

Machine Learning - Lecture 8

Linear Support Vector Machines

24.05.2016

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Course Outline

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



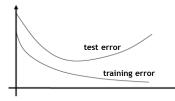


- Discriminative Approaches (5 weeks)
 - Linear Discriminant Functions
 - Statistical Learning Theory & SVMs
 - **Ensemble Methods & Boosting**
 - Randomized Trees, Forests & Ferns
- · Generative Models (4 weeks)
 - Bayesian Networks
 - Markov Random Fields





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!

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.
- ⇒ 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

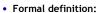
$$R(\alpha) \cdot R_{emp}(\alpha) + \epsilon(N, p^*, h)$$

- where
 - N: number of training examples
 - p^* : probability that the bound is correct
 - h: capacity of the learning machine ("VC-dimension")

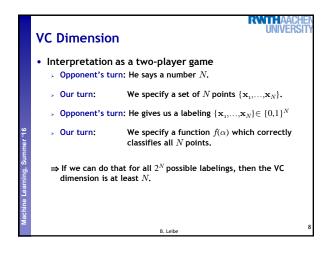
Recap: VC Dimension

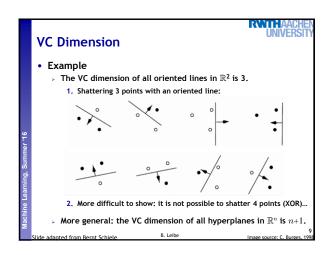


- Measure for the capacity of a learning machine.

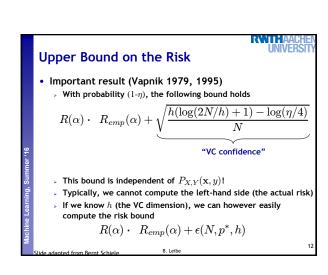


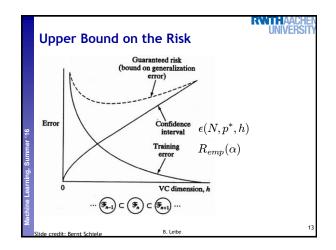
- If a given set of ℓ points can be labeled in all possible 2^{ℓ} ways, and for each labeling, a member of the set $\{f(\alpha)\}$ can be found which correctly assigns those labels, we say that the set of points is shattered by the set of functions.
- The VC dimension for the set of functions $\{f(\alpha)\}$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

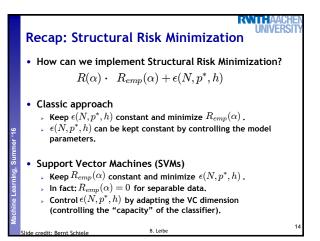




VC Dimension • Intuitive feeling (unfortunately wrong) • The VC dimension has a direct connection with the number of parameters. • Counterexample $f(x;\alpha) = g(\sin(\alpha x))$ $g(x) = \begin{cases} 1, & x > 0 \\ -1, & x \cdot 0 \end{cases}$ • Just a single parameter α . • Infinite VC dimension • Proof: Choose $x_i = 10^{-i}, i = 1, \dots, \ell$







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

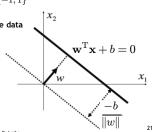
Revisiting Our Previous Example...

- 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 ⇒ Possible to find the globally optimal solution!

Support Vector Machine (SVM)

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

> Hyperplane separating the data



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 ${f w},\,b$ such that $\,d_-=d_+=$

Support Vector Machine (SVM)

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

$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \ge +1$$
 for $t_n = +1$
 $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \cdot -1$ for $t_n = -1$

· Combined in one equation, this can be written as

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

- ⇒ 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)

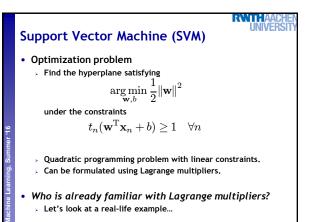
ullet We can choose w such that

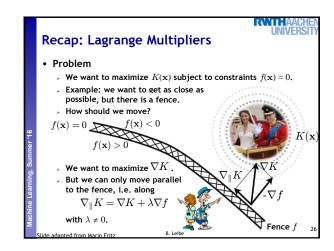
$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b = +1$$
 for one $t_n = +1$
 $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b = -1$ for one $t_n = -1$

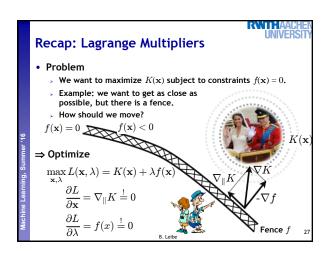
• The distance between those two hyperplanes is then the margin

