

Advanced Machine Learning

Spring 2021

Prof. Joachim M. Buhmann

Final Exam

August 27th, 2021

First and last name: _____

Student ID number: _____

Signature: _____

General Remarks

- Please check that you have all 28 pages of this exam.
- There are 100 points in total.
- The duration of the exam is 180 minutes.
- Do not spend too much time on a single question. You do not need 100 points to get the top grade.
- Remove all material which is not permitted by the examination regulations from your desk.
- Write your answers directly on the exam sheets. If you need more space, make sure you put your student ID number on top of each supplementary sheet.
- Immediately inform an assistant in case that you are not able to take the exam under regular conditions. Later complaints are not accepted.
- Attempts to cheat/defraud lead to immediate notification to the rector's office with a possible exclusion from the examination and it might entail judicial consequences.
- Use a **black** or a **blue** pen to answer the questions. Pencils or red/green colored pens are not allowed.
- Provide only one solution to each exercise. Invalid solutions have to be clearly and unambiguously cancelled.

	Topic	Points	Points achieved	Checked
1	Regression	10		
2	Gauss-Markov	12		
3	Kernels	12		
4	Linear discriminators	10		
5	Maximum likelihood	12		
6	SVMs	10		
7	Ensembles	12		
8	ELBO	12		
9	PAC learning	10		
Total		100		

$$\begin{aligned}
X\beta^r &= X(X^\top X + \lambda I)^{-1} X^\top Y \\
&= UDV^\top (V \underbrace{D^\top U^\top U D}_{=I} V^\top + \lambda I)^{-1} V D^\top U^\top Y \\
&\quad \underbrace{\hspace{10em}}_{=D^2 \text{ (as } D \text{ is diag.)}} \\
&\quad \underbrace{\hspace{10em}}_{=D^2 \underbrace{V V^\top}_{=I} = D^2} \\
&= UDV^\top (D^2 + \lambda I)^{-1} V D^\top U^\top Y \\
\text{As } D \text{ is diagonal, it follows that:} \\
&= UD(D^2 + \lambda I)^{-1} \underbrace{V^\top V}_{=I} D^\top U^\top Y \\
&= UD(D^2 + \lambda I)^{-1} D U^\top Y
\end{aligned}$$

- Briefly explain what the equation above demonstrates about ridge regression and multicollinearity.

2 pts

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In case of multicollinearity, the rank of X is less than full and D^2 cannot be inverted. The equation above shows that by adding λI to D^2 , ridge regression ensures the equation stays solvable even if D^2 is not invertible on its own. (choosing a relatively large λ can also prevent the estimates from having a large variance.)

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Gauss-Markov Theorem:

For any $a \in \mathbb{R}^d$, it holds that

$$\text{Var}(a^\top \tilde{\beta}) \geq \text{Var}(a^\top \hat{\beta})$$

Proof:

1. $\text{Var}(a^\top \tilde{\beta}) \geq a^\top \sigma^2 (X^\top X)^{-1} a$ (inferred from above)
2. $\text{Var}(a^\top \hat{\beta}) = a^\top \text{Cov}(\hat{\beta}) a$ (inferred from above)
- 3.

$$\begin{aligned}\hat{\beta} &= (X^\top X)^{-1} X^\top Y \\ &= (X^\top X)^{-1} X^\top (X\beta + \xi) \\ &= \underbrace{(X^\top X)^{-1} (X^\top X \beta)}_{=\beta} + (X^\top X)^{-1} X^\top \xi \\ &= \beta + (X^\top X)^{-1} X^\top \xi\end{aligned}$$

4.

$$\begin{aligned}\text{Cov}(\hat{\beta}) &= \underbrace{\text{Cov}(\beta)}_{=0} + \text{Cov}((X^\top X)^{-1} X^\top \xi) \\ &= \mathbb{E}[(X^\top X)^{-1} X^\top \xi \xi^\top X (X^\top X)^{-1}] \\ &= (X^\top X)^{-1} X^\top \underbrace{\mathbb{E}[\xi \xi^\top]}_{=\sigma^2 I} X (X^\top X)^{-1} \\ &= (X^\top X)^{-1} X^\top \sigma^2 I X (X^\top X)^{-1} \\ &= \sigma^2 I (X^\top X)^{-1} X^\top X (X^\top X)^{-1} \\ &= \sigma^2 (X^\top X)^{-1}\end{aligned}$$

Hence:

$$\text{Var}(a^\top \tilde{\beta}) \geq a^\top \underbrace{\sigma^2 (X^\top X)^{-1}}_{\text{Cov}(\hat{\beta})} a = a^\top \text{Cov}(\hat{\beta}) a = \text{Var}(a^\top \hat{\beta})$$

Question 3: Kernels (12 pts)

Let $k_1(x, x')$ and $k_2(x, x')$ be valid kernels. Demonstrate that the following functions are also kernels. You are not allowed to use the method of composition from the lecture.

