Deep Learning in Science

This is the first rigorous, self-contained treatment of the theory of deep learning. Starting with the foundations of the theory and building it up, this is essential reading for any scientists, instructors, and students interested in artificial intelligence and deep learning. It provides guidance on how to think about scientific questions, and leads readers through the history of the field and its fundamental connections to neuroscience. The author discusses many applications to beautiful problems in the natural sciences, in physics, chemistry, and biomedicine. Examples include the search for exotic particles and dark matter in experimental physics, the prediction of molecular properties and reaction outcomes in chemistry, and the prediction of protein structures and the diagnostic analysis of biomedical images in the natural sciences. The text is accompanied by a full set of exercises at different difficulty levels and encourages out-of-the-box thinking.

Pierre Baldi is Distinguished Professor of Computer Science at University of California, Irvine. His main research interest is understanding intelligence in brains and machines. He has made seminal contributions to the theory of deep learning and its applications to the natural sciences, and has written four other books.
Deep Learning in Science

PIERRE BALDI
University of California, Irvine
To Cristina, Julia Melody, and Marco Jazz
Contents

Preface  xi

1  Introduction  1
   1.1 Carbon-Based and Silicon-Based Computing  1
   1.2 Early Beginnings Until the Late 1940s  4
   1.3 From 1950 to 1980  10
   1.4 From 1980 to Today  12
   1.5 Roadmap  14
   1.6 Exercises  15

2  Basic Concepts  16
   2.1 Synapses  16
   2.2 Units or Neurons  17
   2.3 Activations  17
   2.4 Transfer Functions  18
   2.5 Discrete versus Continuous Time  22
   2.6 Networks and Architectures  23
   2.7 Functional and Cardinal Capacity of Architectures  26
   2.8 The Bayesian Statistical Framework  28
   2.9 Information Theory  31
   2.10 Data and Learning Settings  33
   2.11 Learning Rules  35
   2.12 Computational Complexity Theory  36
   2.13 Exercises  37

3  Shallow Networks and Shallow Learning  41
   3.1 Supervised Shallow Networks and their Design  41
   3.2 Capacity of Shallow Networks  46
   3.3 Shallow Learning  52
   3.4 Extensions of Shallow Learning  56
   3.5 Exercises  58
## Contents

4 Two-Layer Networks and Universal Approximation 63
  4.1 Functional Capacity 63
  4.2 Universal Approximation Properties 65
  4.3 The Capacity of $A(n, m, 1)$ Architectures 68
  4.4 Exercises 69

5 Autoencoders 71
  5.1 A General Autoencoder Framework 72
  5.2 General Autoencoder Properties 73
  5.3 Linear Autoencoders 75
  5.4 Non-Linear Autoencoders: Unrestricted Boolean Case 84
  5.5 Other Autoencoders and Autoencoder Properties 90
  5.6 Exercises 96

6 Deep Networks and Backpropagation 99
  6.1 Why Deep? 99
  6.2 Functional Capacity: Deep Linear Case 101
  6.3 Functional Capacity: Deep Unrestricted Boolean Case 102
  6.4 Cardinal Capacity: Deep Feedforward Architectures 103
  6.5 Other Notions of Capacity 104
  6.6 Learning by Backpropagation 105
  6.7 The Optimality of Backpropagation 109
  6.8 Architecture Design 111
  6.9 Practical Training Issues 114
  6.10 The Bias–Variance Decomposition 118
  6.11 Dropout 119
  6.12 Model Compression/Distillation and Dark Knowledge 124
  6.13 Multiplicative Interactions: Gating and Attention 125
  6.14 Unsupervised Learning and Generative Models 127
  6.15 Exercises 131

7 The Local Learning Principle 137
  7.1 Virtualization and Learning in the Machine 137
  7.2 The Neuronal View 138
  7.3 The Synaptic View: the Local Learning Principle 139
  7.4 Stratification of Learning Rules 141
  7.5 Deep Local Learning and its Fundamental Limitations 142
  7.6 Local Deep Learning: the Deep Learning Channel 144
  7.7 Local Deep Learning and Deep Targets Equivalence 147
  7.8 Exercises 149

8 The Deep Learning Channel 151
  8.1 Random Backpropagation (RBP) and its Variations 152
  8.2 Simulations of Random Backpropagation 154
## Contents

