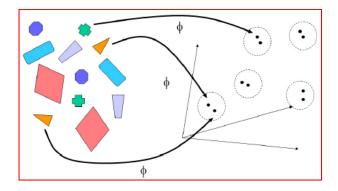
Machine Learning

10-701, Fall 2016

Advanced topics in Max-Margin Learning





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Lecture 7, September 28, 2016
Reading: class handouts

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Recap: the SVM problem

We solve the following constrained opt problem:

$$\max_{\alpha} \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} (\mathbf{x}_{i}^{T} \mathbf{x}_{j})$$
s.t. $\alpha_{i} \geq 0, \quad i = 1, ..., m$

$$\sum_{i=1}^{m} \alpha_{i} y_{i} = 0.$$

- This is a quadratic programming problem.
 - A global maximum of α_i can always be found.

• How to predict:
$$\mathbf{w}^T \mathbf{x}_{\text{new}} + b \leqslant 0$$

The SMO algorithm

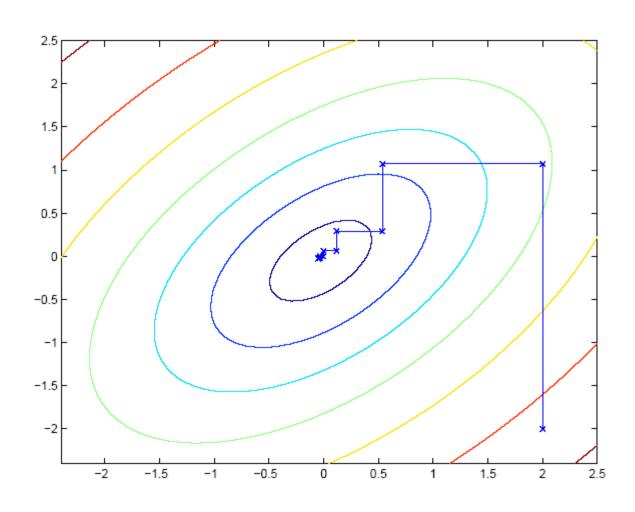


Consider solving the unconstrained opt problem:

$$\max_{\alpha} W(\alpha_1, \alpha_2, \dots, \alpha_m)$$

- We've already see three opt algorithms!
 - Coordinate ascent
 - Gradient ascent
 - Newton-Raphson
- Coordinate ascend:

Coordinate ascend





Sequential minimal optimization

Constrained optimization:

$$\max_{\alpha} \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} (\mathbf{x}_{i}^{T} \mathbf{x}_{j})$$
s.t.
$$0 \le \alpha_{i} \le C, \quad i = 1, ..., m$$

$$\sum_{i=1}^{m} \alpha_{i} y_{i} = 0.$$

• Question: can we do coordinate along one direction at a time (i.e., hold all $\alpha_{[-i]}$ fixed, and update α_i ?)

The SMO algorithm



Repeat till convergence

- 1. Select some pair α_i and α_j to update next (using a heuristic that tries to pick the two that will allow us to make the biggest progress towards the global maximum).
- 2. Re-optimize $J(\alpha)$ with respect to α_i and α_j , while holding all the other α_k 's $(k \neq i; j)$ fixed.

Will this procedure converge?



Convergence of SMO

$$\max_{\alpha} \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

• Let's hold α_3 ,..., α_m fixed and reopt J w.r.t. α_1 and α_2

Convergence of SMO



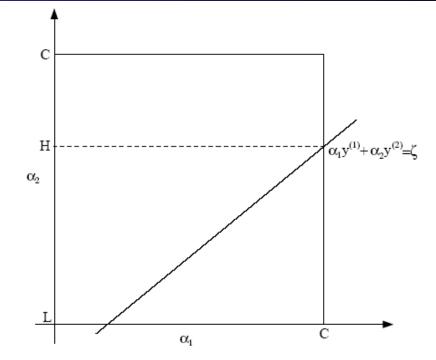
• The constraints:

$$\alpha_1 y_1 + \alpha_2 y_2 = \xi$$

$$0 \le \alpha_1 \le C$$

$$0 \le \alpha_2 \le C$$





$$\mathcal{J}(\alpha_1, \alpha_2, \dots, \alpha_m) = \mathcal{J}((\xi - \alpha_2 y_2) y_1, \alpha_2, \dots, \alpha_m)$$

