RWTH AACHEN UNIVERSITY

Machine Learning – Lecture 9

Support Vector Machines II

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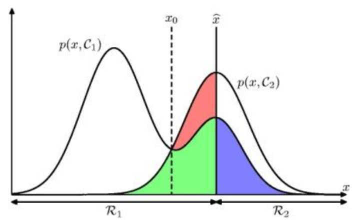
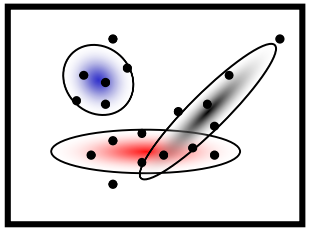
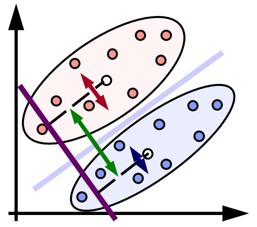
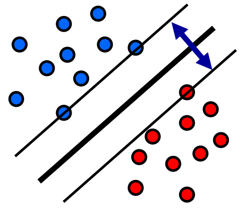
Course Outline

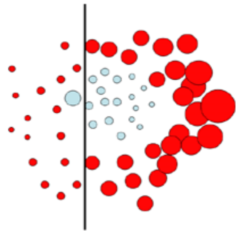
- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation
- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

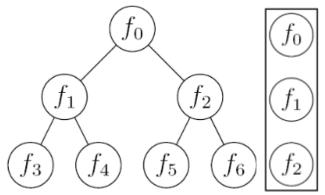


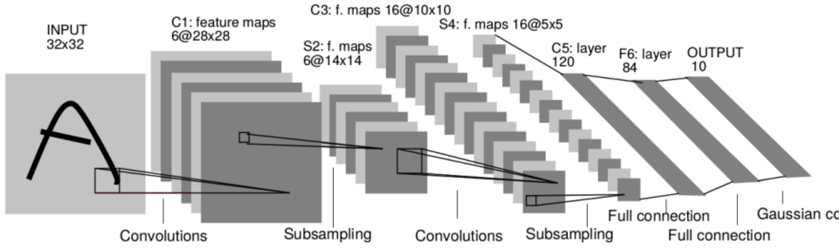












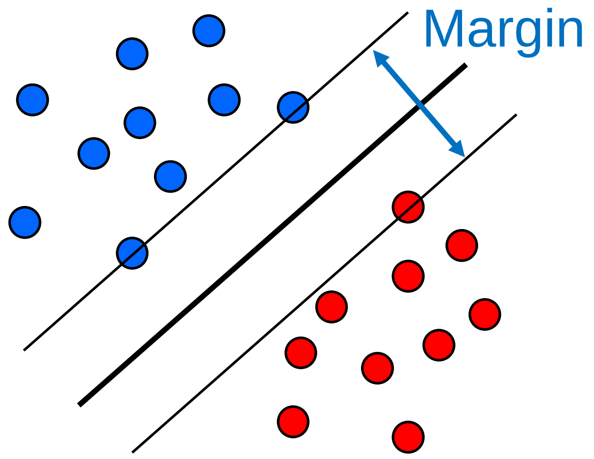
Topics of This Lecture

- Recap: Support Vector Machines
  - Lagrangian (primal) formulation
  - Dual formulation
  - Soft-margin classification
- Nonlinear Support Vector Machines
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Analysis
  - 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 – Lagrangian Formulation

- Find hyperplane minimizing $||\mathbf{w}||^2$ under the constraints

$$t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) - 1 \geq 0 \quad \forall n$$

- Lagrangian formulation
  - Introduce positive Lagrange multipliers: $a_n \geq 0 \quad \forall n$
  - Minimize Lagrangian ("primal form")

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

  - I.e., find $\mathbf{w}$, b, and $\mathbf{a}$ such that

$$\frac{\partial L}{\partial b} = 0 \Rightarrow \boxed{\sum_{n=1}^{N} a_n t_n = 0} \qquad \frac{\partial L}{\partial \mathbf{w}} = 0 \Rightarrow \boxed{\mathbf{w} = \sum_{n=1}^{N} a_n t_n \mathbf{x}_n}$$

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

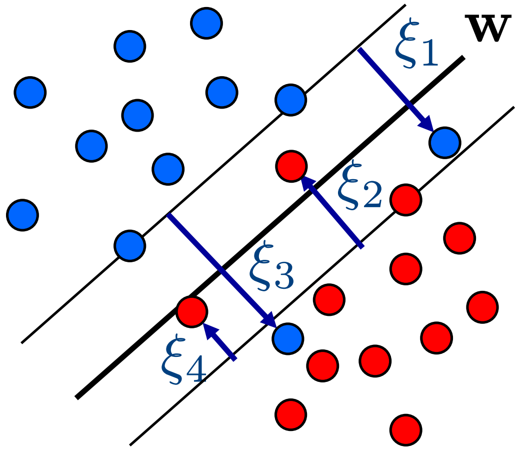
$$\begin{aligned} a_n &\geq 0 \\ t_n y(\mathbf{x}_n) - 1 &\geq 0 \\ a_n \left\{ t_n y(\mathbf{x}_n) - 1 \right\} &= 0 \end{aligned}$$

KKT:

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

Recap: SVM for Non-Separable Data

- 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.



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 $\mathbf{w}$.

Recap: 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

  $\Rightarrow$ Solve as before…

Slide adapted from Bernt Schiele

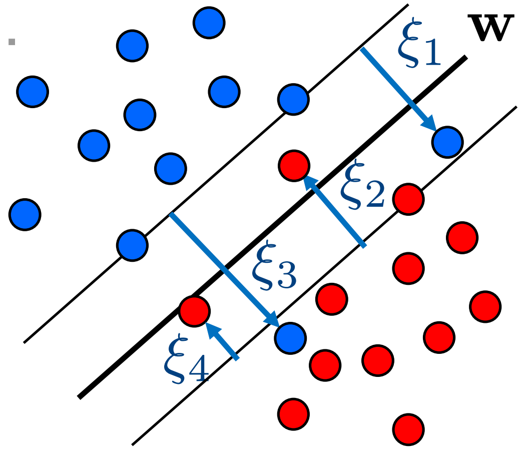
Topics of This Lecture

- Recap: 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
  - Error function
- Applications

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.