8.3 Understanding Random Backpropagation 155
8.4 Mathematical Analysis of Random Backpropagation 157
8.5 Further Remarks About Learning Channels 162
8.6 Circular Autoencoders 164
8.7 Recirculation: Locality in Both Space and Time 165
8.8 Simulations of Recirculation 167
8.9 Recirculation is Random Backpropagation 168
8.10 Mathematical Analysis of Recirculation 170
8.11 Exercises 173

9 Recurrent Networks 177
9.1 Recurrent Networks 177
9.2 Cardinal Capacity of Recurrent Networks 178
9.3 Symmetric Connections: The Hopfield Model 179
9.4 Symmetric Connections: Boltzmann Machines 182
9.5 Exercises 185

10 Recursive Networks 189
10.1 Variable-Size Structured Data 189
10.2 Recursive Networks and Design 190
10.3 Relationships between Inner and Outer Approaches 199
10.4 Exercises 201

11 Applications in Physics 204
11.1 Deep Learning in the Physical Sciences 204
11.2 Antimatter Physics 208
11.3 High Energy Collider Physics 214
11.4 Neutrino Physics 224
11.5 Dark Matter Physics 228
11.6 Cosmology and Astrophysics 230
11.7 Climate Physics 233
11.8 Incorporating Physics Knowledge and Constraints 235
11.9 Conclusion: Theoretical Physics 237

12 Applications in Chemistry 239
12.1 Chemical Data and Chemical Space 240
12.2 Prediction of Small Molecule Properties 242
12.3 Prediction of Chemical Reactions 245

13 Applications in Biology and Medicine 257
13.1 Biomedical Data 257
13.2 Life in a Nutshell 258
13.3 Deep Learning in Proteomics 261
13.4 Deep Learning in Genomics and Transcriptomics 268
Preface

By and large, this book grew out of research conducted in my group as well as classes and lectures given at the University of California, Irvine (UCI) and elsewhere over the years. It can be used as a textbook for an undergraduate or graduate course in machine learning, or as an introduction to the topic for scientists from other fields. Basic prerequisites for understanding the material include college-level algebra, calculus, and probability. Familiarity with information theory, statistics, coding theory, and computational complexity at an elementary level are also helpful. I have striven to focus primarily on fundamental principles and provide a treatment that is both self-contained and rigorous, sometimes referring to the literature for well-known technical results, or to the exercises, which are an integral part of the book.

In writing this book, one of my goals has been to provide a rigorous treatment from first principles, as much as possible, in a still rapidly evolving field. This is one of the meanings of “in science” in the title. In this regard, the flow of the book is dictated primarily by complexity issues, going from shallow networks in their different forms, to deep feedforward networks, to recurrent and recursive networks. Two-layer networks, of which autoencoders are the prototypical example, provide the hinge between shallow and deep learning. For each kind of network, it is useful to consider special “hardware” cases, such as networks of linear units. Contrary to widespread belief, the linear case is often interesting and far from trivial. But this is not the only case where using a particular hardware model is helpful. Another example is the use of unrestricted Boolean units, another model that may seem trivial at first sight, but which leads to useful insights for both autoencoders and deep architectures. Yet another important example is provided by networks of linear or polynomial threshold gates.

A second characteristic of this book is its connection to biology. Neural networks, deep learning, and the entire field of AI are deeply rooted in biology, in trying to understand how the brain works and the space of possible strategies to replicate and surpass its capabilities. This is evident in Turing’s foundational work on Turing machines, guided by the fundamental intuition of a brain capable of having only a finite number of states [736] and in the vocabulary of computer science, which is full of words clearly rooted in biology such as AI, machine learning, memory, computer vision, computer virus, genetic algorithms, and so forth. It is regrettable to see young students and practitioners of machine learning misled to believe that artificial neural networks have little to do with biology, or that machine learning is the set of techniques used to maximize engineering or business goals, such as advertising revenues for search engines. In addition, not only computers and neural networks are inspired by biology, but they are of course also being
Preface

successfully used to analyze biological data, for instance high-throughput omic data, and through one of these surprising self-recursions only mankind seems to have produced, the results of these bioinformatics and systems biology analyses are progressively informing our understanding of the brain, helping to reveal for instance key gene expression and protein mechanisms involved in synaptic formation and biological memory.

