Machine Learning – Lecture 9

Nonlinear SVMs

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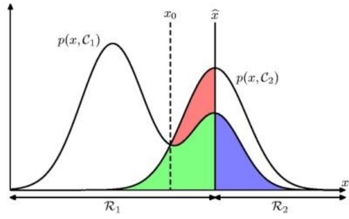
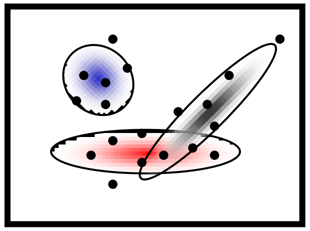
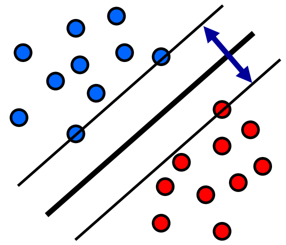
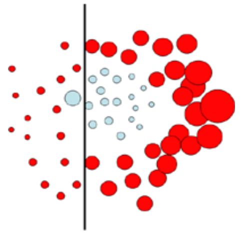
Course Outline

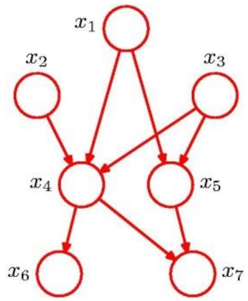
- Fundamentals (2 weeks)
  - Bayes Decision Theory
  - Probability Density Estimation
- Discriminative Approaches (5 weeks)
  - Linear Discriminant Functions
  - Statistical Learning Theory & SVMs
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns
- Generative Models (4 weeks)
  - Bayesian Networks
  - Markov Random Fields

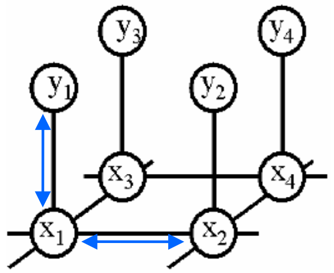












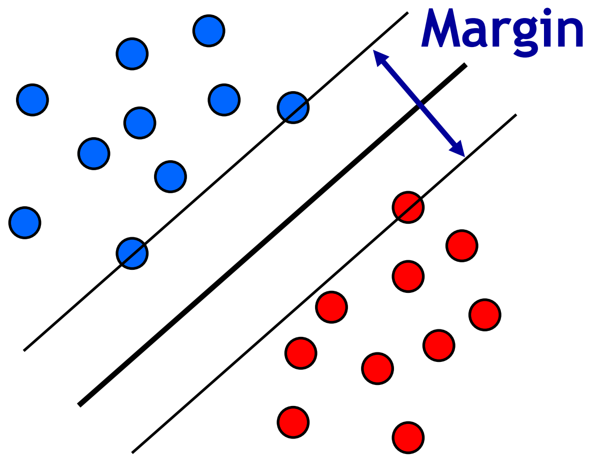
Topics of This Lecture

- Support Vector Machines (Recap)
  - Lagrangian (primal) formulation
  - Dual formulation
  - Soft-margin classification
- Nonlinear Support Vector Machines
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Analysis
  - VC dimensions
  - Error function
- Applications

Recap: Support Vector Machine (SVM)

- Basic idea
  - The SVM tries to find a classifier which maximizes the margin between pos. and neg. data points.
  - Up to now: consider linear classifiers

$$\mathbf{w}^\mathrm{T}\mathbf{x} + b = 0$$



- Formulation as a convex optimization problem
  - Find the hyperplane satisfying

$$\underset{\mathbf{w},b}{\arg\min}\ \frac{1}{2}\|\mathbf{w}\|^2$$

under the constraints

$$t_n(\mathbf{w}^\mathrm{T}\mathbf{x}_n + b) \geq 1 \quad \forall n$$

based on training data points $\mathbf{x}_n$ and target values $t_n \in \{-1, 1\}$.

Recap: SVM - Primal Formulation

- **Lagrangian primal form**

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left\{ t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) - 1 \right\}$$

$$= \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left\{ t_n y(\mathbf{x}_n) - 1 \right\}$$

- **The solution of L_p needs to fulfill the KKT conditions**
  - **Necessary and sufficient conditions**

$$\begin{aligned} a_n &\geq 0 \\ t_n y(\mathbf{x}_n) - 1 &\geq 0 \\ a_n \left\{ t_n y(\mathbf{x}_n) - 1 \right\} &= 0 \end{aligned}$$

KKT:

$$\begin{aligned} \lambda &\geq 0 \\ f(\mathbf{x}) &\geq 0 \\ \lambda f(\mathbf{x}) &= 0 \end{aligned}$$

Recap: SVM – Solution

- Solution for the hyperplane
  - Computed as a linear combination of the training examples

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \mathbf{x}_n$$

  - Sparse solution: $a_n \neq 0$ only for some points, the support vectors

$\Rightarrow$ Only the SVs actually influence the decision boundary!

  - Compute b by averaging over all support vectors:

$$b = \frac{1}{N_{\mathcal{S}}} \sum_{n \in \mathcal{S}} \left(t_n - \sum_{m \in \mathcal{S}} a_m t_m \mathbf{x}_m^{\mathrm{T}} \mathbf{x}_n \right)$$

Recap: SVM – Support Vectors

- The training points for which $a_n > 0$ are called "support vectors".
- Graphical interpretation:
  - The support vectors are the points on the margin.
  - They *define* the margin and thus the hyperplane.

$\Rightarrow$ All other data points can be discarded!

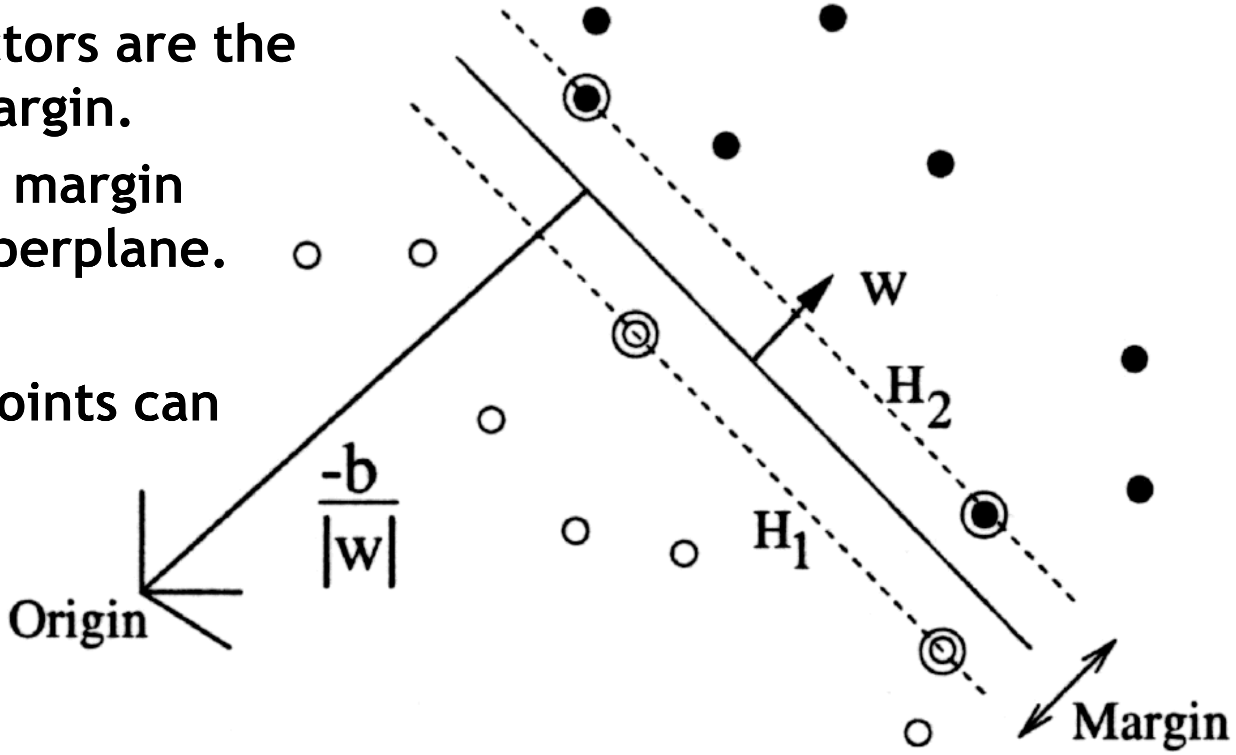


Image source: C. Burges, 1998

Recap: SVM - Dual Formulation

- **Maximize**

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^{\mathrm{T}}\mathbf{x}_n)$$

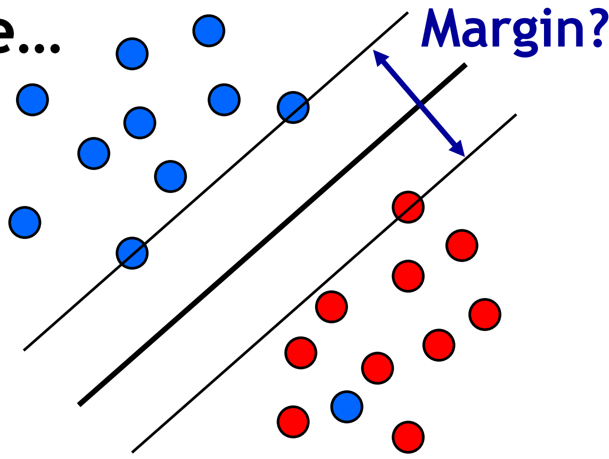
under the conditions

$$\begin{aligned} a_n &\geq 0 \quad \forall n \\ \sum_{n=1}^{N} a_n t_n &= 0 \end{aligned}$$

- **Comparison**
  - L_d **is equivalent to the primal form** L_p**, but only depends on** a_n**.**
  - L_p **scales with** $\mathcal{O}(D^3)$**.**
  - L_d **scales with** $\mathcal{O}(N^3)$ **- in practice between** $\mathcal{O}(N)$ **and** $\mathcal{O}(N^2)$**.**

So Far…

- Only looked at linearly separable case…
  - Current problem formulation has no solution if the data are not linearly separable!
  - Need to introduce some tolerance to outlier data points.



SVM – Non-Separable Data

- Non-separable data
  - I.e. the following inequalities cannot be satisfied for all data points

$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \geq +1 \qquad \text{for} \quad t_n = +1$$
$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \cdot \; -1 \qquad \text{for} \quad t_n = -1$$

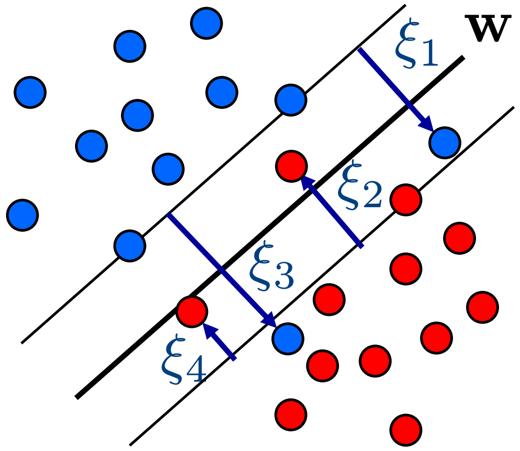
  - Instead use

$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \geq +1 - \xi_n \quad \text{for} \quad t_n = +1$$
$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \cdot \; -1 + \xi_n \quad \text{for} \quad t_n = -1$$

with "slack variables" $\xi_n \geq 0 \quad \forall n$

SVM – Soft-Margin Classification

- Slack variables
  - One slack variable $\xi_n \geq 0$ for each training data point.
- Interpretation
  - $\xi_n = 0$ for points that are on the correct side of the margin.
  - $\xi_n = |t_n - y(\mathbf{x}_n)|$ for all other points (linear penalty).



