## Contents

P	refac	е	1X		
$\mathbf{S}_{\mathbf{J}}$	mbo	ls and Notation	xiii		
1	1 Introduction				
2	Bas	ics of Supervised Learning	5		
	2.1	Introduction	5		
	2.2	Regression	. 7		
		2.2.1 Linear Models			
		2.2.2 Nonlinear Models	8		
		2.2.3 Error Measures	9		
	2.3	Classification	. 11		
	2.4	Time Series Prediction	13		
	2.5	Model Selection	14		
	2.6	Cross-validation	18		
	2.7	Further Reading	19		
3	Basics of Symbolic Regression				
	3.1	Example: Identification of a Polynomial			
		3.1.1 Data Collection and Preprocessing	22		
		3.1.2 Establishing a Baseline	22		
		3.1.3 Modeling Approach	23		
		3.1.4 Modeling Results	24		
	3.2	Example: Discovery of Laws of Physics from Data	26		
	3.3	Example: Approximation of the Gamma Function	29		
	3.4	Extending Symbolic Regression to Classification	32		
		3.4.1 Model Structures for Symbolic Classification	32		
		3.4.2 Evaluation of Symbolic Classification Models	33		
	3.5	Further Reading	34		
4	Evo	olutionary Computation and Genetic Programming	35		
	4.1	General Concepts	39		
		4.1.1 Genotype, Phenotype, and Semantics	39		
		4.1.2 Diversity and Evolvability	40		
		4.1.3 Buffering, Redundancy, and Neutrality	41		
	4.2	Population Initialization	42		

