

Contents

1 Introduction — 1

- 1.1 Basics, Questions, and Motivation — 1**
- 1.2 Machine Learning as Model of the Scientific Process — 4**
 - 1.2.1 Early Approaches to Scientific Discovery — 4
 - 1.2.2 Knowledge Representation – What is a Theory? — 5
 - 1.2.3 Towards Probabilities — 7
 - 1.2.4 The Big Data Move — 8
- 1.3 From the Physical Theory to the Physical Observable — 10**
- 1.4 From the Measured Variable to the Measuring Point — 18**
- 1.5 The Epistemology of Physics in Concert with Machine Learning — 26**
 - 1.5.1 Further Reading in this Book — 28

2 Challenges in Particle and Astroparticle Physics — 31

- 2.1 Physical Motivation, Problems, and Examples — 31**
- 2.2 Astroparticle Physics — 32**
 - 2.2.1 Experiments — 34
- 2.3 Particle Physics — 42**
 - 2.3.1 Experiments — 42

3 Key Concepts in Machine Learning and Data Analysis — 51

- 3.1 Overview of the Field of Machine Learning — 51**
 - 3.1.1 Learning Tasks — 52
 - 3.1.2 Processing Paradigms of Machine Learning — 55
 - 3.1.3 Machine Learning Pipelines — 56
 - 3.1.4 Minimum Redundancy Maximum Relevance (MRMR) — 58
- 3.2 Optimization — 59**
 - 3.2.1 Stochastic Gradient Descent — 60
 - 3.2.2 Newton-Raphson Optimization — 61
- 3.3 Theories of Machine Learning — 62**
 - 3.3.1 Computational Learning Theory — 64
- 3.4 Tree Models — 66**
 - 3.4.1 Ensemble Methods — 67
 - 3.4.2 Implementations and Hardware Considerations — 69
- 3.5 Neural Networks — 70**
 - 3.5.1 Architectures of DNNs — 71
 - 3.5.2 Robustness of DNNs — 73

- 3.5.3 Deep Learning Theory — 73
- 3.5.4 Explanations — 74
- 3.5.5 Hardware Considerations — 75

4 Data Acquisition and Data Structure — 77

- 4.1 Introduction — 77**
- 4.2 Data Acquisition — 79**
 - 4.2.1 Data Acquisition for LHCb — 79
 - 4.2.2 Data Acquisition for Imaging Air Cherenkov Telescopes — 82
 - 4.2.3 Data Acquisition for IceCube — 85
- 4.3 Data Structures — 89**
 - 4.3.1 Data Structures for LHCb — 89
 - 4.3.2 Data Structures for IACTs — 92
 - 4.3.3 Data Structures for IceCube — 96
- 4.4 GPU-Based Trigger Decisions — 98**

5 Monte Carlo Simulations — 103

- 5.1 LHCb: Monte Carlo Simulations and Libraries in Particle Physics — 103**
 - 5.1.1 Astro: Monte Carlo Simulations, Libraries — 105
- 5.2 Simulation Efficiency Studies — 108**
 - 5.2.1 Corsika – Active Learning — 108
 - 5.2.2 Control of the Simulation – Active Sampling — 112
 - 5.2.3 Corsika 8 New Modular Library — 118
 - 5.2.4 ARM-Cluster for Corsika — 120
- 5.3 Validation of the Simulation — 126**
 - 5.3.1 Introduction — 126
 - 5.3.2 Mismatches Between Observed and Simulated Data — 127
 - 5.3.3 Detection of Mismatches — 128
- 5.4 Keynote: The Muon Puzzle — 133**
 - 5.4.1 Introduction — 133
 - 5.4.2 Meta-Analysis of Muon Measurements in Air Showers — 134
 - 5.4.3 Muon Production in Air Showers — 136
 - 5.4.4 Related Measurements at the LHC at CERN — 138
 - 5.4.5 Fixed-Target Experiments at SPS and LHC — 141
 - 5.4.6 Summary and Outlook — 142

6 Data Storage and Access — 145

- 6.1 Introduction — 145**
- 6.2 Research Data Management — 145**

- 6.2.1 Management of Large Amounts of Research Data — 146
- 6.3 The FACT Open Data Project as an Example of Public Data Access — 150**
 - 6.3.1 Available Data — 151
- 6.4 The DeLoreanSystem Architecture as Example of Experiment-Internal Access — 152**
 - 6.4.1 The Data Volume Problem at LHCb — 153
 - 6.4.2 DeLorean: Optimized Scans for Efficient Data Access — 157
 - 6.4.3 Evaluating *DeLorean* — 160
 - 6.4.4 Looking Ahead — 161

