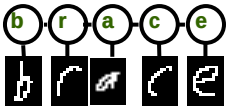
Advanced Machine Learning

Learning Graphical Models

Max-margin learning of GM

Eric Xing

Lecture 16, August 13, 2009



Reading:

Structured Prediction Problem

- Unstructured prediction

$$\mathbf{x} = \begin{pmatrix} x_{11} & x_{12} & \cdots \\ x_{21} & x_{22} & \cdots \\ \vdots & \vdots & \cdots \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \end{pmatrix}$$

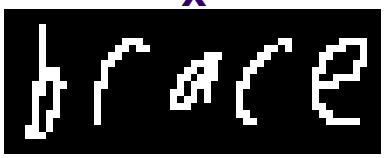
- Structured prediction
  - Part of speech tagging

    $\mathbf{x}$ = "Do you want sugar in it?" $\Rightarrow$ $\mathbf{y}$ =<verb pron verb noun prep pron>
  - Image segmentation

$$\mathbf{x} = \begin{pmatrix} x_{11} & x_{12} & \cdots \\ x_{21} & x_{22} & \cdots \\ \vdots & \vdots & \cdots \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} y_{11} & y_{12} & \cdots \\ y_{21} & y_{22} & \cdots \\ \vdots & \vdots & \cdots \end{pmatrix}$$

OCR example

x



y

brace

Sequential structure

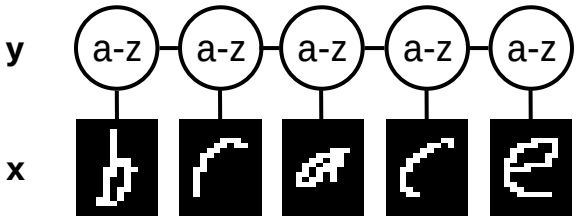
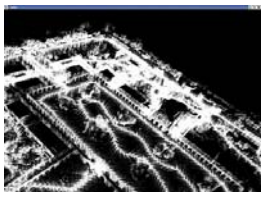
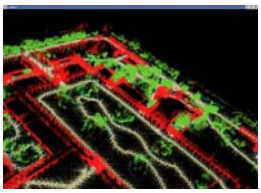


Image segmentation example

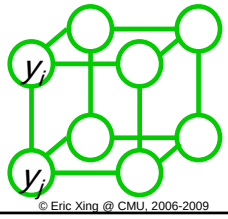
x



y



Spatial structure



Classical Predictive Models

- Inputs:
  - a set of training samples and $\mathcal{D} = \{(\mathbf{x}^i, y^i)\}_{i=1}^N$ $\quad \mathbf{x}^i = [x_1^i, x_2^i, \cdots, x_d^i]^\top$ $\quad y^i \in C \triangleq \{c_1, c_2, \cdots, c_L\}$
- Outputs:
  - a predictive function $h(\mathbf{x})$ $\quad y^\star = h(\mathbf{x}) \triangleq \arg\max_y F(\mathbf{x}, y; \mathbf{w})$
- Examples: $F(\mathbf{x}, y; \mathbf{w}) = g(\mathbf{w}^\top \mathbf{f}(\mathbf{x}, y))$

– Logistic Regression, Bayes classifiers
  - Max-likelihood estimation

E.g.: $\max_{\mathbf{w}} \mathcal{L}(\mathcal{D}; \mathbf{w}) \triangleq \sum_{i=1}^N \log p(y^i|\mathbf{x}^i)$

$$p(y|\mathbf{x}) = \frac{\exp\{\mathbf{w}^\top \mathbf{f}(\mathbf{x}, y)\}}{\sum_{y'} \exp\{\mathbf{w}^\top \mathbf{f}(\mathbf{x}, y')\}}$$

Advantages:
1.Full probabilistic semantics
2.Straightforward Bayesian or direct regularization
3.Hidden structures or generative hierarchy

