RWTH AACHEN UNIVERSITY

Machine Learning – Lecture 8

Linear Support Vector Machines

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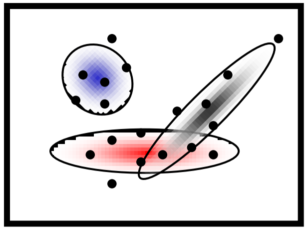
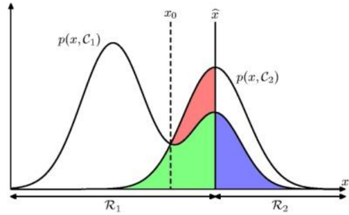
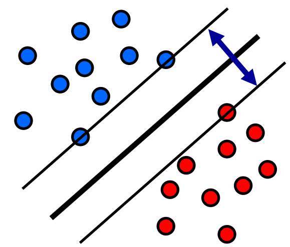
Course Outline

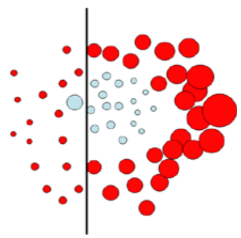
- Fundamentals (2 weeks)
  - Bayes Decision Theory
  - Probability Density Estimation



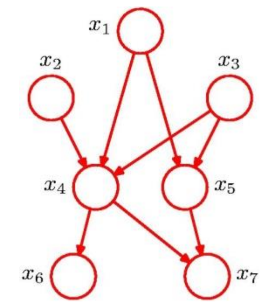


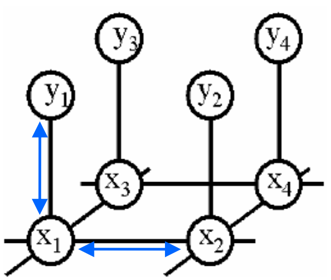
- Discriminative Approaches (5 weeks)
  - Linear Discriminant Functions
  - Statistical Learning Theory & SVMs
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns



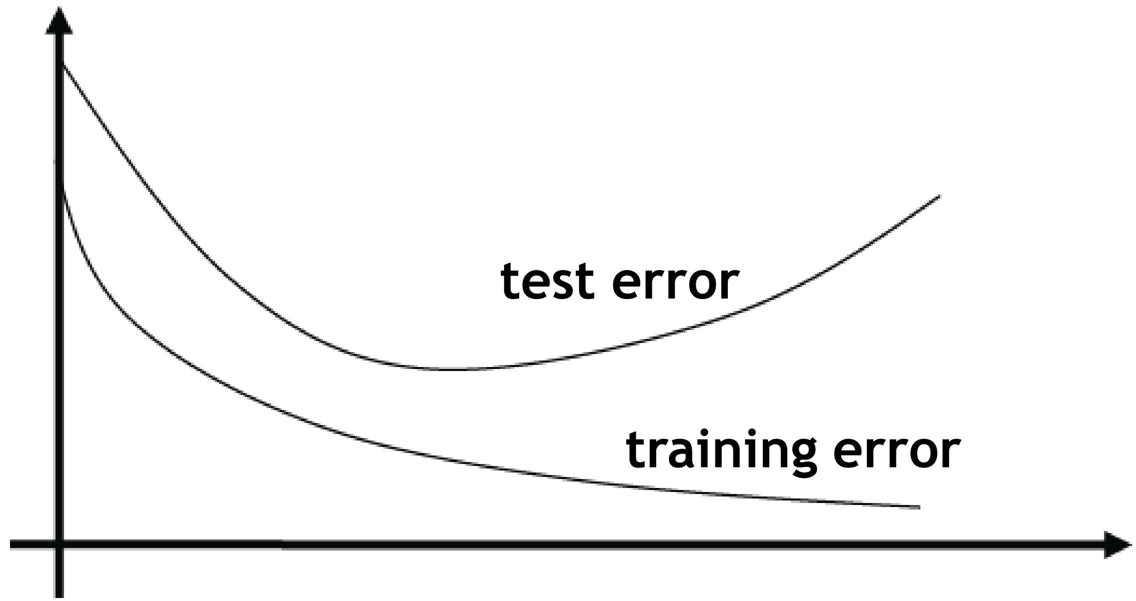


- Generative Models (4 weeks)
  - Bayesian Networks
  - Markov Random Fields





Recap: Generalization and Overfitting



- Goal: predict class labels of new observations
  - Train classification model on limited training set.
  - The further we optimize the model parameters, the more the training error will decrease.
  - However, at some point the test error will go up again.
  - ⇒ *Overfitting to the training set!*

Image source: B. Schiele

Recap: Risk

- **Empirical risk**
  - Measured on the training/validation set

$$R_{emp}(\alpha) = \frac{1}{N}\sum_{i=1}^{N} L(y_i, f(\mathbf{x}_i;\alpha))$$

- **Actual risk** (= **Expected risk**)
  - Expectation of the error on *all* data.

$$R(\alpha) = \int L(y_i, f(\mathbf{x};\alpha))dP_{X,Y}(\mathbf{x},y)$$

  - $P_{X,Y}(\mathbf{x},y)$ is the probability distribution of $(\mathbf{x},y)$. It is fixed, but typically unknown.

$\Rightarrow$ In general, we can't compute the actual risk directly!

Recap: Statistical Learning Theory

- **Idea**
  - Compute an upper bound on the actual risk based on the empirical risk

$$R(\alpha) \cdot \quad R_{emp}(\alpha) + \epsilon(N, p^{*}, h)$$

  - where

    N: number of training examples

    p^{*}: probability that the bound is correct

    h: capacity of the learning machine (“VC-dimension”)

Recap: VC Dimension

see Exercise 2.3

- Vapnik-Chervonenkis dimension
  - Measure for the capacity of a learning machine.

- Formal definition:
  - *If a given set of ℓ points can be labeled in all possible 2^ℓ ways, and for each labeling, a member of the set $\{f(\alpha)\}$ can be found which correctly assigns those labels, we say that the set of points is shattered by the set of functions.*
  - *The VC dimension for the set of functions $\{f(\alpha)\}$ is defined as the maximum number of training points that can be shattered by $\{f(\alpha)\}$.*

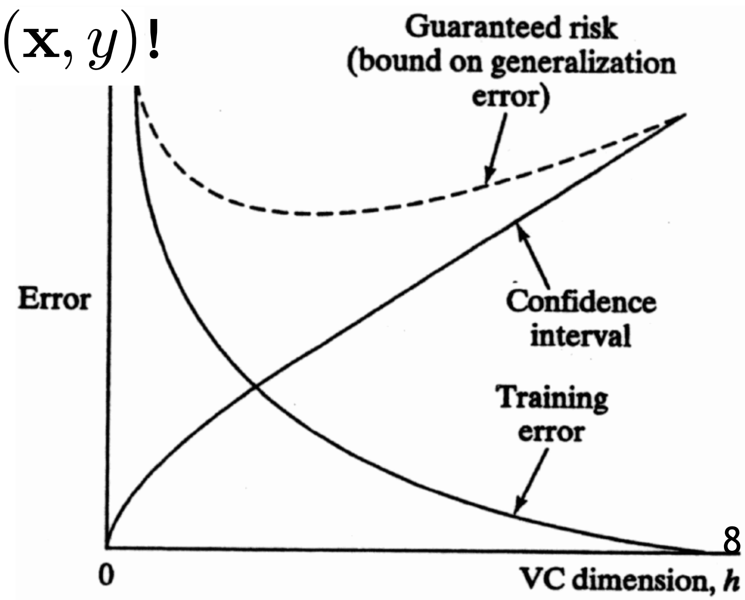
Recap: Upper Bound on the Risk

- **Important result (Vapnik 1979, 1995)**
  - **With probability $(1\text{-}\eta)$, the following bound holds**

$$R(\alpha) \cdot \quad R_{emp}(\alpha) + \underbrace{\sqrt{\frac{h(\log(2N/h)+1) - \log(\eta/4)}{N}}}_{\text{“VC confidence”}}$$

  - **This bound is independent of $P_{X,Y}(\mathbf{x}, y)$!**
  - **If we know h (the VC dimension), we can easily compute the risk bound**

$$R(\alpha) \cdot \quad R_{emp}(\alpha) + \epsilon(N, p^*, h)$$



Recap: Structural Risk Minimization

- How can we implement Structural Risk Minimization?

$$R(\alpha) \cdot \quad R_{emp}(\alpha) + \epsilon(N, p^*, h)$$

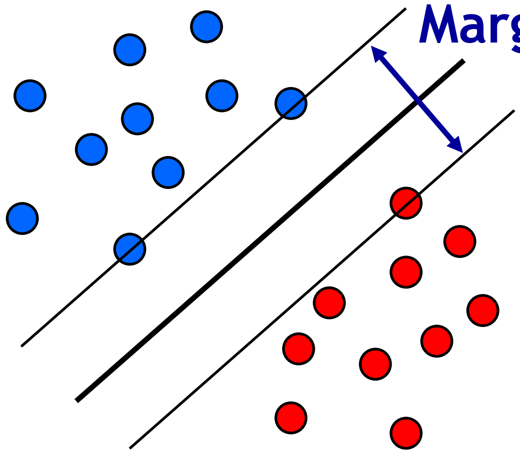
- Classic approach
  - Keep $\epsilon(N, p^*, h)$ constant and minimize $R_{emp}(\alpha)$.
  - $\epsilon(N, p^*, h)$ can be kept constant by controlling the model parameters.

- Support Vector Machines (SVMs)
  - Keep $R_{emp}(\alpha)$ constant and minimize $\epsilon(N, p^*, h)$.
  - In fact: $R_{emp}(\alpha) = 0$ for separable data.
  - Control $\epsilon(N, p^*, h)$ by adapting the VC dimension (controlling the "capacity" of the classifier).

