Machine Learning - Lecture 9

Nonlinear SVMs

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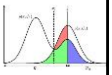
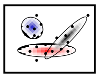
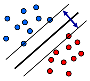
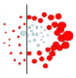
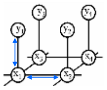
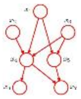
Course Outline

- 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

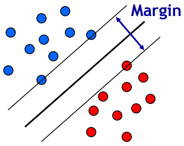
Topics of This Lecture

- 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

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

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

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

- 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:

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

Recap: SVM - Solution

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

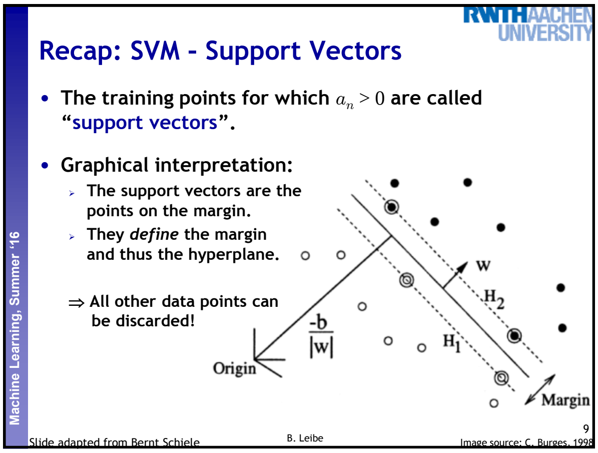
$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \mathbf{x}_n$$

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

⇒ Only the SVs actually influence the decision boundary!

  - Compute b by averaging over all support vectors:

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



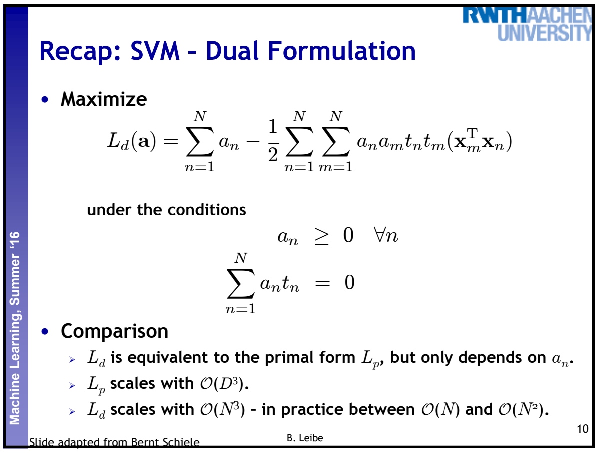
Recap: SVM - Support Vectors

- 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.

  ⇒ All other data points can be discarded!

Slide adapted from Bernt Schiele

Image source: C. Burges, 1998



Recap: SVM - Dual Formulation

- Maximize

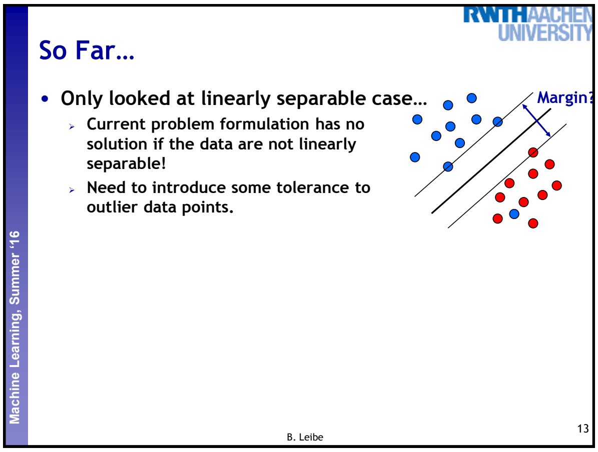
$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^{\mathrm{T}}\mathbf{x}_n)$$