– Support Vector Machines (SVM)
  - Max-margin learning

$$\min_{\mathbf{w},\xi} \frac{1}{2}\mathbf{w}^\top \mathbf{w} + C\sum_{i=1}^N \xi_i;$$
$$\text{s.t. } \mathbf{w}^\top \Delta\mathbf{f}_i(y) \geq 1 - \xi_i, \ \forall i, \forall y \neq y^i.$$

Advantages:
1.Dual sparsity: few support vectors
2.Kernel tricks
3.Strong empirical results

Structured Prediction Models

- Conditional Random Fields (CRFs) (Lafferty et al 2001)
  - Based on Logistic Regression
  - Max-likelihood estimation (point-estimate)

$$\max_{\mathbf{w}} \mathcal{L}(\mathcal{D}; \mathbf{w}) \triangleq \sum_{i=1}^N \log p(\mathbf{y}^i|\mathbf{x}^i)$$

$$p(\mathbf{y}|\mathbf{x}) = \frac{\exp\{\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y})\}}{\sum_{\mathbf{y}'} \exp\{\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}')\}}$$

- Max-margin Markov Networks (M^3Ns) (Taskar et al 2003)
  - Based on SVM
  - Max-margin learning (point-estimate)

$$\text{P0 } (M^3N): \min_{\mathbf{w},\xi} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^N \xi_i$$
$$\text{s.t. } \forall i, \forall \mathbf{y} \neq \mathbf{y}^i : \mathbf{w}^\top \Delta\mathbf{f}_i(\mathbf{y}) \geq \Delta\ell_i(\mathbf{y}) - \xi_i, \ \xi_i \geq 0 \ ,$$

where $\mathbf{w}^\top \Delta\mathbf{f}_i(\mathbf{y}|\mathbf{x}_i)$ denotes the margin and $\Delta\ell_i(\mathbf{y})$ is a loss function.

Structured models

$$h(\mathbf{x}) = \arg\max_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \; s(\mathbf{x}, \mathbf{y})$$

← scoring function

↑ space of feasible outputs

Assumptions:

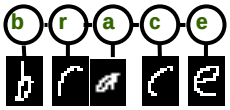
$$score(\mathbf{x}, \mathbf{y}) = \mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}) = \sum_p \mathbf{w}^\top \mathbf{f}(\mathbf{x}_p, \mathbf{y}_p)$$

linear combination of features

sum of part scores:
- index *p* represents a part in the structure

Learning w

- Training examples $(\mathbf{x}_i, \mathbf{y}_i)$



- Probabilistic approach:

$$P_{\mathbf{w}}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z_{\mathbf{w}}(\mathbf{x})} \exp\{\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y})\}$$

- Computing $Z_w(x)$ can be NP-complete
  - Tractable models but intractable estimation
- Large margin approach:
  - Exact and efficient when prediction is tractable

Learning Strategy

- Recall that in CRF
  - We predict based on:

$$y^* \mid x = \arg\max_y p_\theta(y \mid x) = \frac{1}{Z(\theta, x)} \exp\left\{\sum_c \theta_c f_c(x, y_c)\right\}$$

  - And we learn based on:

$$\theta_c^* \mid \{y_n, x_n\} = \arg\max_{\theta_c} \prod_n p_\theta(y_n \mid x_n) = \prod_n \frac{1}{Z(\theta, x_n)} \exp\left\{\sum_c \theta_c f_c(x_n, y_{n,c})\right\}$$

- Max-Margin:
  - We predict based on:

$$y^* \mid x = \arg\max_y \sum_c \theta_c f_c(x, y_c) = \arg\max_y w^T F(x, y)$$

  - And we learn based on:

$$w^* \mid \{y_n, x_n\} = \arg\max_w \left(\max_{y'_n \neq y_n, \forall n} w^T \left(F(y_n, x_n) - F(y'_n, x_n)\right)\right)$$