  $\Rightarrow$ Slack variables. ✓



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

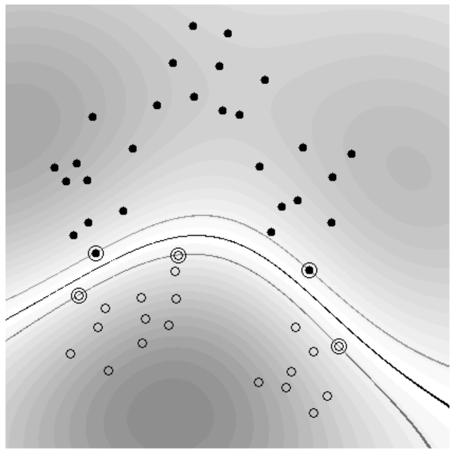
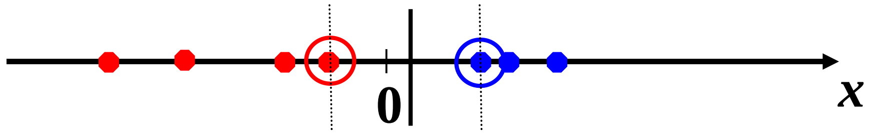


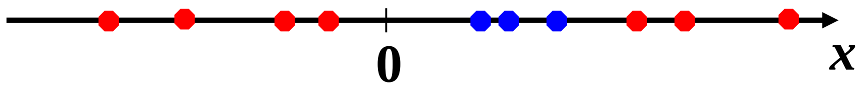
Image source: B. Schoelkopf, A. Smola, 2002

Nonlinear SVM

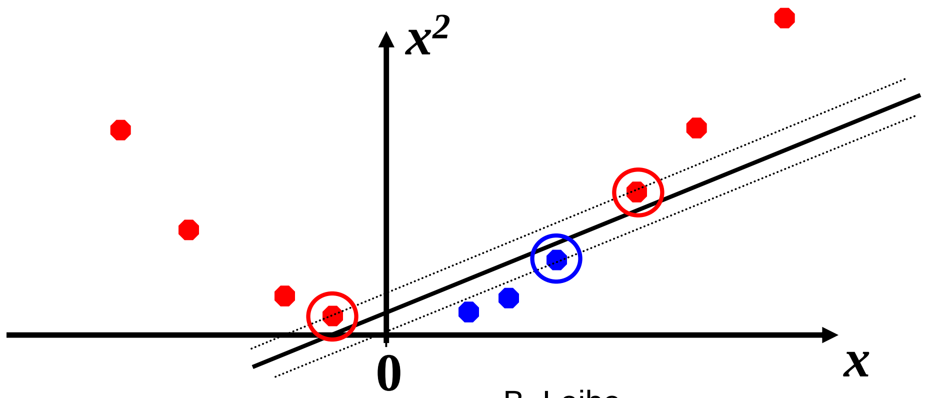
- Linear SVMs
  - Datasets that are linearly separable with some noise work well:



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

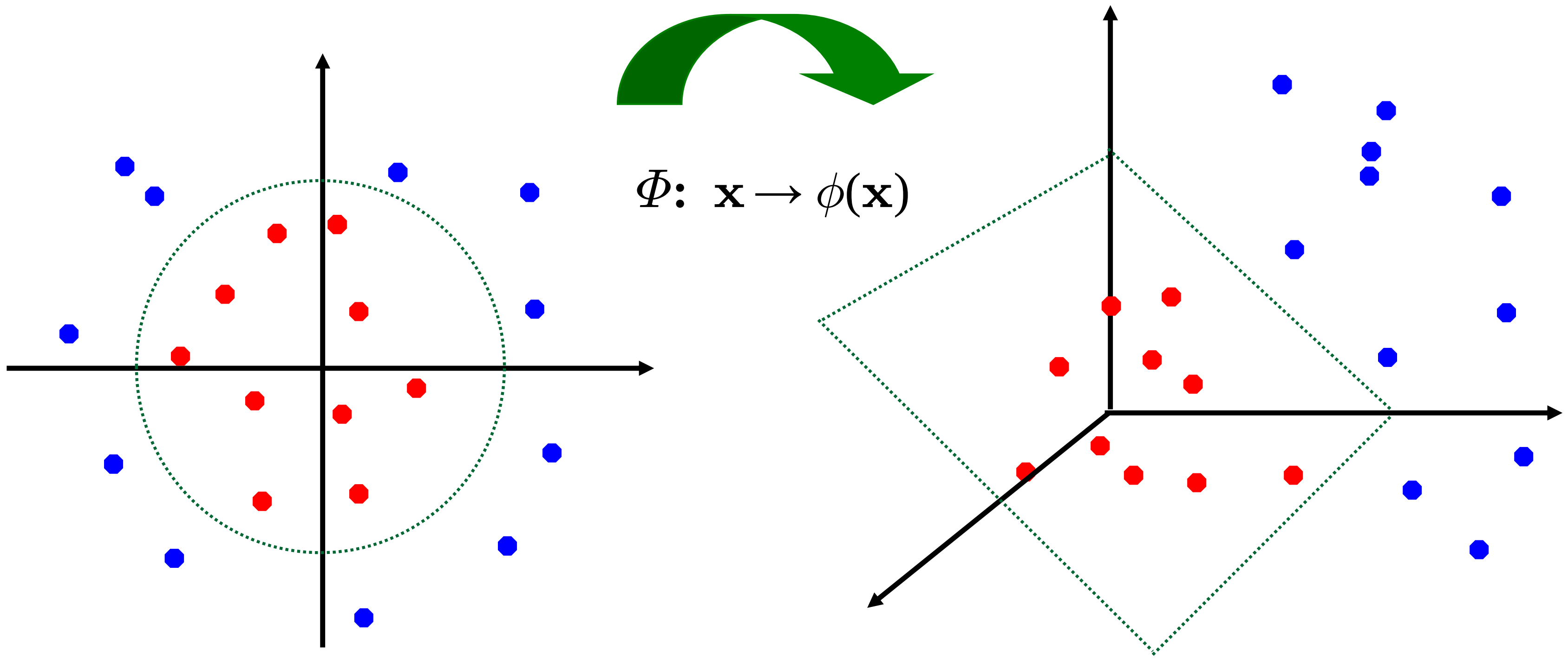


  - How about… mapping data to a higher-dimensional space:



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 $\mathcal{H}$)

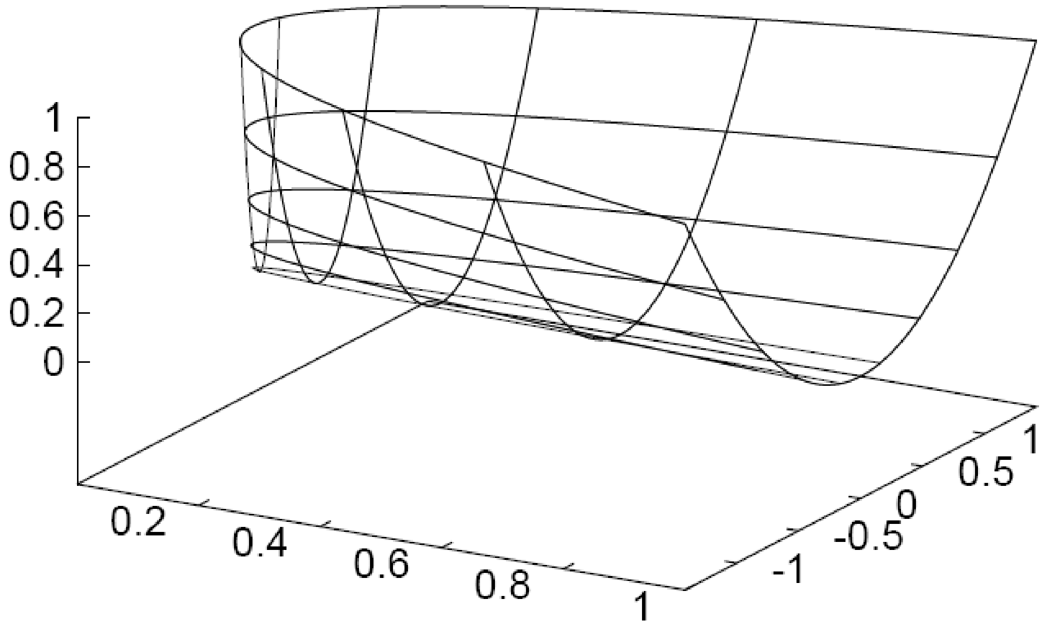
$$\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b = 0$$

