T7 - SVM and Perceptrons

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Based on slides by P. Orbanz & J. Keuchel

Overview

- Supervised/Unsupervised Learning
- Perceptrons
- Support Vector Machines
- Kernels

Supervised vs. Unsupervised Learning

- Task: Apply some machine learning method to data from a given source
- The source has a characteristic distribution, but we don't know what it is.

Supervised vs. Unsupervised Learning

- Def.: Training data
  In a classification/regression problem, a sample from the data source with the correct classification/ regression results already assigned is called ***training data***.
- Example: Training data for a classification problem is a data sample **plus correct class labels**.
- Training data is the knowledge about the data source which we use to construct the classifier/regressor.

Supervised vs. Unsupervised Learning

- Supervised Learning:
  - Use training data to infer model
  - apply model to test data
  - e.g. Maximum likelihood, Perceptron, SVM

we can test our model

- Unsupervised Learning:
  - No training data
  - Model inference and application **both rely on test data exclusively**
  - e.g. k-means

We can **not** test our our model

Supervised vs. Unsupervised Learning

- Fish-example from lecture
- Supervised Learning:
  - One bag with salmons
  - One bag with sea bass
    => build model
  - One mixed bag
    => please classify
- Unsupervised Learning:
  - One mixed bag
    => build model
  - Another mixed bag
    => please classify

Supervised Example: classification

1. Choose a classifier model (e. g. family of functions)
2. Use *training data* (pre-classified reference data) to choose a specific classifier (e. g. compute parameter)
3. Using the classifier on new data (*test data*): Apply classifier function to data value -> Result: Class label

Perceptron

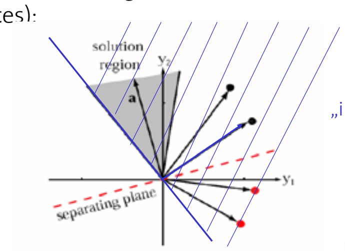
- **Idea:** Separate data points from two classes C_1, C_2 by a **linear** function (hyperplane)
- Identify hyperplane by normal vector a (in generalized coordinates):

$$a^T y_i > 0 \quad \text{for} \quad i \in C_1$$
$$a^T y_i < 0 \quad \text{for} \quad i \in C_2$$

CG: homogeneous coordinates

Perceptron

- Solution is not unique: possible normal vectors define a conic region (= intersection of n half spaces):



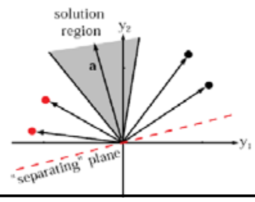
„in" halfspace

Perceptron

- For training: "normalization" of data points by mirroring points from C_2 at the origin:

$$y_i \leftarrow -y_i \quad \text{for} \quad i \in C_2$$

- Linear separation remains!
- New requirement:



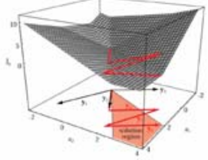
$$a^T y_i > 0 \quad \forall \quad i$$

angle between a and y_i < 90°

Perceptron Algorithm

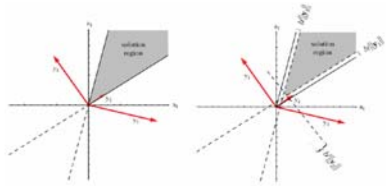
- Sequentially add "normalized" misclassified data points y_i to a
- Moves a in the direction of the wider opening of the solution cone
- Terminates if a lies in the solution cone

→ Aufgabe 3



Perceptron to SVM

- Introduce a margin $a^T y_i >= b$ to reduce the cone of possible solutions (and move the separating hyperplane more to the middle):



SVM

- By definition, SVM is the maximum margin classifier defined in terms of the support vector approach.
- Real-world SVM implementations usually combine three techniques:
  1. Maximum margin classifier (this is where convex optimization comes in).
  2. Soft margin technique (slack variables).
  3. Kernel trick.

Maximum Margin Classifiers

- Background on maximum margin classifiers: Generalization error.
- V. Vapnik: Theory of "Structural risk minimization"
- Approach: Classification error consists of two parts.

classification error = training error + generalization error

Flexible classifiers: small training error, but possibly large generalization error (overfitting).

badly trained does not generalize well

Maximum Margin Classifiers

To keep the generalization error low (prevent from overfitting):

1. Use linear classifier. More complex/flexible classifiers (curved surfaces etc) are more likely to overfit.
2. When placing the hyperplane, choose the position which maximizes the margin.

Note: The only conceptual difference between the basic SVM and the perceptron is the rule for positioning the hyperplane.

Support Vectors

- Support vector idea: The classifier hyperplane is determined only by the points which are closest to it (the *suppport vectors*).
- Background: Region around class boundary is critical for classification. What happens "in the back" of the classes does not matter (classification ≠ density estimation).
- In theory, you may have millions of data points, but only three support vectors.

→ Aufgabe 2

Aufgabe 2

- personal opinion:
  - very nice task
  - good for low level understanding
- a): simply draw a picture
- b) – d): this is not SVM, but LSQ
  - used to illustrate the difference to SVM
- e) + f): SVM

Soft Margin

„maximum margin classifier"

- First problem of the SVM classifier: It requires data to be linearly separable.
- Solution: *Soft margin approach.*
  - We allow training points on the wrong side of the classifier, but such points produce extra costs.
- The margin maximization is rewritten as a minimization problem.
- The two problems are combined.