under the conditions

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

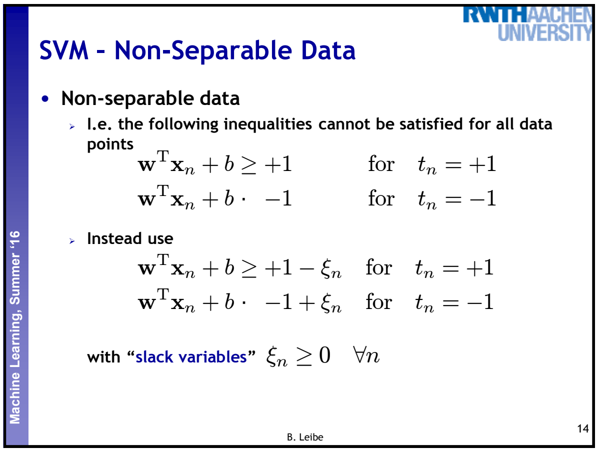
- Comparison
  - L_d is equivalent to the primal form L_p, but only depends on a_n.
  - L_p scales with $\mathcal{O}(D^3)$.
  - L_d scales with $\mathcal{O}(N^3)$ - in practice between $\mathcal{O}(N)$ and $\mathcal{O}(N^2)$.

Slide adapted from Bernt Schiele



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

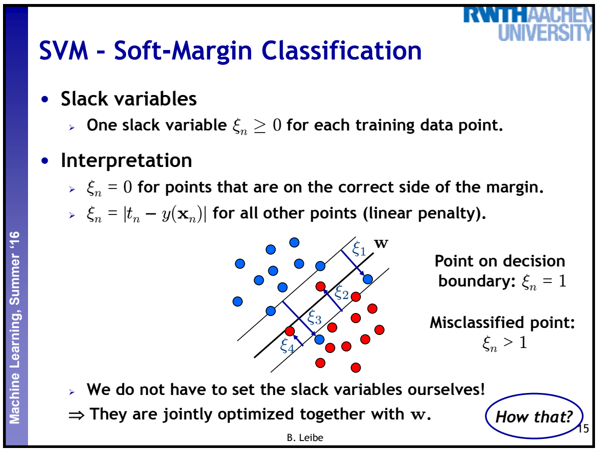
- Non-separable data
  - I.e. the following inequalities cannot be satisfied for all data points

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

  - 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).

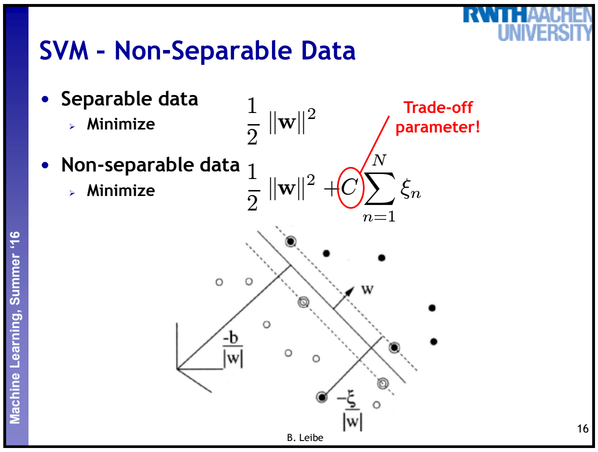
Point on decision boundary: $\xi_n = 1$

Misclassified point: $\xi_n > 1$

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

⇒ 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

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

- KKT conditions

$$\begin{aligned} a_n &\geq 0 & \mu_n &\geq 0 \\ t_n y(\mathbf{x}_n) - 1 + \xi_n &\geq 0 & \xi_n &\geq 0 \\ a_n\left(t_n y(\mathbf{x}_n) - 1 + \xi_n\right) &= 0 & \mu_n\xi_n &= 0 \end{aligned} \qquad \boxed{\begin{array}{rcl} \multicolumn{3}{c}{\text{KKT:}} \\ \lambda & \geq & 0 \\ f(\mathbf{x}) & \geq & 0 \\ \lambda f(\mathbf{x}) & = & 0 \end{array}}$$

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

$$0 \cdot a_n \cdot C$$

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

This is all that changed!

