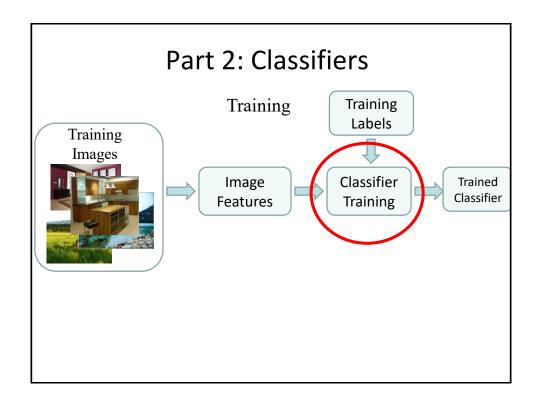
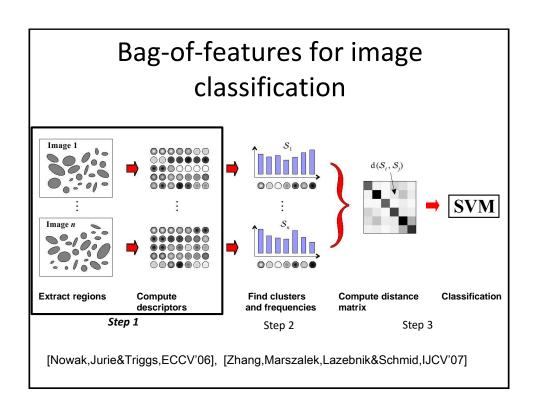
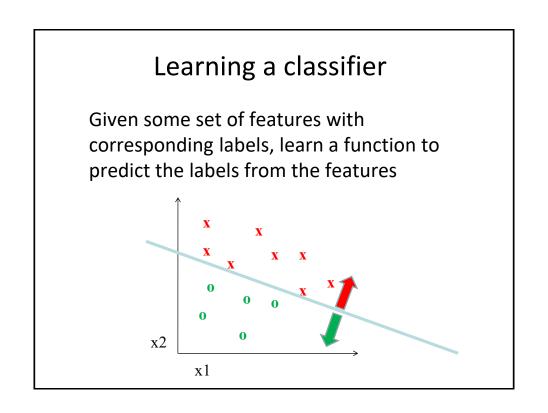
ECS797P - Machine Learning for Visual Data Analysis

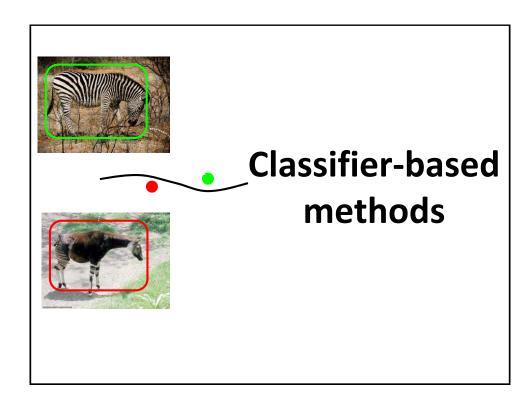
Tao Xiang t.xiang@qmul.ac.uk

Lecture 2









Many classifiers to choose from

- SVM
- Neural networks
- Naïve Bayes
- Bayesian network
- Logistic regression
- Randomized Forests
- Boosted Decision Trees
- K-nearest neighbor
- RBMs
- Etc.

Which is the best one?

The perfect classification algorithm

- Objective function: encodes the right loss for the problem
- <u>Parameterization</u>: makes assumptions that fit the problem
- Regularization: right level of regularization for amount of training data
- <u>Training algorithm</u>: can find parameters that maximize objective on training set
- <u>Inference algorithm</u>: can solve for objective function in evaluation