Topics of This Lecture

- Linear Support Vector Machines
  - Lagrangian (primal) formulation
  - Dual formulation
  - Discussion
- Linearly non-separable case
  - Soft-margin classification
  - Updated formulation
- Nonlinear Support Vector Machines
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- Applications

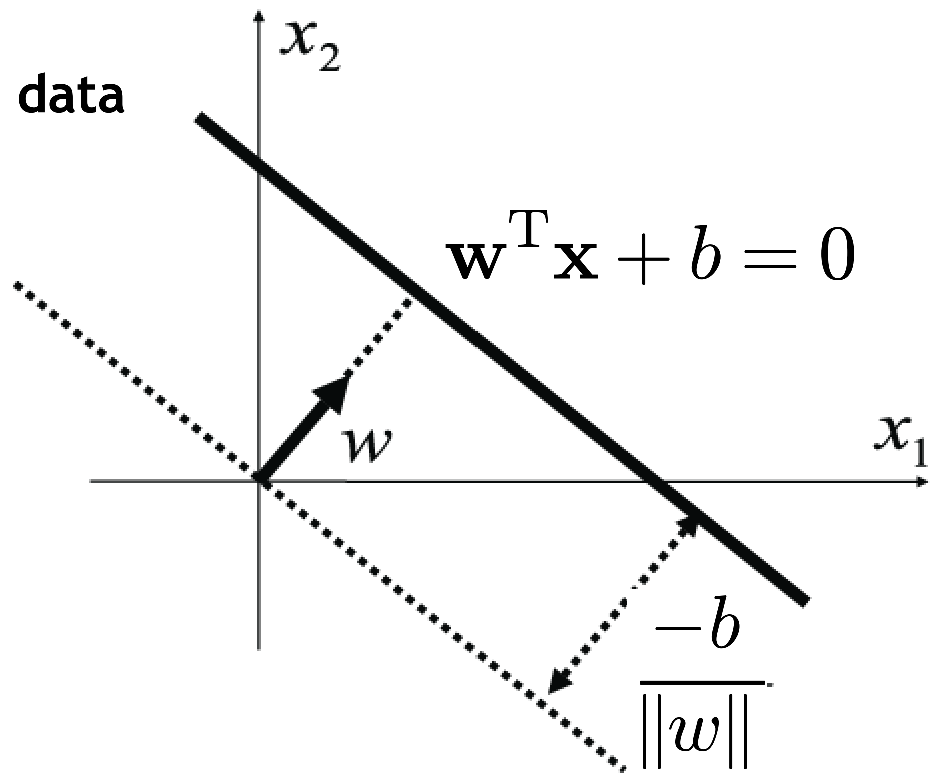
Revisiting Our Previous Example…



- How to select the classifier with the best generalization performance?
  - Intuitively, we would like to select the classifier which leaves maximal "safety room" for future data points.
  - This can be obtained by maximizing the margin between positive and negative data points.
  - It can be shown that the larger the margin, the lower the corresponding classifier's VC dimension.
- The SVM takes up this idea
  - It searches for the classifier with maximum margin.
  - Formulation as a convex optimization problem
    $\Rightarrow$ Possible to find the globally optimal solution!

Support Vector Machine (SVM)

- **Let's first consider linearly separable data**
  - N **training data points** $\{(\mathbf{x}_i, y_i)\}_{i=1}^N \qquad \mathbf{x}_i \in \mathbb{R}^d$
  - **Target values** $\qquad t_i \in \{-1, 1\}$
  - **Hyperplane separating the data**



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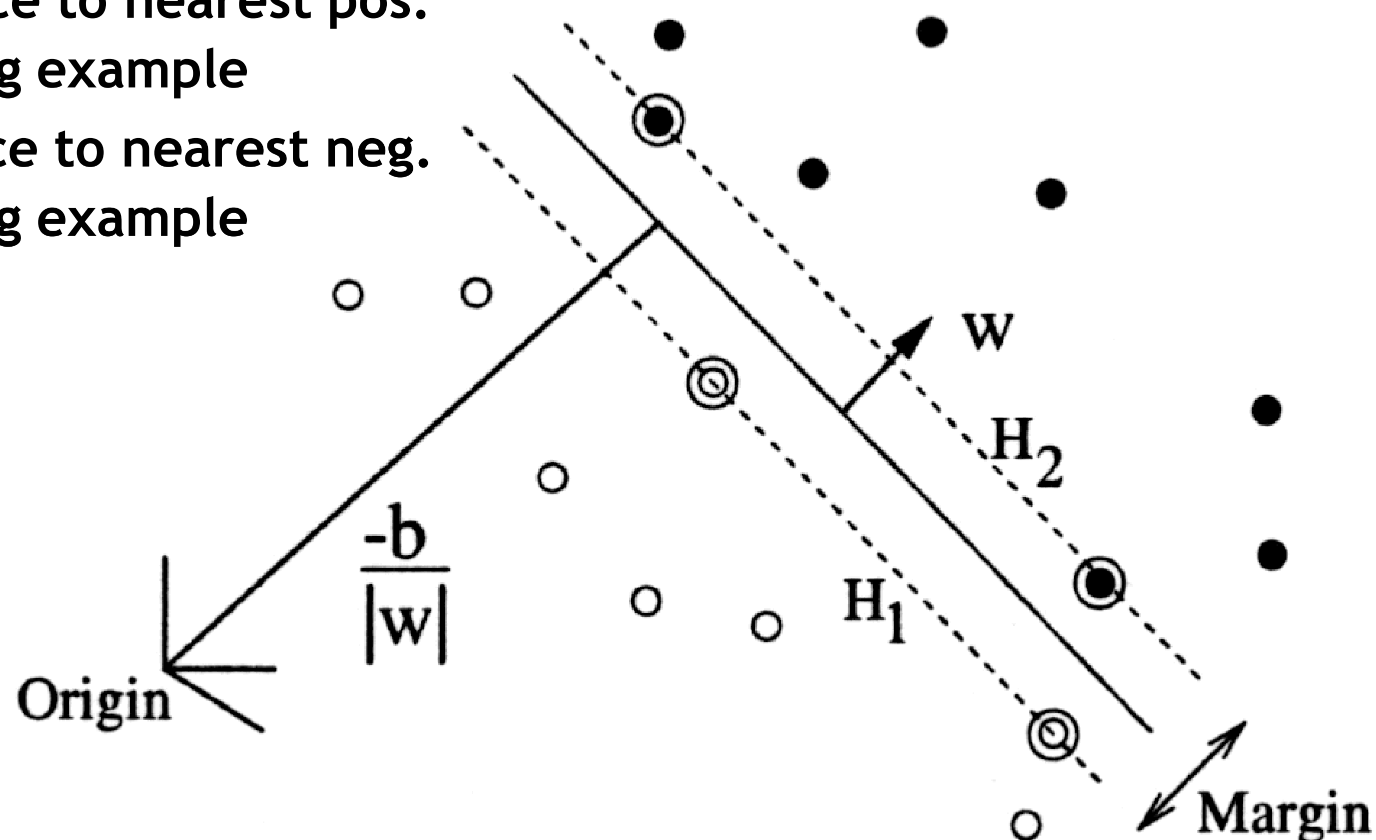
Support Vector Machine (SVM)

- **Margin of the hyperplane:** $d_- + d_+$
  - d_+: **distance to nearest pos. training example**
  - d_-: **distance to nearest neg. training example**



  - **We can always choose** $\mathbf{w}, b$ **such that** $d_- = d_+ = \frac{1}{\|\mathbf{w}\|}$.

Image source: C. Burges, 1998

Support Vector Machine (SVM)

- Since the data is linearly separable, there exists a hyperplane with

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

- Combined in one equation, this can be written as

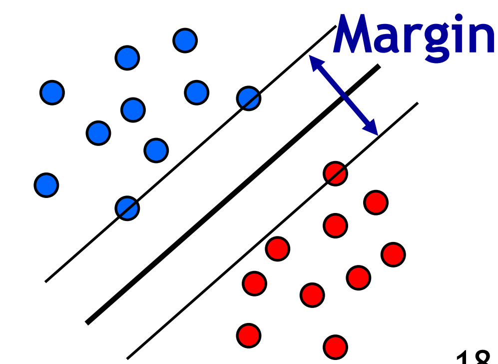
$$t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) \geq 1 \quad \forall n$$

$\Rightarrow$ Canonical representation of the decision hyperplane.

- The equation will hold exactly for the points on the margin

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

- By definition, there will always be at least one such point.



Support Vector Machine (SVM)

- We can choose w such that

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

- The distance between those two hyperplanes is then the margin

$$d_- = d_+ = \frac{1}{\|\mathbf{w}\|}$$
$$d_- + d_+ = \frac{2}{\|\mathbf{w}\|}$$

$\Rightarrow$ We can find the hyperplane with maximal margin by minimizing $\|\mathbf{w}\|^2$.

Support Vector Machine (SVM)

- Optimization problem
  - Find the hyperplane satisfying

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

under the constraints

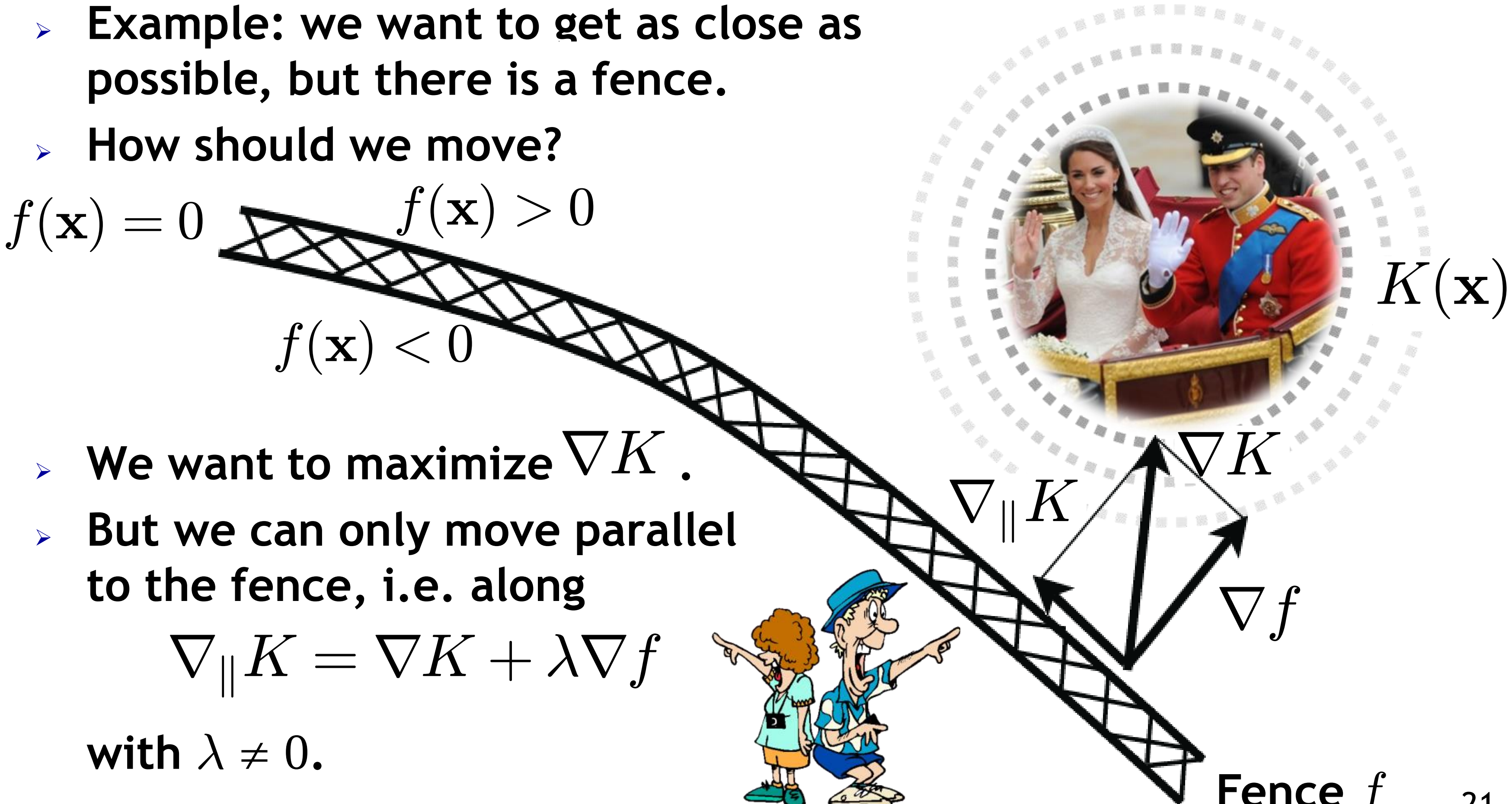
$$t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) \geq 1 \quad \forall n$$

