Machine Learning – Lecture 8

Support Vector Machines

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Announcements

- Exam dates
  - 1st date: Saturday, 29.02., 13:30h – 15:30h
  - 2nd date: Thursday, 19.03., 11:00h – 13:00h

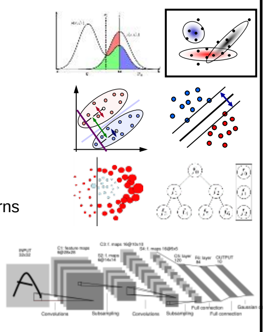
  - The exam dates have been optimized to avoid overlaps with other Computer Science Master lectures as much as possible.
  - If you still have conflicts with *both* exam dates, please tell us.

  - If you're *an exchange student and need to leave RWTH before the first exam date*, we will offer some special oral exam slots
    - Please do NOT contact us about those yet.
    - We will let you sign up for those special exam slots in early January

- *Please do not forget to register for the exam in RWTH online!*

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



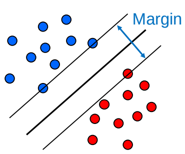
Topics of This Lecture

- Support Vector Machines
  - 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 $t_n \in \{-1, 1\}$

Support Vector Machine (SVM)

- Optimization problem
  - Find the hyperplane satisfying

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

under the constraints

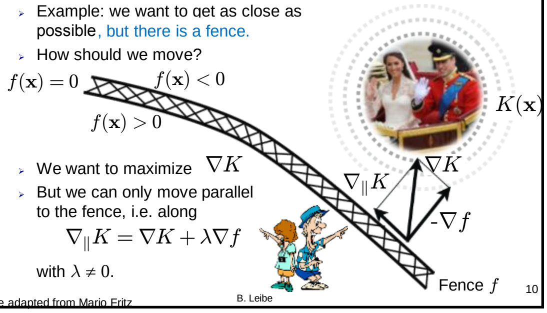
$$t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) \geq 1 \quad \forall n$$

  - Quadratic programming problem with linear constraints.
  - Can be formulated using Lagrange multipliers.

- *Who is already familiar with Lagrange multipliers?*
  - Let's look at a real-life example…

Recap: Lagrange Multipliers

- Problem
  - We want to maximize $K(\mathbf{x})$ subject to constraints $f(\mathbf{x}) = 0$.
  - Example: we want to get as close as possible, but there is a fence.
  - How should we move?



- We want to maximize ∇K
- But we can only move parallel to the fence, i.e. along
  $$\nabla_{\|} K = \nabla K + \lambda \nabla f$$
  with $\lambda \neq 0$.

Slide adapted from Mario Fritz

Recap: Lagrange Multipliers

- Problem
  - We want to maximize $K(\mathbf{x})$ subject to constraints $f(\mathbf{x}) = 0$.
  - Example: we want to get as close as possible, but there is a fence.
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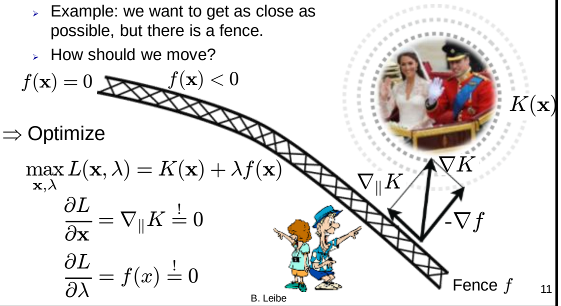


$\Rightarrow$ Optimize

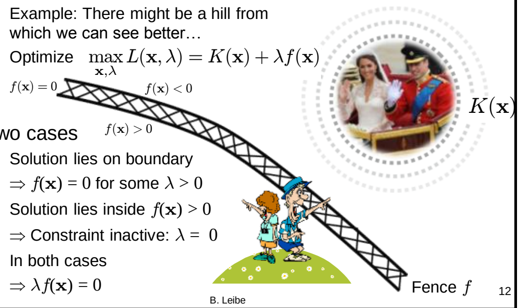
$$\max_{\mathbf{x},\lambda} L(\mathbf{x}, \lambda) = K(\mathbf{x}) + \lambda f(\mathbf{x})$$

