# Data Mining 2023/2024
# List of exercises

I use the following abbreviations to indicate the source of an exercise:

1. ISL = An Introduction to Statistical Learning by G. James et al.
2. ESL = The Elements of Statistical Learning by T. Hastie et al.
3. ...

## 1 Introduction

**Exercise 1 —** Suppose that random variables $X$ and $Y$ are independent. Prove that (1p)

(a) $\mathbb{E}(X+Y) = \mathbb{E}(X) + \mathbb{E}(Y)$,

(b) $\mathbb{V}\mathrm{ar}(X+Y) = \mathbb{V}\mathrm{ar}(X) + \mathbb{V}\mathrm{ar}(Y)$.

**Exercise 2 —** Recall what is the bias and variance of an estimator. Give examples of biased and unbiased estimators. (1p)

**Exercise 3 —** (ESL, p. 223) Suppose that we have a training set of points $(x_1, y_1), \ldots, (x_n, y_n)$. Assume there is an underlying relation $y = f(x) + \epsilon$, where $\epsilon$ represents noise and is a random variable with zero mean and variance $\sigma_\epsilon^2$. We use the training set to find $\hat{f}(x)$ that approximates $f(x)$. Show that we can decompose expected squared error at a new input $x_0$ as:

$$\mathrm{E}\Big[\big(y_0 - \hat{f}(x_0)\big)^2\Big] = \mathrm{Bias}\big[\hat{f}(x_0)\big]^2 + \mathrm{Var}\big[\hat{f}(x_0)\big] + \sigma_\epsilon^2 \ .$$

What is the bias–variance tradeoff? (3p)

**Exercise 4 —** (ISL) For each of parts (a) through (d), indicate whether we would generally expect the performance of a flexible statistical learning method to be better or worse than an inflexible method. Justify your answer. (1p)

(a) The sample size $n$ is extremely large, and the number of predictors $p$ is small.

(b) The number of predictors $p$ is extremely large, and the number of observations $n$ is small.

(c) The relationship between the predictors and response is highly non-linear.

(d) The variance of the error terms, i.e. $\sigma^2 = \mathbb{V}\mathrm{ar}(\epsilon)$, is extremely high.

**Exercise 5 —** (ISL) Provide a sketch of typical squared bias, variance, training error, test error and irreducible error curves, on a single plot, as we go from less flexible statistical learning methods towards more flexible approaches. The x-axis should represent the amount of flexibility in the method, and the y-axis should represent the values for each curve. Explain the shape of each curve. (1p)

**Exercise 6 —** (ISL) Explain whether each scenario is a classification or regression problem, and indicate whether we are most interested in inference or prediction. Finally, provide the sample size $n$ and the number of predictors $p$. (1p)

(a) We collect a set of data on the top 500 firms in the US. For each firm we record profit, number of employees, industry and the CEO salary. We are interested in understanding which factors affect CEO salary.

(b) We are considering launching a new product and wish to know whether it will be a success or a failure. We collect data on 20 similar products that were previously launched. For each product we have recorded whether it was a success or failure, price charged for the product, marketing budget, competition price, and ten other variables.

(c) We are interesting in predicting the percent change in the US dollar in relation to the weekly changes in the world stock markets. Hence we collect weekly data for all of 2012. For each week we record the percent change in the dollar, the percent change in the US market, the percent change in the British market, and the percent change in the German market.

**Exercise 7** — (ISL) You will now think of some real-life applications for statistical learning. (1p)

(a) Describe three real-life applications in which classification might be useful. Describe the response, as well as the predictors. Is the goal of each application inference or prediction? Explain your answer.

(b) Describe three real-life applications in which regression might be useful. Describe the response, as well as the predictors. Is the goal of each application inference or prediction? Explain your answer.

(c) Describe three real-life applications in which cluster analysis might be useful.

