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Data Assimilation – Mathematical Foundation and Applications

Organized by
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20 February – 26 February 2022

Abstract. The field of "Data Assimilation" has been driven by applications from the geosciences where complex mathematical models are interfaced with observational data in order to improve model forecasts. Mathematically, data assimilation is closely related to filtering and smoothing on the one hand and inverse problems and statistical inference on the other. Key challenges of data assimilation arise from the high-dimensionality of the underlying models, combined with systematic spatio-temporal model errors, pure model uncertainty quantification and relatively sparse observation networks. Advances in the field of data assimilation will require combination of a broad range of mathematical techniques from differential equations, statistics, machine learning, probability, scientific computing and mathematical modeling, together with insights from practitioners in the field. The workshop brought together a collection of scientists representing this broad spectrum of research strands.

Mathematics Subject Classification (2020): 37xx, 60xx.

Introduction by the Organizers

The workshop *Data Assimilation – Mathematical Foundation and Applications*, organized by Youssef M. Marzouk, Cambridge MA, Sebastian Reich, Potsdam, and Aretha Teckentrup, Edinburgh was held 20 February – 26 February 2022. The meeting was attended by nearly 25 participants attending in person and about an equal number joining remotely. Participants represented a broad range of mathematical subject areas as well as numerous application areas from the natural sciences. The workshop was the first major meeting on the subject since the emergence of COVID-19 and has been enthusiastically endorsed by all participants.

The field of data assimilation has undergone major developments since the last MFO workshop on this topic in 2016. We mention in particular an emerging strong interplay between data assimilation and machine learning, mathematical statistics, optimisation and optimal control. A further current hot topic has been on interacting particle filters and the stochastic analysis of their McKean–Vlasov mean field equations. The strong trend towards novel applications in, e.g., pharmacology, cognitive science, space weather and biology continued.

A total of 17 talks were presented during the workshop. The talks were selected such as to cover novel mathematical developments on data assimilation algorithms (Dan Crisan, Edriss Titi), theoretical and practical aspects of the ensemble Kalman filter (Alberto Carrassi, Roland Potthast, Geir Evensen, Xin Tong) parameter estimation and optimisation (Claudia Schillings), statistical inference (Markus Reiß), computational methods for Bayesian inference and their theoretical analysis (Jonas Latz, Jacob Zech, Sven Wang, Omar Ghattas, Lassi Rioninen), interacting particle systems, mean-field limits and optimal control (Prashant Mehta, Pierre del Moral, Sahani Pathiraja), random matrix theory (Manfred Opper).

Throughout the workshop a number of spontaneous discussion groups arose triggered by the many different facets of data assimilation presented during the talks. The following discussion groups took place in the central lecture hall of the MFO

- Monday evening: Ensemble Kalman inversion and regularised inverse problems
- Tuesday evening: Statistics of SPDEs
- Wednesday evening: Structures in high-dimensional data assimilation
- Thursday evening: Physics-based and surrogate modelling inspired by machine learning

These discussions were well received and have already led to follow up scientific projects among the participants of the workshop.

Acknowledgement: The MFO and the workshop organizers would like to thank the National Science Foundation for supporting the participation of junior researchers in the workshop by the grant DMS-1641185, “US Junior Oberwolfach Fellows”.

Workshop: Data Assimilation – Mathematical Foundation and Applications

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Abstracts

Uniform in time Error Estimates for Numerical Schemes of Downscaling Data Assimilation Algorithm Employing Coarse Scale Observations

Edriss S. Titi

A downscaling data assimilation algorithm for the Navier-Stokes and other related geophysical models will be presented [1, 3, 8, 22, 23]. Inspired by conventional theory of turbulence, which asserts that instabilities occur at the coarse spatial scales and are dissipated by the viscosity at the fine spatial scales, the algorithm is designed to continuously nudge the large spatial scales of the coarse spatial scales in the algorithm's solutions toward the observed large spatial scales, i.e. the measurements, of the unknown reference solution. The algorithm is also extended to the cases when the measurements are collected discretely, but frequently enough, in time and are possibly contaminated with deterministic or stochastic errors [4, 17, 20]. Moreover, it will be shown that for certain models a modification of the algorithm employing coarse spatial measurements of only part of the state variables are sufficient to recover the full reference solution of all the state variables [9, 10, 11, 12]. The algorithm's solution can be initialized arbitrary and shown to always converge at an exponential rate toward the unique exact reference solution that is corresponding to the coarse scale measurements. This indicates that the dynamics of the algorithm is globally stable in time. Capitalizing on this fact I will demonstrate uniform in time error estimates of numerical discretization of this algorithm, which makes the algorithm reliable upon implementation computationally for arbitrary long intervals of time [18, 24, 21]. Computational implementation of the algorithm demonstrate the remarkable performance of the algorithm beyond what is suggested by the analytical results and in comparison to other nudging algorithms [2, 6, 7, 13, 19, 20]. Furthermore, I will also present some recent advances, employing this algorithm, for recovering the statistics of the solution from those of the corresponding measurements [5, 14, 15, 16, 17].