  - 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 $\lambda \neq 0$.

Recap: Lagrange Multipliers

- **Problem**
  - We want to maximize $K(\mathbf{x})$ subject to constraints $f(\mathbf{x}) = 0$.
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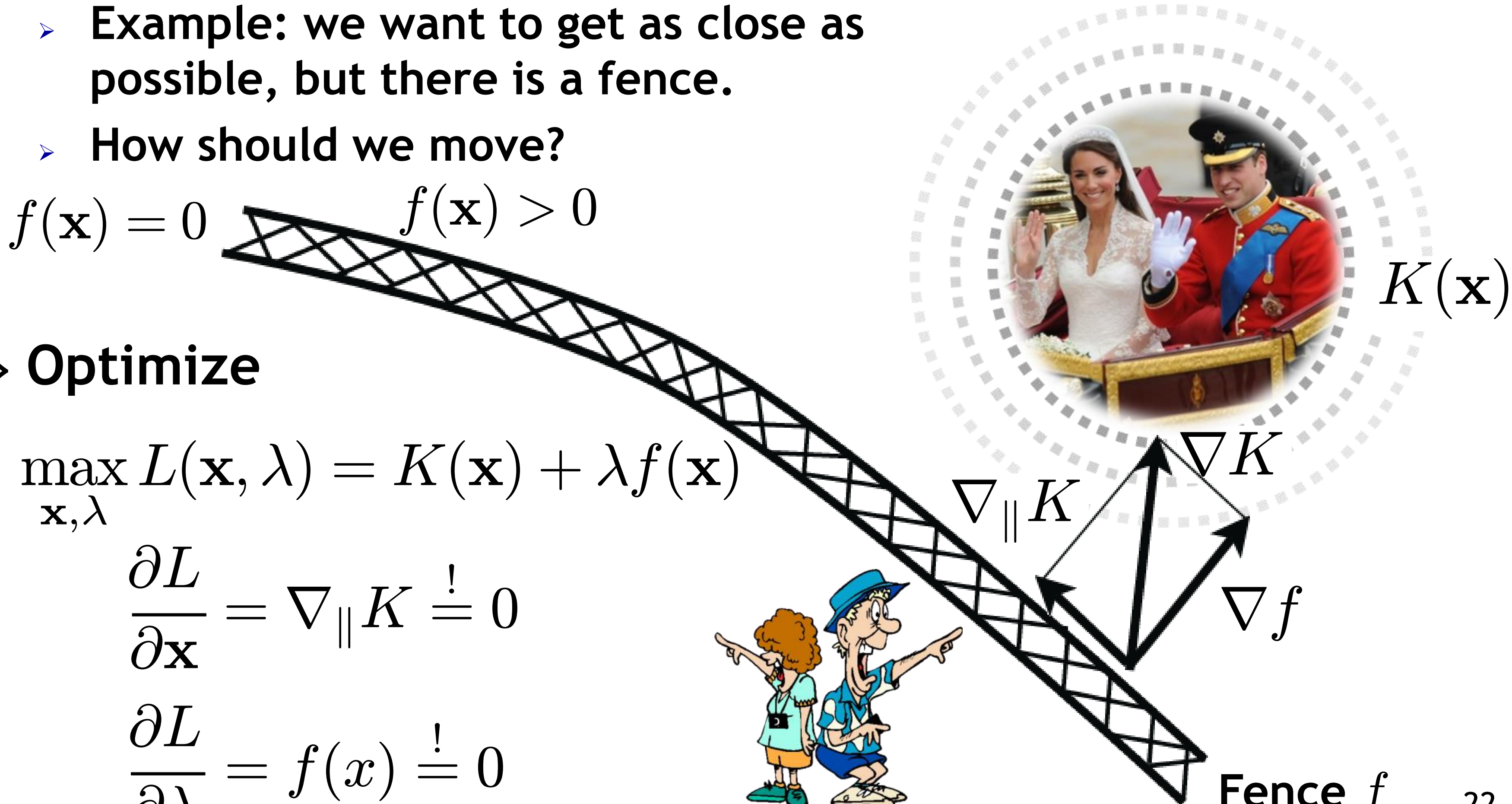


$\Rightarrow$ **Optimize**

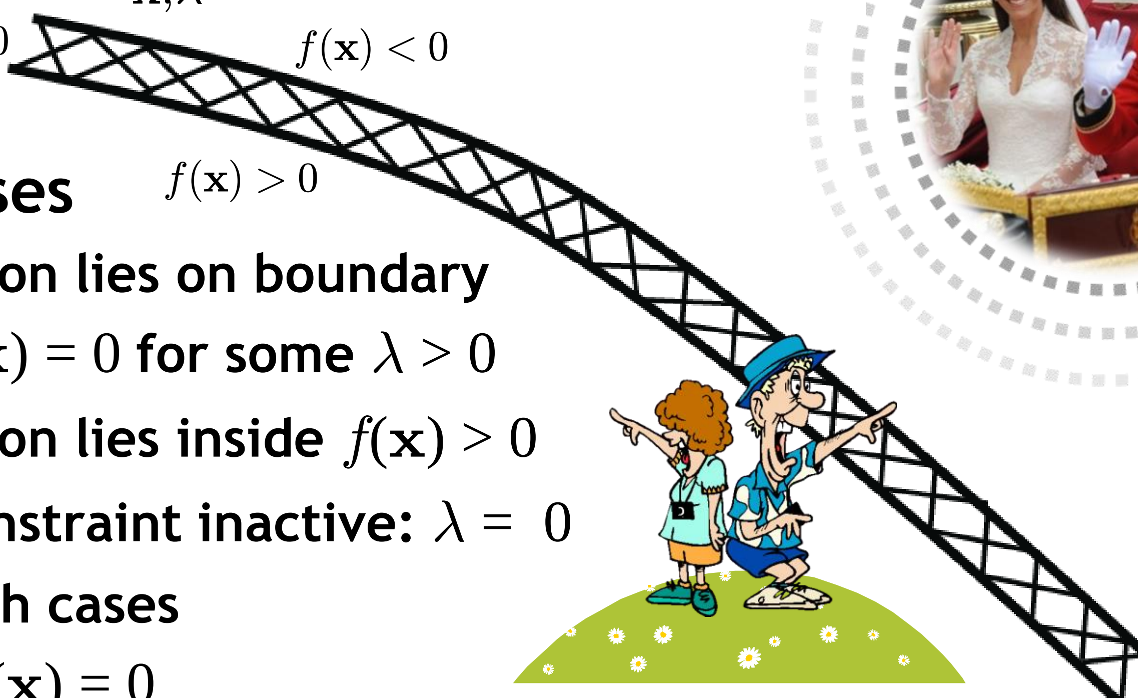
$$\max_{\mathbf{x},\lambda} L(\mathbf{x}, \lambda) = K(\mathbf{x}) + \lambda f(\mathbf{x})$$

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

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

Recap: Lagrange Multipliers

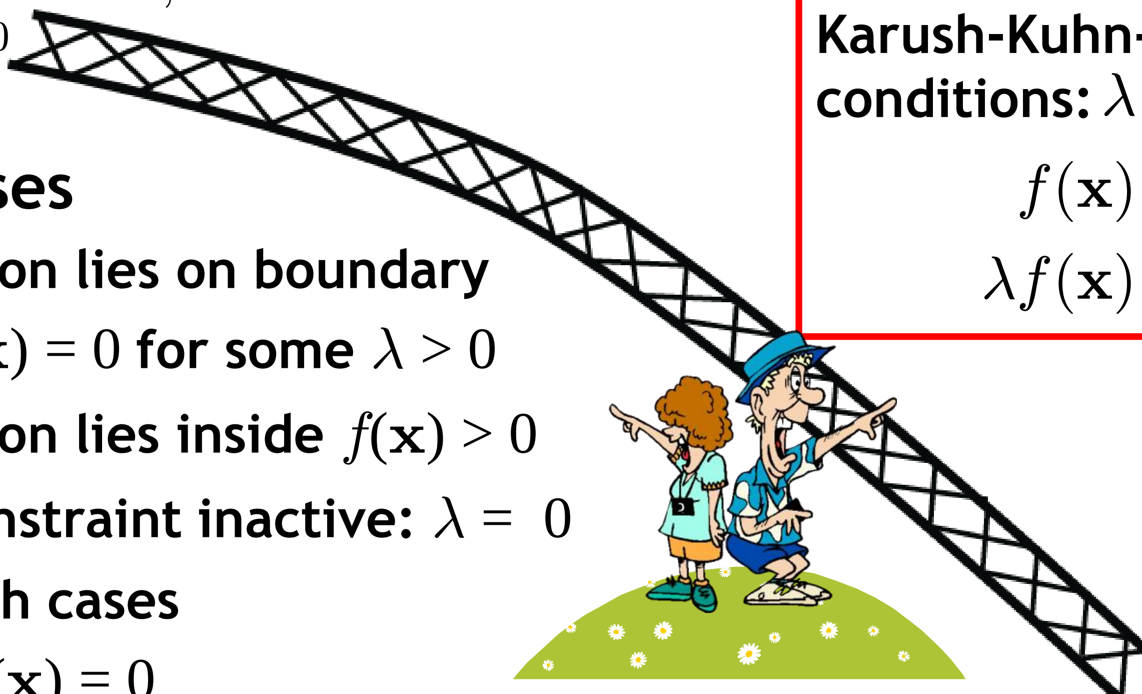
- **Problem**
  - Now let's look at constraints of the form $f(\mathbf{x}) \geq 0$.
  - Example: There might be a hill from which we can see better…
  - Optimize $\max\limits_{\mathbf{x},\lambda} L(\mathbf{x},\lambda) = K(\mathbf{x}) + \lambda f(\mathbf{x})$



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



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  - In both cases
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Karush-Kuhn-Tucker (KKT) conditions:

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

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

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

SVM – Lagrangian Formulation

- Lagrangian primal form

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

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

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

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

KKT:

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

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

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

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!***

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!

