## Machine Learning - Lecture 9

## Nonlinear SVMs

19.05. 2013

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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

$$
t_{n}\left(\mathbf{w}^{\mathrm{T}} \mathbf{x}_{n}+b\right) \geq 1 \quad \forall n
$$

based on training data points $\mathbf{x}_{n}$ and target values $t_{n} \in\{-1,1\}$.

- Lagrangian primal form

$$
\begin{aligned}
L_{p} & =\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{n=1}^{N} a_{n}\left\{t_{n}\left(\mathbf{w}^{\mathrm{T}} \mathbf{x}_{n}+b\right)-1\right\} \\
& =\frac{1}{2}\|\mathbf{w}\|^{2}-\sum_{n=1}^{N} a_{n}\left\{t_{n} y\left(\mathbf{x}_{n}\right)-1\right\}
\end{aligned}
$$

- The solution of $L_{p}$ needs to fulfill the KKT conditions
- Necessary and sufficient conditions

$$
\begin{aligned}
a_{n} & \geq 0 \\
t_{n} y\left(\mathbf{x}_{n}\right)-1 & \geq 0 \\
a_{n}\left\{t_{n} y\left(\mathbf{x}_{n}\right)-1\right\} & =0
\end{aligned}
$$

| KKT: |  |
| ---: | :--- |
| $\lambda$ | $\geq 0$ |
| $f(\mathbf{x})$ | $\geq 0$ |
| $\lambda f(\mathbf{x})$ | $=0$ |



## Recap: SVM - Dual Formulation

- Maximize

$$
L_{d}(\mathbf{a})=\sum_{n=1}^{N} a_{n}-\frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_{n} a_{m} t_{n} t_{m}\left(\mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{n}\right)
$$

under the conditions

$$
\sum_{n=1}^{N} a_{n} t_{n}=0
$$

## - Comparison

, $L_{d}$ is equivalent to the primal form $L_{p}$, but only depends on $a_{n}$.

- $L_{p}$ scales with $O\left(D^{3}\right)$.
- $L_{d}$ scales with $\mathrm{O}\left(N^{3}\right)$ - in practice between $\mathrm{O}(N)$ and $\mathrm{O}\left(N^{2}\right)$.

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| :--- | :--- | :--- |

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## Recap: SVM - New Dual Formulation

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- New SVM Dual: Maximize

$$
L_{d}(\mathbf{a})=\sum_{n=1}^{N} a_{n}-\frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_{n} a_{m} t_{n} t_{m}\left(\mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{n}\right)
$$

under the conditions

$$
\begin{gathered}
0 \cdot a_{n} \cdot C \quad \begin{array}{c}
\text { This is all } \\
\text { that changed! }
\end{array} \\
\sum_{n=1}^{N} a_{n} t_{n}=0
\end{gathered}
$$

- This is again a quadratic programming problem $\Rightarrow$ Solve as before...
, We do not have to set the slack variables ourselves! $\Rightarrow$ They are jointly optimized together with w .


## Interpretation of Support Vectors

- Those are the hard examples!

We can visualize them, e.g. for face detection



## 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:


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


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## 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, $\mathrm{x}, \mathrm{y} \in \mathbb{R}^{2}$ :

- Motivation: Easier to separate data in higher-dimensional space.
- But wait - isn't there a big problem?

How should we evaluate the decision function?

## Solution: The Kernel Trick

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

$$
\begin{aligned}
y(\mathbf{x}) & =\mathbf{w}^{\mathrm{T}} \phi(\mathbf{x})+b \\
& =\sum_{n=1}^{N} a_{n} t_{n} \phi\left(\mathbf{x}_{n}\right)^{\mathrm{T}} \phi(\mathbf{x})+b
\end{aligned}
$$

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

$$
y(\mathbf{x})=\sum_{n=1}^{N} a_{n} t_{n} k\left(\mathbf{x}_{n}, \mathbf{x}\right)+b
$$