$$\frac{\partial L}{\partial \mathbf{x}} = \nabla_{\|} K \stackrel{!}{=} 0$$

$$\frac{\partial L}{\partial \lambda} = f(x) \stackrel{!}{=} 0$$

Recap: Lagrange Multipliers

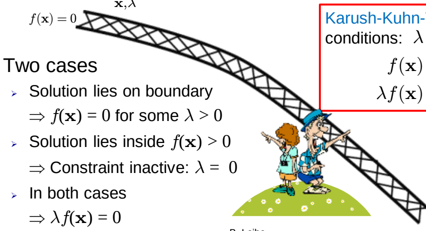
- Problem
  - Now let's look at constraints of the form $f(\mathbf{x}) \geq 0$.
  - Example: There might be a hill from which we can see better…
  - Optimize $\max_{\mathbf{x},\lambda} L(\mathbf{x}, \lambda) = K(\mathbf{x}) + \lambda f(\mathbf{x})$



- Two cases
  - Solution lies on boundary
    $\Rightarrow f(\mathbf{x}) = 0$ for some $\lambda > 0$
  - Solution lies inside $f(\mathbf{x}) > 0$
    $\Rightarrow$ Constraint inactive: $\lambda = 0$
  - In both cases
    $\Rightarrow \lambda f(\mathbf{x}) = 0$

Recap: Lagrange Multipliers

- Problem
  - Now let's look at constraints of the form $f(\mathbf{x}) \geq 0$.
  - Example: There might be a hill from which we can see better…
  - Optimize $\max_{\mathbf{x},\lambda} L(\mathbf{x}, \lambda) = K(\mathbf{x}) + \lambda f(\mathbf{x})$



Karush-Kuhn-Tucker (KKT) conditions:
$$\begin{aligned} \lambda &\geq 0 \\ f(\mathbf{x}) &\geq 0 \\ \lambda f(\mathbf{x}) &= 0 \end{aligned}$$

- Two cases
  - Solution lies on boundary
    $\Rightarrow f(\mathbf{x}) = 0$ for some $\lambda > 0$
  - Solution lies inside $f(\mathbf{x}) > 0$
    $\Rightarrow$ Constraint inactive: $\lambda = 0$
  - In both cases
    $\Rightarrow \lambda f(\mathbf{x}) = 0$

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

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

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

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

$\boxed{\text{KKT: } \lambda f(\mathbf{x}) = 0}$

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

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

$\Rightarrow$ *Only some of the data points actually influence the decision boundary!*

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Slide adapted from Bernt Schiele

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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.

$\Rightarrow$ Robustness to "too correct" points!

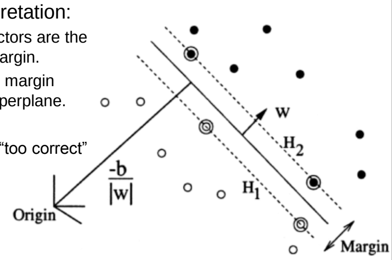

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Image source: C. Burges, 1998

SVM – Solution (Part 2)

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

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

$\boxed{\text{KKT: } f(\mathbf{x}) \geq 0}$

  - Using $t_n^2 = 1$ we can derive: $b = t_n - \sum_{m \in \mathcal{S}} a_m t_m \mathbf{x}_m^{\mathrm{T}} \mathbf{x}_n$
  - In practice, it is more robust to average over all support vectors:

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

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SVM – Discussion (Part 1)

- Linear SVM
  - Linear classifier
  - SVMs have a "guaranteed" generalization capability.
  - Formulation as convex optimization problem.