$\Rightarrow$ 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

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

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

  - 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:

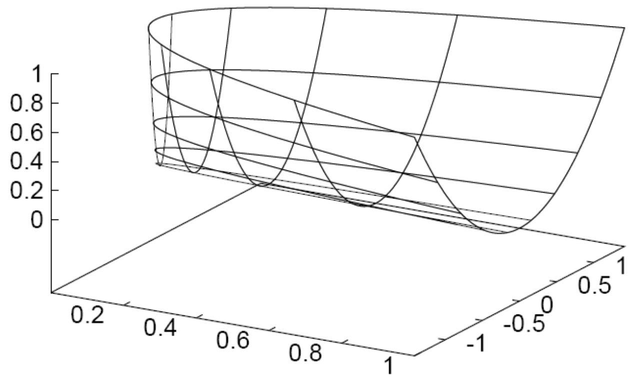
$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

  - 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?

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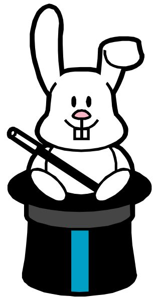
Which Functions are Valid Kernels?



- 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)

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

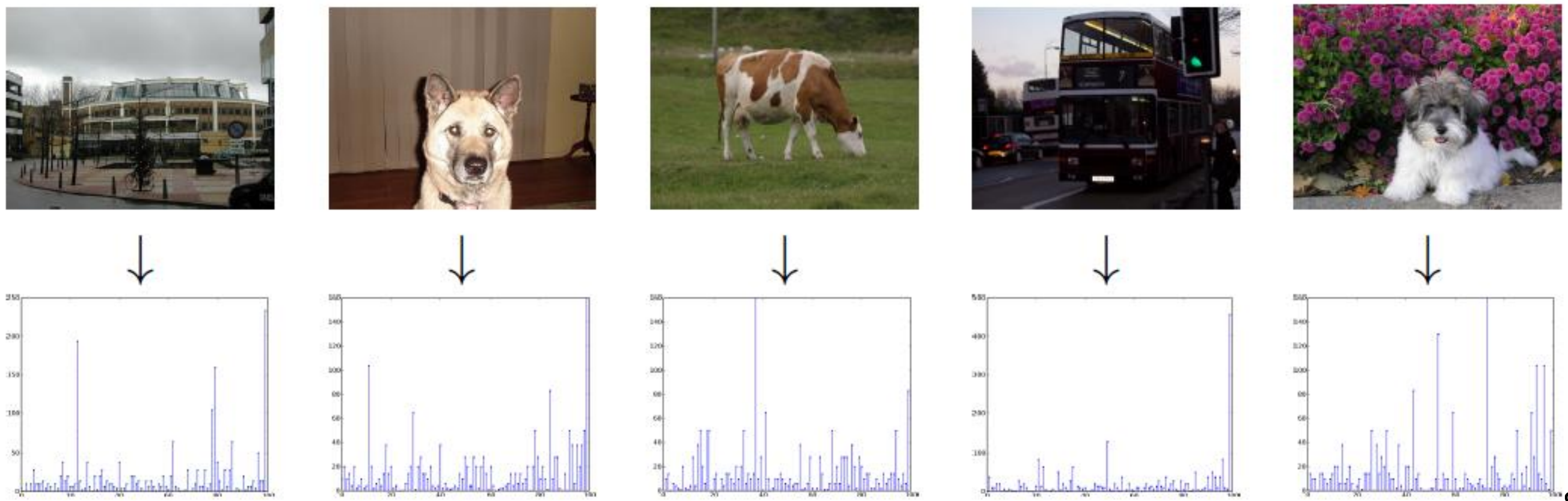
Actually, this was wrong in the original SVM paper...

(and many, many more…)

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

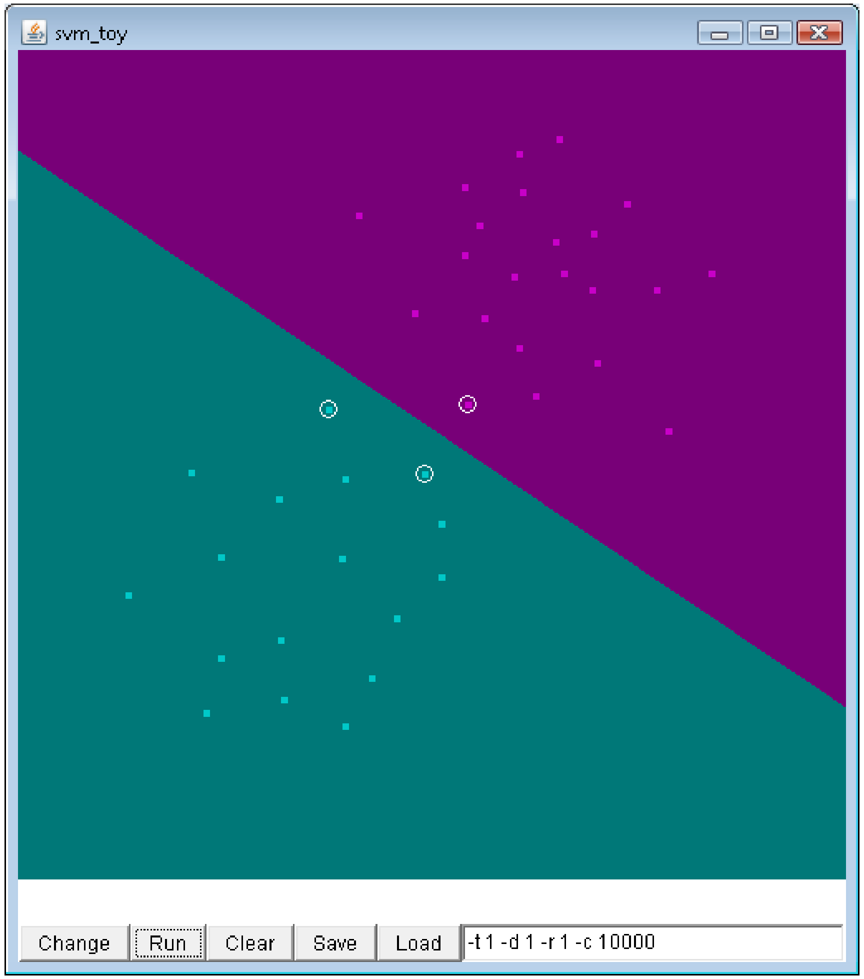
$$0 \cdot \quad a_n \cdot \quad C$$

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

- Classify new data points using

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

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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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"

