

Yanfei Wang
Anatoly G. Yagola
Changchun Yang
Editors

Computational Methods for Applied Inverse Problems

应用反问题中的计算方法



高等教育出版社
HIGHER EDUCATION PRESS

Yanfei Wang
Anatoly G. Yagola
Changchun Yang
Editors

Computational Methods for Applied Inverse Problems

应用反问题中的计算方法

YINGYONG FANWENTI ZHONG DE JISUAN FANGFA



Editors

Prof. Dr. Yanfei Wang
Key Laboratory of Petroleum Resources Research
Institute of Geology and Geophysics
Chinese Academy of Sciences
Beijing 100029, China
e-mail: yfwang@mail.iggcas.ac.cn

Prof. Dr. Anatoly G. Yagola
Department of Mathematics
Faculty of Physics
Lomonosov Moscow State University
Moscow 119991, Russia
e-mail: yagola@inverse.phys.msu.ru

Prof. Dr. Changchun Yang
Key Laboratory of Petroleum Resources Research
Institute of Geology and Geophysics
Chinese Academy of Sciences
Beijing 100029, China
e-mail: ccy@mail.iggcas.ac.cn

©2012 Higher Education Press, 4 Dewai Dajie, Beijing 100120, P. R. China

图书在版编目(CIP)数据

应用反问题中的计算方法 = Computational Methods
for Applied Inverse Problems : 英文 / 王彦飞,

(俄罗斯) 亚哥拉 (Yagola, A. G.), 杨长春编著. — 北
京: 高等教育出版社, 2012. 10

ISBN 978-7-04-034499-8

I. ①应… II. ①王… ②亚… ③杨… III. ①反演算
法—英文 IV. ①O177.6

中国版本图书馆 CIP 数据核字 (2012) 第 214503 号

策划编辑 赵天夫

责任编辑 赵天夫

封面设计 张楠

责任印制 朱学忠

出版发行 高等教育出版社
社址 北京市西城区德外大街 4 号
邮政编码 100120
印刷 涿州市星河印刷有限公司
开本 787mm × 1092mm 1/16
印张 34.5
字数 640 千字
购书热线 010-58581118

咨询电话 400-810-0598
网 址 <http://www.hep.edu.cn>
<http://www.hep.com.cn>
网上订购 <http://www.landraco.com>
<http://www.landraco.com.cn>
版 次 2012 年 10 月第 1 版
印 次 2012 年 10 月第 1 次印刷
定 价 139.00 元

本书如有缺页、倒页、脱页等质量问题, 请到所购图书销售部门联系调换

版权所有 侵权必究

物料号 34499-00

Sales only inside the mainland of China (仅限中国大陆地区销售)

Preface

This volume contains the chapters based on the lectures given by invited speakers of the international workshop “Computational Methods for Applied Inverse Problems”. The workshop was organized under the auspices of the Chinese Academy of Sciences in the Institute of Geology and Geophysics, located in Beijing, the capital of China, and held during July 12–16, 2010. The workshop was sponsored by the National Science Foundation of China (NSFC), China-Russia Cooperative Research Project (NSFC-RFBR), Knowledge Innovation Programs of Chinese Academy of Sciences (CAS) and the Strategic Priority Research Program of the Chinese Academy of Sciences (CAS). The main goal of the workshop is to gather young participants (mostly mathematicians and geophysicists) from China and overseas together to discuss how to solve inverse and ill-posed problems using different solving strategies. Eminent specialists from China, Russia (partially sponsored by the Russian Foundation of Basic Research), USA, India and Norway were invited to present their lectures. Other young scientists also present their recent researches during the conference.

The book covers many directions in the modern theory of inverse and ill-posed problems — mathematical physics, optimal inverse design, inverse scattering, inverse vibration, biomedical imaging, oceanography, seismic imaging and remote sensing; methods including standard regularization, parallel computing for multidimensional problems, Nyström method, numerical differentiation, analytic continuation, perturbation regularization, filtering, optimization and sparse solving methods are fully addressed. This issue attempts to bridge the gap between theoretical studies of ill-posed inverse problems and practical applications. Let us continue our efforts for further progress.

