Faculty: BioScienze e Tecnologie Agro-Alimentari e Ambientali MASTER DEGREE IN FOOD SCIENCE AND TECHNOLOGY I YEAR

> Course: EXPERIMENTAL DESIGN AND CHEMOMETRICS IN FOOD (5 credits – 40 hours)

> > Teacher: Marcello Mascini (mmascini@unite.it)

The Teacher is available to answer questions at the end of the lesson, or on request by mail

### The course is split in 4 units

#### **UNIT 1: Univariate analysis**

Data, information, models, data types, analytical representation of data

Calibration and regression, Introduction to Statistics

Media & Variance

The Normal distribution, theory of measurement errors, the central limit theorem and the theorem of Gauss

Maximum likelihood, method of least squares, Generalization of the method of least squares

Polynomial regression, non-linear regression, the  $\chi 2$  method, Validation of the model

#### **UNIT 2: Multivariate analysis**

Correlation

Multiple linear regression

Principal component analysis (PCA)

Principal component regression (PCR) and Partial least squares regression - (PLS)

### **UNIT 3: Design of Experiments**

Basic design of experiments and analysis of the resulting data

Analysis of variance, blocking and nuisance variables

Factorial designs

Fractional factorial designs

Overview of other types of experimental designs (Plackett– Burman designs, D-optimal designs, Supersaturated designs, Asymmetrical designs)

Response surface methods and designs

Applications of designed experiments from various fields of food science

### **UNIT 4: Elements of Pattern recognition**

cluster analysis

Potential Method normalization

The space representation (PCA) Examples of PCA

Discriminant analysis (DA) PLS-DA

Examples of PLS-DA

### GOALS

The course aims to increase the knowledge of pre and post processing experimental data with multivariate statistical techniques applied to the analysis of foods.

This course will emphasize computer approaches to multivariate statistical analysis. We will discuss how to design, conduct, and analyze experiments in food sciences Various designs will be discussed and their respective differences, advantages, and disadvantages will be noted. We will examine techniques for data reduction (principal components, factor analysis, and cluster analysis) and for discrimination and classification (cluster analysis, discriminant analysis).

In the first part the course will examine how to design experiments, carry them out, and analyze the data they yield. In the second part it will be compared univariate and multivariate statistical techniques (PCA and PLS). Case studies related to research projects will be taken as practical examples and they will be carried out by using academic free software

# **Course Management**

The teacher manage the course through the web platform http://elearning.unite.it/ . After sign up Students can download all electronics materials of the course. Agenda of the practical use of academic-free programs and of multi-choice tests and reports will be planned at the beginning of the course and uploaded on the web platform. Students can download all electronic supplies (pdf files, software, excel files ect) before classes.

# **EVALUATION**

The tests are held during the semester at the end of the units and are a series of 30 multiple choice questions, related to the specific arguments of the units. The correct answer to each question is 1 point. The wrong answer or no date is 0 points.

In case of you can not do the tests during the course, you can do a final multiple choice quiz of 90 questions at the end of the semester.

The score obtained in the tests will be kept up for one year.

An oral presentation is requested in the form of report which will highlight potential, limitations and possible developments of the work performed. Non-attending students are asked to submit a report online evaluated by the teacher and the attending students.

During the lessons, students can check their learning, through the online test simulator, similar to the examination tests .

The Teacher is available to answer questions at the end of the lesson, or on request by mail (mmascini@unite.it)

# BOOKS

Because of the practical application nature of this course there is no mandatory textbook. Instead, you should purchase a text that suits your needs (e.g., practical application versus mathematical statistics). Recommended texts are:

Johnson, Dallas E. (1998). Applied multivariate methods for data analysis. Pacific Grove, CA: Duxbury Press. Good balance between theory and practice.

Tabachnick, B. G. & Fideii, L.S. (2000). Using Multivariate Statistics, 4th Ed. New York: Allyn & Bacon. A traditional and popular text that focuses on practical applications.

Oehlert, Gary W. (2010). A first course in design and analysis of experiments. (<u>http://users.stat.umn.edu/~gary/book/fcdae.pdf</u>)

Barrentine Larry B. (1999) An Introduction to Design of Experiments: A Simplified Approach Amer Society for Quality

# ON THE WEB

http://elearning.unite.it/

YOU CAN FIND ALL INFORMATION & MATERIALS JUST SIGN IN!!!!