

Machine Learning – Lecture 8

Nonlinear Support Vector Machines

15.11.2018

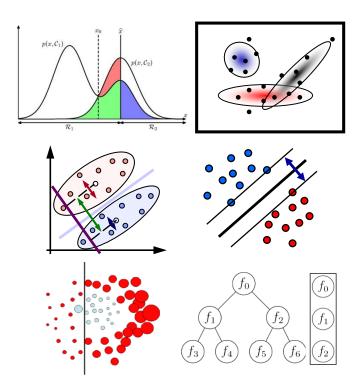
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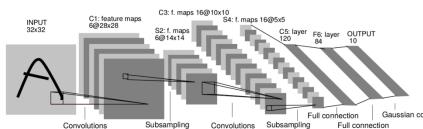
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Course Outline

- 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

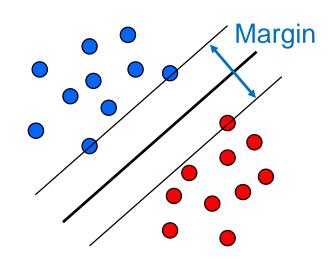
- Support Vector Machines
 - Recap: Lagrangian (primal) formulation
 - Dual formulation
 - Soft-margin classification
- Nonlinear Support Vector Machines
 - Nonlinear basis functions
 - The Kernel trick
 - Mercer's condition
 - Popular kernels
- Analysis
 - Error function
- Applications

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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

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

under the constraints

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

based on training data points \mathbf{x}_n and target values

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



Recap: SVM – Lagrangian Formulation

• Find hyperplane minimizing $\left|\left|\mathbf{w}\right|\right|^2$ under the constraints

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

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

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

 \triangleright I.e., find w, b, and a such that

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



Recap: SVM – Primal Formulation

Lagrangian primal form

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

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

$$a_n \ge 0$$

$$t_n y(\mathbf{x}_n) - 1 \ge 0$$

$$a_n \{t_n y(\mathbf{x}_n) - 1\} = 0$$

KKT:

$$\lambda \geq 0$$

 $f(\mathbf{x}) \geq 0$
 $\lambda f(\mathbf{x}) = 0$

$$\lambda f(\mathbf{x}) = 0$$



SVM – Solution (Part 1)

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

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

Because of the KKT conditions, the following must also hold

$$a_n \left(t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) - 1 \right) = 0$$

 $\begin{array}{c} \text{KKT:} \\ \lambda f(\mathbf{x}) = 0 \end{array}$

 \triangleright This implies that $a_n > 0$ only for training data points for which

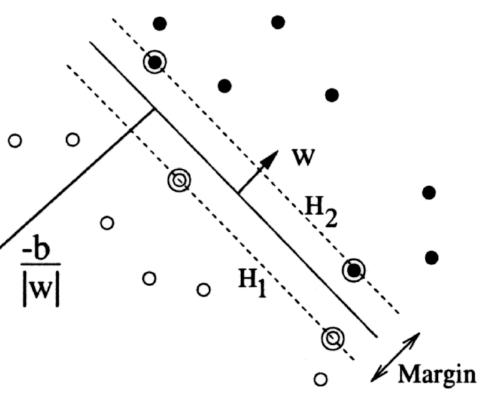
$$(t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) - 1) = 0$$

⇒ Only some of the data points actually influence the decision boundary!



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.
 - ⇒ Robustness to "too correct" points!





SVM – Solution (Part 2)

- Solution for the hyperplane
 - \triangleright To define the decision boundary, we still need to know b.
 - > Observation: any support vector \mathbf{x}_n satisfies

$$t_n y(\mathbf{x}_n) = t_n \left(\sum_{m \in \mathcal{S}} a_m t_m \mathbf{x}_m^{\mathrm{T}} \mathbf{x}_n + b \right) = 1$$
 KKT: $f(\mathbf{x}) \ge 0$

Using
$$t_n^2=1$$
 we can derive: $b=t_n-\sum_{m\in\mathcal{S}}a_mt_m\mathbf{x}_m^T\mathbf{x}_n$

In practice, it is more robust to average over all support vectors:

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



SVM - Discussion (Part 1)

Linear SVM

- Linear classifier
- SVMs have a "guaranteed" generalization capability.
- Formulation as convex optimization problem.
- ⇒ Globally optimal solution!