This book will be helpful to researchers and teachers in developing courses on various inverse and ill-posed problems of mathematical physics, geosciences, designing technology, imaging, high performance computing, inverse scattering and vibration, and so on. It could be also beneficial for senior undergraduate students, graduate and Ph.D. students, recent graduates getting practical experience, engineers and researchers who study inverse and ill-posed problems and solve them in practice.

Editor's Preface

Inverse problem theory and methods are driven by applied problems in sciences and engineering. Studies on inverse problems represent an exciting research area in recent decades. The special importance of inverse problems is that it is an interdisciplinary subject related with mathematics, physics, chemistry, geoscientific problems, biology, financial and business, life science, computing technology and engineering.

Inverse problems consist in using the results of actual observations to infer the values of the (model) parameters characterizing the system under investigation. Inverse problems are typically ill-posed in the sense that one of the three items “existence, uniqueness or stability” of the solution may be violated. Inverse problems use modeling design and solving methods to provide a better, more accurate, and more efficient simulation for practical problems.

Methodologies for solving inverse problems involve regularization, optimization and statistics. No one particular method solves all inverse problems. This book provides a background of using regularization and optimization techniques to solve practical inverse problems for the readers who do research in computational/applied mathematics, physical chemistry, engineering, geophysics, image processing and remote sensing, etc. In particular, recent advances of inversion theory and solution methods with applications to practical inverse problems are addressed.

This book *Computational Methods for Applied Inverse Problems* will comprise the following scientific fields:

- Historical background and key issues of general inverse problems;
- Recent advances in regularization theory and new solution methods;
- Optimal inverse design and optimization methods;
- Recent advances in inverse scattering;
- Inverse vibration and data processing;
- Modeling and inversion of the geoscientific problems;
- Analytic, algebraic, statistical and computational methods.

The five main parts of the book are preceded with the first part of an introductory chapter. Chapter 1 written by S. I. Kabanikhin presents us a general idea about inverse problems and key theories on solving problems.

The second part of this book is devoted to presenting recent advances in regularization theory and solving methods. Chapter 2 written by D. V. Lukyanenko and A. G. Yagola proposes a parallel computing technique on multidimensional ill-posed problems. In this chapter, example of a practical problem of restoring

magnetization parameters over a ship body using parallelization is considered. Chapter 3 written by M. T. Nair talks about the theoretical issues of Nyström approximation method for ill-posed problems, numerical issues and error estimates. Chapter 4 written by T. Y. Xiao, H. Zhang and L. L. Hao discusses about the regularizing theories on numerical differentiation. In this chapter, different regularization schemes are presented and compared with extensive numerical simulations. Chapter 5 written by C. L. Fu, H. Cheng and Y. J. Ma shows readers the analytic continuation and regularization. Convergence properties and error estimates are included. Chapter 6 written by G. S. Li discusses about the perturbation regularization method for function reconstruction problem. Four cases of coefficient determination of an advection diffusion equation are addressed. Chapter 7 written by L. V. Zotov and V. L. Panteleev presents some filtering methods for ill-posed problems.

The third part is devoted to inverse design problems and optimization. Chapter 8 written by G. S. Dulikravich and I. N. Egorov describes the alloy design methodology. The inverse problem is formulated as a constrained multi-objective optimization problem and solved using a robust evolutionary optimizer of IOSO type. Chapter 9 written by Z. H. Xiang discusses both the optimal sensor placement design and the regularization method. Practical methods based on the well-posedness analysis of parameter identification procedures and the adaptive adjusting of a-priori information are developed. Chapter 10 written by Y. H. Dai introduces a stable optimization method, called the BFGS method. A general convergence result about the BFGS algorithm is obtained.

The fourth part is devoted to the field of inverse scattering. Chapter 11 written by X. D. Liu and B. Zhang presents the uniqueness results in inverse acoustic and electromagnetic obstacle scattering problems. Some interesting open problems are posed at the end of the chapter. Chapter 12 written by G. Bao and P. J. Li addresses a shape reconstruction problem of inverse scattering. A continuation method for the inverse obstacle scattering problem is developed and details about solving issues are established.

