<div align="center">Calculation methods in chemistry (INF/01, informatics)</div>

Academic year: 2017-2018
Faculty: Dep. of Chemistry
Study courses: degree in chemistry L-27
Study plans/Curricula:
Type:
Total Credits: 3
Didactic Methods: lessons, direct applications on computers
Didactic Period: second semester
Exam type: the sessions of work of students are saved, if sufficient no exam is needed, otherwise an oral exam is required
Professor in charge: Fulvio Ciriaco

Training objectives: capability to understand and apply the main statistical methods; capability to import data from several sources: files, dbs, network, instruments and manage them to obtain presentable data; capability to solve sample problems in many-variable linear and nonlinear regression; numerical methods for ordinary differential equations; spectra and other scientific data manipulation, scientific plotting; basic high level programming.

Prerequisites: first course in analysis .

Didactic Methods: lessons and contextual application on pcs, based on R, IPython and their scientific libraries.

Course programme
PROGRAMME:
Lectures (12h):
1. Introduction to Python and to general programming logics.
2. Presentation methods for mono and multivariate data.
3. The fourier transform and its properties.
4. Applications of the fourier transform
5. libreries for solving ordinary differential equations.
6. elements of statistics and bayesian inference
7. libraries for variable reduction and data classification
Numerical exercises (27h):
1. fourier transform and IR apodization filters application
2. sample kinetics of chemical reactions
3. monodimensional Schrödinger equation: particle in boxed potential, nuclear motion for biatomic molecules
4. exercises of statistics on the blackboard
5. sample application of bayesian inference on a gayger detector matrix with a model parameterized response

6. data classification problems

Reference Texts

Notes from the teacher and saved sample sessions.