

Effective approach to spectroscopy and spectral analysis techniques using Matlab

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Abstract

With the development of electronic information, computer and network, modern education technology has entered new era, which would give a great impact on teaching process. Spectroscopy and spectral analysis is an elective course for Optoelectronic Information Science and engineering. The teaching objective of this course is to master the basic concepts and principles of spectroscopy, spectral analysis and testing of basic technical means. Then, let the students learn the principle and technology of the spectrum to study the structure and state of the material and the developing process of the technology. MATLAB (matrix laboratory) is a multi-paradigm numerical computing environment and fourth-generation programming language. A proprietary programming language developed by MathWorks, MATLAB allows matrix manipulations, plotting of functions and data, Based on the teaching practice, this paper summarizes the new situation of applying Matlab to the teaching of spectroscopy. This would be suitable for most of the current school multimedia assisted teaching.

Key words: Teaching, spectral analysis, Matlab

1. Introduction

Spectroscopy is the study of the interaction between matter and electromagnetic radiation. Historically, spectroscopy originated through the study of visible light dispersed according to its wavelength, by a prism. Later the concept was expanded greatly to include any interaction with radiative energy as a function of its wavelength or frequency. Spectroscopic data is often represented by an emission spectrum, a plot of the response of interest as a function of wavelength or frequency. Spectral analysis measures and analyzes the properties of matter based on the material's interactions with electromagnetic energy. In chemistry and physics, this process is known as spectroscopy. Spectroscopy is of particular use in astronomy, where it is used to determine the chemical composition of celestial objects. one of the most widely used methods for data analysis in geophysics, oceanography, atmospheric science, astronomy, engineering. Based on the analysis of Matlab, the teaching of spectroscopy is the important link of the theoretical relationship and the reform of the teaching curriculum. On the one hand, the teaching

model is beneficial to the students' understanding and deepening of the theory, and can find the problem in time and solve the problem. On the other hand, the teaching mode is beneficial to the practical ability of the students, which is beneficial to the cultivation of students' innovation and logical analysis ability. The experimental teaching mode effectively adapted to the principle of automatic control course of comprehensive and practical requirements, at the same time, the analysis of the typical features of the spectroscopy study has a very large role in promoting.

2. Course of spectroscopy and spectral analysis

Spectroscopy and spectral analysis is an elective course for Optoelectronic Information Science and engineering^[1,2]. The teaching objective of this course is to master the basic concepts and principles of spectroscopy, spectral analysis and testing of basic technical means. Then, let the students learn the principle and technology of the spectrum to study the structure and state of the material and the developing process of the technology. Through this course, students could consolidate the foundation in the theory and application of optical technology^[3], enhance the detection of light radiation and the processing ability of the radiation understanding, master an analysis method of important scientific research tools and an important qualitative and quantitative. The pre-required courses are Advanced mathematics, college physics, applied optics, physical optics, linear algebra, probability theory and mathematical statistics.

The teaching aim of spectroscopy and spectral analysis is as follow.

- 1) To master the knowledge of mathematics and natural sciences, and be able to model and solve the problems in the field of photoelectric information.
- 2) The basic knowledge of optics can be used to analyze optical design, simulation, analysis and experiment in the field of photoelectric information.
- 3) The basic knowledge of electronic technology can be used to analyze circuit design, analysis and experiment in the field of photoelectric information.
- 4) The basic knowledge of machinery can be used to analyze mechanical design and analysis in the field of photoelectric information.
- 5) The basic knowledge of computers can be used to analyze software and hardware analysis and design in the field of photoelectric information.
- 6) 6. Understanding of the concept of photoelectric information system and its embodiment in the field of engineering, to complex engineering problems in the field of photoelectric information solutions is analyzed, and trying to improve;

- 7) All landowners to master professional knowledge, can choose appropriate mathematical model, is used to describe the photoelectric information system or process, the model of reasoning, analysis, validation, and correct solutions are given.
- 8) Master the basic principles of mathematics, science and engineering science, and can be used to identify, express, analyze and solve complex engineering problems to obtain valid conclusions.

3. Software of Matlab

MATLAB (matrix laboratory) is a multi-paradigm numerical computing environment and fourth-generation programming language. A proprietary programming language developed by MathWorks, MATLAB allows matrix manipulations, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs written in other languages, including C, C++, C#, Java, Fortran and Python. Although MATLAB is intended primarily for numerical computing, an optional toolbox uses the MuPAD symbolic engine, allowing access to symbolic computing abilities. An additional package, Simulink, adds graphical multi-domain simulation and model-based design for dynamic and embedded systems. MATLAB had around one million users across industry and academia. MATLAB users come from various backgrounds of engineering, science, and economics^[4].

