# Machine Learning – Lecture 9

## Support Vector Machines II

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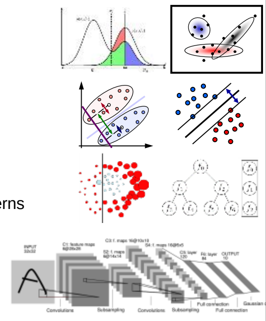
## Course Outline

- 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

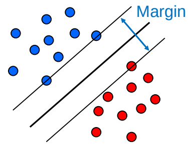
- Recap: Support Vector Machines
  - Lagrangian (primal) formulation
  - Dual formulation
  - Soft-margin classification
- Nonlinear Support Vector Machines
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Analysis
  - Error function
- Applications



## 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

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

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 – 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

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

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

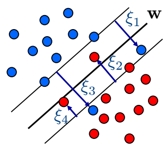
$$\begin{aligned} a_n &\geq 0 \\ t_n y(\mathbf{x}_n) - 1 &\geq 0 \\ a_n \left\{ t_n y(\mathbf{x}_n) - 1 \right\} &= 0 \end{aligned}$$

KKT:

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

## 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…



## Topics of This Lecture

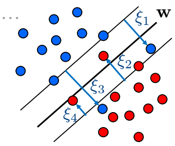
- Recap: Support Vector Machines
  - Recap: Lagrangian (primal) formulation
  - Dual formulation
  - Soft-margin classification
- Nonlinear Support Vector Machines
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Analysis
  - Error function
- Applications



## 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.

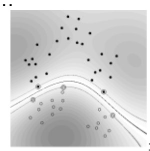
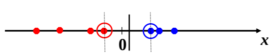


Image source: B. Schoelkopf, A. Smola, 2002

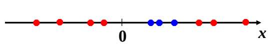


## Nonlinear SVM

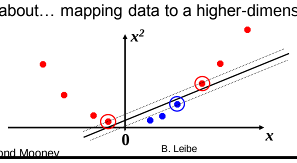
- Linear SVMs
  - Datasets that are linearly separable with some noise work well:




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



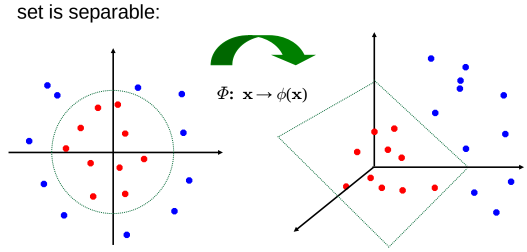

  - How about… mapping data to a higher-dimensional space:






## 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:



## Nonlinear SVM

- General idea
  - Nonlinear transformation $\phi$ 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 $\mathcal{H}$)

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

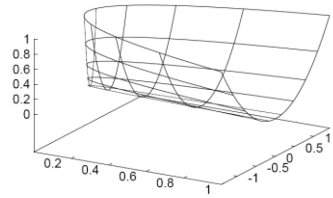
$\Rightarrow$ Nonlinear classifier in $\mathbb{R}^D$.



## 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?



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

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

  - 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:

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

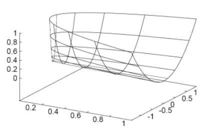
  - The kernel function *implicitly* maps the data to the higher-dimensional space (without having to compute $\phi(\mathbf{x})$ explicitly)!



## 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.



## SVMs with Kernels

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

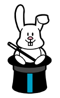
$$\mathbf{x}^{\mathrm{T}}\mathbf{y} \quad \rightarrow \quad k(\mathbf{x}, \mathbf{y})$$

  - …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:

$$K = \begin{array}{|c|c|c|c|c|} \hline k(\mathbf{x}_1,\mathbf{x}_1) & k(\mathbf{x}_1,\mathbf{x}_2) & k(\mathbf{x}_1,\mathbf{x}_3) & \dots & k(\mathbf{x}_1,\mathbf{x}_n) \\ \hline k(\mathbf{x}_2,\mathbf{x}_1) & k(\mathbf{x}_2,\mathbf{x}_2) & k(\mathbf{x}_2,\mathbf{x}_3) & & k(\mathbf{x}_2,\mathbf{x}_n) \\ \hline & & & & \\ \hline \dots & \dots & \dots & \dots & \dots \\ \hline k(\mathbf{x}_n,\mathbf{x}_1) & k(\mathbf{x}_n,\mathbf{x}_2) & k(\mathbf{x}_n,\mathbf{x}_3) & \dots & k(\mathbf{x}_n,\mathbf{x}_n) \\ \hline \end{array}$$

(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

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

e.g. Sigmoid

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

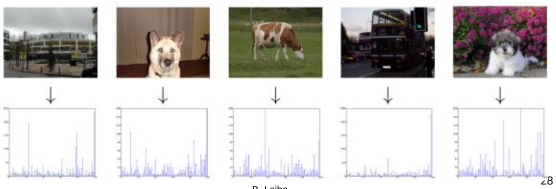
(and many, many more…)