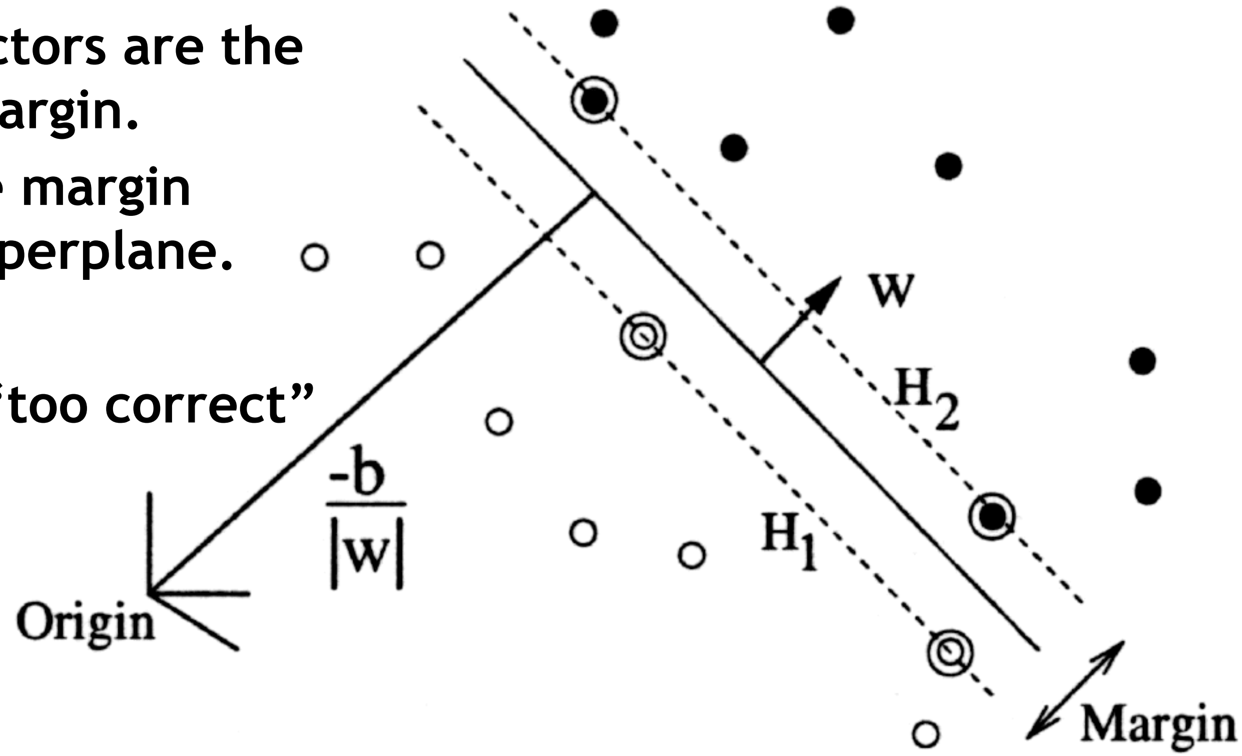


Image source: C. Burges, 1998

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

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

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:

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

SVM – Discussion (Part 1)

- **Linear SVM**
  - Linear classifier
  - Approximative implementation of the SRM principle.
  - In case of separable data, the SVM produces an empirical risk of zero with minimal value of the VC confidence (i.e. a classifier minimizing the upper bound on the actual risk).
  - SVMs thus 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")

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**

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

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

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

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

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

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

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

- **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 $\mathcal{O}(N^2)$.

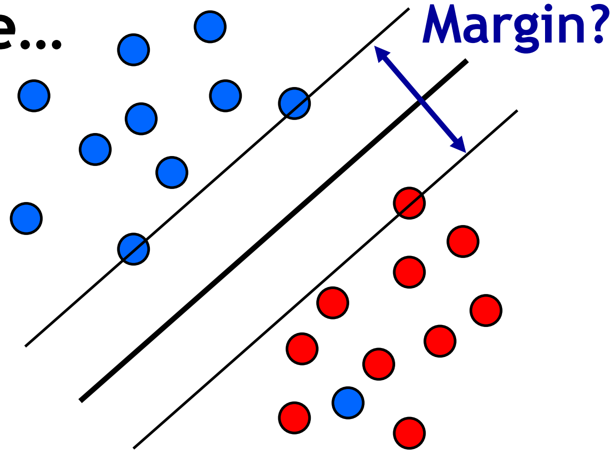
  2. We have avoided the dependency on the dimensionality.

  ⇒ This makes it possible to work with infinite-dimensional feature spaces by using suitable basis functions $\phi(\mathbf{x})$.

  ⇒ We'll see that in a few minutes…

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

$$\begin{aligned} \mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b &\geq +1 && \text{for} \quad t_n = +1 \\ \mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b &\cdot \;\; -1 && \text{for} \quad t_n = -1 \end{aligned}$$

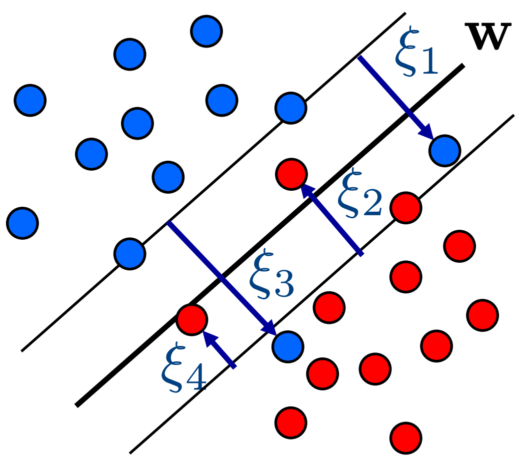
  - Instead use

$$\begin{aligned} \mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b &\geq +1 - \xi_n && \text{for} \quad t_n = +1 \\ \mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b &\cdot \;\; -1 + \xi_n && \text{for} \quad t_n = -1 \end{aligned}$$

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!

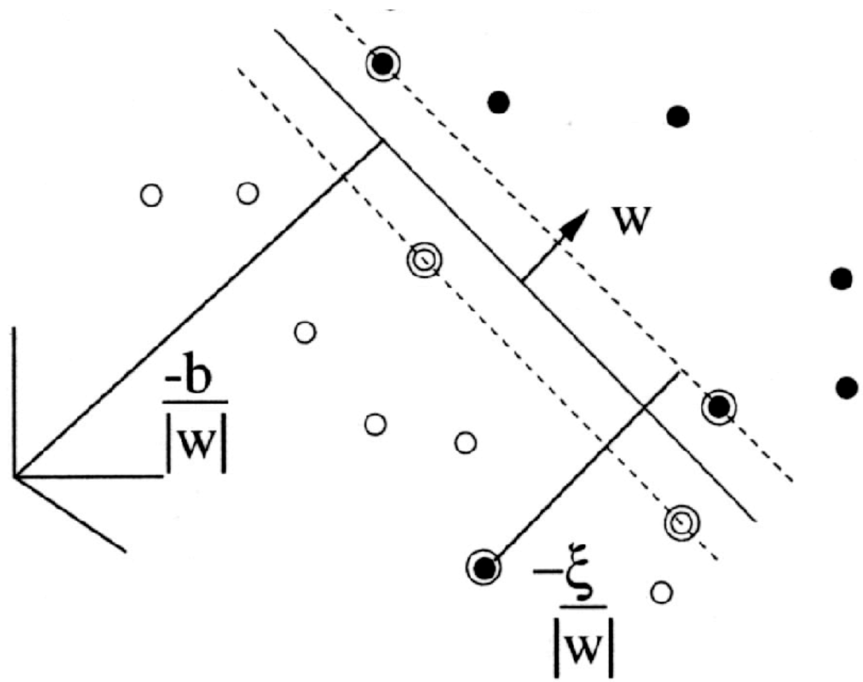
$\Rightarrow$ They are jointly optimized together with $\mathbf{w}$.