• Constrained opt:

Advanced topics in Max-Margin Learning



$$\max_{\alpha} \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$
$$\mathbf{w}^T \mathbf{x}_{\text{new}} + b \leq 0$$

- Kernel
- Point rule or average rule
- Can we predict vec(y)?

Outline



- The Kernel trick
- Maximum entropy discrimination
- Structured SVM, aka, Maximum Margin Markov Networks

(1) Non-linear Decision Boundary



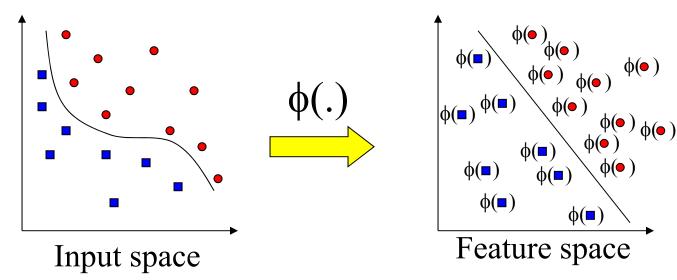
- So far, we have only considered large-margin classifier with a linear decision boundary
- How to generalize it to become nonlinear?
- Key idea: transform x_i to a higher dimensional space to "make life easier"
 - Input space: the space the point x_i are located
 - Feature space: the space of $\phi(\mathbf{x}_i)$ after transformation
- Why transform?
 - Linear operation in the feature space is equivalent to non-linear operation in input space
 - Classification can become easier with a proper transformation. In the XOR problem, for example, adding a new feature of x₁x₂ make the problem linearly separable (homework)



Non-linear Decision Boundary







Note: feature space is of higher dimension than the input space in practice

The Kernel Trick

Recall the SVM optimization problem

$$\max_{\alpha} \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} (\mathbf{x}_{i}^{T} \mathbf{x}_{j})$$
s.t.
$$0 \le \alpha_{i} \le C, \quad i = 1, ..., m$$

$$\sum_{i=1}^{m} \alpha_{i} y_{i} = 0.$$

- The data points only appear as inner product
- As long as we can calculate the inner product in the feature space, we do not need the mapping explicitly
- Many common geometric operations (angles, distances) can be expressed by inner products
- Define the kernel function K by $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$

An Example for feature mapping and kernels



- Consider an input $\mathbf{x} = [x_1, x_2]$
- Suppose $\phi(.)$ is given as follows

$$\phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = 1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2$$

An inner product in the feature space is

$$\left\langle \phi \left[\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right], \phi \left[\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right] \right\rangle =$$

 So, if we define the kernel function as follows, there is no need to carry out φ(.) explicitly

$$K(\mathbf{x}, \mathbf{x}') = (\mathbf{1} + \mathbf{x}^T \mathbf{x}')^2$$

More examples of kernel functions



Linear kernel (we've seen it)

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}'$$

Polynomial kernel (we just saw an example)

$$K(\mathbf{x}, \mathbf{x}') = (\mathbf{1} + \mathbf{x}^T \mathbf{x}')^p$$

where p = 2, 3, ... To get the feature vectors we concatenate all pth order polynomial terms of the components of x (weighted appropriately)

Radial basis kernel

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\|\mathbf{x} - \mathbf{x}'\|^2\right)$$

In this case the feature space consists of functions and results in a nonparametric classifier.

