

Neural networks

Training CRFs - loss function

LINEAR CHAN CRF

Topics: reminder of notation

- Then we have:

$$p(\mathbf{y}|\mathbf{X}) = \exp \left(\sum_{k=1}^K a_u(y_k) + \sum_{k=1}^{K-1} a_p(y_k, y_{k+1}) \right) / Z(\mathbf{X})$$

where

$$Z(\mathbf{X}) = \sum_{y'_1} \sum_{y'_2} \cdots \sum_{y'_K} \exp \left(\sum_{k=1}^K a_u(y'_k) + \sum_{k=1}^{K-1} a_p(y'_k, y'_{k+1}) \right)$$

- Two types of (log-)factors:

- ▶ unary: $a_u(y_k) = a^{(L+1,0)}(\mathbf{x}_k)_{y_k} +$
 $1_{k>1} a^{(L+1,-1)}(\mathbf{x}_{k-1})_{y_k} +$
 $1_{k<K} a^{(L+1,+1)}(\mathbf{x}_{k+1})_{y_k}$
- ▶ pairwise: $a_p(y_k, y_{k+1}) = 1_{1 \leq k < K} V_{y_k, y_{k+1}}$

MACHINE LEARNING

Topics: empirical risk minimization, regularization

- Empirical risk minimization

- ▶ framework to design learning algorithms

$$\arg \min_{\boldsymbol{\theta}} \frac{1}{T} \sum_t l(\mathbf{f}(\mathbf{X}^{(t)}; \boldsymbol{\theta}), \mathbf{y}^{(t)}) + \lambda \Omega(\boldsymbol{\theta})$$

- ▶ $l(\mathbf{f}(\mathbf{X}^{(t)}; \boldsymbol{\theta}), \mathbf{y}^{(t)})$ is a loss function
 - ▶ $\Omega(\boldsymbol{\theta})$ is a regularizer (penalizes certain values of $\boldsymbol{\theta}$)

- Learning is cast as optimization

- ▶ ideally, we'd optimize classification error, but it's not smooth
 - ▶ loss function is a surrogate for what we truly should optimize

MACHINE LEARNING

Topics: stochastic gradient descent (SGD)

- Algorithm that performs updates after each example

- ▶ initialize $\boldsymbol{\theta}$
- ▶ for N iterations

$$\left. \begin{array}{l} \text{- for each training example } (\mathbf{X}^{(t)}, \mathbf{y}^{(t)}) \\ \quad \checkmark \Delta = -\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{X}^{(t)}; \boldsymbol{\theta}), \mathbf{y}^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta}) \\ \quad \checkmark \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \Delta \end{array} \right\} \begin{array}{l} \text{training epoch} \\ = \\ \text{iteration over \textbf{all} examples} \end{array}$$

- To apply this algorithm to a CRF, we need

- ▶ the loss function $l(\mathbf{f}(\mathbf{X}^{(t)}; \boldsymbol{\theta}), \mathbf{y}^{(t)})$
- ▶ a procedure to compute the parameter gradients $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{X}^{(t)}; \boldsymbol{\theta}), \mathbf{y}^{(t)})$
- ▶ the regularizer $\Omega(\boldsymbol{\theta})$ (and the gradient $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)
- ▶ initialization method

LOSS FUNCTION

Topics: loss function for sequential classification with CRF

- CRF estimates $p(\mathbf{y}|\mathbf{X})$
 - ▶ we could maximize the probabilities of $\mathbf{y}^{(t)}$ given $\mathbf{X}^{(t)}$ in the training set
- To frame as minimization, we minimize the negative log-likelihood

$$l(\mathbf{f}(\mathbf{X}), \mathbf{y}) = -\log p(\mathbf{y}|\mathbf{X})$$

- ▶ unlike for non-sequential classification, we never explicitly compute the value of $p(\mathbf{y}|\mathbf{X})$ for all values of \mathbf{y}

Neural networks

Training CRFs - unary log-factor gradient

MACHINE LEARNING

Topics: stochastic gradient descent (SGD)

- Algorithm that performs updates after each example

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- ▶ for N iterations

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PARAMETER GRADIENTS

Topics: loss gradient at unary log-factors

- Partial derivative wrt $a_u(y_k')$:

$$\frac{\partial -\log p(\mathbf{y}|\mathbf{X})}{\partial a_u(y'_k)} = -(1_{y_k=y'_k} - p(y'_k|\mathbf{X}))$$

- Gradient for each unary (log-)factors:

$$\nabla_{\mathbf{a}^{(L+1,0)}(\mathbf{x}_k)} -\log p(\mathbf{y}|\mathbf{X}) = -(\mathbf{e}(y_k) - \mathbf{p}(y_k|\mathbf{X}))$$

$$\nabla_{\mathbf{a}^{(L+1,-1)}(\mathbf{x}_{k-1})} -\log p(\mathbf{y}|\mathbf{X}) = -1_{k>1} (\mathbf{e}(y_k) - \mathbf{p}(y_k|\mathbf{X}))$$

$$\nabla_{\mathbf{a}^{(L+1,+1)}(\mathbf{x}_{k+1})} -\log p(\mathbf{y}|\mathbf{X}) = -1_{k<K} (\mathbf{e}(y_k) - \underbrace{\mathbf{p}(y_k|\mathbf{X})}_{\text{vector of all marginal probabilities}})$$

vector of all
marginal probabilities

$$\frac{\partial - \log p(\mathbf{y}|\mathbf{X})}{\partial a_u(y'_k)} = \frac{\partial}{\partial a_u(y'_k)} - \left(\left(\sum_{k=1}^K a_u(y_k) + \sum_{k=1}^{K-1} a_p(y_k, y_{k+1}) \right) - \log Z(\mathbf{X}) \right)$$

$$\begin{aligned}
\frac{\partial - \log p(\mathbf{y} | \mathbf{X})}{\partial a_u(y'_k)} &= \frac{\partial}{\partial a_u(y'_k)} - \left(\left(\sum_{k=1}^K a_u(y_k) + \sum_{k=1}^{K-1} a_p(y_k, y_{k+1}) \right) - \log Z(\mathbf{X}) \right) \\
&= - \left(1_{y_k=y'_k} - \frac{\partial}{\partial a_u(y'_k)} \log Z(\mathbf{X}) \right)
\end{aligned}$$