Point on decision boundary: $\xi_n = 1$

Misclassified point: $\xi_n > 1$

  - We do not have to set the slack variables ourselves!

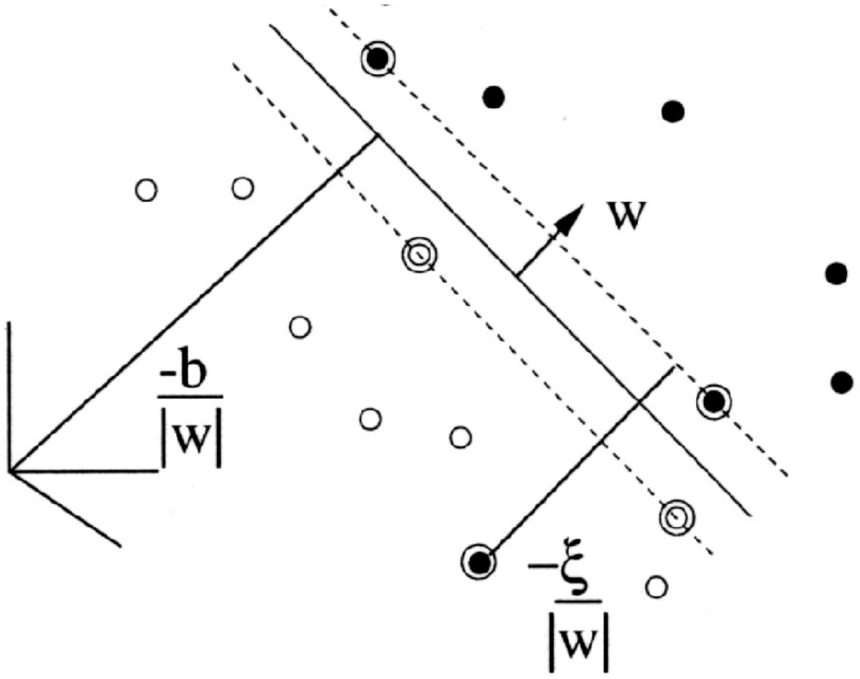
$\Rightarrow$ They are jointly optimized together with $\mathbf{w}$.

How that?

SVM – Non-Separable Data

- Separable data
  - Minimize $$\frac{1}{2}\|\mathbf{w}\|^2$$
- Non-separable data
  - Minimize $$\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

Trade-off parameter!



SVM – New Primal Formulation

- **New SVM Primal: Optimize**

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \underbrace{\sum_{n=1}^{N} a_n\left(t_n y(\mathbf{x}_n) - 1 + \xi_n\right)}_{\substack{\textbf{Constraint} \\ t_n y(\mathbf{x}_n) \geq 1 - \xi_n}} - \underbrace{\sum_{n=1}^{N}\mu_n\xi_n}_{\substack{\textbf{Constraint} \\ \xi_n \geq 0}}$$

- **KKT conditions**

$$\begin{aligned} a_n &\geq 0 \\ t_n y(\mathbf{x}_n) - 1 + \xi_n &\geq 0 \\ a_n\left(t_n y(\mathbf{x}_n) - 1 + \xi_n\right) &= 0 \end{aligned} \qquad \begin{aligned} \mu_n &\geq 0 \\ \xi_n &\geq 0 \\ \mu_n\xi_n &= 0 \end{aligned}$$

KKT:

$$\boxed{\begin{aligned} \lambda &\geq 0 \\ f(\mathbf{x}) &\geq 0 \\ \lambda f(\mathbf{x}) &= 0 \end{aligned}}$$

SVM – New Dual Formulation

- **New SVM Dual: Maximize**

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^{\mathrm{T}}\mathbf{x}_n)$$

under the conditions

$$0 \cdot \quad a_n \cdot \quad C$$

$$\sum_{n=1}^{N} a_n t_n \quad = \quad 0$$

This is all that changed!

- **This is again a quadratic programming problem**
  - $\Rightarrow$ Solve as before... (more on that later)

SVM – New Solution

- Solution for the hyperplane
  - Computed as a linear combination of the training examples

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \mathbf{x}_n$$

  - Again sparse solution: $a_n = 0$ for points outside the margin.

$\Rightarrow$ The slack points with $\xi_n > 0$ are now also support vectors!

  - Compute b by averaging over all $N_{\mathcal{M}}$ points with $0 < a_n < C$:

$$b = \frac{1}{N_{\mathcal{M}}} \sum_{n \in \mathcal{M}} \left(t_n - \sum_{m \in \mathcal{M}} a_m t_m \mathbf{x}_m^{\mathrm{T}} \mathbf{x}_n \right)$$

Interpretation of Support Vectors

- **Those are the hard examples!**
  - **We can visualize them, e.g. for face detection**

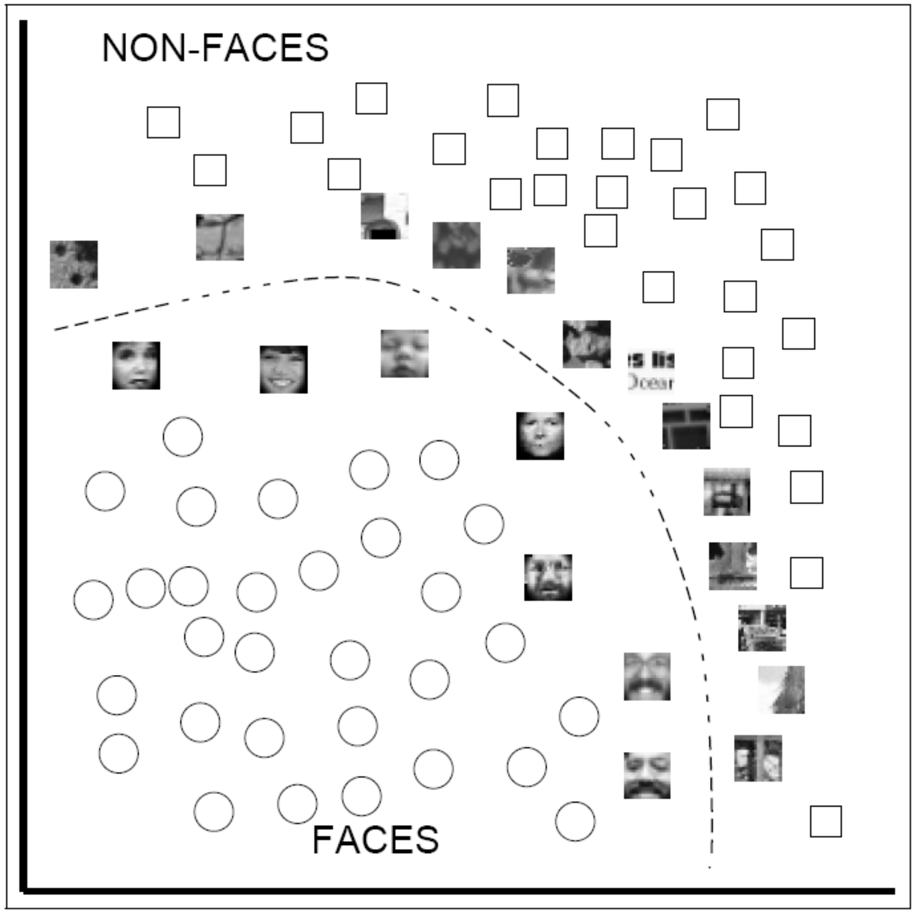


Image source: E. Osuna, F. Girosi, 1997

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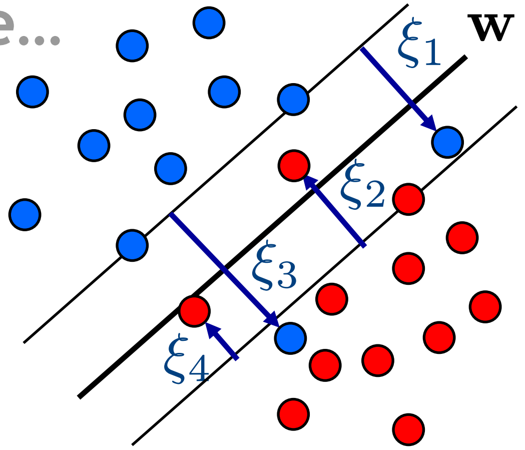
  - Current problem formulation has no solution if the data are not linearly separable!
  - Need to introduce some tolerance to outlier data points.
  - $\Rightarrow$ Slack variables. ✓



- Only looked at linear decision boundaries…
  - This is not sufficient for many applications.
  - Want to generalize the ideas to non-linear boundaries.

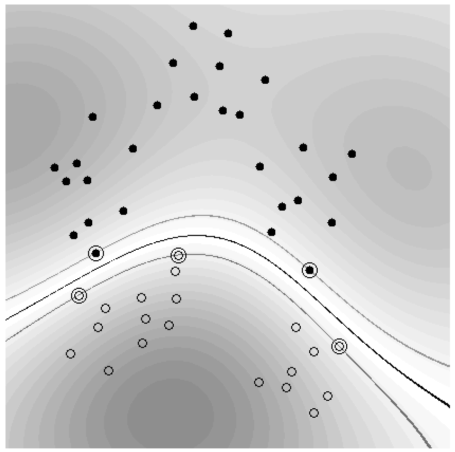
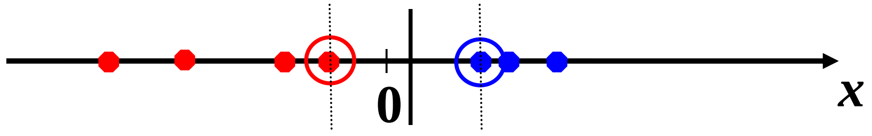


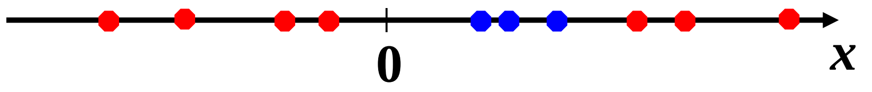
Image source: B. Schoelkopf, A. Smola, 2002

Nonlinear SVM

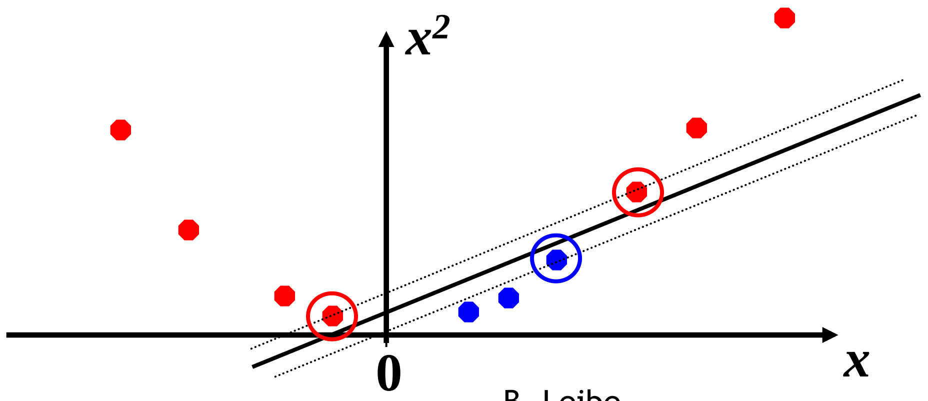
- Linear SVMs
  - Datasets that are linearly separable with some noise work well:



  - But what are we going to do if the dataset is just too hard?



