Preface

The use of Artificial Intelligence within science is growing at a remarkable rate. In the early 1990s, little was known about how Artificial Intelligence could be applied in a practical way to the physical and life sciences; at that stage, few experimental scientists showed any interest in the area. Now, hundreds of research papers are published each year and the numbers are rising rapidly. The change has been dramatic, and yet, despite the growth, the field is still very young.

The upsurge of interest owes much to an increasing understanding of the scientific potential of Artificial Intelligence. This book explains in a lucid and straightforward way how these methods are used by scientists and what we can accomplish with them. Recognizing that not all experimental scientists are computer experts, the approach adopted here assumes no prior knowledge of Artificial Intelligence and no unusual skills in computer science or programming; it does however presume some scientific background. Each chapter is designed to take the reader quickly to the point at which meaningful scientific applications can be investigated.

Computer scientists may use this book to gain a clearer picture of how experimental scientists use Artificial Intelligence tools. Chemists, biochemists, physicists and others in the experimental sciences who have data to analyse or simulations to run will find tools within these pages that may speed up their work or make it more effective. For both groups, the aim of this book is to encourage a broader application of these methods.

Many people have contributed to the production of this book. The final chapter was written by Nawwaf Kharma, following several months on sabbatical at Oxford University; his perceptive and challenging chapter gives a glimpse of the future of AI in science. EJS, a software tool for the construction of simulations in Java, has been used to perform a number of calculations for this book; a complete version of EJS is included on the CD that accompanies it with the permission of Francisco Esquembre, to whom I am most grateful. Most of the figures in this text have been prepared by John Freeman, adding both clarity and humour to it. The editorial staff at CRC Press, particularly Lance Wobus and Pat Roberson, have been a regular source of encouragement and expert advice. Numerous members of my research group, past and present, have contributed to the ideas that are crystallized here, notably “the two Alexes”, whose comments about the interface between Artificial Intelligence and science are often thought-provoking. Finally my wife, Susie, tolerating my long and unsociable working hours, and my daughter Jenny, a distant but engaging email voice, have provided less tangible but invaluable contributions. I am grateful to them all.

Errors are almost unavoidable in a text of this sort and I shall be grateful to be notified of any that may be spotted by readers.

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