

Yanfei Wang  
Anatoly G. Yagola  
Changchun Yang  
*Editors*

# Optimization and Regularization for Computational Inverse Problems and Applications

计算反演问题中的优化与正则化方法及其应用



高等教育出版社  
HIGHER EDUCATION PRESS

Yanfei Wang  
Anatoly G. Yagola  
Changchun Yang  
*Editors*

# Optimization and Regularization for Computational Inverse Problems and Applications

计算反演问题中的优化  
与正则化方法及其应用

With 41 figures



高等教育出版社·北京  
HIGHER EDUCATION PRESS BEIJING

Editors

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

©2010 Higher Education Press, 4 Dewai Dajie, Beijing 100120, P. R. China

图书在版编目 (CIP) 数据

计算反演问题中的优化与正则化方法及其应用 = Optimization and Regularization for Computational Inverse Problems and Applications: 英文/王彦飞, (俄)亚哥拉, 杨长春主编.—北京: 高等教育出版社, 2010.5

ISBN 978-7-04-028515-4

I. ①计… II. ①王…②亚…③杨… III. ①数学物理方法—研究—英文 IV. ①O411.1

中国版本图书馆 CIP 数据核字(2010)第 076526 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 陈伟光

出版发行	高等教育出版社	购书热线	010-58581118
社 址	北京市西城区德外大街 4 号	免费咨询	400-810-0598
邮政编码	100120	网 址	http://www.hep.edu.cn
总 机	010-58581000		http://www.hep.com.cn
		网上订购	http://www.landaco.com
经 销	蓝色畅想图书发行有限公司		http://www.landaco.com.cn
印 刷	涿州市星河印刷有限公司	畅想教育	http://www.widedu.com
开 本	787 × 1092 1/16	版 次	2010 年 5 月第 1 版
印 张	23	印 次	2010 年 5 月第 1 次印刷
字 数	620 000	定 价	79.00 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 28515-00

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

Yanfei Wang  
Anatoly G. Yagola  
Changchun Yang  
*Editors*

**Optimization and Regularization for  
Computational Inverse Problems  
and Applications**

# Preface by Anatoly G. Yagola

This volume contains the papers presented by invited speakers of the first international workshop “Optimization and Regularization for Computational Inverse Problems and Applications”. 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 21–25, 2008, just before the opening of the Olympic Games. The workshop was sponsored by the National Natural Science Foundation of China, China-Russia Cooperative Research Project RFBR-07-01-92103-NFSC and the National “973” Key Basic Research Developments Program of China. The main goal of the workshop was to teach about 60 young Chinese participants (mostly geophysicists) how to solve inverse and ill-posed problems using optimization procedures. Eminent specialists from China, Russia (partially sponsored by the Russian Foundation of Basic Research), USA and Austria were invited to present their lectures. Some of them could not participate personally but all invited speakers found a possibility to write papers especially for this publication.

The book covers many directions in the modern theory of inverse and ill-posed problems – the variational approach, iterative methods, using *a priori* information for constructing regularizing algorithms, etc. But the most important for the papers is to show how these methods can be applied to effectively solving of practical problems in geophysics, astrophysics, vibrational spectroscopy, and image processing. This issue should encourage specialists in the inverse problems field not only to investigate mathematical methods and propose new approaches but also to apply them to processing of real experimental data. I would like to wish all of them great successes!

Lomonosov Moscow State University  
Moscow, Russia  
March 2010

Anatoly G. Yagola

# Preface by Editors

The field of inverse problems has existed in many branches of physics, earth science, engineering and mathematics for a long time. From the beginning of the birth of the inversion theory, inverse problem with its modeling design and optimization becomes a multi-disciplinary subject, which has received much more attention nowadays. The aim of the inverse problems, modeling design and optimization is to provide a better, more accurate, and more efficient simulation in practical applications. Many methodologies for solving inverse problems employ optimization algorithms. At the same time, optimization community that employ methods of inverse modeling design could reduce the number of time-consuming analyses required by the typical optimization algorithms substantially. This book provides readers who do research in computational/applied mathematics, engineering, geophysics, medical science, image processing, remote sensing and atmospheric science a background of using regularization and optimization techniques for solving practical inverse problems.