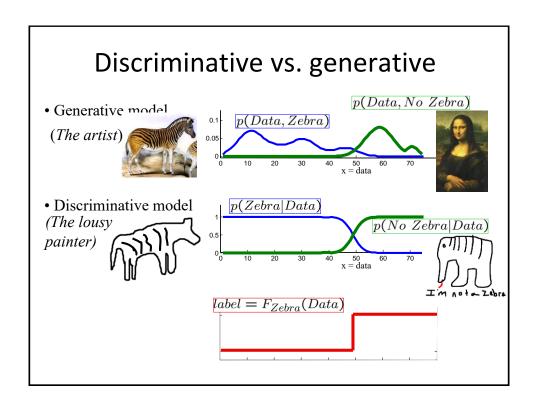
Generative vs. Discriminative Classifiers

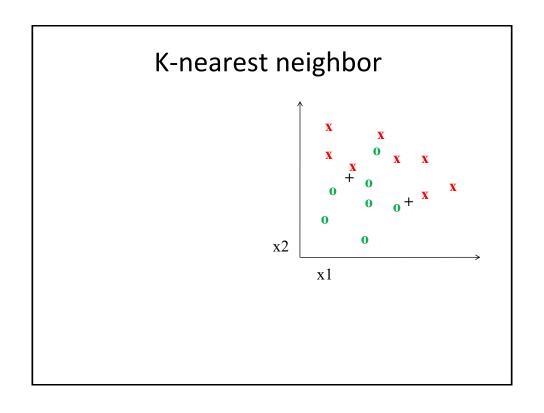
Generative

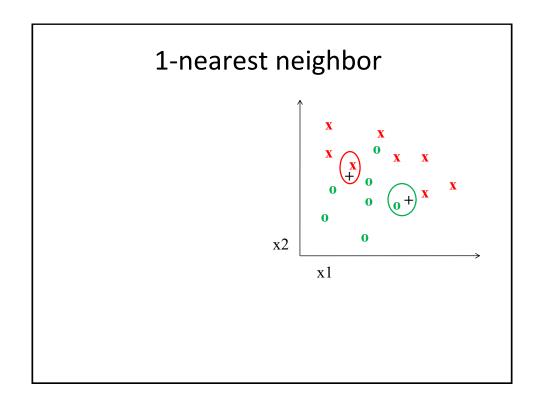
- Training
 - Models the data and the labels
 - Assume (or learn) probability distribution and dependency structure
 - Can impose priors
- Testing
 - P(y=1, x) / P(y=0, x) > t?
- Examples
 - Foreground/background GMM
 - Naïve Bayes classifier
 - Bayesian network

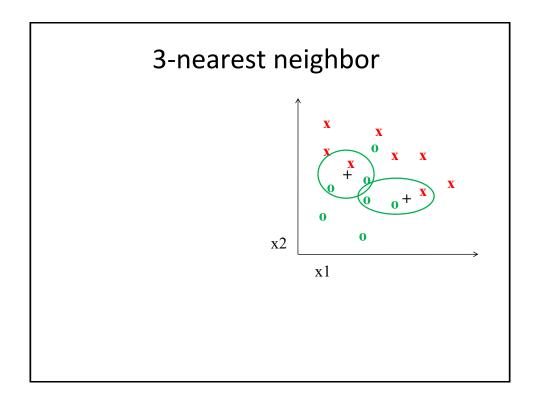
Discriminative

- Training
 - Learn to directly predict the labels from the data
 - Assume form of boundary
 - Margin maximization or parameter regularization
- Testing
 - f(x) > t; e.g., $w^{T}x > t$
- Examples
 - Logistic regression
 - SVM
 - Boosted decision trees

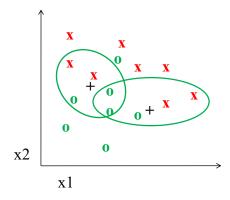








5-nearest neighbor



What is the parameterization? The regularization? The training algorithm? The inference?

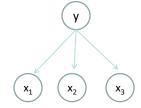
Is K-NN generative or discriminative?