$\Rightarrow$ 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")

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SVM – Dual Formulation

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

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

$$= \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n t_n \mathbf{w}^{\mathrm{T}} \mathbf{x}_n - b \underbrace{\cancel{\sum_{n=1}^{N} a_n t_n}}_{=0} + \sum_{n=1}^{N} a_n$$

  - Using the constraint $\sum_{n=1}^{N} a_n t_n = 0$ we obtain $\boxed{\frac{\partial L_p}{\partial b} = 0}$

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

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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 $\mathbf{w} = \sum_{n=1}^{N} a_n t_n \mathbf{x}_n$ we obtain $\boxed{\frac{\partial L_p}{\partial \mathbf{w}} = 0}$

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

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

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SVM – Dual Formulation

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

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

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

- 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

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

- The hyperplane is given by the N_S support vectors:

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

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!

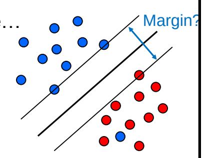
     ⇒ This makes it possible to construct efficient algorithms
     - e.g. Sequential Minimal Optimization (SMO)
     - Effective runtime between $\mathcal{O}(N)$ and $\mathcal{O}(N^2)$.
  2. We have avoided the dependency on the dimensionality.

     ⇒ 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

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

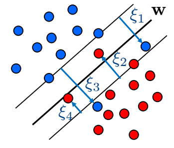
  - Instead use

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

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

SVM – Soft-Margin Classification

- Slack variables
  - One slack variable $\xi_n \geq 0$ for each training data point.
- Interpretation
  - $\xi_n = 0$ for points that are on the correct side of the margin.
  - $\xi_n = |t_n - y(\mathbf{x}_n)|$ for all other points (linear penalty).



Point on decision boundary: $\xi_n = 1$

Misclassified point: $\xi_n > 1$

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

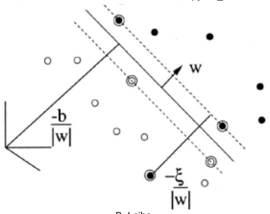
⇒ They are jointly optimized together with $\mathbf{w}$.

How that?

SVM – Non-Separable Data

- Separable data
  - Minimize $\frac{1}{2}\|\mathbf{w}\|^2$
- Non-separable data
  - Minimize $\frac{1}{2}\|\mathbf{w}\|^2 + C \sum_{n=1}^{N} \xi_n$

Trade-off parameter!



SVM – New Primal Formulation

- New SVM Primal: Optimize

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

- KKT conditions

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

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

SVM – New Dual Formulation

- New SVM Dual: Maximize

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

under the conditions

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

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

This is all that changed!

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

Slide adapted from Bernt Schiele

SVM – New Solution

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

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

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

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

Interpretation of Support Vectors

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

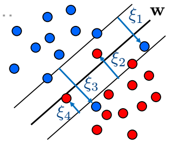
Image source: E. Osuna, F. Girosi, 1997

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

So Far…

- Only looked at linearly separable case…
  - Current problem formulation has no solution if the data are not linearly separable!
  - Need to introduce some tolerance to outlier data points.
  - ⇒ Slack variables.



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

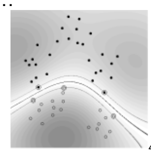
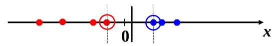


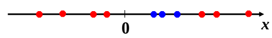
Image source: B. Schoelkopf, A. Smola, 2002

Nonlinear SVM

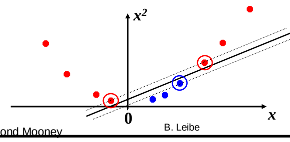
- Linear SVMs
  - Datasets that are linearly separable with some noise work well:



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



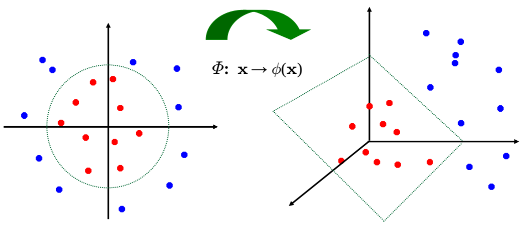
  - How about… mapping data to a higher-dimensional space:



Slide credit: Raymond Mooney

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 $\mathcal{H}$)

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

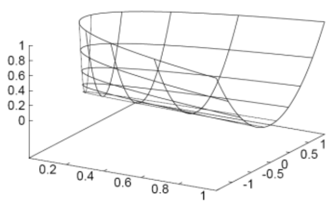
  - ⇒ Nonlinear classifier in $\mathbb{R}^D$.

