Book of abstracts

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Invited talks

Levenberg-Marquardt and Other Regularisations for Ill-Posed Nonlinear Systems

List of authors:

<u>S. Bellavia</u> [1]

It is well known that inverse problems typically lead to mathematical models that are ill-posed. This means especially that their solution is unstable under data perturbations. Numerical methods that can cope with these problems are so-called regularisation methods. The analysis of such methods for linear problems is relatively complete. The theory for nonlinear problems is developed to a much lesser extent. In this talk we will analyse a class of algorithms for nonlinear ill-posed problems, which includes Levenberg-Marquardt approaches as well as trust-regions and quadratic regularization methods. The noise-free case as well as the realistic situation where noisy data are set will be considered and conditions under which these methods can be seen as regularizing methods for ill-posed problems will be given.

We will eventually show that in these approaches, by properly choosing regularizing terms not only global convergence can be reached but the ill-posedness of the problems can be managed.

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Variational and Ensemble Data Assimilation at Météo-France

List of authors:

L. Berre [2]

G. Desroziers [3]

H. Varella [4]

L. Raynaud [5]

This talk will address recent research developments and associated operational implementations in the Météo-France data assimilation system. On the one hand, variational methods are being used in order to handle e.g. a large number of satellite radiances, and in order to account for the temporal dimension of data assimilation, using a 4D-Var formalism. On the other hand, ensemble techniques are also being developed and employed in order to provide realistic flow-dependent estimates of error covariances at the beginning of the 4D-Var time window.

It will be shown that these two approaches can be combined in a consistent way. Recent achievements in this context will be presented, regarding the estimation of model error contributions, the use of flow-dependent wavelet-based error correlations, and preconditioning issues. These developments, which are detailed in references [1, 2, 3, 4], have benefitted from collaborations associated to the ADTAO project in particular.

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Reasons to Study Derivative-Free Algorithms

List of authors:

J. Dennis [6]

Over the course of my career, continuous nonlinear optimization has come into its own as a crucial area of computational and applied mathematics. When I got my degree in 1966, it was generally true that the available algorithms could not solve the problems encountered by an industrial design engineer. I do not think this is true any longer. A large part of this advancement has been the resurgence of interest in derivative-free algorithms.

I will introduce you to, or remind you of, the class of problems we can now solve using derivative-free methods. These problems are small, very expensive, and they have some universal properties not usually mentioned in polite conversation in the halls of academe. I will not talk about our approaches to these problems, but I will give some practical successes of our algorithms as evidence of the importance of this class of problems, and I will outline two extensions needed now for this class of problems by industrial designers. Specifically, I will mention nonlinear robust optimization and optimization with conflicting objectives. Although I have worked on the really hard and important areas of multidisciplinary design optimization and distributed optimization, these are beyond the scope of a single talk.

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Parallelising 4D-Var using a Saddle Point Formulation

List of authors:

M. Fisher [7]

Four-dimensional variational data assimilation (4D-Var) is a highly sequential algorithm. Iterations of a minimisation algorithm are performed sequentially. Within each iteration, there is an integration of a linear model followed by an integration of its adjoint, and each of these integrations performs a number of sequential timesteps.

Currently, parallelisation of 4D-Var for Numerical Weather Prediction (NWP) is achieved using a spatial distribution of the problem over processors. However, as computer architectures evolve, a purely spatial parallelisation is unlikely to remain sufficient. To exploit highly parallel machines, new dimensions of parallelism must be found.

In this talk, I consider parallelisation of weak-constraint 4DVar in the time dimension. Variants of the 4D-Var algorithm will be categorised according to whether or not they admit such parallelisation. I will present a new, highly-parallel formulation of weak-constraint 4D-Var, based on a saddle point representation of the underlying optimisation problem. Numerical experiments using a simplified analogue of an NWP system will be presented.

References

[1] Fisher M. Parallelisation in the Time Dimension of Four-Dimensional Variational Data Assimilation *submitted to: Quarterly Journal of the Royal Meteorological Society*, 2013.

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Low-rank Tensor Recovery: Theory and Algorithms

List of authors:

D. Goldfarb [8]

C. Mu [9] B. Huang [10] J. Wright [11]

Recovering a low-rank tensor from incomplete or corrupted observations is a recurring problem in signal processing and machine learning. To exploit the structure of data that is intrinsically more than three-dimensional, convex models such low-rank completion and robust principal component analysis (RPCA) have been extended to tensors. In this work, we rigorously establish the recovery guarantees for both tensor completion and tensor RPCA. We also demonstrate that using the most popular convex relaxation for the tensor Tucker rank can be substantially suboptimal in terms of the number of observations needed for exact recovery. We introduce a very simple, new convex relaxation which is shown, both theoretically and empirically, to be greatly superior to the previous model. Moreover, we propose algorithms to solve these low-rank tensor recovery models based on the Accelerated Linearized Bregman (ALB) method and the Alternating Direction Augmented Lagrangian (ADAL) method. Finally, we empirically investigate the recoverability properties of the convex models, and compare the computational performance of the algorithms on both simulated and real data.

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The ADTAO Project on Variational Data Assimilation

List of authors:

S. Gratton [12]

The ADTAO project funded by RTRA-STAE involves several partners in Toulouse who are internationally recognized experts in environmental modelling, data assimilation and applied mathematics: "Laboratoire de Dynamique Terrestre et Planétaire" of the "Observatoire Midi-Pyrénées" (space research), the "Géodésie Spatiale" Team of CNES (geodesy), Météo-France (meteorology), CERFACS (mathematical algorithms and oceanography), IRIT (computer science) and IMT (applied mathematics). These partners share a common objective: to enhance the performance of operational data assimilation systems by improving the representation of model errors in large, multi-scale and highly nonlinear dynamical systems and by designing optimisation algorithms able to solve maximum likelhood optimization problems involving millions of degrees of freedom.

In this talk, we describe the general organisation of the project and outline the main results obtained by the scientific teams and by the visiting senior scientists in the last four years.

