Training CRFs - loss function

### LINEAR CHAIN 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:  $a_p(y_k, y_{k+1}) = 1_{1 \le k < K} V_{y_k, y_{k+1}}$

## MACHINE LEARNING

#### Topics: empirical risk minimization, regularization

- Empirical risk minimization
  - framework to design learning algorithms

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

- $l(\mathbf{f}(\mathbf{X}^{(t)}; \boldsymbol{\theta}), \mathbf{y}^{(t)})$  is a loss function
- $m \Omega(m heta)$  is a regularizer (penalizes certain values of m heta )
- 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
  - ightharpoonup initialize  $oldsymbol{ heta}$
  - for N iterations
    - for each training example  $(\mathbf{X}^{(t)}, \mathbf{y}^{(t)})$   $\checkmark \ \Delta = -\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{X}^{(t)}; \boldsymbol{\theta}), \mathbf{y}^{(t)}) \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$  =  $\checkmark \ \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \ \Delta$ iteration over **all** examples
- To apply this algorithm to a CRF, we need
  - the loss function  $l(\mathbf{f}(\mathbf{X}^{(t)}; \boldsymbol{\theta}), \mathbf{y}^{(t)})$
  - lacktriangle a procedure to compute the parameter gradients  $abla_{m{ heta}}l(\mathbf{f}(\mathbf{X}^{(t)};m{ heta}),\mathbf{y}^{(t)})$
  - lack the regularizer  $\Omega(oldsymbol{ heta})$  (and the gradient  $abla_{oldsymbol{ heta}}\Omega(oldsymbol{ heta})$  )
  - initialization method

## LOSS FUNCTION

Topics: loss function for sequential classification with CRF

- CRF estimates  $p(\mathbf{y}|\mathbf{X})$ 
  - $oldsymbol{ iny}$  we could maximize the probabilities of  $oldsymbol{y}^{(t)}$  given  $oldsymbol{X}^{(t)}$  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  $\mathbf{y}$ 

Training CRFs - unary log-factor gradient

### MACHINE LEARNING

### Topics: stochastic gradient descent (SGD)

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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:

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

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

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

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

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$$= -\left( 1_{y_k = y_k'} - \frac{\partial}{\partial a_u(y_k')} \log Z(\mathbf{X}) \right)$$

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$$= \frac{1}{Z(\mathbf{X})} \frac{\partial}{\partial a_{u}(y_{k}')} \sum_{y_{1}''} \sum_{y_{2}''} \cdots \sum_{y_{K}''} \exp \left( \sum_{k=1}^{K} a_{u}(y_{k}'') + \sum_{k=1}^{K-1} a_{p}(y_{k}'', y_{k+1}'') \right)$$

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$$\frac{\partial}{\partial a_{u}(y'_{k})} \log Z(\mathbf{X}) = \frac{1}{Z(\mathbf{X})} \frac{\partial}{\partial a_{u}(y'_{k})} Z(\mathbf{X})$$

$$= \frac{1}{Z(\mathbf{X})} \frac{\partial}{\partial a_{u}(y'_{k})} \sum_{y''_{1}} \sum_{y''_{2}} \cdots \sum_{y''_{K}} \exp\left(\sum_{k=1}^{K} a_{u}(y''_{k}) + \sum_{k=1}^{K-1} a_{p}(y''_{k}, y''_{k+1})\right)$$

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$$= \frac{1}{Z(\mathbf{X})} \sum_{y''_{1}} \sum_{y''_{2}} \cdots \sum_{y''_{K}} 1_{y'_{k} = y''_{k}} \exp\left(\sum_{k=1}^{K} a_{u}(y''_{k}) + \sum_{k=1}^{K-1} a_{p}(y''_{k}, y''_{k+1})\right)$$