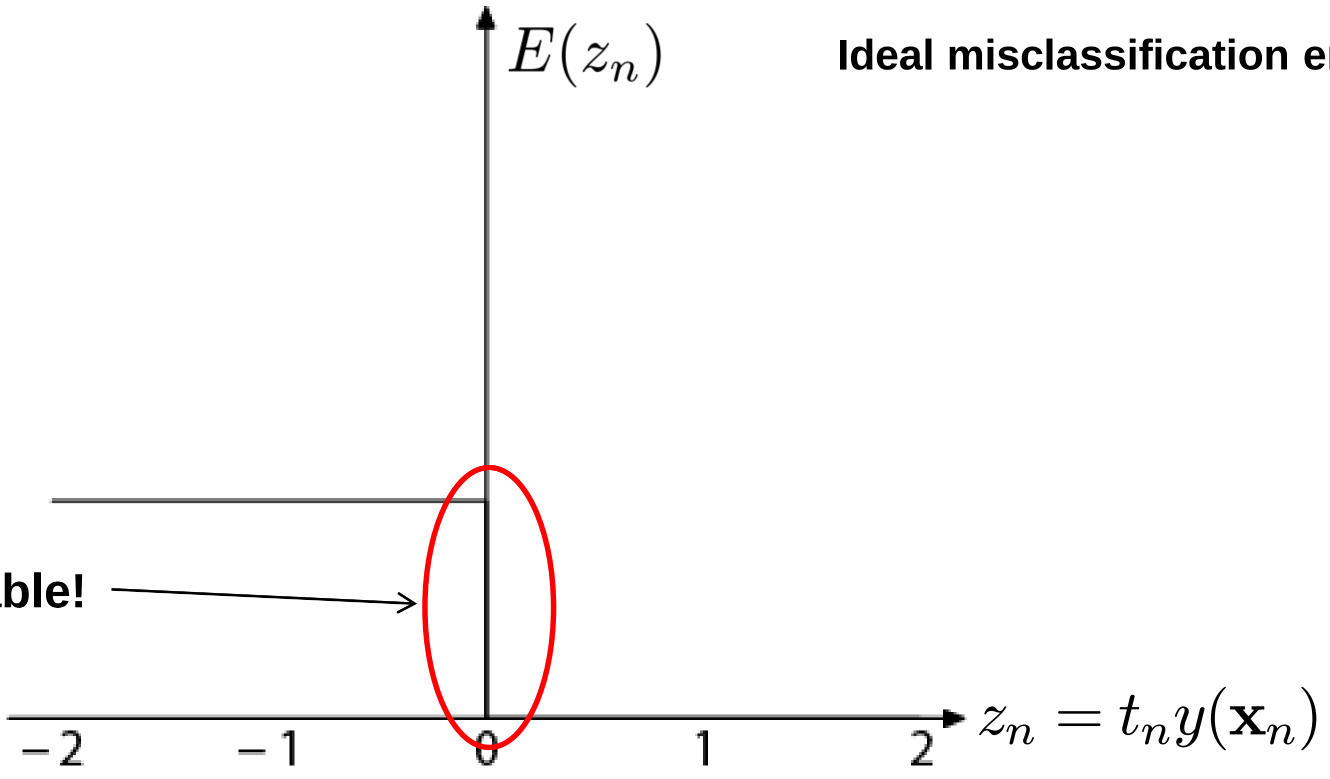
- Different way of looking at it
  - We can reformulate the constraints into the objective function.

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{L_2 \text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+}_{\text{“Hinge loss”}}$$

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

Recap: Error Functions

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



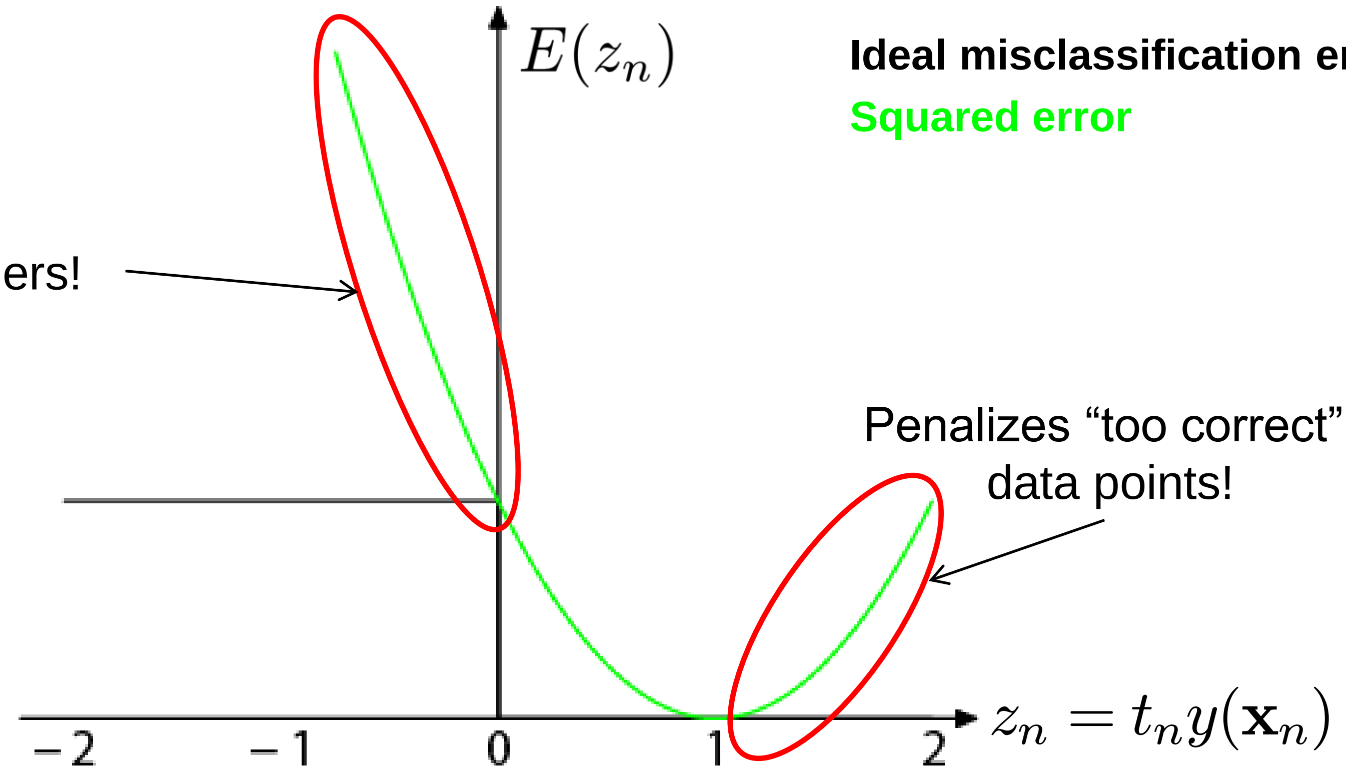
- Ideal misclassification error function (black)
  - This is what we want to approximate,
  - Unfortunately, it is not differentiable.
  - The gradient is zero for misclassified points.