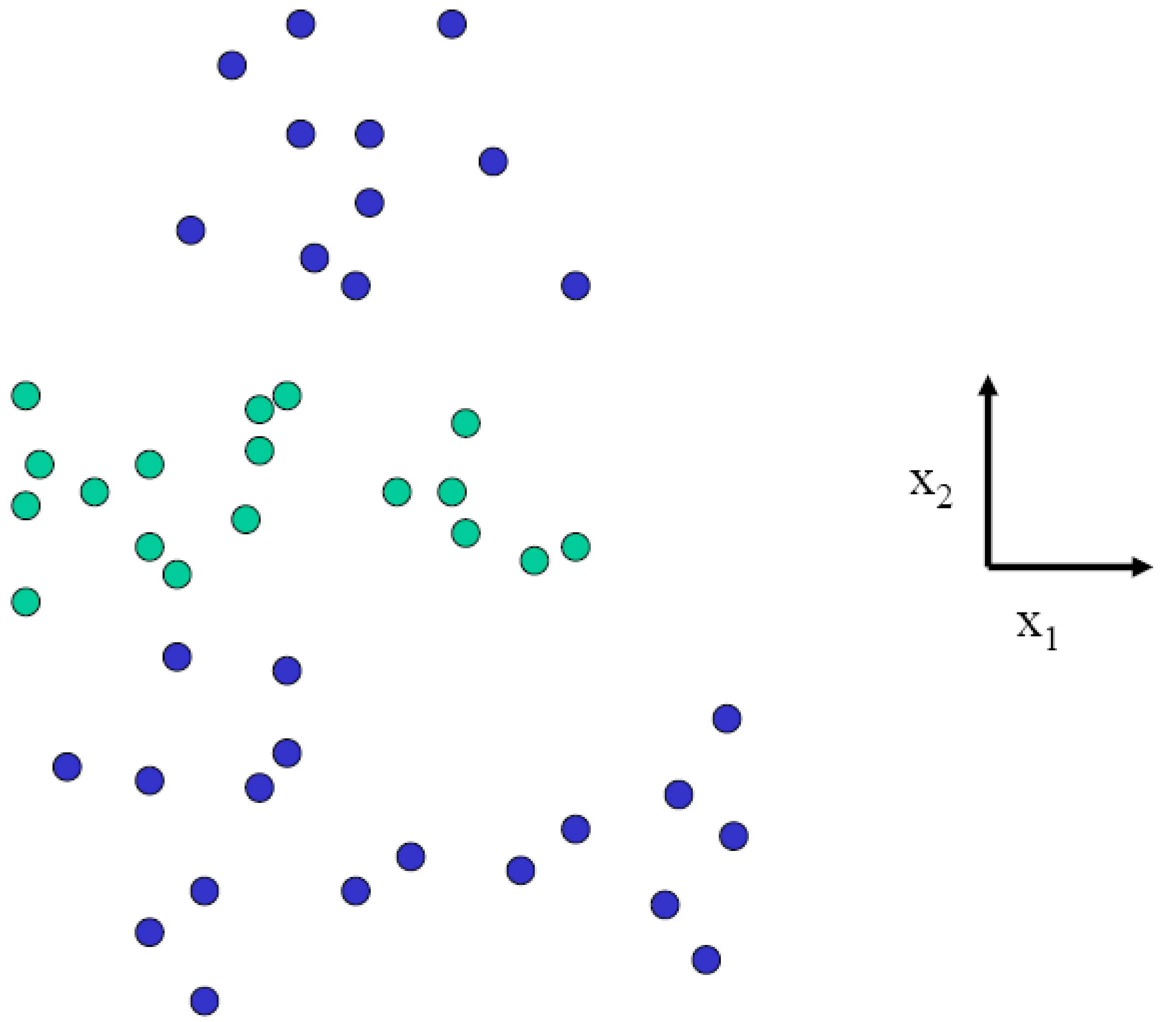
  - How about… mapping data to a higher-dimensional space:



Slide credit: Raymond Mooney

Another Example

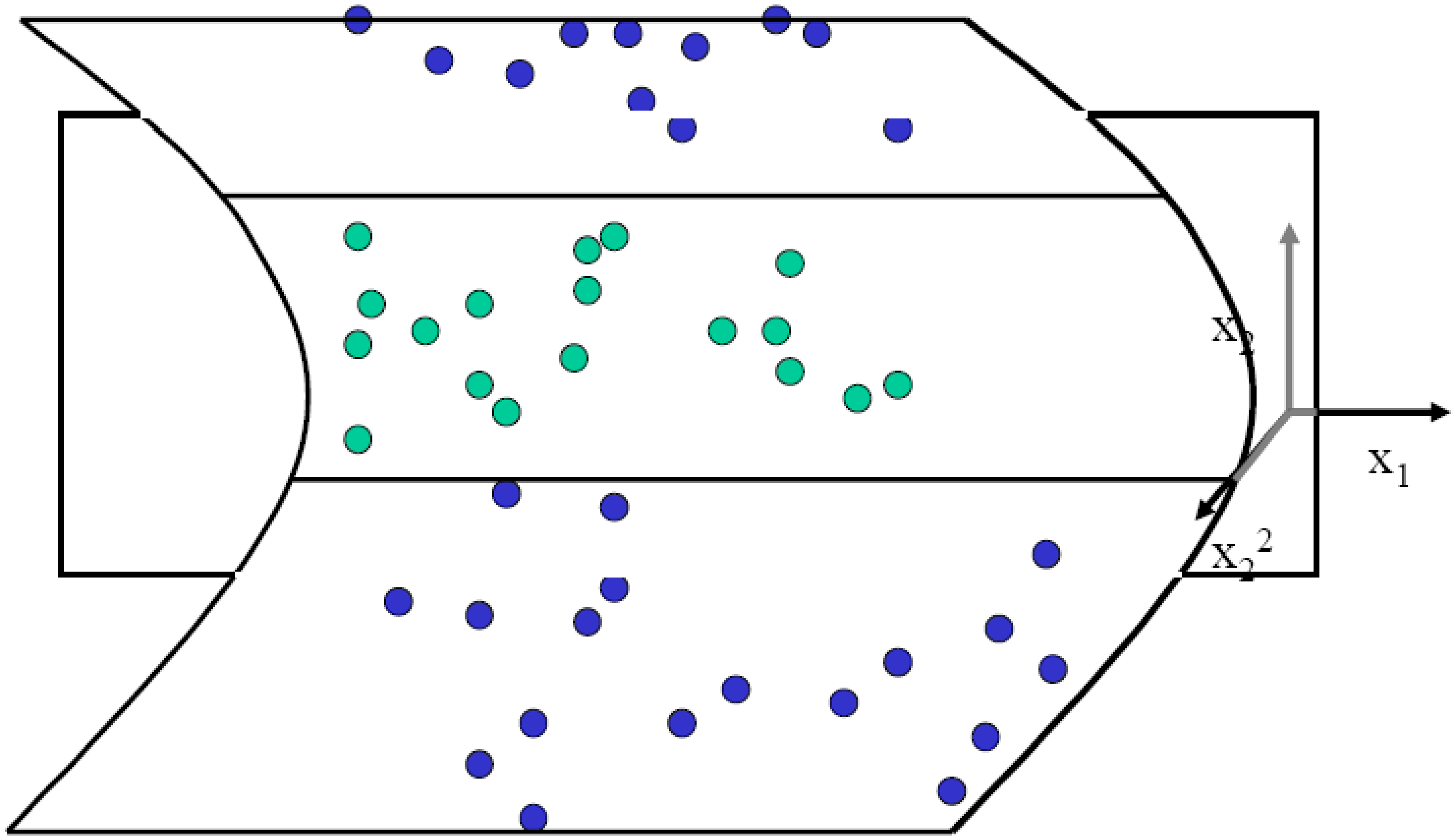
- Non-separable by a hyperplane in 2D



Slide credit: Bill Freeman

Another Example

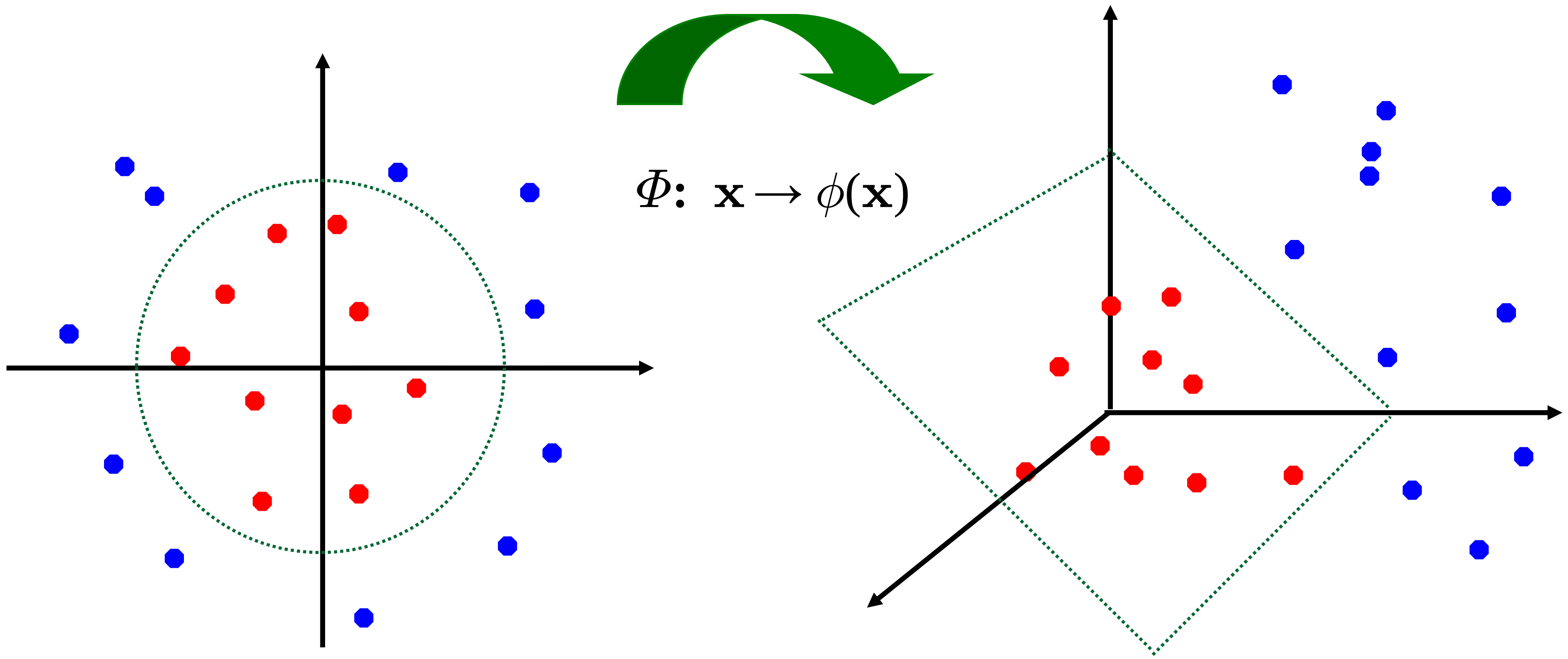
- Separable by a surface in 3D



Slide credit: Bill Freeman

Nonlinear SVM – Feature Spaces

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



Slide credit: Raymond Mooney

Nonlinear SVM

- **General idea**
  - **Nonlinear transformation ϕ of the data points $\mathbf{x}_n$:**

$$\mathbf{x} \in \mathbb{R}^D \quad \phi : \mathbb{R}^D \rightarrow \mathcal{H}$$

