

Joint French-Czech Workshop on Krylov Methods for Inverse Problems

July 19 - 20, 2010 Institute of Computer Science (room 318), Pod Vodárenskou věží 2, Praha 8

Inverse problems of imaging present numerous theoretical and numerical challenges, and the multitude of their applications place these problems between various scientific domains. Their formulation leads generally to the resolution of large linear systems. The objective of this workshop is to gather Czech and French specialists to present their last developments in this domain and review the state of the art in the numerical resolution of inverse problems. Particular attention will be devoted to problems of imaging, whose importance in the current scientific landscape does not need to be further demonstrated.

Xavier Bonnefond (*Mathematical Institute of Toulouse*):
The ThermoAcoustic Tomography Inverse Problem

Jurjen Duintjer Tebbens (*ICS AS CR*):
Matrix Inversion and Condition Estimation with Triangular Factors

Serge Gratton (*CERFACS*):
Nonlinear Least Squares Problem Minimization Using Subspace Preconditioners with an Application to Data Assimilation

Didier Henrion (*LAAS-CNRS, University of Toulouse & FEE CTU*):
Recovering Semialgebraic Shapes from Their Moments with Semidefinite Programming

Iveta Hnětynková (*MFF Charles University*):
Revealing the Noise in the Data via the Golub-Kahan Iterative Bidiagonalization

Pavel Jiránek (*CERFACS*):
How to Estimate the Backward Error in LSQR

Pierre Maréchal (*Mathematical Institute of Toulouse*):
Survey of Regularization by Mollification

Zdeněk Strakoš (*MFF Charles University*):
Moments, Model Reduction and Nonlinearity in Solving Linear Algebraic Problems

Petr Tichý (*ICS AS CR*):
On Efficient Numerical Approximation of the Bilinear Form $c^*A^{-1}b$



Mathematical Institute of Toulouse



CERFACS - Centre Européen
de Recherche et Formation
Avancées en Calcul Scientifique



Institute of Computer Science AS CR
Department of Computational Methods

PROGRAMME

MONDAY, July 19

- 9.25 - 9.30 Opening
- 9.30 - 10.30 **Pierre Maréchal** (*Mathematical Institute of Toulouse*):
Survey of Regularization by Mollification
- 10.30 - 10.45 Coffee Break
- 10.45 - 11.45 **Xavier Bonnefond** (*Mathematical Institute of Toulouse*):
The ThermoAcoustic Tomography Inverse Problem
- 11.45 - 12.00 Coffee Break
- 12.00 - 13.00 **Jurjen Duintjer Tebbens** (*ICS AS CR*):
Matrix Inversion and Condition Estimation with Triangular Factors
- 13.00 - 14.30 Lunch Break
- 14.30 - 15.30 **Serge Gratton** (*CERFACS*):
Nonlinear Least Squares Problem Minimization Using Subspace
Preconditioners with an Application to Data Assimilation
- 15.30 - 15.45 Coffee Break
- 15.45 - 16.45 **Pavel Jiránek** (*CERFACS*):
How to Estimate the Backward Error in LSQR

TUESDAY, July 20

- 9.30 - 10.30 **Zdeněk Strakoš** (*MFF Charles University*):
Moments, Model Reduction and Nonlinearity in Solving Linear
Algebraic Problems
- 10.30 - 10.45 Coffee Break
- 10.45 - 11.45 **Iveta Hnětynková** (*MFF Charles University*):
Revealing the Noise in the Data via the Golub-Kahan Iterative
Bidiagonalization
- 11.45 - 12.00 Coffee Break
- 12.00 - 13.00 **Petr Tichý** (*ICS AS CR*):
On Efficient Numerical Approximation of the Bilinear Form $c^*A^{-1}b$
- 13.00 - 14.30 Lunch Break
- 14.30 - 15.30 **Didier Henrion** (*LAAS-CNRS, University of Toulouse & FEE CTU*):
Recovering Semialgebraic Shapes from Their Moments with
Semidefinite Programming

