Prof. J. M. Buhmann

Final Exam

February 10th, 2010

First and Last name: ______________________________

ETH number: ______________________________

Signature: ______________________________

General Remarks

- Please check that you have all 21 pages of this exam.
- Remove all material from your desk which is not permitted by the examination regulations.
- Fill in your first and last name and your ETH number and sign the exam. Place your student ID in front of you.
- You have 2 hours for the exam. There are five questions, where you can earn a total of 150 points. Scoring 120 points (equivalent to solving four questions) guarantees you a grade of six.
- Write your answers directly on the exam sheets. If you need more space, put your name and ETH number on top of each supplementary sheet.
- Answer the questions in English. Do not use a pencil or red color pen.
- You may provide at most one valid answer per question. Invalid solutions must be canceled out clearly.

	Topic	Max. Points	Points Achieved	Visum
1	Density Estimation	30		
2	PCA	30		
3	Classifiers	30		
4	Regression	30		
5	Boosting	30		
Total		150		

Grade: ....

Question 1: Parametric Density Estimation (30 pts.)

When estimating densities from data, we assume that the data distribution is well approximated by a parametric model $P(x; \boldsymbol{\theta})$, where $\boldsymbol{\theta}$ denotes the parameters of the model. Estimation of the density then reduces to estimation of the parameter $\boldsymbol{\theta}$.

a) In maximum-likelihood estimation (MLE), we usually start by assuming that the data is given as an i.i.d. sample $x_1, x_2, ..., x_N \sim P(x; \theta)$. Please explain how this assumption simplifies the calculations.
Answer:

2 pts.

b) We model a coin flip as a random variable X, where $X = 1$ denotes the outcome 'heads', and $X = 0$ denotes 'tails'. We model this event using the Bernoulli distribution, parametrized by μ that denotes $P(X = 1)$.

$$\text{Bern}(x|\mu) = \mu^x (1 - \mu)^{1-x}.$$

Given a data set $\mathcal{X}_N = \{x_1, ..., x_N\}$ of N i.i.d. observations of X, show us step by step how to compute the MLE for μ. Comment your calculations where necessary.
Answer:

8 pts.

c) We flip our coin three times and obtain the dataset $\mathcal{X}_3 = \{1, 1, 1\}$.

1. What is the MLE for $\hat{\mu}$ for dataset $\mathcal{X}_3$?
   Answer:

2. State one problem with this estimate. What is a possible remedy (solution)?
   Answer:

3 pts.

d) Assume that there are a total of m heads in $\mathcal{X}_N$, i.e., $\sum_{i=1}^{N} x_i = m$.

1. In terms of μ, N and m only, what is the probability of obtaining this dataset $P(\mathcal{X}_N|\mu)$? Explain the terms of your solution.
   Answer:

2. What is the expected value of m? (*Hint: For independent random variables, the expectation of a sum is the sum of expectations*)
   Answer:
   $\mathbb{E}[m] =$

5 pts.

We now turn to Bayesian estimation of μ given a data set $\mathcal{X}$, by introducing a prior distribution $P(\mu)$. Here, we use the (conjugate) prior given by the Beta distribution:

$$\text{Beta}(\mu|\alpha,\beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\mu^{\alpha-1}(1-\mu)^{\beta-1},$$

where $\Gamma(x)$ denotes the gamma function (not necessary). Some useful properties:

1. Mean $\mathbb{E}(\mu) = \frac{\alpha}{\alpha+\beta}$
2. Variance $\mathbb{V}(\mu) = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$

e) With the mean and variance of μ, we can understand how the parameters influence the prior. Select the best (α_0, β_0) pair for the prior that emphasizes the following beliefs.