MLE of Feature Based UGMs

- Scaled likelihood function

$$\tilde{\ell}(\theta; D) = \ell(\theta; D)/N = \frac{1}{N}\sum_n \log p(x_n \mid \theta)$$
$$= \sum_x \tilde{p}(x) \log p(x \mid \theta)$$
$$= \sum_x \tilde{p}(x) \sum_i \theta_i f_i(x) - \log Z(\theta)$$

- Instead of optimizing this objective directly, we attack its lower bound
  - The logarithm has a linear upper bound …

$$\log Z(\theta) \leq \mu Z(\theta) - \log \mu - 1$$

  - This bound holds for all μ, in particular, for $\mu = Z^{-1}(\theta^{(t)})$

  - Thus we have

$$\tilde{\ell}(\theta; D) \geq \sum_x \tilde{p}(x) \sum_i \theta_i f_i(x) - \frac{Z(\theta)}{Z(\theta^{(t)})} - \log Z(\theta^{(t)}) + 1$$

Generalized Iterative Scaling (GIS)

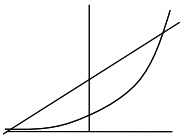
- Lower bound of scaled loglikelihood

$$\tilde{\ell}(\theta;D) \geq \sum_x \tilde{p}(x)\sum_i \theta_i f_i(x) - \frac{Z(\theta)}{Z(\theta^{(t)})} - \log Z(\theta^{(t)}) + 1$$

- Define $\Delta\theta_i^{(t)} \overset{\text{def}}{=} \theta_i - \theta_i^{(t)}$

$$\begin{aligned}\tilde{\ell}(\theta;D) &\geq \sum_x \tilde{p}(x)\sum_i \theta_i f_i(x) - \frac{1}{Z(\theta^{(t)})}\sum_x \exp\left\{\sum_i \theta_i f_i(x)\right\} - \log Z(\theta^{(t)}) + 1 \\ &= \sum_i \theta_i \sum_x \tilde{p}(x) f_i(x) - \frac{1}{Z(\theta^{(t)})}\sum_x \exp\left\{\sum_i \theta_i^{(t)} f_i(x)\right\}\exp\left\{\sum_i \Delta\theta_i^{(t)} f_i(x)\right\} - \log Z(\theta^{(t)}) + 1 \\ &= \sum_i \theta_i \sum_x \tilde{p}(x) f_i(x) - \sum_x p(x\,|\,\theta^{(t)})\exp\left\{\sum_i \Delta\theta_i^{(t)} f_i(x)\right\} - \log Z(\theta^{(t)}) + 1\end{aligned}$$

- Relax again
  - Assume $f_i(x) \geq 0, \quad \sum_i f_i(x) = 1$
  - Convexity of exponential: $\exp\left(\sum_i \pi_i x_i\right) \leq \sum_i \pi_i \exp(x_i)$



- We have:

$$\tilde{\ell}(\theta;D) \geq \sum_i \theta_i \sum_x \tilde{p}(x) f_i(x) - \sum_x p(x\,|\,\theta^{(t)})\sum_i f_i(x)\exp\left(\Delta\theta_i^{(t)}\right) - \log Z(\theta^{(t)}) + 1 \overset{\text{def}}{=} \Lambda(\theta)$$

GIS

- Lower bound of scaled loglikelihood

$$\tilde{\ell}(\theta;D) \geq \sum_i \theta_i \sum_x \tilde{p}(x) f_i(x) - \sum_x p(x\,|\,\theta^{(t)})\sum_i f_i(x)\exp\left(\Delta\theta_i^{(t)}\right) - \log Z(\theta^{(t)}) + 1 \overset{\text{def}}{=} \Lambda(\theta)$$