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[12]IRIT, University of Toulouse and CERFACS, France

Nonsmooth Optimization and Equation Solving via Algorithmic Piecewise Linearization

List of authors:

A. Griewank [13]

Most nonsmooth problem functions are in fact piecewise smooth, which means that their generalized Jacobians are finitely generated. Then the functions can be locally approximated up to second order discrepancies by piecewise linear models. These can be generated in an AD like fashion and manipulated using standard techniques of numerical linear algebra. We discuss the iterative solution of Lipschitzian systems of equations by piecewise Newton and the unconstrained optimization of Lipschitzian functions by true steepest descent. Convergence is guaranteed in under the additional assumptions of coherent orientation and convexity, respectively.

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Introducing PENLAB, an MATLAB code for nonlinear (and) semidefinite optimization

List of authors:

M. Kocvara [14]

[14]University of Birmingham, UK

Do You Trust Your Algorithms?

List of authors:

J. Moré [15]

S. Wild [16]

We have been studying the accuracy and stability of algorithms for at least the last fifty years, but new issues arise as algorithms and computational environments evolve. In this talk we explore these issues and show that the accuracy and uncertainty of algorithms should be viewed in terms of computational noise.

We define computational noise for a function and present examples that illustrate sources of computational noise: large-scale calculations, iterative and adaptive algorithms, and mixed-precision calculations. We present a new algorithm, ECnoise, for quantifying the noise level of a computed function, and show that ECnoise produces reliable results in few function evaluations and offers new insights into building blocks of large scale simulations.

We discuss two applications of computational noise. We show how computational noise can destroy the accuracy of derived calculations, in particular, derivatives. We also show that the noise level can be used to obtain near-optimal finite difference estimates of the derivatives of a noisy deterministic function.

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Preconditioner Updates for Solving Sequences of Indefinite Linear Systems in Optimization

List of authors:

B. Morini [17]

The problem of solving sequences of indefinite linear systems is a key issue in many optimization techniques. Recently, in the iterative solution of large-scale systems there has been a growing interest in improving the solution of the overall sequence by sharing some computational effort throughout the sequence. To this end, cheap updates of an existing preconditioner for one matrix of the sequence have been proposed in order to build preconditioners for subsequent matrices.

In this talk we address the problem of preconditioning two classes of indefinite systems: KKT systems arising in large-scale optimization methods for quadratic programming and possibly nonsymmetric systems arising from large nonlinear systems of equations. We present and analyse new strategies which are based on the availability of the factorization of a preconditioner for a reference matrix of the sequence and attempt to cheaply approximate the ideal update to such preconditioner. Numerical results showing the performance of these techniques are presented.

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Inexact Second-Order Methods for Machine Learning

List of authors:

 J. Nocedal [18]

F. Oztoprak [19]

R. Byrd [20]

In many machine learning applications, it is imperative that the optimization algorithm make fast initial progress toward the solution as this may be sufficient to obtain a good generalization error. For this reason, first-order optimization methods, like the stochastic gradient method and variants that employ Nesterov acceleration, have become very popular. In this talk we consider a second-order method that we call inexact sequential Lasso method. It achieves fast initial progress and enjoys the benefits of second-order iterations. We discuss the theoretical convergence properties of this iteration and illustrate its numerical performance on a variety of applications.

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[19]Istanbul Technical University, Turkey
[20]University of Colorado, Boulder, USA

A Fast Method for Generating Trust Region Steps subject to Linear Constraints

List of authors:

M.J.D. Powell [21]

The speaker is developing the LINCOA software for minimization without derivatives when there are general linear constraints on the variables. An exact trust region step would minimize a quadratic model within a trust region subject to the linear constraints, but LINCOA generates an estimate of this step in only of magnitude $n2$ operations, where n is the number of variables, in order that n can be quite large. Active sets of constraints are employed, which reduce the number of degrees of freedom in the variables until the active set is updated. A piecewise path is generated from the trust region centre, each piece being a conjugate gradient step or a move round the trust region boundary. The conjugate gradient steps are restarted at the best point so far when the active set is changed. The calculations for the new active set are analogous to applying conjugate gradients without linear constraints when the starting point is not at the trust region centre. We address this problem briefly, and find that the Krylov subspace view of conjugate gradients has a severe disadvantage. Finally, some numerical experiments investigate whether the trust region procedure of LINCOA is suitable for linearly constrained optimization with hundreds of variables.

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Using Spectral Information to Precondition Saddle-Point Systems

List of authors:

A. Sartenaer [22]

D. Ruiz [23]

Ch. Tannier [24]

For nonsingular indefinite matrices of saddle-point (or KKT) form, Murphy, Golub and Wathen [1] have proposed an ideal block diagonal preconditioner based on the exact Schur complement. In this talk, assuming a zero (2,2) block, we focus on the case where the (1,1) block is symmetric positive definite and (eventually) very badly conditionned, but with only a few very small eigenvalues. Under the assumption that a good approximation of these eigenvalues and their associated eigenvectors is available, we consider different approximations of the block diagonal preconditioner of Murphy, Golub and Wathen. We analyze the spectral properties of the preconditioned matrices and show how it is possible to appropriately recombine the available spectral information from the (1,1) block through a particular Schur complement approximation that allows to build an efficient block diagonal preconditioner with little extra cost. We finally illustrate the performance of the proposed preconditioners with some numerical experiments, showing that the resulting technique actually reduces to efficiently solve problems associated to the blocks, separately.

References

[1] M. Murphy, G. Golub, and A. Wathen A Note on Preconditioning for Indefinite Linear Systems *SIAM Journal on Scientific Computing*, 21(6):1969–1972, 2000.

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[22]University of Namur, Belgium
[23]ENSEEIHT-IRIT, France
[24]University of Namur, Belgium

CG versus MINRES on Positive Definite Systems

List of authors:

M. A. Saunders [25]

For symmetric positive definite systems $Ax = b$, the CG iterates $\{x_k\}$ are known to have three desirable properties:

P1:	$\|x - x_k\|$	decreases monotonically,
P2:	$\|x - x_k\|_A$	decreases monotonically,
P3:	$\|x_k\|$	increases monotonically,

where $\frac{1}{2}\|x - x_k\|_A = \frac{1}{2}x_k^T A x_k - b^T x_k + \text{constant}$. P1 was shown by Hestenes and Stiefel [5], P2 follows by design [5], and P3 was shown by Steihaug [6]. For the large-scale trust-region problem with A possibly indefinite, P2 and P3 are vital for the CG-based Steihaug-Toint method [6, 7] (until negative curvature is encountered) and for the Lanczos-based method GLTR (Gould et al. [4]).