THE THERMOACOUSTIC TOMOGRAPHY INVERSE PROBLEM

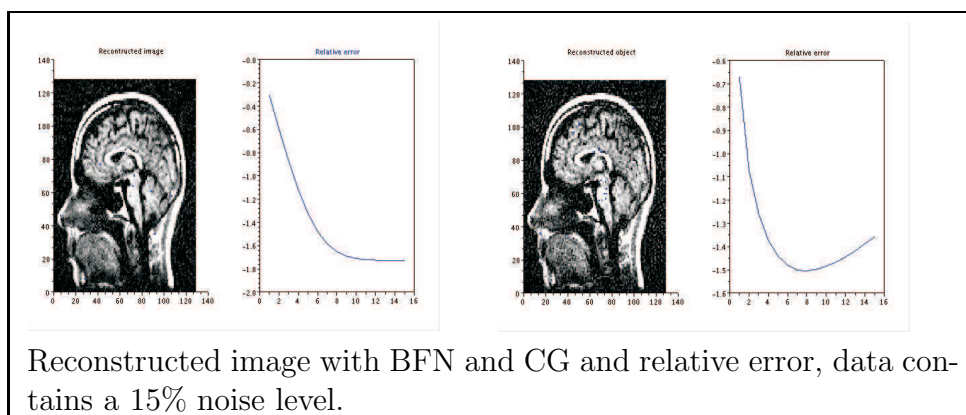
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ThermoAcoustic Tomography (TAT) is a non invasive hybrid imaging technique which uses ultrasound waves emitted from a body submitted to a radio frequency impulse. The absorption of this initial energy causes an amount of thermal expansion, leading to the propagation of a pressure wave outside the body to investigate. This wave is then measured all around the body and the absorption of the initial impulse is highly related to the physiological properties of the tissue, as a result the magnitude of the ultrasonic emission (i.e. thermoacoustic signal), which is proportional to the local energy deposition, reveals physiologically specific absorption contrast. See [1] for an interesting overview.

Most of recent works dedicated to TAT efficiently solve the inverse problem but requires approximations of the model (no attenuation of the wave, measurement all around the body, etc) which may not be appropriate to real-life measurement conditions. That is why we will propose a particular data assimilation method based on a nudging technique: given a evolution model of the state and direct observation (our data), it consists in adding, inside the model equation, a newtonian recall of the state solution to the observations (or data), which is usually called the recall, feedback or nudging term.



References

- [1] P. Kuchment and L. Kunyansky, Mathematics of Thermoacoustic Tomography, *arXiv:0704.0286v2*,(2007).
- [2] D. Auroux and J. Blum, A nudging-based data assimilation method: the Back and Forth Nudging (BFN) algorithm, *Nonlinear Processes in Geophysics*, **15** (2008) 305–319.

MATRIX INVERSION AND CONDITION ESTIMATION WITH TRIANGULAR FACTORS

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Explicit computation of matrix inverses arises in several applications, for instance image reconstruction or signal processing. The computational process can be particularly challenging with ill-conditioned matrices, in which case an accurate condition estimator may play a crucial role. In this talk we restrict ourselves to methods of matrix inversion based on LU or Cholesky decomposition. We start with a brief overview of the properties of classical methods of this type and describe a recently introduced decomposition method which computes the inverse triangular factors as a by-product. In the second part of the talk we discuss condition estimation based on LU or Cholesky decomposition. We concentrate on so-called incremental condition estimation and show how the presence of inverse factors can be exploited to obtain an accurate condition estimator.

This is joint work with **Miroslav Tůma** (ICS AS CR).

NONLINEAR LEAST SQUARES PROBLEM MINIMIZATION USING SUBSPACE PRECONDITIONERS WITH AN APPLICATION TO DATA ASSIMILATION

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We consider parameter estimation problems involving a set of m physical observations, where an unknown vector of n parameters is defined as the solution of a nonlinear least-squares problem regularized by a quadratic penalty term. A Gauss-Newton process is used to solve this large scale optimization problem. The main purpose of this work is to design an efficient algorithm to compute the successive steps of this algorithm, by using a warm-started truncated conjugate gradient approach that take into account problem structure.