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

## 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

$$
\mathbf{w}=\sum_{n=1}^{N} a_{n} t_{n} \phi\left(\mathbf{x}_{n}\right)
$$

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

## Back to Our Previous Example...

- $2^{\text {nd }}$ degree polynomial kernel:

$$
\phi(\mathbf{x})^{\mathrm{T}} \phi(\mathbf{y})=\left[\begin{array}{c}
x_{1}^{2} \\
\sqrt{2} x_{1} x_{2} \\
x_{2}^{2}
\end{array}\right] \cdot\left[\begin{array}{c}
y_{1}^{2} \\
\sqrt{2} y_{1} y_{2} \\
y_{2}^{2}
\end{array}\right]
$$

$$
\begin{aligned}
& \qquad=x_{1}^{2} y_{1}^{2}+2 x_{1} x_{2} y_{1} y_{2}+x_{2}^{2} y_{2}^{2} \\
& \qquad=\left(\mathbf{x}^{\mathrm{T}} \mathbf{y}\right)^{2}=: k(\mathbf{x}, \mathbf{y}) \\
& \text { Whenever we evaluate the kernel function } k(\mathbf{x}, \mathbf{y})=\left(\mathbf{x}^{\top} \mathbf{y}\right)^{2} \text {, we } \\
& \text { implicitly compute the dot product in the higher-dimensional } \\
& \text { feature space. }
\end{aligned}
$$

## 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 higherdimensional (potentially infinite dimensional!) space, where the data is more easily separable.
- 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?


## "Sounds like magic..."



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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:

$K=$| $k\left(\mathbf{x}_{1}, \mathbf{x}_{1}\right)$ | $k\left(\mathbf{x}_{1}, \mathbf{x}_{2}\right)$ | $k\left(\mathbf{x}_{1}, \mathbf{x}_{3}\right)$ | $\ldots$ | $k\left(\mathbf{x}_{1}, \mathbf{x}_{n}\right)$ |
| :---: | :---: | :---: | :---: | :---: |
| $k\left(\mathbf{x}_{2}, \mathbf{x}_{1}\right)$ | $k\left(\mathbf{x}_{2}, \mathbf{x}_{2}\right)$ | $k\left(\mathbf{x}_{2}, \mathbf{x}_{3}\right)$ |  | $k\left(\mathbf{x}_{2}, \mathbf{x}_{n}\right)$ |
|  |  |  |  |  |
| $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |
| $k\left(\mathbf{x}_{n}, \mathbf{x}_{1}\right)$ | $k\left(\mathbf{x}_{n}, \mathbf{x}_{2}\right)$ | $k\left(\mathbf{x}_{n}, \mathbf{x}_{3}\right)$ | $\ldots$ | $k\left(\mathbf{x}_{n}, \mathbf{x}_{n}\right)$ |

(positive definite $=$ all eigenvalues are $>0$ )

## Kernels Fulfilling Mercer's Condition

- Polynomial kernel

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

- Radial Basis Function kernel

$$
k(\mathbf{x}, \mathbf{y})=\exp \left\{-\frac{(\mathbf{x}-\mathbf{y})^{2}}{2 \sigma^{2}}\right\} \quad \text { e.g. Gaussian }
$$

- Hyperbolic tangent kernel

$$
\left.k(\mathbf{x}, \mathbf{y})=\tan \quad{ }^{T}+-\delta\right) \quad \text { e.g. Sigmoid }
$$

Actually, this was wrong in the original SVM paper...
(and many, many more...)

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Untyle:Rs
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

$$
k_{\chi^{2}}\left(h, h^{\prime}\right)=\exp \left(-\frac{1}{\gamma} \sum_{j} \frac{\left(h_{j}-h_{j}^{\prime}\right)^{2}}{h_{j}+h_{j}^{\prime}}\right)
$$



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Nonlinear SVM - Dual Formulation

- SVM Dual: Maximize

$$
L_{d}(\mathbf{a})=\sum_{n=1}^{N} a_{n}-\frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_{n} a_{m} t_{n} t_{m} k\left(\mathbf{x}_{m}, \mathbf{x}_{n}\right)
$$

under the conditions

$$
\begin{gathered}
0 \cdot a_{n} \cdot C \\
\sum_{n=1}^{N} a_{n} t_{n}=0
\end{gathered}
$$

- Classify new data points using

$$
y(\mathbf{x})=\sum_{n=1}^{N} a_{n} t_{n} k\left(\mathbf{x}_{n}, \mathbf{x}\right)+b
$$