We now know that P1, P2, P3 also hold for MINRES on positive definite systems. P1 and P2 were proved by Hestenes and Stiefel for their CR method [5] (which is equivalent to MINRES when A is definite). P3 was shown by Fong [2, 3], and it implies that the backward errors for the MINRES iterates are monotonic when A is definite (see Theorems 1 and 2 below).

With these results in mind, we compare CG and MINRES on a range of positive definite systems from the UFL sparse matrix collection [1]. While MINRES is generally reserved for indefinite systems, we feel it should be considered even if A is definite.

THEOREM 1 (Titley-Peloquin [8], restated in terms of ψ_k). For given tolerances $\alpha, \beta \geq 0$ with $\psi_k \equiv \alpha\|A\|\|x_k\| + \beta\|b\|$ and $r_k \equiv b - Ax_k$, the optimization problem

$$\min_{\xi, E, f} \xi \quad \text{st} \quad (A + E)x_k = b + f, \qquad \frac{\|E\|}{\|A\|} \leq \alpha\xi, \qquad \frac{\|f\|}{\|b\|} \leq \beta\xi$$

has solution ξ_k, E_k, f_k given by

$$\xi_k = \frac{\|r_k\|}{\psi_k}, \qquad E_k = \frac{\alpha\|A\|}{\psi_k\|x_k\|}r_k x_k^T, \qquad f_k = -\frac{\beta\|b\|}{\psi_k}r_k, \qquad \frac{\|E_k\|}{\|A\|} = \alpha\xi_k, \qquad \frac{\|f_k\|}{\|b\|} = \beta\xi_k.$$

Comment. We define ξ_k to be the *normwise relative backward error* for x_k, and say that x_k is an *acceptable* solution of $Ax = b$ iff $\xi_k \leq 1$ (i.e. if $\|r_k\| \leq \psi_k = \alpha\|A\|\|x_k\| + \beta\|b\|$).

THEOREM 2 (Fong [2, 3]). For any $\alpha \geq 0$, $\beta \geq 0$ (with $\alpha + \beta > 0$), the relative backward errors ξ_k (and their components $\|E_k\|/\|A\|$ and $\|f_k\|/\|b\|$) decrease monotonically when MINRES is applied to positive definite $Ax = b$.

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Joint work with David Fong

Proof. With $\|r_k\|$ decreasing monotonically and property P3 holding, we see that ξ_k is monotonic.

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[1] T. A. Davis. *University of Florida Sparse Matrix Collection*, 2013. `http://www.cise.ufl.edu/research/sparse/`.

[2] D. C.-L. Fong. *Minimum-Residual Methods for Sparse Least-Squares Using Golub-Kahan Bidiagonalization*, PhD thesis, ICME, Stanford University, Dec 2011.

[3] D. C.-L. Fong and M. A. Saunders. CG versus MINRES: An empirical comparison, *SQU Journal for Science*, 17(1):44–62, 2012. `http://www.stanford.edu/group/SOL/reports/SOL-2011-2R.pdf`.

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[6] T. Steihaug. The conjugate gradient method and trust regions in large scale optimization, *SINUM*, 20(3):626–637, 1983.

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[8] D. Titley-Peloquin. *Backward Perturbation Analysis of Least Squares Problems*, PhD thesis, School of Computer Science, McGill University, 2010.

Probabilistic Model Based Derivative Free Methods

List of authors:

K. Scheinberg [26]

A. S. Bandereira [27]

L. N. Vicente [28]

R. Chen [29]

Traditional analysis of model based derivative free optimization methods relies on the worst case behavior of the algorithmic steps and the models involved. There are conditions that the models and the iterates have to satisfy to guarantee convergence. Such requirements are difficult or costly to satisfy in practice and are often ignored in practical implementations. We will present a probabilistic view point for such algorithms, showing that convergence still holds even if some properties fail with some small enough probability. We will discuss several settings where this approach useful and we will discuss advantages of using regularized models in the derivative free setting.

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Optimization for Bayesian Estimation. The case of Variational Assimilation of Meteorological Observations

List of authors:

O. Talagrand [30]

M. Jardak [31]

Optimization is at the basis of *Variational Assimilation* of meteorological observations, which adjusts a numerical model of the atmospheric flow to observations distributed over a period of time. Variational Assimilation is used operationally in several major meteorological centres. Adjustment is achieved by numerical minimization of a scalar objective function (most often of gaussian form) which measures the misfit between the observations and a model solution.

All the available data (model and observations) are affected with some uncertainty, and it is natural to consider assimilation as a problem in Bayesian estimation. Specifically, determine the probability distribution for the state of the flow, conditioned by the available data. In the linear and (additive) gaussian case, a simple numerical algorithm, called *Ensemble Variational Assimilation* (*EnsVar*), produces an ensemble of independent realizations of the conditional probability distribution. Specifically, perturb the data according to their own error probability law, perform the assimilation on the perturbed data, and repeat the process.

This simple algorithm has been heuristically implemented on two small dimension chaotic systems, the Lorenz-96 system and the Kuramuto-Sivashinsky equation. The size of the ensembles is 30. For long assimilation periods, over which a linear local approximation is not valid, the objective function can possess distinct minima. The absolute minimum is then obtained through the process of *Quasi-Static Variational Assimilation (QSVA)*, in which the length of the assimilation period is progressively increased.