1. $ck_1(x, x')$, for $c > 0$.

3 pts

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$k(x, x') = ck_1(x, x') = ck_1(x', x) = k(x', x)$ as $k_1(x, x')$ is a valid kernel and hence symmetric.

$$\begin{aligned} \int_{\Omega} \int_{\Omega} f(x)k(x, x') f(x') dx dx' &= \int_{\Omega} \int_{\Omega} f(x)ck_1(x, x') f(x') dx dx' = \\ &= c \int_{\Omega} \int_{\Omega} f(x)k_1(x, x') f(x') dx dx' \geq 0 \end{aligned}$$

as $c > 0$, $\int_{\Omega} \int_{\Omega} f(x)k_1(x, x') f(x') dx dx' \geq 0$ since $k_1(x, x')$ is a valid kernel.

2. $k_1(x, x') + k_2(x, x')$.

3 pts

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 $k(x, x') = k_1(x, x') + k_2(x, x') = k_1(x', x) + k_2(x', x) = k(x', x)$ as $k_1(x, x'), k_2(x, x')$ are both valid kernels and hence symmetric.

$$\begin{aligned} \int_{\Omega} \int_{\Omega} f(x)k(x, x') f(x')dxdx' &= \int_{\Omega} \int_{\Omega} f(x) (k_1(x, x') + k_2(x, x')) f(x')dxdx' = \\ &= \int_{\Omega} \int_{\Omega} f(x)k_1(x, x') f(x')dxdx' + \int_{\Omega} \int_{\Omega} f(x)k_2(x, x') f(x')dxdx' \geq 0 \\ \text{as } \int_{\Omega} \int_{\Omega} f(x)k_1(x, x') f(x')dxdx' &\geq 0, \int_{\Omega} \int_{\Omega} f(x)k_2(x, x') f(x')dxdx' \geq 0 \\ &\text{since } k_1(x, x'), k_2(x, x') \text{ are valid kernels.} \end{aligned}$$

3. $k_1(x, x') k_2(x, x')$.

3 pts



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$k(x, x') = k_1(x, x') k_2(x, x') = k_1(x', x) k_2(x', x) = k(x', x)$ as $k_1(x, x')$, $k_2(x, x')$ are both valid kernels and hence symmetric.

Since $k_1(x, x')$, $k_2(x, x')$ they admit an inner product representation. Let $\phi(x)$ be a feature map for $k_1(x, x')$ and let $\psi(x)$ be a feature map for $k_2(x, x')$.

$$\begin{aligned}
 k(x, x') &= k_1(x, x') k_2(x, x') = (\phi(x)^\top \phi(x')) (\psi(x)^\top \psi(x')) = \\
 &= \left(\sum_i \phi_i(x) \phi_i(x') \right) \left(\sum_j \psi_j(x) \psi_j(x') \right) = \left(\sum_i \sum_j \phi_i(x) \phi_i(x') \psi_j(x) \psi_j(x') \right) = \\
 &= \left(\sum_i \sum_j \phi_i(x) \psi_j(x) \phi_i(x') \psi_j(x') \right) = \left(\sum_{ij} \eta_{ij}(x) \eta_{ij}(x') \right) = \eta(x)^\top \eta(x')
 \end{aligned}$$

where $\eta_{ij}(x) = \phi_i(x) \psi_j(x)$

So $k(x, x')$ can be represented as an inner product with a feature map $\eta(x)$ and, hence, is a valid kernel (Mercer Theorem).

4. Show that if A is symmetric and positive definite, then $k(x, x') = x^\top A x'$ is a valid kernel.

3 pts

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$k(x, x') = x^\top A x' = (x^\top A x')^\top = x'^\top A^\top x = x'^\top A x = k(x', x)$ as $x^\top A x' \in \mathbb{R}$ and A is positive definite and, therefore, symmetric.