Using K-NN

- Simple, and a good one to try first
- With infinite examples, 1-NN provably has error that is at most twice Bayes optimal error

Naïve Bayes

- Objective
- Parameterization
- Regularization
- Training
- Inference



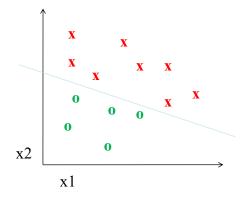
Naïve Bayes Classifier wikipedia link

Using Naïve Bayes

- Simple thing to try for categorical data
- Very fast to train/test

Classifiers: Logistic Regression

- Objective
- Parameterization
- Regularization
- Training
- Inference

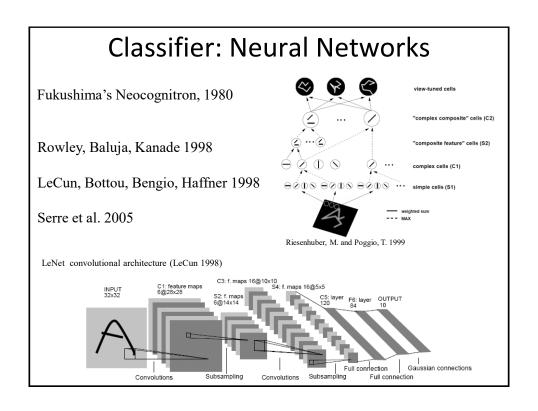


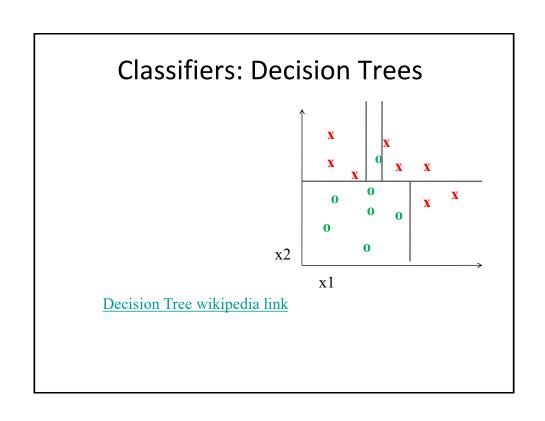
Logistic Regression wikipedia link

A document on how to use Logistic Regression as a classifier

Using Logistic Regression

- Quick, simple classifier (try it first)
- Use L2 or L1 regularization
 - L1 does feature selection and is robust to irrelevant features but slower to train



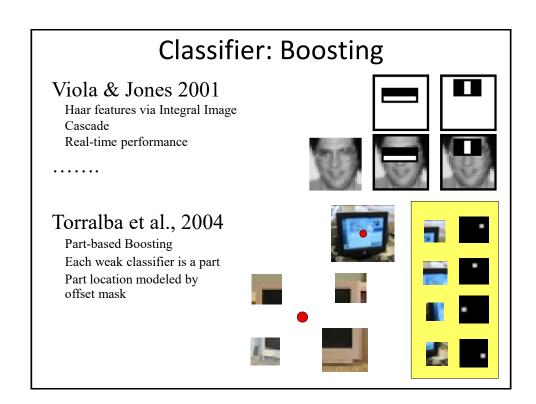


Ensemble Methods: Boosting

Discrete AdaBoost(Freund & Schapire 1996b)

- 1. Start with weights $w_i = 1/N$, i = 1, ..., N.
- 2. Repeat for $m=1,2,\ldots,M$:
 - (a) Fit the classifier $f_m(x) \in \{-1,1\}$ using weights w_i on the training data.
 - (b) Compute $\operatorname{err}_m = E_w[1_{(y \neq f_m(x))}], c_m = \log((1 \operatorname{err}_m)/\operatorname{err}_m).$
 - (c) Set $w_i \leftarrow w_i \exp[c_m \cdot 1_{(y_i \neq f_m(x_i))}], \ i=1,2,\dots N,$ and renormalize so that $\sum_i w_i=1.$
- 3. Output the classifier $\mathrm{sign}[\sum_{m=1}^M c_m f_m(x)]$

figure from Friedman et al. 2000



Two ways to think about classifiers

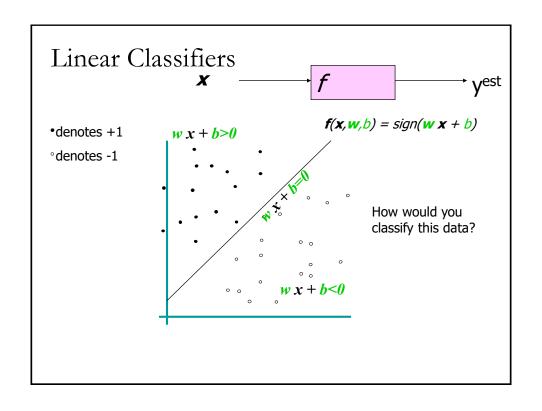
- 1. What is the objective? What are the parameters? How are the parameters learned? How is the learning regularized? How is inference performed?
- 2. How is the data modeled? How is similarity defined? What is the shape of the boundary?

