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Organisations

Postdoc, Department of Informatics and Mathematical Modeling
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CERE – Center for Energy Resources Engineering
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Publications:

An Implementation of the Frequency Matching Method
During the last decade multiple-point statistics has become increasingly popular as a tool for incorporating complex prior information when solving inverse problems in geosciences. A variety of methods have been proposed but often the implementation of these is not straightforward. One of these methods is the recently proposed Frequency Matching method to compute the maximum a posteriori model of an inverse problem where multiple-point statistics, learned from a training image, is used to formulate a closed form expression for an a priori probability density function. This paper discusses aspects of the implementation of the Frequency Matching method and the techniques adopted to make it computationally feasible also for large-scale inverse problems. The source code is publicly available at GitHub and this paper also provides an example of how to apply the Frequency Matching method to a linear inverse problem.

General information
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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, CERE – Center for Energy Resources Engineering
Authors: Lange, K. (Intern), Frydendall, J. (Intern), Hansen, T. M. (Intern), Zunino, A. (Intern), Mosegaard, K. (Intern)
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Assimilation of OMI NO2 retrievals into the limited-area chemistry-transport model DEHM (V2009.0) with a 3-D OI algorithm
Data assimilation is the process of combining real-world observations with a modelled geophysical field. The increasing abundance of satellite retrievals of atmospheric trace gases makes chemical data assimilation an increasingly viable method for deriving more accurate analysed fields and initial conditions for air quality forecasts.

We implemented a three-dimensional optimal interpolation (OI) scheme to assimilate retrievals of NO2 tropospheric columns from the Ozone Monitoring Instrument into the Danish Eulerian Hemispheric Model (DEHM, version V2009.0), a three-dimensional, regional-scale, offline chemistry-transport model. The background error covariance matrix, B, was estimated based on differences in the NO2 concentration field between paired simulations using different meteorological inputs. Background error correlations were modelled as non-separable, horizontally homogeneous and isotropic. Parameters were estimated for each month and for each hour to allow for seasonal and diurnal patterns in NO2.
concentrations.

Three experiments were run to compare the effects of observation thinning and the choice of observation errors. Model performance was assessed by comparing the analysed fields to an independent set of observations: ground-based measurements from European air-quality monitoring stations. The analysed NO2 and O3 concentrations were more accurate than those from a reference simulation without assimilation, with increased temporal correlation for both species. Thinning of satellite data and the use of constant observation errors yielded a better balance between the observed increments and the prescribed error covariances, with no appreciable degradation in the surface concentrations due to the observation thinning. Forecasts were also considered and these showed rather limited influence from the initial conditions once the effects of the diurnal cycle are accounted for.

The simple OI scheme was effective and computationally feasible in this context, where only a single species was assimilated, adjusting the three-dimensional field for this compound. Limitations of the assimilation scheme are discussed.

**General information**

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Aarhus University, Danish Ministry of the Environment
Authors: Silver, J. D. (Ekstern), Brandt, J. (Ekstern), Hvidberg, M. (Ekstern), Frydendall, J. (Intern), Christensen, J. H. (Ekstern)
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**Bibliographical note**

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A Frequency Matching Method: Solving Inverse Problems by Use of Geologically Realistic Prior Information

The frequency matching method defines a closed form expression for a complex prior that quantifies the higher order statistics of a proposed solution model to an inverse problem. While existing solution methods to inverse problems are capable of sampling the solution space while taking into account arbitrarily complex a priori information defined by sample algorithms, it is not possible to directly compute the maximum a posteriori model, as the prior probability of a solution model cannot be expressed. We demonstrate how the frequency matching method enables us to compute the maximum a posteriori solution model to an inverse problem by using a priori information based on multiple point statistics learned from training images. We demonstrate the applicability of the suggested method on a synthetic tomographic crosshole inverse problem.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, CERE – Center for Energy Resources Engineering
Authors: Lange, K. (Intern), Frydendall, J. (Intern), Cordua, K. S. (Intern), Hansen, T. M. (Intern), Melnikova, Y. (Intern), Mosegaard, K. (Intern)
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Scopus rating (2004): SJR 0.962 SNIP 1.181
Efficient Iterated Filtering