vi Contents

		4.2.1 Operators	43
	4.3	Fitness Calculation	45
	4.4	Parent Selection	45
		4.4.1 Operators	45
		4.4.2 Selection Pressure	46
	4.5	Bloat and Introns	47
	4.6	Crossover and Mutation	49
	4.7	Power of the Hypothesis Space	50
	4.8	GP Dynamics	54
		4.8.1 Fitness	56
		4.8.2 Variable Relevance	56
		4.8.3 Model Complexity	58
		4.8.4 Diversity	59
	4.9	v v	64
		4.9.1 Brood Selection and Offspring Selection	64
		4.9.2 Age-layered Population Structures	69
			70
			73
		4.9.5 Restricting Expressions: Syntax and Types	74
		4.9.6 Semantics-aware GP	76
	4.10	Conclusions	77
			78
	4.11	Further Reading	10
5		el Validation, Inspection, Simplification, and Selection & Model Validation	<b>81</b> 82
5	Mod	el Validation, Inspection, Simplification, and Selection  Model Validation	81 82 83
5	Mod	el Validation, Inspection, Simplification, and Selection  Model Validation	81 82 83
5	<b>Mod</b> 5.1	validation, Inspection, Simplification, and Selection         8           Model Validation         8           5.1.1 Visual Tools         8           5.1.2 Explaining Models         9           5.1.3 Model Interpretability         9	81 82 83 90
5	Mod	el Validation, Inspection, Simplification, and Selection       8         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10	81 82 83 90 99
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection       8         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10	81 83 90 99
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection       8         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10         5.2.2 Hold-out Set for Validation       10	81 82 83 90 99 00 01
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection       8         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10         5.2.2 Hold-out Set for Validation       10         5.2.3 Cross-validation       10	81 82 83 90 99 00 01
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection       8         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10         5.2.2 Hold-out Set for Validation       10         5.2.3 Cross-validation       10         5.2.4 Akaike's Information Criterion       10	81 82 83 90 99 00 01 01
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection       8         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10         5.2.2 Hold-out Set for Validation       10         5.2.3 Cross-validation       10         5.2.4 Akaike's Information Criterion       10         5.2.5 Bayesian Information Criterion       10	81 82 83 90 99 00 01 01 02 04
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10         5.2.2 Hold-out Set for Validation       10         5.2.3 Cross-validation       10         5.2.4 Akaike's Information Criterion       10         5.2.5 Bayesian Information Criterion       10         5.2.6 Minimum Description Length Principle       10	81 82 83 90 99 00 01 01 02 04
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10         5.2.2 Hold-out Set for Validation       10         5.2.3 Cross-validation       10         5.2.4 Akaike's Information Criterion       10         5.2.5 Bayesian Information Criterion       10         5.2.6 Minimum Description Length Principle       10         5.2.7 Comparison of Model Selection Criteria       10	81 82 83 90 99 00 01 01 02 04 04
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10         5.2.2 Hold-out Set for Validation       10         5.2.3 Cross-validation       10         5.2.4 Akaike's Information Criterion       10         5.2.5 Bayesian Information Criterion       10         5.2.6 Minimum Description Length Principle       10         5.2.7 Comparison of Model Selection Criteria       10         Model Simplification       10	81 82 83 90 99 00 01 01 02 04 06 08
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection         8           Model Validation         8           5.1.1 Visual Tools         8           5.1.2 Explaining Models         9           5.1.3 Model Interpretability         9           Model Selection         10           5.2.1 Criteria for Model Selection         10           5.2.2 Hold-out Set for Validation         10           5.2.3 Cross-validation         10           5.2.4 Akaike's Information Criterion         10           5.2.5 Bayesian Information Criterion         10           5.2.6 Minimum Description Length Principle         10           5.2.7 Comparison of Model Selection Criteria         10           Model Simplification         10           5.3.1 Nested Models         10	81 82 83 90 99 00 01 01 04 04 06 08
5	5.1 5.2	el Validation, Inspection, Simplification, and Selection         8           Model Validation         8           5.1.1 Visual Tools         8           5.1.2 Explaining Models         9           5.1.3 Model Interpretability         9           Model Selection         10           5.2.1 Criteria for Model Selection         10           5.2.2 Hold-out Set for Validation         10           5.2.3 Cross-validation         10           5.2.4 Akaike's Information Criterion         10           5.2.5 Bayesian Information Criterion         10           5.2.6 Minimum Description Length Principle         10           5.2.7 Comparison of Model Selection Criteria         10           Model Simplification         10           5.3.1 Nested Models         10           5.3.2 Removal of Subexpressions         12	81 82 83 90 99 00 01 01 02 04 06 08 09
5	<b>Mod</b> 5.1	el Validation, Inspection, Simplification, and Selection         Model Validation       8         5.1.1 Visual Tools       8         5.1.2 Explaining Models       9         5.1.3 Model Interpretability       9         Model Selection       10         5.2.1 Criteria for Model Selection       10         5.2.2 Hold-out Set for Validation       10         5.2.3 Cross-validation       10         5.2.4 Akaike's Information Criterion       10         5.2.5 Bayesian Information Criterion       10         5.2.6 Minimum Description Length Principle       10         5.2.7 Comparison of Model Selection Criteria       10         5.3.1 Nested Models       10         5.3.2 Removal of Subexpressions       11         Example: Boston Housing       12	81 82 83 99 99 00 01 01 04 04 06 08 11
5	5.1 5.2	el Validation, Inspection, Simplification, and Selection         8           Model Validation         8           5.1.1 Visual Tools         8           5.1.2 Explaining Models         9           5.1.3 Model Interpretability         9           Model Selection         10           5.2.1 Criteria for Model Selection         10           5.2.2 Hold-out Set for Validation         10           5.2.3 Cross-validation         10           5.2.4 Akaike's Information Criterion         10           5.2.5 Bayesian Information Criterion         10           5.2.6 Minimum Description Length Principle         10           5.2.7 Comparison of Model Selection Criteria         10           5.3.1 Nested Models         10           5.3.2 Removal of Subexpressions         12           Example: Boston Housing         12           5.4.1 Data Preprocessing         12	81 82 83 90 99 00 01 01 02 04 06 08 09
5	5.1 5.2	el Validation, Inspection, Simplification, and Selection         8           Model Validation         8           5.1.1 Visual Tools         8           5.1.2 Explaining Models         9           5.1.3 Model Interpretability         9           Model Selection         10           5.2.1 Criteria for Model Selection         10           5.2.2 Hold-out Set for Validation         10           5.2.3 Cross-validation         10           5.2.4 Akaike's Information Criterion         10           5.2.5 Bayesian Information Criterion         10           5.2.6 Minimum Description Length Principle         10           5.2.7 Comparison of Model Selection Criteria         10           5.3.1 Nested Models         10           5.3.2 Removal of Subexpressions         11           5.4.1 Data Preprocessing         12           5.4.2 Model Generation and Selection for Median Values of	81 82 83 99 99 00 01 01 04 04 08 09 11 13
5	5.1 5.2	el Validation, Inspection, Simplification, and Selection  Model Validation	81 82 83 90 99 00 01 01 02 04 08 09 11 13
5	5.1 5.2	el Validation, Inspection, Simplification, and Selection  Model Validation  5.1.1 Visual Tools  5.1.2 Explaining Models  5.1.3 Model Interpretability  Model Selection  5.2.1 Criteria for Model Selection  5.2.2 Hold-out Set for Validation  5.2.3 Cross-validation  5.2.4 Akaike's Information Criterion  5.2.5 Bayesian Information Criterion  5.2.6 Minimum Description Length Principle  5.2.7 Comparison of Model Selection Criteria  Model Simplification  5.3.1 Nested Models  5.3.2 Removal of Subexpressions  Example: Boston Housing  5.4.1 Data Preprocessing  Model Generation and Selection for Median Values of Homes  Model Generation and Selection for NO <sub>X</sub> Concentrations  15  16  17  18  19  19  10  10  10  10  10  10  10  10	81 82 83 90 99 00 01 01 02 04 08 09 11 13