Since A is PS, it allows Cholesky decomposition $A = L^\top L$. Therefore, $k(x, x') = x^\top A x' = x^\top L^\top L x' = (Lx)^\top (Lx') = \phi(x)^\top \phi(x')$, where $\phi(x) = Lx$. According to Mercer Theorem, $k(x, x')$ is a valid kernel.

Question 4: Linear discriminators (10 pts)

Consider two random variables (X, Y) taking values in $\mathbb{R}^d \times \{-1, +1\}$, such that

- $P(Y = +1) = P(Y = -1)$,
- $X | Y = +1 \sim \mathcal{N}(\mu_+, \Sigma)$, and
- $X | Y = -1 \sim \mathcal{N}(\mu_-, \Sigma)$, for some $\mu_+, \mu_- \in \mathbb{R}^d$ and some symmetric positive definite $\Sigma \in \mathbb{R}^{d \times d}$.

Formally demonstrate that

$$P(Y = +1 | X = x) = \sigma(\beta^\top x + \beta_0), \tag{4}$$

for some $\beta \in \mathbb{R}^d$ and $\beta_0 \in \mathbb{R}$. Here, σ is the sigmoid function $\sigma(t) = \frac{1}{1+e^{-t}}$.

Derive formulas for β and β_0 .

10 pts

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$$\begin{aligned}
 P(Y = +1 | x) &= \frac{p(x | +1)P(+1)}{p(x | +1)P(+1) + p(x | -1)P(-1)} = \frac{1}{1 + \frac{p(x|-1)P(-1)}{p(x|+1)P(+1)}} \\
 \frac{p(x|-1)P(-1)}{p(x|+1)P(+1)} &= \frac{p(x|-1)}{p(x|+1)} = e^{-\frac{1}{2}(x-\mu_-)^T \Sigma (x-\mu_-) + \frac{1}{2}(x-\mu_+)^T \Sigma (x-\mu_+)} \\
 \beta^\top x + \beta_0 &= \frac{1}{2}(x-\mu_-)^T \Sigma (x-\mu_-) - \frac{1}{2}(x-\mu_+)^T \Sigma (x-\mu_+) = \mu_-^T \Sigma x - \mu_+^T \Sigma x + \frac{1}{2}\mu_-^T \Sigma \mu_- - \frac{1}{2}\mu_+^T \Sigma \mu_+ \\
 \beta &= \Sigma(\mu_- - \mu_+), \quad \beta_0 = \frac{1}{2}\mu_-^T \Sigma \mu_- - \frac{1}{2}\mu_+^T \Sigma \mu_+.
 \end{aligned}$$

Question 5: Constrained optimization and maximum likelihood (12 pts)

Assume given a partition of $[0, 1]$ into M disjoint intervals B_1, \dots, B_M . A *piecewise constant pdf* is a pdf $p : [0, 1] \rightarrow \mathbb{R}^+$ that is constant on each B_j , for $j \leq M$. That is, for all $x \in B_j$, $p(x) = c_j$, for some $c_j \in \mathbb{R}^+$.

Assume that the intervals B_1, \dots, B_M are fixed and that you are given a sample $\{x_1, \dots, x_n\} \subseteq [0, 1]$. Your task is to estimate c_1, \dots, c_M using maximum likelihood.

- a) Let $b : [0, 1] \rightarrow \{1, \dots, M\}$ be the function that maps points in $[0, 1]$ to their corresponding interval in the partition, i.e. $b(x) = j$ iff $x \in B_j$, for $j \leq M$. Write the log likelihood of the sample with respect to c_1, \dots, c_M and b .

2 pts

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$$\sum_{i=1}^n \log c_{b(x_i)}$$

- b) For $j \leq M$, let V_j be the length of the interval B_j . Formulate the problem of computing c_1, \dots, c_M that maximize the sample's log likelihood as a constrained optimization problem.