The results are interpreted in terms of the properties of the ensembles produced by EnsVar, considered as defining probability distributions. There is no general criterion for objectively checking the Bayesian character of probability distributions. The weaker property of *reliability, i.e.* statistical consistency between the reality and the distributions, is used instead. Even in the case of strong nonlinearities, the ensembles show almost perfect reliability. The corresponding *resolution, i.e.* the capability of producing different probability distributions for different situations, is also high. But, as can be expected, it degrades with fewer observations. In addition, the ensembles, at the degree of accuracy defined by their size, are gaussian. These various conclusions are valid in both cases of *strong constraint* assimilation, in which the assimilating model is exact, and the objective function measures only misfit to the observations, and *weak constraint* assimilation, in which the assimilating model is inexact, and a corresponding misfit term is included in the objective function. In the latter

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case, the additional misfit term actually acts as a regularizing term in the minimization.

Comparison, made at constant ensemble size, with two other algorithms for "ensemble assimilation", namely the *Ensemble Kalman Filter* and the *Particle Filters*, shows higher performance, in particular higher reliability, for EnsVar. However, this is obtained, in the present setting, at a higher numerical cost.

The significance of these results is discussed, in particular in the perspective of Bayesian estimation.

Inexact Range Space Methods

List of authors:

Ph. L. Toint [32]

S. Gratton [33]

J. Tshimanga [34]

In this talk we present range-space variants of standard Krylov iterative solvers for unsymmetric and symmetric linear systems and to discuss how inexact matrix-vector products may be used in this context. The new range-space variants are characterized by possibly much lower storage and computational costs than their full-space counterparts, which is crucial in data assimilation applications and other inverse problems. However, this gain is achieved without sacrificing the inherent monotonicity properties of the original algorithms, which are of paramount importance in data assimilation applications. The use of inexact matrix-vector products is shown to further reduce computational cost in a controlled manner. We refer to [1] for further detail.

References

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Global Rates for Zero-Order Methods

List of authors:
L. N. Vicente [35]

In some derivative-free methods, it is possible to develop worst case complexity bounds in terms of the number of iterations or function evaluations to reach some level of stationarity. Such global rates complement existing analyses of global convergence by providing additional insight and comparisons.

We show that the broad class of direct-search methods of directional type, based on imposing sufficient decrease to accept new iterates, exhibits the same global rates or worst case complexity bounds of the gradient method for the unconstrained minimization of a smooth function, both in the nonconvex and convex cases. A smoothing direct search approach is also discussed capable of deliver a global rate in the nonsmooth nonconvex setting.

We will also discuss some recent interesting discoveries in probabilistic direct-search methods where polling does not rely necessarily on positive spanning sets and global rates are developed for certain positive probability.

This is joint work with M. Dodangeh, R. Garmanjani, S. Gratton, C. Royer, and Z. Zhang.

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Covariance Modelling and Minimization for Variational Ocean Data Assimilation

List of authors:

A. Weaver [36]

S. Gratton [37]

S. Gürol [38]

I. Mirouze [39]

A. Moore [40]

A. Piacentini [41]

O. Titaud [42]

This talk will describe research developments made in the ADTAO project in variational data assimilation (VDA) for ocean applications. Theoretical and practical advances have been made in the modelling of the background (prior) error covariances and in the minimization algorithms used to solve the VDA problem.

The background error covariance matrix ($\mathbf{B}$) is modelled using a diffusion operator. Computational aspects of the method are discussed within the context of a global ocean VDA system. The potential of the method for representing general (anisotropic, inhomogeneous) covariances from an ensemble is also discussed.

In global ocean applications the number of observations is far fewer than the number of control variables that need to be estimated. A dual formulation of a $\mathbf{B}$-preconditioned conjugate gradient algorithm, which performs the minimization in a space spanned by vectors of the size of the observation vector, is shown to bring significant practical benefits in two operational ocean VDA systems.

More details can be found in [1] and [2].

References

[1] Weaver, A. T. and I. Mirouze. On the diffusion equation and its application to isotropic and anisotropic correlation modelling in variational assimilation. *Quarterly Journal of the Royal Meteorological Society*, 139:3605–3625, 2013.

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[36]CERFACS, Toulouse, France
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[38]ECMWF, Reading, UK
[39]Met Office, Exeter, UK
[40]University of California, Santa Cruz. USA
[41]CERFACS, France
[42]CERFACS, France

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Randomized Algorithms in Optimization

List of authors:

S. Wright [43]

J. Liu [44]

Modern optimization algorithms are making use more and more of randomization as a means of reducing the amount of information needed to perform each step of the algorithm, while eventually accessing enough information about the problem to identify a good approximate solution. Stochastic gradient methods, which obtain gradient estimates from small samples of a full data set, are one example of such methods. Related techniques include the Kaczmarz method for linear algebraic systems and coordinate descent methods in optimization. In this talk, we focus on parallel versions of these methods that are suited to asynchronous implementation on multicore processors. Convergence theory for these methods is described, along with some computational experience.

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[44]University of Wisconsin-Madison, USA

An Augmented Lagrangian Trust Region Method for Equality Constrained Optimization

List of authors:

Y.-X. Yuan [45]

In this talk, we present a trust region method for solving equality constrained optimization problems, which is motivated by the famous augmented Lagrangian function. It is different from standard augmented Lagrangian methods where the augmented Lagrangian function is minimized at each iteration. This method, for fixed Lagrange multiplier and penalty parameters, tries to minimize an approximate model of the augmented Lagrangian function to generate the next iterate. A condition is introduced to decide whether the Lagrange multiplier should be updated. We also suggest a new strategy for adjusting the penalty parameters. Global convergence of this method is established under mild conditions. Furthermore, we analyze the behavior of penalty parameters and figure out in which case they will be bounded from above. Numerical experiments on problems from the CUTEr set collection reveal that our method is very promising.

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[45]Chinese Academy of Sciences, China

Contributed talks

Optimizing City Traffic using Time-Expanded Graphs

List of authors:

S. Felix [46]

J. Galtier [47]

In the case of car trafic networks and vehicle routing, we have a set of journey requests in a network incomming from some vehicles. Each vehicle wants to travel from a given origin to a given destination starting at a given departure time. We choose to model such a network as a time-expanded graph and journeys as paths in this graph. Our goal is to find a minimum cost collection of paths that satisfy all requests. Since two vehicles cannot be at the same time and at the same place without implying a collision, we want our collection of paths to be vertex-disjoint. Moreover, we want to forbid overtakings in our solution. In this paper, we formulate our problem as an integer linear program. All the properties wanted (vertex-disjoint paths, no overtakings) give raise to some incompatibilities in the simultaneous use of some edges of the graph, and could be modelled as constraints. We provide methods to reduce the number of constraints and solve the given integer linear program. We show that savings in the model size can be up to 95% depending on the particular city.