- Take derivative: $\frac{\partial\Lambda}{\partial\theta_i} = \sum_x \tilde{p}(x) f_i(x) - \exp\left(\Delta\theta_i^{(t)}\right)\sum_x p(x\,|\,\theta^{(t)}) f_i(x)$
- Set to zero

$$e^{\Delta\theta_i^{(t)}} = \frac{\sum_x \tilde{p}(x) f_i(x)}{\sum_x p(x\,|\,\theta^{(t)}) f_i(x)} = \frac{\sum_x \tilde{p}(x) f_i(x)}{\sum_x p^{(t)}(x) f_i(x)} Z(\theta^{(t)})$$

  - where $p^{(t)}(x)$ is the unnormalized version of $p(x|\theta^{(t)})$

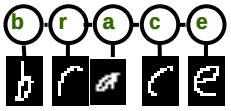
- Update

$$\theta_i^{(t+1)} = \theta_i^{(t)} + \Delta\theta_i^{(t)} \Rightarrow p^{(t+1)}(x) = p^{(t)}(x) e^{\Delta\theta_i^{(t)} f_i(x)}$$

$$\begin{aligned}p^{(t+1)}(x) &= \frac{p^{(t)}(x)}{Z(\theta^{(t)})}\prod_i \left(\frac{\sum_x \tilde{p}(x) f_i(x)}{\sum_x p^{(t)}(x) f_i(x)} Z(\theta^{(t)})\right)^{f_i(x)} \\ \Rightarrow \quad &= \frac{p^{(t)}(x)}{Z(\theta^{(t)})}\prod_i \left(\frac{\sum_x \tilde{p}(x) f_i(x)}{\sum_x p^{(t)}(x) f_i(x)}\right)^{f_i(x)} \left(Z(\theta^{(t)})\right)^{\sum_i f_i(x)} \\ &= p^{(t)}(x)\prod_i \left(\frac{\sum_x \tilde{p}(x) f_i(x)}{\sum_x p^{(t)}(x) f_i(x)}\right)^{f_i(x)}\end{aligned}$$

Learning w

- Training examples $(\mathbf{x}_i, \mathbf{y}_i)$



- Probabilistic approach:

$$P_{\mathbf{w}}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z_{\mathbf{w}}(\mathbf{x})} \exp\{\mathbf{w}^{\top}\mathbf{f}(\mathbf{x}, \mathbf{y})\}$$

- Computing $Z_{\mathbf{w}}(\mathbf{x})$ can be NP-complete
  - Tractable models but intractable estimation
- Large margin approach:
  - Exact and efficient when prediction is tractable

OCR Example

- We want:

  argmax$_{\text{word}}$ $\mathbf{w}^{\top}\mathbf{f}($  , **word**$) =$ **"brace"**

- Equivalently:

  $\mathbf{w}^{\top}\mathbf{f}($  ,**"brace"**$) > \mathbf{w}^{\top}\mathbf{f}($  ,**"aaaaa"**$)$

  $\mathbf{w}^{\top}\mathbf{f}($  ,**"brace"**$) > \mathbf{w}^{\top}\mathbf{f}($  ,**"aaaab"**$)$

  ...

  $\mathbf{w}^{\top}\mathbf{f}($  ,**"brace"**$) > \mathbf{w}^{\top}\mathbf{f}($  ,**"zzzzz"**$)$

a lot!

Large Margin Estimation

- Given training example (**x**, **y***), we want:

$$\arg\max_{\mathbf{y}} \mathbf{w}^\top \mathbf{f}(\mathbf{x},\mathbf{y}) = \mathbf{y}^*$$

$$\mathbf{w}^\top \mathbf{f}(\mathbf{x},\mathbf{y}^*) > \mathbf{w}^\top \mathbf{f}(\mathbf{x},\mathbf{y}) \quad \forall \mathbf{y} \neq \mathbf{y}^*$$

$$\mathbf{w}^\top \mathbf{f}(\mathbf{x},\mathbf{y}^*) \geq \mathbf{w}^\top \mathbf{f}(\mathbf{x},\mathbf{y}) + \gamma\, \ell(\mathbf{y}^*,\mathbf{y}) \quad \forall \mathbf{y}$$