Parameter estimation in general state space models is not trivial as the likelihood is unknown. We propose a recursive estimator for general state space models, and show that the estimates converge to the true parameters with probability one. The estimates are also asymptotically Cramer-Rao efficient. The proposed estimator is easy to implement as it only relies on non-linear filtering. This makes the framework flexible as it is easy to tune the implementation to achieve computational efficiency. This is done by using the approximation of the score function derived from the theory on Iterative Filtering as a building block within the recursive maximum likelihood estimator.

General information
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Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing, CERE – Center for Energy Resources Engineering, Mathematical Statistics
Authors: Lindström, E. (Ekstern), Ionides, E. (Ekstern), Frydendall, J. (Intern), Madsen, H. (Intern)
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Improving multiple-point-based a priori models for inverse problems by combining Sequential Simulation with the Frequency Matching Method

In order to move beyond simplified covariance based a priori models, which are typically used for inverse problems, more complex multiple-point-based a priori models have to be considered. By means of marginal probability distributions ‘learned’ from a training image, sequential simulation has proven to be an efficient way of obtaining multiple realizations that honor the same multiple-point statistics as the training image. The frequency matching method provides an alternative way of formulating multiple-point-based a priori models. In this strategy the pattern frequency distributions (i.e. marginals) of the training image and a subsurface model are matched in order to obtain a solution with the same multiple-point statistics as the training image. Sequential Gibbs sampling is a simulation strategy that provides an efficient way of applying sequential simulation based algorithms as a priori information in probabilistic inverse problems. Unfortunately, when this strategy is applied with the multiple-point-based simulation algorithm SNESIM the reproducibility of training image patterns is violated. In this study we suggest to combine sequential simulation with the frequency matching method in order to improve the pattern reproducibility while maintaining the efficiency of the sequential Gibbs sampling strategy. We compare realizations of three types of a priori models. Finally, the results are exemplified through crosshole travel time tomography.

General information
Oil Reservoir Production Optimization using Single Shooting and ESDIRK Methods

Conventional recovery techniques enable recovery of 10-50% of the oil in an oil field. Advances in smart well technology and enhanced oil recovery techniques enable significant larger recovery. To realize this potential, feedback model-based optimal control technologies are needed to manipulate the injections and oil production such that flow is uniform in a given geological structure. Even in the case of conventional water flooding, feedback based optimal control technologies may enable higher oil recovery than with conventional operational strategies. The optimal control problems that must be solved are large-scale problems and require specialized numerical algorithms. In this paper, we combine a single shooting optimization algorithm based on sequential quadratic programming (SQP) with explicit singly diagonally implicit Runge-Kutta (ESDIRK) integration methods and the a continuous adjoint method for sensitivity computation. We demonstrate the procedure on a water flooding example with conventional injectors and producers.
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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Capolei, A. (Intern), Völcker, C. (Intern), Frydendall, J. (Intern), Jørgensen, J. B. (Intern)
Publication date: 2012

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**Single Shooting and ESDIRK Methods for adjoint-based optimization of an oil reservoir**

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
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**A Frequency Matching Method for Generation of a Priori Sample Models from Training Images**

This paper presents a Frequency Matching Method (FMM) for generation of a priori sample models based on training images and illustrates its use by an example. In geostatistics, training images are used to represent a priori knowledge or expectations of models, and the FMM can be used to generate new images that share the same multi-point statistics as a given training image. The FMM proceeds by iteratively updating voxel values of an image until the frequency of patterns in the image matches the frequency of patterns in the training image; making the resulting image statistically indistinguishable from the training image.