4 pts

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Using Lagrange multipliers, we obtain the objective function:

$$J(c_i; \lambda) := \sum_{i=1}^n \log c_{b(x_i)} + \lambda \left(\sum_{j=1}^M c_j V_j - 1 \right)$$

Writing the first order condition wrt c_j we obtain:

$$\frac{K_j}{c_j} + \lambda V_j \stackrel{!}{=} 0$$

It follows that:

$$c_j = \frac{-K_j}{\lambda V_j},$$

and from the constraint we get that:

$$-\sum_{j=1}^M \frac{K_j}{\lambda} = 1 \Rightarrow \lambda = -\sum_{j=1}^M K_j \Rightarrow \lambda = -n$$

Introducing λ in the first order condition gives the final result:

$$c_j = \frac{K_j}{nV_j}, \forall j \in \{1, \dots, M\}$$

Question 6: SVMs (10 pts)

Let $\{(x_1, y_1), \dots, (x_n, y_n)\} \subseteq \mathbb{R}^d \times \{+1, -1\}$. Consider the standard problem of training an SVM:

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{1}{2} \|w\|^2 \tag{6}$$

$$\text{s.t. } y_i (w^\top x_i + b) \geq 1, \text{ for } i \leq n. \tag{7}$$

1. Formulate the Lagrangian for this constrained optimization problem.

2 pts

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2. Formulate the dual for this optimization problem and rewrite it so that w never appears.

3 pts

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3. Prove that if there exists $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$ that fulfil the constraints of this problem, then this problem satisfies Slater's condition.

3 pts

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4. Suppose that Slater's condition is not fulfilled. What is the consequence of this for strong duality? Briefly explain.

2 pts

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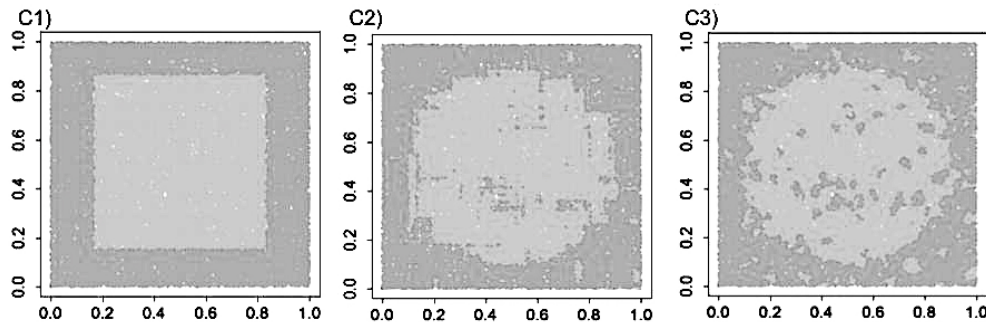
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Question 7: Ensembles (12 pts)

1. The following figure, from the paper “Explaining the Success of AdaBoost and Random Forests as Interpolating Classifiers”, by Wyler et al, depicts a dataset for binary classification and three ensembles trained on that set. Match the classifiers to their corresponding plots ($C1, C2, C3$).

3 pts



- AdaBoost with deep decision trees ...
 - A shallow decision tree ...
 - A 1NN classifier ...
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- [AdaBoost with deep decision trees C2](#)
 - [A shallow decision tree C1](#)
 - [A 1NN classifier C3](#)
2. Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and p be a distribution over \mathbb{R}^d . Suppose that we draw a sample $Z = \{X_1, \dots, X_n\}$ from p and train M regression functions f_1, \dots, f_M by repeatedly running some randomized algorithm on $\{(X_1, f(X_1)), \dots, (X_n, f(X_n))\}$. Assume that $\mathbb{E}_Z[f_i(x)] = f(x)$, for all $x \in \mathbb{R}^d$ and $i \leq M$.

Let

$$\bar{f}(x) := \frac{1}{M} \sum_{i \leq M} f_i(x). \quad (8)$$

Demonstrate that the ensemble \bar{f} is a better estimator of f than any f_i . That is, for any $i \in 1, \dots, M$:

$$\mathbb{E}_Z \left[(f(x) - \bar{f}(x))^2 \right] \leq \mathbb{E}_Z \left[(f(x) - f_i(x))^2 \right], \text{ for any } x \in \mathbb{R}^d. \quad (9)$$

9 pts

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Proof 1.