**Exercise 8** — (ISL) What are the advantages and disadvantages of a very flexible (versus a less flexible) approach for regression or classification? Under what circumstances might a more flexible approach be preferred to a less flexible approach? When might a less flexible approach be preferred? (1p)

**Exercise 9** — (ISL) Describe the differences between a parametric and a non-parametric statistical learning approach. What are the advantages of a parametric approach to regression or classification (as opposed to a nonparametric approach)? What are its disadvantages? (1p)

**Exercise 10** — (ISL) The table below provides a training data set containing six observations, three predictors, and one qualitative response variable.

| Obs. | $X_1$ | $X_2$ | $X_3$ | $Y$ |
|---|---|---|---|---|
| 1 | 0 | 3 | 0 | Red |
| 2 | 2 | 0 | 0 | Red |
| 3 | 0 | 1 | 3 | Red |
| 4 | 0 | 1 | 2 | Green |
| 5 | −1 | 0 | 1 | Green |
| 6 | 1 | 1 | 1 | Red |

Suppose we wish to use this data set to make a prediction for $Y$ when $X1 = X2 = X3 = 0$ using K-nearest neighbors. (1p)

(a) Compute the Euclidean distance between each observation and test point $X1 = X2 = X3 = 0$ .

(b) What is our prediction with K = 1? Why?

(c) What is our prediction with K = 3? Why?

(d) If the Bayes decision boundary in this problem is highly nonlinear, then would we expect the best value for K to be large or small? Why?

## 2 Linear Regression

**Exercise 11 —** Assume we have $n$ observations $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ and we consider a linear model $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$. We estimate parameters $\beta_0$ and $\beta_1$ by minimizing mean squared error:

$$MSE(\hat{\beta}_0, \hat{\beta}_1) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{\beta}_0 + \hat{\beta}_1 x))^2 \ .$$

Show that in such a case

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \ ,$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

where $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$ are sample means. Argue that the obtained line always passes through the point $(\bar{x}, \bar{y})$. (2p)

**Exercise 12 —** Derive the bias, variance and standard error for estimators $\hat{\beta}_0$ and $\hat{\beta}_1$. We assume that $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$ , $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ and all $\varepsilon_i$ for $i \in \{1, \ldots, n\}$ are independent. (2p)

**Exercise 13 —** Recall how to prove that the sum of two independent normally distributed random variables is normally distributed. (2p)

**Exercise 14 —** Explain why there is approximately a 95% chance that the interval

$$\hat{\beta}_1 \pm 2\sqrt{\mathbb{V}\mathrm{ar}\left(\hat{\beta}_1\right)}$$

contains the true value of $\beta_1$. (2p)

**Exercise 15 —** Recall that for $RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ and $TSS = \sum_{i=1}^{n}(y_i - \bar{y}_i)^2$ we define $R^2$ as

$$R^2 = 1 - \frac{RSS}{TSS} \ .$$

What's the interpretation for $R^2$? Show that if we consider a model $Y = \beta_0 + \beta_1 X + \varepsilon$ we have

$$R^2 = Corr(X, Y)^2 \ ,$$

where $Corr(X, Y)$ is correlation coefficient. (3p)

**Exercise 16 —** Recall what's t-statistic and how we can use it in the context of linear regression. What's p-value? (3p)

**Exercise 17 —** Show that for a linear regression model with $k+1$ parameters we can obtain estimations of

$$\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k)$$

as

$$\hat{\beta} = (XX^T)^{-1} X^T \vec{y} \ ,$$

where $X$ is data matrix and $\vec{y}$ is vector of responses (see e.g. here ). (3p)

# 3 Classification

**Exercise 18 —** Explain what are the elements of the boxplot. (1p)

**Exercise 19 —** Explain what is Naive Bayes classifier. Explain and prove the following formula:

$$p(C_k \mid x_1, \ldots, x_n) = \frac{1}{p(\mathbf{x})} p(C_k) \prod_{i=1}^{n} p(x_i \mid C_k)$$

where

$$p(\mathbf{x}) = \sum_k p(\mathbf{x} \mid C_k) p(C_k) \quad \text{and} \quad \mathbf{x} = (x_1, \ldots, x_n) \ . \ (1p)$$