- Maximize margin γ
- Mistake weighted margin: $\gamma \ell(\mathbf{y}^*,\mathbf{y})$

$\ell(\mathbf{y}^*,\mathbf{y}) = \sum_i I(y_i^* \neq y_i)$ # of mistakes in **y**

*Taskar et al. 03

Large Margin Estimation

- Recall from SVMs:
  - Maximizing margin γ is equivalent to minimizing the square of the L2-norm of the weight vector **w**:
- New objective function:

$$\min_{\mathbf{w}} \quad \frac{1}{2}||\mathbf{w}||^2$$
$$s.t.\ \mathbf{w}^\top \mathbf{f}(\mathbf{x}_i,\mathbf{y}_i) \geq \mathbf{w}^\top \mathbf{f}(\mathbf{x}_i,\mathbf{y}_i') + \ell(\mathbf{y}_i,\mathbf{y}_i'), \quad \forall i, \mathbf{y}_i' \in \mathcal{Y}_i$$

Min-max Formulation

- Brute force enumeration of constraints:

$$\min \quad \frac{1}{2}||\mathbf{w}||^2$$
$$\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}^*) \geq \mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}) + \ell(\mathbf{y}^*, \mathbf{y}), \quad \forall \mathbf{y}$$

  - The constraints are exponential in the size of the structure
- Alternative: min-max formulation
  - add only the most violated constraint

$$\mathbf{y}' = \arg\max_{\mathbf{y} \neq \mathbf{y}^*} [\mathbf{w}^\top \mathbf{f}(\mathbf{x}^i, \mathbf{y}) + \ell(\mathbf{y}^i, \mathbf{y})]$$
$$\text{add to QP}: \ \mathbf{w}^\top \mathbf{f}(\mathbf{x}^i, \mathbf{y}^i) \geq \mathbf{w}^\top \mathbf{f}(\mathbf{x}^i, \mathbf{y}') + \ell(\mathbf{y}^i, \mathbf{y}')$$

  - Handles more general loss functions
  - Only polynomial # of constraints needed

Min-max formulation

$$\min \quad \frac{1}{2}||\mathbf{w}||^2$$
$$\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}^*) \geq \max_{\mathbf{y} \neq \mathbf{y}^*} \ \mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}) + \ell(\mathbf{y}^*, \mathbf{y})$$

- Key step: convert the maximization in the constraint from discrete to continuous
  - This enables us to plug it into a QP

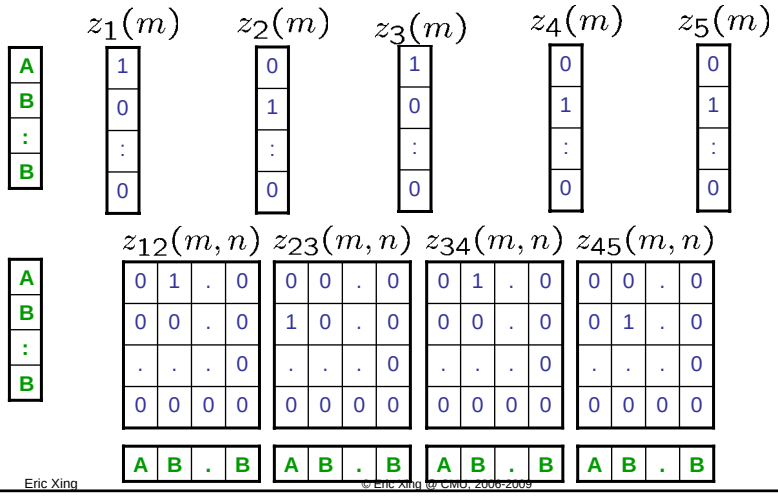
$$\max_{\mathbf{y} \neq \mathbf{y}^*} \ \mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}) + \ell(\mathbf{y}^*, \mathbf{y}) \iff \max_{\mathbf{z} \in \mathcal{Z}} \ (\mathbf{F}^\top \mathbf{w} + \ell)^\top \mathbf{z}$$

discrete optim. ⟺ continuous optim.