**General information**
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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
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Kriging in High Dimensional Attribute Space using Principal Component Analysis

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Lange, K. (Intern), Fernández Martínez, J. L. (Ekstern), Frydendall, J. (Intern), Mosegaard, K. (Intern)
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Data Assimilation in Marine Models
This thesis consists of six research papers published or submitted for publication in the period 2006-2009 together with a summary report. The main topics of this thesis are nonlinear data assimilation techniques and estimation in dynamical models. The focus has been on the nonlinear filtering techniques for large scale geophysical numerical models and making them feasible to work with in the data assimilation framework. The filtering techniques investigated are all Monte Carlo simulation based. Some very nice features that can be exploited in the Monte Carlo based data assimilation framework from a computational point of view, e.g. low storage cost, no linearizations of the numerical models, etc. However, this also gives rise to many unforeseen difficulties, e.g. the curse of dimensionality, huge computational costs, etc. The challenge faced in this thesis was finding filters that could handle the nonlinearities encountered in data assimilation and at the same time are robust and reliable enough given the constraints and difficulties that can arise. These problems were addressed in the papers A, E and D. The other topic of this thesis is estimation in dynamical geophysical numerical models. The challenge of estimating model parameters for well establish geophysical dynamical systems is that these models are not formulated in a way that incorporates the necessary stochastic assumptions that make estimation possible in a maximum likelihood sense. The maximum likelihood approach is selected due to its unique performance in data rich situations. The estimations are often based on output from the model and the raw observations which lead to suboptimal estimates. The challenge is to give a meaningful description of the model errors through diffusion processes that can be identified and incorporated into the existing maximum likelihood framework. These issues are discussed in paper B. The third part of the thesis falls a bit out of the above context is work published in papers C, F. In the first paper, a simple data assimilation scheme was investigated to examine the potential benefits of incorporating a data assimilation concept into an atmospheric chemical transport model. This paper deals with the results and conclusions obtained through some of the first experiments with the Optimal Interpolation filter in a geophysical model. The second paper F, deals with the construction of a finite element solver for the Fokker-Planck equation on a 2 dimensional flexible mesh system. The report details the construction of the finite element solver and investigates the potential benefits of a parallel FORTRAN implementation through a series of experiments.

General information
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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Mathematical Statistics
Authors: Frydendall, J. (Intern), Madsen, H. (Intern), Sørensen, J. V. T. (Intern)
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A parallel implementation of a finite element solver: for statistical methods

Implementation and testing of a simple data assimilation algorithm in the regional air pollution forecast model, DEOM

A simple data assimilation algorithm based on statistical interpolation has been developed and coupled to a long-range chemistry transport model, the Danish Eulerian Operational Model (DEOM), applied for air pollution forecasting at the National Environmental Research Institute (NERI), Denmark. In this paper, the algorithm and the results from experiments designed to find the optimal setup of the algorithm are described. The algorithm has been developed and optimized via eight different experiments where the results from different model setups have been tested against measurements from the EMEP (European Monitoring and Evaluation Programme) network covering a half-year period, April-September 1999. The best performing setup of the data assimilation algorithm for surface ozone concentrations has been found, including the combination of determining the covariances using the Hollingsworth method, varying the correlation length according to the number of adjacent observation stations and applying the assimilation routine at three successive hours during the morning. Improvements in the correlation coefficient in the range of 0.1 to 0.21 between the results from the reference and the optimal configuration of the data assimilation algorithm, were found. The data assimilation algorithm will in the future be used in the operational THOR integrated air pollution forecast system, which includes the DEOM.
Particle filters with applications

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Organisations: Mathematical Statistics, Department of Informatics and Mathematical Modeling
Authors: Frydendall, J. (Intern)
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Data Assimilation in Marine Modelling

Department of Informatics and Mathematical Modeling
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Number of participants: 6
Phd Student:
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Main Supervisor:
Madsen, Henrik (Intern)
Examiner:
Poulsen, Niels Kjølstad (Intern)
Carstensen, Niels Jacob (Intern)
Heemink, Arnold Willem (Ekstern)

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