We exhibit a subspace of dimension m that contains the solution of these linear least-squares problems, and derive a new variant of the conjugate gradient algorithm (CG) that is more efficient in terms of memory and computational costs than its standard form, whenever m is smaller than n , which is often the case for ill-posed problems arising in Earth observation systems. This CG variant, called Restricted Preconditioned Conjugate Gradient (RPCG), is able to keep all vectors from the standard recurrence in subspaces of dimension m and is algebraically equivalent to CG in exact arithmetics. Interestingly enough, techniques like full re-orthogonalization and subspace preconditioning that could be considered as expensive in CG for large n , become completely affordable in RPCG provided that m is small enough. In particular, we focus on Quasi-Newton preconditioners and show a possible implementation of this technique that uses only by-products of RPCG. We also derived a convergence theory for RPCG, that improves known convergence bounds by restraining the iterates to the appropriate subspace. We also consider a class of preconditioners, known as Limited Memory Pre- conditioners, that generalizes Quasi-Newton preconditioners to Ritz directions and derive preconditioner formulas involving dimension m subspaces. To illustrate all the above theoretical results, numerical experiments are shown on academic problems. The presented algorithms are currently being implemented in an ocean data assimilation system built on the NEMO Global Ocean Circulation Model and experiments on problems with more than 107 unknowns will be presented.

Joint work with **Selime Gurol** (CERFACS), **Jean Tshimanga** (ENSEEIH), **Philippe Toint** (Universit de Namur).

RECOVERING SEMIALGEBRAIC SHAPES FROM THEIR MOMENTS WITH SEMIDEFINITE PROGRAMMING

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Moments of a shape convey key geometric information. For instance, the volume, center of mass, and moments of inertia of an object give an idea of how large it is, where it is located, how round it is, and in which direction it is elongated. Reconstructing a domain from the values of its moments is a well-known inverse problem with applications in probability and statistics, signal processing, tomography or potential theory. In this talk we focus on semialgebraic shapes, i.e. polynomial sublevel sets which are not necessarily convex or connected. We show that a semidefinite programming approach to the generalised problem of moments can be followed to address the reconstruction problem using convex optimisation.

Joint work with **Jean-Bernard Lasserre** (LAAS-CNRS).

REVEALING THE NOISE IN THE DATA VIA THE GOLUB-KAHAN ITERATIVE BIDIAGONALIZATION

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Consider a linear ill-posed problem $Ax \approx b$ with a right-hand side b (observation vector) contaminated by *white noise*, where the noise level is unknown. In each step of the Golub-Kahan iterative bidiagonalization, the original problem is projected onto a lower dimensional subspace, which represents a form of regularization by projection. The projected problem, however, inherits a part of the ill-posedness of the original problem, and therefore some form of inner regularization must be applied. Stopping criteria for the whole process are then based on the regularization of the projected (small) problem.

It was shown in (I. Hnětynková, M. Plešinger, Z. Strakoš: The regularizing effect of the Golub-Kahan iterative bidiagonalization and revealing the noise level in the data, BIT **49**, pp. 669–696 (2009)) that the information from the Golub-Kahan iterative bidiagonalization can be used for *estimating the noise level* in the data. In this presentation we examine a problem whether a similar approach can be used for approximating the unknown noise vector. Such information could further be used for improving accuracy of a regularized solution.

Joint work with **Martin Plešinger** (FM TU Liberec), **Zdeněk Strakoš** (MFF Charles University).

HOW TO ESTIMATE THE BACKWARD ERROR IN LSQR

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We propose efficiently computable stopping criteria for the LSQR method for solving large and sparse linear least squares problems. The original implementation of LSQR allows a cheap estimation of the backward error of the actual approximate solution which can be however much conservative. We present new stopping criteria based on the norm of the actual residual vector projected onto the column-space of the data matrix. We recall its connection to the backward error in least squares problems and show how it can be cheaply estimated at each iteration of LSQR. We also introduce estimates on the size of the optimal backward perturbation of Karlson, Waldn, and Sun using the quantities computed during the LSQR iterations.