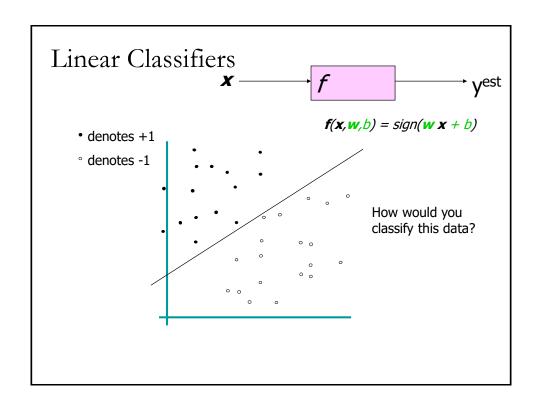
Comparison		
Learning Objective	Training	Inference
$\begin{aligned} & \operatorname{maximize} \sum_{i} \left[\sum_{j} \log P \left(\boldsymbol{x}_{ij} \mid \boldsymbol{y}_{i}; \boldsymbol{\theta}_{j} \right) \\ & + \log P \left(\boldsymbol{y}_{i}; \boldsymbol{\theta}_{0} \right) \end{aligned} \right] \qquad \boldsymbol{\theta}_{k} \end{aligned}$	$j = \frac{\sum_{i} \delta(x_{ij} = 1 \land y_{i} = k) + r}{\sum_{i} \delta(y_{i} = k) + Kr}$	$\begin{aligned} & \theta_{i}^{T}\mathbf{x} + \theta_{o}^{T}(1 - \mathbf{x}) > 0 \\ & \text{where } \theta_{ij} = \log \frac{P(x_{i} = 1 \mid y = 1)}{P(x_{j} = 1 \mid y = 0)}, \\ & \theta_{oj} = \log \frac{P(x_{j} = 0 \mid y = 1)}{P(x_{j} = 0 \mid y = 0)} \end{aligned}$
$\begin{aligned} & \text{maximize} \sum_{i} \log(P(y_{i} \mid \mathbf{x}, \mathbf{\theta})) + \lambda \ \mathbf{\theta}\ \\ & \text{where } P(y_{i} \mid \mathbf{x}, \mathbf{\theta}) = 1/(1 + \exp(-y_{i}\mathbf{\theta}^{T}\mathbf{x})) \end{aligned}$	Gradient ascent	$\boldsymbol{\theta}^T \mathbf{x} > 0$
minimize $\lambda \sum_{i} \xi_{i} + \frac{1}{2} \ \mathbf{\theta}\ $ such that $y_{i} \mathbf{\theta}^{T} \mathbf{x} \ge 1 - \xi_{i} \forall i$	Linear programming	$\boldsymbol{\theta}^T \mathbf{x} > 0$
complicated to write	Quadratic programming	$\sum_{i} y_{i} \alpha_{i} K(\hat{\mathbf{x}}_{i}, \mathbf{x}) > 0$
most similar features → same label	Record data	y_i where $i = \underset{i}{\operatorname{argmin}} K(\hat{\mathbf{x}}_i, \mathbf{x})$
	Learning Objective $\max \sum_{i} \left[\sum_{j} \log P(x_{ij} \mid y_i; \theta_j) \right] \qquad \theta_k$ $\max \sum_{i} \log(P(y_i \mid \mathbf{x}, \mathbf{\theta})) + \lambda \ \mathbf{\theta}\ $ where $P(y_i \mid \mathbf{x}, \mathbf{\theta}) = 1/(1 + \exp(-y_i \mathbf{\theta}^T \mathbf{x}))$ $\min \sum_{i} \lambda \sum_{i} \xi_i + \frac{1}{2} \ \mathbf{\theta}\ $ such that $y_i \mathbf{\theta}^T \mathbf{x} \ge 1 - \xi_i \forall i$ complicated to write	Learning Objective Training $\max \sum_{i} \left[\sum_{j=1}^{j} \log P(x_{ij} \mid y_{i}; \theta_{j}) \right] \qquad \theta_{kj} = \frac{\sum_{i} \delta(x_{ij} = 1 \land y_{i} = k) + r}{\sum_{i} \delta(y_{i} = k) + Kr}$ $\max \sum_{i} \log(P(y_{i} \mid \mathbf{x}, \mathbf{\theta})) + \lambda \ \mathbf{\theta}\ \qquad \text{Gradient ascent}$ $\text{where } P(y_{i} \mid \mathbf{x}, \mathbf{\theta}) = 1/(1 + \exp(-y_{i}\mathbf{\theta}^{T}\mathbf{x}))$ $\min \sum_{i} \lambda \sum_{j} \xi_{i} + \frac{1}{2} \ \mathbf{\theta}\ \qquad \text{Linear programming}$ $\text{such that } y_{i}\mathbf{\theta}^{T}\mathbf{x} \ge 1 - \xi_{i} \forall i$ $\text{Complicated to write}$ $\text{Quadratic programming}$