  - **Hyperplane in higher-dim. space $\mathcal{H}$ (linear classifier in $\mathcal{H}$)**

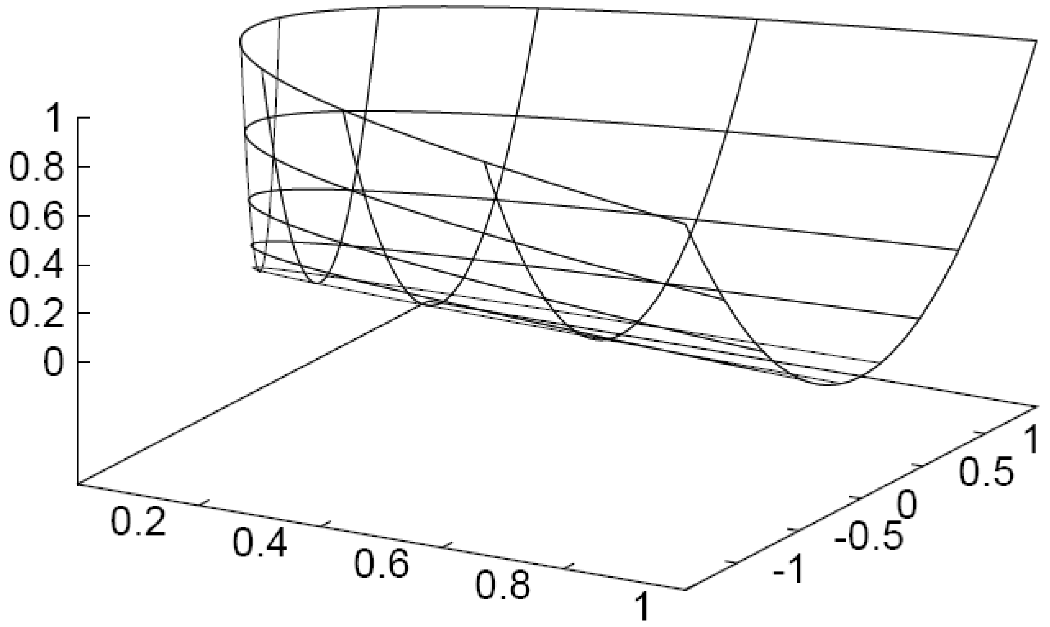
$$\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b = 0$$

$\Rightarrow$ **Nonlinear classifier in $\mathbb{R}^D$.**

What Could This Look Like?

- **Example:**
  - **Mapping to polynomial space, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$:**

$$\phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix}$$



  - **Motivation: Easier to separate data in higher-dimensional space.**
  - **But wait - isn't there a big problem?**
    - How should we evaluate the decision function?

Image source: C. Burges, 1998

Problem with High-dim. Basis Functions

- Problem
  - In order to apply the SVM, we need to evaluate the function

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b$$

  - Using the hyperplane, which is itself defined as

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n)$$

$\Rightarrow$ What happens if we try this for a million-dimensional feature space $\phi(\mathbf{x})$?

  - Oh-oh…

Solution: The Kernel Trick

- **Important observation**
  - $\phi(\mathbf{x})$ only appears in the form of dot products $\phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{y})$:

$$\begin{aligned} y(\mathbf{x}) &= \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b \\ &= \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n)^{\mathrm{T}}\phi(\mathbf{x}) + b \end{aligned}$$

  - Trick: Define a so-called **kernel function** $k(\mathbf{x},\mathbf{y}) = \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{y})$.
  - Now, in place of the dot product, use the kernel instead:

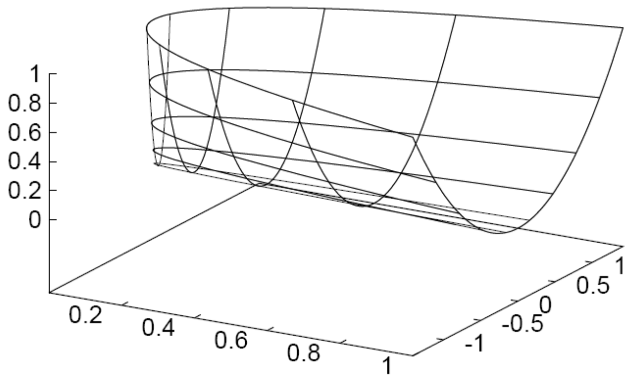
$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

  - The kernel function *implicitly* maps the data to the higher-dimensional space (without having to compute $\phi(\mathbf{x})$ explicitly)!

Back to Our Previous Example…

- 2nd degree polynomial kernel:

$$\phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{y}) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \cdot \begin{bmatrix} y_1^2 \\ \sqrt{2}y_1y_2 \\ y_2^2 \end{bmatrix}$$



$$= x_1^2y_1^2 + 2x_1x_2y_1y_2 + x_2^2y_2^2$$

$$= (\mathbf{x}^{\mathrm{T}}\mathbf{y})^2 =: k(\mathbf{x},\mathbf{y})$$

  - Whenever we evaluate the kernel function $k(\mathbf{x},\mathbf{y}) = (\mathbf{x}^{\mathsf{T}}\mathbf{y})^2$, we implicitly compute the dot product in the higher-dimensional feature space.

Image source: C. Burges, 1998

SVMs with Kernels

- Using kernels
  - Applying the kernel trick is easy. Just replace every dot product by a kernel function…

$$\mathbf{x}^{\mathrm{T}}\mathbf{y} \quad \rightarrow \quad k(\mathbf{x},\mathbf{y})$$

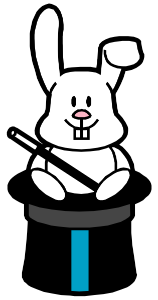
  - …and we're done.
  - Instead of the raw input space, we're now working in a higher-dimensional (potentially infinite dimensional!) space, where the data is more easily separable.

"Sounds like magic…"

- Wait - does this always work?
  - The kernel needs to define an implicit mapping to a higher-dimensional feature space $\phi(\mathbf{x})$.
  - When is this the case?

Which Functions are Valid Kernels?

- Mercer's theorem (modernized version):
  - *Every positive definite symmetric function is a kernel.*



- Positive definite symmetric functions correspond to a positive definite symmetric Gram matrix:

$K =$

$k(\mathbf{x}_1,\mathbf{x}_1)$	$k(\mathbf{x}_1,\mathbf{x}_2)$	$k(\mathbf{x}_1,\mathbf{x}_3)$	$\ldots$	$k(\mathbf{x}_1,\mathbf{x}_n)$
$k(\mathbf{x}_2,\mathbf{x}_1)$	$k(\mathbf{x}_2,\mathbf{x}_2)$	$k(\mathbf{x}_2,\mathbf{x}_3)$		$k(\mathbf{x}_2,\mathbf{x}_n)$
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$
$k(\mathbf{x}_n,\mathbf{x}_1)$	$k(\mathbf{x}_n,\mathbf{x}_2)$	$k(\mathbf{x}_n,\mathbf{x}_3)$	$\ldots$	$k(\mathbf{x}_n,\mathbf{x}_n)$

(positive definite = all eigenvalues are > 0)

Slide credit: Raymond Mooney

Kernels Fulfilling Mercer's Condition

- **Polynomial kernel**

$$k(\mathbf{x},\mathbf{y}) = (\mathbf{x}^{\mathrm{T}}\mathbf{y} + 1)^p$$

- **Radial Basis Function kernel**

$$k(\mathbf{x},\mathbf{y}) = \exp\left\{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}\right\}$$

e.g. Gaussian

- **Hyperbolic tangent kernel**

$$\cancel{k(\mathbf{x},\mathbf{y}) = \tanh(\kappa\mathbf{x}^{\mathrm{T}}\mathbf{y} + \delta)}$$

e.g. Sigmoid

Actually, this was wrong in the original SVM paper...

(and many, many more...)

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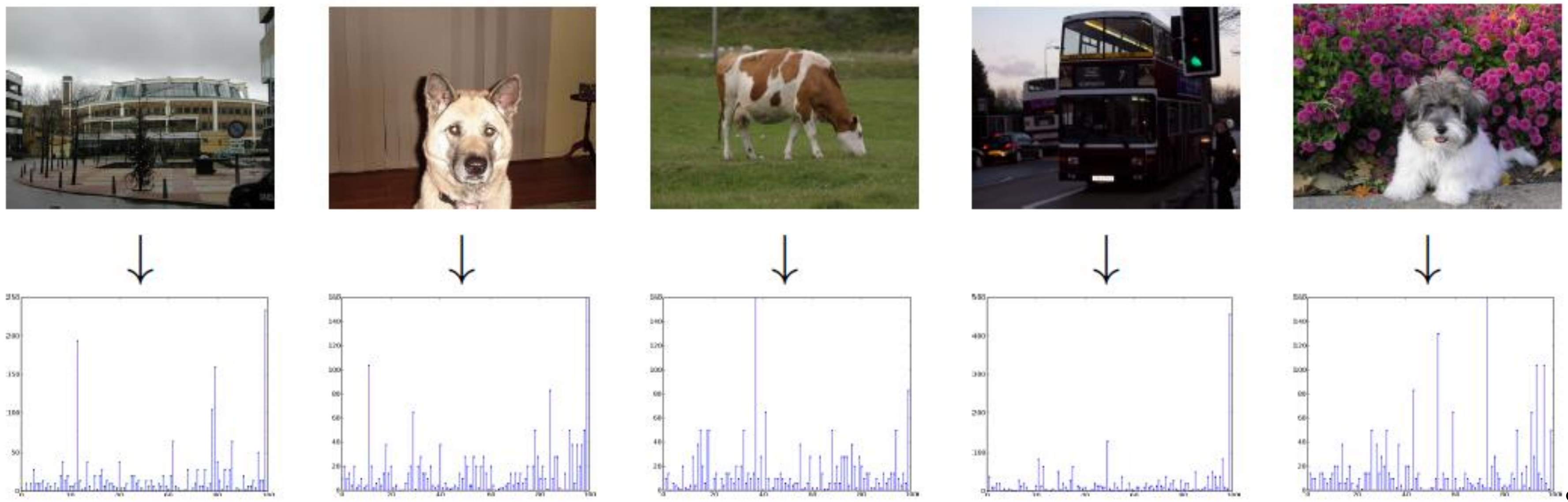
Example: Bag of Visual Words Representation

- General framework in visual recognition
  - Create a codebook (vocabulary) of prototypical image features
  - Represent images as histograms over codebook activations
  - Compare two images by any histogram kernel, e.g. χ^2 kernel

$$k_{\chi^2}(h, h') = \exp\left(-\frac{1}{\gamma}\sum_j \frac{(h_j - h'_j)^2}{h_j + h'_j}\right)$$