Primal form formulation

- > Solution to quadratic prog. problem in M variables is in $\mathcal{O}(M^3)$.
- > Here: D variables $\Rightarrow \mathcal{O}(D^3)$
- Problem: scaling with high-dim. data ("curse of dimensionality")



SVM – Dual Formulation

• Improving the scaling behavior: rewrite L_p in a dual form

> Using the constraint $\sum_{n=1}^{\infty}a_nt_n=0$ we obtain

$$\frac{\partial L_p}{\partial b} = 0$$

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



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SVM - Dual Formulation

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

> Using the constraint $\mathbf{w=}\sum_{\mathbf{1}}a_{n}t_{n}\mathbf{x}_{n}$ we obtain

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0$$

$$L_p = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n t_n \sum_{m=1}^{N} a_m t_m \mathbf{x}_m^T \mathbf{x}_n + \sum_{n=1}^{N} a_n$$
$$= \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^T \mathbf{x}_n) + \sum_{n=1}^{N} a_n$$





SVM – Dual Formulation

$$L = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^T \mathbf{x}_n) + \sum_{n=1}^{N} a_n$$

> Applying $\frac{1}{9} \|\mathbf{w}\|^2 = \frac{1}{9} \mathbf{w}^{\mathrm{T}} \mathbf{w}$ and again using $\mathbf{w} = \sum_{n=1}^{\infty} a_n t_n \mathbf{x}_n$

$$\frac{1}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} = \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}a_{n}a_{m}t_{n}t_{m}(\mathbf{x}_{m}^{\mathrm{T}}\mathbf{x}_{n})$$

Inserting this, we get the Wolfe dual

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



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

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

 \succ The hyperplane is given by the N_S support vectors:

$$\mathbf{w} = \sum_{n=1}^{N_{\mathcal{S}}} a_n t_n \mathbf{x}_n$$



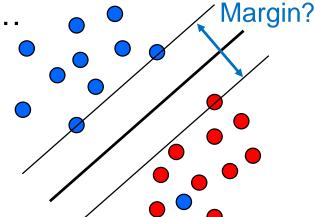
SVM – Discussion (Part 2)

- Dual form formulation
 - In going to the dual, we now have a problem in N variables (a_n) .
 - Isn't this worse??? We penalize large training sets!
- However...
 - 1. SVMs have sparse solutions: $a_n \neq 0$ only for support vectors!
 - ⇒ This makes it possible to construct efficient algorithms
 - e.g. Sequential Minimal Optimization (SMO)
 - Effective runtime between $\mathcal{O}(N)$ and $\mathcal{O}(N^2)$.
 - 2. We have avoided the dependency on the dimensionality.
 - \Rightarrow This makes it possible to work with infinite-dimensional feature spaces by using suitable basis functions $\phi(\mathbf{x})$.
 - ⇒ We'll see that later in today's lecture...



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

$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_{n} + b \ge +1$$
 for $t_{n} = +1$
 $\mathbf{w}^{\mathrm{T}}\mathbf{x}_{n} + b \cdot -1$ for $t_{n} = -1$

Instead use

$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_{n} + b \ge +1 - \xi_{n}$$
 for $t_{n} = +1$
 $\mathbf{w}^{\mathrm{T}}\mathbf{x}_{n} + b \cdot -1 + \xi_{n}$ for $t_{n} = -1$

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



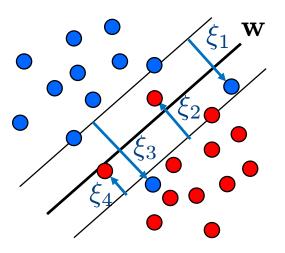
SVM – Soft-Margin Classification

Slack variables

> One slack variable $\xi_n \geq 0$ for each training data point.

Interpretation

- $\xi_n = 0$ for points that are on the correct side of the margin.
- > $\xi_n = |t_n y(\mathbf{x}_n)|$ for all other points (linear penalty).