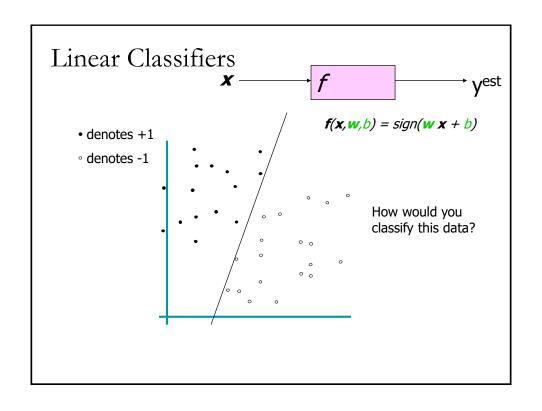
What to remember about classifiers

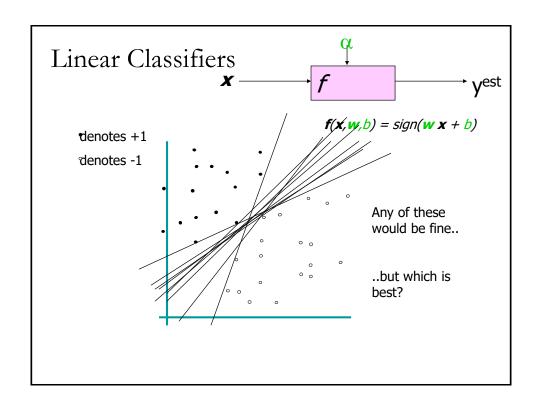
- No free lunch: machine learning algorithms are tools, not dogmas
- Try simple classifiers first
- Better to have smart features and simple classifiers than simple features and smart classifiers
- Use increasingly powerful classifiers with more training data (bias-variance tradeoff)

