y}_k|\mathcal{X}^n,\mathbf{w})$ can be calculated efficiently (e.g., with BP)

Probabilistic Inference to the Rescue



Similarly, the **feature expectation simplifies** as:

$$\sum_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \psi(\mathcal{X}^{n}, \mathcal{Y}) = \mathbb{E}_{\mathcal{Y} \sim p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w})} \sum_{k} \psi_{k}(\mathcal{X}^{n}, \mathcal{Y}_{k})$$

$$= \sum_{k} \mathbb{E}_{\mathcal{Y} \sim p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w})} \psi_{k}(\mathcal{X}^{n}, \mathcal{Y}_{k})$$

$$= \sum_{k} \mathbb{E}_{\mathcal{Y}_{k} \sim p(\mathcal{Y}_{k}|\mathcal{X}^{n}, \mathbf{w})} \psi_{k}(\mathcal{X}^{n}, \mathcal{Y}_{k})$$

$$= \sum_{k} \underbrace{\sum_{\mathcal{Y}_{k}} p(\mathcal{Y}_{k}|\mathcal{X}^{n}, \mathbf{w})}_{\text{marginal}} \psi_{k}(\mathcal{X}^{n}, \mathcal{Y}_{k})$$

- ► K: number of potentials, C: max. number of labels, F: largest order
- ► Marginals can be calculated efficiently in polynomial time (e.g., with BP)

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle - \log \sum_{\mathcal{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \sum_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

Computational complexity: $O(NC^{M}D) \rightarrow O(NKC^{F}D)$

- ▶ N: number of samples in dataset (\approx 100 to 1,000,000)
- ► M: number of output nodes (\approx 100 to 1,000,000)
- ► C: maximal number of labels per output node (\approx 2 to 100)
- ▶ D: dim. of feature space, K: number of factors, F: order of largest factor (\approx 2-3)

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle - \log \sum_{\mathcal{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \sum_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

Computational complexity: $O(NKC^FD)$

- ▶ N: number of samples in dataset (\approx 100 to 1,000,000)
- ► M: number of output nodes (\approx 100 to 1,000,000)
- ► C: maximal number of labels per output node (\approx 2 to 100)
- ▶ *D*: dim. of feature space, *K*: number of factors, *F*: order of largest factor

Learning on large datasets:

- lacktriangleright Processing all N training samples for one gradient update is slow
- ► Furthermore, often not all data fits into memory (as in deep learning)

How can we estimate parameters in this setting?

- ► Simplify model to make gradient updates faster ⇒ results get worse
- ► Train model on subsampled dataset ⇒ ignores information
- ▶ Parallelize across CPUs/GPUs ⇒ bottlenecks, doesn't save computation
- ► Stochastic gradient descent

Stochastic Gradient Descent (SGD)

Stochastic Gradient Descent:

- ► In each gradient step:
 - ► Create random subset $\mathcal{D}' \subset \mathcal{D}$ (typically $\mathcal{D}' \leq 256$)
 - ► Follow approximate gradient:

$$\nabla_{\mathbf{w}} \approx -\sum_{(\mathcal{X}^n, \mathcal{Y}^n) \in \mathcal{D}'} \left[\psi(\mathcal{X}^n, \mathcal{Y}^n) - \mathbb{E}_{\mathcal{Y} \sim p(\mathcal{Y}|\mathcal{X}^n, \mathbf{w})} \psi(\mathcal{X}^n, \mathcal{Y}) \right]$$

Comments:

- lackbox Line search no longer possible \Rightarrow extra step-size hyper-parameter η
- ► SGD converges to $\operatorname{argmin}_{\mathbf{w}} \mathcal{L}(\mathbf{w})!$ (if η chosen right)
- ► SGD needs more iterations, but each one is faster
- ► See also: Bottou & Bousquet: The Tradeoffs of Large Scale Learning, NIPS 2007