Point on decision boundary: $\xi_n = 1$

Misclassified point:

$$\xi_n > 1$$

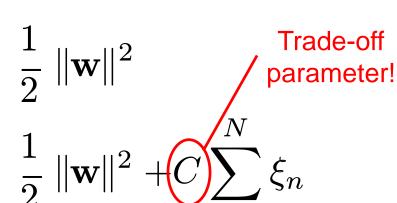
- We do not have to set the slack variables ourselves!
- \Rightarrow They are jointly optimized together with w.

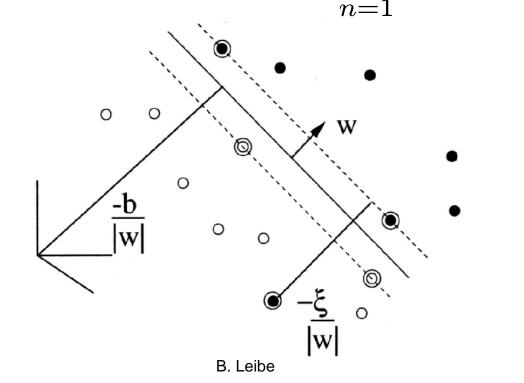




SVM - Non-Separable Data

- Separable data
 - Minimize
- Non-separable data
 - Minimize







SVM - New Primal Formulation

New SVM Primal: Optimize

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

KKT conditions

$$a_n \geq 0$$
 $\mu_n \geq 0$ $t_n y(\mathbf{x}_n) - 1 + \xi_n \geq 0$ $\xi_n \geq 0$ $a_n (t_n y(\mathbf{x}_n) - 1 + \xi_n) = 0$ $\mu_n \xi_n = 0$ λ

$$\lambda \geq 0$$

$$f(\mathbf{x}) \geq 0$$

$$\lambda f(\mathbf{x}) = 0$$



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

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

This is all that changed!

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



SVM - New Solution

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

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

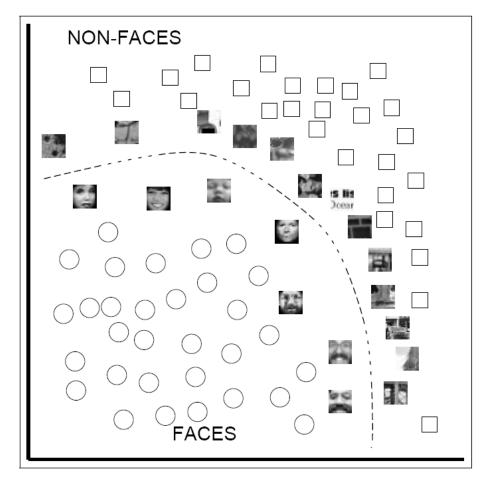
- Again sparse solution: $a_n=0$ for points outside the margin.
- \Rightarrow The slack points with $\xi_n > 0$ are now also support vectors!
- > Compute b by averaging over all $N_{\mathcal{M}}$ points with $0 < a_n < C$:

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



Interpretation of Support Vectors

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





Topics of This Lecture

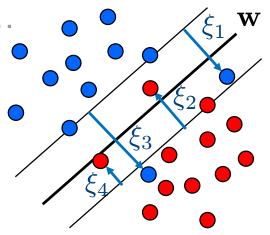
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 - Recap: Lagrangian (primal) formulation
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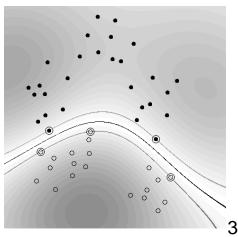
So Far...

- 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.

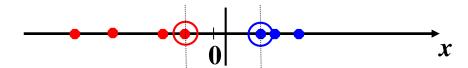




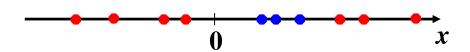
Nonlinear SVM

Linear SVMs

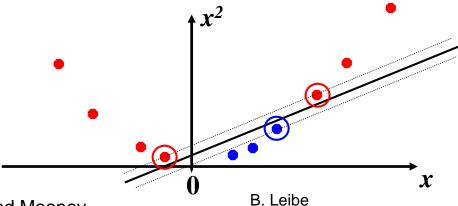
Datasets that are linearly separable with some noise work well:



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



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



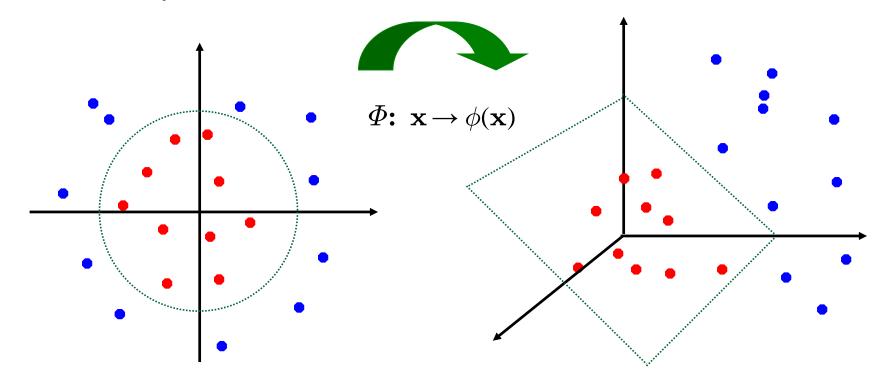
Slide credit: Raymond Mooney

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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 ϕ of the data points \mathbf{x}_n :

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

 \rightarrow 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, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$:

$$\phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \begin{bmatrix} 0.8 \\ 0.6 \\ 0.4 \\ 0.2 \\ 0 \end{bmatrix}$$

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

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

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

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

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



Back to Our Previous Example...

2nd degree polynomial kernel:

$$\phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{y}) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \cdot \begin{bmatrix} y_1^2 \\ \sqrt{2}y_1y_2 \\ y_2^2 \end{bmatrix}^{\frac{0.8}{0.4}}$$

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

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

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



SVMs with Kernels

Using kernels

Applying the kernel trick is easy. Just replace every dot product by a kernel function...

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

- ...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.

"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:

	$k(\mathbf{x}_1,\mathbf{x}_1)$	$k(\mathbf{x}_1,\mathbf{x}_2)$	$k(\mathbf{x}_1,\mathbf{x}_3)$		$k(\mathbf{x}_1,\mathbf{x}_n)$
	$k(\mathbf{x}_2,\mathbf{x}_1)$	$k(\mathbf{x}_2,\mathbf{x}_2)$	$k(\mathbf{x}_2,\mathbf{x}_3)$		$k(\mathbf{x}_2,\mathbf{x}_n)$
K =					
		•••	• • •	•••	•••
	$k(\mathbf{x}_n,\mathbf{x}_1)$	$k(\mathbf{x}_n,\mathbf{x}_2)$	$k(\mathbf{x}_n,\mathbf{x}_3)$	•••	$k(\mathbf{x}_n, \mathbf{x}_n)$

(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

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

e.g. Sigmoid

(and many, many more...)

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

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Example: Bag of Visual Words Representation

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

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

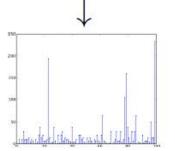


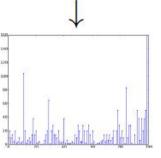


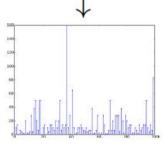


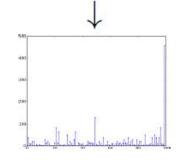


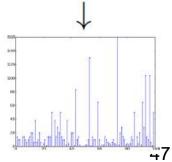












Slide adapted from Christoph Lampert

B. Leibe



Nonlinear SVM – Dual Formulation

SVM Dual: Maximize

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

under the conditions

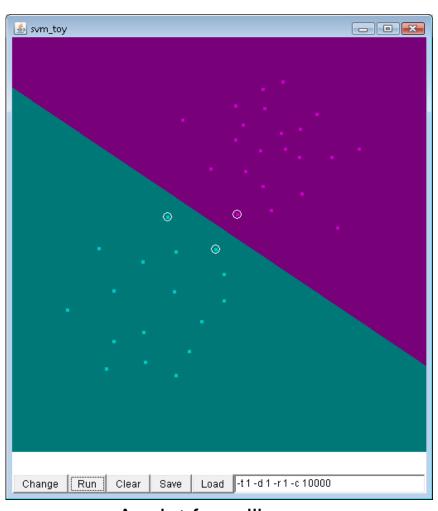
$$\sum_{n=1}^{N} a_n t_n = 0$$

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/)

B. Leibe



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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SVM – Analysis

Traditional soft-margin formulation

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

"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.