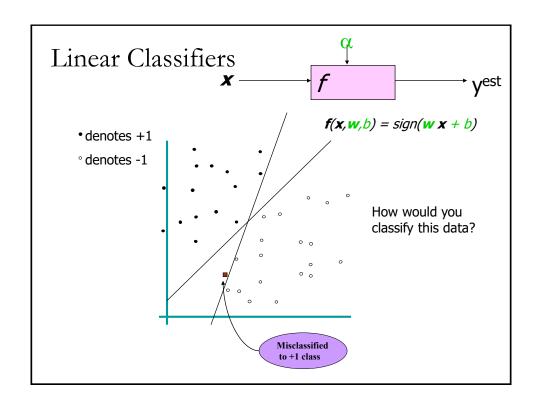
SUPPORT VECTOR MACHINES

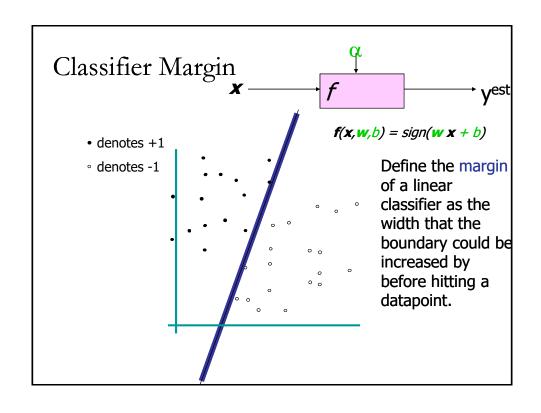


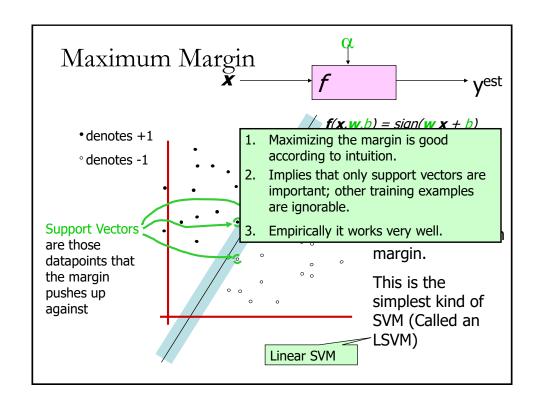


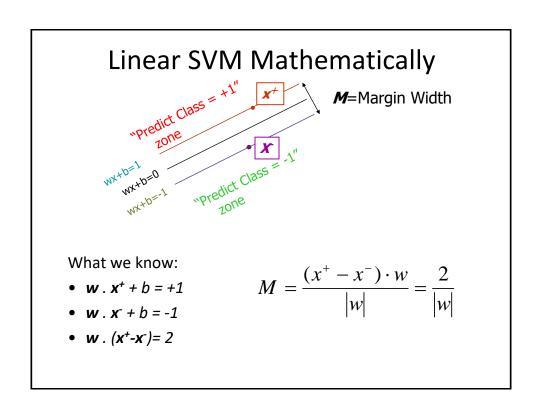












Linear SVM Mathematically

Goal: 1) Correctly classify all training data

$$wx_i + b \ge 1 \text{ if } y_i = +1$$

$$wx_i + b \le -1 \text{ if } y_i = -1$$

$$y_i(wx_i + b) \ge 1 \text{ for all i}$$
2) Maximize the Margin
$$M = \frac{2}{|w|}$$
same as minimize
$$\frac{1}{2}w^t w$$

- We can formulate a Quadratic Optimization Problem and solve for w and b

Minimize
$$\Phi(w) = \frac{1}{2} w^t w$$

$$|_{\text{subject to}} \quad y_i(wx_i + b) \ge 1 \qquad \forall i$$

Solving the Optimization Problem

Find w and b such that

 $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$ is minimized;

and for all $\{(\mathbf{x_i}, y_i)\}: y_i(\mathbf{w^T}\mathbf{x_i} + b) \ge 1$

- Need to optimize a *quadratic* function subject to *linear* constraints.
- Quadratic optimization problems are a well-known class of mathematical programming problems, and many (rather intricate) algorithms exist for solving them.
- The solution involves constructing a dual problem where a Lagrange multiplier α_i is associated with every constraint in the primary problem:

Find $\alpha_1 ... \alpha_N$ such that

 $\mathbf{Q}(\mathbf{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_i y_i y_i \mathbf{x_i}^T \mathbf{x_i}$ is maximized and

- (1) $\sum \alpha_i y_i = 0$
- (2) $\alpha_i \ge 0$ for all α_i

The Optimization Problem Solution

The solution has the form:

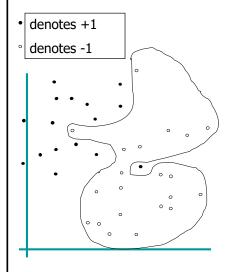
$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x_i} \qquad b = y_k^{-} \mathbf{w}^{\mathrm{T}} \mathbf{x_k} \text{ for any } \mathbf{x_k} \text{ such that } \alpha_k \neq 0$$

- Each non-zero α_i indicates that corresponding $\mathbf{x_i}$ is a support vector.
- Then the classifying function will have the form:

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x_i}^{\mathsf{T}} \mathbf{x} + b$$

- Notice that it relies on an *inner product* between the test point \mathbf{x} and the support vectors \mathbf{x}_i we will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products $\mathbf{x_i}^T \mathbf{x_j}$ between all pairs of training points.