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\end{aligned}$$

$$\frac{\partial}{\partial a_u(y'_k)} \log Z(\mathbf{X}) = \frac{1}{Z(\mathbf{X})} \frac{\partial}{\partial a_u(y'_k)} Z(\mathbf{X})$$

$$\begin{aligned}
\frac{\partial - \log p(\mathbf{y}|\mathbf{X})}{\partial a_u(y'_k)} &= \frac{\partial}{\partial a_u(y'_k)} - \left(\left(\sum_{k=1}^K a_u(y_k) + \sum_{k=1}^{K-1} a_p(y_k, y_{k+1}) \right) - \log Z(\mathbf{X}) \right) \\
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&= \frac{1}{Z(\mathbf{X})} \frac{\partial}{\partial a_u(y'_k)} \sum_{y''_1} \sum_{y''_2} \cdots \sum_{y''_K} \exp \left(\sum_{k=1}^K a_u(y''_k) + \sum_{k=1}^{K-1} a_p(y''_k, y''_{k+1}) \right) \\
&\quad \ddots \quad \ddots \quad \ddots
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&= \sum_{y''_1} \sum_{y''_2} \cdots \sum_{y''_K} \mathbf{1}_{y'_k=y''_k} p(y''_1, \dots, y''_K | \mathbf{X})
\end{aligned}$$

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\frac{\partial - \log p(\mathbf{y}|\mathbf{X})}{\partial a_u(y'_k)} &= \frac{\partial}{\partial a_u(y'_k)} - \left(\left(\sum_{k=1}^K a_u(y_k) + \sum_{k=1}^{K-1} a_p(y_k, y_{k+1}) \right) - \log Z(\mathbf{X}) \right) \\
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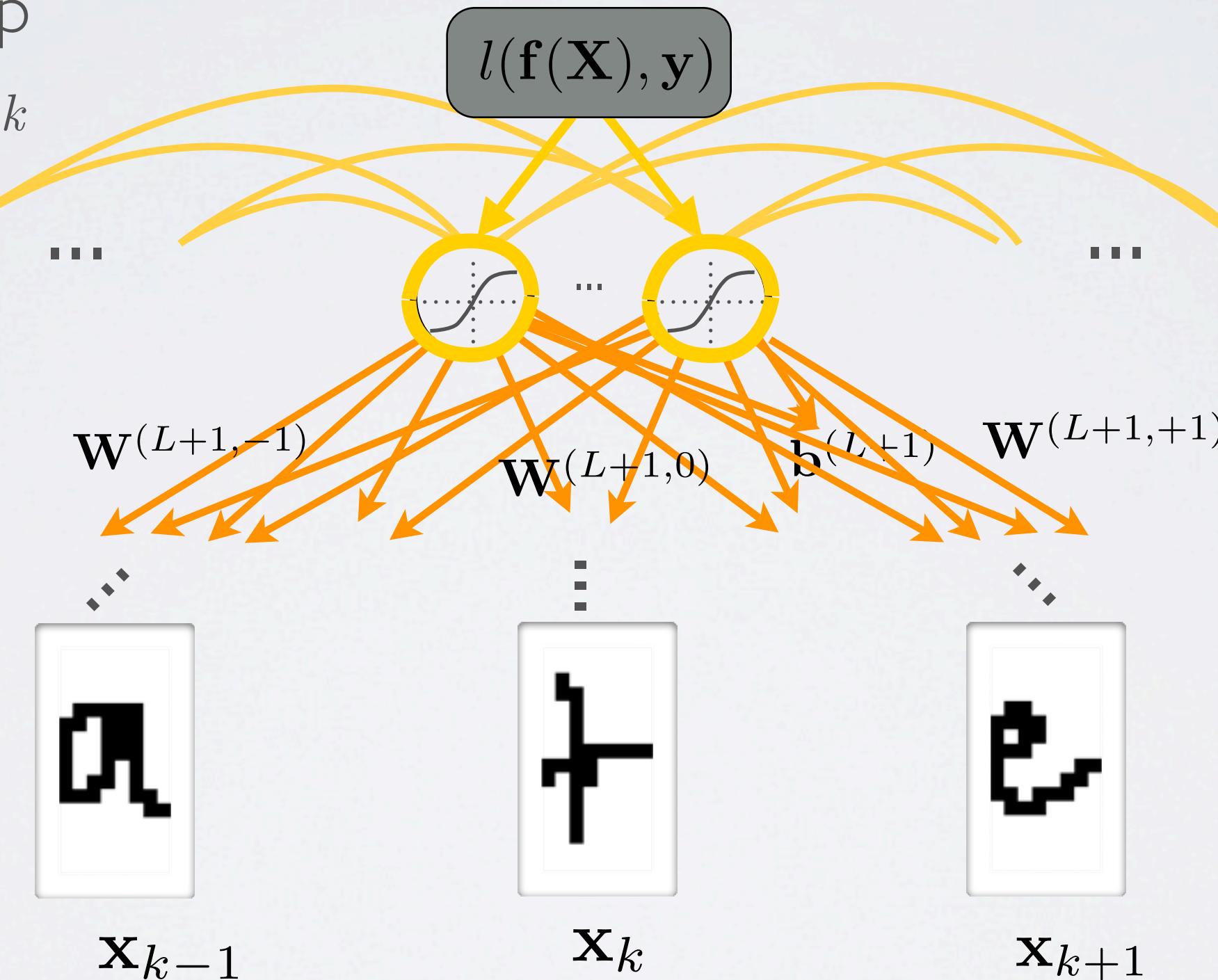
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&= \sum_{y''_1} \sum_{y''_2} \cdots \sum_{y''_K} \mathbf{1}_{y'_k=y''_k} p(y''_1, \dots, y''_K | \mathbf{X}) \\
&= p(y'_k | \mathbf{X})
\end{aligned}$$

