

Contents

Preface — V

Acknowledgment — VII

Alexandre Caboussat, Maude Girardin, and Marco Picasso

A framework to solve inverse problems for parametric PDEs using adaptive finite elements and neural networks — 1

Olivier Cots, Rémy Dutto, Sophie Jan, and Serge Laporte

Generation of value function data for bilevel optimal control and application to hybrid electric vehicle — 17

Rohit Pochampalli and Nicolas R. Gauger

Graph neural networks to predict strokes from blood flow simulations — 29

Alexander Sikorski, Robert Julian Rabben, Surahit Chewle, and Marcus Weber

Capturing the macroscopic behavior of molecular dynamics with membership functions — 41

Phillip Semler and Martin Weiser

Adaptive gradient-enhanced Gaussian process surrogates for inverse problems — 59

Alexander Heinlein, Amanda A. Howard, Damien Beecroft, and Panos Stinis

Multifidelity domain decomposition-based physics-informed neural networks and operators for time-dependent problems — 79

Timo Kreimeier, Andrea Walther, and Andreas Griewank

Constrained piecewise linear optimization by an active signature method — 93

Ken Trotti, Samuel A. Cruz Alegría, Alena Kopaničáková, and Rolf Krause

Parallel trust-region approaches in neural network training — 107

Pascal Van Hentenryck

Trustworthy optimization learning: a brief overview — 121

Max Zimmer, Christoph Spiegel, and Sebastian Pokutta

Compression-aware training of neural networks using Frank-Wolfe — 137

X — Contents

Antonio Carlucci, Ion Victor Gosea, and Stefano Grivet-Talocia
Approximation of generalized frequency response functions via vector fitting — 169

Ganna Shyshkanova, Timo Kreimeier, Lukas Baumgärtner, Franz Bethke, and Andrea Walther
On the nonsmooth regularity condition LIKQ for different abs-normal representations — 181

Philippe L. Toint
Divergence of the ADAM algorithm with fixed-stepsizes: a (very) simple example — 195

Index — 199