The book covers advances of inversion theory and recent developments with practical applications. Particularly, it emphasizes combining optimization and regularization for solving inverse problems. The methods include standard regularization theory, Fejér processes for linear and nonlinear problems, balancing principle, extrapolated regularization, nonstandard regularization, nonlinear gradient method, nonmonotone (Barzilai-Borwein) method, subspace method and Lie group method. The practical applications include reconstruction problem for inverse scattering, molecular spectra data processing, quantitative remote sensing inversion, seismic inversion by Lie group method and gravitational lensing problem.

Uniqueness of this book is that it provides novel methods for both standard and nonstandard regularization and practical applications in frontiers of sciences. Each chapter is written by renown researchers in their research field respectively. Illustrations and tables are provided for better understanding of their ideas. Scientists, researchers, engineers and as well as graduate students engaged in applied mathematics, engineering, geophysics, medical science, image processing, remote sensing and atmospheric science will benefit from the contents of the book since

the book incorporates a background of using regularization and optimization techniques for solving practical inverse problems.

Chinese Academy of Sciences, Beijing  
Lomonosov Moscow State University, Moscow  
Chinese Academy of Sciences, Beijing  
May 2010

*Yanfei Wang*  
*Anatoly G. Yagola*  
*Changchun Yang*

# List of Contributors

Boris Artamonov

Sternberg Astronomical Institute of Moscow State University,  
Universitetskiy prospekt, 19, Moscow, Russia.

e-mail: bartamon@sai.msu.ru

Hui Cao

Johann Radon Institute for Computational and Applied Mathematics (RICAM),  
Austrian Academy of Science,  
Altenbergstrasse 69, 4040 Linz, Austria.

e-mail: hui.cao@ricam.oeaw.ac.at

Jin Cheng

Department of Mathematics,  
Fudan University, Shanghai 200433, China.

e-mail: jcheng@fudan.edu.cn

Yuhong Dai

State Key Laboratory of Scientific and Engineering Computing,  
Institute of Computational Mathematics and Scientific/Engineering Computing,  
Academy of Mathematics and Systems Science, Chinese Academy of Sciences,  
P.O.Box 2719, Beijing 100190, China.

e-mail: dyh@lsec.cc.ac.cn

Ekaterina Koptelova

Sternberg Astronomical Institute of Moscow State University,  
Universitetskiy prospekt, 19, Moscow, Russia.

e-mail: koptelova@xray.sai.msu.ru

Gulnara Kuramshina

Department of Physical Chemistry, Faculty of Chemistry,  
Lomonosov Moscow State University,  
Moscow 119991, Russia.

e-mail: kuramshi@phys.chem.msu.ru



Xiaowen Li  
Research Center for Remote Sensing and GIS,  
Beijing Normal University,  
Beijing, 100875, China.  
e-mail: lix@bnu.edu.cn

Hong Liu  
Key Laboratory of Petroleum Geophysics,  
Institute of Geology and Geophysics, Chinese Academy of Sciences,  
Beijing 100029, China.  
e-mail: liuhong@mail.igcas.ac.cn

Jijun Liu  
Department of Mathematics,  
Southeast University,  
Nanjing, 210096, China.  
e-mail: jjliu@seu.edu.cn

Shiqian Ma  
Department of Industrial Engineering and Operations Research,  
Columbia University,  
New York, NY 10027-6902, USA.  
e-mail: sm2756@columbia.edu

Qinghua Ma  
College of Art and Science,  
Beijing Union University,  
Beijing, 100083, China.  
e-mail: qinghua@ygi.edu.cn

Sergei Pereverzyev  
Johann Radon Institute for Computational and Applied Mathematics (RICAM),  
Austrian Academy of Science,  
Altenbergstrasse 69, 4040 Linz, Austria.  
e-mail: sergei.pereverzev@ricam.oeaw.ac.at

Elena Shimanovskaya  
Sternberg Astronomical Institute of Moscow State University,  
Universitetskiy prospekt, 19, Moscow, Russia.  
e-mail: eshim@sai.msu.ru