PARAMETER GRADIENTS

Topics: loss gradient at unary log-factor parameters

- Use regular backprop

- ▶ backprop at all positions k
- ▶ accumulate all gradients, from every position, into parameters



PARAMETER GRADIENTS

Topics: loss gradient at unary log-factor parameters

- For linear log-factors:
 - ▶ the log-factors are directly connected to the input:

$$\mathbf{a}^{(1,0)}(\mathbf{x}_k) = \mathbf{b}^{(1)} + \mathbf{W}^{(1,0)}\mathbf{x}_k$$

$$\mathbf{a}^{(1,-1)}(\mathbf{x}_k) = \mathbf{W}^{(1,-1)}\mathbf{x}_k$$

$$\mathbf{a}^{(1,+1)}(\mathbf{x}_k) = \mathbf{W}^{(1,+1)}\mathbf{x}_k$$

PARAMETER GRADIENTS

Topics: loss gradient at unary log-factor parameters

- For linear log-factors:

- ▶ the gradients are:

$$\nabla_{\mathbf{b}^{(1)}} - \log p(\mathbf{y}|\mathbf{X}) = \sum_{k=1}^K (\nabla_{\mathbf{a}^{(1,0)}(\mathbf{x}_k)} - \log p(\mathbf{y}|\mathbf{X})) = \sum_{k=1}^K -(\mathbf{e}(y_k) - \mathbf{p}(y_k|\mathbf{X}))$$

$$\nabla_{\mathbf{W}^{(1,0)}} - \log p(\mathbf{y}|\mathbf{X}) = \sum_{k=1}^K (\nabla_{\mathbf{a}^{(1,0)}(\mathbf{x}_k)} - \log p(\mathbf{y}|\mathbf{X})) \mathbf{x}_k^\top = \sum_{k=1}^K -(\mathbf{e}(y_k) - \mathbf{p}(y_k|\mathbf{X})) \mathbf{x}_k^\top$$

$$\nabla_{\mathbf{W}^{(1,-1)}} - \log p(\mathbf{y}|\mathbf{X}) = \sum_{k=2}^K (\nabla_{\mathbf{a}^{(1,-1)}(\mathbf{x}_k)} - \log p(\mathbf{y}|\mathbf{X})) \mathbf{x}_{k-1}^\top = \sum_{k=2}^K -(\mathbf{e}(y_k) - \mathbf{p}(y_k|\mathbf{X})) \mathbf{x}_{k-1}^\top$$

$$\nabla_{\mathbf{W}^{(1,+1)}} - \log p(\mathbf{y}|\mathbf{X}) = \sum_{k=1}^{K-1} (\nabla_{\mathbf{a}^{(1,+1)}(\mathbf{x}_k)} - \log p(\mathbf{y}|\mathbf{X})) \mathbf{x}_{k+1}^\top = \sum_{k=1}^{K-1} -(\mathbf{e}(y_k) - \mathbf{p}(y_k|\mathbf{X})) \mathbf{x}_{k+1}^\top$$

Neural networks

Training CRFs - pairwise log-factor gradient

MACHINE LEARNING

Topics: stochastic gradient descent (SGD)

- Algorithm that performs updates after each example

- ▶ initialize $\boldsymbol{\theta}$
- ▶ for N iterations

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- ▶ initialization method

PARAMETER GRADIENTS

Topics: loss gradient at pairwise log-factor and parameters

- Partial derivative for log-factor:

$$\frac{\partial -\log p(\mathbf{y}|\mathbf{X})}{\partial a_p(y'_k, y'_{k+1})} = -(1_{y_k=y'_k, y_{k+1}=y'_{k+1}} - p(y'_k, y'_{k+1}|\mathbf{X}))$$

- Partial derivative of log-factor parameters:

$$\frac{\partial -\log p(\mathbf{y}|\mathbf{X})}{\partial V_{y'_k, y'_{k+1}}} = \sum_{k=1}^{K-1} -(1_{y_k=y'_k, y_{k+1}=y'_{k+1}} - p(y'_k, y'_{k+1}|\mathbf{X}))$$

- Gradient of log-factor parameters

$$\begin{aligned} \nabla_{\mathbf{V}} -\log p(\mathbf{y}|\mathbf{X}) &= \sum_{k=1}^{K-1} -(\mathbf{e}(y_k) \mathbf{e}(y_{k+1})^\top - \underbrace{\mathbf{p}(y_k, y_{k+1}|\mathbf{X})}_{\text{matrix of all pairwise marginal probabilities}}) \\ &= - \left(\underbrace{\text{freq}(y_k, y_{k+1})}_{\text{matrix of all pairwise label frequencies}} - \sum_{k=1}^{K-1} \mathbf{p}(y_k, y_{k+1}|\mathbf{X}) \right) \end{aligned}$$

