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Optimization Program Inverse Problems Workshop
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SPEAKER TITLES/ABSTRACTS

Ahmed Attia
SAMSI

"Goal-Oriented Optimal Experimental Design"

Computer models play an essential role in forecasting complicated phenomena such as the atmosphere, ocean dynamics, volcanic eruptions among others. These models however are usually imperfect due to various sources of uncertainty. Measurements are snapshots of reality that are collected as an additional source of information. Parameter inversion and data assimilation are means to fusing information obtained from measurement, model, prior knowledge, and other available sources to produce reliable and accurate description (the analysis) of the underlying physical system. The accuracy of the analysis is greatly influenced by the quality of the observational grid design used to collect measurements. Sensor placement can be viewed as optimal experimental design (OED) problem, where the locations of the sensors define an experimental design. There are many criteria for choosing an optimal experimental design, such as minimization of the uncertainty in the output (e.g., minimization of the trace of the posterior covariance). Including the end-goal (predictions) in the experimental design leads to a goal-oriented OED approach that can be used in several applications. In this talk, we outline the idea of goal-oriented optimal design of experiments for PDE based Bayesian linear inverse problems with infinite-dimensional parameters.

John Bardsley
University of Montana

"Markov Chain Monte Carlo Algorithms for Linear Inverse Problems"

In this talk, I will begin with a review of the basic characteristics of inverse problems before moving into Bayesian methods for inverse problems. The connection between the choice of the regularization function in classical inverse problems and the choice of the prior probability density function (or simply the prior) in Bayesian inverse problems is well-known. Less well-known is that in imaging, Gaussian priors (quadratic regularization functions) can be derived from pixel-level statistical assumptions about the unknown image using Gaussian Markov random fields (GMRFs). GMRFs and their use in modeling the prior will be a focus of the first half of the talk. With the prior in hand, in order to perform uncertainty quantification, one often must sample from the posterior density function (or simply the posterior). In cases where both the measurement error and prior variances are unknown, which is typical, a so-called hierarchical model assumes hyper-prior probabilities on these scalar parameters, resulting in a non-Gaussian posterior. The problem of sampling from this posterior is the focus of the second half of the talk. We will begin by presenting a basic Gibbs sampler, discuss its drawbacks in terms of algorithmic performance, and then present alternative MCMC methods that have better performance characteristics, and that make use of a technique known as marginalization. We will also present techniques developed in a current SAMSI working group for improving these methods when the discretized forward model has low rank structure.

Andrew Brown
Clemson University

"Computationally Efficient Markov Chain Monte Carlo Methods for Hierarchical Bayesian Inverse Problems"

In Bayesian inverse problems, the posterior distribution can be used to quantify uncertainty about the reconstructed solution. In practice, approximating the posterior requires Markov chain Monte Carlo (MCMC) algorithms, but these can be computationally expensive. We present a computationally efficient MCMC sampling scheme for ill-posed Bayesian inverse problems. The forward map is assumed to be linear with additive Gaussian noise, and the goal is to reconstruct the solution as well as to estimate regularization parameters. We employ a Metropolis-Hastings-within-Gibbs (MHwG) sampler with a proposal distribution based on a low-rank approximation of the prior-preconditioned Hessian. We show the dependence of the acceptance rate on the number of eigenvalues retained and discuss conditions under which the acceptance rate is high. We demonstrate our proposed sampler through numerical experiments in electroencephalography and computerized tomography.

Julianne Chung
Virginia Tech

"Hybrid Iterative Methods for Large-Scale Bayesian Inverse Problems"

Hybrid iterative methods are increasingly being used to solve large, ill-posed inverse problems, due to their desirable properties of (1) avoiding semi-convergence, whereby later reconstructions are no longer dominated by noise, and (2) enabling adaptive and automatic regularization parameter selection. In this talk, we develop a generalized hybrid iterative approach for computing solutions to large-scale Bayesian inverse problems. We consider a hybrid algorithm based on the generalized Golub-Kahan bidiagonalization for computing Tikhonov regularized solutions to problems where explicit computation of the square root and inverse of the covariance kernel for the prior covariance matrix is not feasible. This is useful for large-scale problems where covariance kernels are defined on irregular grids or are only available via matrix-vector multiplication, e.g., those from the Matern class. We show that iterates are equivalent to LSQR iterates applied to a directly regularized Tikhonov problem, after a transformation of variables, and we provide connections to a generalized singular value decomposition filtered solution. Numerical examples from image processing demonstrate the effectiveness of the described approaches. We will discuss some ongoing work on the use of these generalized hybrid methods for PAT reconstruction and for uncertainty quantification.