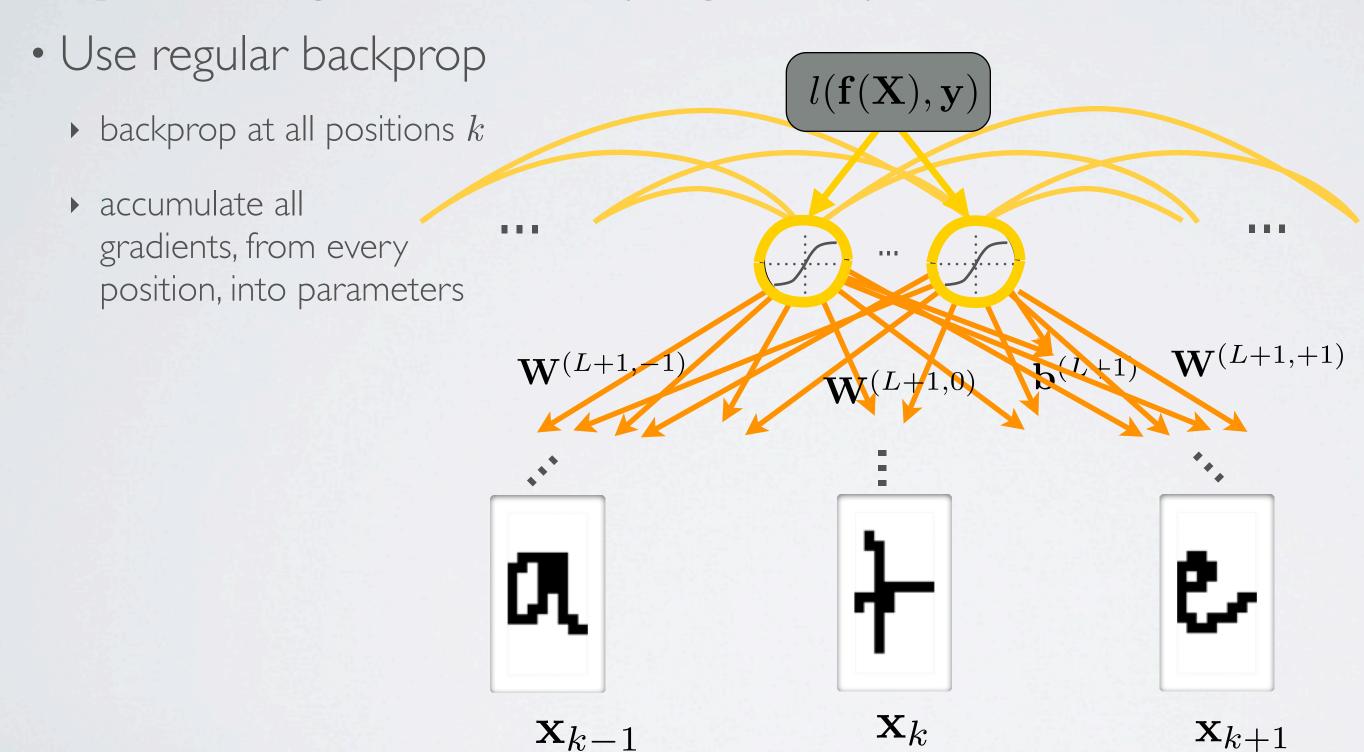
$$= \sum_{y''_{1}} \sum_{y''_{2}} \cdots \sum_{y''_{K}} 1_{y'_{k} = y''_{k}} p(y''_{1}, \dots, y''_{K} | \mathbf{X})$$

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

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= \sum_{y''_{1}} \sum_{y''_{2}} \cdots \sum_{y''_{K}} 1_{y'_{k} = y''_{k}} p(y''_{1}, \dots, y''_{K} | \mathbf{X}) 
= p(y'_{k} | \mathbf{X})$$

Topics: loss gradient at unary log-factor parameters



Topics: loss gradient at unary log-factor parameters

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

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

Topics: loss gradient at unary log-factor parameters

- For linear log-factors:
  - the gradients are:

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

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

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

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

Training CRFs - pairwise log-factor gradient

### MACHINE LEARNING

### Topics: stochastic gradient descent (SGD)

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  - initialization method

matrix of all pairwise

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

$$\nabla_{\mathbf{V}} - \log p(\mathbf{y}|\mathbf{X}) = \sum_{k=1}^{K-1} -(\mathbf{e}(y_k) \mathbf{e}(y_{k+1})^{\top} - \mathbf{p}(y_k, y_{k+1}|\mathbf{X}))$$
marginal probabilities

matrix of all pairwise label frequencies 
$$= -\left(\underbrace{\operatorname{freq}(y_k,y_{k+1})}_{\text{label frequencies}} - \sum_{k=1}^{K-1} \mathbf{p}(y_k,y_{k+1}|\mathbf{X})\right)$$

### 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
- ullet We could scale  $\lambda$  by the sequence size

• With the loss and regularization gradients, we have all the ingredients to perform stochastic gradient descent

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:



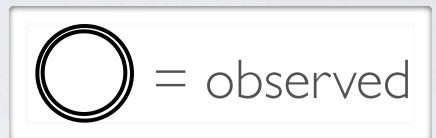
- See these papers for more details:
  - On Discriminative vs. Generative classifiers: A comparison of logistic regression and naive Bayes. Andrew Ng and Michael Jordan, 2001

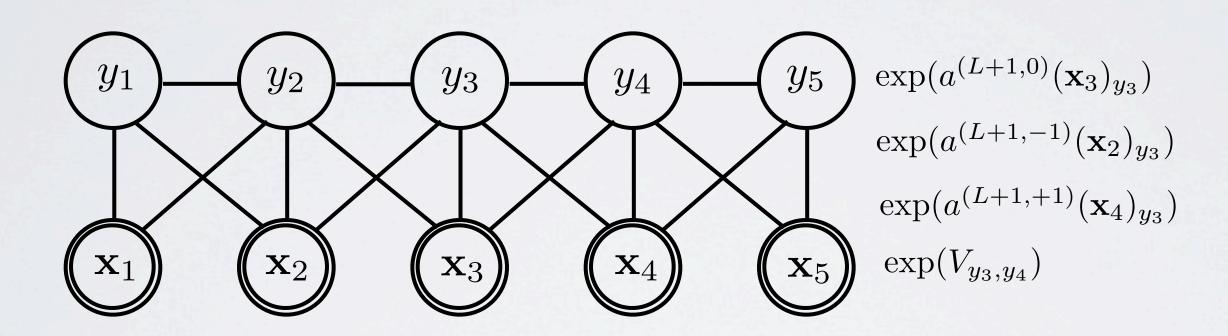
Training CRFs - maximum-entropy Markov model

## LINEAR CHAIN CRF

#### Topics: Markov network

• Illustration for K=5



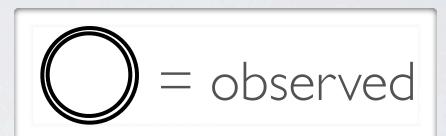


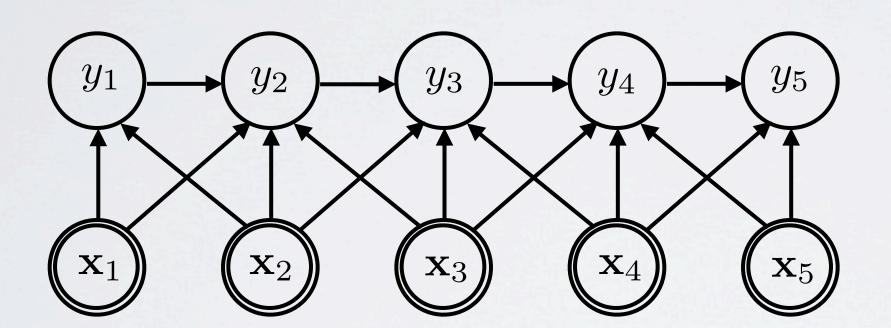
- Conditional random field are discriminatively trained, which should work better with more data
- Other alternative discriminatively trained sequence model?

## MAXIMUM-ENTROPY MARKOV MODEL

#### Topics: MEMM

MEMM is directed and discriminative:



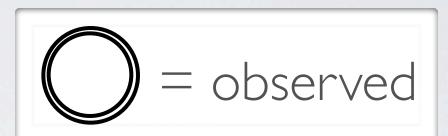


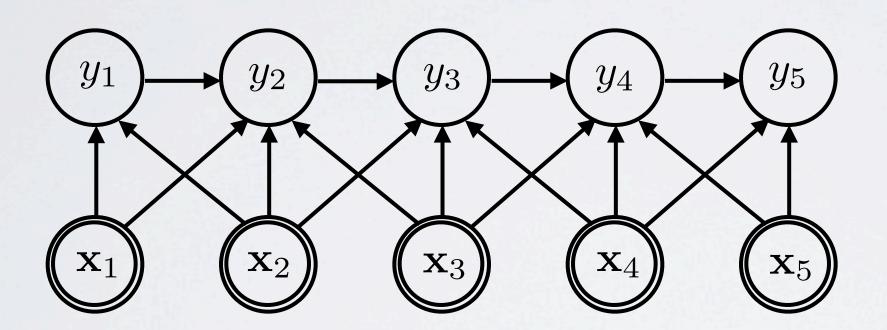
- it's a Markov model where the transition probabilities are given by logistic regressors (or neural networks):
  - $p(\mathbf{y}|\mathbf{X}) = \prod_{k=1}^{K} p(y_k|y_{k-1}, \mathbf{X})$
  - $p(y_k|y_{k-1}, \mathbf{X}) = \frac{1}{Z(y_{k-1}, \mathbf{X})} \exp\left(a_u(y_k) + a_p(y_{k-1}, y_k)\right)$