Soft Margin

$$
\begin{aligned}
\text{minimize} \quad & T(\mathbf{w},\boldsymbol{\xi}) = \tfrac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{n}\xi_i \\
\text{subject to} \quad & z_i(\mathbf{w}^T\mathbf{y}_i + w_0) \geq 1 - \xi_i \\
& \xi_i \geq 0
\end{aligned}
$$

slack vars: the more the **original** constraint is violated, the larger they get

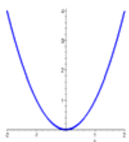
- There are many ways to combine two cost terms into a cost function: Every expression that becomes larger as either of the two terms increases is valid.
- Note: Slack variables apply only to training data. Classification of test points depends only on which side of the hyperplane they are on.

Optimization Theory

- The theory about convex optimization (KKT conditions etc) only comes in because the maximum margin problem (with and without slack variables) can be cast in terms of a quadratic optimization problem.
- In machine learning, the convex optimization part is usually used as a black box. To program SVMs, we use libraries or matlab functions.

Optimization Theory

- Why formulation as a convex optimization problem is so appealing:
  - Convex problems have the best possible optimization properties (clearly defined optimum, no catches to confuse computer algorithms).
  - Convex structure allows to tie in constraints in a very neat fashion.
- The meaning of „can be formulated as convex optimization problem" is roughly equivalent to „the optimization involved will not give us any trouble".



Kernel trick: Motivation

- Problem with **linear** classifiers: Not very flexible.
- Two types of errors:
  1. Classes overlap.
  2. Boundary between classes is obviously non-linear.

  The use of slack variables should be reserved for case (1).
- Consequence: We would like to be able to use "curved" classifiers.
- Curved classifiers: Nonlinear objects ! much more difficult mathematics.

„classifier still linear, but space transformed"

Kernel Trick

Observation: Imagine some high-dimensional vector space

- Projection of a linear object (say, a hyperplane) onto a linear subspace is again linear.
- Projection of the same object onto a non-linear subset (e. g. a curved surface) is non-linear.
- If we regard our data space as a non-linear subset of some high-dimensional space, we can "simulate" non-linear operations in data space by doing linear operations in the highdimensional space.

Kernel Trick

High-dimensional computations the hard way:

- Define transformation into high-dim. space $\mathbb{R}^H$.
- Parameterize data space $\mathbb{R}^L$ (e. g. as parametric differentiable manifold).
- Perform linear classifier training in high-dim space $\mathbb{R}^H$.
- Project the classifier back onto $\mathbb{R}^L$.

$$\mathbb{R}^L \xrightarrow{T} \mathbb{R}^H \xrightarrow{C} \mathbb{R}^H \xrightarrow{T^{-1}(C)} \mathbb{R}^L$$

Nobody would think about this, if it was the only way and would not lead to...

Kernel Trick

- The key operation of our linear methods is the scalar product:
  - Computes projections (needed for classification). $a^T y_i > 0 \;\; \forall \;\; i$
  - Computes orientations (determines orthogonality/direction of hyperplanes). $a || n$
- Check the slides on optimization for SVMs: The only vector operation that appears is the scalar product.
- So: If we can represent the scalar product in $\mathbb{R}^H$ as a function in $\mathbb{R}^L$, we can simulate linear classification in $\mathbb{R}^H$ without actually leaving $\mathbb{R}^L$.

=> we compute the scalar product of $\mathbb{R}^L$ vectors in $\mathbb{R}^H$

Kernel Trick

Recall linear algebra:

- A matrix A defines a scalar product if it is symmetric positive definite:

brackets: scalar prod.

$$a(x, y) := \langle x, Ay \rangle$$

has all the properties of a scalar product.

- For a function $k(x, y)$, what do we have to require such that there is *some* space $\mathbb{R}^H$ in which k is a scalar product?

  Meaning: When do we have

$$k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathbb{R}^H}$$
$$\phi : \mathbb{R}^L \rightarrow \mathbb{R}^H$$

Kernel Trick

- Answer: Mercer's theorem.
  If K: $G \subset \mathbb{R}^L \times \mathbb{R}^L \rightarrow \mathbb{R}$ continuous and symmetric for which

$$\forall f \in L_2(G): \qquad \int_G K(x, y) f(x) f(y) \, dx \geq 0$$

  then K represents a scalar product in some high-dimensional space.
- The Mercer condition is the functional analogy of positive definiteness for matrices (prev. slide)

$\longrightarrow$ We can use all these functions **instead** of the scalar product

Kernel Trick

Using the kernel trick:

- Start with some function K.
- Check whether it fulfills Mercer's condition.
- Replace all scalar products in algorithm by K.
- The important part: See whether it works.
  Most of the time (i. e. for most kernels), it will not ☺

Why do SVM work so well?

- First of all: It's an unsolved research problem.
- Some claims: Because of…
  1. the maximum margin classifier.
  2. the compression property (solution represented by small subset of points, the support vectors).
  3. certain (still largely unproved) convergence properties of the kernel operator eigenvalues.

Why do SVM work so well?

- Three very simple reason why SVMs are so popular:
  1. Of proven merit.
  2. Lots of experience, literature etc exists.
  3. Several easy-to-use, freely accessible, well-tested implementations are available (libsvm, svmlite etc.)