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Derivative-Free Optimization via Proximal Point Methods

List of authors:

Y. Lucet [48]

W. Hare [49]

Many standard techniques in Derivative-Free Optimization (DFO) are based on using model functions to approximate the objective function, and then applying classic optimization methods on the model function. For example, the details behind adapting steepest descent, conjugate gradient, and quasi-Newton methods to DFO have been studied in this manner. In this paper we demonstrate that the proximal point method can also be adapted to DFO. To that end, we provide a derivative-free proximal point (DFPP) method and prove convergence of the method in a general sense. In particular, we give conditions under which the gradient values of the iterates converge to 0, and conditions under which an iterate corresponds to a stationary point of the objective function. More details can be found in [1].

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A Subspace Decomposition Framework for Nonlinear Optimization: Global Convergence and Global Rates

List of authors:

Z. Zhang [50]

S. Gratton [51]

L. N. Vicente [52]

We discuss a general subspace decomposition framework for optimization (for the moment without constraints). Two versions of the framework are presented, namely a Levenberg-Marquardt version and a trust-region one. We establish global (asymptotic) convergence and derive global rates for both of them. We also discuss how to exploit the framework to design parallel and multilevel derivative-free algorithms for large-scale problems.

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Posters

A Decomposition-based Optimal Control Method for Aircraft Conflict Avoidance Problem

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Aircraft conflict avoidance is crucial in air traffic management, and it is even more challenging as the air traffic is continuously increasing. The problem is to keep a given minimum safety distance for aircraft along their trajectories. To guarantee aircraft separation, various maneuvers can be performed: heading changes, level assigments, speed variations or some combinations of these three possibilities.

We address the aircraft conflict avoidance problem through velocity regulation maneuvers. We propose optimal control-based model and approaches by considering that the aircraft acceleration are the commands. We choose to minimize a quadratic-energy cost function depending on speed variations. We propose a problem decomposition strategy which identifies different regions with respect to the importance to check the crucial separation condition.

Based on this decomposition, we apply direct and indirect numerical shooting optimal control methods depending on the regions. The direct method is based on time-discretization and the use of numerical integrators to replace the differential equations. This transformation leads to a large-scale nonlinear continuous optimization problem. When the separation constraint is not necessary, an indirect method via the Pontryagin maximum principle provides the analytical solution. The insertion of this analytical solution into the criterion significantly reduces the number of variables and constraints involved in the nonlinear problem to solve. The proposed combination of optimal control methods, tailored on the aircraft con ict avoidance problem, yields efficient numerical results.

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Globally Convergent Evolution Strategies and CMA-ES

List of authors:

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In this work, we show how to modify a large class of evolution strategies (ES) to rigorously achieve a form of global convergence, meaning convergence to stationary points independently of the starting point. The type of ES under consideration recombine the parents by means of a weighted sum, around which the offsprings are computed by random generation. One relevant instance of such ES is CMA-ES.

The modifications consist essentially of the reduction of the size of the steps whenever a sufficient decrease condition on the function values is not verified. When such a condition is satisfied, the step size can be reset to the step size maintained by the ES themselves, as long as this latter one is sufficiently large. We suggested in [1] a number of ways of imposing sufficient decrease for which global convergence holds under reasonable assumptions (in particular density of certain limit directions in the unit sphere).

Given a limited budget of function evaluations, our numerical experiments [1] have shown that the modified CMA-ES is capable of further progress in function values. Moreover, we have observed that such an improvement in efficiency comes without deteriorating the behavior of the underlying method in the presence of nonconvexity.

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The ID4CS Project: Integrative Design for Complex Systems using a Self-Adaptive Multi-Agent System

List of authors:

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A nine partner strong ANR funded research project for a 4.8 M euros total budget, currently in the last validation phase. Application of the Self-Adaptive Multi-Agent Systems Technology for an innovative approach to Multi-Disciplinary Optimization by distributing and decentralizing the optimization process with a natural expression of complex design problems. Test Cases include turbo fan optimization and preliminary aircraft design.

Further details and reference can be found in [1].

References

[1] The ID4CS Consortium : IRIT, Airbus, Snecma, Artal, Upetec, IMT, ICA, EMSE, INRIA http://www.irit.fr/id4cs/

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Preconditioning the Saddle Point Systems Arising from Variational Data Assimilation

List of authors:

S. Gürol [60]

M. Fisher [61]

This poster will address the numerical solution of the saddle point system arising from four dimensional variational (4D-Var) data assimilation, including a study of preconditioning and its convergence properties. This new saddle point formulation [3] of 4D-Var allows parallelization in time dimension. Therefore, it represents a crucial step towards higher computational efficiency, since 4D-Var approaches otherwise require many sequential computations.

In recent years, there has been increasing interest in saddle point problems which arise in many other applications such as constrained optimization, computational fluid dynamics, optimal control and so forth. The key issue of solving saddle point systems with Krylov subspace methods is to find efficient preconditioners [1]. This poster focuses on the inexact constrained preconditioner proposed by [2] and presents numerical results obtained from the Object Oriented Prediction System (OOPS) developed by ECMWF.

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Recent Advance in Global Optimization
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The existing methods in global optimization can be classified as deterministic and probabilistic. Deterministic methods include: Lipschitzian methods, Branch and Bound methods, Cutting Plane methods, Difference of Convex Function methods, Outer Approximation methods, Reformulation- Linearization methods, Interval methods. These methods demand the exponential number of iterations for finding the global extreme.

The probabilistic methods include among others: random searches, genetic and evolutionary methods. However, these methods allow to find a global extreme only with some probability.