Matlab was originally designed for working efficiently with large matrices of numbers, and was adopted therefore by scientists and engineers. (A matrix is implemented as a two-dimensional array of numbers, but operations on matrices such as multiplication follow specific mathematical rules.) In this course, we'll use Matlab not so much for its abilities with matrices, but for the ease with which it handles and displays visual data (images and graphs). Of course, an image can also be seen as a matrix or set of matrices^[5].

Matlab provides various toolbox for users, which make spectral analysis very convenient. Among those Matlab toolboxes, the Signal Processing Toolbox and Statistics and Machine Learning Toolbox are the most useful ones for spectral analysis.

Signal Processing Toolbox provides functions and apps to generate, measure, transform, filter, and visualize signals. The toolbox includes algorithms for resampling, smoothing, and synchronizing signals, designing and analyzing filters, estimating power spectra, and measuring peaks, bandwidth, and distortion. The toolbox also includes parametric and linear predictive modeling algorithms. You can use Signal Processing Toolbox to analyze and compare signals in time, frequency, and time-frequency domains, identify patterns and trends, extract features, and develop and validate custom algorithms to gain insight into your data.

Statistics and Machine Learning Toolbox provides functions and apps to describe, analyze, and model data. You can use descriptive statistics and plots for exploratory data analysis, fit probability distributions to data, generate random numbers for Monte Carlo simulations, and perform hypothesis tests. Regression and classification algorithms let you draw inferences from data and build predictive models. Figure 1 shows the main algorithm provided in this toolbox.

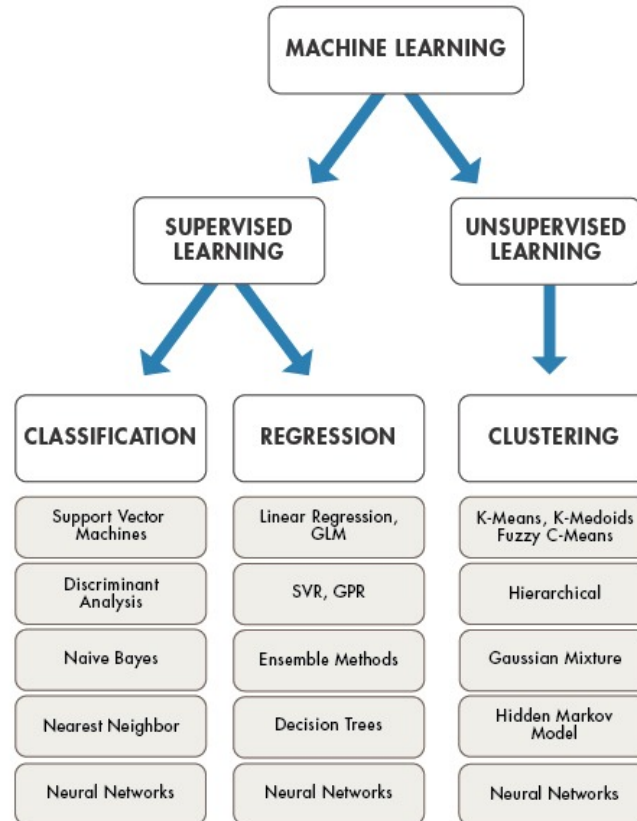


Fig. 1 Statistics and Machine Learning Toolbox

For multidimensional data analysis, Statistics and Machine Learning Toolbox provides feature selection, stepwise regression, principal component analysis (PCA), regularization, and other dimensionality reduction methods that let you identify variables or features that impact your model.

4. Application of Matlab in spectral analysis teaching

To bring students without programming experience up to speed, we start with a two-week introduction to visual programming, using the multi-media environment from the Bistu Media Lab. Following that simplified lesson, students would begin to program for spectral analysis. After introducing the MATLAB environment, including matrices and operators, we teach procedural

programming, beginning with a lesson on functions. Students learn the importance of well-defined interfaces and how to use functions to create reusable software components. In the following weeks, we cover selection (also known as branching) using if and switch statements, loops, data types, and file input/output. We then take a more in-depth look at functions, introducing functions with a variable number of arguments and recursion. The course then covers linear algebra, including the MATLAB regression operator and inconsistent, overdetermined, and underdetermined equations. The final lessons cover most functions of Signal Processing Toolbox and Statistics and Machine Learning Toolbox. concludes with a project in which the students apply the concepts they have learned throughout the semester. Past projects have included processing and analyzing spectral data in MATLAB and calculating the content of mixture.

5 Conclusion

Spectroscopy and spectral analysis is an elective course for Optoelectronic Information Science and engineering. The course is also popular among science majors and other non-engineering students, and about 60 students enrolled each semester take the course as an elective. In addition to its growing popularity among students, the course has garnered the approval of engineering faculty across departments. Because students now learn MATLAB in their in our course, professors in upper-level courses no longer have to spend valuable class time teaching MATLAB basics. Besides, students also enjoy the course and as a result, work harder and learn more.

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