Co-author: tArvind Saibaba, North Carolina State University

Matthias Chung
Virginia Tech

"Stochastic Newton and Quasi-Newton Methods for Large Linear Least-squares Problems"

In this work, we describe stochastic Newton and stochastic quasi-Newton approaches to efficiently solve large linear least-squares problems, for applications where the size of the data exceeds the memory capabilities or for problems with time-dependent data acquisition. In our proposed framework, stochasticity is introduced as a means to overcome these computational limitations, and probability distributions that can exploit structure and/or sparsity are considered. Two stochastic approximation methods are developed for approximating solutions. Theoretical results on consistency of estimators for both the stochastic Newton and the stochastic quasi-Newton methods are provided and reveal that stochastic Newton iterates, in contrast to stochastic quasi-Newton iterates, may not converge to the desired least-squares solution. Numerical examples demonstrate the potential benefits of these methods.

This is joined work with Julianne Chung, Tanner Slagel, and Luis Tenorio.

Dirk Lorenz
TU Braunschweig

“Gaussian Scale Mixtures for Inverse Problems in Imaging”

We investigate inverse problems in imaging from a probabilistic viewpoint. Images need special priors that respect the existence of edges and especially, Gaussian smoothness priors are not appropriate. We propose to use Gaussian scale mixtures which incorporate a new latent variable to encode the edge strength.

We investigate different algorithms to infer information from the corresponding posterior. Specifically, we derive an expectation-maximization method and show that this is equivalent to the lagged diffusivity algorithm for the Perona-Malik problem. We also discuss methods based on mean-field approximations and show that these lead to adaptions of the lagged diffusivity scheme that better capture the uncertainties in the restoration process. Finally, we derive sampling methods for Gaussian scale mixtures which allow to calculate, for example, conditional mean estimates. Our methods rely on the formulation of the posterior as a so-called exponential pair, slightly generalizing the notion of the exponential family.

Lars Ruthotto
Emory University

“Optimal Experimental Design for Constrained Inverse Problems”

This talk presents recent progress towards efficient numerical methods for Optimal Experimental Design (OED) for inverse problems in the presence of constraints. We consider ill-posed linear inverse problems where the measurement matrix depends on design parameters. In addition to Tikhonov regularization we assume that additional linear equality and/or bound constraints are present. A common goal in these OED problems is to enforce sparse sampling in the design parameters. We will discuss two OED formulations to achieve sparse designs. First, we use a fine discretization of the parameter space and develop a subsampling strategy in the design problem with a sparsity enforcing term. Second, we fix the number of non-zero design parameters and identify them by solving the corresponding nonlinear and non-convex optimization problem.

We present both a Bayes and an empirical Bayes framework for solving the OED problems. In the Bayes framework, we consider the unconstrained inverse state problem and exploit a closed form solution for the inner problem to efficiently compute derivatives for the outer OED problem. For the empirical Bayes formulation, we derive a bilevel optimization problem in which the objective function is the sum of the reconstruction errors for the given training data and the costs of the design. The constraints are given by the inverse problems which need to be solved for all training models. Derivative-based methods are a key to efficiently optimize the typically high-dimensional design parameters. We discuss challenges associated with inequality constraints and how to overcome them using relaxed formulations of the problem.

The talk is joint work with Julianne and Matthias Chung, Virginia Tech.

Adrian Sandu
Virginia Tech

"Computational Methodologies for Large Data Assimilation Problems"

Data assimilation is the process of fusing information from priors, models, and observations, in order to obtain best estimates of the state of a physical system such as the atmosphere. Data assimilation relies on comprehensive physical models with large numbers of variables, and on complex observational data sets. The resulting large scale inverse problems need to be solved in faster than real time in order to, for example, meet the demands of weather forecasting. In this talk we introduce variational and statistical estimation approaches to data assimilation. We discuss important computational aspects including the construction of efficient models for (background) errors, the construction and analysis of discrete adjoint models, solving the optimization problem using reduced order model surrogates, estimating the information content of observations, and methodologies that are robust with respect to error in data.

Georg Stadler
New York University

"Mitigating the Influence of the Boundary on PDE-based Covariance Operators"

Elliptic PDE operators are commonly used to construct covariance operators for Gaussian random fields over infinite-dimensional Hilbert spaces. PDE operators require a choice of boundary conditions, and this choice can have a strong and usually undesired influence on the Gaussian random field. I will illustrate the problem and propose two techniques that allow to ameliorate these boundary effects. The first approach combines the elliptic PDE operator with a Robin boundary condition, where a varying Robin coefficient is computed from an optimization problem. The second approach normalizes the pointwise variance by rescaling the covariance operator. The performance of these approaches is studied numerically.

This is joint work with Yair Daon (NYU).