Ludwig-Maximilians-Universitaet Muenchen

19.06.2020

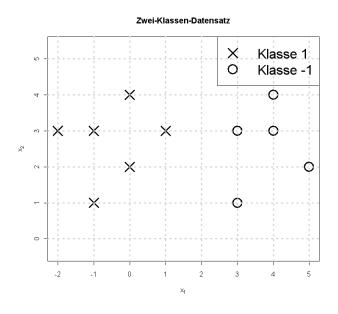
Institute for Informatics

Prof. Dr. Volker Tresp Rajat Koner Andreas Lohrer Sebastian Schmoll

Machine Learning Summer 2021 Exercise Sheet 9

Exercise 9-1 Optimal Separating Hyperplane 1

Consider the following dataset consisting of points $\binom{x_1}{x_2}$ in \mathbb{R}^2 . Using a hyperplane, points marked by \times are to be mapped onto ≥ 1 , points marked by \bigcirc are to be mapped onto ≤ -1 .



- (a) Find the support vectors.
- (b) Determine the equation of one separating hyperplane $h = \mathbf{x}^T \mathbf{w}$, optimize it and draw it within the figure.
- (c) Compute the margin \mathcal{C} .

Exercise 9-2 Optimal Separating Hyperplane 2

Determine the optimal separating hyperplane of the following dataset, partitioned into two classes A and B:

$$A = \left\{ p_1 = \begin{pmatrix} 2 \\ 4 \end{pmatrix}, \ p_2 = \begin{pmatrix} 3 \\ -1 \end{pmatrix}, \ p_3 = \begin{pmatrix} 1 \\ 0.5 \end{pmatrix}, \ p_4 = \begin{pmatrix} 2.5 \\ 3 \end{pmatrix}, \ p_5 = \begin{pmatrix} 2 \\ 2 \end{pmatrix} \right\},$$

$$B = \left\{ p_6 = \begin{pmatrix} 0.5 \\ 1.5 \end{pmatrix}, \ p_7 = \begin{pmatrix} -1 \\ 3 \end{pmatrix}, \ p_8 = \begin{pmatrix} 0 \\ 0.5 \end{pmatrix} \right\}$$

Instances of class A shall be labeled with 1, instances of class B with -1.

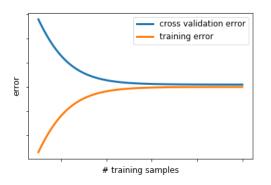
Name the support vectors, compute the optimal separating hyperplane and visualize the result. How wide is the margin?

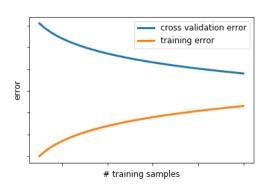
Exercise 9-3 Failure of k-fold cross validation

Consider a case in that the label is chosen at random according to $P[y=1] = P[y=0] = \frac{1}{2}$. Consider a learning algorithm that outputs the constant predictor h(x) = 1 if the parity of the labels on the training set is 1 and otherwise the algorithm outputs the constant predictor h(x) = 0. Prove that the difference between the leave-one-out estimate and the true error in such a case is always $\frac{1}{2}$.

Exercise 9-4 Bias vs. Variance - General

Consider the following learning curves showing training and cross-validation error for two different models when the respective model is trained on an increasing amount of data. For both cases, discuss bias and variance. What are indicators for a high variance or a high bias problem?





Exercise 9-5 Bias-Variance Decomposition

Assume a fixed distribution P(x) over x and a dependent variable $y = f(x) + \epsilon$ with $\epsilon \sim \mathcal{N}(0, \sigma^2)$. We try to model this relationship by a function $\hat{f}(x, w)$ whose parameter w we learn. For short, we write f(x) = f and $\hat{f}(x, w) = \hat{f}$. Consider the expected square loss $\mathbb{E}[L] = \mathbb{E}[(\hat{f} - y)^2]$.

(a) Show that: $\mathbb{E}[(\hat{f}-y)^2] = \mathbb{E}[(\hat{f}-f)^2] + \mathbb{E}[(f-y)^2]$ with $\mathbb{E}[(f-y)^2] = \text{Var}[y] = \sigma^2$ being the intrinsic noise of the data.

Hint: Make use of the calculation rules for the expected value: For two random variables X and Y and a constant c it holds that: $\mathbb{E}[cX + Y] = c\mathbb{E}[X] + \mathbb{E}[Y]$. Moreover, if X and Y are independent: $\mathbb{E}[X \cdot Y] = \mathbb{E}[X] \cdot \mathbb{E}[Y]$.

- (b) Now show that: $\mathbb{E}[(\hat{f} f)^2] = \mathbb{E}[(\hat{f} \mathbb{E}[\hat{f}])^2] + (\mathbb{E}[\hat{f}] f)^2$ where $\mathbb{E}[(\hat{f} \mathbb{E}[\hat{f}])^2]$ is the variance and $(\mathbb{E}[\hat{f}] f)^2$ the squared bias of our estimation \hat{f} . Hint: Substract and add $\mathbb{E}[\hat{f}]$ to the squared term in the loss and simplify.
- (c) With that we have:

$$\mathbb{E}[L] = \mathbb{E}[(\hat{f} - y)^2] = \mathbb{E}[(\hat{f} - \mathbb{E}[\hat{f}])^2] + (\mathbb{E}[\hat{f}] - f)^2 + \mathbb{E}[(f - y)^2]$$
$$= \text{Var}[\hat{f}] + (\text{Bias}(\hat{f}))^2 + \sigma^2.$$

What is the minimum of the expected loss?