The fifth part is devoted to the inverse vibration problems, data processing and some mathematical problems in biomedical imaging. Chapter 13 written by G. M. Kuramshina, I. V. Kochikov and A. V. Stepanova talks about molecular force field calculations. In particular, they discuss how a-priori model assumptions and *ab initio* quantum mechanical calculations are used for constructing regularizing algorithms for the calculation of molecular force fields. Chapter 14 written by J. J. Liu and H. L. Xu discusses about the mathematical models and image reconstruction realizations of magnetic resonance electrical impedance tomography (MREIT), the harmonic B_z algorithm and the integral equation method are presented.

The last part is devoted to the modeling and inversion problems occurred in geophysics, oceanography, and remote sensing. Chapter 15 written by S. I. Kabanikhin and M. A. Shishlenin discusses about iterative regularization method for solving the inverse hyperbolic problems. Chapter 16 written by H. B. Song, X. H. Huang, L. M. Pinheiro, Y. Song, C. Z. Dong and Y. Bai focuses on a new cross discipline between seismology and physical oceanography. Chapter 17 written by L. J. Gelius provides a framework of understanding and analyzing both diffraction-limited imaging as well as super-resolution. Chapter 18 written by Y. F. Wang, Z. H. Li and C. C. Yang makes a short review seismic migration methods and develops a preconditioned regularizing least squares migration method. Chapter 19 written by Y. F. Wang, J. J. Cao, T. Sun and C. C. Yang extends the conception of compressive sensing to seismic wavefields interpolation, sparse optimization and regularization methods are fully described. Chapter 20 written by H. Yang presents a quantitative model to characterize the reflectance of land surfaces, regularizing and optimizing issues and multistage inversion strategies are discussed.

The special features of the book are that it provides both novel methods for standard and nonstandard regularization and practical applications in science and engineering. Each chapter is written by respective researchers in their research fields. Illustrations and tables are provided for better understanding of their ideas. Scientists, researchers, engineers, as well as graduate students engaged in applied/computational mathematics, engineering, physical chemistry, geophysics, medical science, image processing, computer science and remote sensing, will benefit from this book.

Finally, we hope that this book will stimulate and inspire new research efforts and the intensive exploration of new promising directions.

Chinese Academy of Sciences, Beijing
Lomonosov Moscow State University, Moscow
Chinese Academy of Sciences, Beijing
June 2012

Yanfei Wang
Anatoly G. Yagola
Changchun Yang

Contents

Preface	v
Editor's Preface	vii
I Introduction	1
1 <i>S. I. Kabanikhin</i>	
Inverse Problems of Mathematical Physics	3
1.1 Introduction	3
1.2 Examples of Inverse and Ill-posed Problems	12
1.3 Well-posed and Ill-posed Problems	24
1.4 The Tikhonov Theorem	26
1.5 The Ivanov Theorem: Quasi-solution	29
1.6 The Lavrentiev's Method	33
1.7 The Tikhonov Regularization Method	35
References	44
II Recent Advances in Regularization Theory and Methods	47
2 <i>D. V. Lukyanenko and A. G. Yagola</i>	
Using Parallel Computing for Solving Multidimensional Ill-posed Problems	49
2.1 Introduction	49
2.2 Using Parallel Computing	51
2.2.1 Main idea of parallel computing	51
2.2.2 Parallel computing limitations	52
2.3 Parallelization of Multidimensional Ill-posed Problem	53
2.3.1 Formulation of the problem and method of solution	53
2.3.2 Finite-difference approximation of the functional and its gradient	56
2.3.3 Parallelization of the minimization problem	58
2.4 Some Examples of Calculations	61
2.5 Conclusions	63
References	63