**Exercise 20 —** (ISL) When the number of features $p$ is large, there tends to be a deterioration in the performance of k-nearest neighbors (KNN) and other local approaches that perform prediction using only observations that are near the test observation for which a prediction must be made. This phenomenon is known as the curse of dimensionality and it ties into the fact that non-parametric approaches often perform poorly when $p$ is large. We will now investigate this curse. (1p)

a) Suppose that we have a set of observations, each with measurements on $p = 1$ feature, $X$. We assume that $X$ is uniformly distributed on $[0, 1]$. Associated with each observation is a response value. Suppose that we wish to predict a test observation's response using only observations that are within 10% of the range of $X$ closest to that test observation. For instance, in order to predict the response for a test observation with $X = 0.6$, we will use observations in the range $[0.55, 0.65]$. On average, what fraction of the available observations will we use to make the prediction?

b) Now suppose that we have a set of observations, each with measurements on $p = 2$ features, $X_1$ and $X_2$. We assume that $(X_1, X_2)$ are uniformly distributed on $[0, 1] \times [0, 1]$. We wish to predict a test observation's response using only observations that are within 10% of the range of $X_1$ and within 10% of the range of $X_2$ closest to that test observation. For instance, in order to predict the response for a test observation with $X_1 = 0.6$ and $X_2 = 0.35$, we will use observations in the range $[0.55, 0.65]$ for $X_1$ and in the range $[0.3, 0.4]$ for $X_2$. On average, what fraction of the available observations will we use to make the prediction?

c) Now suppose that we have a set of observations on $p = 100$ features. Again the observations are uniformly distributed on each feature, and again each feature ranges in value from 0 to 1. We wish to predict a test observation's response using observations within the 10% of each feature's range that is closest to that test observation. What fraction of the available observations will we use to make the prediction?

d) Using your answers to parts (a)–(c), argue that a drawback of KNN when $p$ is large is that there are very few training observations "near" any given test observation.

e) Now suppose that we wish to make a prediction for a test observation by creating a $p$-dimensional hypercube centered around the test observation that contains, on average, 10% of the training observations. For $p = 1$, 2 and 100, what is the length of each side of the hypercube? Comment on your answer.

**Exercise 21** — Assume we have single predictor $X$ and binary response $Y$ and we would like to create a parametric model for $p(X) = Pr(Y = 1|X)$. (1p)

a) We might try using the linear regression model. Why it is not very good idea?

b) In the binary logistic regression algorithm we model the probability $p(X)$ with the logistic function

$$p(X) = \frac{e^{\beta_0+\beta_1 X}}{1 + e^{\beta_0+\beta_1 X}} \ .$$

Prove that above equation is equivalent to the following log-odds (logit) representation:

$$\ln\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X \ .$$

What's the connection between the logistic $\sigma(x) = \frac{e^x}{1+e^x}$ and logit $l(p) = \ln\left(\frac{p}{1-p}\right)$ function?

**Exercise 22** — (ISL) This problem has to do with odds. (1p)

a) On average, what fraction of people with an odds of 0.37 of defaulting on their credit card payment will in fact default?

b) Suppose that an individual has a 16% chance of defaulting on her credit card payment. What are the odds that she will default?

**Exercise 23** — (ISL) Suppose we collect data for a group of students in a statistics class with variables $X_1$="hours studied", $X_2$="average grade", and $Y$ = "receive 5.0". We fit a logistic regression and produce estimated coefficient, $\hat{\beta}_0 = -6$, $\hat{\beta}_1 = 0.05$, $\hat{\beta}_2 = 1$. (1p)

a) Estimate the probability that a student who studies for $40h$ and has an average grade 3.5 gets 5.0 in the class.

b) How many hours would the student in part a) need to study to have a 50% chance of getting 5.0 in the class?