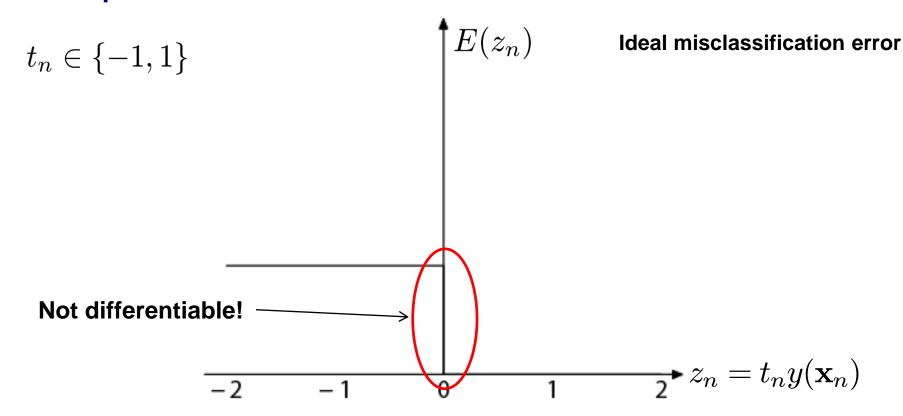
$$\min_{\mathbf{w} \in \mathbb{R}^D} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N [1 - t_n y(\mathbf{x}_n)]_+$$
L₂ regularizer "Hinge loss"

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

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Recap: Error Functions

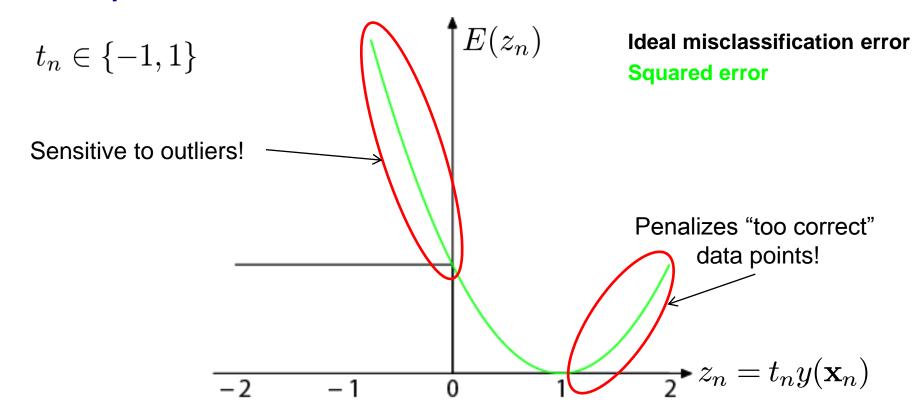


- Ideal misclassification error function (black)
 - This is what we want to approximate,
 - Unfortunately, it is not differentiable.
 - The gradient is zero for misclassified points.
 - ⇒ We cannot minimize it by gradient descent.

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Recap: Error Functions

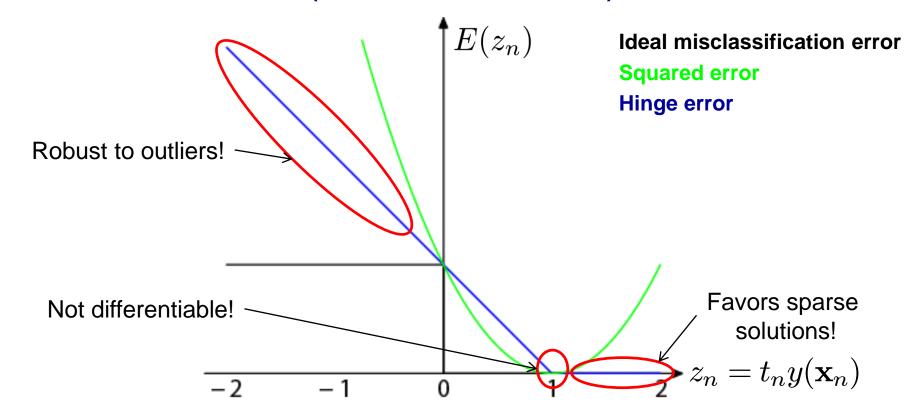


- Squared error used in Least-Squares Classification
 - Very popular, leads to closed-form solutions.
 - However, sensitive to outliers due to squared penalty.
 - Penalizes "too correct" data points
 - ⇒ Generally does not lead to good classifiers.