Contents vii

	5.6	Furth	er Reading	125
6	Adv	anced	Techniques	127
	6.1	Integr	ration of Knowledge	127
		6.1.1	Example Applications	128
		6.1.2	Knowledge Integration Methods	128
		6.1.3	Knowledge Integration via Customized Fitness Evalua-	
			tion	129
		6.1.4	Shape Constraints	131
		6.1.5	Knowledge Integration via the Hypothesis Space	133
	6.2	Optin	nization of Coefficients	138
		6.2.1	Linear Scaling	139
		6.2.2	Nonlinear Optimization of Coefficients	141
	6.3		ction Intervals	143
	0.0	6.3.1	Prediction intervals for Linear Models	146
		6.3.2	Approximate Prediction Intervals for Nonlinear Models	147
		6.3.3	Bayesian Prediction Intervals	152
	6.4		ling System Dynamics	153
	0.1	6.4.1	Basics of Differential Equations	154
		6.4.2	Finding Differential Equations with Symbolic Regression	
	6.5	_	numeric Data	166
	6.6		evolutionary Symbolic Regression	168
	0.0	6.6.1	Fast Function Extraction	168
		6.6.2	Sparse Identification of Nonlinear Dynamics (SINDy)	169
		6.6.3	Prioritized Grammar Enumeration	169
		6.6.4	Exhaustive Symbolic Regression	169
		6.6.5	Grammar-guided Exhaustive Equation Search	170
		6.6.6	Equation Learner	171
		6.6.7	Deep Symbolic Regression	
		6.6.8	AI Feynman	172
		0.0.0	Ti Teyimian	112
7			and Applications	173
	7.1		Hydrodynamics	173
	7.2		trial Chemical Processes	179
		7.2.1	Correlation Analysis	180
		7.2.2	Experimental Setup	
		7.2.3	Results for the Chemical Dataset	182
		7.2.4		183
	7.3	Intera	tomic Potentials	187
	7.4	Friction	on	189
	7.5	Lithiu	um-ion Batteries	197
		7.5.1	NASA PCoE Battery Datasets	197
		7.5.2	First Version of the State-of-charge Model	199
		7.5.3	Extended Version of the State-of-charge Model $ \ldots  \ldots$	203
		7.5.4	Predicting the Discharge Voltage Curve	209

viii	Contents
------	----------

	7.6	Biomedical Problems	214
		7.6.1 Identification of Virtual Tumor Markers	216
	7.7	Function Approximation	219
	7.8	Atmospheric CO <sub>2</sub> Concentration	223
	7.9	Flow Stress	225
	7.10	Dynamics of Simple Mechanical Systems	229
		7.10.1 Oscillator	230
		7.10.2 Pendulum	233
		7.10.3 Double Oscillator	236
		7.10.4 Double Pendulum	239
	7.11	Conclusions	. 247
8	Con	clusion	249
	8.1	Unique Selling Points of Symbolic Regression	249
	8.2	Limitations and Caveats	250
9	Δnn	pendix	253
J	9.1	Benchmarks	253
	9.2	Open-source Software for Genetic Programming	253
	9.4	9.2.1 HeuristicLab	254
		9.2.2 Operon	254
		9.2.3 PySR	$\frac{255}{255}$
		9.2.4 DEAP	256
		9.2.5 FEAT	256
		9.2.6 ECJ	256
		9.2.7 GPTIPS	
	9.3	Commercial Software for Genetic Programming	258
	0.0	9.3.1 Evolved Analytics DataModeler	258
		9.3.2 Eureqa Formulize	258
D:	blica	raphy	259
וט	Bonra	таршу	<b>4</b> 99
In	$\operatorname{dex}$		285