1. My coin is biased towards 'tails'.
   $\square(0.5, 0.5)$ $\square(1, 4)$ $\square(4, 1)$ $\square(2, 2)$
2. My coin is most probably biased (but I don't know heads or tails)
   $\square(0.5, 0.5)$ $\square(1, 4)$ $\square(4, 1)$ $\square(2, 2)$

3 pts.

f) Show that if the prior is Beta distributed

$$P(\mu) = \text{Beta}(\alpha_0, \beta_0),$$

then the posterior takes again the same functional dependency on μ as the prior, i.e.,

$$P(\mu|\mathcal{X}_N) \propto \mu^{\alpha_0+m-1}(1-\mu)^{\beta_0+N-m-1}.$$

Answer:

5 pts.

g) In fact, the posterior is again a Beta distribution, and we obtain $P(X = 1|\mathcal{X}) = \frac{m+\alpha_0}{N+\alpha_0+\beta_0}$.

1. For $\mathcal{X}_3 = \{1, 1, 1\}$, use a choice of (α_0, β_0) which assumes a fair coin, and obtain your estimate for $P(X = 1|\mathcal{X})$. How does this estimate differ from the MLE?
   Answer:

2. What happens to the posterior as $N \to \infty$? How does this relate to the MLE?
   Answer:

4 pts.

Question 2: Principal Component Analysis (PCA) (30 pts.)

Principal component analysis is a widely applied method in data analysis and dimensionality reduction. Given a dataset $\mathbf{X} \in \mathbb{R}^{D \times N}$ (observations as columns), where D is the number of dimensions and N is the number of observations, a linear transformation using an orthonormal matrix $\mathbf{P} \in \mathbb{R}^{M \times D}$ is applied to make a *change of basis*, to obtain a (usually) lower-dimensional dataset $\mathbf{Y} \in \mathbb{R}^{M \times N}$.

a) We begin by reviewing the steps of applying PCA to a dataset $\mathbf{X}$. Please complete each step below by providing the appropriate formula to compute the desired quantity.

   1. Define the zero-mean dataset $\tilde{\mathbf{X}}$ in terms of the original dataset $\mathbf{X}$. For this purpose, introduce the data mean as a column-vector $\boldsymbol{\mu} \in \mathbb{R}^{D \times 1}$.
      Answer:

   2. Define the covariance matrix $\mathbf{C}_{\tilde{\mathbf{X}}}$ in terms of the zero-mean dataset $\tilde{\mathbf{X}}$.
      Answer:

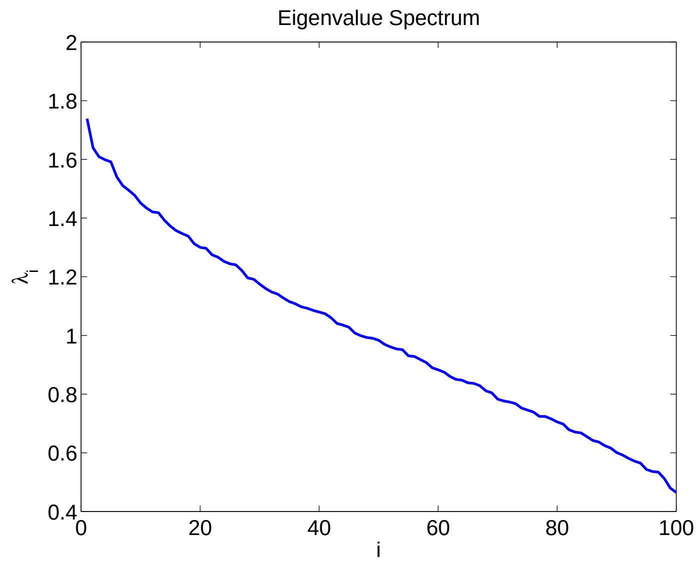
   3. Write down the eigen-decomposition of the covariance matrix $\mathbf{C}_{\tilde{\mathbf{X}}}$, in terms of the eigenvector matrix $\mathbf{E}$ (eigenvectors as columns) and the diagonal matrix of eigenvalues $\mathbf{D}$.
      Answer:

   4. Define the PCA transformation matrix $\mathbf{P}$ in terms of the eigenvector matrix $\mathbf{E}$. (Note: assume we don't want to reduce the dimensionality of the transformed dataset. Further assume that the eigenvectors in $\mathbf{E}$ have already been sorted according to the corresponding eigenvalues, in decreasing order.)
      Answer:

   5. Define the transformed dataset $\mathbf{Y}$ in terms of the original dataset $\mathbf{X}$ and the transformation matrix $\mathbf{P}$.
      Answer:

6 pts.

b) Assume we have applied PCA to some dataset ($D = 100$). We observe the following eigenvalue spectrum of the covariance matrix of the data. (λ_i: eigenvalues)



1. Is the intrinsic dimensionality of this dataset low or high? Why?
   Answer:

2. Can this dataset be expressed in few dimensions with low approximation error? Why?
   Answer:

3. If yes, which dimensionality (approximately) should be chosen for the transformed dataset and why?
   Answer:

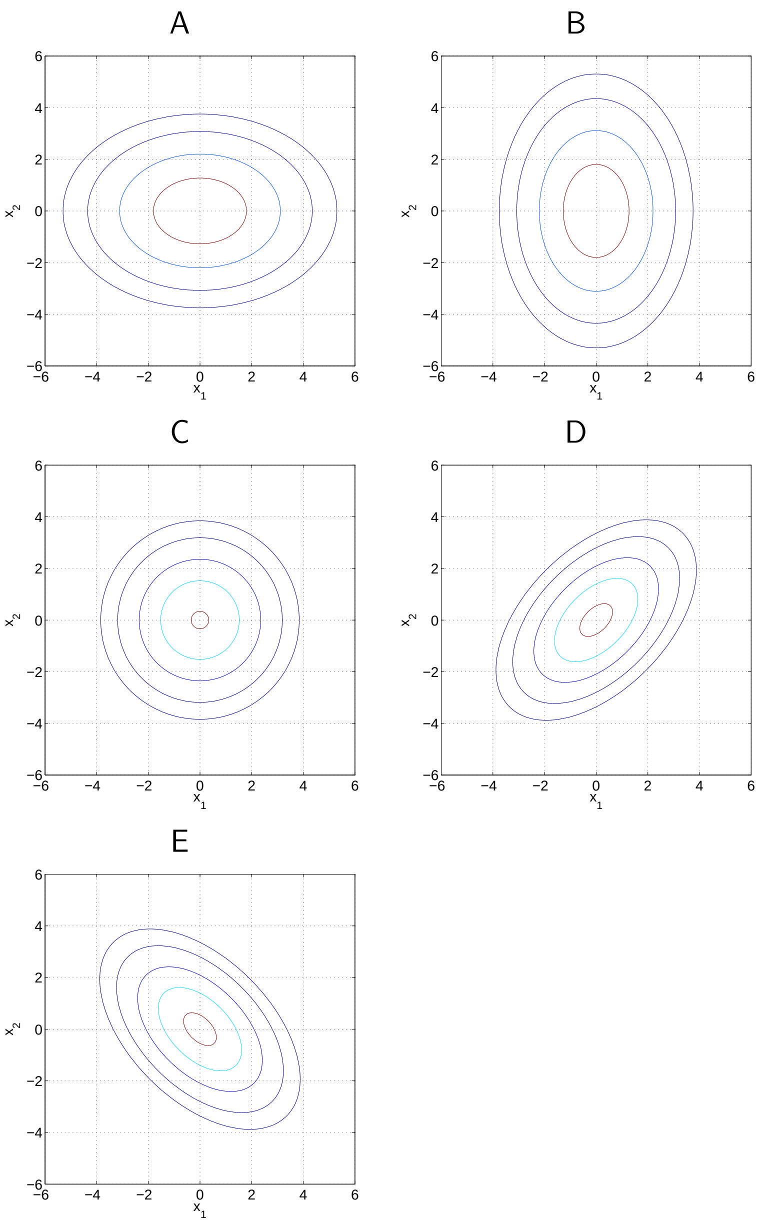
5 pts.

c) Assume you have observed 2D data $\mathbf{X} \in \mathbb{R}^{2 \times N}$ (observations as columns). The first row of $\mathbf{X}$ corresponds to the first dimension x_1, the second row corresponds to x_2. For each of the three covariance matrices $\mathbf{C}_\mathbf{X}$ below, please choose the iso-line plot (A-E) corresponding to the covariance matrix. (Note the axis labels on the figures)

1. $\begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$ Answer: ( )

2. $\begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix}$ Answer: ( )

3. $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ Answer: ( )



3 pts.

d) PCA can be derived as follows: Given a dataset $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\} \in \mathbb{R}^{D \times N}$, find a new set of basis vectors such that the variance of the projected dataset is maximized. We begin by finding the first projection direction $\mathbf{e}_1 \in \mathbb{R}^D$, $||\mathbf{e}_1||_2 = 1$, which satisfies our goal.