REGULARIZATION

Topics: regularization

- For regularization, we can use the same regularizers as for a non-sequential neural network
 - ▶ add a regularizing term for all connection matrices
 - ▶ do not regularize the bias vectors
- We could scale λ by the sequence size
- With the loss and regularization gradients, we have all the ingredients to perform stochastic gradient descent

Neural networks

Training CRFs - discriminative vs. generative learning

GENERATIVE VS. DISCRIMINATIVE

Topics: discriminative learning, generative learning

- In discriminative learning, we optimize the conditional likelihood $-\log p(\mathbf{y}|\mathbf{X})$
 - ▶ CRFs are discriminative
- In generative learning, we optimize the joint log-likelihood:
$$-\log p(\mathbf{y}, \mathbf{X}) = -\log (p(\mathbf{y}|\mathbf{X})p(\mathbf{X})) = -\log p(\mathbf{y}|\mathbf{X}) - \log p(\mathbf{X})$$
 - ▶ HMMs are usually trained generatively
 - ▶ $-\log p(\mathbf{X})$ is similar to a regularizer

GENERATIVE VS. DISCRIMINATIVE

Topics: generative learning, discriminative learning

- It can be shown that:
 - ▶ if model is well-specified (i.e. is the true model) generative learning is better



GENERATIVE VS. DISCRIMINATIVE

Topics: generative learning, discriminative learning

- It can be shown that:
 - ▶ if model is not well-specified (i.e. most of the time), it depends:



- ▶ See these papers for more details:
 - On Discriminative vs. Generative classifiers: A comparison of logistic regression and naive Bayes. Andrew Ng and Michael Jordan, 2001

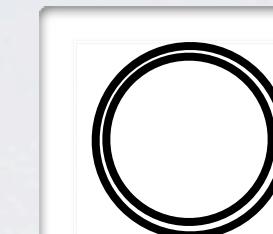
Neural networks

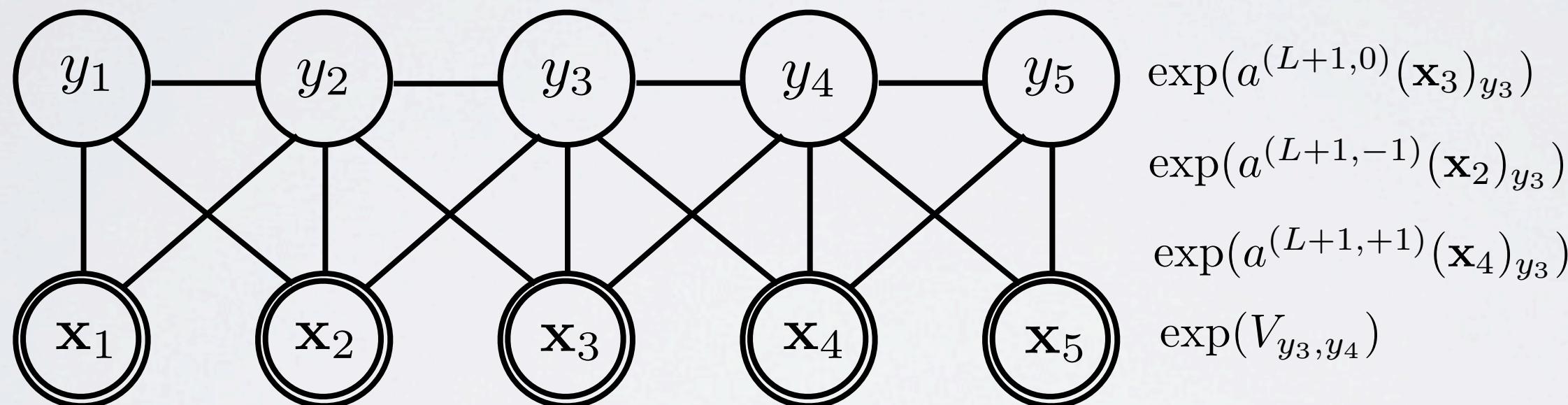
Training CRFs - maximum-entropy Markov model