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) \rangle - \log \sum_{\mathcal{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^{n}, \mathcal{Y}) \rangle \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}) - \sum_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \psi(\mathcal{X}^{n}, \mathcal{Y}) \right]$$

Computational complexity: $O(NKC^FD)$

- ▶ N: number of samples in dataset (\approx 100 to 1,000,000)
- ► M: number of output nodes (\approx 100 to 1,000,000)
- ► C: maximal number of labels per output node (\approx 2 to 100)
- ightharpoonup D: dim. of feature space, K: number of factors, F: order of largest factor

Semantic Segmentation:

- $\psi_i(\mathcal{X}, y_i) \in \mathbb{R}^{\approx 1000}$: local image features (e.g., bag of words, deep features)
 - $\rightarrow \langle \mathbf{w}_i, \psi_i(\mathcal{X}, y_i) \rangle$: local classifier (like logistic regression)
- $lackbox{}\psi_{ij}(y_i,y_j)=[y_i=y_j]\in\mathbb{R}^1$: test for same label
 - $\rightarrow \langle w_{ij}, \psi_{ij}(y_i, y_j) \rangle$: penalizer for label changes (if $w_{ij} > 0$)
- ightharpoonup combined: $\operatorname{argmax}_{\mathcal{V}} p(\mathcal{Y}|\mathcal{X}, \mathbf{w})$ is smoothed version of local cues



original



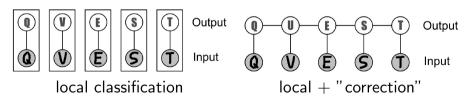
local classification



local + smoothness

Handwriting Recognition:

- $\psi_i(\mathcal{X}, y_i) \in \mathbb{R}^{\approx 1000}$: image representation (e.g., pixels, gradients) • $\langle \mathbf{w}_i, \psi_i(\mathcal{X}, y_i) \rangle$: local classifier for letters
- $\psi_{ij}(y_i, y_j) = \mathbf{e}_{y_i} \mathbf{e}_{y_j}^{\top} \in \mathbb{R}^{26 \times 26}$: letter/letter indicator (matrix with one element = 1) $\rightarrow \langle \mathbf{w}_{ij}, \psi_{ij}(y_i, y_j) \rangle$: encourage/suppress letter combinations
- ightharpoonup Combined: $\operatorname{argmax}_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}, \mathbf{w})$ is "corrected" version of local cues



Pose Estimation:

- ▶ $\psi_i(\mathcal{X}, y_i) \in \mathbb{R}^{\approx 1000}$: image representation (e.g., HoG, deep features) $\rightarrow \langle \mathbf{w}_i, \psi_i(\mathcal{X}, y_i) \rangle$: local confidence map
- $\psi_{ij}(y_i, y_j) = \text{fit}(y_i, y_j) \in \mathbb{R}^1$: test for geometric fit / pose prior $\rightarrow \langle w_{ij}, \psi_{ij}(y_i, y_j) \rangle$: penalizer for unrealistic poses
- ightharpoonup Combined: $\operatorname{argmax}_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}, \mathbf{w})$ is sanitized version of local cues





original

local classification

local + geometry

Typical feature functions for CRFs in computer vision:

- ▶ Unary terms $\psi_i(\mathcal{X}, y_i)$: local representation, high-dimensional $\rightarrow \langle \mathbf{w}_i, \psi_i(\mathcal{X}, y_i) \rangle$: local classifier
- Pairwise terms $\psi_{ij}(y_i,y_j)$: prior knowledge, typically low-dimensional $\rightarrow \langle w_{ij}, \psi_{ij}(y_i,y_j) \rangle$: penalize inconsistencies
- lacktriangle Pairwise terms sometimes also depend on \mathcal{X} : $\psi_{ij}(\mathcal{X}, y_i, y_j)$

Learning adjusts parameters:

- lackbox Unary weights \mathbf{w}_i : learn local linear classifiers
- lacktriangle Pairwise weights w_{ij} : learn importance of smoothing/penalization
- lacktriangledown $lpha \operatorname{argmax}_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}, \mathbf{w})$ is cleaned up version of local prediction