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

Image source: Bishop, 2006

Recap: Error Functions

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



Ideal misclassification error

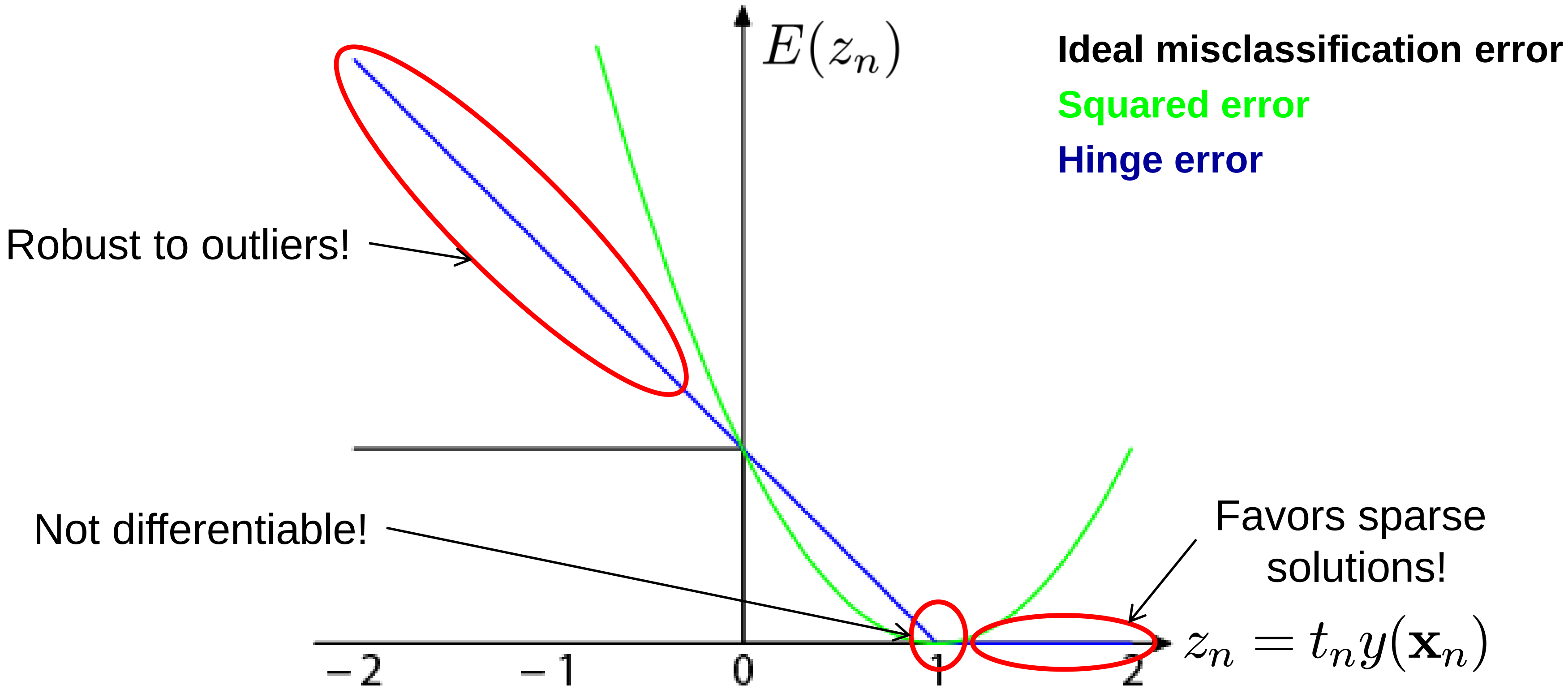
Squared error

- 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 $z_n = 1 \Rightarrow$ Harder to optimize directly.

Image source: Bishop, 2006

SVM – Discussion

- SVM optimization function

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

- 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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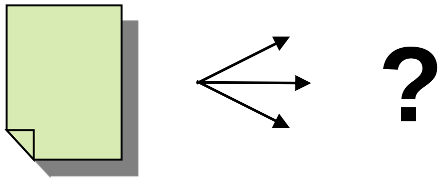
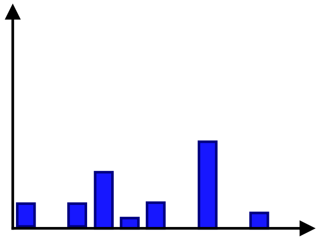
Example Application: Text Classification

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



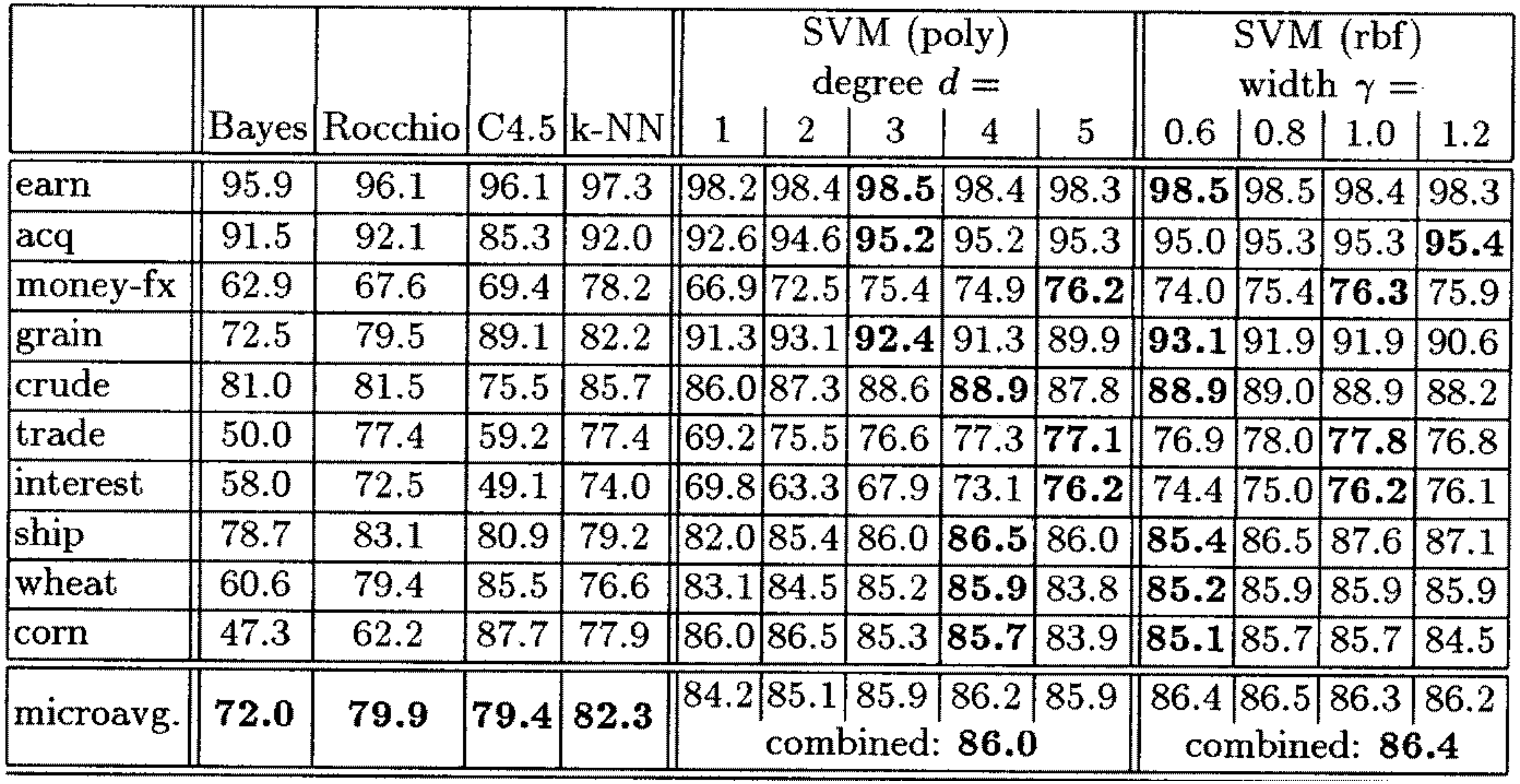
- Representation:
  - "Bag-of-words" approach
  - Histogram of word counts (on learned dictionary)
    - Very high-dimensional feature space (~10.000 dimensions)
    - Few irrelevant features



