**Total possible marks: 100.** Explain all your answers concisely. This set covers chapters 1–5 of the textbook *Introduction to Machine Learning*, 3rd. ed., by E. Alpaydin.

Exercise 1: Bayes' rule (6 points). Suppose that 5% of competitive athletes use performance-enhancing drugs and that a particular drug test has a 2% false positive rate and a 1.5% false negative rate.

- 1. (3 points) Athlete A tests positive for drug use. What is the probability that Athlete A is using drugs?
- 2. (3 points) Athlete B tests negative for drug use. What is the probability that Athlete B is not using drugs?

Exercise 2: Bayesian decision theory: losses and risks (11 points). Consider a classification problem with K classes, using a loss  $\lambda_{ik} \geq 0$  if we choose class i when the input actually belongs to class k, for  $i, k \in \{1, ..., K\}$ .

1. (2 points) Write the expression for the expected risk  $R_i(\mathbf{x})$  for choosing class i as the class for a pattern  $\mathbf{x}$ , and the rule for choosing the class for  $\mathbf{x}$ .

Consider a two-class problem with losses given by the matrix  $\lambda_{ik} = \begin{pmatrix} 0 & 1 \\ \lambda_{21} & 0 \end{pmatrix}$ .

- 2. (3 points) Give the optimal decision rule in the form " $p(C_1|\mathbf{x}) > \dots$ " as a function of  $\lambda_{21}$ .
- 3. (3 points) Imagine we consider both misclassification errors as equally costly. When is class 1 chosen (for what values of  $p(C_1|\mathbf{x})$ )?
- 4. (3 points) Imagine we want to be very conservative when choosing class 2 and we seek a rule of the form " $p(C_2|\mathbf{x}) > 0.99$ " (i.e., choose class 2 when its posterior probability exceeds 99%). What should  $\lambda_{21}$  be?

Exercise 3: association rules (6 points). Given the following data of transactions at a supermarket, calculate the support and confidence values of the following association rules: meat  $\rightarrow$  avocado, avocado  $\rightarrow$  meat, yogurt  $\rightarrow$  avocado, avocado  $\rightarrow$  yogurt, meat  $\rightarrow$  yogurt, yogurt  $\rightarrow$  meat. What is the best rule to use in practice?

transaction #	items in basket
1	meat, avocado
2	yogurt, avocado
3	meat
4	yogurt, meat
5	avocado, meat, yogurt
6	meat, avocado

Exercise 4: true- and false-positive rates (10 points). Consider the following table, where  $\mathbf{x}_n$  is a pattern,  $y_n$  its ground-truth label (1 = positive class, 2 = negative class) and  $p(C_1|\mathbf{x}_n)$  the posterior probability produced by some probabilistic classification algorithm:

$\overline{n}$	1	2	3	4	5
$\overline{y_n}$	1	2	2	1	2
$p(C_1 \mathbf{x}_n)$	0.6	0.7	0.5	0.9	0.2

We use a classification rule of the form " $p(C_1|\mathbf{x}) > \theta$ " where  $\theta \in [0,1]$  is a threshold.

- 1. (8 points) Give, for all possible values of  $\theta \in [0,1]$ , the predicted labels and the corresponding confusion matrix and classification error.
- 2. (2 points) Plot the corresponding pairs (fp, tp) as an ROC curve.

Exercise 5: ROC curves (8 points). Imagine we have a classifier A that has false-positive and true-positive rates  $fp_A, tp_A \in [0, 1]$  such that  $fp_A > tp_A$  (that is, this classifier is below the diagonal on the ROC space). Now consider a classifier B that negates the decision of A, that is, whenever A predicts the positive class then B predicts the negative class and vice versa. Compute the false-positive and true-positive rates  $fp_B, tp_B$  for classifier B. Where is this point in the ROC space?