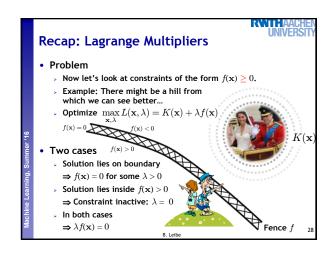
 $d_- = d_+ = \frac{1}{\|\mathbf{w}\|}$ $d_- + d_+ = \frac{2}{\|\mathbf{w}\|}$

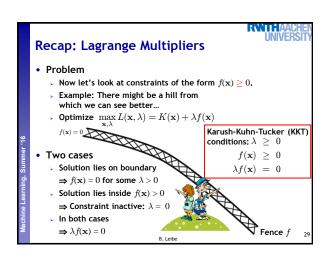
⇒ We can find the hyperplane with maximal margin by minimizing $\|\mathbf{w}\|^2$

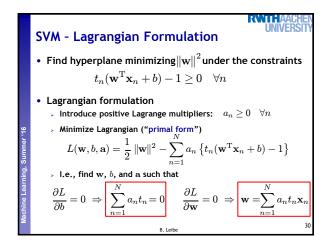












SVM - Lagrangian Formulation

· 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 \mathcal{L}_{p} needs to fulfill the KKT conditions

> Necessary and sufficient conditions

$$a_n \ge 0$$

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

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

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

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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

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

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

adapted from Bornt 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. ⇒ Robustness to "too correct" points!

SVM - Solution (Part 2)

• Solution for the hyperplane

ightarrow To define the decision boundary, we still need to know b.

> Observation: any support vector \mathbf{x}_n satisfies

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

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

> 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
- > 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.
- ⇒ Globally optimal solution!

Primal form formulation

- ightharpoonup 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 $L_{\scriptscriptstyle p}$ in a dual form

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

. Using the constraint $\displaystyle \sum_{n=1}^N a_n t_n = 0$, we obtain

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

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

Slide adapted from Bernt Schiele

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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 $\,\,{\bf w}=\!\!\sum^{N}a_{n}t_{n}{\bf x}_{n}\,$, we obtain

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

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

SVM - Dual Formulation

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

 $\,\,$ Applying $\frac{1}{2} \, \|\mathbf{w}\|^2 = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$ and again using $\, \mathbf{w} = \! \sum^{N} a_n t_n \mathbf{x}_n$

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

> Inserting this, we get the Wolfe dual

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

SVM - Dual Formulation

Maximize

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

under the conditions

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

 $\,\,$ The hyperplane is given by the N_S support vectors:

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

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 O(N) and $O(N^2)$.
 - 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 $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \geq +1$ for $t_n = +1$ $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \cdot -1$ for $t_n = -1$

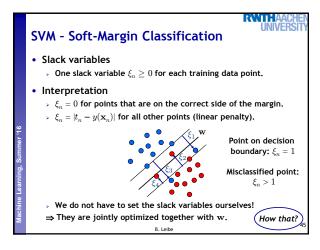
$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \ge +1$$

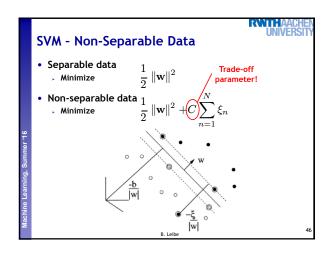
for
$$t_n = +1$$

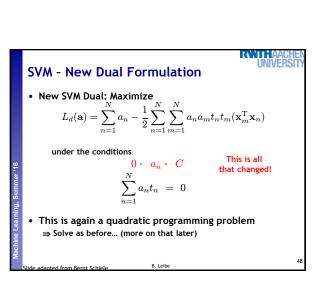
for
$$t_n = -1$$

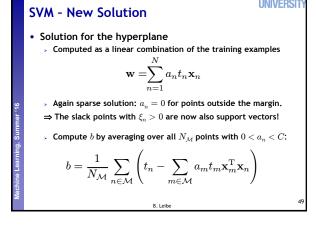
$$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \ge +1 - \xi_n$$
 for $t_n = +1$
 $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b \cdot -1 + \xi_n$ for $t_n = -1$

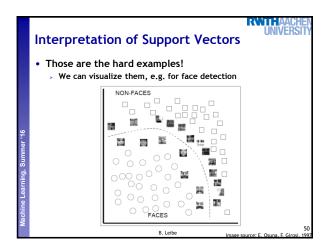
with "slack variables" $\xi_n \geq 0 \quad \forall n$











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

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