- This is again a quadratic programming problem
  - ⇒ Solve as before… (more on that later)

Slide adapted from Bernt Schiele

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.
  - ⇒ 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

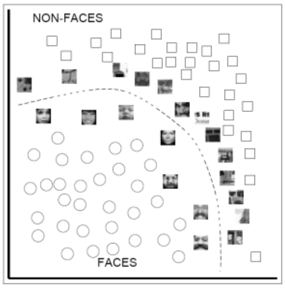


Image source: E. Osuna, F. Girosi, 1997

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  - Popular kernels
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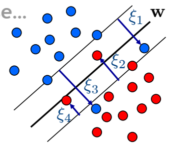
So Far…

- 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.
  - ⇒ Slack variables. ✓



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

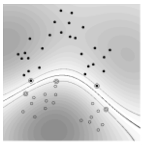
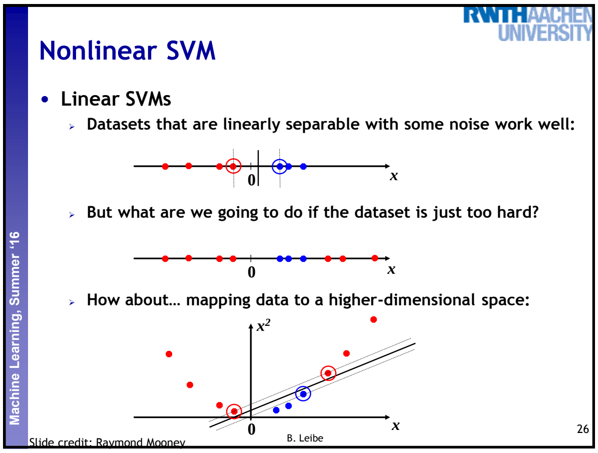


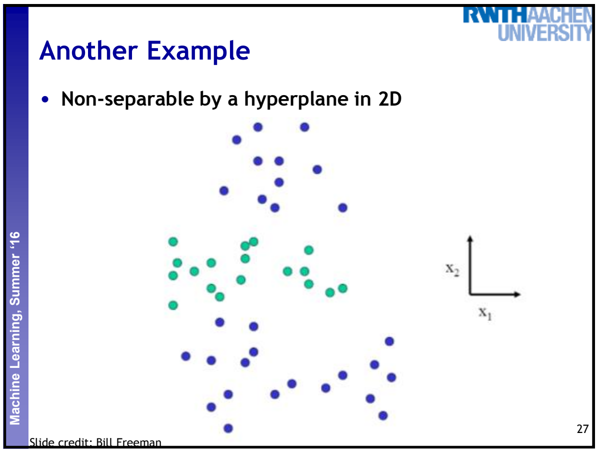
Image source: B. Schoelkopf, A. Smola, 2002



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:

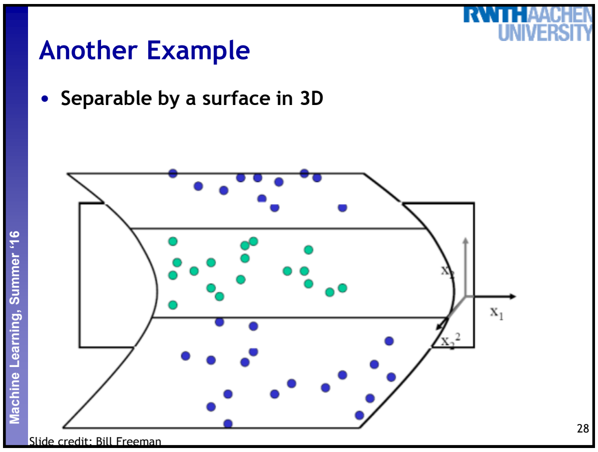
Slide credit: Raymond Mooney



Another Example

- Non-separable by a hyperplane in 2D

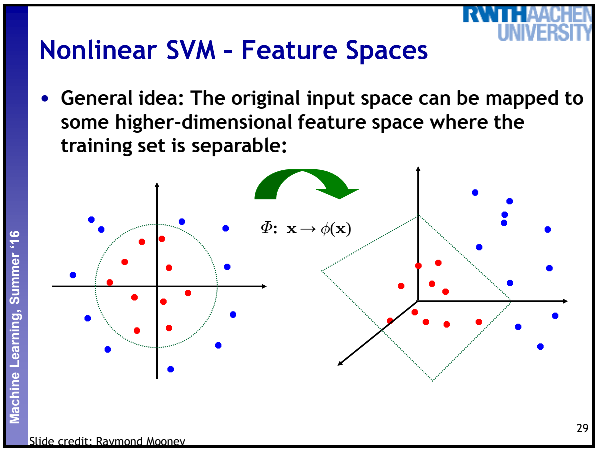
Slide credit: Bill Freeman



Another Example

- Separable by a surface in 3D

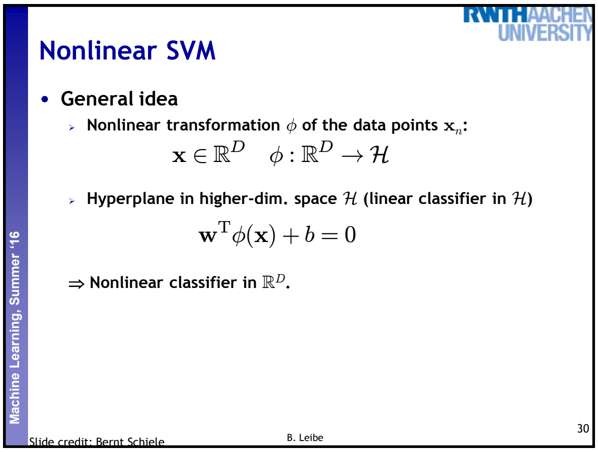
Slide credit: Bill Freeman



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 $\mathbf{x}_n$:

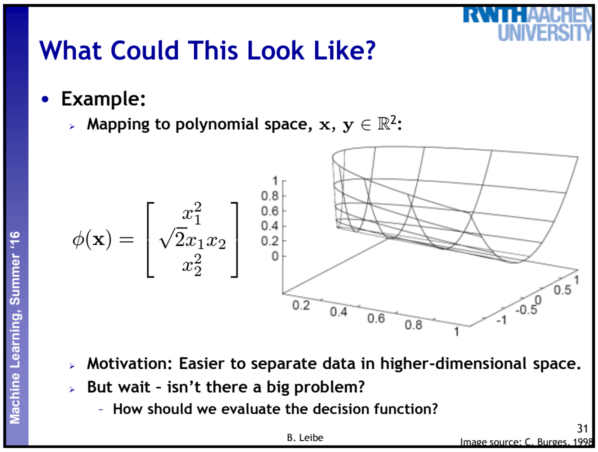
$$\mathbf{x} \in \mathbb{R}^D \quad \phi : \mathbb{R}^D \rightarrow \mathcal{H}$$

  - 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 $\mathbb{R}^D$.

Slide credit: Bernt Schiele



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

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

⇒ 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 $\phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{y})$:

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

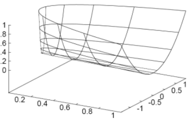
  - Trick: Define a so-called kernel function $k(\mathbf{x},\mathbf{y}) = \phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{y})$.
  - Now, in place of the dot product, use the kernel instead:

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

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

Image source: C. Burges, 1998

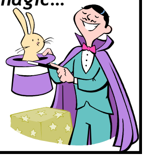
SVMs with Kernels

- 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:

$K =$

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

(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

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

e.g. Sigmoid

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

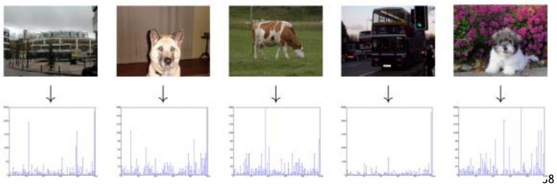
(and many, many more…)

Slide credit: Bernt Schiele

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

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



Slide adapted from Christoph Lampert

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

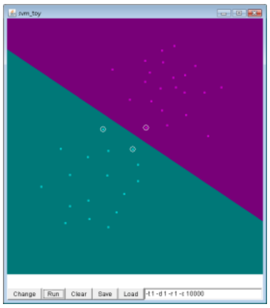
$$0 \cdot \; a_n \cdot \; C$$

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

- 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



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.
    - ⇒ 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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e.g. Gaussian

- Hyperbolic tangent kernel

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

e.g. Sigmoid

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

(and many, many more...)