Guozhong Su  
School of Sciences, Hebei University of Technology,  
Tianjin 300130, China.  
e-mail: guozhong-su@hebut.edu.cn

Vladimir V. Vasin  
Department of the Ill-posed Problems,  
Institute of Mathematics and Mechanics UB RAS,

Ekaterinburg, 620219, Russia  
e-mail: vasin@imm.uran.ru

Haibing Wang  
School of Mathematics and Computational Science,  
Hunan University of Science and Technology,  
Xiangtan 411201, China.  
e-mail: wanghb845@yahoo.com.cn

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

Tingyan Xiao  
School of Sciences, Hebei University of Technology,  
Tianjin 300130, China.  
e-mail: ty\_xiao@hebut.edu.cn

Pingli Xie  
School of Sciences,  
Henan University of Technology,  
Zhengzhou 450001, China.  
e-mail: plxie@fudan.edu.cn

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

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

Yaxiang Yuan  
State Key Laboratory of Scientific/Engineering Computing,  
Institute of Computational Mathematics and Scientific/Engineering Computing,  
Academy of Mathematics and Systems Science, Chinese Academy of Sciences,  
Zhong Guan Cun Donglu 55, Beijing, 100190, China.  
e-mail: yyx@lsec.cc.ac.cn

Yuan Zhao  
School of Sciences, Hebei University of Technology,  
Tianjin 300130, China.  
e-mail: zhaoyuan135821@163.com

# Contents

## Part I Introduction

<b>1 Inverse Problems, Optimization and Regularization: A Multi-Disciplinary Subject</b> .....	3
<i>Yanfei Wang and Changchun Yang</i>	
1.1 Introduction .....	3
1.2 Examples about mathematical inverse problems .....	4
1.3 Examples in applied science and engineering .....	5
1.4 Basic theory .....	12
1.5 Scientific computing .....	12
1.6 Conclusion .....	13
References .....	13

## Part II Regularization Theory and Recent Developments

<b>2 Ill-Posed Problems and Methods for Their Numerical Solution</b> .....	17
<i>Anatoly G. Yagola</i>	
2.1 Well-posed and ill-posed problems .....	18
2.2 Definition of the regularizing algorithm .....	22
2.3 Ill-posed problems on compact sets .....	25
2.4 Ill-posed problems with sourcewise represented solutions .....	27
2.5 Variational approach for constructing regularizing algorithms ...	28
2.6 Nonlinear ill-posed problems .....	32
2.7 Iterative and other methods .....	33
References .....	34
<b>3 Inverse Problems with <i>A Priori</i> Information</b> .....	35
<i>Vladimir V. Vasin</i>	
3.1 Introduction .....	35

3.2	Formulation of the problem with <i>a priori</i> information . . . . .	39
3.3	The main classes of mappings of the Fejér type and their properties . . . . .	41
3.4	Convergence theorems of the method of successive approximations for the pseudo-contractive operators . . . . .	46
3.5	Examples of operators of the Fejér type . . . . .	50
3.6	Fejér processes for nonlinear equations . . . . .	53
3.7	Applied problems with <i>a priori</i> information and methods for solution . . . . .	57
3.7.1	Atomic structure characterization . . . . .	57
3.7.2	Radiolocation of the ionosphere . . . . .	58
3.7.3	Image reconstruction . . . . .	59
3.7.4	Thermal sounding of the atmosphere . . . . .	60
3.7.5	Testing a wellbore/reservoir . . . . .	61
3.8	Conclusions . . . . .	62
	References . . . . .	62
<b>4</b>	<b>Regularization of Naturally Linearized Parameter Identification Problems and the Application of the Balancing Principle . . . . .</b>	<b>65</b>
	<i>Hui Cao and Sergei Pereverzyev</i>	
4.1	Introduction . . . . .	65
4.2	Discretized Tikhonov regularization and estimation of accuracy . . . . .	68
4.2.1	Generalized source condition . . . . .	68
4.2.2	Discretized Tikhonov regularization . . . . .	70
4.2.3	Operator monotone index functions . . . . .	71
4.2.4	Estimation of the accuracy . . . . .	73
4.3	Parameter identification in elliptic equation . . . . .	75
4.3.1	Natural linearization . . . . .	75
4.3.2	Data smoothing and noise level analysis . . . . .	77
4.3.3	Estimation of the accuracy . . . . .	78
4.3.4	Balancing principle . . . . .	80
4.3.5	Numerical examples . . . . .	83
4.4	Parameter identification in parabolic equation . . . . .	85
4.4.1	Natural linearization for recovering $b(x) = a(u(T, x))$ . . . . .	86
4.4.2	Regularized identification of the diffusion coefficient $a(u)$ . . . . .	89
4.4.3	Extended balancing principle . . . . .	92
4.4.4	Numerical examples . . . . .	99
	References . . . . .	103
<b>5</b>	<b>Extrapolation Techniques of Tikhonov Regularization . . . . .</b>	<b>107</b>
	<i>Tingyan Xiao, Yuan Zhao and Guozhong Su</i>	
5.1	Introduction . . . . .	107
5.2	Notations and preliminaries . . . . .	109