We propose new methods for deterministic global optimization: The Semidefinite Programming (SDP), Polyconvex Optimization (PO) and Exact Quadratic Regularization (EQR).We offer new methods for solution of the problems SDP and PO. EQR – is recent essential advance in global optimization. Let's consider these new methods for the solution of the problem of global optimization.

The semidefinite simplex-method is developed for the solution of the semidefinite optimization problems

$$\min\{C \bullet X | A_i \bullet X = b_i, i = 1, ..., m, X \succeq 0\}$$

This method allows to find the solution of a problem SDP in the form of a convex combination of matrixes of a rank unit

$$X = \sum \alpha_i x_i x_i^T$$

where new vector x_k is the solution of the problem

$$\min\{x^T Q x | ||x||^2 = 1\}$$

and

$$Q = C - \sum_i C \bullet x_i x_i^T \sum_{j=1}^m b_{ij}^{-1} A_j,$$

b_{ij}^{-1} is the element of the inverse basic matrix of simplex method. The problem SDP is solved if the matrix Q is positive definite. Usually semidefinite relaxation is used

$$x^T A x = A \bullet x x^T = A \bullet X$$

for the solution of global optimization problems.

The problems of PO can be transformed into convex one with reverse convex constraint

$$\min\{c^T x | g_i(x) \leq 0, i = 1, ..., m, h(x) \leq 0, x \geq 0\}$$

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where all $g_i(x)$, $h(x)$ are convex functions. We construct a polyhedral cone that contains a convex set $\{x|h(x) \leq 0\}$. The generatrices of polyhedral cone define the cutting plane $p^T x \geq q$. Let's solve convex problem

$$\min\{c^T x|g_i(x) \leq 0, i = 1, ..., m, h(x) \leq 0, p^T x \geq q, x \geq 0\}$$

If its solution is feasible, then it is optimum. Otherwise, we construct a new polyhedral cone.

The exact quadratic regularization allows to construct the most effective method in global optimization. We transform the problem

$$\min\{f_0(x)|f_i(x) \leq 0, i = 1, ..., m, x \in E^n\} \tag{1}$$

where all functions $f_i(x)$ are twice differentiable, x is a vector in n-dimensional Euclidean space E^n. Let the solution of a problem (1) exist, its feasible domain is bounded and x^* – the point of global minimum (1). We transform the problem (1) to the following one

$$\min\{x_{n+1}|f_0(x) + s \leq x_{n+1}, f_i(x) \leq 0, i = 1, ..., m\} \tag{2}$$

where the value s is chosen so that $f_0(x^*) + s \geq ||x^*||^2$. The solution of the problem (2) is the point (x^*, x_{n+1}^*) where $x_{n+1}^* = f_0(x^*) + s \geq 0$. Further, using the replacement $x = Az$ where matrix A of the order $(n+1) \times (n+1)$ is given by

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ z_1 & z_2 & \dots & z_{n+1} \end{pmatrix}$$

The problem (2) is transformed to the following one

$$\min\{||z||^2|f_0(\bar{z}) + s \leq ||z||^2, f_i(\bar{z}) \leq 0, i = 1, ..., m, z \in E^{n+1}\} \tag{3}$$

where $\bar{z} = (z_1, ..., z_n)$. Thus the problem (1) transformed to the minimization of a norm of a square vector. The value $r > 0$ exists so that all functions $f_i(\bar{z}) + r||z||^2$ are convex on the bounded feasible domain of the problem (1). It follows from the fact that Hessians of these functions are positively defined matrixes (matrixes with a dominant main diagonal). Let's use the quadratic regularization to transform the problem (3) in to the following convex problem

$$\min\{d|g_i(z) \leq d, i = 0, 1, ..., m, r||z||^2 \leq d\} \tag{4}$$

or

$$\max\{||z||^2|g_i(z) \leq d, i = 0, 1, ..., m\} \tag{5}$$

where all $g_i(z)$ are strong convex functions

$$g_0(z) = f_0(\bar{z}) + s + (r-1)||z||^2$$

and

$$g_i(z) = f_i(\bar{z}) + r||z||^2, i = 1, ..., m.$$

Let (z^*, d^*) is the solution of the problem (4). If $r||z^*||^2 = d^*$ holds then z^* is the solution of the problem (1). Let's notice that the feasible domain of the problem (5) approximate to intersection of spheres if $r \to \infty$. But the solution of the problem

$$\max\{||x||^2 | ||x - a^i||^2 \le r_i^2, i = 1, ..., m\} \tag{6}$$

can be found by a dual method. As a result we have

$$\min\{\frac{||\sum_{i=1}^m \lambda_i a^i||^2}{\sum_{i=1}^m \lambda_i - 1} - \sum_{i=1}^m \lambda_i(||a^i||^2 - r_i^2)\} \tag{7}$$

subject to

$$||\frac{\sum_{i=1}^m \lambda_i a^i}{\sum_{i=1}^m \lambda_i - 1} - a^i||^2 \le r_i^2, i = 1, ..., m, \sum_{i=1}^m \lambda_i - 1 \ge 0, \lambda \ge 0. \tag{8}$$

We put the solution of the dual problem (7–8) into the formula

$$x = \frac{\sum_{i=1}^m \lambda_i a^i}{\sum_{i=1}^m \lambda_i - 1}$$

and find the solution of the problem (6). Let's notice, that the problem (6) can have the duality gap is nonzero.

The EQR allows to find the best solutions for a lot of known test problems in global optimization. New methods are simple for making up the software. The EQR can be used for the solution of discrete problems. The comparative numerical experiments have shown that new methods are very efficient and promising.

Nonsmooth Nonconvex Optimization Approach to Clusterwise Linear Regression Problems

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In this paper we consider the clusterwise linear regression problem. A new approach for solving the clusterwise linear regression problems is proposed based on a nonsmooth nonconvex formulation. We present an algorithm for minimizing this nonsmooth nonconvex function. This is an incremental algorithm that gradually finds clusters and linear regression functions within these clusters and minimizes the overall fit function. A special procedure is introduced to generate a good starting point for solving global optimization problems at each iteration of the incremental algorithm. Such an approach allows one to find global or near global solution to the problem when the data sets are sufficiently dense. The algorithm is compared with the multistart Spath algorithm on several publicly available data sets for regression analysis.