The essence of kernel

- Feature mapping, but "without paying a cost"
 - E.g., polynomial kernel

$$K(x,z) = (x^T z + c)^d$$

- How many dimensions we've got in the new space?
- How many operations it takes to compute K()?
- Kernel design, any principle?
 - K(x,z) can be thought of as a similarity function between x and z
 - This intuition can be well reflected in the following "Gaussian" function (Similarly one can easily come up with other K() in the same spirit)

$$K(x,z) = \exp\left(-\frac{\|x - z\|^2}{2\sigma^2}\right)$$

Is this necessarily lead to a "legal" kernel?
 (in the above particular case, K() is a legal one, do you know how many dimension φ(x) is?

Kernel matrix

- Suppose for now that K is indeed a valid kernel corresponding to some feature mapping ϕ , then for x_1, \ldots, x_m , we can compute an $m \times m$ matrix $K = \{K_{i,j}\}$, where $K_{i,j} = \phi(x_i)^T \phi(x_j)$
- This is called a kernel matrix!
- Now, if a kernel function is indeed a valid kernel, and its elements are dot-product in the transformed feature space, it must satisfy:
 - Symmetry $K=K^T$ proof $K_{i,j}=\phi(x_i)^T\phi(x_j)=\phi(x_j)^T\phi(x_i)=K_{j,i}$
 - Positive –semidefinite $y^T K y \ge 0 \quad \forall y$ proof?

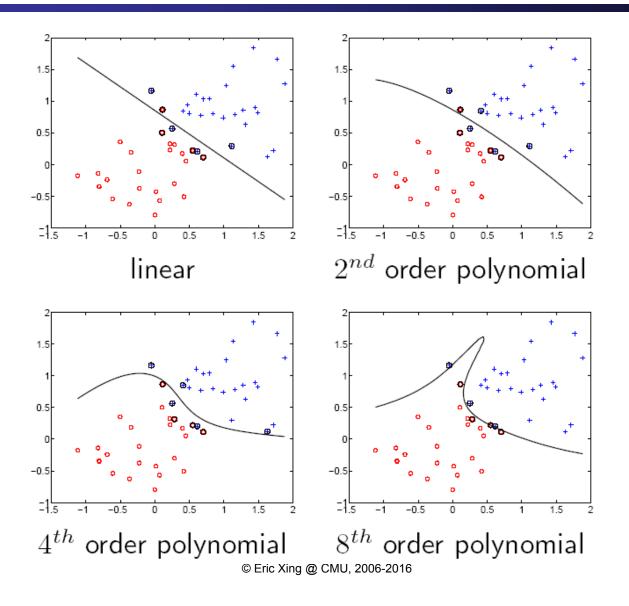




Theorem (Mercer): Let $K: \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}$ be given. Then for K to be a valid (Mercer) kernel, it is necessary and sufficient that for any $\{x_i, \ldots, x_m\}$, $(m < \infty)$, the corresponding kernel matrix is symmetric positive semi-denite.