Slide credit: Bernt Schiele

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!

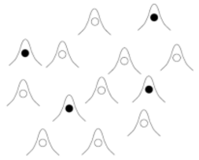
$$\exp(\mathbf{x}) = 1 + \frac{\mathbf{x}}{1!} + \frac{\mathbf{x}^2}{2!} + \ldots + \frac{\mathbf{x}^n}{n!} + \ldots$$

  - 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.

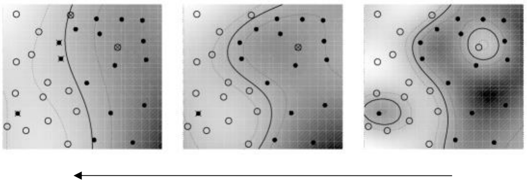


  - However, this also means that we can get finite VC-dimension if we set a lower limit to the RBF radius.

Image source: C. Burges

Example: RBF Kernels

- Decision boundary on toy problem



RBF Kernel width (σ)

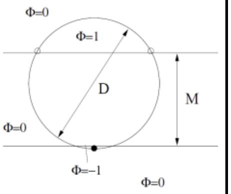
Image source: B. Schoelkopf, A. Smola, 2002

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**
  - $M \leq 3/4\ D$ ⇒ 3 points can be shattered
  - $3/4\ D < M < D$ ⇒ 2 points can be shattered
  - $M \geq D$ ⇒ 1 point can be shattered

⇒ 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.

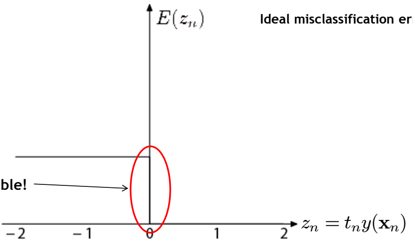
$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\text{L}_2\text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+}_{\text{“Hinge loss”}}$$

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

Slide adapted from Christoph Lampert

Recap: Error Functions

$t_n \subset \{\ \ 1, 1\}$



Ideal misclassification error

Not differentiable!

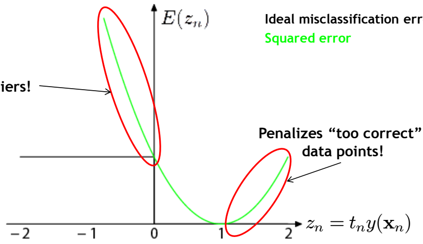
- **Ideal misclassification error function (black)**
  - This is what we want to approximate,
  - Unfortunately, it is not differentiable.
  - The gradient is zero for misclassified points.

⇒ We cannot minimize it by gradient descent.

Image source: Bishop, 2006

Recap: Error Functions

$t_n \subset \{\ \ 1, 1\}$



Ideal misclassification error

Squared error

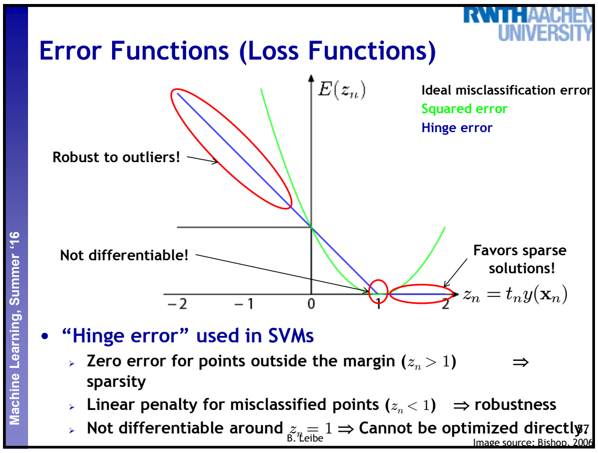
Sensitive to outliers!

Penalizes "too correct" data points!

- 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

⇒ Generally does not lead to good classifiers.