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Spectral Theory of Some Copositive Matrices

List of authors:

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A symmetric matrix A is called copositive if the quadratic form $x^T A x$ is nonnegative for all nonnegative values of the variables $x^T = (x_1, x_2, \ldots, x_n,)$. In this talk, we give a spectral constructive characterizations of some copositive matrices: If $\lambda_1 < \lambda_2$ are the eigenvalues of A and $\lambda_1 < 0 < \lambda_2$ then

$$A \ \text{copositive} \quad \Leftrightarrow \quad \|P_{E_-}(x)\|^2 \leq -\frac{\lambda_2}{\lambda_1}\|P_{E_+}(x)\|^2 \quad \forall \ x \geq 0$$

where $E_- = \{x \ | \ Ax = \lambda_1 x\}$, $E_+ = \{x \ | \ Ax = \lambda_2 x\}$. P_{E_-} and P_{E_+} are the orthogonal projections in these spaces.

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On the Numerical Solution of Constrained Eigenvalue Problems in Structural Engineering

List of authors:

M. Porcelli [68]

V. Binante [69] M. Girardi [70] C. Padovani [71] G. Pasquinelli [72] D. Pellegrini [73]

The poster is devoted to the analysis of the numerical linear algebra issues arising in the modal analysis of structures with application to masonry construction of historical interest. Although the constitutive equation adopted for masonry [1] is nonlinear, modal analysis gives important qualitative information on the dynamic behavior of masonry structures and allows for assessing their seismic vulnerability, while taking Italian regulations into account.

Modal analysis consists in the solution of a constrained eigenvalue problem arising from the solution of the free vibration equilibrium equations in a finite-element setting and involves the mass and stiffness matrices and a set of constraints which enforce relationships between degrees of freedom. A simple example of a constraint, is the imposition of the Dirichlet boundary conditions which usually consists in setting certain degrees of freedom to zero (single-point or fixed constraints). A further example is given by the so called master-slave constraints which impose that the displacement of a node (called the slave)depends linearly on the displacements of other nodes (called the masters). These constraints are crucial, e.g., in modeling the contact interaction between masonry and reinforcement.

We propose an efficient implementation of numerical methods for constrained eigenvalue problems, specialized for the modal analysis of structures taking into account both the sparsity of the matrices and the features of master-slave constraints. The implementation will be based on open-source packages embedded in the finite-element code NOSA-ITACA developed in the framework of a research project funded by the Region of Tuscany (www.nosaitaca.it/en/).

Numerical examples will be shown on the Project case study "Voltone" - a large vaulted masonry structure located beneath Piazza della Repubblica in Livorno, Italy.

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Efficient Solution of the Optimization Problem in Model-Reduced Gradient-Based History Matching

List of authors:

M. Rojas [74]

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In this poster, we present preliminary results of a performance evaluation study of several gradient-based state-of-the-art optimization methods for solving the nonlinear minimization problem arising in model-reduced gradient-based history matching. The issues discussed in this work also apply to other problems, such as production optimization in closed-loop reservoir management. This work is based on [1]

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Topology Optimization of Electromagnetic Devices: Resolution of Inverse Problems

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In this work, we deal with **T**opology **O**ptimization to solve *Inverse Problems* of Electric and Electromagnetic Circuits. This poster will address plasma hall effect thruster. On this poster, we shall show the main used materials and imposed caracteristics for designing an electrical thruster. We will give some mathematical formulations to solve optimization problem about optimal electric circuit of Hall effect thrusters.

In general the *Direct Problem* is considered. It consists to use Magnetic Circuit where the characteristics (Dimensions, Materials, Sources, $\cdots$) are known. Then, some physical values such as values of fields, intensity of electromagnetic forces at some points are computed. For such problems, the resolution is in general known. Indeed, we can analytically approximate the solutions of them (Direct Problem) with Ampère theorem or flux conservation laws. They can also be solved Numerically with Finite Element Methods [2]. But here, we deal with the *Inverse Problem* which consists to impose a magnetic fields or force distributions on some given points of the device and also to determine what circuit can provide this electromagnetic imposed effects.

For designing a device, the engineer generally solves inverse problem by defining the device structure and its parameters and then he procceeds to deal with the technical specifications. The obtained solutions are based on intuitions and empirically studies with previous experiences.

We bring methods and approaches to formulate mathematicaly the Inverse Problem like an Optimization one. For example, with a given magnetic induction or field $\mathbf{B}_0$, we want to design a device which will be able to produce this value at some fixed points. In this case, the objective is to *minimize* the gap between a computed value $\mathbf{B}$ and $\mathbf{B}_0$ at these points. For such a problem the variables are material properties and sources. In this work, we consider as variables the material properties, and the process is to fill the design domain with *iron* (associated to value 1) and *void* (associated to value 0); This type of problem is a *0-1 Optimization problem*. The magnetic field $\mathbf{B}$ values are obtained by solving **Maxwell's Equations** via the Finite Element software: **FEMM** (**F**inite **E**lement **M**ethod **M**agnetics).

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This *0-1 Optimization problem* is relaxed into the interval $[0, 1]$, then the obtained continuous problem is solved with classical algorithms such as a *steepest descent algorithm*. Hence, the need to provide the first derivative of the criterion is necessary. We compute it by using the *adjoint variable method* [1].

Numerical resolutions of our Topological Optimization is performed with a function of *Matlab's* Optimization Toolbox: *fmincon*. In general, the numerical results contain some *intermediary values* and these solutions are not manufacturable. Then, we avoid these intermediary values by using the **SIMP method** (**S**olid **I**sotropic **M**aterial with **P**enalization). This method combined with the relaxed problem give us binary solutions. Figure 1 presents some reslutats of our **Topology Optimization** *method* applied on a small example with 2×500 variables.

Figure 1 shows some numerical results:

- Figure 1(a) depicts the coordonates of the researched magnetic induction $\mathbf{B}_0$. To obtain it, we solve:
$$\min_{x \in [0,1]} F = \int_{\Omega} \|\mathbf{B}(x) - \mathbf{B}_0\|^2 d\Omega.$$

  With Ω the considered domain and $x \in [0, 1]$ corresponds to permeability $\mu \in [1, 1000]$.