Piece-wise Training

Sometimes, training the entire model at once is not easy:

- ► If terms actually depend on parameters in non-linear fashion
- ► If features are high-dimensional, learning can be very slow

Alternative: Piece-wise Training

- ▶ Pre-train classifiers $p(y_i|\mathcal{X})$; set $\psi_i(\mathcal{X}, y_i) = \log p(y_i|\mathcal{X}) \in \mathbb{R}$
- ▶ Learn one-dimensional weight per classifier: $\langle w_i, \psi_i(\mathcal{X}, y_i) \rangle$

Advantage:

- lacktriangledown Lower dimensional feature vector during training/inference ightarrow faster
- $ightharpoonup \log p(y_i|\mathcal{X})$ can be stronger classifiers, e.g., non-linear SVMs, CNNs, ..

Disadvantage

► If local classifiers are bad, CRF training cannot fix this

Summary

Given:

- $\blacktriangleright \text{ Training set } \mathcal{D} = \{(\mathcal{X}^1, \mathcal{Y}^1), \dots, (\mathcal{X}^N, \mathcal{Y}^N)\} \text{ with } (\mathcal{X}^n, \mathcal{Y}^n) \overset{\text{i.i.d.}}{\sim} p_{data}(\mathcal{X}, \mathcal{Y})$
- ▶ Feature function: $\psi(\mathcal{X}, \mathcal{Y}) : \mathbb{X} \times \mathbb{R}^M \to \mathbb{R}^D$

Task:

lacktriangle Find parameter vector $\hat{\mathbf{w}}_{ML}$ such that

$$p_{model}(\mathcal{Y}|\mathcal{X}, \hat{\mathbf{w}}_{ML}) = \frac{1}{Z(\mathcal{X}, \hat{\mathbf{w}}_{ML})} \exp\left\{ \langle \hat{\mathbf{w}}_{ML}, \psi(\mathcal{X}, \mathcal{Y}) \rangle \right\} \approx p_{data}(\mathcal{Y}|\mathcal{X})$$

Minimize negative conditional log-likelihood:

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^n, \mathcal{Y}^n) \rangle - \log \sum_{\mathcal{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^n, \mathcal{Y}) \rangle \right\} \right]$$

- lacktriangle Convex optimization problem ightarrow gradient descent leads to global optimum
- lacktriangle Training needs repeated runs of probabilistic inference \Rightarrow must be fast

Summary

Gradient of negative conditional log-likelihood:

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\langle \mathbf{w}, \psi(\mathcal{X}^n, \mathcal{Y}^n) \rangle - \log \sum_{\mathcal{Y} \in \mathbb{Y}} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}^n, \mathcal{Y}) \rangle \right\} \right]$$

Problem	Solution	Method
¥ too large	exploit structure	belief propagation
N too large	mini-batches	stochastic gradient descent
${\it D}$ too large	trained ψ	piece-wise training

7.3

Deep Structured Models

Motivation

Log-Linear Models:

$$p(\mathcal{Y}|\mathcal{X}, \mathbf{w}) = \frac{1}{Z(\mathcal{X}, \mathbf{w})} \exp \left\{ \langle \mathbf{w}, \psi(\mathcal{X}, \mathcal{Y}) \rangle \right\}$$

- \blacktriangleright Log-linear in the parameters $\mathbf{w} \Rightarrow$ features must do all the heavy lifting
- Only linear combination of features is learned

Deep Structured Models:

$$p(\mathcal{Y}|\mathcal{X}, \mathbf{w}) = \frac{1}{Z(\mathcal{X}, \mathbf{w})} \exp \{ \psi(\mathcal{X}, \mathcal{Y}, \mathbf{w}) \}$$

- Potential functions directly parametrized via w
- ightharpoonup Results in a much more flexible model (ψ can represent, e.g., a neural network)