Nonlinear SVM – Dual Formulation

- **SVM Dual: Maximize**

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_m, \mathbf{x}_n)$$

under the conditions

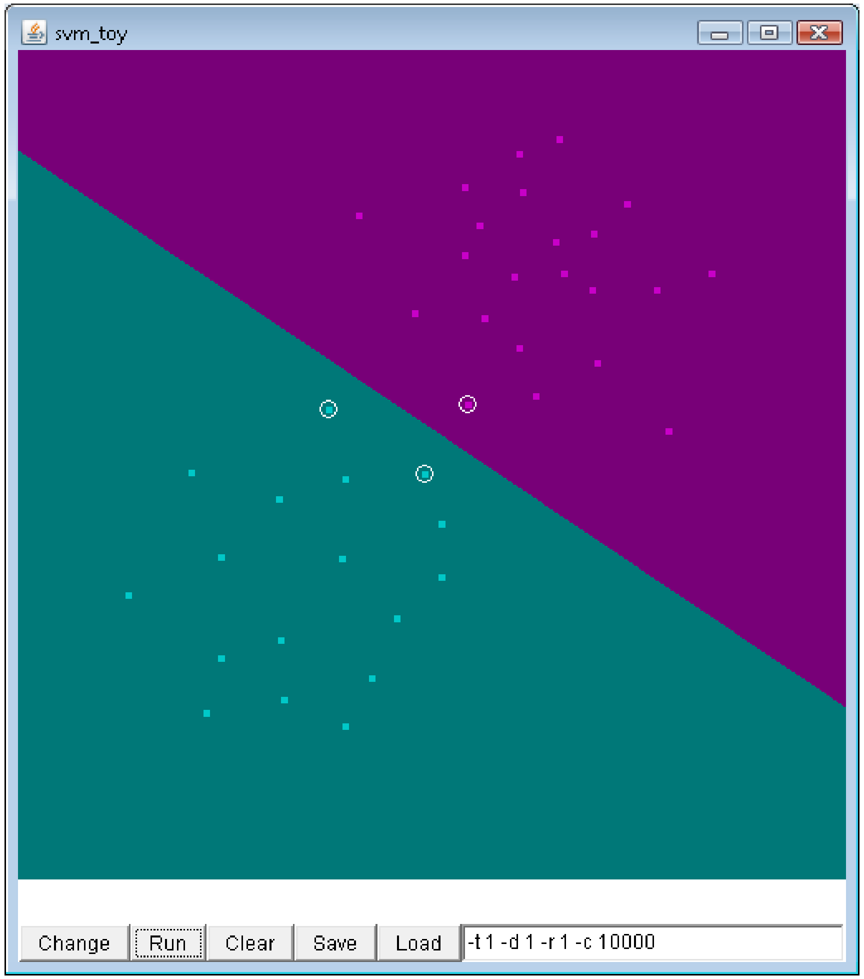
$$0 \cdot a_n \cdot C$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

- **Classify new data points using**

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

SVM Demo



-t 1 -d 1 -r 1 -c 10000

Applet from libsvm
(http://www.csie.ntu.edu.tw/~cjlin/libsvm/)

Summary: SVMs

- Properties
  - Empirically, SVMs work very, very well.
  - SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
  - SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.
  - SVM techniques have been applied to a variety of other tasks
    - e.g. SV Regression, One-class SVMs, …
  - The kernel trick has been used for a wide variety of applications. It can be applied wherever dot products are in use
    - e.g. Kernel PCA, kernel FLD, …
    - Good overview, software, and tutorials available on http://www.kernel-machines.org/

Summary: SVMs

- Limitations
  - How to select the right kernel?
    - Best practice guidelines are available for many applications
  - How to select the kernel parameters?
    - (Massive) cross-validation.
    - Usually, several parameters are optimized together in a grid search.
  - Solving the quadratic programming problem
    - Standard QP solvers do not perform too well on SVM task.
    - Dedicated methods have been developed for this, e.g. SMO.
  - Speed of evaluation
    - Evaluating $y(\mathbf{x})$ scales linearly in the number of SVs.
    - Too expensive if we have a large number of support vectors.

    $\Rightarrow$ There are techniques to reduce the effective SV set.
  - Training for very large datasets (millions of data points)
    - Stochastic gradient descent and other approximations can be used

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Recap: Kernels Fulfilling Mercer's Condition

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e.g. Gaussian

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(and many, many more...)

VC Dimension for Polynomial Kernel

- **Polynomial kernel of degree p:**

$$k(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^{\mathrm{T}} \mathbf{y})^p$$

  - **Dimensionality of $\mathcal{H}$:** $\binom{D+p-1}{p}$

  - **Example:**

$$\begin{aligned} D &= 16 \times 16 = 256 \\ p &= 4 \\ \dim(\mathcal{H}) &= 183.181.376 \end{aligned}$$

  - **The hyperplane in $\mathcal{H}$ then has VC-dimension**

$$\dim(\mathcal{H}) + 1$$

VC Dimension for Gaussian RBF Kernel

- **Radial Basis Function:**

$$k(\mathbf{x},\mathbf{y}) = \exp\left\{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}\right\}$$

  - **In this case, $\mathcal{H}$ is infinite dimensional!**

$$\exp(\mathbf{x}) = 1 + \frac{\mathbf{x}}{1!} + \frac{\mathbf{x}^2}{2!} + \ldots + \frac{\mathbf{x}^n}{n!} + \ldots$$

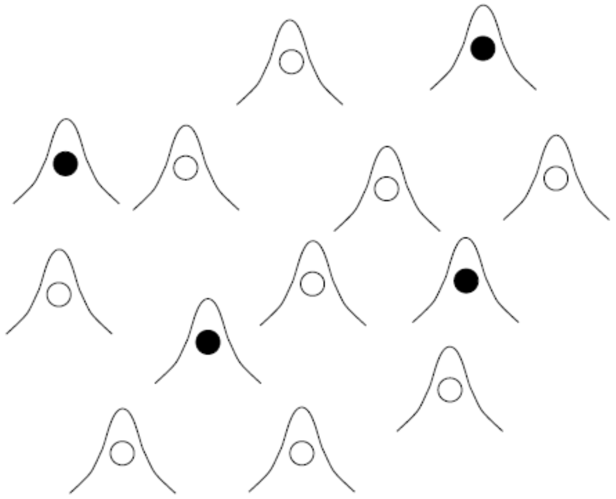
  - **Since only the kernel function is used by the SVM, this is no problem.**

  - **The hyperplane in $\mathcal{H}$ then has VC-dimension**

$$\dim(\mathcal{H}) + 1 = \infty$$

VC Dimension for Gaussian RBF Kernel

- Intuitively
  - If we make the radius of the RBF kernel sufficiently small, then each data point can be associated with its own kernel.

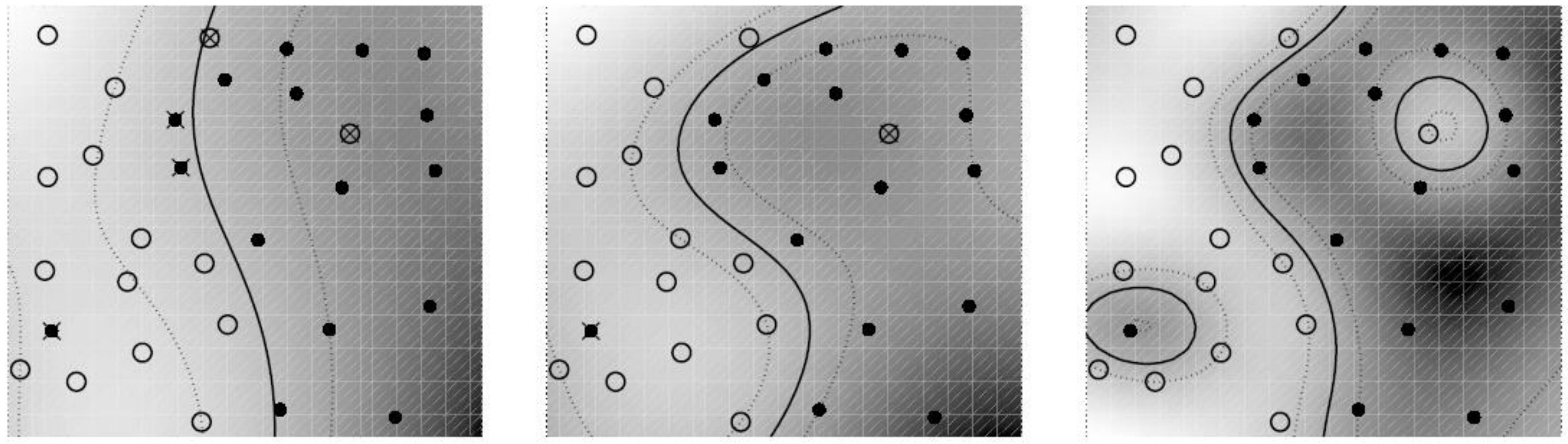


  - However, this also means that we can get finite VC-dimension if we set a lower limit to the RBF radius.

Image source: C. Burges

Example: RBF Kernels

- Decision boundary on toy problem



RBF Kernel width (σ)

Image source: B. Schoelkopf, A. Smola, 2002

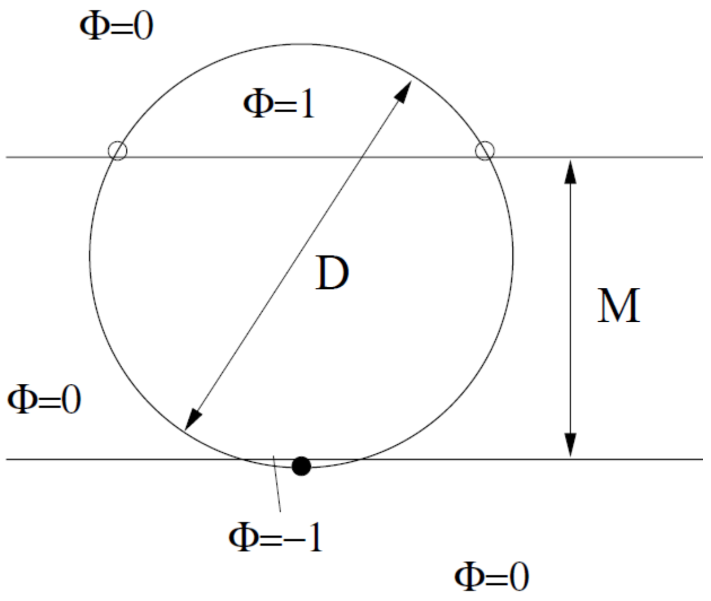
But... but... but...

- Don’t we risk overfitting with those enormously high-dimensional feature spaces?
  - No matter what the basis functions are, there are really only up to N parameters: a_1, a_2,..., a_N and most of them are usually set to zero by the maximum margin criterion.
  - The data effectively lives in a low-dimensional subspace of $\mathcal{H}$.

- What about the VC dimension? I thought low VC-dim was good (in the sense of the risk bound)?
  - Yes, but the maximum margin classifier “magically” solves this.
  - Reason (Vapnik): by maximizing the margin, we can reduce the VC-dimension.
  - Empirically, SVMs have very good generalization performance.

Theoretical Justification for Maximum Margins

- Gap Tolerant Classifier
  - Classifier is defined by a ball in $\mathbb{R}^d$ with diameter D enclosing all points and two parallel hyperplanes with distance M (the margin).
  - Points in the ball are assigned class $\{$-1,1$\}$ depending on which side of the margin they fall.



- VC dimension of this classifier depends on the margin
  - $M \leq 3/4\ D$ $\Rightarrow$ 3 points can be shattered
  - $3/4\ D < M < D$ $\Rightarrow$ 2 points can be shattered
  - $M \geq D$ $\Rightarrow$ 1 point can be shattered

  $\Rightarrow$ By maximizing the margin, we can minimize the VC dimension

Image source: C. Burges

Theoretical Justification for Maximum Margins

- For the general case, Vapnik has proven the following:
  - *The class of optimal linear separators has VC dimension h bounded from above as*

$$h \leq \min\left\{\left\lceil \frac{D^2}{\rho^2} \right\rceil, m_0\right\} + 1$$

where ρ is the margin, D is the diameter of the smallest sphere that can enclose all of the training examples, and m_0 is the dimensionality.

- Intuitively, this implies that regardless of dimensionality m_0 we can minimize the VC dimension by maximizing the margin ρ.
- Thus, complexity of the classifier is kept small regardless of dimensionality.