## MAXIMUM-ENTROPY MARKOV MODEL

#### Topics: MEMM

MEMM is directed and discriminative:





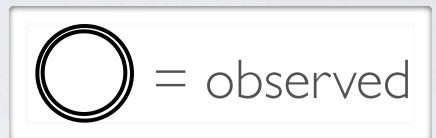
- «label bias» problem: observations far away don't impact early predictions
  - example:  $p(y_3|\mathbf{X}) = p(y_3|\mathbf{x}_1, \dots, \mathbf{x}_4)$
  - observations after  $\mathbf{x}_4$  do not change our decision about  $y_3!$

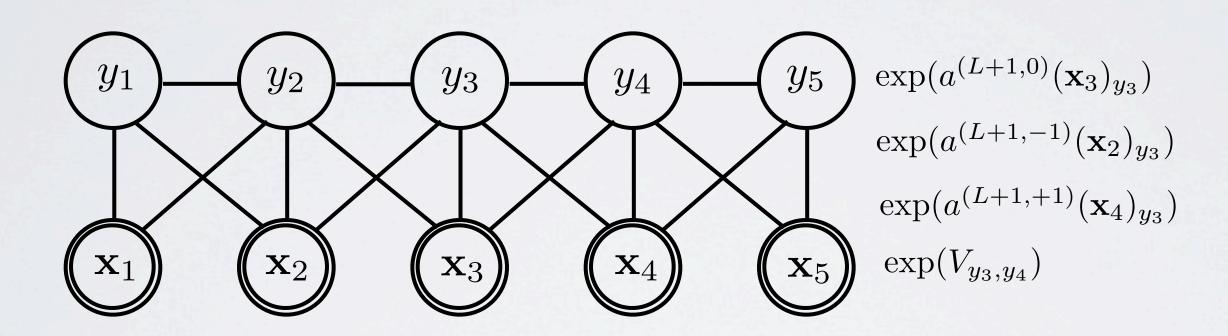
Training CRFs - hidden Markov model

## LINEAR CHAIN CRF

#### Topics: Markov network

• Illustration for K=5



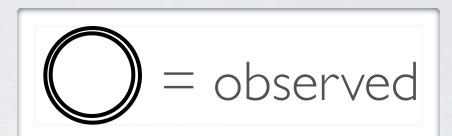


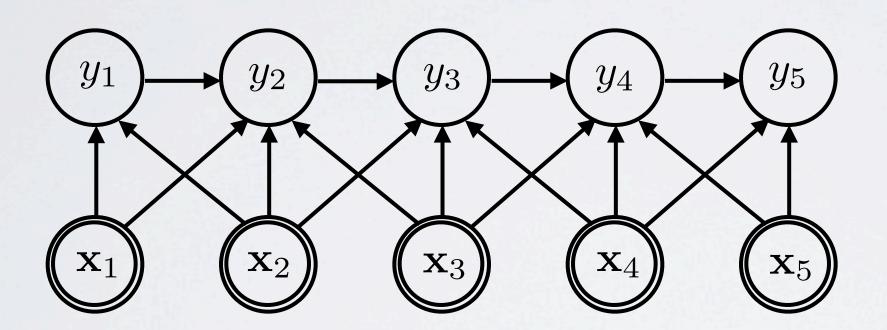
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## MAXIMUM-ENTROPY MARKOV MODEL

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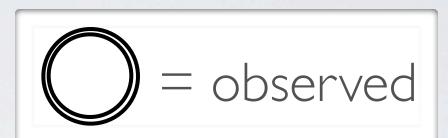


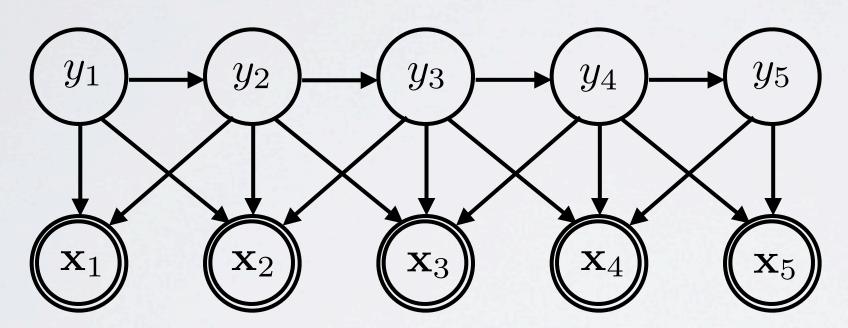
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## HIDDEN MARKOV MODEL