Slide credit: Bernt Schiele

What Could This Look Like?

- Example:
  - Mapping to polynomial space, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$:

$$\phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix}$$



  - Motivation: Easier to separate data in higher-dimensional space.
  - But wait – isn't there a big problem?
    - How should we evaluate the decision function?

Image source: C. Burges, 1998

Problem with High-dim. Basis Functions

- Problem
  - In order to apply the SVM, we need to evaluate the function

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

  - Using the hyperplane, which is itself defined as

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

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

Solution: The Kernel Trick

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

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

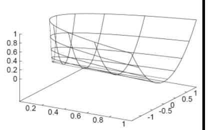
  - Trick: Define a so-called kernel function $k(\mathbf{x},\mathbf{y}) = \phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{y})$.
  - Now, in place of the dot product, use the kernel instead:

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

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

Back to Our Previous Example…

- 2nd degree polynomial kernel:



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

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

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

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

Image source: C. Burges, 1998

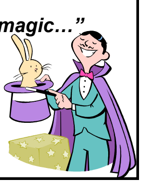
SVMs with Kernels

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

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

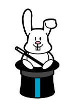
  - …and we're done.
  - Instead of the raw input space, we're now working in a higher-dimensional (potentially infinite dimensional!) space, where the data is more easily separable.

"Sounds like magic…"



- Wait – does this always work?
  - The kernel needs to define an implicit mapping to a higher-dimensional feature space $\phi(\mathbf{x})$.
  - When is this the case?

Which Functions are Valid Kernels?



- Mercer's theorem (modernized version):
  - *Every positive definite symmetric function is a kernel.*
- Positive definite symmetric functions correspond to a positive definite symmetric Gram matrix:

$K =$

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

(positive definite = all eigenvalues are > 0)

Slide credit: Raymond Mooney

Kernels Fulfilling Mercer's Condition

- Polynomial kernel

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

- Radial Basis Function kernel

$$k(\mathbf{x},\mathbf{y}) = \exp\left\{-\frac{(\mathbf{x}-\mathbf{y})^2}{2\sigma^2}\right\}$$

e.g. Gaussian

- Hyperbolic tangent kernel

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

e.g. Sigmoid

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

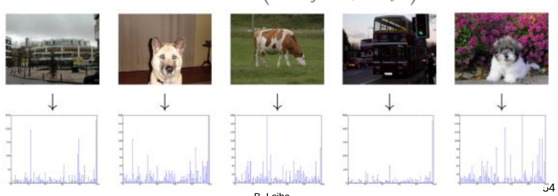
(and many, many more…)

Slide credit: Bernt Schiele

Example: Bag of Visual Words Representation

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

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



Slide adapted from Christoph Lampert

Nonlinear SVM – Dual Formulation

- SVM Dual: Maximize

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

under the conditions

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

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

- Classify new data points using

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

SVM Demo

Applet from libsvm
(http://www.csie.ntu.edu.tw/~cjlin/libsvm/)

Summary: SVMs

- Properties
  - Empirically, SVMs work very, very well.
  - SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
  - SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.
  - SVM techniques have been applied to a variety of other tasks
    - e.g. SV Regression, One-class SVMs, …
  - The kernel trick has been used for a wide variety of applications. It can be applied wherever dot products are in use
    - e.g. Kernel PCA, kernel FLD, …
    - Good overview, software, and tutorials available on http://www.kernel-machines.org/

Summary: SVMs

- Limitations
  - How to select the right kernel?
    - Best practice guidelines are available for many applications
  - How to select the kernel parameters?
    - (Massive) cross-validation.
    - Usually, several parameters are optimized together in a grid search.
  - Solving the quadratic programming problem
    - Standard QP solvers do not perform too well on SVM task.
    - Dedicated methods have been developed for this, e.g. SMO.
  - Speed of evaluation
    - Evaluating $y(\mathbf{x})$ scales linearly in the number of SVs.
    - Too expensive if we have a large number of support vectors.
    - ⇒ There are techniques to reduce the effective SV set.
  - Training for very large datasets (millions of data points)
    - Stochastic gradient descent and other approximations can be used