LINEAR CHAN CRF

Topics: Markov network

- Illustration for $K=5$

 = observed

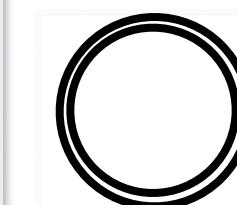


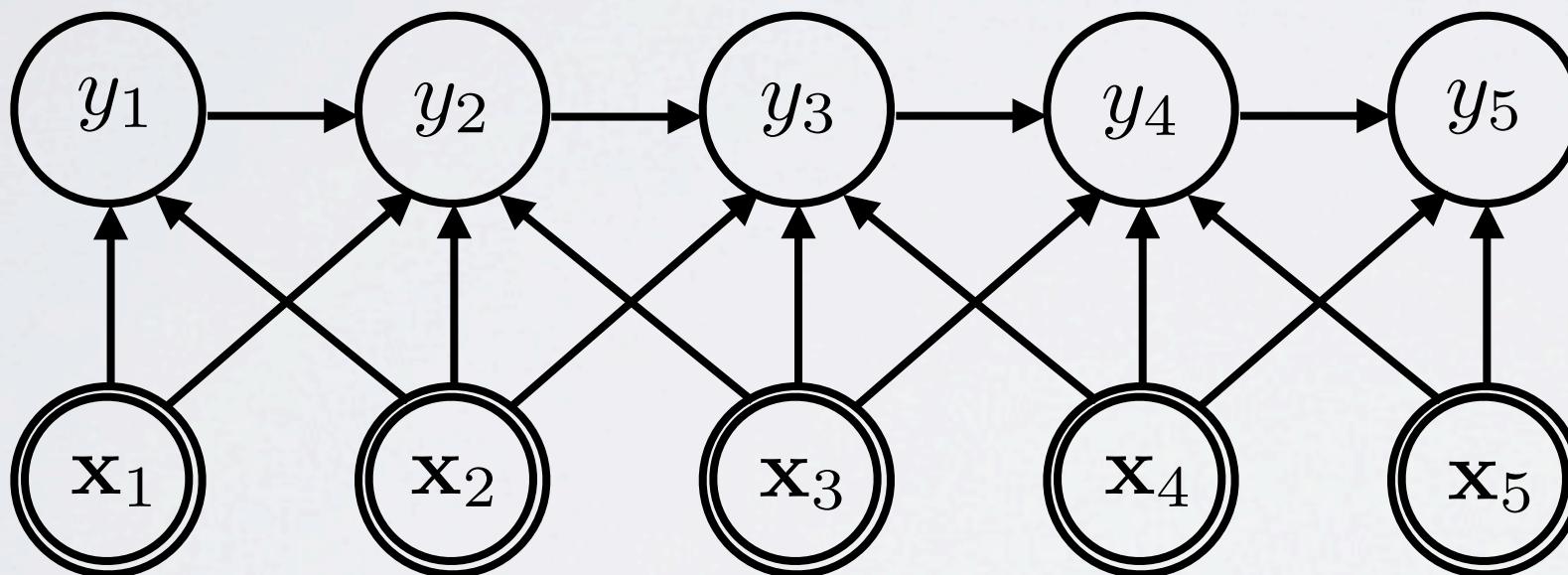
- Conditional random field are discriminatively trained, which should work better with more data
- Other alternative discriminatively trained sequence model?

MAXIMUM-ENTROPY MARKOV MODEL

Topics: MEMM

- MEMM is directed and discriminative:

 = observed



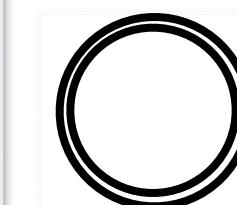
- ▶ it's a Markov model where the transition probabilities are given by logistic regressors (or neural networks):

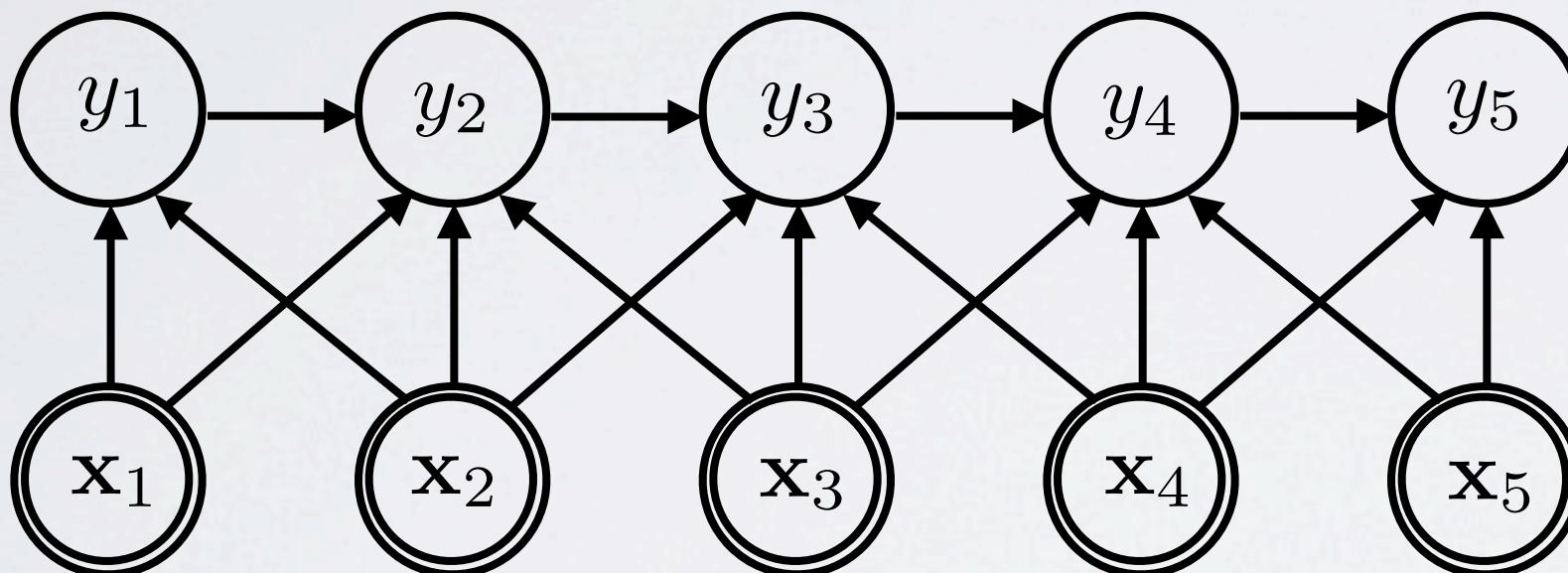
- $p(\mathbf{y}|\mathbf{X}) = \prod_{k=1}^K p(y_k|y_{k-1}, \mathbf{X})$
- $p(y_k|y_{k-1}, \mathbf{X}) = \frac{1}{Z(y_{k-1}, \mathbf{X})} \exp(a_u(y_k) + a_p(y_{k-1}, y_k))$

MAXIMUM-ENTROPY MARKOV MODEL

Topics: MEMM

- MEMM is directed and discriminative:

 = observed



- ▶ «label bias» problem: observations far away don't impact early predictions
 - example: $p(y_3|\mathbf{X}) = p(y_3|\mathbf{x}_1, \dots, \mathbf{x}_4)$
 - observations after \mathbf{x}_4 do not change our decision about y_3 !