#### Topics: discriminative HMM

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





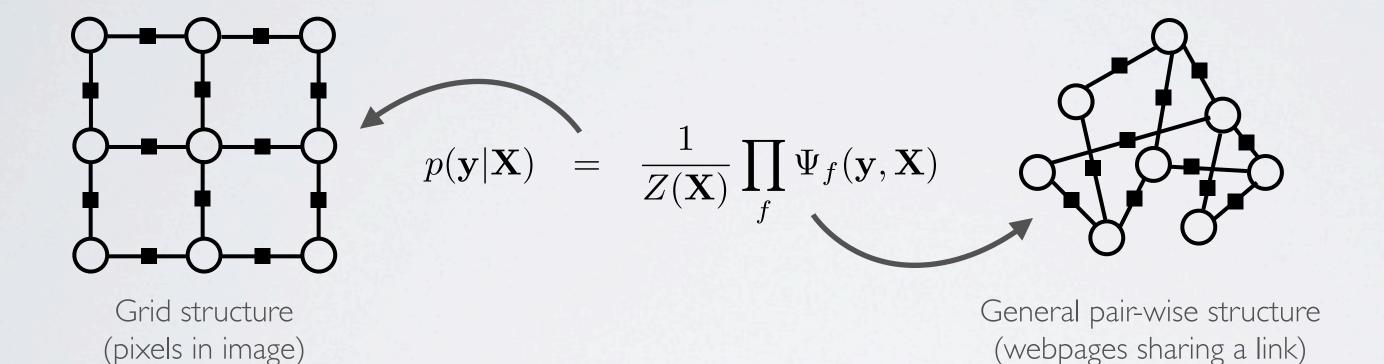
- used a lot in speech recognition (called «maximum mutual information training»)
- we don't have the same label bias anymore
- however, optimization might be more complicated, since factors most correspond to normalized probabilities

Training CRFs - general conditional random field

## GENERAL CRF

#### Topics: CRFs in general

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



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

### GENERAL CRF

#### Topics: CRFs in general

• Gradients in general CRFs always take the form:

make 
$$y^{(t)}$$
 more likely

$$\frac{\partial -\log p(\mathbf{y}^{(t)}|\mathbf{X}^{(t)})}{\partial \theta} = -\left(\sum_{f} \frac{\partial}{\partial \theta} \log \Psi_f(\mathbf{y}^{(t)}, \mathbf{X}^{(t)})\right)$$

$$- \operatorname{E}_{\mathbf{y}} \left[ \sum_{f} \frac{\partial}{\partial \theta} \log \Psi_{f}(\mathbf{y}, \mathbf{X}^{(t)}) \left| \mathbf{X}^{(t)} \right] \right)$$

make everything less likely

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

# (LOOPY) BELIEF PROPAGATION

#### Topics: CRFs in general

• Marginals can be approximated with:

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

- In general, an approximated marginal is computed by
  - I. 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

Training CRFs - pseudolikelihood

### GENERAL CRF

#### Topics: CRFs in general

• Gradients in general CRFs always take the form:

make 
$$y^{(t)}$$
 more likely

$$\frac{\partial -\log p(\mathbf{y}^{(t)}|\mathbf{X}^{(t)})}{\partial \theta} = -\left(\sum_{f} \frac{\partial}{\partial \theta} \log \Psi_f(\mathbf{y}^{(t)}, \mathbf{X}^{(t)})\right)$$

$$- \operatorname{E}_{\mathbf{y}} \left[ \sum_{f} \frac{\partial}{\partial \theta} \log \Psi_{f}(\mathbf{y}, \mathbf{X}^{(t)}) \left| \mathbf{X}^{(t)} \right] \right)$$

make everything less likely

- The expectation over  $\mathbf{y}$  will often need to be approximated, using loopy belief propagation
  - ightharpoonup 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

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

- lacktriangle predict, in turn, each  $y_k$  not just from  ${f X}$ , but also all the other elements of  ${f y}$
- 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