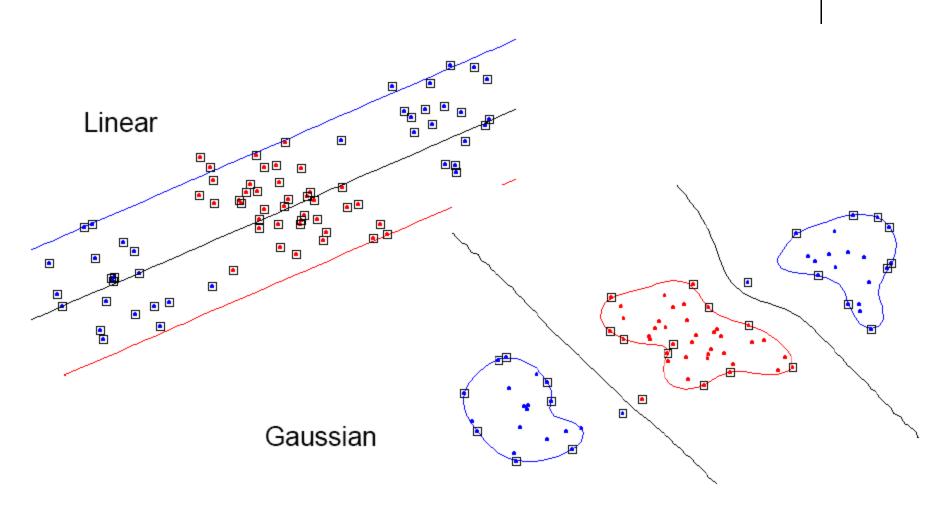






Examples for Non Linear SVMs – Gaussian Kernel

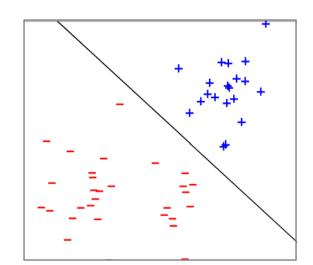








- Inputs x, class y = +1, -1
- data $D = \{ (x_1, y_1), ..., (x_m, y_m) \}$
- Point Rule:
 - learn f^{opt}(x) discriminant function
 from F = {f} family of discriminants
 - classify $y = sign f^{opt}(x)$



• E.g., SVM

$$f^{\text{opt}}(\mathbf{x}) = \mathbf{w}^T \mathbf{x}_{\text{new}} + b$$

Model averaging

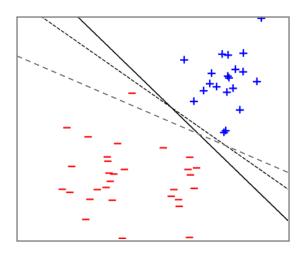
- There exist many f with near optimal performance
- Instead of <u>choosing</u> f^{opt}, <u>average</u> over all f in F

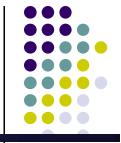
$$y(x) = \operatorname{sign} \int_{F} Q(f)f(x)df$$

= $\operatorname{sign}\langle f(x)\rangle_{Q}$



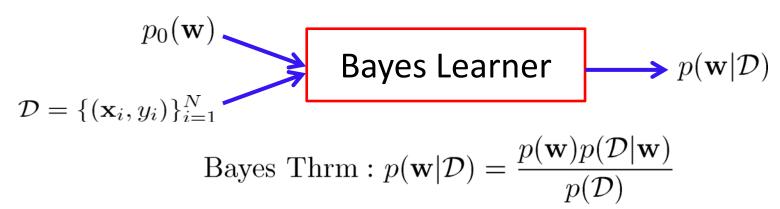
How to learn Q(f) distribution over F?





Recall Bayesian Inference

Bayesian learning:



Bayes Predictor (model averaging):

$$h_1ig(\mathbf{x}; p(\mathbf{w})ig) = rg\max_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \int p(\mathbf{w}) f(\mathbf{x}, \mathbf{y}; \mathbf{w}) d\mathbf{w}$$

Recall in SVM:
$$h_0(\mathbf{x}; \mathbf{w}) = \arg \max_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} F(\mathbf{x}, \mathbf{y}; \mathbf{w})$$

• What p_0 ?

How to score distributions?



Entropy

Entropy H(X) of a random variable X

$$H(X) = -\sum_{i=1}^{N} P(x=i) \log_2 P(x=i)$$

- H(X) is the expected number of bits needed to encode a randomly drawn value of X (under most efficient code)
- Why?