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

Example Application: Text Classification

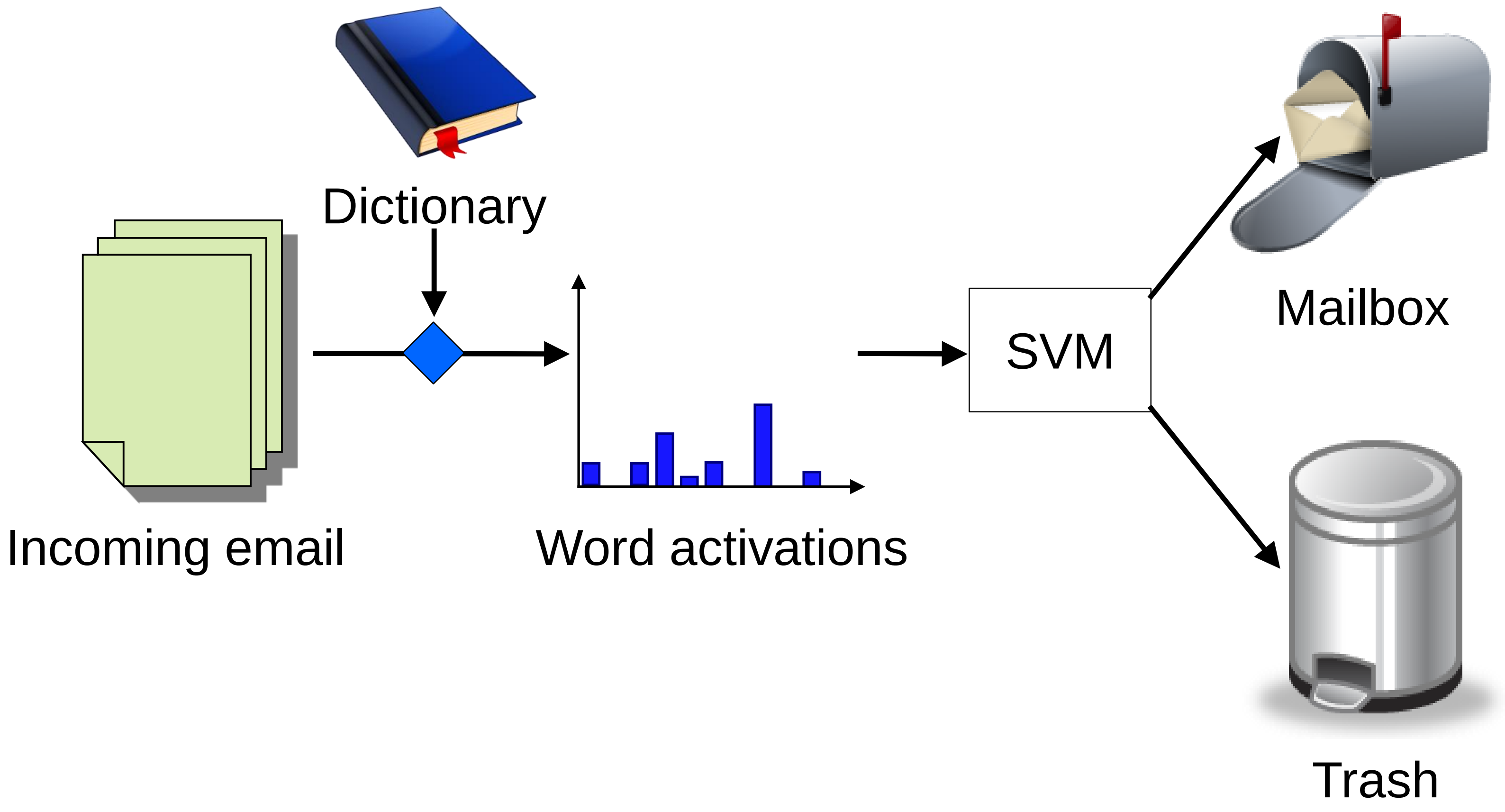
- Results:



					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**			

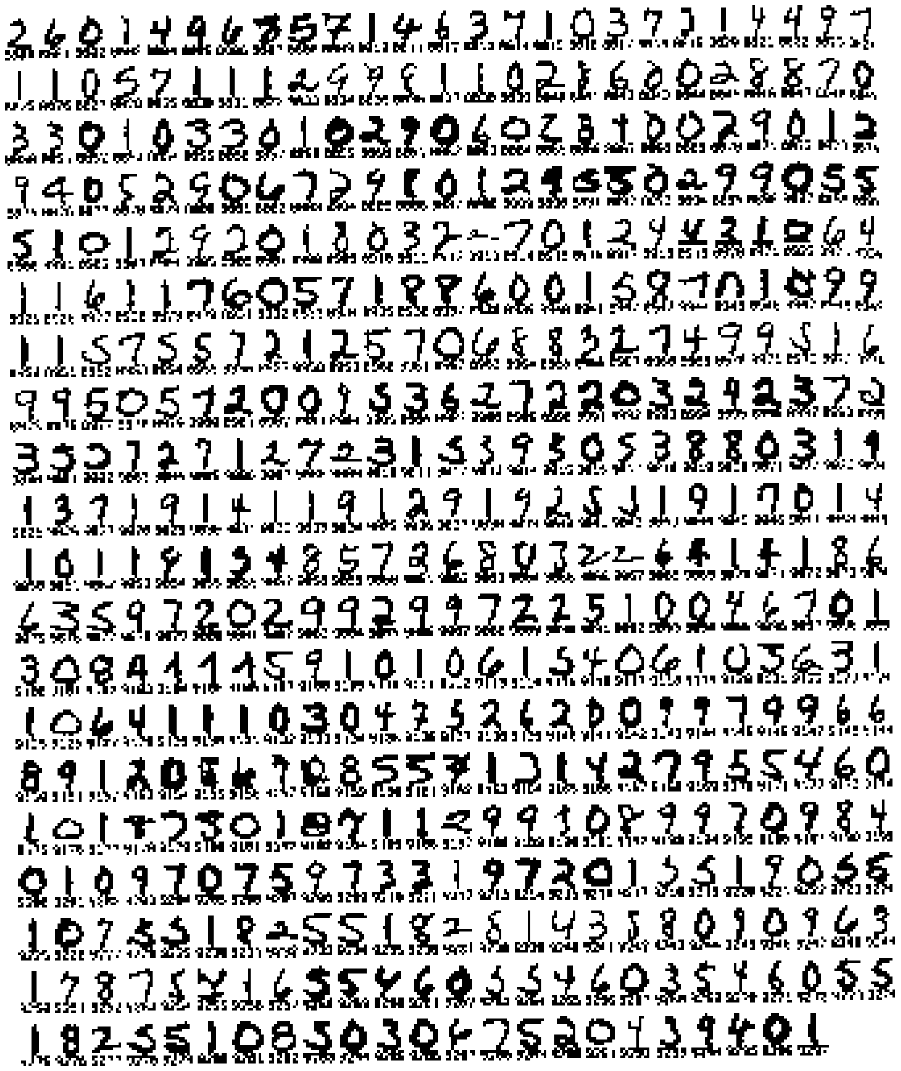
Example Application: Text Classification