Dataset with noise

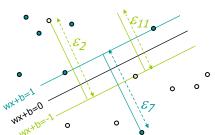


- Hard Margin: So far we require all data points be classified correctly
 - No training error
- What if the training set is noisy?
- Solution 1: use very powerful kernels

Overfitting?

Soft Margin Classification

Slack variables ξi can be added to allow misclassification of difficult or noisy examples.



What should our quadratic optimization criterion be?

Minimize

$$\frac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_{k=1}^{R} \varepsilon_k$$

Hard Margin v.s. Soft Margin

The old formulation:

```
Find w and b such that \Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} is minimized and for all \{(\mathbf{X_i}, y_i)\} y_i(\mathbf{w}^{\mathrm{T}} \mathbf{x_i} + \mathbf{b}) \ge 1
```

The new formulation incorporating slack variables:

```
Find w and b such that \mathbf{\Phi}(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} + C \sum_{i} \xi_{i} \quad \text{is minimized and for all } \{(\mathbf{x_{i}}, y_{i})\}
y_{i}(\mathbf{w}^{\mathrm{T}} \mathbf{x_{i}} + b) \ge 1 - \xi_{i} \quad \text{and} \quad \xi_{i} \ge 0 \text{ for all } i
```

Parameter C can be viewed as a way to control overfitting.

Linear SVMs: Overview

- The classifier is a separating hyperplane.
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points x_i are support vectors with non-zero Lagrangian multipliers α_i
- Both in the dual formulation of the problem and in the solution training points appear only inside dot products:

Find $\alpha_1...\alpha_N$ such that

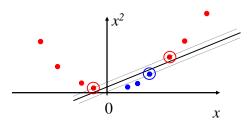
 $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \alpha_i \alpha_i y_i y_i x_i^T x_i$ is maximized and

- (1) $\Sigma \alpha_i y_i = 0$
- (2) $0 \le \alpha_i \le C$ for all α_i

$$f(\mathbf{x}) = \sum \alpha_i \mathbf{y}_i \mathbf{x}_i^{\mathrm{T}} \mathbf{x} + \mathbf{b}$$

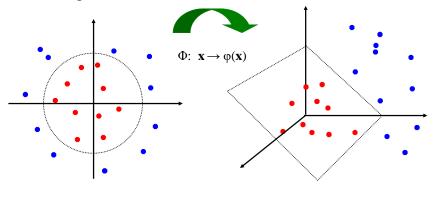
Non-linear SVMs

- Datasets that are linearly separable with some noise work out great:
- But what are we going to do if the dataset is just too hard?
- How about... mapping data to a higher-dimensional space:



Non-linear SVMs: Feature spaces

General idea: the original input space can always be mapped to some higher-dimensional feature space where the training set is separable:



The "Kernel Trick"

- The linear classifier relies on dot product between vectors $K(\mathbf{x_i}, \mathbf{x_j}) = \mathbf{x_i}^T \mathbf{x_j}$
- If every data point is mapped into highdimensional space via some transformation

 Φ : $x \to \phi(x)$, the dot product becomes:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

■ A *kernel function* is some function that corresponds to an inner product in some expanded feature space.

What Functions are Kernels?

