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Volume 5   Issue 2   *November 2004*

Physical Sciences Educational Reviews

The journal of the Physical Sciences Centre   Number 9

Reviewed in this issue:

2 software packages
1 web site
22 books

Intelligent Data Analysis in Science

Subject area
Analytical Chemistry, Computer Science.

Description
This book is a graduate text in the interdisciplinary area between computer science and analytical chemistry.

Authors
H Cartwright (editor).

Publishers/Suppliers
Oxford University Press (http://www.oup.co.uk).

Date/Edition
2000/1st Edition.

ISBN
0-19-850233-8.

Level
Undergraduate.

Price
£47.50.

"Intelligent Data Analysis in Science" is intended for senior undergraduate students and graduates 'as they progress... to leadership in research'. The book gives an overview of the area, describing what the various artificial intelligence (AI) methods can do and how they can be used. In keeping with the stated aims, there is insufficient detail to build or run an AI system, as a research team leader would probably not be involved in the hands-on day-to-day operation of the group.

Summary Review	
range: * poor to ***** good	
Academic content	*****
Usefulness to student	****
Usefulness to teacher	*****
Meets objectives	*****
Accuracy	*****

The book reviews the use of AI in analytical chemistry and related fields. Topics include expert systems (ESs), simple genetic algorithms (sGA), structured genetic algorithms (stGA), fuzzy logic, artificial neural networks (ANNs), and genetic programming (GP). These are intended to analyse data with minimal or no human supervision. In a typical analysis such as the spectrometric measurement of some analyte, a student or researcher would be expected to calibrate the instrument or method using known standards (a *learning set*) and then to convert measurements of one or more unknown samples to useful information. Often we would want to know properties or quantities such as the amount of substance, but increasingly we want a qualitative judgment, for example, if a sample meets specifications or is safe to eat. AI allows automation of the analysis and critical evaluation of data. Many expert systems require human intervention for the *learning* process, through the construction of rules or criteria, which summarise the *known* facts. On the other hand, artificial neural networks can use unsupervised learning to extract features or characteristics from the *learning set* before applying that information to the evaluation of data. The scope, advantages and limitations of the different methods are explained.

In some areas, the practice of using AI has departed from the original theoretical concepts in computer science. For example, Chapter 5 explains how and why binary numbers were used by pioneers of genetic algorithms, followed by a description of the disadvantages of binary data for real-world problems and the use of alternative representative schemes. However, such in-depth coverage of subtleties has not been given for each of the AI methods.

"Intelligent Data Analysis in Science" is not intended to be a 'how-do-I-do-this?' textbook. There are no revision questions or problem sets. The book is a 'what-can-this-technique-do' reference text. Each chapter has an extensive bibliography, totalling 23 pages of references or more than 10% of the book.

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November 2004

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