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



Example Application: OCR

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

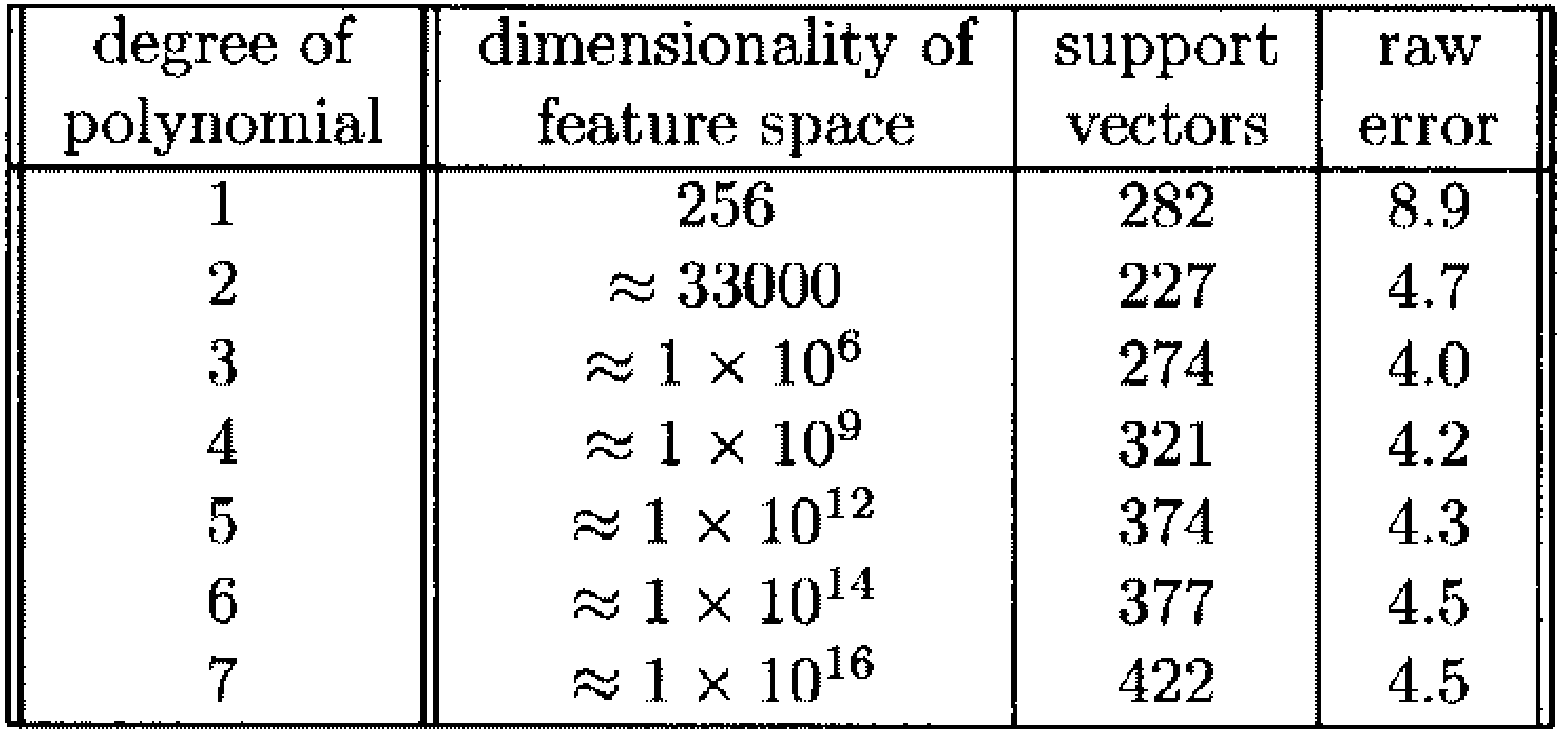


Historical Importance

- 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.

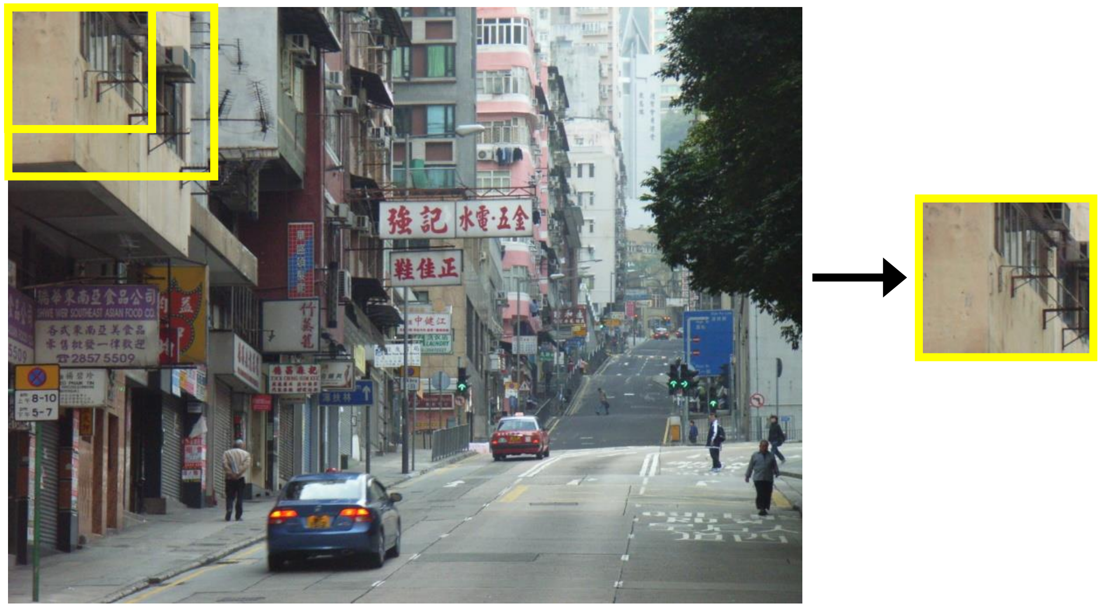


degree of polynomial	dimensionality of feature space	support vectors	raw error
1	256	282	8.9
2	≈ 33000	227	4.7
3	$\approx 1 \times 10^6$	274	4.0
4	$\approx 1 \times 10^9$	321	4.2
5	$\approx 1 \times 10^{12}$	374	4.3
6	$\approx 1 \times 10^{14}$	377	4.5
7	$\approx 1 \times 10^{16}$	422	4.5

