#### POLITECNICO DI MILANO — COMO CAMPUS



# PATTERN ANALYSIS AND MACHINE INTELLIGENCE 2015-2016 prof. Matteo Matteucci

# Exams 2014-2015 Summary

## Project Repository

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## Contents

1	Sta	tistical learning (8 points)	<b>2</b>
	1.1	ex 2015-02-09	2
	1.2	ex 2015-02-23	2
	1.3	ex 2015-07-06	2
	1.4	ex 2015-09-14	3
	1.5	ex 2015-09-30	4
2	Line	ear regression (8 points)	4
	2.1	ex 2015-02-09	4
	2.2	ex 2015-02-23	5
	2.3	ex 2015-07-06	5
	2.4	ex 2015-09-14	5
	2.5	ex 2015-09-30	6
3	Cla	ssification (8 points)	6
	3.1	ex 2015-02-09	6
	3.2	ex 2015-02-23	6
	3.3	ex 2015-07-06	7
	3.4	ex 2015-09-14	7
	3.5	ex 2015-09-30	8
4	Clu	stering (8 points)	8
	4.1	ex 2015-02-09	8
	4.2	ex 2015-02-23	9
	4.3	ex 2015-07-06	9
	4.4	ex 2015-09-14	10
	4.5	ex 2015-09-30	10
5	Sun	nmary on topics	12
	5.1	Statistical learning	12
	5.2		12
	5.3	Classification	13
	5.4	Clustering	13

## 1 Statistical learning (8 points)

#### $1.1 \quad \text{ex } 2015-02-09$

Answer the following questions:

- 1. Describe what are the bias, variance, and irreducible error of a model, how are they related with its complexity, how they are related to the expected prediction error, and what is the meaning of bias-variance tradeoff?
- 2. Draw a plot of (1) bias, (2) variance, (3) training error, (4) test error, and (5) irreducible error curves as a function of increasing amount of flexibility in a statistical learning method. Explain the reason of their shapes and highlight the relationships among them.

#### 1.2 ex 2015-02-23

In statistical learning theory, Test and Training set Mean Squared Errors are related by the so called Bias-Variance trade-off:

1. Write and comment the formula representing the Bias-Variance trade off for the Expected Prediction Error in Regression

The previous formula does not hold for Classification, but a useful result exists for the Classification Error Rate as well

2. Write and comment what statistical learning theory states about the minimum achievable average test error rate.

Provided the previous result for Classification, answer the following questions

- 3. Describe in detail how the previous result for the optimal classifier is used to derive the Logistic Regression classifier; provide a detailed description of the underlining model for Logistic Regression and derive the shape of the decision boundary for Logistic Regression.
- 4. Describe in detail how the previous result for the optimal classifier is used to derive Linear Discriminant Analysis; provide a detailed description of the underlining model for Linear Discriminant Analysis and derive the shape of the decision boundary for Linear Discriminant Analysis.

#### $1.3 \quad \text{ex } 2015-07-06$

- (a) Both classification and regression problems can be solved by simple but restrictive methods as well as more complex but flexible ones. Explain which ones are better:
  - 1. when doing inference or prediction;

- 2. when the irreducible error is extremely high;
- 3. when the number of observations is very large and the number of predictors is small;
- 4. when the function we need to estimate is highly non-linear.
- (b) What are the Bayes classifier and the Bayes error rate? Define them and explain why the latter is defined as analogous to the irreducible error.

#### 1.4 ex 2015-09-14

In statistical learning theory, Test and Training set Mean Squared Errors are related by the so called Bias-Variance trade-off:

- (a) Write and comment the formula representing the Bias-Variance trade off for the Expected Prediction Error in Regression
- (b) The previous formula does not hold for Classification, but a useful result exists for the Classification Error Rate; write and comment what statistical learning theory states about the minimum achievable average test error rate.
- (c) Describe in detail how the previous result for the optimal classifier is used to derive Linear Discriminant Analysis (LDA) classifier providing a detailed description of the underlining model and the shape of its decision boundary (derive it from the model).
- (d) Train a LDA classifier using the data provided in the table and provide the classification error achieved by this classifier on the training data

X	Class
0	A
1	A
2	A
1	A
3	A
1	В
2	В
3	В
4	В
4	С
6	С
6	С
6	С

#### $1.5 \quad \text{ex } 2015 \text{-} 09 \text{-} 30$

Answer the following questions

- 1. Describe (1) what are the bias, variance, and irreducible error of a model, (2) how are they related with its complexity, (3) how they are related to the expected prediction error, and (4) what is the meaning of bias-variance tradeoff?
- 2. Draw a plot of (1) bias, (2) variance, (3) training error, (4) test error, and (5) irreducible error curves as a function of increasing amount of flexibility in a statistical learning method. Explain the reason of their shapes and highlight the relationships among them.