Image source: Bishop, 2006

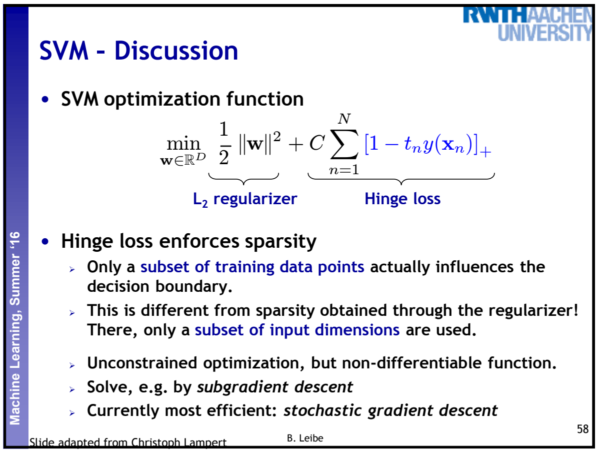


Error Functions (Loss Functions)

$E(z_n)$
Ideal misclassification error
Squared error
Hinge error
Robust to outliers!
Not differentiable!
Favors sparse solutions!
$z_n = t_n y(\mathbf{x}_n)$
−2
−1
0
1
2

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

Image source: Bishop, 2006



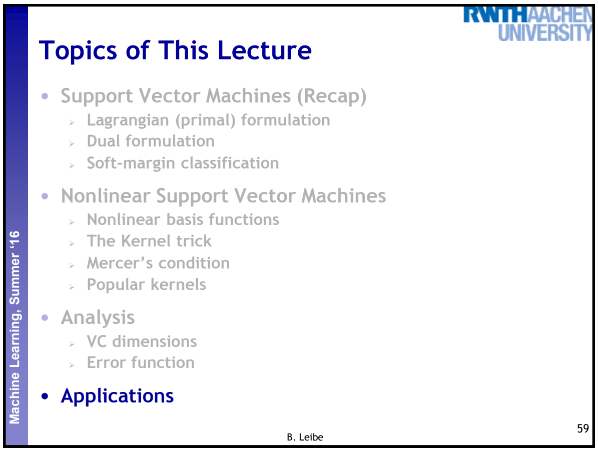
SVM - Discussion

- SVM optimization function

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

- 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*

Slide adapted from Christoph Lampert



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- Nonlinear Support Vector Machines
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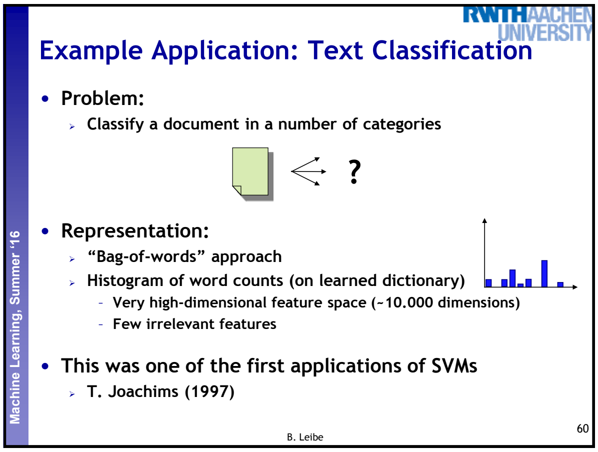
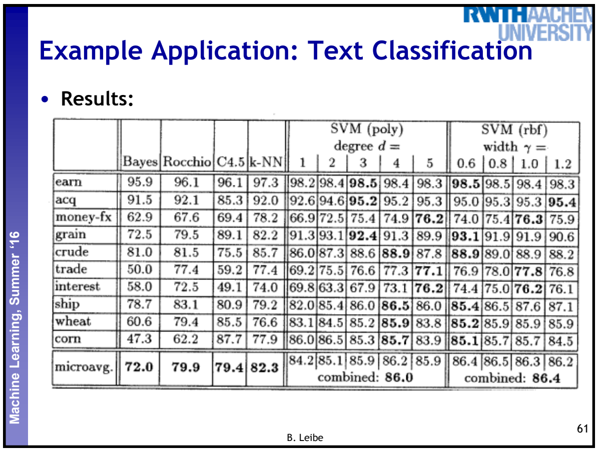
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Analysis
  - VC dimensions
  - Error function
- **Applications**