3 *M. T. Nair*

Regularization of Fredholm Integral Equations of the First Kind using Nyström Approximation	65
3.1 Introduction	65
3.2 Nyström Method for Regularized Equations	68
3.2.1 Nyström approximation of integral operators	68
3.2.2 Approximation of regularized equation	69
3.2.3 Solvability of approximate regularized equation	70
3.2.4 Method of numerical solution	73
3.3 Error Estimates	74
3.3.1 Some preparatory results	74
3.3.2 Error estimate with respect to $\ \cdot\ _2$	77
3.3.3 Error estimate with respect to $\ \cdot\ _\infty$	77
3.3.4 A modified method	78
3.4 Conclusion	80
References	81

4 *T. Y. Xiao, H. Zhang and L. L. Hao*

Regularization of Numerical Differentiation: Methods and Applications	83
4.1 Introduction	83
4.2 Regularizing Schemes	87
4.2.1 Basic settings	87
4.2.2 Regularized difference method (RDM)	88
4.2.3 Smoother-Based regularization (SBR)	89
4.2.4 Mollifier regularization method (MRM)	90
4.2.5 Tikhonov's variational regularization (TiVR)	92
4.2.6 Lavrentiev regularization method (LRM)	93
4.2.7 Discrete regularization method (DRM)	94
4.2.8 Semi-Discrete Tikhonov regularization (SDTR)	96
4.2.9 Total variation regularization (TVR)	99
4.3 Numerical Comparisons	102
4.4 Applied Examples	105
4.4.1 Simple applied problems	106
4.4.2 The inverse heat conduct problems (IHCP)	107
4.4.3 The parameter estimation in new product diffusion model	108
4.4.4 Parameter identification of Sturm-Liouville operator	110
4.4.5 The numerical inversion of Abel transform	112
4.4.6 The linear viscoelastic stress analysis	114
4.5 Discussion and Conclusion	115
References	117

5	<i>C. L. Fu, H. Cheng and Y. J. Ma</i>	
	Numerical Analytic Continuation and Regularization	121
5.1	Introduction	121
5.2	Description of the Problems in Strip Domain and Some Assumptions	124
5.2.1	Description of the problems	124
5.2.2	Some assumptions	125
5.2.3	The ill-posedness analysis for the Problems 5.2.1 and 5.2.2	125
5.2.4	The basic idea of the regularization for Problems 5.2.1 and 5.2.2	126
5.3	Some Regularization Methods	126
5.3.1	Some methods for solving Problem 5.2.1	126
5.3.2	Some methods for solving Problem 5.2.2	133
5.4	Numerical Tests	135
	References	140
6	<i>G. S. Li</i>	
	An Optimal Perturbation Regularization Algorithm for Function Reconstruction and Its Applications	143
6.1	Introduction	143
6.2	The Optimal Perturbation Regularization Algorithm	144
6.3	Numerical Simulations	147
6.3.1	Inversion of time-dependent reaction coefficient	147
6.3.2	Inversion of space-dependent reaction coefficient	149
6.3.3	Inversion of state-dependent source term	151
6.3.4	Inversion of space-dependent diffusion coefficient	157
6.4	Applications	159
6.4.1	Determining magnitude of pollution source	159
6.4.2	Data reconstruction in an undisturbed soil-column experiment	162
6.5	Conclusions	165
	References	166
7	<i>L. V. Zotov and V. L. Panteleev</i>	
	Filtering and Inverse Problems Solving	169
7.1	Introduction	169
7.2	SLAE Compatibility	170
7.3	Conditionality	171
7.4	Pseudosolutions	173
7.5	Singular Value Decomposition	175
7.6	Geometry of Pseudosolution	177

7.7	Inverse Problems for the Discrete Models of Observations . . .	178
7.8	The Model in Spectral Domain	180
7.9	Regularization of Ill-posed Systems	181
7.10	General Remarks, the Dilemma of Bias and Dispersion	181
7.11	Models, Based on the Integral Equations	184
7.12	Panteleev Corrective Filtering	185
7.13	Philips-Tikhonov Regularization	186
	References	194