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**

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

- **KKT conditions**

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

KKT:

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

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)

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**

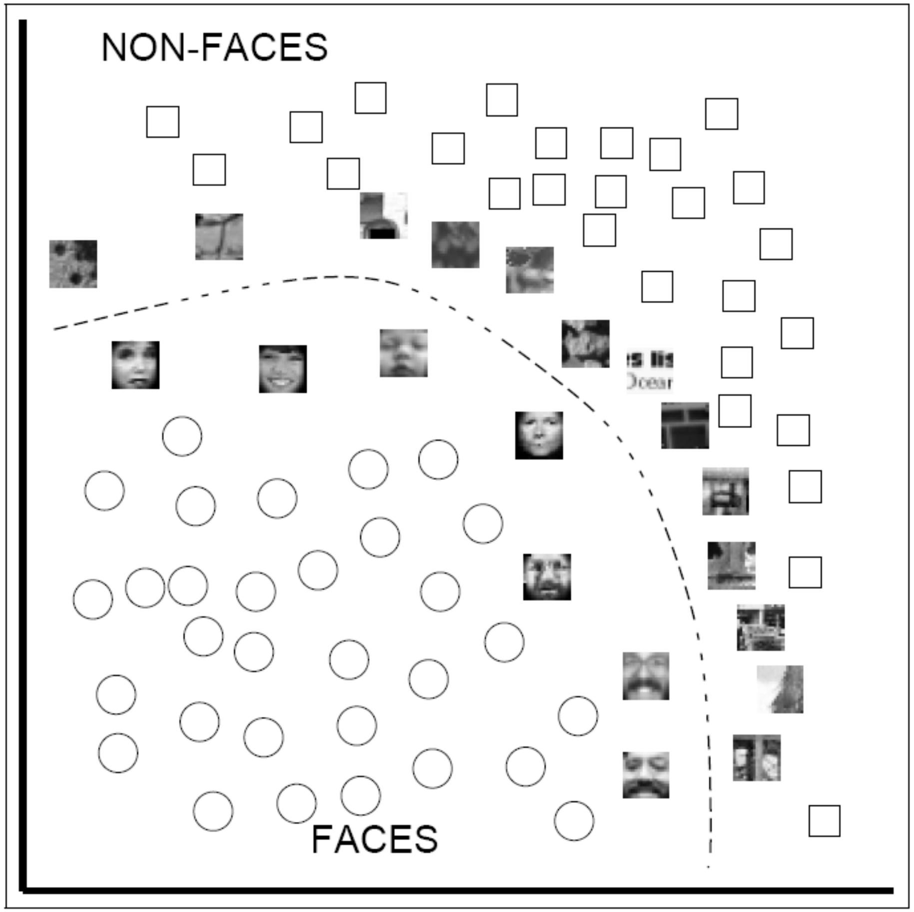
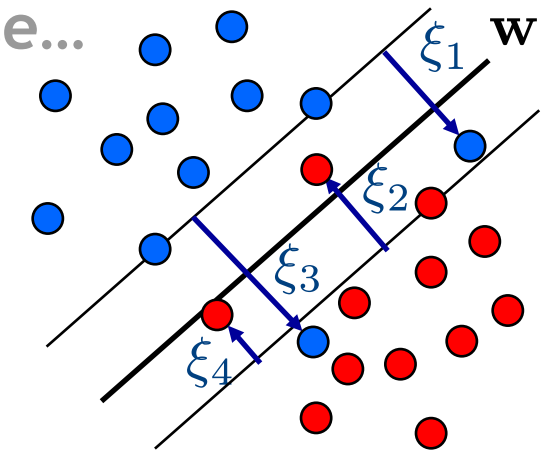


Image source: E. Osuna, F. Girosi, 1997

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.

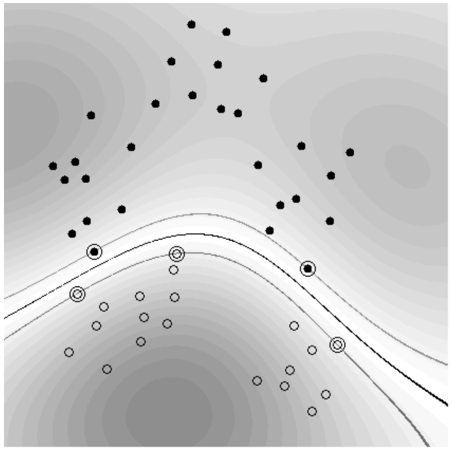
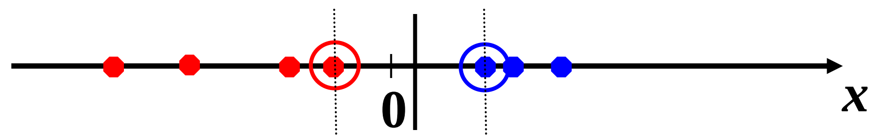


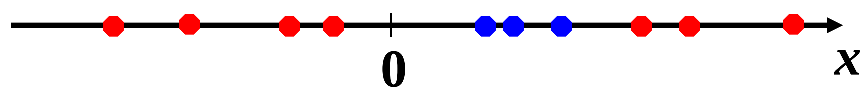
Image source: B. Schoelkopf, A. Smola, 2002

Nonlinear SVM

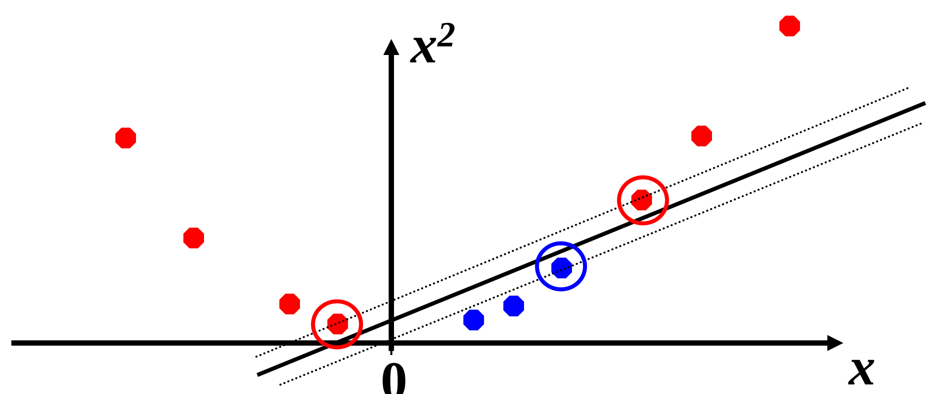
- Linear SVMs
  - Datasets that are linearly separable with some noise work well:



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

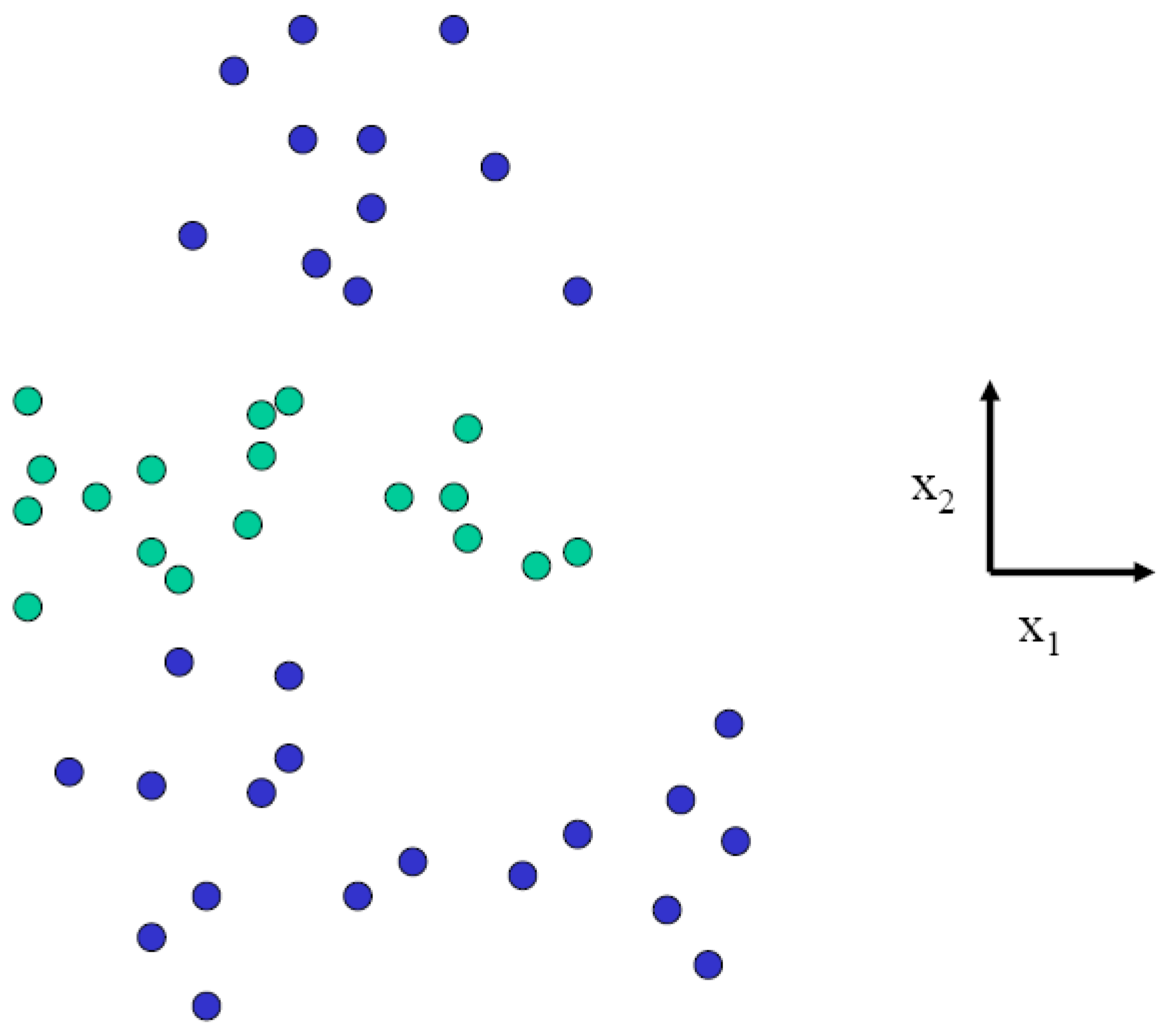


  - How about… mapping data to a higher-dimensional space:



Another Example

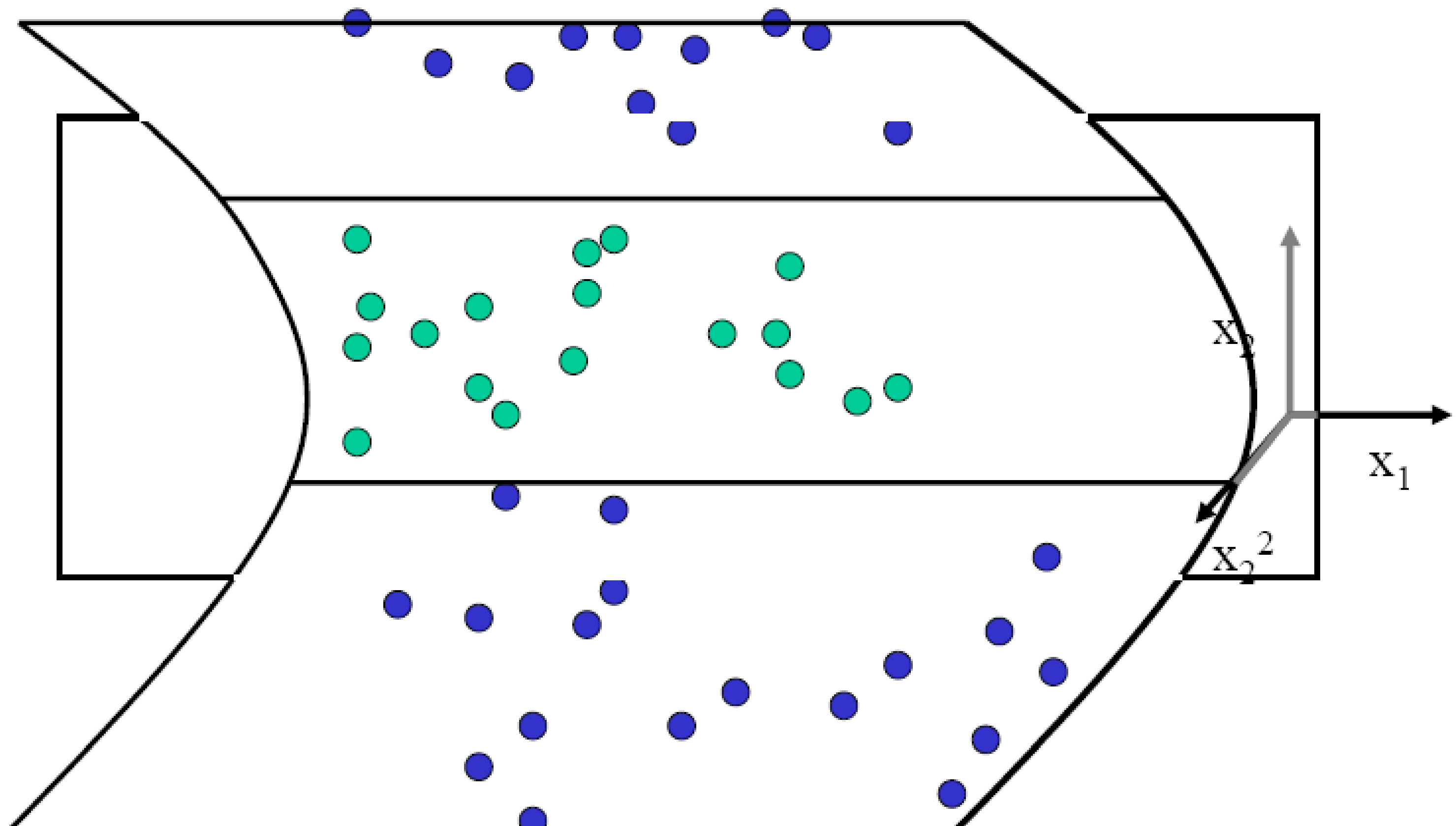
- Non-separable by a hyperplane in 2D



Slide credit: Bill Freeman

Another Example

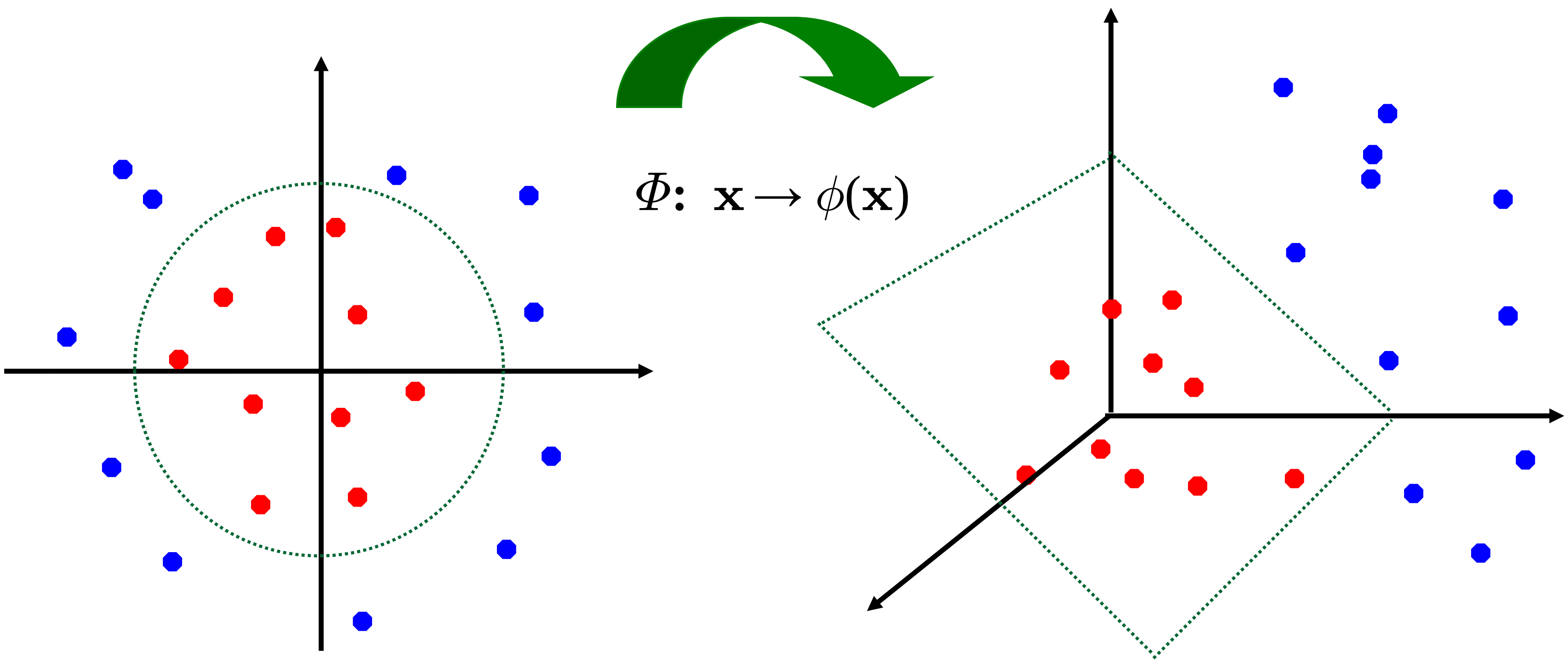
- **Separable by a surface in 3D**



Slide credit: Bill Freeman

Nonlinear SVM – Feature Spaces

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



Slide credit: Raymond Mooney

Nonlinear SVM

- **General idea**
  - Nonlinear transformation ϕ of the data points $\mathbf{x}_n$:

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

  - Hyperplane in higher-dim. space $\mathcal{H}$ (linear classifier in $\mathcal{H}$)

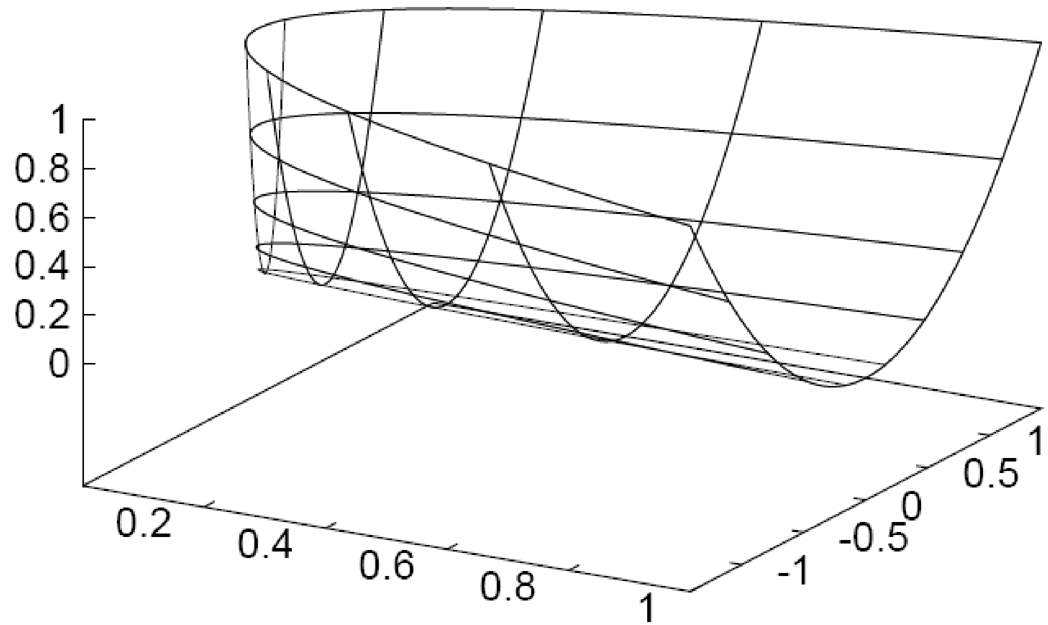
$$\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b = 0$$

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

What Could This Look Like?

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

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



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

Image source: C. Burges, 1998

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

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

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

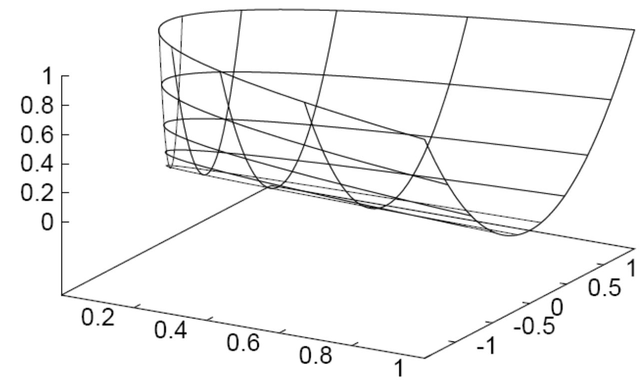
$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

  - 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:**

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



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

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

  - **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…

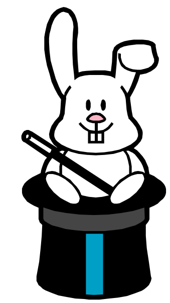
$$\mathbf{x}^{\mathrm{T}}\mathbf{y} \quad \rightarrow \quad k(\mathbf{x}, \mathbf{y})$$

  - …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:**

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

(positive definite = all eigenvalues are > 0)

Recap: 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...)