SURVEY OF REGULARIZATION BY MOLLIFICATION

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Mollification has been used in approximation theory for a long time, but (to the best of our knowledge) it was introduced in the field of inverse problems only in the 1980's. Notably, a variational formulation of it appeared in the specific context of deconvolution and Fourier synthesis (see reference [4]). Another (non variational) formulation was given shortly after and independently for linear operator equations of the first kind (see reference [5]). In a recent series of papers, asymptotic theorems were exhibited for the variational formulation, first in Fourier synthesis, and then in a more general setting (see references [1] and [2]).

The first part of this talk will be an attempt to give a survey of ideas around the regularization by mollification, with particular attention to the aforementioned asymptotic analysis. The second part will be a speculative discussion on possible numerical strategies for the implementations of the regularization by mollification.

References

- [1] N. Alibaud, P. Maréchal and Y. Saesor, *A variational approach to the inversion of truncated Fourier operators*, Inverse Problems 25 (2009).
- [2] X. Bonnefond, P. Maréchal, *A variational approach to the inversion of some compact operators*, Pacific Journal of Optimization 5(1) (2009), 97-110.
- [3] M. Haltmeier, T. Schuster, O. Scherzer, *Filtered backprojection for thermoacoustic computed tomography in spherical geometry*, Math. Meth. Appl. Sci., 2005.
- [4] A. Lannes, S. Roques, M.-J. Casanove, *Stabilized reconstruction in signal and image processing; Part I: partial deconvolution an spectral extrapolation with limited field*, J. Mod. Opt. 34 (1987), 161-226.
- [5] A.K. Louis, P. Maass, *A mollifier method for linear operator equations of the first kind*, Inverse Problems, 1990.

MOMENTS, MODEL REDUCTION AND NONLINEARITY IN SOLVING LINEAR ALGEBRAIC PROBLEMS

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Krylov subspace methods play an important role in many areas of scientific computing, including numerical solution of linear algebraic systems arising from discretisation of partial differential or integral equations. By their nature they represent *model reductions based on matching moments*. Such view naturally complements, in our opinion, the standard description using the projection processes framework, and it shows their highly nonlinear character.

We present three examples that link algebraic views of problems with views from related areas of mathematics:

- Matching moments reduced order modeling in approximation of large-scale linear dynamical systems is linked with the classical work on moments and continued fractions by Chebyshev and Stieltjes, and with development of the conjugate gradient method by Hestenes and Stiefel.
- We show that Gauss-Christoffel quadrature for a small number of quadrature nodes can be highly sensitive to small changes in the distribution function, and we relate the sensitivity of Gauss-Christoffel quadrature to the convergence properties of the CG and Lanczos methods in exact and in finite precision arithmetic.
- Based on the method of moments, we show how the information from the Golub-Kahan iterative bidiagonalization can be used for estimating the noise level in discrete ill-posed problems.

Joint work with **Iveta Hnětynková** (MFF Charles University), **Dianne Prost O’Leary** (University of Maryland), **Martin Plešinger** (FM TU Liberec), **Petr Tichý** (ICS AS CR).

ON EFFICIENT NUMERICAL APPROXIMATION OF THE BILINEAR FORM $c^*A^{-1}b$

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This talk presents results on efficient and numerically well-behaved approximation of the bilinear form $c^*A^{-1}b$. We briefly outline the matching moment property of the Lanczos and Arnoldi methods, and specify techniques for approximating $c^*A^{-1}b$ with A non-Hermitian, including a new algorithm based on the BiCG method. We show its mathematical equivalence to the existing estimates which use a complex generalization of Gauss quadrature, and discuss its numerical properties. The proposed estimate will be compared with existing approaches using analytic arguments and numerical experiments on a practically important problem that arises from the computation of diffraction of light on media with periodic structure.

Joint work with **Zdeněk Strakoš** (MFF Charles University).