1. Please describe in words why we are interested to find a projection direction such that the projected data has large variance.
   Answer:

2. Write down formally the objective function for maximizing the variance of the projected dataset. For this purpose, define the variance of the projected dataset in terms of the original data $\mathbf{x}_n$ and the first projection direction $\mathbf{e}_1$. (Hint: introduce the mean $\boldsymbol{\mu}$ of the data $\mathbf{X}$.)
   Answer:

5 pts.

e) PCA transforms a dataset $\mathbf{X}$ into a dataset $\mathbf{Y}$ by defining a new basis using the eigenvectors of the covariance matrix $\mathbf{C_X}$ of the dataset $\mathbf{X}$. With this particular choice of a new basis, the covariance matrix $\mathbf{C_Y}$ of the transformed dataset $\mathbf{Y}$ is *diagonalized*. (Note: For this exercise, assume a zero-mean dataset.)

1. Please explain in words, why we desire the covariance matrix of the transformed dataset to be diagonal.
   Answer:

2. Show that $\mathbf{C_Y} = \mathbf{P}\mathbf{C_X}\mathbf{P}^T$, i.e., that the covariance matrix $\mathbf{C_Y}$ of the transformed dataset can be written in terms of the covariance matrix $\mathbf{C_X}$ of the original dataset.
   Answer:

3. Show that the choice $\mathbf{P} = \mathbf{E}^T$ for the PCA transformation matrix, where $\mathbf{E}$ is the matrix of eigenvectors of the covariance matrix $\mathbf{C_X}$, actually diagonalizes the covariance matrix $\mathbf{C_Y}$ of the transformed dataset $\mathbf{Y}$. Use the eigen decomposition of $\mathbf{C_X}$ and the fact that $\mathbf{P}^{-1} = \mathbf{P}^T$.
   Answer:

11 pts.

Question 3: Linear Classifiers (30 pts.)

The simplest representation of a linear discriminant function is obtained by taking a linear function of the input vector $\boldsymbol{x}$ so that

$$y(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + b$$

a) Define the term decision boundary. Explain what is the relation between the vector $\boldsymbol{w}$ and the decision boundary.
Answer:

2 pts.

b) Consider the following set $S \subseteq \mathbb{R}^2 \times \{+1, -1\}$:

$$S = \{((3,3),+1),((1,4),+1),((2,1),-1),((5,1),-1),((6,2),+1),((4,3),+1),((4,1),-1)\}$$

Prove that there exist no homogeneous half-space that separates S with no errors (recall that a half-space is homogeneous if its separating hyperplane passes through the origin). Assume that the classification of a point is given by $y(\boldsymbol{x}) = \mathrm{sign}(\boldsymbol{w}^T \boldsymbol{x} + b)$.
Answer:

5 pts.

The simple form of the online perceptron algorithm is defined as follows:

Initialize by setting $\boldsymbol{w}^{(0)} = \mathbf{0}$.

$$\text{Update } \boldsymbol{w}^{(t+1)} = \begin{cases} \boldsymbol{w}^{(t)} & y_k({\boldsymbol{w}^{(t)}}^T \boldsymbol{x}_k) > 0 \\ \boldsymbol{w}^{(t)} + y_k \boldsymbol{x}_k & \text{otherwise.} \end{cases}$$

c) We would like to use the perceptron algorithm to find a separating half-space that makes no errors on the set S. Recall that you have just proven that this is impossible using a homogeneous half-space. Make the necessary adjustments and perform 7 iterations of the perceptron algorithm. For each iteration write down the training example and the current vector $\boldsymbol{w}^{(t)}$. Assume that the points are given in the same order as they appear in S.
Answer:

5 pts.