Slide credit: Raymond Mooney

Topics of This Lecture

- Support Vector Machines (Recap)
  - Lagrangian (primal) formulation
  - Dual formulation
  - Soft-margin classification
- Nonlinear Support Vector Machines
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Analysis
  - VC dimensions
  - Error function
- Applications

SVM - Analysis

- **Traditional soft-margin formulation**

$$\min_{\mathbf{w}\in\mathbb{R}^D,\, \xi_n\in\mathbb{R}^+} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

"Maximize the margin"

subject to the constraints

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n$$

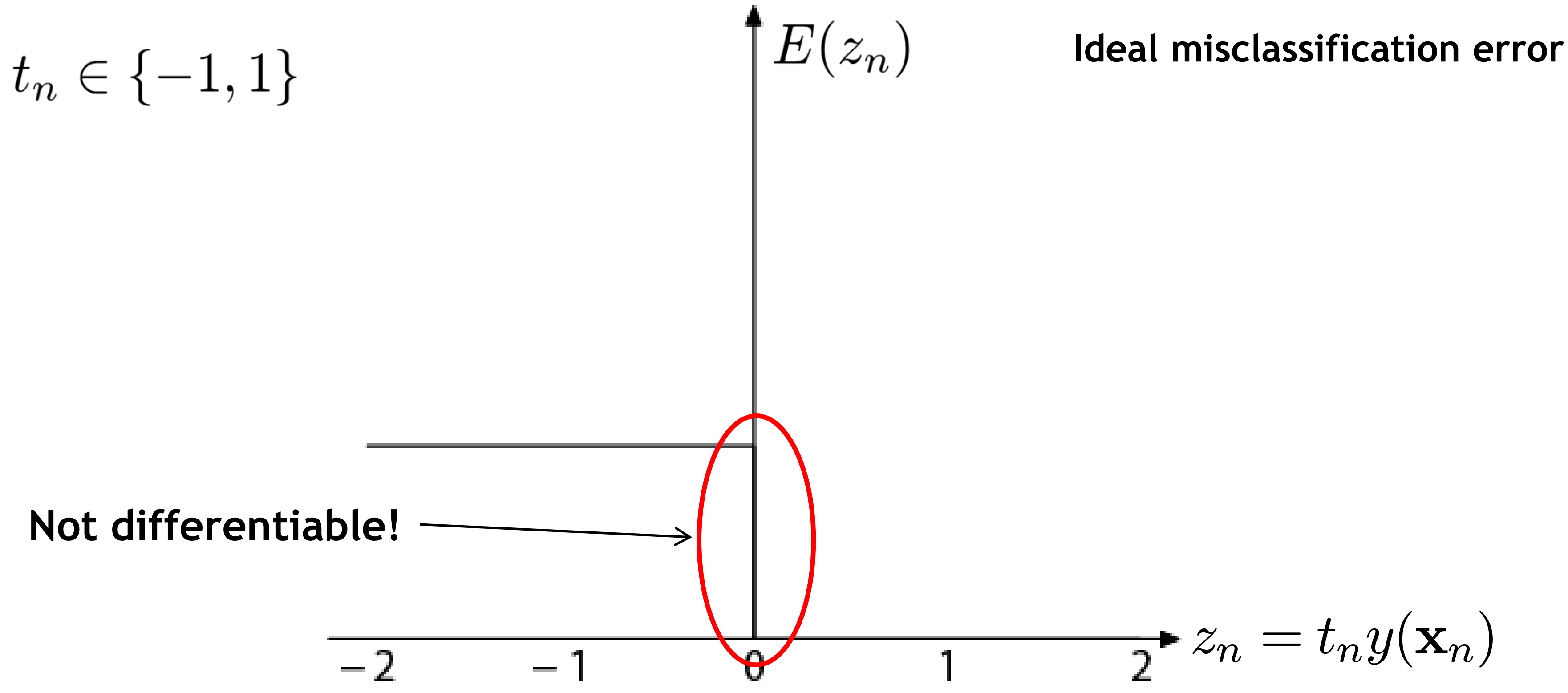
"Most points should be on the correct side of the margin"

- **Different way of looking at it**
  - **We can reformulate the constraints into the objective function.**

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\text{L}_2\text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+}_{\text{"Hinge loss"}}$$

where $[x]_+ := \max\{0,x\}$.

Recap: Error Functions



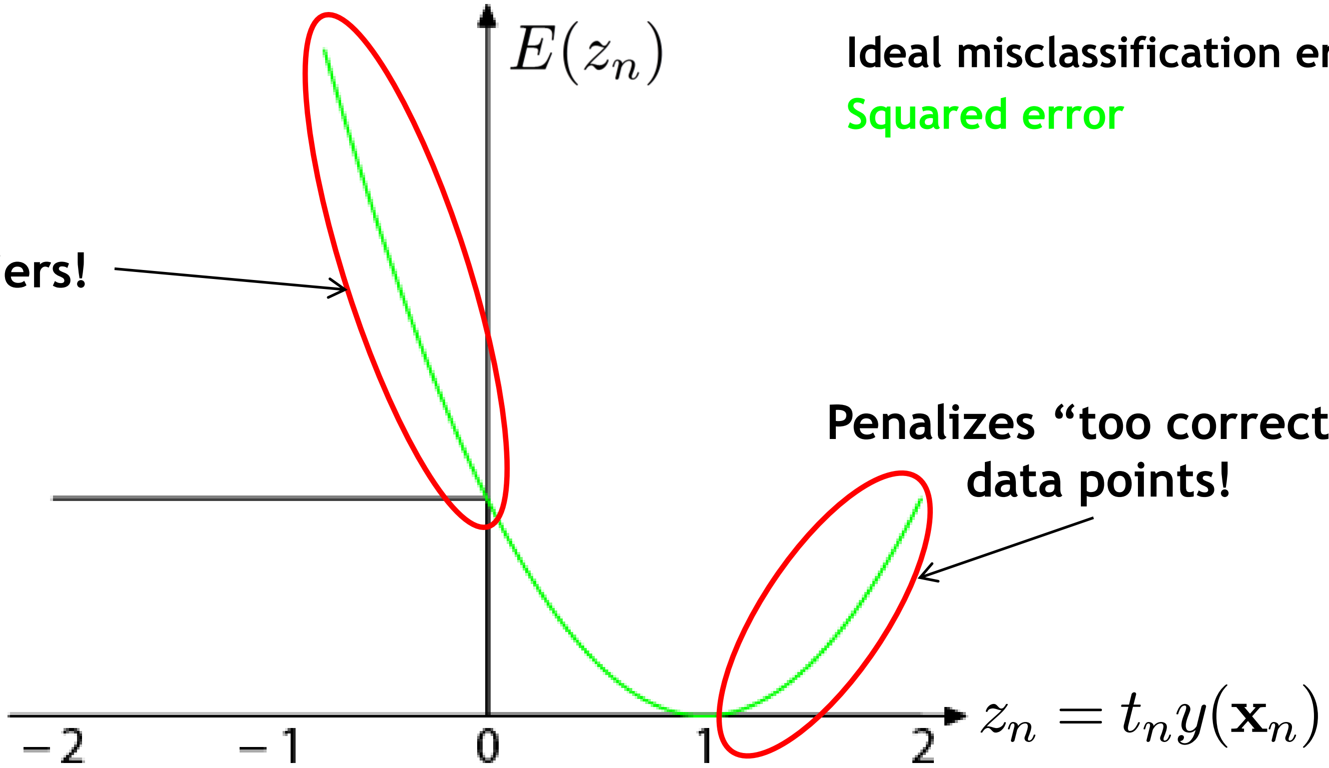
- Ideal misclassification error function (black)
  - This is what we want to approximate,
  - Unfortunately, it is not differentiable.
  - The gradient is zero for misclassified points.

  $\Rightarrow$ We cannot minimize it by gradient descent.

Image source: Bishop, 2006

Recap: Error Functions

$t_n \in \{-1, 1\}$



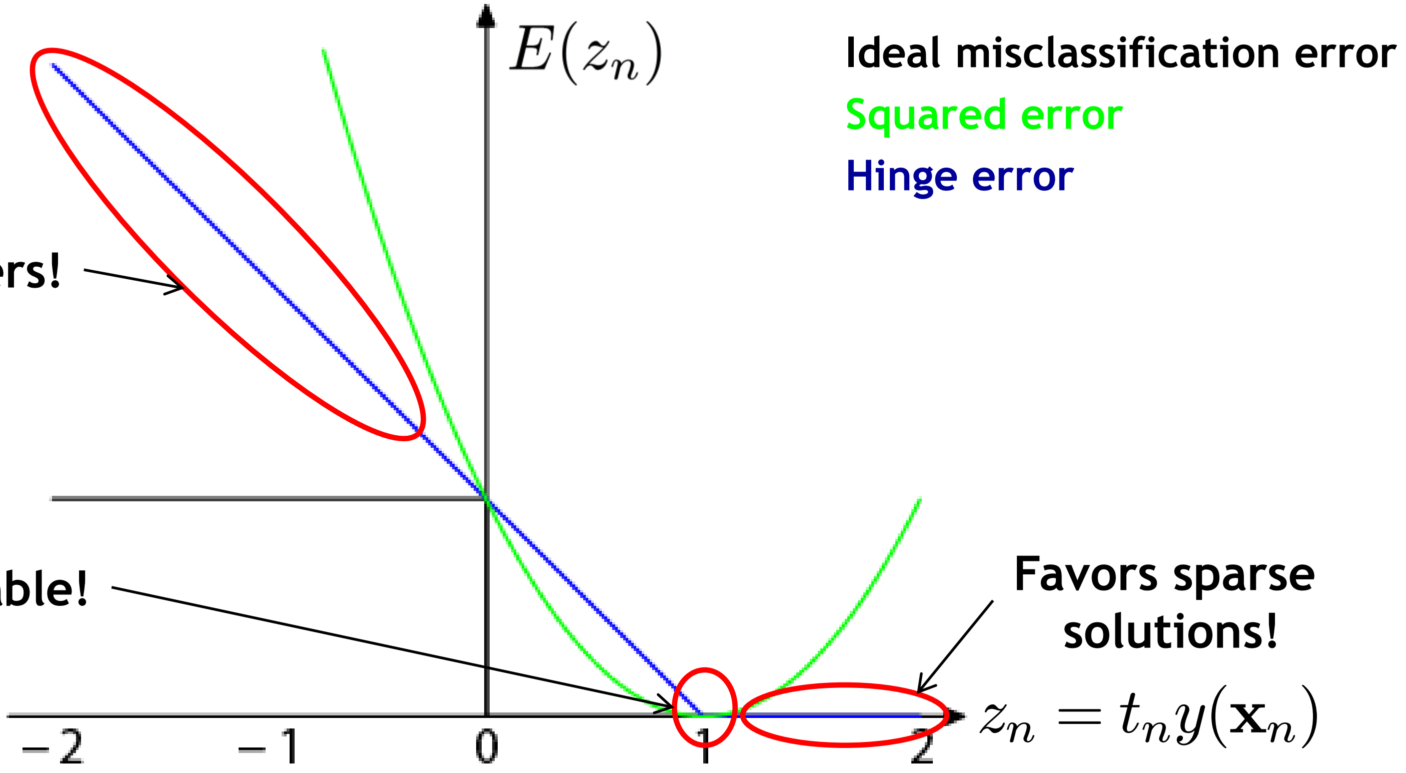
Ideal misclassification error
Squared error

- Squared error used in Least-Squares Classification
  - Very popular, leads to closed-form solutions.
  - However, sensitive to outliers due to squared penalty.
  - Penalizes "too correct" data points

$\Rightarrow$ Generally does not lead to good classifiers.