Information theory:

Most efficient code assigns $-\log_2 P(X=i)$ bits to encode the message X=I, So, expected number of bits to code one random X is:

$$-\sum_{i=1}^{N} P(x=i) \log_2 P(x=i)$$





• Given data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$, find

$$Q_{\mathrm{ME}} = rg \max \quad \mathrm{H}(Q)$$
 s.t. $y^i \langle f(\mathbf{x}^i) \rangle_{Q_{\mathrm{ME}}} \geq \xi_i, \quad \forall i$ $\xi_i \geq 0 \quad \forall i$

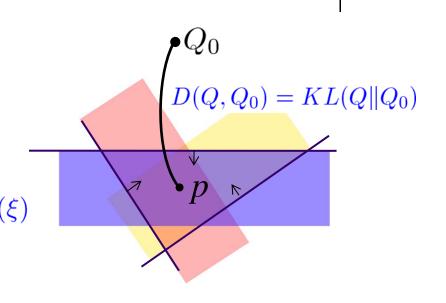
- solution Q_{ME} correctly classifies
- among all admissible Q, Q_{MF} has max entropy
- max entropy \longrightarrow "minimum assumption" about f

Introducing Priors



- Prior $Q_0(f)$
- Minimum Relative Entropy
 Discrimination

$$Q_{\mathrm{MRE}} = \underset{}{\mathrm{arg\,min}} \quad \mathrm{KL}(Q\|Q_0) + U(\xi)$$
 s.t. $y^i \langle f(\mathbf{x}^i) \rangle_{Q_{\mathrm{ME}}} \geq \xi_i, \quad \forall i$ $\xi_i \geq 0 \quad \forall i$



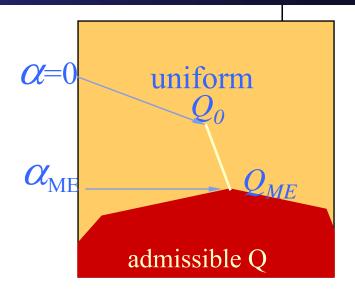
- Convex problem: Q_{MRE} unique solution
- MER \longrightarrow "minimum additional assumption" over Q_0 about f

Solution: Q_{ME} as a projection



- Convex problem: Q_{ME} unique
- Theorem:

$$Q_{\text{MRE}} \propto \exp\{\sum_{i=1}^{N} \alpha_i y_i f(x_i; w)\} Q_0(w)$$



 $\alpha_i \ge 0$ Lagrange multipliers

• finding Q_M : start with $\alpha_i = 0$ and follow gradient of unsatisfied constraints

Solution to MED



- Theorem (Solution to MED):
 - Posterior Distribution:

$$Q(\mathbf{w}) = \frac{1}{Z(\alpha)} Q_0(\mathbf{w}) \exp \left\{ \sum_i \alpha_i y_i [f(\mathbf{x}_i; \mathbf{w})] \right\}$$

– Dual Optimization Problem:

D1:
$$\max_{\alpha} -\log Z(\alpha) - U^{\star}(\alpha)$$
s.t. $\alpha_i(\mathbf{y}) \ge 0, \ \forall i,$

$$U^{\star}(\cdot)$$
 is the conjugate of the $U(\cdot)$, i.e., $U^{\star}(\alpha) = \sup_{\xi} \left(\sum_{i,y} \alpha_i(y) \xi_i - U(\xi) \right)$

- Algorithm: to computer α_t , t = 1,...T
 - start with $\alpha_t = 0$ (uniform distribution)
 - iterative ascent on $J(\alpha)$ until convergence

Examples: SVMs

Theorem

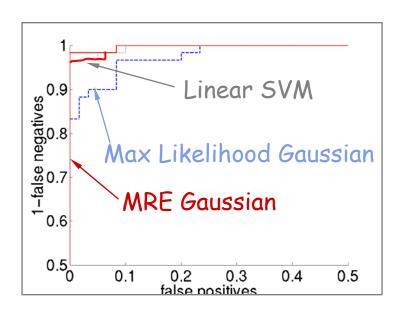
For $f(x) = w^T x + b$, $Q_0(w) = \text{Normal}(0, I)$, $Q_0(b) = \text{non-informative prior}$, the Lagrange multipliers α are obtained by maximizing $J(\alpha)$ subject to $0 \le \alpha_t \le C$ and $\sum_t \alpha_t y_t = 0$, where

$$J(\alpha) = \sum_{t} \left[\alpha_t + \log(1 - \alpha_t/C) \right] - \frac{1}{2} \sum_{s,t} \alpha_s \alpha_t y_s y_t x_s^T x_t$$