## 2 Linear regression (8 points)

#### $2.1 ext{ ex } 2015-02-09$

Given the variables  $x = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$  and  $y = \{3.3, 3.6, 5.2, 5.6, 7.4, 8.3, 8.7, 9.7, 11.2\}$ 

- 1. Manually compute the parameters  $\hat{\beta}_0$  and  $\hat{\beta}_1$  of a linear model  $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$  which fits the given data
- 2. What is the value of MSE calculated between the values of y and the ones returned by the  $\hat{y}$  function?
- 3. How can we compute if the trend identified by  $\hat{\beta}_1$  is significant or it is just due to spurious correlations?

To ease your computation, you can follow the following steps:

- calculate the mean  $\bar{x}$  of x
- calculate the mean  $\bar{y}$  of y
- $\bullet\,$  calculate  $x-\bar{x}$  (a vector where each value is  $x_i-\bar{x}$  )
- calculate  $y \bar{y}$  (as above)
- calculate  $\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i \bar{x})(y_i \bar{y})}{\sum_{i=1}^n (x_i \bar{x})^2}$
- calculate  $\hat{\beta}_o = \hat{y} \hat{\beta}_1 x$

#### $2.2 ext{ ex } 2015-02-23$

Provide detailed answers to the following

- 1. Let assume you have a dataset with n=1000 observations and you try to fit different models on the data:
  - A linear regression model, i.e.  $Y = \beta_0 + \beta_1 X + \epsilon$
  - The polynomial regression model  $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 X^4 + \epsilon$
  - A smoothing spline (i.e. an even more flexible model than the previous two)

For each of the three models, you calculate both training and test RSS. How would you expect the values of RSS to be (both in the training and in the test case), supposing that the true relationship between X and Y is (a) linear or (b) cubic?

2. What is the additive assumption in a linear regression model? Show how you would detect and quantify a possible interaction between the variables in a regression model and how you would model it from a statistical perspective. Finally explain, with an example, how your model would take this interaction into account (e.g. explain how, given a change in the input, the dependent variable and consequently the output change).

#### $2.3 \quad \text{ex } 2015-07-06$

Given the variables  $x_1 = \{14, 1, 13, 8, 11, 19, 0, 9\}$ ,  $x_2 = \{12, 13, 7, 10, 8, 11, 16, 10\}$ , and  $y = \{26, 7, 24, 15, 24, 38, 2, 13\}$ , manually calculate the parameters  $\hat{\beta}_0$  and  $\hat{\beta}_1$  of the two linear functions  $\hat{y} = \beta_0 + \beta_1 x_1$  and  $\hat{y} = \beta_0 + \beta_1 x_2$  which fit the given data. To ease your calculations, take the following steps:

- 1. calculate the mean  $\bar{x}$  of x and the mean  $\bar{y}$  of y
- 2. calculate  $x \bar{x}$  (a vector where each value is  $x_i \bar{x}$ ) and  $y \bar{y}$
- 3. calculate  $\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i \bar{x})(y_i \bar{y})}{\sum_{i=1}^n (x_i \bar{x})^2}$ , then  $\hat{\beta}_o = \hat{y} \hat{\beta}_1 x$

Measure the quality of your predictions in terms of MSE, compare the results of the two linear regressions, and justify them.

#### 2.4 ex 2015-09-14

- (a) What is the standard error and how is it used to calculate a confidence interval? For instance, what does it mean to have a 95% confidence interval on the parameter  $\beta_1$  of a linear regression?
- (b) Explain what the null hypothesis is in the context of linear regression and how it is verified.

#### $2.5 \quad \text{ex } 2015 - 09 - 30$

Given the following observations  $x = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$  and  $y = \{12, 11.2, 9.7, 8.7, 8.3, 7.4, 5.6, 5.2, 3.6, 3.3\}$ 

- 1. Manually compute the parameters  $\hat{\beta}_0$  and  $\hat{\beta}_1$  of a linear model  $\hat{y} = \beta_0 + \beta_1 x$  which fits the given data
- 2. What is the value of MSE calculated between the values of y and the ones returned by the  $\hat{y}$  function?
- 3. Is the trend identified by  $\hat{\beta}_1$  significant or it is just due to spurious correlations? You have to provide supporting computations and justifications for your answer.