Image source: Bishop, 2006

Error Functions (Loss Functions)



- “Hinge error” used in SVMs
  - Zero error for points outside the margin ($z_n > 1$) $\Rightarrow$ sparsity
  - Linear penalty for misclassified points ($z_n < 1$) $\Rightarrow$ robustness
  - Not differentiable around $z_n = 1$ $\Rightarrow$ Cannot be optimized directly.

Image source: Bishop, 2006

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SVM – Discussion

- SVM optimization function

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\text{L}_2\text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1-t_n y(\mathbf{x}_n)]_+}_{\text{Hinge loss}}$$

- Hinge loss enforces sparsity
  - Only a subset of training data points actually influences the decision boundary.
  - This is different from sparsity obtained through the regularizer! There, only a subset of input dimensions are used.
  - Unconstrained optimization, but non-differentiable function.
  - Solve, e.g. by *subgradient descent*
  - Currently most efficient: *stochastic gradient descent*

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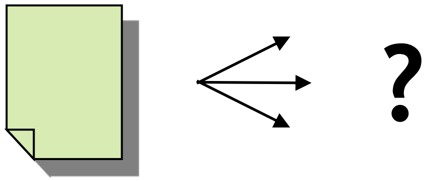
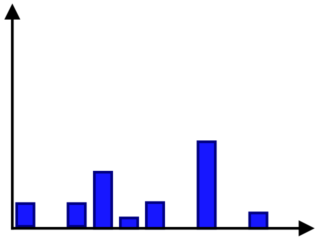
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Analysis
  - VC dimensions
  - Error function
- **Applications**

Example Application: Text Classification

- Problem:
  - Classify a document in a number of categories



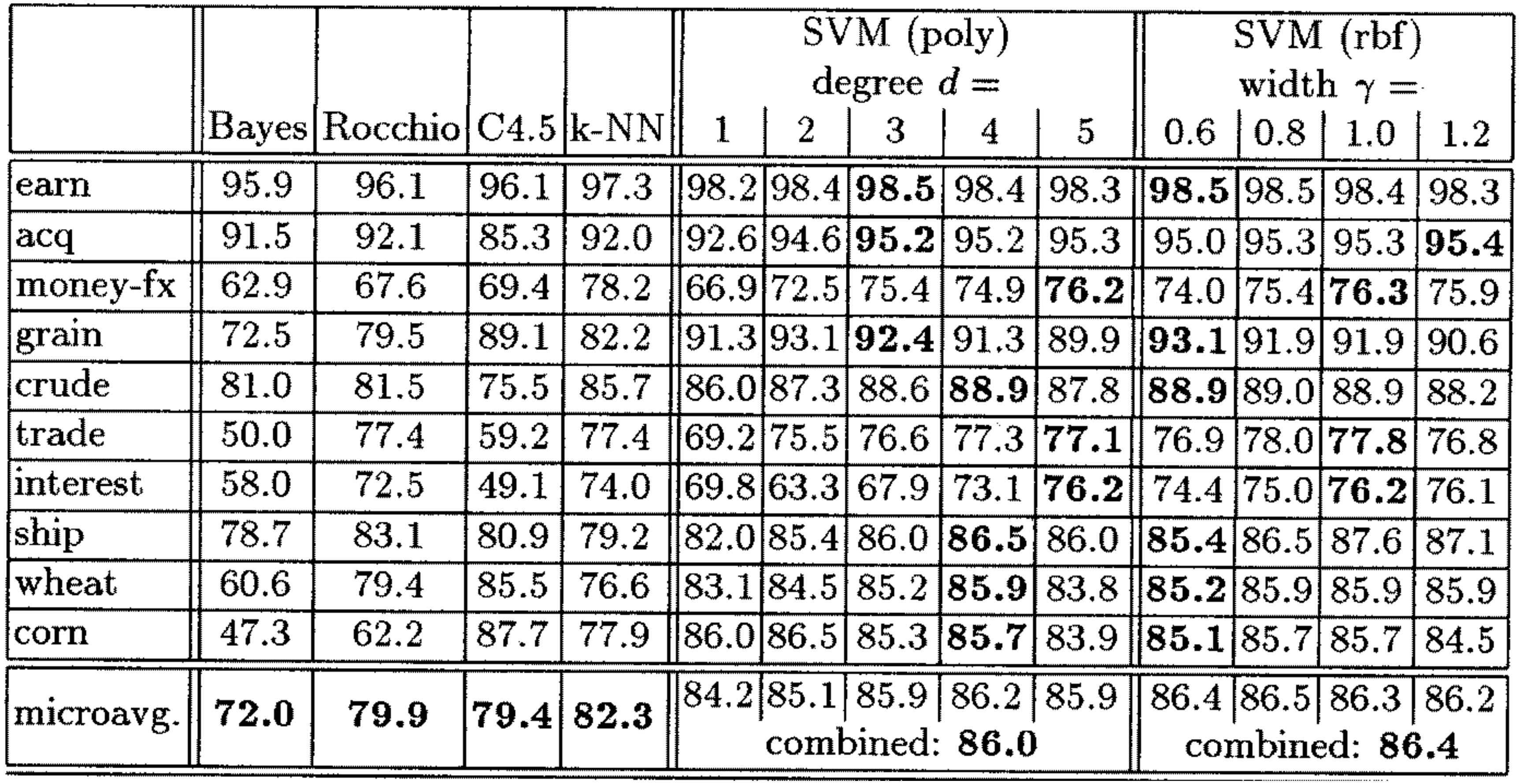
- Representation:
  - "Bag-of-words" approach
  - Histogram of word counts (on learned dictionary)
    - Very high-dimensional feature space (~10.000 dimensions)
    - Few irrelevant features



- This was one of the first applications of SVMs
  - T. Joachims (1997)

Example Application: Text Classification

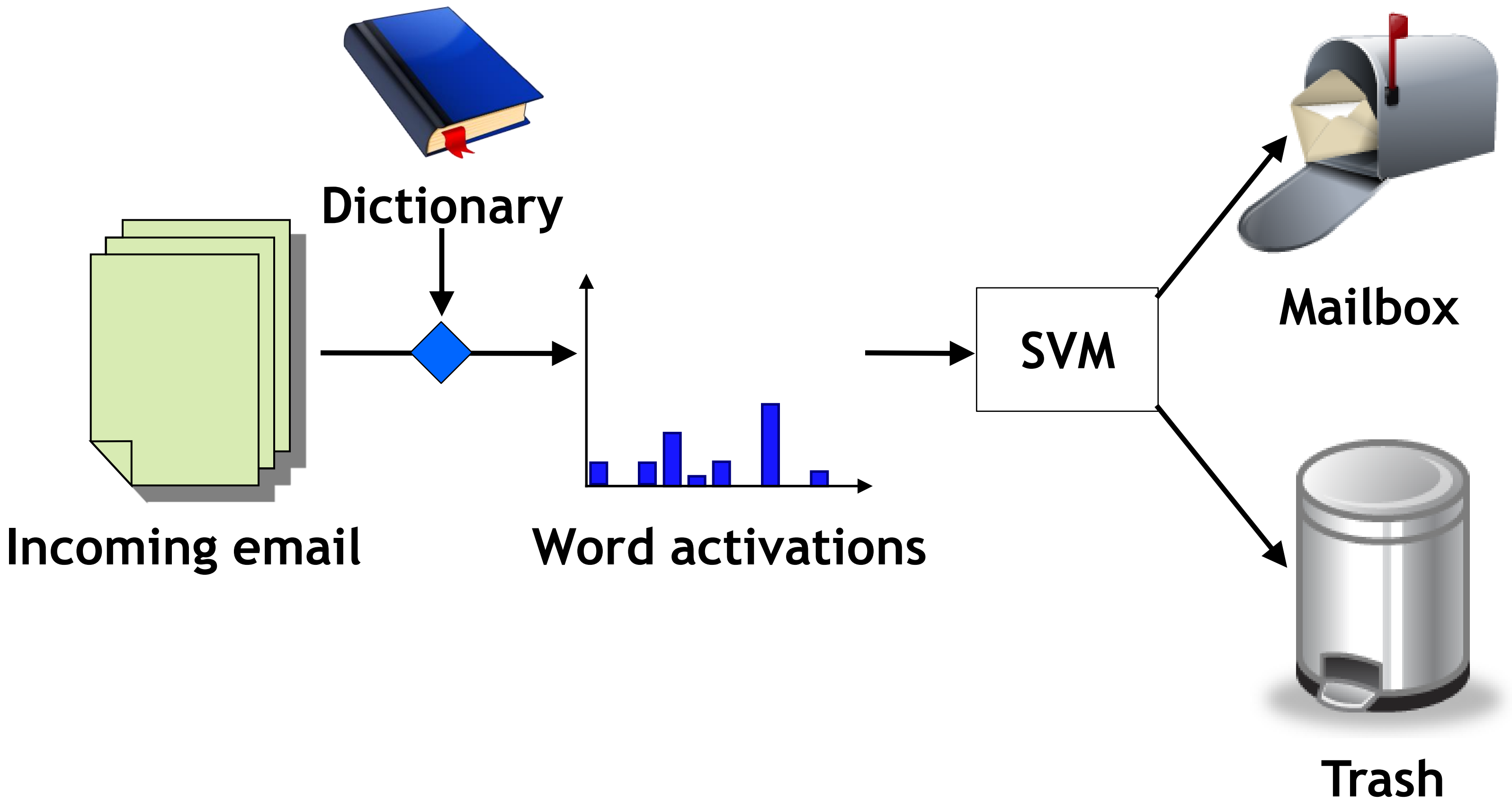
- **Results:**



					SVM (poly) degree $d =$					SVM (rbf) width $\gamma =$			
	Bayes	Rocchio	C4.5	k-NN	1	2	3	4	5	0.6	0.8	1.0	1.2
earn	95.9	96.1	96.1	97.3	98.2	98.4	**98.5**	98.4	98.3	**98.5**	98.5	98.4	98.3
acq	91.5	92.1	85.3	92.0	92.6	94.6	**95.2**	95.2	95.3	95.0	95.3	95.3	**95.4**
money-fx	62.9	67.6	69.4	78.2	66.9	72.5	75.4	74.9	**76.2**	74.0	75.4	**76.3**	75.9
grain	72.5	79.5	89.1	82.2	91.3	93.1	**92.4**	91.3	89.9	**93.1**	91.9	91.9	90.6
crude	81.0	81.5	75.5	85.7	86.0	87.3	88.6	**88.9**	87.8	**88.9**	89.0	88.9	88.2
trade	50.0	77.4	59.2	77.4	69.2	75.5	76.6	77.3	**77.1**	76.9	78.0	**77.8**	76.8
interest	58.0	72.5	49.1	74.0	69.8	63.3	67.9	73.1	**76.2**	74.4	75.0	**76.2**	76.1
ship	78.7	83.1	80.9	79.2	82.0	85.4	86.0	**86.5**	86.0	**85.4**	86.5	87.6	87.1
wheat	60.6	79.4	85.5	76.6	83.1	84.5	85.2	**85.9**	83.8	**85.2**	85.9	85.9	85.9
corn	47.3	62.2	87.7	77.9	86.0	86.5	85.3	**85.7**	83.9	**85.1**	85.7	85.7	84.5
microavg.	**72.0**	**79.9**	**79.4**	**82.3**	84.2	85.1	85.9	86.2	85.9	86.4	86.5	86.3	86.2
					combined: **86.0**					combined: **86.4**			