Deep Structured Models

Negative Log-Likelihood and its Gradient:

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}, \mathbf{w}) - \log \sum_{\mathcal{Y}} \exp \left\{ \psi(\mathcal{X}^{n}, \mathcal{Y}, \mathbf{w}) \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\nabla_{\mathbf{w}} \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}, \mathbf{w}) - \sum_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \nabla_{\mathbf{w}} \psi(\mathcal{X}^{n}, \mathcal{Y}, \mathbf{w}) \right]$$

- ► Similar form as for log-linear models
- ► Differences to log-linear model highlighted in red

Deep Structured Models

Negative Log-Likelihood and its Gradient:

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\psi(\mathcal{X}^{n}, \mathcal{Y}^{n}, \mathbf{w}) - \log \sum_{\mathcal{Y}} \exp \left\{ \psi(\mathcal{X}^{n}, \mathcal{Y}, \mathbf{w}) \right\} \right]$$

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} \left[\nabla_{\mathbf{w}} \psi(\mathcal{X}^{n}, \mathcal{Y}^{n}, \mathbf{w}) - \sum_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}^{n}, \mathbf{w}) \nabla_{\mathbf{w}} \psi(\mathcal{X}^{n}, \mathcal{Y}, \mathbf{w}) \right]$$

Again, sums can be efficiently computed as features decompose

$$\psi(\mathcal{X}, \mathcal{Y}, \mathbf{w}) = (\psi_1(\mathcal{X}, \mathcal{Y}_1, \mathbf{w}), \dots, \psi_K(\mathcal{X}, \mathcal{Y}_K, \mathbf{w}))$$

Deep Structured Models

Algorithm:

- ► Forward pass to compute $\psi_k(\mathcal{X}, \mathcal{Y}_k, \mathbf{w})$
- ▶ Backward pass to obtain gradients $\nabla_{\mathbf{w}}\psi(\mathcal{X}^n, \mathcal{Y}, \mathbf{w})$
- ► Compute marginals using message passing
- ► Update parameters w

What is the problem with this approach?

 Very slow as forward and backward pass are required to calculate features and gradients for GM inference in every gradient update step

Alternatives:

- ► Interleave learning and inference [Chen et al., ICML 2015], but still slow
- ► Unrolled inference (simple, but we loose probabilistic interpretation)

Inference Unrolling

Inference Unrolling

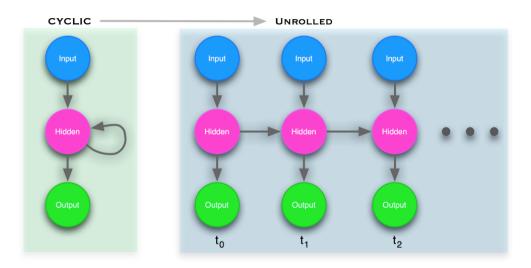
Idea:

- ► Consider inference as sequence of small computations
- ▶ "Unroll" a **fixed** number of inference iterations similar to RNN
- ► Compute gradients using automatic differentiation

Remarks:

- ► Now: empirical risk minimization
- ► Thus purely deterministic approach, giving up probabilistic viewpoint
- ▶ But often fast enough for efficient training in deep models
- ► Effectively integrates structure of the problem into architecture of the network
- ► Can be thought of as a form of regularization (hard constraint)

Inference Unrolling



Automatic Differentiation

Automatic Differentiation:

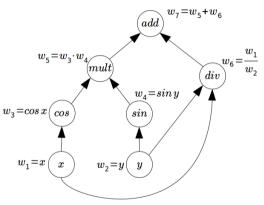
Rewrite complicated function as composition of simple functions:

$$f = f_0 \circ f_1 \circ \cdots \circ f_n$$

- ► Each simple function f_k has a simple derivative
- ▶ Use chain rule: $\frac{\partial f_0}{\partial f_1} \frac{\partial f_1}{\partial f_2} \dots \frac{\partial f_n}{\partial x}$
- **►** Example:

$$f(x,y) = \cos(x)\sin(y) + \frac{x}{y}$$

Computation Graph:

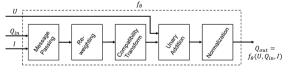


Examples

Conditional Random Fields as Recurrent Neural Networks

$$E(\mathbf{x}) = \sum_{i} \psi_u(x_i) + \sum_{i < j} \psi_p(x_i, x_j), \tag{1}$$

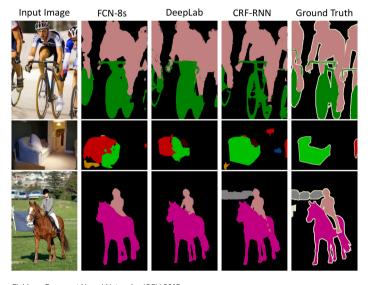
$$\psi_p(x_i, x_j) = \mu(x_i, x_j) \sum_{m=1}^{M} w^{(m)} k_G^{(m)}(\mathbf{f}_i, \mathbf{f}_j), \quad (2)$$



Algorithm 1 Mean-field in dense CRFs [29], broken down to common CNN operations.

$$\begin{array}{c|c} Q_i(l) \leftarrow \frac{1}{Z_i} \exp{(U_i(l))} \text{ for all } i & \triangleright \text{Initialization} \\ \textbf{while not converged do} \\ & \hat{Q}_i^{(m)}(l) \leftarrow \sum_{j \neq i} k^{(m)}(\mathbf{f}_i, \mathbf{f}_j) Q_j(l) \text{ for all } m \\ & \triangleright \text{Message Passing} \\ & \hat{Q}_i(l) \leftarrow \sum_m w^{(m)} \hat{Q}_i^{(m)}(l) & \triangleright \text{Weighting Filter Outputs} \\ & \hat{Q}_i(l) \leftarrow \sum_{l' \in \mathcal{L}} \mu(l, l') \check{Q}_i(l') & \triangleright \text{Compatibility Transform} \\ & \check{Q}_i(l) \leftarrow U_i(l) - \hat{Q}_i(l) & \triangleright \text{Adding Unary Potentials} \\ & Q_i \leftarrow \frac{1}{Z_i} \exp{\left(\check{Q}_i(l)\right)} & \triangleright \text{Normalizing} \\ & \text{end while} & \end{array}$$

Conditional Random Fields as Recurrent Neural Networks



RayNet: Learning Volumetric 3D Reconstruction

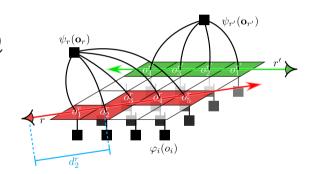
Distribution over voxel occupancies:

$$p(\mathbf{o}) = \frac{1}{Z} \prod_{i \in \mathcal{X}} \underbrace{\varphi_i(o_i)}_{\text{unary}} \prod_{r \in \mathcal{R}} \underbrace{\psi_r(\mathbf{o}_r)}_{\text{ray}}$$

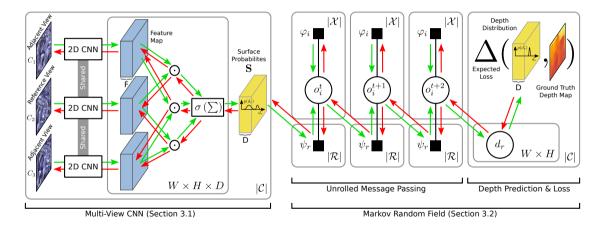
$$\varphi_i(o_i) = \gamma^{o_i} (1 - \gamma)^{1 - o_i}$$

$$\psi_r(\mathbf{o}_r) = \sum_{i=1}^{N_r} o_i^r \prod_{j < i} (1 - o_j^r) s_i^r$$

Corresponding factor graph:



RayNet: Learning Volumetric 3D Reconstruction



RayNet: Learning Volumetric 3D Reconstruction