- Inseparable D SVM recovered with different misclassification penalty

SVM extensions

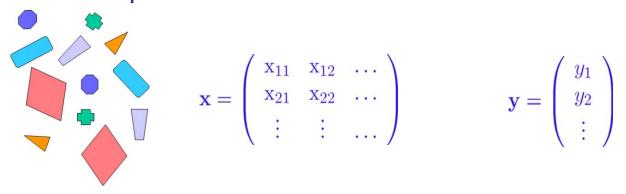
• Example: Leptograpsus Crabs (5 inputs, T_{train}=80, T_{test}=120)







Unstructured prediction



$$\mathbf{x} = \begin{pmatrix} x_{11} & x_{12} & \dots \\ x_{21} & x_{22} & \dots \\ \vdots & \vdots & \dots \end{pmatrix}$$

$$\mathbf{y} = \left(\begin{array}{c} y_1 \\ y_2 \\ \vdots \end{array}\right)$$

- Structured prediction
 - Part of speech tagging

 ${f x}=$ "Do you want sugar in it?" \Rightarrow ${f y}=$ verb pron verb noun prep pron>

Image segmentation

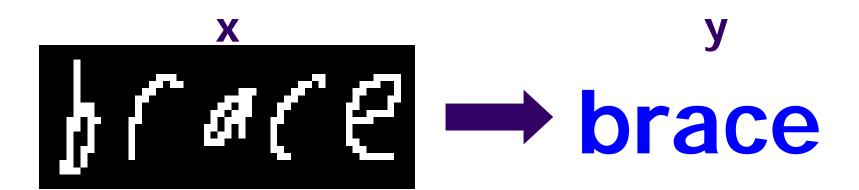


$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_{11} & \mathbf{x}_{12} & \dots \\ \mathbf{x}_{21} & \mathbf{x}_{22} & \dots \\ \vdots & \vdots & \dots \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} y_{11} & y_{12} & \dots \\ y_{21} & y_{22} & \dots \\ \vdots & \vdots & \dots \end{pmatrix}$$

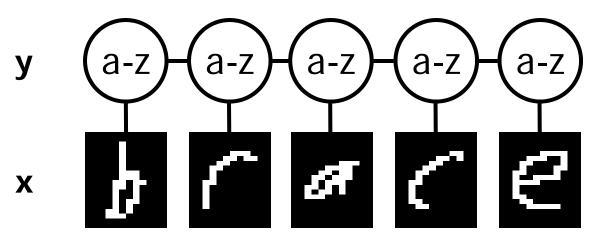
$$\mathbf{y} = \begin{pmatrix} y_{11} & y_{12} & \dots \\ y_{21} & y_{22} & \dots \\ \vdots & \vdots & \dots \end{pmatrix}$$

OCR example





Sequential structure



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Classical Classification Models

- Inputs:
 - a set of training samples $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$, where $\mathbf{x}_i = [x_i^1, x_i^2, \cdots, x_i^d]^\top$ and $y_i \in C \triangleq \{c_1, c_2, \cdots, c_L\}$
- Outputs:
 - a predictive function $h(\mathbf{x})$: $y^* = h(\mathbf{x}) \triangleq \arg \max_y F(\mathbf{x}, y)$ $F(\mathbf{x}, y) = \mathbf{w}^{\top} \mathbf{f}(\mathbf{x}, y)$
- Examples:
 - SVM: $\max_{\mathbf{w}, \xi} \frac{1}{2} \mathbf{w}^{\top} \mathbf{w} + C \sum_{i=1}^{N} \xi_{i}; \text{ s.t. } \mathbf{w}^{\top} \Delta \mathbf{f}_{i}(y) \geq 1 \xi_{i}, \ \forall i, \forall y.$
 - Logistic Regression: $\max_{\mathbf{w}} \mathcal{L}(\mathcal{D}; \mathbf{w}) \triangleq \sum_{i=1}^{N} \log p(y_i | \mathbf{x}_i)$