- For some functions $K(\mathbf{x}_i, \mathbf{x}_j)$ checking that $K(\mathbf{x}_i, \mathbf{x}_i) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_i)$ can be cumbersome.
- Mercer's theorem:

Every semi-positive definite symmetric function is a kernel

Semi-positive definite symmetric functions correspond to a semi-positive definite symmetric Gram matrix:

Examples of Kernel Functions

- Linear: $K(\mathbf{x_i}, \mathbf{x_j}) = \mathbf{x_i}^T \mathbf{x_j}$
- Polynomial of power $p: K(\mathbf{x_i}, \mathbf{x_j}) = (1 + \mathbf{x_i}^T \mathbf{x_j})^p$
- Gaussian (radial-basis function network):

$$K(\mathbf{x_i}, \mathbf{x_j}) = \exp(-\frac{\|\mathbf{x_i} - \mathbf{x_j}\|^2}{2\sigma^2})$$

• Sigmoid: $K(\mathbf{x_i}, \mathbf{x_i}) = \tanh(\beta_0 \mathbf{x_i}^T \mathbf{x_i} + \beta_1)$

Non-linear SVMs Mathematically

Dual problem formulation:

Find $\alpha_1...\alpha_N$ such that $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j K(\mathbf{x_i}, \mathbf{x_j})$ is maximized and (1) $\sum \alpha_i y_i = 0$ (2) $\alpha_i \geq 0$ for all α_i

The solution is:

$$f(\mathbf{x}) = \sum \alpha_i y_i K(\mathbf{x_i}, \mathbf{x}) + b$$

• Optimization techniques for finding α_i 's remain the same!

Nonlinear SVM - Overview

- SVM locates a separating hyperplane in the feature space and classify points in that space
- It does not need to represent the space explicitly, simply by defining a kernel function
- The kernel function plays the role of the dot product in the feature space.

Properties of SVM

- · Flexibility in choosing a similarity function
- Sparseness of solution when dealing with large data sets
 - only support vectors are used to specify the separating hyperplane
- Ability to handle large feature spaces
 - complexity does not depend on the dimensionality of the feature space
- Overfitting can be controlled by soft margin approach
- Nice math property: a simple convex optimization problem which is guaranteed to converge to a single global solution

Some Issues

Choice of kernel

- Gaussian or polynomial kernel is default
- if ineffective, more elaborate kernels are needed
- domain experts can give assistance in formulating appropriate similarity measures

Choice of kernel parameters

- e.g. σ in Gaussian kernel
- σ is the distance between closest points with different classifications
- In the absence of reliable criteria, applications rely on the use of a validation set or cross-validation to set such parameters.

References

 An excellent tutorial on VC-dimension and Support Vector Machines:

C.J.C. Burges. A tutorial on support vector machines for pattern recognition. Data Mining and Knowledge Discovery, 2(2):955-974, 1998.

• The VC/SRM/SVM Bible:

Statistical Learning Theory by Vladimir Vapnik, Wiley-Interscience; 1998

The most widely used code library:

http://www.csie.ntu.edu.tw/~cjlin/libsvm/

• A good link:

http://www.kernel-machines.org/

Summary: SVMs for image classification

- 1. Pick an image representation (in our case, bag of features)
- 2. Pick a kernel function for that representation
- 3. Compute the matrix of kernel values between every pair of training examples
- 4. Feed the kernel matrix into your favorite SVM solver to obtain support vectors and weights
- 5. At test time: compute kernel values for your test example and each support vector, and combine them with the learned weights to get the value of the decision function

Category classification – CalTech101

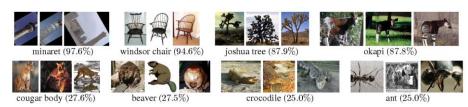


L	Single-level	Pyramid
0(1x1)	41.2±1.2	
1(2x2)	55.9±0.9	57.0 ±0.8
2(4x4)	63.6±0.9	64.6 ±0.8
3(8x8)	60.3±0.9	64.6 ±0.7

Bag-of-features approach by Zhang et al.'07: 54 %

CalTech101

Easiest and hardest classes



- · Sources of difficulty:
 - Lack of texture
 - Camouflage
 - Thin, articulated limbs
 - Highly deformable shape

Evaluation of image classification

- Averaged classification accuracy
- Confusion matrix

		Predicted class		
		Cat	Dog	Rabbit
Actual class	Cat	5	3	0
	Dog	2	3	1
	Rabbit	0	2	11