## 3 Classification (8 points)

#### $3.1 \quad \text{ex } 2015-02-09$

Given the two sets of samples from classes RED =  $\{(1, 3), (2, 2), (3.5, 1), (5, 4), (1.5, 4), (4, 2)\}$  and GREEN =  $\{(2, 3), (3, 0.5), (4, 3), (3.5, 2), (1, 2), (2, 1)\}$ , and the three unclassified elements a = (4, 1), b = (2, 3.5), and c = (3, 4)

- 1. Use the KNN approach to classify the unknown items for k = 1, 3, 5. Apply the Euclidean distance as a metric (note that you can skip the actual distance calculations if you can tell the nearest neighbours at a glance).
- 2. Describe in details the Linear Discriminant Analysis and Logistic Regression techniques for classification and discuss how these techniques perform, in general, with respect to the KNN classifiers.

#### $3.2 ext{ ex } 2015-02-23$

Consider the following dataset with three classes and the Linear Discriminant Analysis model (LDA hereafter)

X1	X2	Class
1	1	A
2	2	A
2	3	Α
3	1	A
4	1	A
1	4	В
2	5	В
3	4	В
4	5	В
4	3	С
6	1	С
6	2	$\mathbf{C}$
6	3	С

- 1. Compute the parameters of a LDA classifier
- 2. Compute the discriminant functions for the LDA classifier
- 3. Compute the equations of the boundaries between the three classes according to the classifier
- 4. Draw the dataset and the boundaries between the classes according to the classifier
- 5. Compute the parameters in case of a Quadratic Discriminant Analysis model

#### $3.3 \quad \text{ex } 2015-07-06$

- (a) Given the subset of Iris dataset in figure, classify the three points identified with white triangles (at coordinates (5.85, 2.3), (4.7, 2.4), and (6.5, 2.5) respectively), using the KNN algorithm with k = 3, 5, 7. Note: if your point has the same amount of neighbors for each class, you can assign it the class of the closest one.
- (b) Explain what the curse of dimensionality is. How would you address this problem? {PIC1}

#### 3.4 ex 2015-09-14

- (a) What is the difference between Discriminative and Generative methods for classification? Provide one example for each category explaining why it can be considered as Discriminative/Generative.
- (b) Provide a detailed description of the Generative method you previously introduced, the underlining model, the training algorithm, and derive the shape of its decision boundary.

(c) Provide a detailed description of the Discriminative method you previously introduced, the underlining model, the training algorithm, and describe the shape of its decision boundary.

#### $3.5 \quad \text{ex } 2015 - 09 - 30$

- (a) Given the dataset in figure, classify the three points identified with white triangles (at coordinates (21, 5), (24, 20), and (26.5, 11.5) respectively), using the KNN algorithm with k = 2, 3, 5. Note: if your point has the same amount of neighbors for each class, you can assign it the class of the closest one.
- (b) A hospital collected data for a group of patients to study the relationship between Heart-attack Risk Index (HRI =  $X_1$ ), weekly hours of physical activity (PHY =  $X_2$ ), and the probability Y of having a heart attack. Roughly, for a heart attack probability to be low the HRI should be below 5, and the more hours one spends exercising the better it is.

After fitting a logistic regression, the following coefficients were estimated:  $\hat{\beta}_0 = -9.7$ ,  $\hat{\beta}_0 = 1.05$ , and  $\hat{\beta}_2 = -0.29$ .

- estimate the probability for a patient with HRI=5 and PHY=2 to have a heart attack;
- estimate how many hours of PHY a patient with HRI=7.5 should do to have that same probability.

{PIC1}

## 4 Clustering (8 points)

#### $4.1 \quad \text{ex } 2015-02-09$

Suppose you want to evaluate the results of some clustering algorithms using SSE and Accuracy.

- 1. Which of these measures is defined as internal, which is external, and what does this mean?
- 2. After running your function, you obtain the result SSE=21.5. How can you evaluate whether this is a good or bad result? What would you compare this result with?
- 3. One of the clustering algorithms allows you to choose the number of clusters in advance. You calculate SSE after different executions of this algorithm, using K=2, 3, ..., 10. SSE for K=10 provides the lowest value: what can you deduce from this?
- 4. Now suppose you have ground truth for your dataset. You run two different clustering algorithms on the same data and obtain the following results:

	SSE	Accuracy
Algorithm1	115.3	87%
Algorithm2	1285	95%

What is the meaning of these results? Which algorithm is better?