A third characteristic of this book is precisely in the applications. The second meaning of “in science” in the title is “for science”. I have focused on applications of deep learning to the natural sciences – primarily physics, chemistry, and biology for the past three decades or so. These applications are expanding rapidly today, but were almost nonexistent in the 1980s. Plenty of textbooks and other material can be found dealing with applications of neural networks to problems in engineering and other related areas.

A fourth characteristic is the emphasis placed on storage, specifically on the neural-style of information storage, in fundamental contrast to the Turing-style of information storage, ironically introduced by Turing precisely while thinking about the brain. This theme goes together with the importance of recognizing the virtualization process hidden behind most of today’s neural network applications. In most applications of neural networks today, there are no neurons and no synapses, only their digital mirage. This comes at a price that can only be understood by thinking about “learning in the machine”, as opposed to machine learning. In a physical neural system, learning rules must be local both in space and time. Among other things, this locality principle helps clarify the relationship between Hebbian learning and backpropagation and explains why Hebbian learning applied to feedforward convolutional architectures has never worked. It also naturally leads to random backpropagation and recirculation algorithms, important topics that are poorly known because they are not particularly useful for current applications. For readers primarily interested in applications, or for courses with tight time limitations, I recommend using the abbreviated sequence of chapters: 2, 3, 6, and 10, covering most of the practical aspects.

Finally, the field of neural networks has been polluted by fads and a significant amount of cronyism and collusion over the past few decades, that a fragmented, multigenerational, and often unaware community could do little to stop. Cronyism and collusion are nothing new in human affairs, but they have distorted and slowed down the development of the field through the subtle control and manipulation of conferences, publications, academic and corporate research departments, and other avenues of power and dissemination. Readers should read more widely, check what has been published – where and when – and decide for themselves which results are supported by mathematical proofs or sound simulations, and which are not. In the end, towering over human affairs, all that matters are the beauty of deep learning and the underlying mysteries it is intimately connected to: from whether silicon can be conscious to the fundamental nature of the universe.

About the Exercises

The exercises vary in difficulty substantially. Should you become frustrated at trying to solve one of them, remind yourself that it is only when you are struggling with a problem that your brain is really learning something.
In order to solve some of the problems in the book, or more broadly to think about scientific and other questions, I recommend that my students systematically try at least four different approaches. The first of course is to simplify. When a question seems too difficult at first, look for special or simpler cases. When trying to understand a theorem, look at the case of “small $n$”, or fix the values of certain parameters, or switch to the linear case, or try to interpolate. The second is the opposite way of thinking: generalize, abstract, or extrapolate. Are there other situations that bear some similarity to the current problem? How can a result be applied to more general cases? Can the conditions under which a theorem is true be relaxed? The third way of thinking is “to take the limit”, to look at what happens at the boundaries of a certain domain, under extreme conditions, to let $n$ go to zero, or to infinity. And finally, the fourth way is always to invert, look at things somehow from an opposite perspective. Thus, for example, when thinking about an autoencoder, one may want first to simplify it by studying how to solve the top layer given the lower layer, which is usually an easier problem; and then to invert this approach by studying how the lower layer can be solved given the top layer, which is usually a harder problem.

Of course these four principles are not a panacea to every situation and, for instance, identifying the right form of “inversion” in a given situation may not be obvious. However, the discipline of trying to apply these four principles in a systematic manner can be helpful and, incidentally, remains a major challenge for Artificial Intelligence (AI).

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- As a graduate student at Caltech (1983-1986) and visiting lecturer at UCSD (1986-1988), I was fortunate to be able to participate and contribute to the early beginnings of neural networks in the 1980s. Being at those two universities, which were the hotbeds of neural networks research at the time, resulted to a large extent from a series of chance encounters with several individuals, of whom I can only mention two: Brian Ekin and Gill Williamson. Brian, who I met by chance in Paris, told me to apply to Caltech, a name I had never heard before. And while bartending for an alumni reunion in the basement of the Caltech Athenaeum, I met Gill Williamson who was a Professor at UCSD and, while still sober, offered me my first academic job.

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