III Optimal Inverse Design and Optimization Methods 195

8 *G. S. Dulikravich and I. N. Egorov*

	Inverse Design of Alloys' Chemistry for Specified Thermo-Mechanical Properties by using Multi-objective Optimization	197
8.1	Introduction	198
8.2	Multi-Objective Constrained Optimization and Response Surfaces	199
8.3	Summary of IOSO Algorithm	201
8.4	Mathematical Formulations of Objectives and Constraints . . .	203
8.5	Determining Names of Alloying Elements and Their Concentra- tions for Specified Properties of Alloys	212
8.6	Inverse Design of Bulk Metallic Glasses	214
8.7	Open Problems	215
8.8	Conclusions	218
	References	219

9 *Z. H. Xiang*

	Two Approaches to Reduce the Parameter Identification Errors	221
9.1	Introduction	221
9.2	The Optimal Sensor Placement Design	223
9.2.1	The well-posedness analysis of the parameter identifica- tion procedure	223
9.2.2	The algorithm for optimal sensor placement design . . .	226
9.2.3	The integrated optimal sensor placement and parameter identification algorithm	229
9.2.4	Examples	229
9.3	The Regularization Method with the Adaptive Updating of A- priori Information	233

9.3.1	Modified extended Bayesian method for parameter identification	234
9.3.2	The well-posedness analysis of modified extended Bayesian method	234
9.3.3	Examples	236
9.4	Conclusion	238
	References	238
10	<i>Y. H. Dai</i>	
	A General Convergence Result for the BFGS Method	241
10.1	Introduction	241
10.2	The BFGS Algorithm	243
10.3	A General Convergence Result for the BFGS Algorithm	244
10.4	Conclusion and Discussions	246
	References	247
IV	Recent Advances in Inverse Scattering	249
11	<i>X. D. Liu and B. Zhang</i>	
	Uniqueness Results for Inverse Scattering Problems	251
11.1	Introduction	251
11.2	Uniqueness for Inhomogeneity n	256
11.3	Uniqueness for Smooth Obstacles	256
11.4	Uniqueness for Polygon or Polyhedra	262
11.5	Uniqueness for Balls or Discs	263
11.6	Uniqueness for Surfaces or Curves	265
11.7	Uniqueness Results in a Layered Medium	265
11.8	Open Problems	272
	References	276
12	<i>G. Bao and P. J. Li</i>	
	Shape Reconstruction of Inverse Medium Scattering for the Helmholtz Equation	283
12.1	Introduction	283
12.2	Analysis of the scattering map	285
12.3	Inverse medium scattering	290
12.3.1	Shape reconstruction	291
12.3.2	Born approximation	292
12.3.3	Recursive linearization	294
12.4	Numerical experiments	298
12.5	Concluding remarks	303
	References	303

V Inverse Vibration, Data Processing and Imaging 307

13 *G. M. Kuramshina, I. V. Kochikov and A. V. Stepanova*

Numerical Aspects of the Calculation of Molecular Force Fields from Experimental Data	309
13.1 Introduction	309
13.2 Molecular Force Field Models	311
13.3 Formulation of Inverse Vibration Problem	312
13.4 Constraints on the Values of Force Constants Based on Quantum Mechanical Calculations	314
13.5 Generalized Inverse Structural Problem	319
13.6 Computer Implementation	321
13.7 Applications	323
References	327

14 *J. J. Liu and H. L. Xu*

Some Mathematical Problems in Biomedical Imaging	331
14.1 Introduction	331
14.2 Mathematical Models	334
14.2.1 Forward problem	334
14.2.2 Inverse problem	336
14.3 Harmonic B_z Algorithm	339
14.3.1 Algorithm description	340
14.3.2 Convergence analysis	342
14.3.3 The stable computation of ΔB_z	344
14.4 Integral Equations Method	348
14.4.1 Algorithm description	348
14.4.2 Regularization and discretization	352
14.5 Numerical Experiments	354
References	362

VI Numerical Inversion in Geosciences 367

15 *S. I. Kabanikhin and M. A. Shishlenin*

Numerical Methods for Solving Inverse Hyperbolic Problems	369
15.1 Introduction	369
15.2 Gel'fand-Levitan-Krein Method	370
15.2.1 The two-dimensional analogy of Gel'fand-Levitan-Krein equation	374
15.2.2 N -approximation of Gel'fand-Levitan-Krein equation	377