#### $4.2 ext{ ex } 2015-02-23$

Given the two datasets shown in figure (where blue diamonds are data points and red circles different centroids starting points), calculate and show the different steps of the K-Means algorithm for both the examples in the following way:

- At each step, specify the initial positions of the centroids
- Without actually calculating it (unless it is needed to verify distances you cannot tell apart at a glance), for each step specify which centroid the various dataset points belong to
- After you have assigned data points to the different centroids, calculate their new positions and proceed to next step

Tell how many iterations the algorithm needs to converge, compare its behavior in the two cases and write a comment about it: is the final situation the one you might expect/desire? If not, explain why.

{PIC1 } {PIC2 }

#### $4.3 \quad \text{ex } 2015-07-06$

Given the following algorithms:

- 1. K-means
- 2. Hierarchical
- 3. Mixture of Gaussians
- 4. DBSCAN
- 5. K-medoids
- 6. Fuzzy C-means
- 7. Jarvis-Patrick

complete the following sentences matching them with one (or more!) of the algorithms, answering the questions in parentheses and providing detailed explanations to motivate your choices. (NOTE: although sentences refer to a single algorithm, there may be more than one valid choice. In these cases, provide and motivate all of them).

- (a) This algorithm relies on a self-scaling neighborhood (what does this mean? How can this be accomplished?)
- (b) This algorithm builds new clusters by merging or splitting existing ones (describe the differences between the two approaches and provide the computational complexity of this approach)
- (c) This algorithm provides a soft classification (what does this mean?)
- (d) This algorithm can provide good results even if noise is present in the dataset (is it also able to detect which points are noise?)

#### $4.4 \quad \text{ex } 2015-09-14$

Given the dataset shown in figure, execute the steps of a hierarchical (agglomerative) algorithm using the single linkage technique, showing the new links you create at each step of the algorithm (labeling them with a number) and stopping when you obtain two clusters.

{PIC1}

Then, calculate and show the different steps of a K-Means algorithm run on the same dataset with the starting centroid positions  $C_1 = (1, 1)$  and  $C_2 = (5, 3.5)$ , in the following way:

- at each step, specify the initial positions of the centroids
- without actually calculating it (unless it is needed to verify distances you cannot tell apart at a glance), for each step specify which centroid the various dataset points belong to
- after you have assigned points to the different centroids, calculate their new positions and proceed to next step

Are there any differences between the two algorithms? If so, how could you explain their different behavior?

#### $4.5 \quad \text{ex } 2015 - 09 - 30$

- a) Hierarchical clustering is not a single algorithm but rather a family of different clustering algorithms. Explain (1) how this family is composed, (2) how these algorithms work, and (3) what metrics exist to measure the distance between clusters.
- b) Invent a clustering problem (for example, clustering of students according to their grades, news articles according to the words they contain, or images according to their visual descriptors). Describe the problem in detail, specifying e.g. what kind of application you are doing clustering for, the dataset size and dimensionality, what problems

you might have while clustering, and so on. Then choose any two of the algorithms we have studied, and try to sell us one of the two, describing the characteristics of both and explaining why using one is better than the other (for instance, in terms of speed, quality of results, etc.).

## 5 Summary on topics

### 5.1 Statistical learning

- Bias, Variance, irreducible error, expected prediction error
- Flexibility, complexity
- Bias-variance trade-off (the relations among MSE (test & trainig), Expected prediction error) (regr)
- minimum avg. test error rate (class)
- Plots
- LDA, decision boundaries
- $\bullet$  inference vs prediction, # of observations vs # of predictors
- non-linear functions
- Bayes classifier and bayes error rate
- Example of a solution for LDA

## 5.2 Linear regression

- MSE
- Manual computations for linear model  $(\bar{},\bar{},\beta,$  etc)
- training & test RSS
- convenience intervals
- null hypothesis

#### 5.3 Classification

- Discriminative methods
- Generative methods
- KNN
- Euclidean distance
- LDA, logistic regression
- Manual computations (discriminants, boundary equations, drawings)

- QDA (parameters)
- the curse of dimensionality
- ullet estimation of probabilities

## 5.4 Clustering

- SSE, accuracy (internal/external),
- K-Means
- Hierarchical (agglomerative)
- Mixture of Gaussians
- DBSCAN
- K-medoids
- Fuzzy C-means
- Jarvis-Patrick
- linkage techniques
- metrics for the distance between clusters