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Error Functions (Loss Functions)



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



SVM – Discussion

SVM optimization function

$$\min_{\mathbf{w} \in \mathbb{R}^D} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N \left[1 - t_n y(\mathbf{x}_n)\right]_+$$

$$\mathsf{L}_2 \text{ regularizer} \qquad \mathsf{Hinge loss}$$

- 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



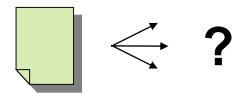
Topics of This Lecture

- 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
 - Error function
- Applications



Example Application: Text Classification

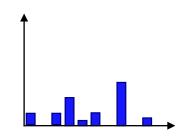
- Problem:
 - Classify a document in a number of categories



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



T. Joachims (1997)



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Example Application: Text Classification

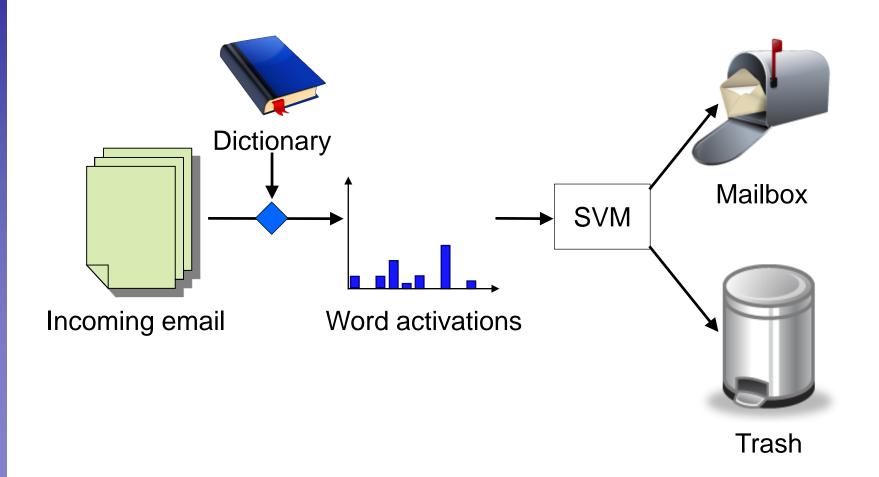
Results:

					SVM (poly)				SVM (rbf)				
					degree $d =$			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)
 - \rightarrow 4.1% error: Gaussian kernel (σ =0.3, 291 support vectors)



Example Application: OCR

Results

Almost no overfitting with higher-degree kernels.

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

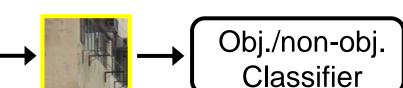
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Real-time capable!

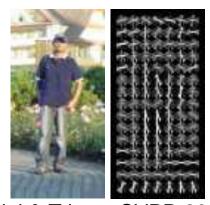
Example Application: Object Detection

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]

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Example Application: Pedestrian Detection



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



Many Other Applications

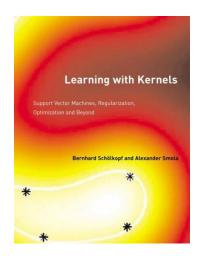
- Lots of other applications in all fields of technology
 - > OCR
 - Text classification
 - Computer vision
 - > . . .
 - High-energy physics
 - Monitoring of household appliances
 - Protein secondary structure prediction
 - Design on decision feedback equalizers (DFE) in telephony

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

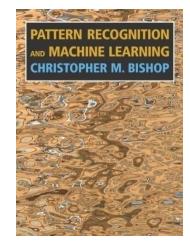


References and Further Reading

 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, <u>A Tutorial on Support Vector Machines for Pattern</u>
 <u>Recognition</u>, Data Mining and Knowledge Discovery, Vol. 2(2), pp.
 121-167 1998.