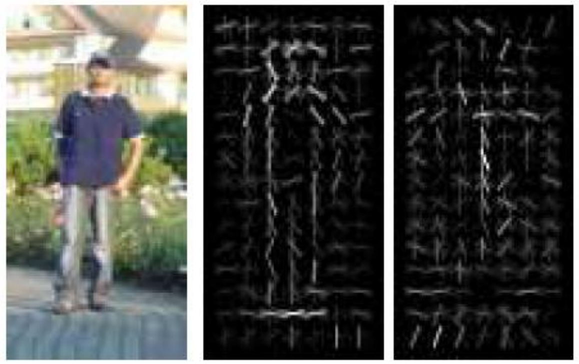
Example Application: Object Detection

Real-time capable!

- Sliding-window approach

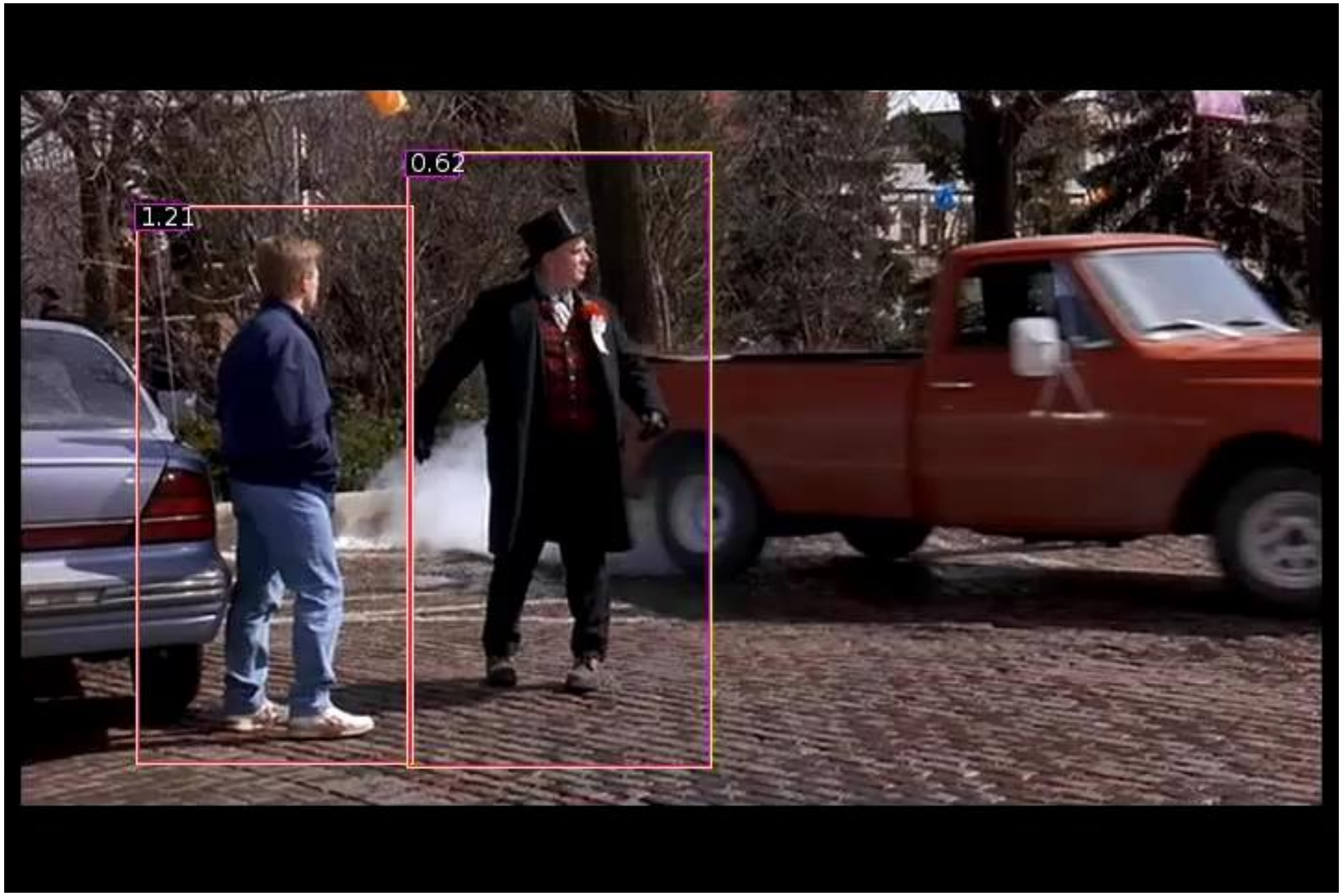


- E.g. histogram representation (HOG)
  - Map each grid cell in the input window to a histogram of gradient orientations.
  - Train a linear SVM using training set of pedestrian vs. non-pedestrian windows.



[Dalal & Triggs, CVPR 2005]

Example Application: Pedestrian Detection



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

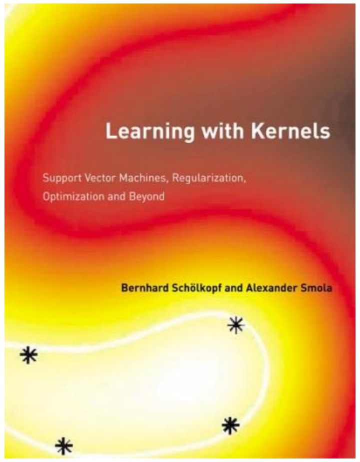
Many Other Applications

- 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

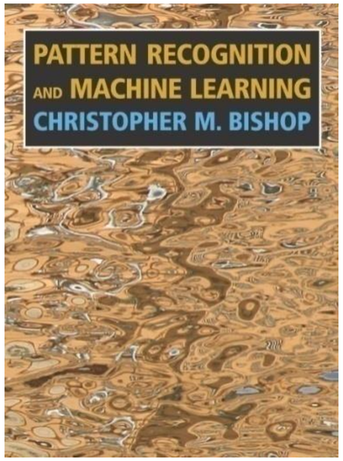
(Detailed references in Schoelkopf & Smola, 2002, pp. 221)

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.