**Exercise 24** — Explain how we may get the multinomial (multi-class) logistic model for $K$ classes by running $K-1$ independent binary logistic regression models. Hint: see here. (1p)

## 4 Maximum likelihood estimation, cross-entropy, tree models

**Exercise 25** — Recall what is a maximum likelihood estimator and what you can say about its consistency and efficiency. (1p)

**Exercise 26** — Assume that you have $n$ observations $x_1, \ldots, x_n$ from the normally distributed random variable $X \sim N(\mu, \sigma^2)$ with unknown parameters $\mu$ and $\sigma^2$. Derive maximum likelihood estimator for the parameter $\mu$. (1p)

**Exercise 27** — Recall what is entropy, cross entropy and Kullback–Leibler divergence. Explain how these three measures are connected to each other. (1p)

**Exercise 28** — During the lecture we have shown that for binary classification problems the log-likelihood function can be expressed in terms of cross-entropy. Show the similar result for multi-class classification problems. You may look at this hint. (1p)

**Exercise 29** — For decision trees we usually use entropy or Gini index as the loss function. Explain how the entropy and Gini index can be interpreted. See e.g. ESL book, page 310. (1p)

**Exercise 30** — (ESL, page 309) Suppose we use a decision tree for two-class problem with 400 observations in each class (denote this by (400, 400)) and suppose one split created nodes (300, 100) and (100, 300), while the other created nodes (200, 400) and (200, 0). Both splits produce a misclassification rate of 0.25, but the second split produces a pure node and is probably preferable. Show that both the Gini index and cross-entropy are lower for the second split. (1p)

**Exercise 31** — Suppose we try to use a decision tree to data with a categorical predictor having $q$ possible unordered values. What might be the problem? Hint: show there are $2^{q-1}-1$ possible partitions of the $q$ values into two groups. (1p)

**Exercise 32** — Provide a pseudo-code of Random Forest algorithm and its detailed explanation (for both classification and regression problem). (1p)

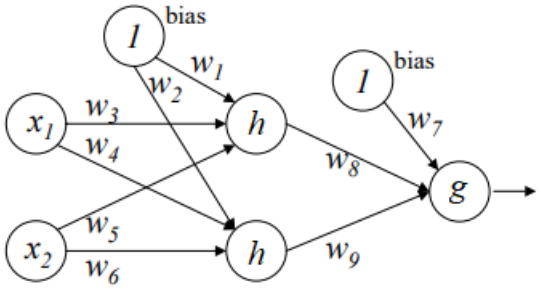
**Exercise 33** — (ISL) Suppose we produce ten bootstrapped samples from a data set containing red and green classes. We then apply a classification tree to each bootstrapped sample and, for a specific value of X, produce 10 estimates of $Pr(Class\ is\ Red|X)$:

$$0.1, 0.15, 0.2, 0.2, 0.55, 0.6, 0.6, 0.65, 0.7\ and\ 0.75.$$

There are two common ways to combine these results together into a single class prediction. One is the majority vote approach discussed earlier. The second approach is to classify based on the average probability. In this example, what is the final classification under each of these two approaches? (1p)

# 5 Neural Networks

**Exercise 34** — Suppose we solve a binary classification problem using a neural network with one hidden layer as shown in the figure below. The network models probability $P(y = 1|\mathbf{x})$, where $y \in \{0, 1\}$ and $\mathbf{x} = (x_1, x_2)$. At hidden units we use a linear activation function $h(z) = c \cdot z$ with constant $c$. At the output unit we use a sigmoid activation function $g(z) = \frac{1}{1+e^{-z}}$.




1. Express the output probability from the above neural network in terms of $x_i$, $w_i$ and $c$.
2. Express classification decision boundary as an equation in terms of $x_i$, $w_i$ and $c$.
   Is this decision boundary linear or non-linear in terms of input values $x_1$ and $x_2$?
3. Explain how you can use cross-entropy to evaluate the above neural network. (1p)

**Exercise 35** — Draw a neural net with no hidden layer which is equivalent to the neural net given in the previous exercise. Express weights $v_1, v_2, \ldots$ of this new neural net in terms of weights $w_i$ and $c$.