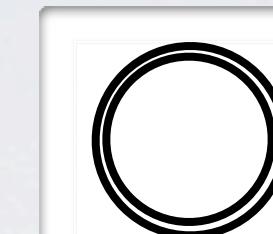
Neural networks

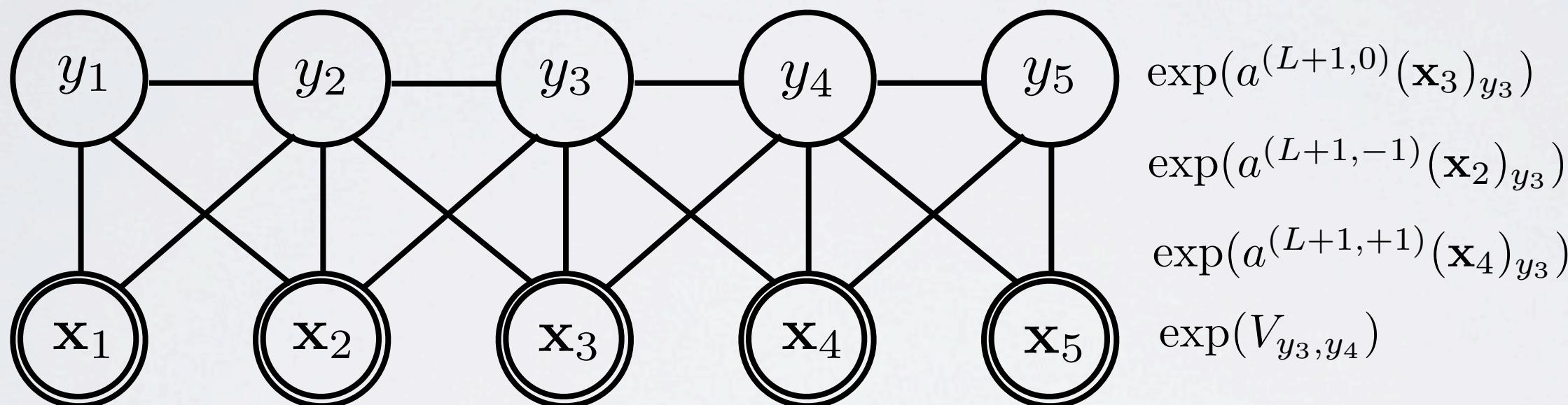
Training CRFs - hidden Markov model

LINEAR CHAN CRF

Topics: Markov network

- Illustration for $K=5$

 = observed

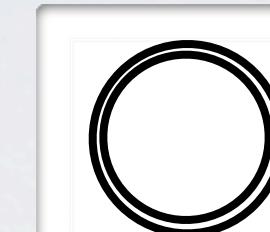


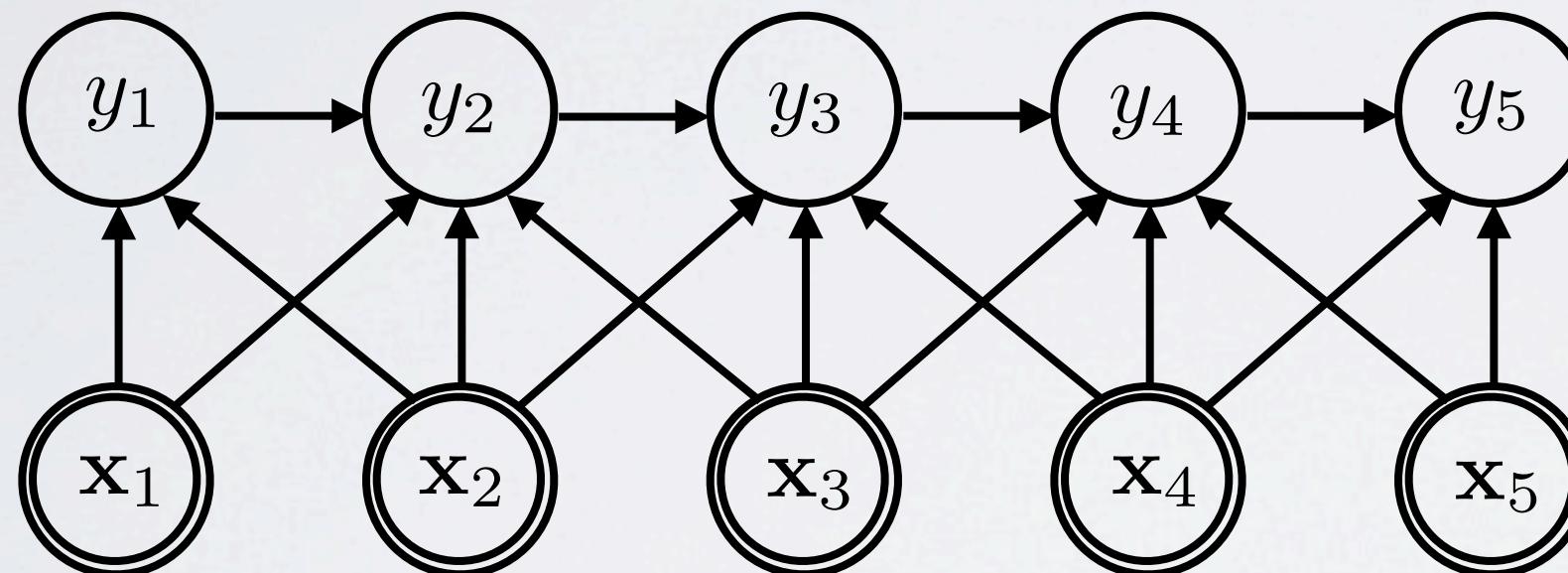
- Conditional random field are discriminatively trained, which should work better with more data
- Other alternative discriminatively trained sequence model?