Example Application: Text Classification

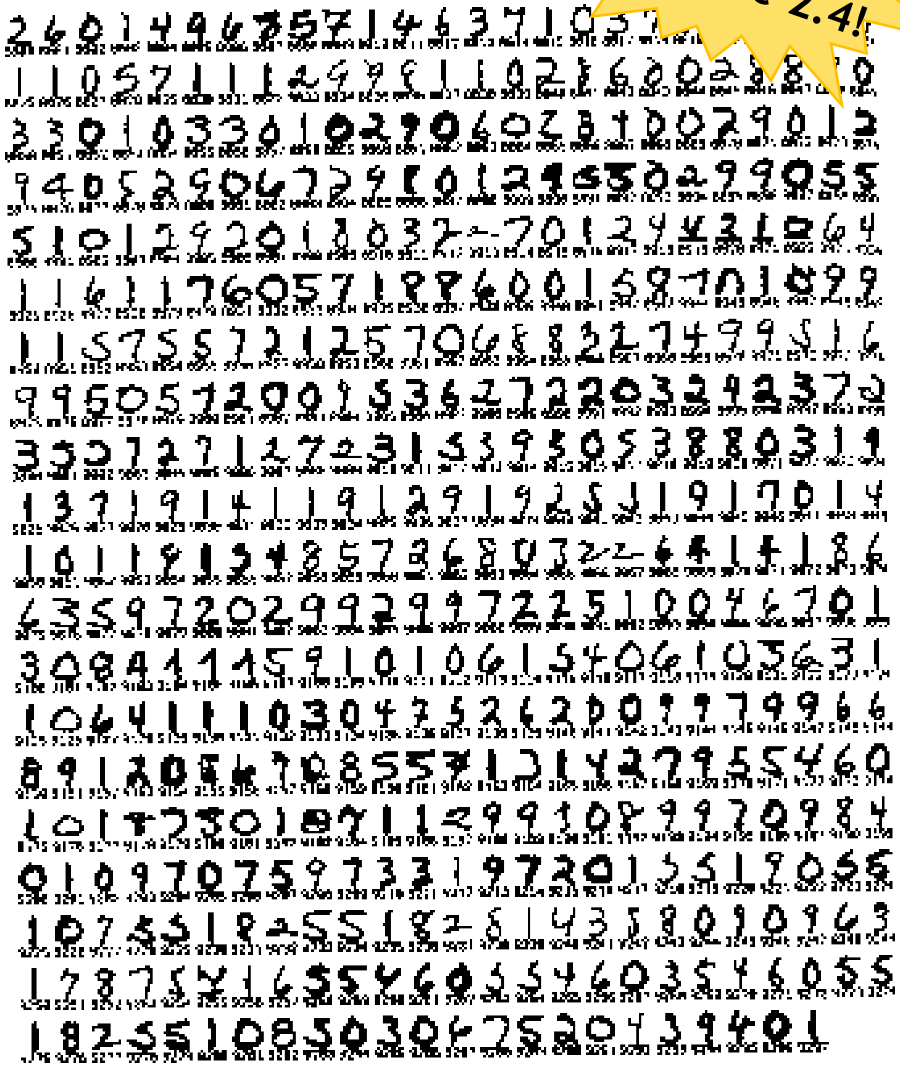
- This is also how you could implement a simple spam filter...



Example Application: OCR

see Exercise 2.4!

- Handwritten digit recognition
  - US Postal Service Database
  - Standard benchmark task for many learning algorithms



Historical Importance

- USPS benchmark
  - 2.5% error: human performance

- Different learning algorithms
  - 16.2% error: Decision tree (C4.5)
  - 5.9% error: (best) 2-layer Neural Network
  - 5.1% error: LeNet 1 - (massively hand-tuned) 5-layer network

- Different SVMs
  - 4.0% error: Polynomial kernel (p=3, 274 support vectors)
  - 4.1% error: Gaussian kernel (σ=0.3, 291 support vectors)

Example Application: OCR

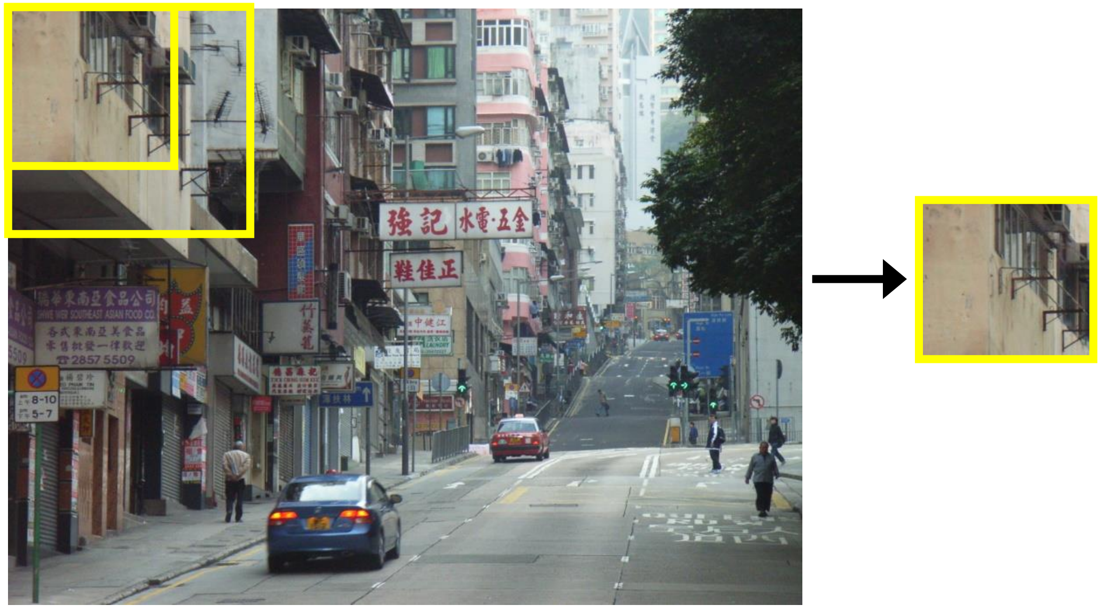
- **Results**
  - Almost no overfitting with higher-degree kernels.

degree of polynomial	dimensionality of feature space	support vectors	raw error
1	256	282	8.9
2	≈ 33000	227	4.7
3	$\approx 1 \times 10^{6}$	274	4.0
4	$\approx 1 \times 10^{9}$	321	4.2
5	$\approx 1 \times 10^{12}$	374	4.3
6	$\approx 1 \times 10^{14}$	377	4.5
7	$\approx 1 \times 10^{16}$	422	4.5

Example Application: Object Detection

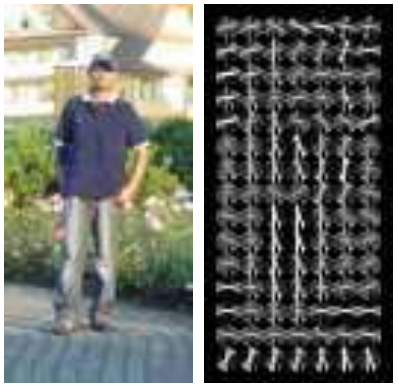
Real-time capable!

- Sliding-window approach



Obj./non-obj. Classifier

- E.g. histogram representation (HOG)
  - Map each grid cell in the input window to a histogram of gradient orientations.
  - Train a linear SVM using training set of pedestrian vs. non-pedestrian windows.



[Dalal & Triggs, CVPR 2005]

Example Application: Pedestrian Detection

N. Dalal, B. Triggs, Histograms of Oriented Gradients for Human Detection, CVPR 2005

Many Other Applications

- Lots of other applications in all fields of technology
  - OCR
  - Text classification
  - Computer vision
  - …
  - High-energy physics
  - Monitoring of household appliances
  - Protein secondary structure prediction
  - Design on decision feedback equalizers (DFE) in telephony

(Detailed references in Schoelkopf & Smola, 2002, pp. 221)

Topics of This Lecture

- Support Vector Machines (Recap)
  - Lagrangian (primal) formulation
  - Dual formulation
  - Soft-margin classification
  - Nonlinear Support Vector Machines
- Analysis
  - VC dimensions
  - Error function
- Applications
- **Extensions**
  - **One-class SVMs**

Summary: SVMs

- Properties
  - Empirically, SVMs work very, very well.
  - SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
  - SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.
  - SVM techniques have been applied to a variety of other tasks
    - e.g. SV Regression, One-class SVMs, …
  - The kernel trick has been used for a wide variety of applications. It can be applied wherever dot products are in use
    - e.g. Kernel PCA, kernel FLD, …
    - Good overview, software, and tutorials available on http://www.kernel-machines.org/

Summary: SVMs

- Limitations
  - How to select the right kernel?
    - Requires domain knowledge and experiments…
  - How to select the kernel parameters?
    - (Massive) cross-validation.
    - Usually, several parameters are optimized together in a grid search.
  - Solving the quadratic programming problem
    - Standard QP solvers do not perform too well on SVM task.
    - Dedicated methods have been developed for this, e.g. SMO.
  - Speed of evaluation
    - Evaluating $y(\mathbf{x})$ scales linearly in the number of SVs.
    - Too expensive if we have a large number of support vectors.

    $\Rightarrow$ There are techniques to reduce the effective SV set.
  - Training for very large datasets (millions of data points)
    - Stochastic gradient descent and other approximations can be used

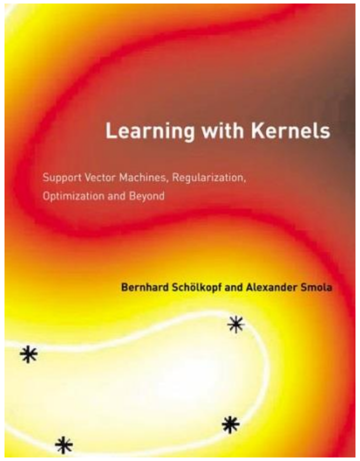
You Can Try It At Home…

- Lots of SVM software available, e.g.
  - svmlight (http://svmlight.joachims.org/)
    - Command-line based interface
    - Source code available (in C)
    - Interfaces to Python, MATLAB, Perl, Java, DLL,…
  - libsvm (http://www.csie.ntu.edu.tw/~cjlin/libsvm/)
    - Library for inclusion with own code
    - C++ and Java sources
    - Interfaces to Python, R, MATLAB, Perl, Ruby, Weka, C+ .NET,…
  - Both include fast training and evaluation algorithms, support for multi-class SVMs, automated training and cross-validation, …

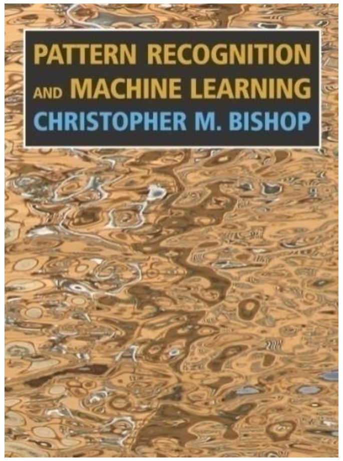
    ⇒ Easy to apply to your own problems!

References and Further Reading

- More information on SVMs can be found in Chapter 7.1 of Bishop's book. You can also look at Schölkopf & Smola (some chapters available online).


Learning with Kernels
Support Vector Machines, Regularization, Optimization and Beyond
Bernhard Schölkopf and Alexander Smola

Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006



B. Schölkopf, A. Smola
Learning with Kernels
MIT Press, 2002
http://www.learning-with-kernels.org/

- A more in-depth introduction to SVMs is available in the following tutorial:
  - C. Burges, A Tutorial on Support Vector Machines for Pattern Recognition, Data Mining and Knowledge Discovery, Vol. 2(2), pp. 121-167 1998.