Can any multi-layered neural net with linear activation functions at hidden layers be represented as a neural net without any hidden layer? Justify your answer. (1p)

**Exercise 36** — Assume we transform some vector $\vec{z} = (z_1, \ldots, z_n)$ using softmax function and we get vector $\vec{p} = (p_1(\vec{z}), \ldots, p_n(\vec{z}))$ where

$$p_j(\vec{z}) = \frac{e^{z_j}}{\sum_{k=1}^{n} e^{z_k}}.$$

1. Describe the Jacobian matrix of the softmax function.

2. Show that $\frac{\partial p_j}{\partial z_k}$ is positive if $j = k$ and negative if $j \neq k$. What are the consequences? (1p)

**Exercise 37 —** Assume we transform a vector $\vec{z} = (z_1, \ldots, z_n)$ using softmax function and we get vector $\vec{p} = (p_1(\vec{z}), \ldots, p_n(\vec{z}))$. Assume also that we have some one-hot encoded vector $\vec{y}$ and we would like to minimize the cross-entropy loss function with respect to $\vec{z}$:

$$L(\vec{z}) = -\sum_{k=1}^{n} y_j \log p_j(\vec{z}) \ .$$

Find the formula for $\frac{\partial L}{\partial z_i}$. Recall how we can use this to iteratively minimize loss function. (1p)

**Exercise 38 —** Rectifier is an activation function defined as $f(x) = max(0, x)$. The unit in the neural network employing the rectifier is called a Rectified Linear Unit (ReLU).

1. What you can say about the derivative of $f(x)$?
2. A smooth approximation to the rectifier is softplus function defined as $s(x) = \ln(1 + e^x)$. Sketch a graph of $s(x)$ and find its derivative.
3. In Deep Learning book in Section 6.3.3 it is written that:

   > „The use of the softplus is generally discouraged. The softplus demonstrates that the performance of hidden unit types can be very counterintuitive—one might expect it to have an advantage over the rectifier due to being differentiable everywhere or due to saturating less completely, but empirically it does not."

   What does it mean that function is saturated? What problem saturation can cause for the learning process? How you could deal with the saturation of rectifier? See e.g. Leaky ReLU. (1p)

# 6 Convolutional neural networks

**Exercise 39 —** What are the parameters and hyperparameters of Conv, MaxPooling, Dense and Dropout layers. For Conv explain what's stride and padding. How to set padding to ensure that the input and output of Conv layer will have the same width and height for stride $S = 1$ and $S = 2$? (1p)

**Exercise 40 —** What's filter (kernel) in CNN and what determines its width, height and depth? Suppose an input to some Conv layer has size $16 \times 16 \times 20$, where the last number is depth.

1. Define some filter and find the number of connections from a single element of the feature map to the input. Explain what's locally-connected layer.
2. If all elements of the feature map share the same filter what is the total number of parameters to learn? Explain what is parameter sharing and when it might be useful. (1p)

**Exercise 41 —** Assume that Conv layer accepts an input of size $W_1 \times H_1 \times D_1$ and let the number of filters be $K$, filter width and hight be $F$, stride be $S$ and padding be $P$. (1p)

1. What's the shape of the output $W_2 \times H_2 \times D_2$ in terms of the input shape and hyperparameters? What are constraints for hyperparameters?
2. What's the number of parameters to be set per filter and in total if we use parameter sharing?
3. How we obtain $d$th depth slice of size $W2 \times H2$ in the output?

**Exercise 42 —** What's might be the role of a filter with width and hight equal to 1? (1p)

**Exercise 43 —** Explain the role of MaxPooling layer. Give a practical example. (1p)

**Exercise 44 —** Explain why feature scaling of the input features is important. (1p)

**Exercise 45 —** Explain what is a regularization technique. You can split these techniques into three general groups:

1. modifying training procedure,
2. modifying loss function,
3. generating „new" training data from data you have.