MAXIMUM-ENTROPY MARKOV MODEL

Topics: MEMM

- MEMM is directed and discriminative:

 = observed

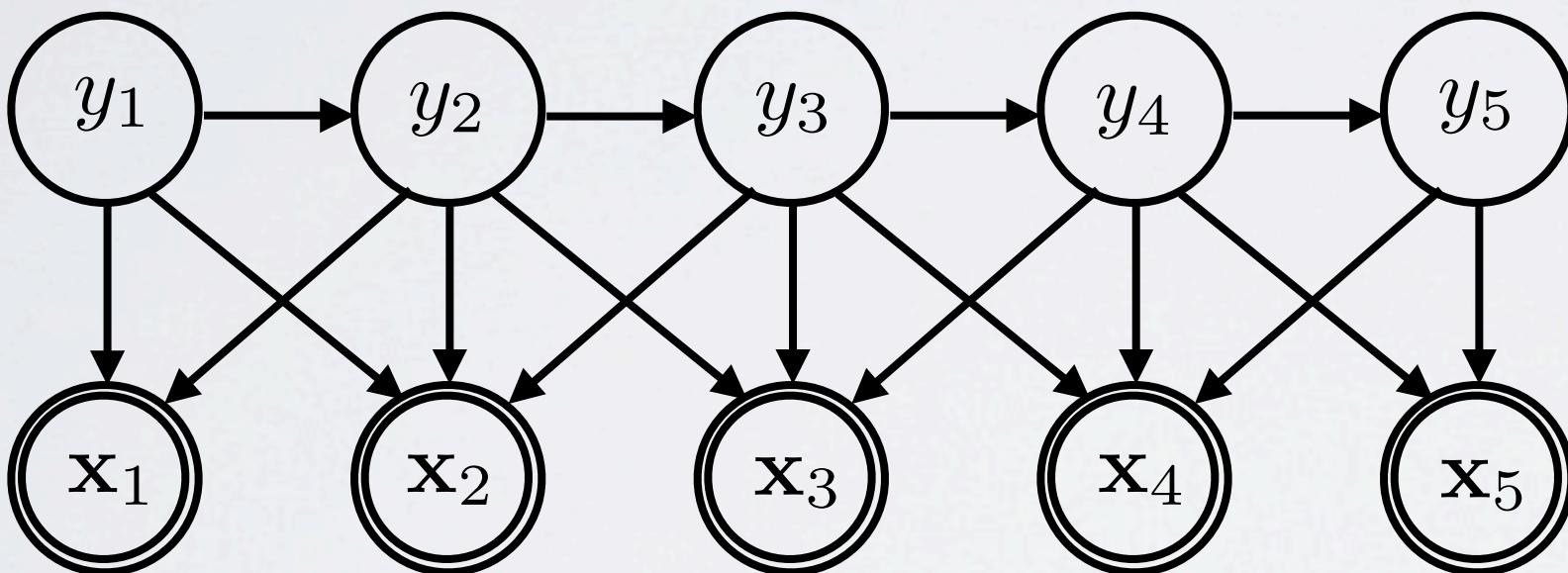
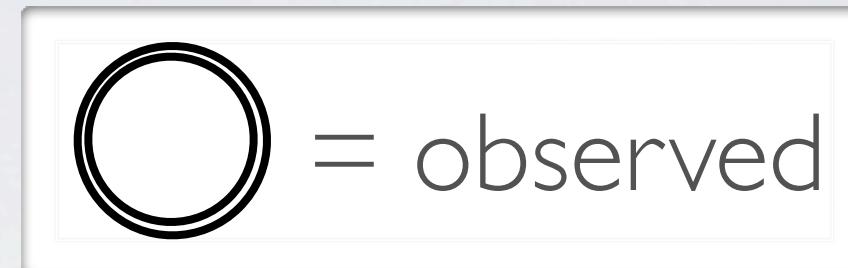


- ▶ «label bias» problem: observations far away don't impact early predictions
 - example: $p(y_3|\mathbf{X}) = p(y_3|\mathbf{x}_1, \dots, \mathbf{x}_4)$
 - observations after \mathbf{x}_4 do not change our decision about y_3 !