Consider the primal form of the soft margin SVM

$$\begin{aligned} &\min \tfrac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{n} \xi_i \\ &s.t. \qquad y_i(\boldsymbol{w}^T \boldsymbol{x}_i + b) \geq 1 - \xi_i, \qquad i = 1, \ldots, n \end{aligned}$$

d) Indicate which of the following statements hold as we increase the value of the parameter C (relative to any starting value, $C > 0$). Use

D - if the validity of the statement depends on the situation,
T - if the statement is necessary true
N - if the statement is never true

[ ] b will not increase

[ ] $\|\boldsymbol{w}\|$ increases

[ ] $\|\boldsymbol{w}\|$ will not decrease

[ ] more points will be misclassified

[ ] The geometric margin will not increase

10 pts.

The dual soft margin SVM is given below

$$\max \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)$$
$$s.t. \qquad 0 \leq \alpha_i \leq C, \qquad i = 1, \ldots, n$$

We would like to solve the SVM problem using the kernel $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = 1 + (\boldsymbol{x}_i^T \boldsymbol{x}_j)^2$.

e) What is the feature representation $\phi(\boldsymbol{x})$ corresponding to this kernel for $\boldsymbol{x} \in \mathbb{R}^2$?
Answer:

2 pts.

f) Using the dual variables α's and $\phi(\boldsymbol{x})$, give an explicit form for the primal variable $\boldsymbol{w}$.
Answer:

2 pts.

We solved the dual SVM problem with the above kernel. We used the following training set $\boldsymbol{x}_1 = (1, 1), y_1 = +1$, $\boldsymbol{x}_2 = (3, 0), y_2 = -1$, $\boldsymbol{x}_3 = (-2, 1), y_3 = -1$.
Below are the α's and b values
$\alpha_1 = 0.1$, $\alpha_2 = 0$, $\alpha_3 = 0.1$, $b = 1.5$

g) Use these values to compute the kernelized discriminant function $y(\boldsymbol{x})$.
Answer:

4 pts.

Question 4: Regression (30 pts.)

In *univariate regression analysis*, we study the *statistical* dependency of the output variable $y \in \mathbb{R}$ on the input variable $x \in \mathbb{R}$.

a) Complete the equation

$$y = \qquad + \qquad \tag{1}$$

where the right hand side consists of two terms. Define each term in the equation.
Note: Be general, don't restrict yourself to linear least-squares regression.
Answer:

3 pts.

b) Regression analysis is only meaningful if there actually is a true dependency between x and y. Prove that if x and y are *statistically independent*, there is no linear dependency:

1. Assume that x and y are statistically independent.
2. Begin with the definition of *covariance*,

$$\mathrm{cov}(x, y) = \mathbb{E}\left[(x - \mu_x)(y - \mu_y)\right],$$

where $\mathbb{E}$ is the expectation operator and μ_x is the mean of x.

3. Show that x and y are uncorrelated.

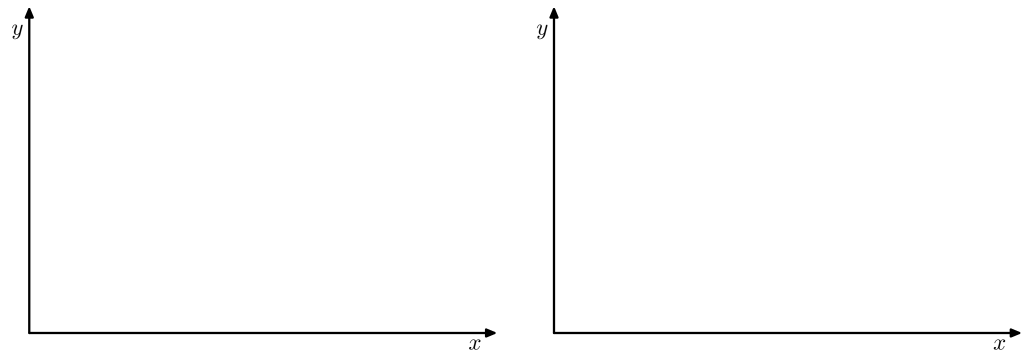
Note: Comment your calculations where necessary.
Answer:

5 pts.

c) You have shown that eq. (1) consists of two terms. Illustrate two conceptually different cases where a linear least-squares fit is inappropriate for the true dependency between x and y, one related to the first term in eq. (1), and one related to the second term in eq. (1):

1. Draw a scatter plot of a data sample.
2. Fit the linear least-squares solution into the sample (qualitatively).
3. Explain why the solution does not capture the true dependency between x and y.

Answer:



4 pts.

So far, we considered a single input variable x. In multivariate linear regression, we assume a weighted linear functional dependency

$$y = w_0 + w_1 x_1 + \cdots + w_D x_D \tag{2}$$

between D input variables $x_1, \ldots, x_D \in \mathbb{R}$ and output variable y.

d) Define the input data matrix $\mathbf{X}$, weight vector $\mathbf{w}$ and output data vector $\mathbf{y}$ such that eq. (2) for all N data points of the sample $(x_1^n, x_2^n, \ldots, x_D^n, y^n), n = 1, \ldots, N$ can be written as

$$\mathbf{y} = \mathbf{X}\mathbf{w}.$$

Answer:

$\mathbf{X} :=$ $\mathbf{w} :=$ $\mathbf{y} :=$

3 pts.

The linear least-squares prediction $\hat{\mathbf{y}}$ is the *orthogonal projection* of $\mathbf{y}$ onto the space spanned by the columns of $\mathbf{X}$, and can be written as

$$\hat{\mathbf{y}} = \mathbf{P}\mathbf{y}.$$

e) Analytically derive $\mathbf{P}$, where $\hat{\mathbf{y}}$ is the least-squares prediction vector. To achieve this:

1. Derive the optimal weight vector $\hat{\mathbf{w}}$ that minimizes the least-squares objective function

$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 \tag{3}$$

Note: we have $\frac{\partial}{\partial \mathbf{w}} \mathbf{w}^\top \mathbf{S} \mathbf{w} = 2\mathbf{S}\mathbf{w}$ *for symmetric matrix* $\mathbf{S}$*, and* $\frac{\partial}{\partial \mathbf{w}} \mathbf{w}^\top \mathbf{a} = \mathbf{a}$.

2. Using your result for $\hat{\mathbf{w}}$, give the definition for $\mathbf{P}$.

Answer:

5 pts.

f) Prove that $\mathbf{P}$ is an orthogonal projector, by showing that $\mathbf{P} = \mathbf{P}\mathbf{P}$ and $\mathbf{P} = \mathbf{P}^\top$.

Answer:

2 pts.

g) Computing $\hat{\mathbf{w}}$ involves the inversion of the symmetric matrix $\mathbf{S} := \mathbf{X}^\top \mathbf{X}$, which we assume to be *positive definite*. Give a mathematical condition (in terms of the eigenvalues of $\mathbf{S}$), when this inversion is numerically unstable.

Answer:

2 pts.

h) Ridge regression finds the regularized weight vector $\hat{\mathbf{w}}_{\text{ridge}}$ that minimizes eq. (3) with an additional norm penalty,

$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 + \lambda \|\mathbf{w}\|_2^2 .$$

Explain why choosing $\lambda > 0$ improves stability of the inversion:

1. Derive the regularized optimal weight vector $\hat{\mathbf{w}}_{\text{ridge}}$.
   Answer:

2 pts.

2. What is the effect of increasing λ on
   (a) the norm $\|\hat{\mathbf{w}}_{\text{ridge}}\|_2$ and
   (b) the numerical stability of computing $\hat{\mathbf{w}}_{\text{ridge}}$?

   Provide **arguments** for your answers.
   Answer:

4 pts.

Question 5: Bagging and AdaBoost (30 pts.)