# 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. $\chi^2$ 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

$$0 \cdot a_n \cdot C$$

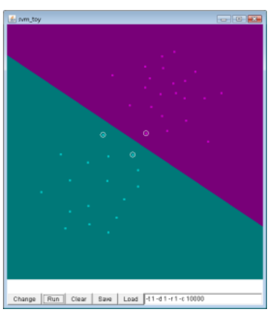
$$\sum_{n=1}^{N} a_n t_n = 0$$

- 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



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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  - Soft-margin classification
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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.

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

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

Slide adapted from Christoph Lampert

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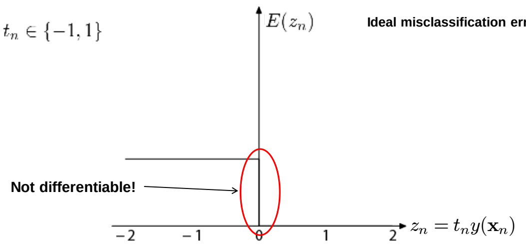
## Recap: Error Functions

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




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

Image source: Bishop, 2006

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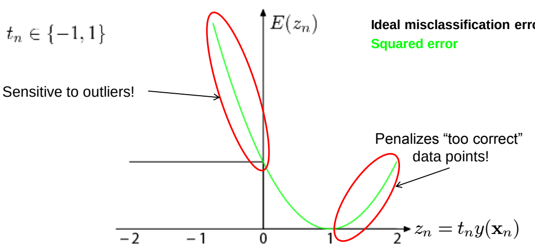
## Recap: Error Functions

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




- 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

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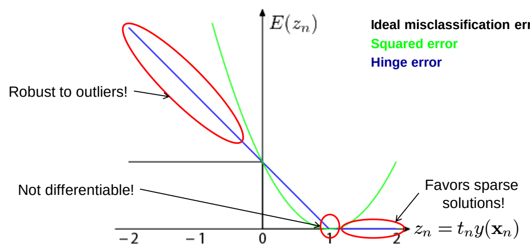
## Error Functions (Loss Functions)




- "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 $z_n = 1$ ⇒ Harder to optimize directly.

Image source: Bishop, 2006

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## SVM – Discussion

- SVM optimization function

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

- 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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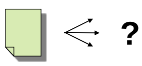
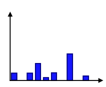
## Example Application: Text Classification

- 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

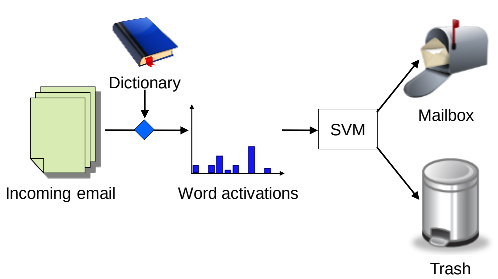
- Results:

| | 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

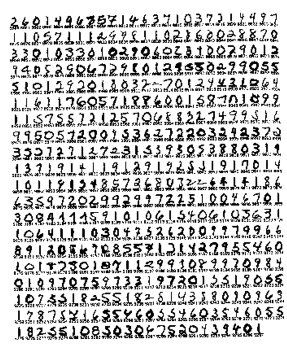
- This is also how you could implement a simple spam filter…






## 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 ($\sigma$=0.3, 291 support vectors)



## Example Application: OCR

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

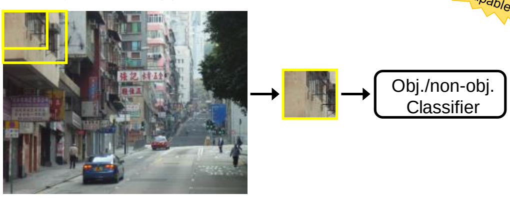
| degree of polynomial | dimensionality of feature space | support vectors | raw error |
|---|---|---|---|
| 1 | 256 | 282 | 8.9 |
| 2 | $\approx 33000$ | 227 | 4.7 |
| 3 | $\approx 1 \times 10^6$ | 274 | 4.0 |
| 4 | $\approx 1 \times 10^9$ | 321 | 4.2 |
| 5 | $\approx 1 \times 10^{12}$ | 374 | 4.3 |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

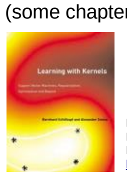
- Lots of other applications in all fields of technology
  - OCR
  - Text classification
  - Computer vision
  - …
  - High-energy physics
  - Monitoring of household appliances
  - Protein secondary structure prediction
  - Design on decision feedback equalizers (DFE) in telephony

(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).




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.