HIDDEN MARKOV MODEL

Topics: discriminative HMM

- HMMs can be trained discriminatively
(i.e. minimize $-\log p(\mathbf{y}|\mathbf{X})$)



- ▶ used a lot in speech recognition (called «maximum mutual information training»)
- ▶ we don't have the same label bias anymore
- ▶ however, optimization might be more complicated, since factors most correspond to normalized probabilities

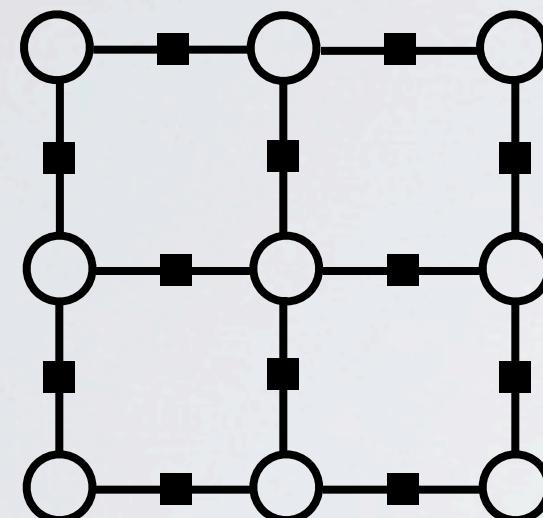
Neural networks

Training CRFs - general conditional random field

GENERAL CRF

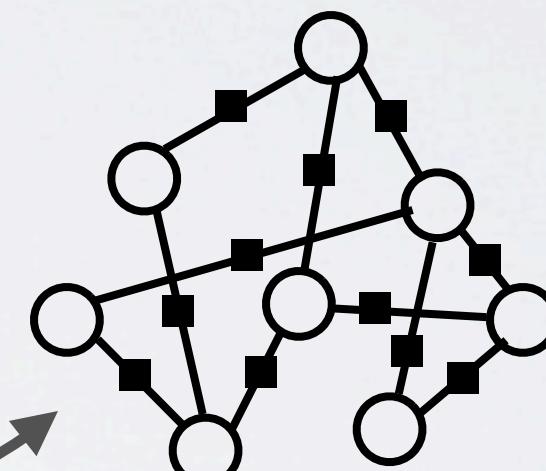
Topics: CRFs in general

- We don't have to restrict the CRF structure to linear chains



Grid structure
(pixels in image)

$$p(\mathbf{y}|\mathbf{X}) = \frac{1}{Z(\mathbf{X})} \prod_f \Psi_f(\mathbf{y}, \mathbf{X})$$



General pair-wise structure
(webpages sharing a link)

- We could also have n -ary factors, with $n > 2$

GENERAL CRF

Topics: CRFs in general

- Gradients in general CRFs always take the form:

$$\frac{\partial -\log p(\mathbf{y}^{(t)} | \mathbf{X}^{(t)})}{\partial \theta} = - \left(\overbrace{\sum_f \frac{\partial}{\partial \theta} \log \Psi_f(\mathbf{y}^{(t)}, \mathbf{X}^{(t)})}^{\text{make } y^{(t)} \text{ more likely}} \right. \\ \left. - \underbrace{\mathbb{E}_{\mathbf{y}} \left[\sum_f \frac{\partial}{\partial \theta} \log \Psi_f(\mathbf{y}, \mathbf{X}^{(t)}) \mid \mathbf{X}^{(t)} \right]}_{\text{make everything less likely}} \right)$$

- The expectation over \mathbf{y} will often need to be approximated, using loopy belief propagation
 - ▶ it will often involve only a few of the y_k variables

(LOOPY) BELIEF PROPAGATION

Topics: CRFs in general

- Marginals can be approximated with:

$$p(y_k | \mathbf{X}) = \frac{\exp(\log \phi_f(y_k) + \sum_{f' \in \text{Ne}(k) \setminus f} \log \mu_{f' \rightarrow k}(y_k))}{\sum_{y'_k} \exp(\log \phi_f(y'_k) + \sum_{f' \in \text{Ne}(k) \setminus f} \log \mu_{f' \rightarrow k}(y'_k))}$$

- In general, an approximated marginal is computed by
 1. summing all the log-factors that involve only the y_k variables of interest
 2. summing all the log-messages coming into the y_k variables from other factors
 3. exponentiating
 4. renormalizing

Neural networks

Training CRFs - pseudolikelihood

GENERAL CRF

Topics: CRFs in general

- Gradients in general CRFs always take the form:

$$\frac{\partial -\log p(\mathbf{y}^{(t)} | \mathbf{X}^{(t)})}{\partial \theta} = - \left(\overbrace{\sum_f \frac{\partial}{\partial \theta} \log \Psi_f(\mathbf{y}^{(t)}, \mathbf{X}^{(t)})}^{\text{make } y^{(t)} \text{ more likely}} \right. \\ \left. - \underbrace{\mathbb{E}_{\mathbf{y}} \left[\sum_f \frac{\partial}{\partial \theta} \log \Psi_f(\mathbf{y}, \mathbf{X}^{(t)}) \mid \mathbf{X}^{(t)} \right]}_{\text{make everything less likely}} \right)$$

- The expectation over \mathbf{y} will often need to be approximated, using loopy belief propagation
 - ▶ it will often involve only a few of the y_k variables

GENERAL CRF

Topics: pseudolikelihood

- Why not just change the loss function to a tractable one

$$-\sum_{k=1}^K \log p(y_k | y_1, \dots, y_{k-1}, y_{k+1}, \dots, y_K, \mathbf{X})$$

- ▶ predict, in turn, each y_k not just from \mathbf{X} , but also all the other elements of \mathbf{y}
- ▶ can compute the exact gradients
 - the probabilities only require normalizing y_k individually, like in a regular softmax
 - each conditional often only depend on few variables (local Markov property)
- ▶ however, often tends to work less well
- ▶ we still need to compute $p(y_k | \mathbf{X})$ to do predictions anyways