- How to do this conversion?
  - Linear chain example in the next slides →

y ⇒ z map for linear chain structures

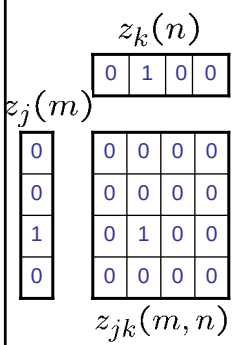
OCR example: y = 'ABABB';
z's are the indicator variables for the corresponding classes (alphabet)



y ⇒ z map for linear chain structures

Rewriting the maximization function in terms of indicator variables:

$$\max_{\mathbf{z}} \sum_{j,m} z_j(m)\left[\mathbf{w}^\top \mathbf{f}_{\text{node}}(\mathbf{x}_j, m) + \ell_j(m)\right] + \sum_{jk,m,n} z_{jk}(m,n)\left[\mathbf{w}^\top \mathbf{f}_{\text{edge}}(\mathbf{x}_{jk}, m, n) + \ell_{jk}(m,n)\right] \Big\} (\mathbf{F}^\top \mathbf{w} + \ell)^\top \mathbf{z}$$



$z_j(m) \geq 0;\ z_{jk}(m,n) \geq 0;$

normalization $\sum_m z_j(m) = 1$

agreement $\sum_n z_{jk}(m,n) = z_j(m)$

$\Big\} \mathbf{A}\mathbf{z} = \mathbf{b}$

$$\max_{A\mathbf{z}=\mathbf{b}} (\mathbf{F}^\top \mathbf{w} + \ell)^\top \mathbf{z}$$

Min-max formulation

- Original problem:

$$\min \quad \frac{1}{2}||\mathbf{w}||^2$$
$$\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}^*) \geq \max_{\mathbf{y}} \ \mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}) + \ell(\mathbf{y}^*, \mathbf{y})$$

- Transformed problem:

$$\min \quad \frac{1}{2}||\mathbf{w}||^2$$
$$\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}^*) \geq \max_{\mathbf{z}\geq 0;\ \mathbf{A}\mathbf{z}=\mathbf{b};} \mathbf{q}^\top \mathbf{z} \quad \text{where } \mathbf{q}^\top = \mathbf{w}^\top \mathbf{F} + \ell^\top$$

  - Has integral solutions **z** for chains, trees
  - Can be fractional for untriangulated networks

Min-max formulation

- Using strong Lagrangian duality:
  (beyond the scope of this lecture)

$$\max_{\mathbf{z}\geq 0;\ \mathbf{A}\mathbf{z}=\mathbf{b};} \mathbf{q}^\top \mathbf{z} \ = \ \min_{\mathbf{A}^\top \mu \geq \mathbf{q}} \mathbf{b}^\top \mu$$

- Use the result above to minimize jointly over **w** and μ:

$$\min_{\mathbf{w},\mu} \ \frac{1}{2}||\mathbf{w}||^2$$
$$\text{s.t.} \ \ \mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}^*) \geq \mathbf{b}^\top \mu;$$
$$\mathbf{A}^\top \mu \geq \mathbf{q};$$