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

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"

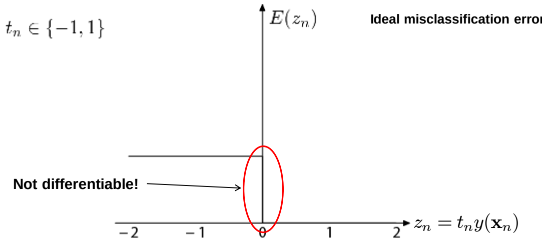
- Different way of looking at it
  - We can reformulate the constraints into the objective function.

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

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

Slide adapted from Christoph Lampert

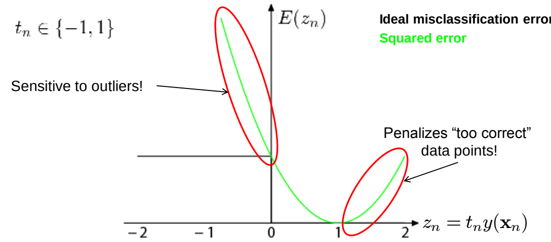
Recap: Error Functions



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

Image source: Bishop, 2006

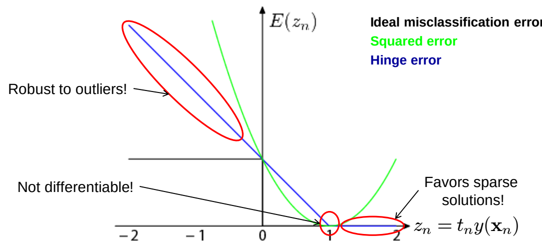
Recap: Error Functions



- 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
  - $\Rightarrow$ 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 $z_n = 1$ $\Rightarrow$ Cannot be optimized directly.

Image source: Bishop, 2006

SVM – Discussion

- SVM optimization function

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

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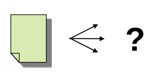
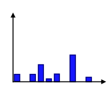
  - Soft-margin classification
- Nonlinear Support Vector Machines
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Analysis
  - Error function
- Applications

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



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

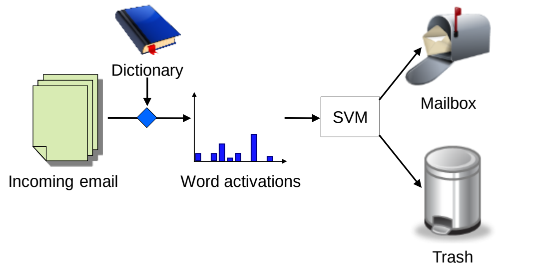
Example Application: Text Classification

- 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**			

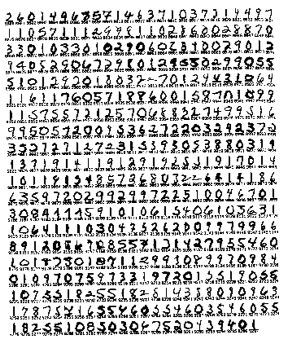
Example Application: Text Classification

- 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 (σ=0.3, 291 support vectors)

Example Application: OCR

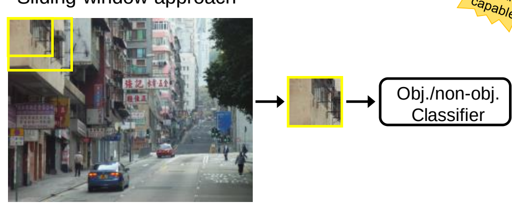
- Results
  - Almost no overfitting with higher-degree kernels.

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

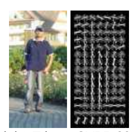
Example Application: Object Detection

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

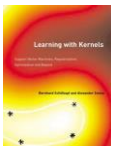
Many Other Applications

- 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

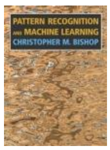
  (Detailed references in Schoelkopf & Smola, 2002, pp. 221)

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).



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.