List regularization techniques for deep neural networks, explain how each technique works and to which group it belongs. (1p)

**Exercise 46 —** By referring to convolutional neural networks describe transfer learning and fine-tuning technique. Give a practical example. (1p)

**Exercise 47 —** When you try to use transfer learning and fine tuning you need to decide which part of the original model will be used and which part will be frozen. Describe the procedure in four cases when you have small/large new dataset and this set is similar/not similar to the original dataset. (1p)

**Exercise 48 —** Describe the main differences between VGG, ResNet and Inception models. Explain the ideas behind each model. You may read for example this post about the evolution of the Inception model. In particular explain what for we may need residual connections, what is "salient parts problem" and why it might be better to use two consecutive layers with 3x3 filters rather than one layer with 5x5 filter. (1p)

# 7 Unsupervised learning

**Exercise 49 —** Describe k-means clustering algorithm and explain why it will always stop. Explain also way we need to run the algorithm many times. (1p)

**Exercise 50 —** With the use k-means algorithm try to discover clusters for a dataset of your choice (e.g. you may use some dataset used at the laboratory). Use KMeans method from sklearn library (see lab9.ipynb). Plot the value of the total within cluster variation for different values of parameter $k$. How you can use this plot? Hint: look for the Elbow Method. (1p)

**Exercise 51 —** Explain how the hierarchical clustering works and how based on the dendrogram you can establish the appropriate number of clusters. Given points $p_1 = 1$; $p_2 = 3$; $p_3 = 8$; $p_4 = 10$; $p_5 = 16$ perform hierarchical clustering using single linkage and complete linkage. Show the resulting dendrograms with distances on the y-axis. (1p)

**Exercise 52 —** Which of the following methods will cluster the data in panel (a) of the figure below into the two clusters (red circle and blue horizontal line) shown in panel (b)? Every dot in the circle and the line is a data point. In all the options that involve hierarchical clustering, the algorithm is run until we obtain two clusters. (1p)


1. Hierarchical agglomerative clustering with Euclidean distance and complete linkage.
2. Hierarchical agglomerative clustering with Euclidean distance and single linkage.
3. Hierarchical agglomerative clustering with Euclidean distance and centroid linkage.
4. k-means clustering with k = 2.

**Exercise 53 —** (PCA) Given are the following values of two variables (X, Y) for five observations: (2, 3), (3, 4), (4, 5), (5, 6), (6, 7). (1p)

1. Calculate the mean of each variable.
2. Compute the covariance matrix.
3. Find the eigenvalues and eigenvectors of the covariance matrix.
4. Interpret the results, indicating which principal components should be chosen for further analysis and why. What if we move the point (6, 7) to (6,107) ?

**Exercise 54 —** Let's assume that we have a data matrix $X$ and the covariance matrix $C$ of this data matrix. Show that the eigenvectors of the matrix $C$ corresponding to different eigenvalues $\lambda_i \neq \lambda_j$ are orthogonal. (1p)

**Exercise 55 —** Which of the following are true about PCA? Assume that no two eigenvectors of the covariance matrix have the same eigenvalue. (1p)

1. Appending a 1 to the end of every sample point doesn't change the results of performing PCA (except that there's one extra useless component with eigenvalue zero).
2. If you use PCA to project d-dimensional points down to j principal coordinates, and then you run PCA again to project those j-dimensional coordinates down to k principal coordinates, with d > j > k, you always get the same result as if you had just used PCA to project the d-dimensional points directly down to k principle coordinates.
3. If you perform an arbitrary rigid rotation of the sample points as a group in feature space before performing PCA, the principal component directions do not change.
4. If you perform an arbitrary rigid rotation of the sample points as a group in feature space before performing PCA, the largest eigenvalue of the sample covariance matrix does not change.

⋮

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