$$\begin{aligned}
 \mathbb{E}_Z \left[(f(x) - \bar{f}(x))^2 \right] &= \mathbb{E}_Z \left[(\mathbb{E}_Z [\bar{f}(x)] - \bar{f}(x))^2 \right] = \text{Var}_Z (\bar{f}(x)) \\
 &= \frac{1}{M^2} \sum_i \text{Var}_Z (f_i(x)) = \frac{1}{M} \text{Var}_Z (f_i(x)) \leq \text{Var}_Z (f_i(x)) \\
 &= \mathbb{E}_Z \left[(\mathbb{E}_Z [f_i(x)] - f_i(x))^2 \right] = \mathbb{E}_Z \left[(f(x) - f_i(x))^2 \right]
 \end{aligned}$$

Proof 2.

$$\begin{aligned}
 \mathbb{E}_Z \left[(f(x) - \bar{f}(x))^2 \right] &= \mathbb{E}_Z \left[\left(\frac{1}{M} \sum_i (f(x) - f_i(x)) \right)^2 \right] \\
 &= \frac{1}{M^2} \mathbb{E}_Z \left[\sum_{i,j} (f(x) - f_i(x)) (f(x) - f_j(x)) \right] \\
 &= \frac{1}{M^2} \underbrace{\sum_{i \neq j} \mathbb{E}_Z [(f(x) - f_i(x)) (f(x) - f_j(x))]}_0 + \frac{1}{M^2} \sum_i \mathbb{E}_Z [(f(x) - f_i(x))^2] \\
 &= \frac{1}{M} \text{Var}(f_i(x)) \leq \text{Var}(f_i(x))
 \end{aligned}$$

Question 8: Evidence lower bound (12 pts)

Recall the notation from the lecture:

- $p_{\theta'}(\cdot)$ is a distribution over a representation space \mathcal{Z} , parametrized by $\theta' \in \Theta'$.
- For $z \in \mathcal{Z}$, $p_{\theta}(\cdot|z)$ is a conditional distribution over a measurement space \mathcal{X} , parametrized by $\theta \in \Theta$.
- For $x \in \mathcal{X}$, $q_{\phi}(\cdot|x)$ is a tractable distribution over \mathcal{Z} , parametrized by $\phi \in \Phi$. It is intended to approximate $p_{\theta, \theta'}(\cdot|x) \propto p_{\theta'}(\cdot)p_{\theta}(x|\cdot)$.

Let $\{x_1, \dots, x_m\} \subseteq \mathcal{X}$. Demonstrate that:

$$\sum_{i \leq n} \log p_{\theta, \theta'}(x_i) \geq \sum_{i \leq n} \text{elbo}_{\theta', \theta, \phi}(x_i), \quad (10)$$

where

$$\text{elbo}_{\theta', \theta, \phi}(x_i) := \mathbb{E}_{z \sim q_{\phi}(\cdot|x_i)}[\log(p_{\theta}(x_i|z))] + \mathbb{E}_{z \sim q_{\phi}(\cdot|x_i)}\left[\log\left(\frac{p_{\theta'}(z)}{q_{\phi}(z|x_i)}\right)\right] \quad (11)$$

Hints:

- Prove that $\mathbb{E}_{z \sim q_{\phi}(\cdot|x_i)}[\log p_{\theta, \theta'}(x_i)] = \mathbb{E}_{z \sim q_{\phi}(\cdot|x_i)}\left[\log\left(\frac{p_{\theta, \theta'}(x_i, z) q_{\phi}(z|x_i)}{p_{\theta', \theta}(z|x_i) q_{\phi}(z|x_i)}\right)\right]$
- Recall that $D_{KL}(P_1||P_2) = \int P_1(z) \log \frac{P_1(z)}{P_2(z)} dz \geq 0$

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Solution:

$$\log p_{\theta, \theta'}(x_i) = \mathbb{E}_{z \sim q_\phi(\cdot|x_i)} [\log p_{\theta, \theta'}(x_i)] = \mathbb{E}_{z \sim q_\phi(\cdot|x_i)} \left[\log \left(\frac{p_{\theta, \theta'}(x_i, z) q_\phi(z|x_i)}{p_{\theta', \theta}(z|x_i) q_\phi(z|x_i)} \right) \right] = \quad (12)$$

$$= \mathbb{E}_{z \sim q_\phi(\cdot|x_i)} \left[\log \left(\frac{p_{\theta, \theta'}(x_i, z)}{q_\phi(z|x_i)} \right) \right] + \mathbb{E}_{z \sim q_\phi(\cdot|x_i)} \left[\log \left(\frac{q_\phi(z|x_i)}{p_{\theta', \theta}(z|x_i)} \right) \right] = \quad (13)$$

$$= \text{elbo}_{\theta', \theta, \phi}(x_i) + D_{KL}(q_\phi(z|x_i) || p_{\theta', \theta}(z|x_i)) \geq \quad (14)$$

$$\geq \text{elbo}_{\theta', \theta, \phi}(x_i) \quad (15)$$

Q.E.D

Question 9: PAC Learning (10 pts)