7 Monitoring and Feature Extraction — 163

- 7.1 Introduction — 163
- 7.2 Feature Extraction and Selection in IceCube — 163
- 7.3 Feature Extraction for IACTs — 172
 - 7.3.1 Introduction — 173
 - 7.3.2 Image Extraction — 173
 - 7.3.3 Image Cleaning — 174
 - 7.3.4 Image Parametrization — 175
- 7.4 Monitoring the Telescope via Data Summarization — 178
 - 7.4.1 Introduction — 178
 - 7.4.2 Data Summarization with Submodular Functions — 179
 - 7.4.3 Dimensionality Reduction with Autoencoders — 183
 - 7.4.4 Submodular Autoencoders — 185
 - 7.4.5 Experiments — 187
 - 7.4.6 Discussion and Outlook — 191

8 Event Property Estimation and Signal Background Separation — 193

- 8.1 Introduction — 193
- 8.2 Boosted Decision Trees LHC — 194
- 8.3 Event Selection in IceCube — 202
 - 8.3.1 Muon Neutrino Selection — 204
 - 8.3.2 Tau Neutrino Selection — 212
- 8.4 Estimation of Event Properties for IACTs — 218
 - 8.4.1 Labeled Training Data — 220
 - 8.4.2 Particle Classification — 222
 - 8.4.3 Energy Estimation — 223
 - 8.4.4 Origin Estimation — 224
 - 8.4.5 Combining Multiple Telescopes — 226

8.4.6	Final Event Selection — 228
8.5	Keynote: Data Analysis at ATLAS — 228
8.5.1	Introduction — 229
8.5.2	Rare Top-Quark Processes: Searching for FCNC Processes — 231
8.5.3	Searching for New Heavy Particles: Vector-Like Quarks — 236
8.5.4	Conclusions — 243

9 Deep Learning Applications — 245

9.1	Introduction — 245
9.2	Deep Learning for IceCube — 245
9.2.1	Domain Knowledge in IceCube — 246
9.2.2	Convolutional Neural Networks in IceCube — 248
9.2.3	Combining Deep Learning with Maximum-Likelihood — 254
9.2.4	Model Performance and Applications — 257
9.3	Flavor Tagging with Deep Learning LHC — 258
9.3.1	Neutral B Meson Oscillations and CP -Violation — 259
9.3.2	Flavor Tagging Technique — 260
9.3.3	Flavor Tagging Formalism — 262
9.3.4	Flavor Tagging Algorithms — 263
9.3.5	Inclusive Flavor Tagging — 264
9.4	A Deep Learning Analysis Pipeline for Gamma Ray Astronomy — 268
9.4.1	Introduction — 269
9.4.2	Event-Tagging Pipeline — 269
9.4.3	Multi-Task Deep Neural Networks — 270
9.4.4	Model Performance and Applications — 273
9.4.5	Discussion — 278

10 Inverse Problems — 279

10.1	Introduction — 279
10.2	Keynote: Introduction to Inverse Problems — 281
10.2.1	Information — 282
10.2.2	The Effect of the Response Function — 284
10.2.3	Supplementary Remarks — 290
10.2.4	Mathematical Appendix: Integrals Over Cosine Functions — 291
10.3	Likelihood-Based Deconvolution — 292
10.3.1	Introduction — 292
10.3.2	Discretization of the Observable Quantities — 294
10.3.3	Optimization — 295
10.3.4	Regularization with a Fixed Number of Degrees of Freedom — 296

10.3.5	Regularization with Minimum Global Correlation —	298
10.4	Deconvolution as a Classification Task —	298
10.4.1	Introduction —	299
10.4.2	Quantification with Classify-and-Count Methods —	300
10.4.3	Accurate Estimates Through Iterative Reweighting —	300
10.4.4	Classifier Choice —	301
10.4.5	Leveraging Eventwise Contributions —	302
10.4.6	Excursion: Document Analysis in Political Science —	303
10.5	Deconvolution of IACT Data —	304
10.5.1	IACT Instrument Response Functions —	305
10.5.2	Application of the Regularized Likelihood Deconvolution —	308
10.6	Deconvolution of Atmospheric Neutrino Spectra —	310
 Bibliography — 319		
 Index — 343		
 List of Contributors — 347		