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

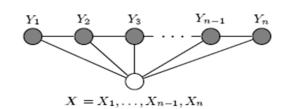
Structured Models



Assumptions:

$$F(\mathbf{x}, \mathbf{y}) = \mathbf{w}^{\top} \mathbf{f}(\mathbf{x}, \mathbf{y}) = \sum_{p} \mathbf{w}^{\top} \mathbf{f}(\mathbf{x}_{p}, \mathbf{y}_{p})$$

- Linear combination of teatures
- Sum of partial scores: index p represents a part in the structure
- Random fields or Markov network features:





Discriminative Learning Strategies

- Max Conditional Likelihood
 - We predict based on:

$$\mathbf{y}^* \mid \mathbf{x} = \arg\max_{\mathbf{y}} \ p_{\mathbf{w}}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\mathbf{w}, \mathbf{x})} \exp \left\{ \sum_{c} w_{c} f_{c}(\mathbf{x}, \mathbf{y}_{c}) \right\}$$

And we learn based on:

$$\mathbf{w}^* \mid \{\mathbf{y}_i, \mathbf{x}_i\} = \arg\max_{\mathbf{w}} \prod_i p_{\mathbf{w}}(\mathbf{y}_i \mid \mathbf{x}_i) = \prod_i \frac{1}{Z(\mathbf{w}, \mathbf{x}_i)} \exp\left\{\sum_c w_c f_c(\mathbf{x}_i, \mathbf{y}_i)\right\}$$

- Max Margin:
 - We predict based on:

$$\mathbf{y}^* \mid \mathbf{x} = \arg \max_{\mathbf{y}} \sum_{c} w_c f_c(\mathbf{x}, \mathbf{y}_c) = \arg \max_{\mathbf{y}} \mathbf{w}^T f(\mathbf{x}, \mathbf{y})$$

And we learn based on:

$$\mathbf{w}^* \mid \{\mathbf{y}_i, \mathbf{x}_i\} = \arg\max_{\mathbf{w}} \left(\min_{\mathbf{y} \neq \mathbf{y}^i, \forall i} \mathbf{w}^T (f(\mathbf{y}_i, \mathbf{x}_i) - f(\mathbf{y}, \mathbf{x}_i)) \right)$$

E.g. Max-Margin Markov Networks



Convex Optimization Problem:

P0 (M³N):
$$\min_{\mathbf{w}, \xi} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{i=1}^{N} \xi_i$$
s.t. $\forall i, \forall \mathbf{y} \neq \mathbf{y}_i$: $\mathbf{w}^{\top} \Delta \mathbf{f}_i(\mathbf{x}, \mathbf{y}) \geq \Delta \ell_i(\mathbf{y}) - \xi_i, \ \xi_i \geq 0$,

Feasible subspace of weights:

$$\mathcal{F}_0 = \{ \mathbf{w} : \mathbf{w}^{\top} \Delta \mathbf{f}_i(\mathbf{x}, \mathbf{y}) \ge \Delta \ell_i(\mathbf{y}) - \xi_i; \ \forall i, \forall \mathbf{y} \ne \mathbf{y}_i \}$$

Predictive Function:

$$h_0(\mathbf{x}; \mathbf{w}) = \arg \max_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} F(\mathbf{x}, \mathbf{y}; \mathbf{w})$$





• We want:

```
\operatorname{argmax}_{\operatorname{word}} \mathbf{w}^{\mathsf{T}} \mathbf{f}(\mathbf{b} \cap \mathbf{e}) = \text{`brace'}
```

Equivalently:

a lot!