15.2.3 Numerical results and remarks	379
15.3 Linearized Multidimensional Inverse Problem for the Wave Equation	379
15.3.1 Problem formulation	381
15.3.2 Linearization	382
15.4 Modified Landweber Iteration	384
15.4.1 Statement of the problem	385
15.4.2 Landweber iteration	387
15.4.3 Modification of algorithm	388
15.4.4 Numerical results	389
References	390
16 <i>H. B. Song, X. H. Huang, L. M. Pinheiro, Y. Song, C. Z. Dong and Y. Bai</i>	
Inversion Studies in Seismic Oceanography	395
16.1 Introduction of Seismic Oceanography	395
16.2 Thermohaline Structure Inversion	398
16.2.1 Inversion method for temperature and salinity	398
16.2.2 Inversion experiment of synthetic seismic data	399
16.2.3 Inversion experiment of GO data (Huang et al., 2011)	402
16.3 Discussion and Conclusion	406
References	408
17 <i>L. J. Gelius</i>	
Image Resolution Beyond the Classical Limit	411
17.1 Introduction	411
17.2 Aperture and Resolution Functions	412
17.3 Deconvolution Approach to Improved Resolution	417
17.4 MUSIC Pseudo-Spectrum Approach to Improved Resolution	424
17.5 Concluding Remarks	434
References	436
18 <i>Y. F. Wang, Z. H. Li and C. C. Yang</i>	
Seismic Migration and Inversion	439
18.1 Introduction	439
18.2 Migration Methods: A Brief Review	440
18.2.1 Kirchhoff migration	440
18.2.2 Wave field extrapolation	441
18.2.3 Finite difference migration in $\omega - X$ domain	442
18.2.4 Phase shift migration	443
18.2.5 Stolt migration	443
18.2.6 Reverse time migration	446

18.2.7	Gaussian beam migration	447
18.2.8	Interferometric migration	447
18.2.9	Ray tracing	449
18.3	Seismic Migration and Inversion	452
18.3.1	The forward model	454
18.3.2	Migration deconvolution	456
18.3.3	Regularization model	457
18.3.4	Solving methods based on optimization	458
18.3.5	Preconditioning	462
18.3.6	Preconditioners	464
18.4	Illustrative Examples	465
18.4.1	Regularized migration inversion for point diffraction scatterers	465
18.4.2	Comparison with the interferometric migration	468
18.5	Conclusion	468
	References	471

19 *Y. F. Wang, J. J. Cao, T. Sun and C. C. Yang*

Seismic Wavefields Interpolation Based on Sparse Regularization and Compressive Sensing		475
19.1	Introduction	475
19.2	Sparse Transforms	477
19.2.1	Fourier, wavelet, Radon and ridgelet transforms	477
19.2.2	The curvelet transform	480
19.3	Sparse Regularizing Modeling	481
19.3.1	Minimization in l_0 space	481
19.3.2	Minimization in l_1 space	481
19.3.3	Minimization in l_p - l_q space	482
19.4	Brief Review of Previous Methods in Mathematics	482
19.5	Sparse Optimization Methods	485
19.5.1	l_0 quasi-norm approximation method	485
19.5.2	l_1 -norm approximation method	487
19.5.3	Linear programming method	489
19.5.4	Alternating direction method	491
19.5.5	l_1 -norm constrained trust region method	493
19.6	Sampling	496
19.7	Numerical Experiments	497
19.7.1	Reconstruction of shot gathers	497
19.7.2	Field data	498
19.8	Conclusion	503
	References	503

20 *H. Yang***Some Researches on Quantitative Remote Sensing Inversion 509**

20.1 Introduction 509

20.2 Models 511

20.3 A Priori Knowledge 514

20.4 Optimization Algorithms 516

20.5 Multi-stage Inversion Strategy 520

20.6 Conclusion 524

References 525

Index 529

Part I

Introduction