Example: Bag of Visual Words Representation

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

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

Nonlinear SVM – Dual Formulation

- **SVM Dual: Maximize**

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

under the conditions

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

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

- **Classify new data points using**

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

VC Dimension for Polynomial Kernel

- **Polynomial kernel of degree p:**

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

  - **Dimensionality of $\mathcal{H}$:** $\binom{D+p-1}{p}$

  - **Example:**

$$\begin{aligned} D &= 16 \times 16 = 256 \\ p &= 4 \\ \dim(\mathcal{H}) &= 183.181.376 \end{aligned}$$

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

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

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!**

$$\exp(\mathbf{x}) = 1 + \frac{\mathbf{x}}{1!} + \frac{\mathbf{x}^2}{2!} + \ldots + \frac{\mathbf{x}^n}{n!} + \ldots$$

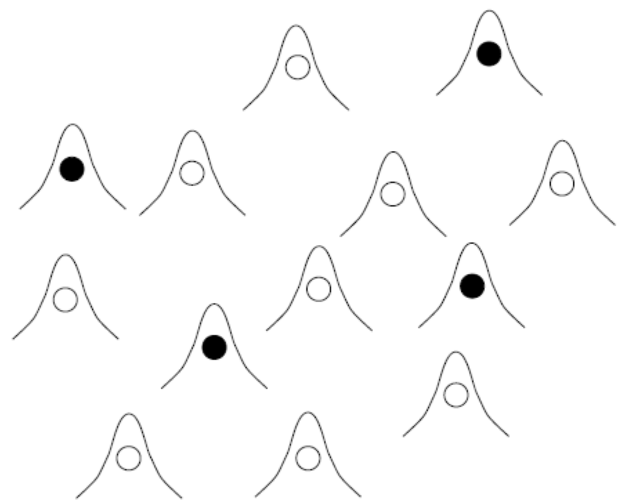
  - **Since only the kernel function is used by the SVM, this is no problem.**

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

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

VC Dimension for Gaussian RBF Kernel

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



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

Example: RBF Kernels

- Decision boundary on toy problem

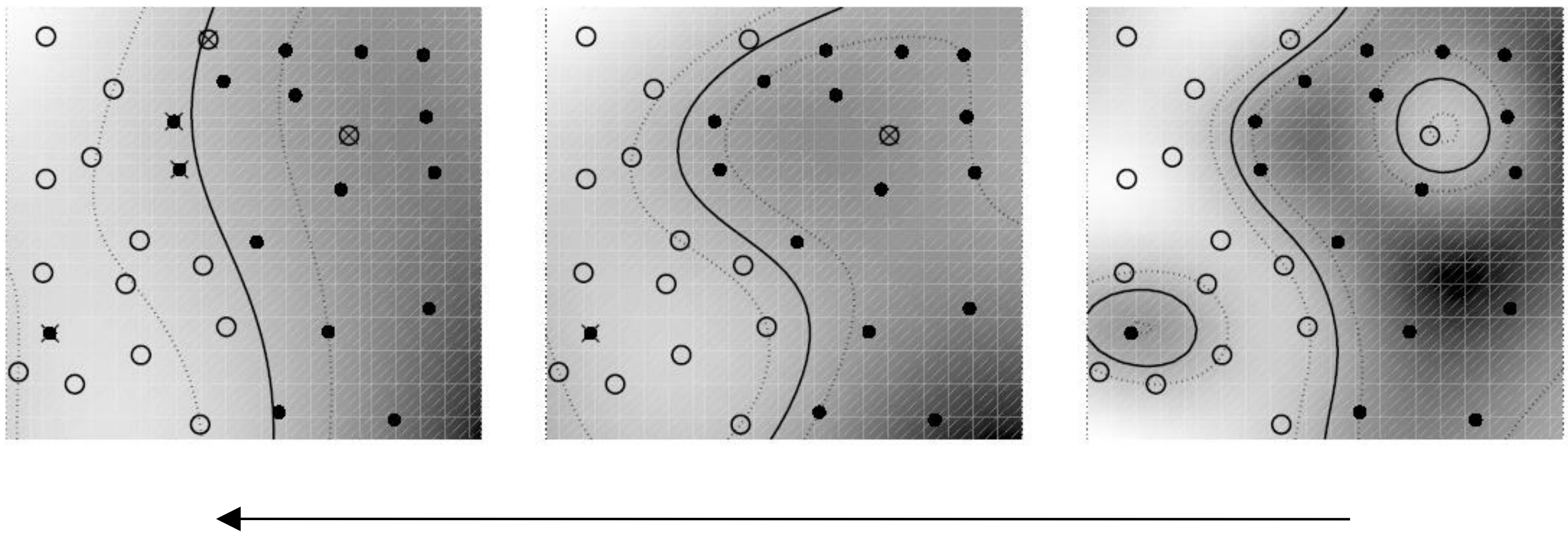


Image source: B. Schoelkopf, A. Smola, 2002

But… but… but…

- Don't we risk overfitting with those enormously high-dimensional feature spaces?
  - No matter what the basis functions are, there are really only up to N parameters: a_1, a_2,…, 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.

Theoretical Justification for Maximum Margins

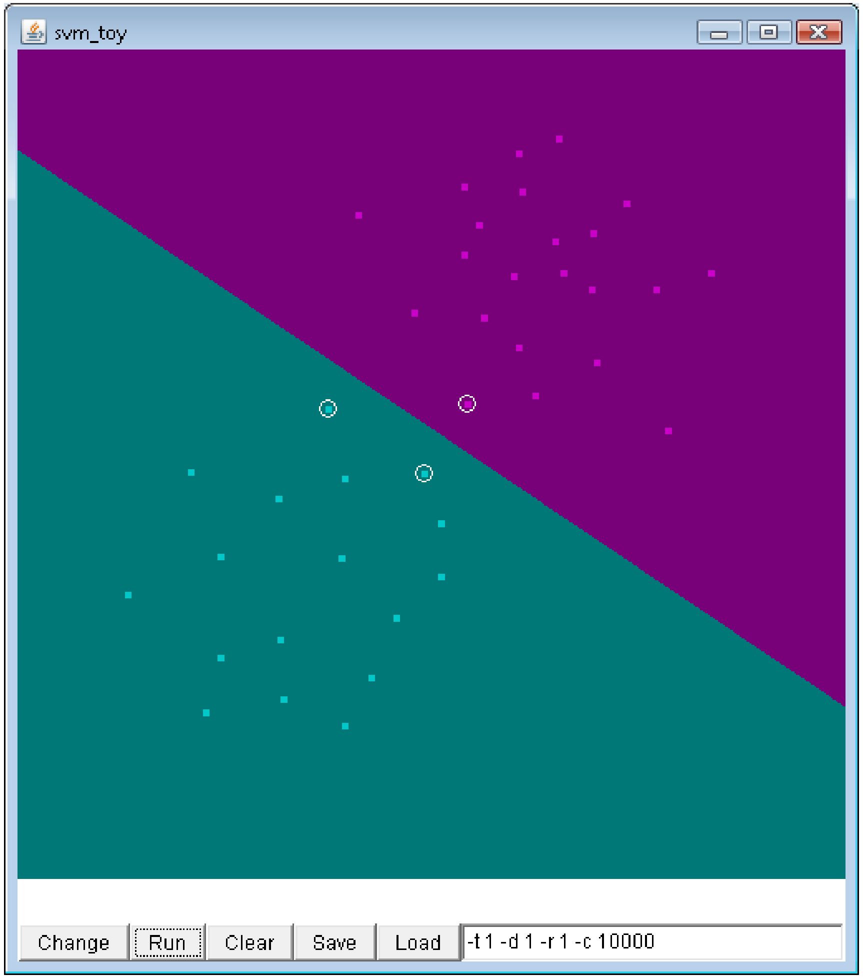
- Vapnik has proven the following:
  - *The class of optimal linear separators has VC dimension h bounded from above as*

$$h \leq \min\left\{\left\lceil \frac{D^2}{\rho^2} \right\rceil, m_0\right\} + 1$$

where ρ 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_0 we can minimize the VC dimension by maximizing the margin ρ.
- Thus, complexity of the classifier is kept small regardless of dimensionality.

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?
    - Still something of a black art...
  - 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.

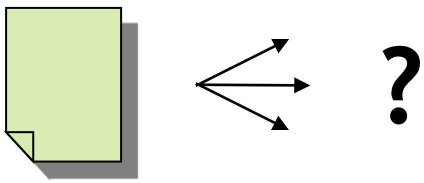
    $\Rightarrow$ There are techniques to reduce the effective SV set.
  - Training for very large datasets (millions of data points)
    - Stochastic gradient descent and other approximations can be used

Topics of This Lecture

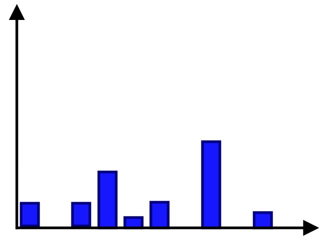
- Linear Support Vector Machines (Recap)
  - Lagrangian (primal) formulation
  - Dual formulation
  - Discussion
- Linearly non-separable case
  - Soft-margin classification
  - Updated formulation
- Nonlinear Support Vector Machines
  - Nonlinear basis functions
  - The Kernel trick
  - Mercer's condition
  - Popular kernels
- **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)