Min-max formulation

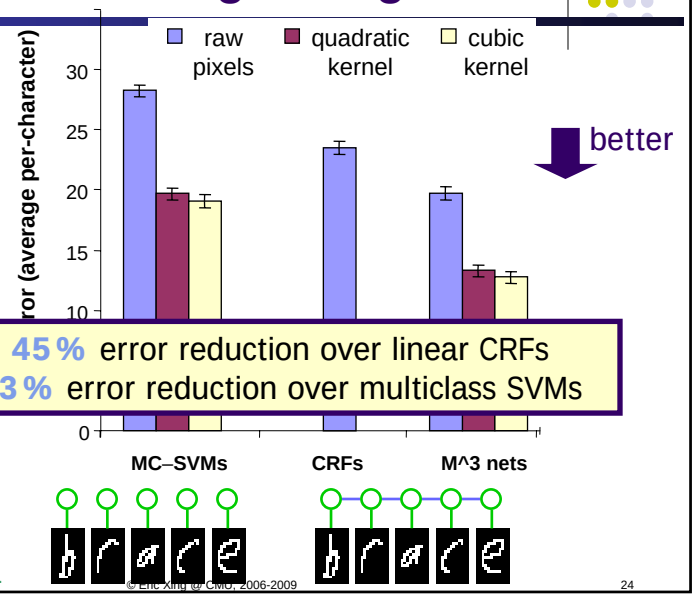
$$\min_{\mathbf{w},\mu} \ \frac{1}{2}||\mathbf{w}||^2$$
$$\text{s.t.} \ \ \mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}^*) \geq \mathbf{b}^\top \mu;$$
$$\mathbf{A}^\top \mu \geq (\mathbf{w}^\top \mathbf{F} + \ell)^\top$$

- Formulation produces compact QP for
  - Low-treewidth Markov networks
  - Associative Markov networks
  - Context free grammars
  - Bipartite matchings
  - Any problem with compact LP inference

Results: Handwriting Recognition

Length: ~8 chars
Letter: 16x8 pixels
10-fold Train/Test
5000/50000 letters
600/6000 words

Models:
Multiclass-SVMs*
CRFs
M³ nets

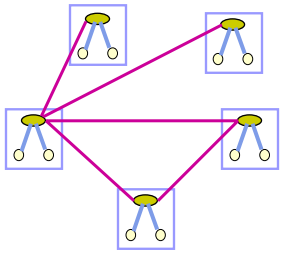


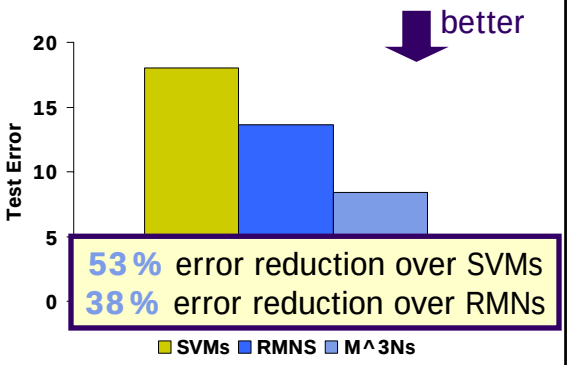
45 % error reduction over linear CRFs
33 % error reduction over multiclass SVMs

*Crammer & Singer 01

Results: Hypertext Classification

- WebKB dataset
  - Four CS department websites: 1300 pages/3500 links
  - Classify each page: faculty, course, student, project, other
  - Train on three universities/test on fourth





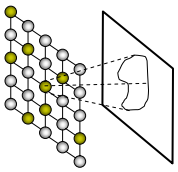
*Taskar et al 02

Summary

- Structured Maximum Margin Networks
  - Concise representation
  - Efficient QP algorithms
  - Applications:
    - Sequences
    - Trees
    - Matchings ….
  - Strong empirical results
- Acknowledgments:
  - Adopted from two different presentations given by Ben Taskar.

Open Problems

- Unsupervised CRF learning and MaxMargin Learning
  - Only X, but not Y (sometimes part of Y), is available
  - We want to recognize a pattern that is maximally different from the rest!



  - What does margin or conditional likelihood mean in these cases? Given only $\{X_n\}$, how can we define the cost function?

$$\text{margin} = w^T\left(F(y_n, x_n) - F(y'_n, x_n)\right) \qquad p_\theta(y \mid x) = \frac{1}{Z(\theta, x)}\exp\left\{\sum_c \theta_c f_c(x, y_c)\right\}$$

  - Algorithmic challenge
  - Stay tuned for lecture 19!