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## SVM Demo



## 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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- 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


## VC Dimension for Polynomial Kernel

- Polynomial kernel of degree $p$ :

$$
\begin{array}{r}
k(\mathbf{x}, \mathbf{y})=\left(\mathbf{x}^{\mathrm{T}} \mathbf{y}\right)^{p} \\
\text {, Dimensionality of } \mathcal{H}:\binom{D+p-1}{p}
\end{array}
$$

, Example:

$$
\begin{aligned}
D & =16 \times 16=256 \\
p & =4 \\
\operatorname{dim}(\mathcal{H}) & =183.181 .376
\end{aligned}
$$

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

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

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Recap: Kernels Fulfilling Mercer's Condition

- Polynomial kernel

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

- Radial Basis Function kernel

$$
k(\mathbf{x}, \mathbf{y})=\exp \left\{-\frac{(\mathbf{x}-\mathbf{y})^{2}}{2 \sigma^{2}}\right\} \quad \text { e.g. Gaussian }
$$

- Hyperbolic tangent kernel

$$
k(\mathbf{x}, \mathbf{y})=\tan \quad \text { e.g. Sigmoid }
$$

Actually, that was wrong in the original SVM paper...
(and many, many more...)
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## 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

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

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## Example: RBF Kernels

- Decision boundary on toy problem

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

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

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

- Don't we risk overfitting with those enormously highdimensional feature spaces?
. No matter what the basis functions are, there are really only up to $N$ parameters: $a_{1}, a_{2}, \ldots, a_{N}$ 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.
- For the general case, Vapnik has proven the following:

The class of optimal linear separators has VC dimension $h$ bounded from above as

$$
h \leq \min \left\{\left[\frac{D^{2}}{\rho^{2}}\right\rceil, m_{0}\right\}+1
$$

where $\rho$ 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 $m_{o}$ we can minimize the VC dimension by maximizing the margin $\rho$.
- Thus, complexity of the classifier is kept small regardless of dimensionality.

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

| . $M \leq 3 / 4 D$ | $\Rightarrow \mathbf{3}$ points can be shattered |
| :--- | :--- |
| 又 $3 / 4 D<M<D$ | $\Rightarrow \mathbf{2}$ points can be shattered |
| > $M \geq D$ | $\Rightarrow \mathbf{1}$ point can be shattered |

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

## SVM - Analysis

- Traditional soft-margin formulation

$$
\min _{\mathbf{w} \in \mathbb{R}^{D}, \xi_{n} \in \mathbb{R}^{+}} \frac{1}{2}\|\mathbf{w}\|^{2}+C \sum_{n=1}^{N} \xi_{n} \quad \begin{gathered}
\text { "Maximize } \\
\text { the margin" }
\end{gathered}
$$

subject to the constraints

$$
t_{n} y\left(\mathbf{x}_{n}\right) \geq 1-\xi_{n}
$$

"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.

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

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


$$
\begin{aligned}
& \text { SVM - Discussion } \\
& \text { - SVM optimization function } \\
& \min _{\mathbf{w} \in \mathbb{R}^{D}}^{\operatorname{L}_{2}} \underbrace{\frac{1}{2}\|\mathbf{w}\|^{2}}_{\text {regularizer }}+\underbrace{C \sum_{n=1}^{N}\left[1-t_{n} y\left(\mathbf{x}_{n}\right)\right]_{+}}_{\text {Hinge loss }}
\end{aligned}
$$

- 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 B. Leibe 51

## 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 ( $\sim 10.000$ dimensions) Few irrelevant features
- This was one of the first applications of SVMs - T. Joachims (1997)



|  | Example Application: OCR <br> - Results <br> . Almost no overfitting with higher-degree kernels. |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | degree of polynomial | dimensionality of feature space | support vectors | $\begin{aligned} & \text { raw } \\ & \text { error } \end{aligned}$ |
|  | plo | 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 |

## 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)


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Nonlinear Support Vector Machines

- Analysis

VC dimensions
Error function

- Applications
- Extensions
, One-class SVMs
$\qquad$



## 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).

- Both include fast training and evaluation algorithms, support for multi-class SVMs, automated training and cross-validation, ... $\Rightarrow$ Easy to apply to your own problems!