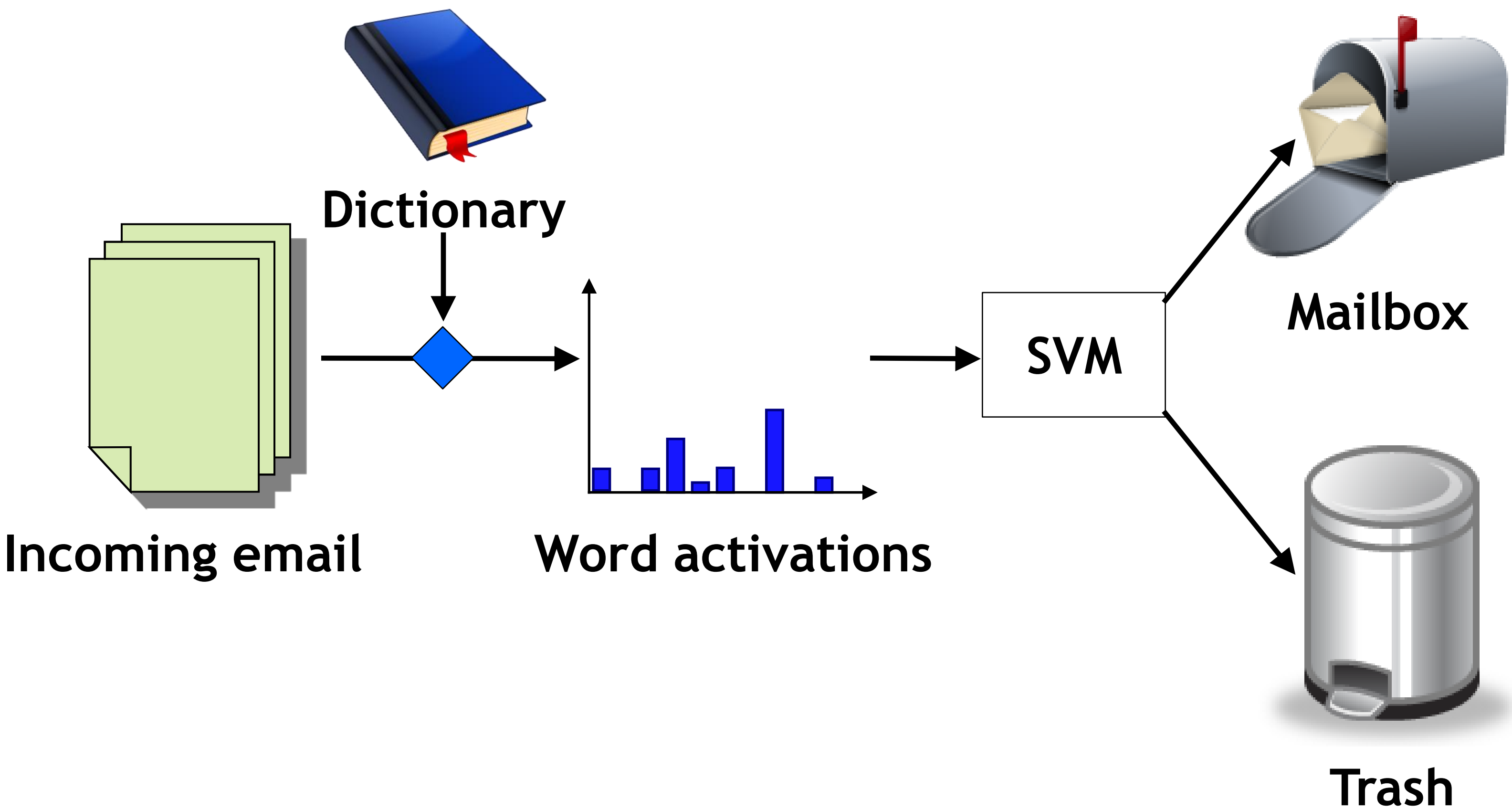
Example Application: Text Classification

- **Results:**

					SVM (poly) degree $d =$					SVM (rbf) width $\gamma =$			
	Bayes	Rocchio	C4.5	k-NN	1	2	3	4	5	0.6	0.8	1.0	1.2
earn	95.9	96.1	96.1	97.3	98.2	98.4	**98.5**	98.4	98.3	**98.5**	98.5	98.4	98.3
acq	91.5	92.1	85.3	92.0	92.6	94.6	**95.2**	95.2	95.3	95.0	95.3	95.3	**95.4**
money-fx	62.9	67.6	69.4	78.2	66.9	72.5	75.4	74.9	**76.2**	74.0	75.4	**76.3**	75.9
grain	72.5	79.5	89.1	82.2	91.3	93.1	**92.4**	91.3	89.9	**93.1**	91.9	91.9	90.6
crude	81.0	81.5	75.5	85.7	86.0	87.3	88.6	**88.9**	87.8	**88.9**	89.0	88.9	88.2
trade	50.0	77.4	59.2	77.4	69.2	75.5	76.6	77.3	**77.1**	76.9	78.0	**77.8**	76.8
interest	58.0	72.5	49.1	74.0	69.8	63.3	67.9	73.1	**76.2**	74.4	75.0	**76.2**	76.1
ship	78.7	83.1	80.9	79.2	82.0	85.4	86.0	**86.5**	86.0	**85.4**	86.5	87.6	87.1
wheat	60.6	79.4	85.5	76.6	83.1	84.5	85.2	**85.9**	83.8	**85.2**	85.9	85.9	85.9
corn	47.3	62.2	87.7	77.9	86.0	86.5	85.3	**85.7**	83.9	**85.1**	85.7	85.7	84.5
microavg.	**72.0**	**79.9**	**79.4**	**82.3**	84.2	85.1	85.9	86.2	85.9	86.4	86.5	86.3	86.2
					combined: **86.0**					combined: **86.4**			

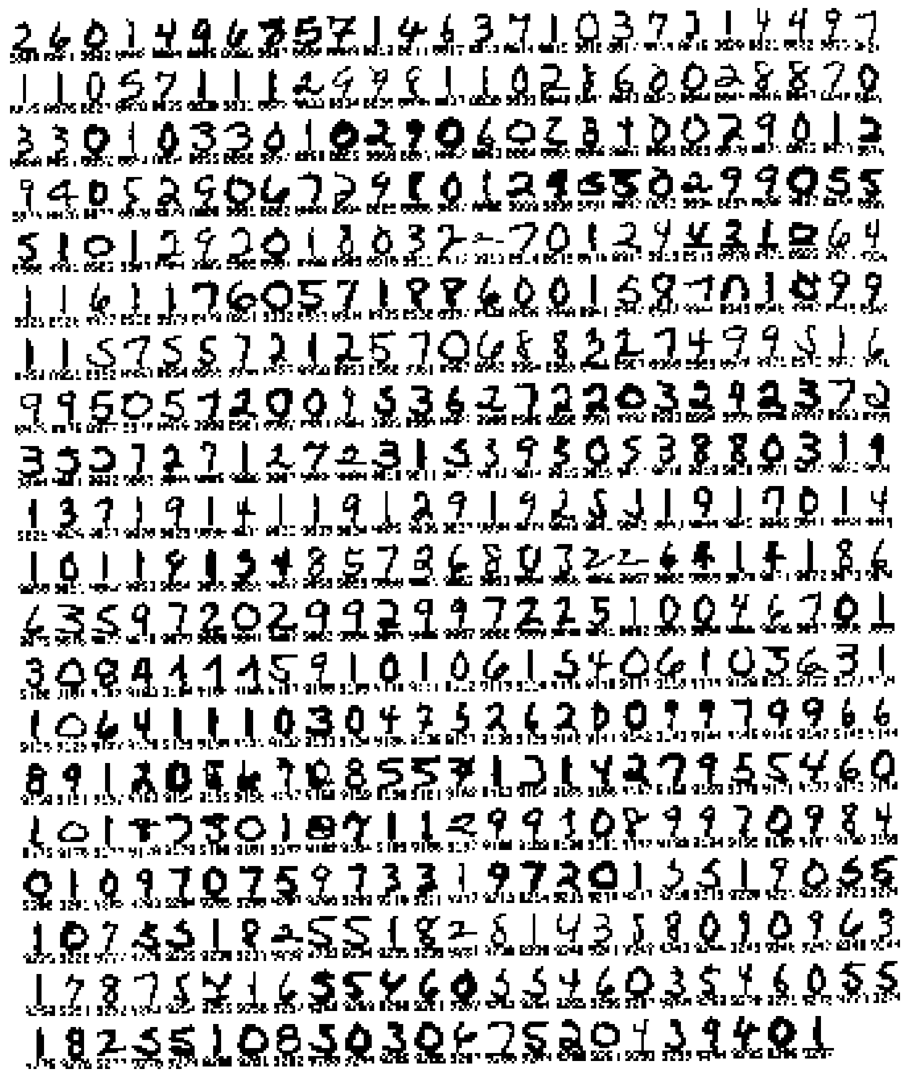
Example Application: Text Classification

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



Example Application: OCR

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



Historical Importance

- USPS benchmark
  - 2.5% error: human performance
- Different learning algorithms
  - 16.2% error: Decision tree (C4.5)
  - 5.9% error: (best) 2-layer Neural Network
  - 5.1% error: LeNet 1 - (massively hand-tuned) 5-layer network
- Different SVMs
  - 4.0% error: Polynomial kernel (p=3, 274 support vectors)
  - 4.1% error: Gaussian kernel (σ=0.3, 291 support vectors)

Example Application: OCR

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

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

Example Application: Object Detection

Real-time capable!

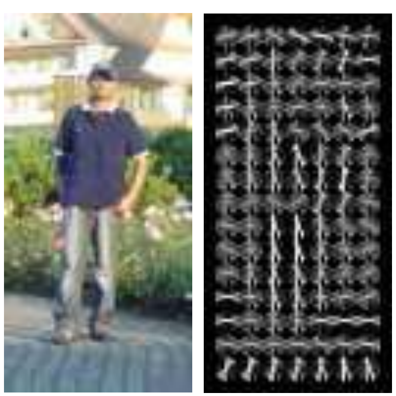
- Sliding-window approach

→

→

Obj./non-obj. Classifier

- 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)

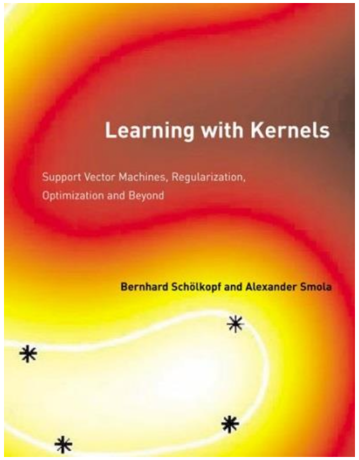
You Can Try It At Home…

- Lots of SVM software available, e.g.
  - svmlight (http://svmlight.joachims.org/)
    - Command-line based interface
    - Source code available (in C)
    - Interfaces to Python, MATLAB, Perl, Java, DLL,…
  - libsvm (http://www.csie.ntu.edu.tw/~cjlin/libsvm/)
    - Library for inclusion with own code
    - C++ and Java sources
    - Interfaces to Python, R, MATLAB, Perl, Ruby, Weka, C+ .NET,…
  - Both include fast training and evaluation algorithms, support for multi-class SVMs, automated training and cross-validation, …

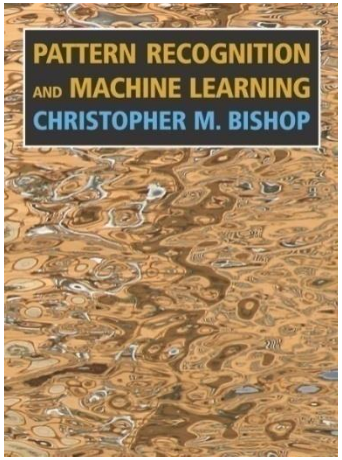
    $\Rightarrow$ Easy to apply to your own problems!

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.