Bagging and AdaBoost are two ensemble methods used frequently in classification.

a) State two essential differences between bagging and AdaBoost.
Answer:

2 pts.

b) Explain how bagging reduces the variance of an estimator?
Answer:

3 pts.

c) State two factors that may influence the performance of AdaBoost?
Answer:

2 pts.

d) How can we use AdaBoost to detect outliers (mislabeled or ambiguously labeled examples)?
Answer:

2 pts.

For a binary classification problem (± 1), assume we have $c_1, ..., c_B$ successive base classifiers obtained via AdaBoost, and let $\alpha_1, ..., \alpha_B$ be the corresponding weights. The ensemble classifier is $\hat{c}_B(x) = \text{sgn}(\sum_{b=1}^{B} \alpha_b c_b(x))$.

Reusing the same base classifiers $c_1, ..., c_B$, we now train a *linear* classifier, by finding *new* $\tilde{\alpha}_b$'s that minimize the average exponential loss on the training examples, and obtain $\tilde{\hat{c}}_B(x) = \text{sgn}(\sum_{b=1}^{B} \tilde{\alpha}_b c_b(x))$.

e) Is $\tilde{\hat{c}}_B$ equivalent to $\hat{c}_B$? Justify your answer.
Answer:

4 pts.

Consider the following simplified ensemble learning algorithm:

We consider a dataset $\{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}$ of N i.i.d. samples, where $y_n \in \{-1, +1\}$. After each iteration b of this algorithm, each training sample x_n has an associated weight $w_{b,n}$. At the beginning, $w_{0,n} = 1$ for $n = 1, ..., N$. Let $0 < \gamma < \frac{1}{2}$ and $\beta = \frac{1+2\gamma}{1-2\gamma}$.

For each iteration $b = 1$ to B:

- The algorithm finds a new weak learner c_b on the weighted training set that is guaranteed to have an error of at most $\frac{1}{2} - \gamma$ on the weighted training set.
- We then update the weights of the training samples:
  - If x_n is misclassified by c_b, i.e., if $c_b(x_n) \neq y_n$: Set $w_{b,n} := \beta w_{b-1,n}$.
  - Otherwise the weight remains unchanged: $w_{b,n} := w_{b-1,n}$.

The ensemble classifier decides by combining the weak learners as follows:

$$\hat{c}_B(x) = \text{sgn}(\sum_{b=1}^{B} c_b(x)).$$

Let $W_b = \sum_{n=1}^{N} w_{b,n}$ be the sum of the weights at the end of iteration b.

f) What is the difference between AdaBoost and this algorithm in the way they combine the weak learners?
Answer:

2 pts.

g) Derive a bound on W_B, the sum of the weights after the final iteration. Given that at each iteration b, the sum of the weights increases by at most a factor of $1 + 2\gamma$:

$$\frac{W_b}{W_{b-1}} \leq 1 + 2\gamma,$$

show that for the final sum of weights it holds that

$$W_B \leq N(1 + 2\gamma)^B.$$

Answer:

4 pts.

h) Prove the following lower bound on the final weight of a training sample, if it is misclassified by the ensemble:

If $\hat{c}_B(x_n) \neq y_n$, then $w_{B,n} \geq \beta^{B/2}$.

Answer:

4 pts.

i) Finally, we will show a bound on the empirical error rate on the training data. Let $M = |\{n : \hat{c}_B(x_n) \neq y_n\}|$ be the number of training samples misclassified by the ensemble classifier.

1. Plugging the two previous bounds together, we have

$$M\beta^{B/2} \leq \sum_{n=1}^{N} w_{n,B} = W_B \leq N(1+2\gamma)^B.$$

   Starting from this inequality, show that the empirical error rate on the training data is bounded by the following:

$$\frac{M}{N} \leq e^{-2B\gamma^2}.$$

   (*Hint: note that* $(1+a)^c \leq e^{ac}$ *for* $c \geq 0$, *and recall that* $\beta = \frac{1+2\gamma}{1-2\gamma}$)
   Answer:

2. Explain what happens to this bound when we
   (a) increase B (the number of training iterations),
   (b) increase γ (have a very good learner).
   Answer:

7 pts.

This page has been intentionally left blank.

Supplementary Sheet

Supplementary Sheet