Exercise 6: least-squares regression (14 points). Consider the following model, with parameters  $\Theta = \{\theta_1, \theta_2, \theta_3\} \subset \mathbb{R}$  and an input  $x \in \mathbb{R}$ :

$$h(x; \mathbf{\Theta}) = \theta_1 + \theta_2 \sin 2x + \theta_3 \sin 4x \in \mathbb{R}.$$

- 1. (2 points) Write the general expression of the least-squares error function of a model  $h(x; \Theta)$  with parameters  $\Theta$  given a sample  $\{(x_n, y_n)\}_{n=1}^N$ .
- 2. (2 points) Apply it to the above model, simplifying it as much as possible.
- 3. (6 points) Find the least-squares estimate for the parameters.
- 4. (4 points) Assume the values  $\{x_n\}_{n=1}^N$  are uniformly distributed in the interval  $[0, 2\pi]$ . Can you find a simpler, approximate way to find the least-squares estimate? *Hint*: approximate  $\frac{1}{N} \sum_{n=1}^{N} f(x_n)$  by an integral.

Exercise 7: maximum likelihood estimate (15 points). A discrete random variable  $x \in \{0, 1, 2...\}$  follows a Poisson distribution if it has the following probability mass function:

$$p(x;\theta) = \frac{e^{-\theta}\theta^x}{x!}$$

where the parameter is  $\theta > 0$ .

- 1. (2 points) Verify that  $\sum_{x=0}^{\infty} p(x) = 1$ .
- 2. (2 points) Write the general expression of the log-likelihood of a probability mass function  $p(x; \Theta)$  with parameters  $\Theta$  for an iid sample  $x_1, \ldots, x_N$ .
- 3. (5 points) Apply it to the above distribution, simplifying it as much as possible.
- 4. (6 points) Find the maximum likelihood estimate for the parameter  $\theta$ .

Exercise 8: multivariate Bernoulli distribution (20 points). Consider a multivariate Bernoulli distribution where  $\theta \in [0, 1]^D$  are the parameters and  $\mathbf{x} \in \{0, 1\}^D$  the binary random vector:

$$p(\mathbf{x}; \boldsymbol{\theta}) = \prod_{d=1}^{D} \theta_d^{x_d} (1 - \theta_d)^{1 - x_d}.$$

1. (5 points) Compute the maximum likelihood estimate for  $\theta$  given a sample  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ .

Let us do document classification using a D-word dictionary (element d in  $\mathbf{x}_n$  is 1 if word d is in document n and 0 otherwise) using a multivariate Bernoulli model for each class. Assume we have K document classes for which we have already obtained the values of the optimal parameters  $\boldsymbol{\theta}_k = (\theta_{k1}, \dots, \theta_{kD})^T$  and prior distribution  $p(C_k) = \pi_k$ , for  $k = 1, \dots, K$ , by maximum likelihood.

- 2. (2 points) Write the discriminant function  $g_k(\mathbf{x})$  for a probabilistic classifier in general (not necessarily Bernoulli), and the rule to make a decision.
- 3. (5 points) Apply it to the multivariate Bernoulli case with K classes. Show that  $g_k(\mathbf{x})$  is linear on  $\mathbf{x}$ , i.e., it can be written as  $g_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}$  and give the expression for  $\mathbf{w}_k$  and  $w_{k0}$ .
- 4. (3 points) Consider K = 2 classes. Show the decision rule can be written as "if  $\mathbf{w}^T \mathbf{x} + w_0 > 0$  then choose class 1", and give the expression for  $\mathbf{w}$  and  $w_0$ .
- 5. (5 points) Compute the numerical values of  $\mathbf{w}$  and  $w_0$  for a two-word dictionary where  $\pi_1 = 0.7$ ,  $\boldsymbol{\theta}_1 = \begin{pmatrix} 0.2 \\ 0.8 \end{pmatrix}$  and  $\boldsymbol{\theta}_2 = \begin{pmatrix} 0.3 \\ 0.6 \end{pmatrix}$ . Plot in 2D all the possible values of  $\mathbf{x} \in \{0,1\}^D$  and the boundary corresponding to this classifier.

Exercise 9: Gaussian classifiers (10 points). Consider a binary classification problem for  $\mathbf{x} \in \mathbb{R}^D$  where we use Gaussian class-conditional probabilities  $p(\mathbf{x}|C_1) \sim \mathcal{N}(\boldsymbol{\mu}, \sigma_1^2 \mathbf{I})$  and  $p(\mathbf{x}|C_2) \sim \mathcal{N}(\boldsymbol{\mu}, \sigma_2^2 \mathbf{I})$ . That is, they have the same mean and the covariance matrices are isotropic but different. Compute the expression for the class boundary. What shape is it?