- Figure 1(b) is the design domain to be optimized with an initial distribution of material property. It is the starting point given to *fmincon*.

- Figure 1(c) shows the optimal design found by *fmincon* with *FEMM*, it is obtainted in 10 hours. This results contains some intermediate values (cells with purple color).

- Figure 1(d) represent a part the evolution of the criterion during the iteration.
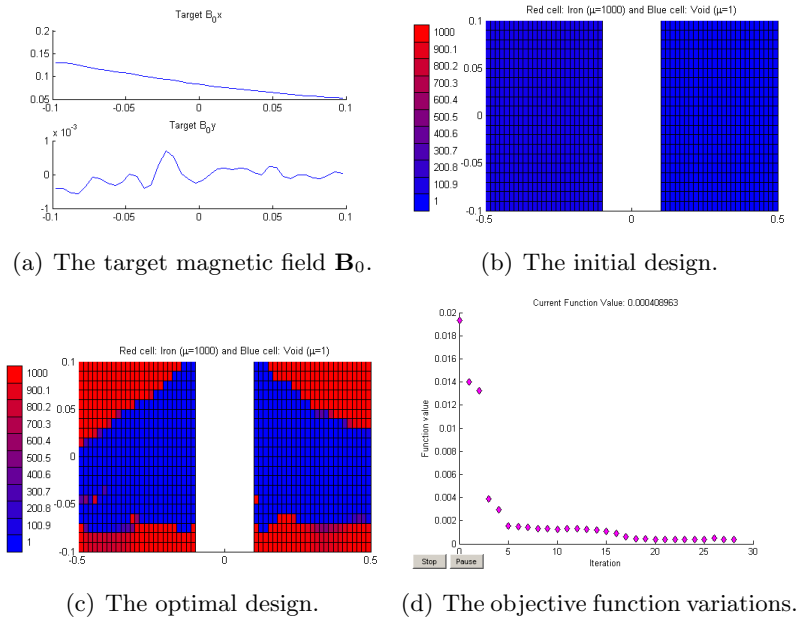
(a) The target magnetic field $\mathbf{B}_0$.

(b) The initial design.

(c) The optimal design.

(d) The objective function variations.

Figure 1: Topology Optimization with SIMP method.

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Inexact Coordinate Descent

List of authors:

R. Tappenden [81]

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In this poster we introduce a new algorithm called inexact coordinate descent (ICD) that can be applied to the problem of minimizing an unconstrained convex composition function. The algorithm uses an *inexact* update at each iteration and we present convergence guarantees in the form of iteration complexity results. The theoretical guarantees are complemented by practical considerations: the use of iterative techniques to determine the update as well as the use of preconditioning for further acceleration. A more detailed can be found in [1].

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Differentiating the Method of Conjugate Gradients

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The method of conjugate gradients (CG) is widely used for the iterative solution of large sparse systems of equations $Ax = b$, where A is symmetric positive definite. For a fixed matrix A, initial guess x_0, and iteration number k, the CG iterate $x_k(b)$ is a nonlinear, differentiable function of b. This poster presents expressions for the Jacobian matrix of $x_k(b)$ with respect to b, as well as data assimilation applications in which the Jacobian is used for first-order propagation of error covariance matrices. The poster is based on the technical report [1].

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A New Algorithm for Derivative-Free Equality- and Bound-Constrained Optimization

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A. Tröltzsch [88]

This poster will present a new algorithm for equality- and bound-constrained nonlinear optimization without derivatives. A trust-region SQP framework is used to handle the constraints. The algorithm can be viewed as an extension of the algorithm BCDFO [1] as it also applies the technique of self-correcting geometry (introduced in [2]) and an active-set strategy to handle bound constraints. We present numerical results on a test set of equality-constrained problems from the CUTEr problem collection.

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Cooperation of Interval Analysis and Evolutionary Algorithms for Reliable Global Optimization

List of authors:

<u>C. Vanaret</u> [89]

N. Durand [90] J-B. Gotteland [91] J-M. Alliot [92]

Highly nonlinear and ill-conditioned numerical optimization problems take their toll on the convergence of existing resolution methods. Stochastic methods such as Evolutionary Algorithms carry out an efficient exploration of the search-space at low cost, but get often trapped in local minima and do not prove the optimality of the solution. Deterministic methods such as Interval Branch and Bound algorithms guarantee bounds on the solution, yet struggle to converge within a reasonable time on high-dimensional problems.

In this talk, we propose to explain how these techniques can be combined [1, 2] to (i) prevent premature convergence toward local optima (ii) outperform both deterministic and stochastic existing approaches and (iii) achieve proof of optimality to problems that were up to now deemed as unsolvable. We demonstrate the efficiency of this approach on highly multimodal benchmark functions for which extensive tests are available, and more practical applications in the field of aeronautics.

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Sequentially Semi-Separable Block Preconditioners for PDE-Constrained Optimization Problems

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Sequentially Semi-Separable matrices are structured matrices with off-diagonal blocks of low rank. By exploiting this structure, it is possible to formulate computationally efficient algorithms for a wide range of problems [1].

In this poster, we present results for iterative solution algorithms for PDE-constrained optimization problems. Discretization of such problems, using for example the Finite Element Method, yields a saddle-point system whose submatrices have a Sequentially Semi-Separable structure. We study block-preconditioners for the saddle-point system, where the Schur complements are approximated using the low-rank structure of the submatrices. We illustrate the performance of our approach on a number of test problems.

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Optimization Challenges in Resting State fMRI Data Analysis

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Analyzing of interaction between different regions of brain for investigating the role of functional connectivity in the brain disorders is an interesting area for researchers in the neuroscience area. However, sometimes it is necessary to solve an optimization problem to get better results from clustering algorithm for estimation of these regions. In this paper we addressed some of optimization challenges in data analyzing of resting state functional magnetic resonance imaging data. We compare results of different methods and discuss about some applications of rsfMRI data analysis.

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