Example Application: Text Classification

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

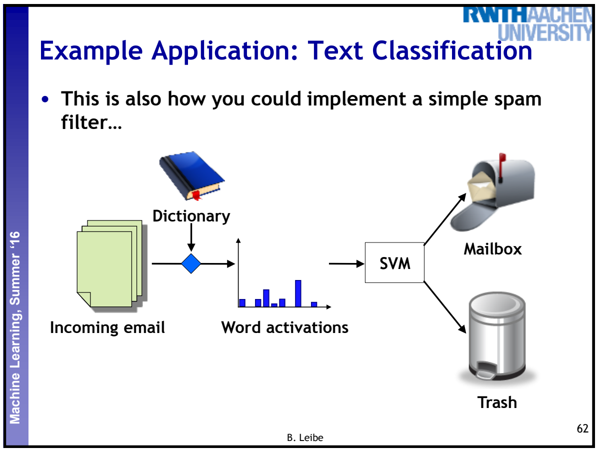
- Representation:
  - "Bag-of-words" approach
  - Histogram of word counts (on learned dictionary)
    - Very high-dimensional feature space (~10.000 dimensions)
    - Few irrelevant features
- This was one of the first applications of SVMs
  - T. Joachims (1997)



Example Application: Text Classification

- Results:

	Bayes	Rocchio	C4.5	k-NN	SVM (poly) degree $d =$ 1	2	3	4	5	SVM (rbf) width $\gamma =$ 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...

Dictionary

Incoming email

Word activations

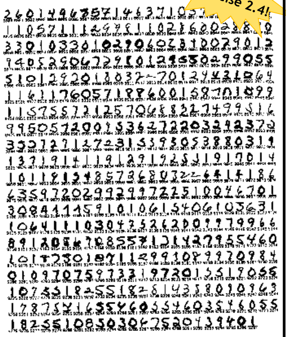
SVM

Mailbox

Trash

Example Application: OCR

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



see Exercise 2.4!

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

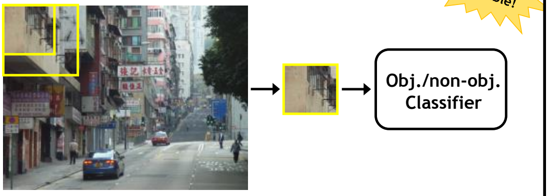
- Results
  - Almost no overfitting with higher-degree kernels.

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

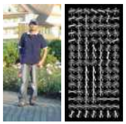
Real-time capable!

- Sliding-window approach



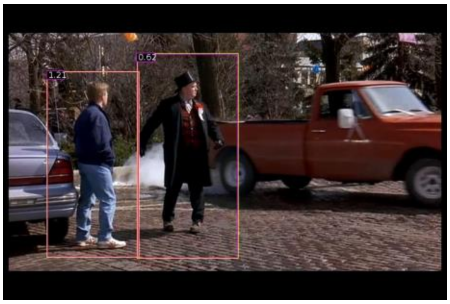
Obj./non-obj. Classifier

- 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

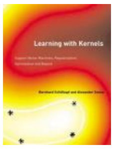
- Limitations
  - How to select the right kernel?
    - Requires domain knowledge and experiments…
  - How to select the kernel parameters?
    - (Massive) cross-validation.
    - Usually, several parameters are optimized together in a grid search.
  - Solving the quadratic programming problem
    - 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.
    - ⇒ 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…

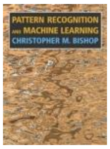
- Lots of SVM software available, e.g.
  - svmlight (http://svmlight.joachims.org/)
    - Command-line based interface
    - Source code available (in C)
    - Interfaces to Python, MATLAB, Perl, Java, DLL,…
  - libsvm (http://www.csie.ntu.edu.tw/~cjlin/libsvm/)
    - Library for inclusion with own code
    - 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).



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.