5.3	Extrapolated regularization based on vector-valued function approximation .....	111
5.3.1	Extrapolated scheme based on Lagrange interpolation ...	112
5.3.2	Extrapolated scheme based on Hermitian interpolation ...	114
5.3.3	Extrapolation scheme based on rational interpolation ...	116
5.4	Extrapolated regularization based on improvement of regularizing qualification .....	118
5.5	The choice of parameters in the extrapolated regularizing approximation .....	119
5.6	Numerical experiments .....	122
5.7	Conclusion .....	125
	References .....	126
<b>6</b>	<b>Modified Regularization Scheme with Application in Reconstructing Neumann-Dirichlet Mapping</b> .....	<b>127</b>
	<i>Pingli Xie and Jin Cheng</i>	
6.1	Introduction .....	127
6.2	Regularization method .....	129
6.3	Computational aspect .....	131
6.4	Numerical simulation results for the modified regularization.....	131
6.5	The Neumann-Dirichlet mapping for elliptic equation of second order .....	135
6.6	The numerical results of the Neumann-Dirichlet mapping .....	136
6.7	Conclusion .....	138
	References .....	138
<b>Part III Nonstandard Regularization and Advanced Optimization Theory and Methods</b>		
<b>7</b>	<b>Gradient Methods for Large Scale Convex Quadratic Functions</b> 141	
	<i>Yaziang Yuan</i>	
7.1	Introduction .....	141
7.2	A generalized convergence result .....	143
7.3	Short BB steps .....	147
7.4	Numerical results .....	149
7.5	Discussion and conclusion .....	154
	References .....	155
<b>8</b>	<b>Convergence Analysis of Nonlinear Conjugate Gradient Methods</b> .....	<b>157</b>
	<i>Yuhong Dai</i>	
8.1	Introduction .....	157
8.2	Some preliminaries .....	160
8.3	A sufficient and necessary condition on $\beta_k$ .....	161

8.3.1	Proposition of the condition	161
8.3.2	Sufficiency of (8.3.5)	163
8.3.3	Necessity of (8.3.5)	166
8.4	Applications of the condition (8.3.5)	168
8.4.1	Property (#)	168
8.4.2	Applications to some known conjugate gradient methods	170
8.4.3	Application to a new conjugate gradient method	175
8.5	Discussion	178
	References	180

<b>9</b>	<b>Full Space and Subspace Methods for Large Scale Image Restoration</b>	<b>183</b>
	<i>Yanfei Wang, Shiqian Ma and Qinghua Ma</i>	
9.1	Introduction	183
9.2	Image restoration without regularization	185
9.3	Image restoration with regularization	186
9.4	Optimization methods for solving the smoothing regularized functional	187
9.4.1	Minimization of the convex quadratic programming problem with projection	187
9.4.2	Limited memory BFGS method with projection	188
9.4.3	Subspace trust region methods	191
9.5	Matrix-Vector Multiplication (MVM)	193
9.5.1	MVM: FFT-based method	193
9.5.2	MVM with sparse matrix	194
9.6	Numerical experiments	197
9.7	Conclusions	200
	References	200