Min-max Formulation

Brute force enumeration of constraints:

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

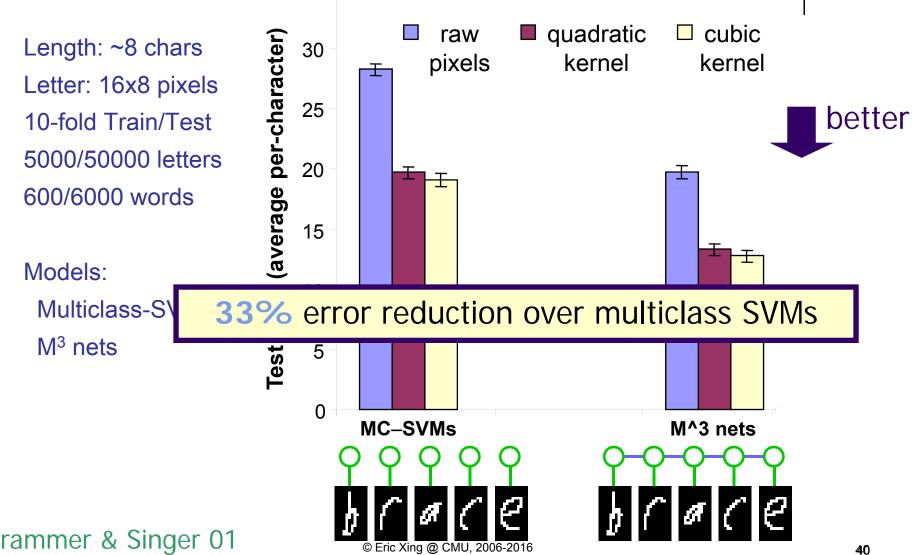
- The constraints are exponential in the size of the structure
- Alternative: min-max formulation
 - add only the most violated constraint

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

- Handles more general loss functions
- Only polynomial # of constraints needed
- Several algorithms exist ...

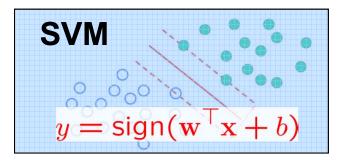
Results: Handwriting Recognition







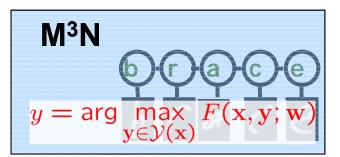




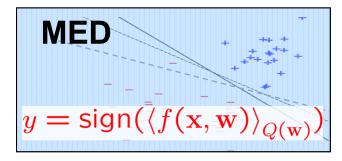
$$\min_{\mathbf{w}, \xi} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{i=1}^m \xi_i$$
$$y^i(\mathbf{w}^\top \mathbf{x}^i + b) \ge 1 - \xi_i, \quad \forall i$$

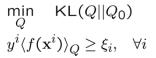






$$\min_{\mathbf{w}, \xi} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{i=1}^m \xi_i \\ \mathbf{w}^{\top} [\mathbf{f}(\mathbf{x}^i, \mathbf{y})] \ge \ell(\mathbf{y}^i, \mathbf{y}) - \xi_i, \quad \forall i, \forall \mathbf{y} \ne \mathbf{y}^i$$







MED-MN

= SMED + Bayesian M³N

See [Zhu and Xing, 2008]

Summary



- Maximum margin nonlinear separator
 - Kernel trick
 - Project into linearly separatable space (possibly high or infinite dimensional)
 - No need to know the explicit projection function
- Max-entropy discrimination
 - Average rule for prediction,
 - Average taken over a posterior distribution of w who defines the separation hyperplane
 - P(w) is obtained by max-entropy or min-KL principle, subject to expected marginal constraints on the training examples
- Max-margin Markov network
 - Multi-variate, rather than uni-variate output Y
 - Variable in the outputs are not independent of each other (structured input/output)
 - Margin constraint over every possible configuration of Y (exponentially many!)