1. Consider the definition of PAC learnability:

A concept class \mathcal{C} is PAC learnable from a hypothesis class \mathcal{H} if there is an algorithm \mathcal{A} s.t. for all $0 < \epsilon, \delta < \frac{1}{2}$, for any distribution on the instance space \mathcal{X} , and for any $c \in \mathcal{C}$, there is a polynomial function $poly(\cdot, \cdot, \cdot)$ s.t. if \mathcal{A} receives a sample \mathcal{Z} of size $n \geq poly(\frac{1}{\epsilon}, \frac{1}{\delta}, size(c))$, then \mathcal{A} outputs a hypothesis \hat{c} such that $\mathbf{P}(\mathcal{R}(\hat{c}) \leq \epsilon) \geq 1 - \delta$.

Fill in the gaps to complete the definition of *efficient PAC learnability*:

We say that \mathcal{A} is an efficient PAC algorithm if it runs in time _____ in _____ and _____.

3 pts

We say that \mathcal{A} is an efficient PAC algorithm if it runs in time *polynomial* in $\frac{1}{\epsilon}$ and $\frac{1}{\delta}$.

Schema:

- ? points for each correctly filled in gap.

2. Let \mathbf{P} be a distribution over $\mathcal{X} \subseteq \mathbb{R}^2$. Let \mathcal{C} be a set of functions mapping $\mathbb{R}^2 \rightarrow \{-1, +1\}$.

- For $c \in \mathcal{C}$, a *c-dataset of size n* is a set of the form $\mathcal{Z} = \{(X_1, c(X_1)), \dots, (X_n, c(X_n))\}$ with X_1, \dots, X_n a sample drawn from \mathbf{P} .
- Assume that you are given an algorithm with the following specification:
 - It takes as input any *c-dataset* of size $n \in \mathbb{N}$, for an arbitrary function $c \in \mathcal{C}$.
 - The output is a function $\hat{c}^* \in \mathcal{C}$ such that

$$\mathbf{P}(\mathcal{R}(\hat{c}^*) \leq \epsilon) \geq 1 - 4 \exp\left(-\frac{n\epsilon}{4}\right), \text{ for any } 0 < \epsilon < \frac{1}{2}. \quad (16)$$

Show that the class \mathcal{C} above is PAC-learnable from itself. You may assume that $size(c) = 1$, for any $c \in \mathcal{C}$.

7 pts

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Fix $\delta = 4 \exp\left(-\frac{n\epsilon}{4}\right)$. Choose $n = \frac{4}{\epsilon} \log\left(\frac{4}{\delta}\right)$, then $\mathbf{P}(\mathcal{R}(\hat{c}^*) \leq \epsilon) \geq 1 - \delta$. Observe that $\frac{4}{\epsilon} \log\left(\frac{4}{\delta}\right)$ is polynomial in $\frac{1}{\epsilon}$, $\frac{1}{\delta}$, and $size(c) = 1$. Thus, we have an algorithm \mathcal{A} which returns $\hat{c}^*(\cdot)$ s. t. $\mathbf{P}(\mathcal{R}(\hat{c}^*) \leq \epsilon) \geq 1 - \delta$, for all $0 < \epsilon, \delta < \frac{1}{2}$, for $n \geq poly\left(\frac{1}{\epsilon}, \frac{1}{\delta}, size(c)\right)$. Hence, \mathcal{C} is PAC-learnable from itself.

Schema:

- ? point for defining δ ;
- ? points for deriving $n = \frac{4}{\epsilon} \log\left(\frac{4}{\delta}\right)$;
- ? point for stating that $\frac{4}{\epsilon} \log\left(\frac{4}{\delta}\right)$ is polynomial in $\frac{1}{\epsilon}$, $\frac{1}{\delta}$, and $size(c)$.

Supplementary Sheet

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