## Part IV Numerical Inversion in Geoscience and Quantitative Remote Sensing

<b>10</b>	<b>Some Reconstruction Methods for Inverse Scattering Problems</b>	<b>205</b>
	<i>Jijun Liu and Haibing Wang</i>	
10.1	Introduction	206
10.2	Iterative methods and decomposition methods	210
10.2.1	Iterative methods	210
10.2.2	Decomposition methods	212
10.2.3	Hybrid method	217
10.3	Singular source methods	218
10.3.1	Probe method	218
10.3.2	Singular sources method	220
10.3.3	Linear sampling method	227

10.3.4	Factorization method .....	228
10.3.5	Range test method .....	231
10.3.6	No response test method .....	233
10.4	Numerical schemes .....	235
	References .....	244
<b>11</b>	<b>Inverse Problems of Molecular Spectra Data Processing .....</b>	<b>249</b>
	<i>Gulnara Kuramshina</i>	
11.1	Introduction .....	249
11.2	Inverse vibrational problem .....	250
11.3	The mathematical formulation of the inverse vibrational problem .....	253
11.4	Regularizing algorithms for solving the inverse vibrational problem .....	255
11.5	Model of scaled molecular force field .....	259
11.6	General inverse problem of structural chemistry .....	261
11.7	Intermolecular potential .....	265
11.8	Examples of calculations .....	266
11.8.1	Calculation of methane intermolecular potential .....	266
11.8.2	Prediction of vibrational spectrum of fullerene $C_{240}$ .....	267
	References .....	271
<b>12</b>	<b>Numerical Inversion Methods in Geoscience and Quantitative Remote Sensing .....</b>	<b>273</b>
	<i>Yanfei Wang and Xiaowen Li</i>	
12.1	Introduction .....	274
12.2	Examples of quantitative remote sensing inverse problems: land surface parameter retrieval problem .....	275
12.3	Formulation of the forward and inverse problem .....	277
12.4	What causes ill-posedness .....	278
12.5	Tikhonov variational regularization .....	279
12.5.1	Choices of the scale operator $D$ .....	279
12.5.2	Regularization parameter selection methods .....	281
12.6	Solution methods .....	282
12.6.1	Gradient-type methods .....	282
12.6.2	Newton-type methods .....	286
12.7	Numerical examples .....	292
12.8	Conclusions .....	297
	References .....	297
<b>13</b>	<b>Pseudo-Differential Operator and Inverse Scattering of Multidimensional Wave Equation .....</b>	<b>301</b>
	<i>Hong Liu, Li He</i>	
13.1	Introduction .....	302
13.2	Notations of operators and symbols .....	303
13.3	Description in symbol domain .....	305

13.4	Lie algebra integral expressions . . . . .	307
13.5	Wave equation on the ray coordinates . . . . .	308
13.6	Symbol expression of one-way wave operator equations . . . . .	310
13.7	Lie algebra expression of travel time . . . . .	312
13.8	Lie algebra integral expression of prediction operator . . . . .	316
13.9	Spectral factorization expressions of reflection data . . . . .	319
13.10	Conclusions . . . . .	323
	References . . . . .	323
<b>14</b>	<b>Tikhonov Regularization for Gravitational Lensing Research .</b>	<b>327</b>
	<i>Boris Artamonov, Ekaterina Koptelova, Elena Shimanovskaya and Anatoly G. Yagola</i>	
14.1	Introduction . . . . .	328
14.2	Regularized deconvolution of images with point sources and smooth background . . . . .	330
14.2.1	Formulation of the problem . . . . .	330
14.2.2	Tikhonov regularization approach . . . . .	333
14.2.3	<i>A priori</i> information . . . . .	335
14.3	Application of the Tikhonov regularization approach to quasar profile reconstruction . . . . .	341
14.3.1	Brief introduction to microlensing . . . . .	341
14.3.2	Formulation of the problem . . . . .	342
14.3.3	Implementation of the Tikhonov regularization approach .	343
14.3.4	Numerical results of the Q2237 profile reconstruction . . . .	345
14.4	Conclusions . . . . .	345
	References . . . . .	346
	<b>Index . . . . .</b>	<b>349</b>



# Part I

## Introduction