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Cauchy Markov Random Field Priors for Bayesian Inversion

Lassi Roininen

(joint work with Jarkko Suuronen, Neil Chada, Angelina Senchukova)

We consider using Cauchy Markov random field priors for Bayesian inversion with applications in sawmill log X-ray imaging. Using Cauchy fields leads to posterior distributions which are non-Gaussian, high-dimensional, multimodal and heavy-tailed. Thus, we need sophisticated optimization and Markov chain Monte Carlo (MCMC) methods. We firstly propose a one-dimensional second order Cauchy difference prior, and construct new first and second order two-dimensional isotropic Cauchy difference priors. Another new Cauchy prior is based on the stochastic partial differential equation approach, derived from Matérn type Gaussian presentation. We consider maximum a posteriori and conditional mean estimation. We exploit state-of-the-art MCMC methodologies such as Metropolis-within-Gibbs, Repelling-Attracting Metropolis, and No-U-Turn sampler variant of Hamiltonian Monte Carlo. We demonstrate the applicability of the models and methods with two one and two-dimensional synthetic deconvolution problems, and with real data example arising from the sawmill X-ray imaging with extremely sparse measurement geometry requiring sophisticated prior constructions and efficient samping methods.

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Space-Time Particle Filters

Dan Crisan

(joint work with Ömer Deniz Akyildiz, Joaquin Miguez)

Particle filters (PF) are known to be robust approximations with regard to the time parameter. In earlier work of the author [1], a particle filter was developed that moved "vertically" along the space index and horizontally in the time component. Heuristically, rather than performing the sampling importance resampling procedure for a d-dimensional model (here d is assumed large) in one step, one does this in several consecutive steps, through a local particle filter running along the space dimension. In data assimilation language, each forecast/assimilation step for a high dimensional state space is decomposed into several intermediate low-dimensional forecast/assimilation steps. Since the generic particle filter is typically well behaved on low to moderate dimensions, the proposed procedure gives

good results well beyond the domain of applicability for the standard particle filter. This particle filter is termed a spacetime particle filter (STPF).

The results in [1] required a specific form the signal transition kernel as well as that of the likelihood function. This restricted considerably the range of applications of the STPF. In recent work with Joaquin Miguez and Deniz Akyildiz, we show how one can lift these constraints to allow for the applicability of the STPF to a wide class of problems. The new framework includes problems where the signal is approximated by a certain semi-implicit Euler method that is appropriately modified to exhibit Markovianity in the space component. The methodology is theoretically grounded in the understanding of the topological structure of optimal filters. The topological structure of optimal filters is natural and has the property that the subset of stable filters is dense in the whole set, see [3] for details.

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The approximations made when deriving data-assimilation methods

Geir Evensen

This presentation gives an overview of our approximations when deriving data-assimilation methods starting from Bayes's theorem. We discuss the assumptions of a Markov model and independent measurements, which allows us to solve the data assimilation problem on a sequence of data assimilation windows. We can, after that, solve for the MAP estimate or use randomized maximum sampling where we minimize an ensemble of cost functions to sample approximately the Bayesian posterior. Then introducing additional approximations, such as linearizations and ensemble-averaged model sensitivities, we can devise the most popular data-assimilation methods in use today. The presentation follows the outline of a new **open access** book on data assimilation [1] that will appear May 3rd, 2022. Hence, we refer to this book for the full story and theory on this presentation.

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Adaptive Tikhonov strategies for stochastic ensemble Kalman inversion

Claudia Schillings

(joint work with Neil Chada, Simon Weissmann, Xin Tong)

Ensemble Kalman inversion (EKI) is a generalization of the ensemble Kalman filter (EnKF) for inverse problems of the form

$$y = G(u) + \eta, \quad \eta \sim N(0, \Gamma)\,, \tag{1}$$

i.e. EKI is used to recover the unknown parameter $u \in X$ from noisy measurements $y \in \mathbb{R}^K$. In (1), $G : X \to \mathbb{R}^K$ is the forward operator mapping the parameters to the observations, and η denotes Gaussian noise with zero mean and known positive definite covariance $\Gamma \in \mathbb{R}^{K\times K}$. We refer to [7, 8] for more details on the derivation of ensemble Kalman filters and inversion. As EKI is known to be not a consistent approximation of the posterior distribution in the Bayesian setting for non-Gaussian problems, most of the EKI analysis views the method as a derivative-free optimizer of the data misfit

$$\mathcal{I}(u; y) := \frac{1}{2}\big\|y - G(u)\big\|_\Gamma^2$$

and studies properties of the continuous time limit of the method

$$\mathrm{d}u^{(j)} = C^{up}(u)\Gamma^{-1}(y - G(u^{(j)}))\mathrm{d}t + C^{up}(u)\Gamma^{-\frac{1}{2}}\mathrm{d}W^{(j)}\,, \tag{2}$$

where $\{u^{(j)}(t)\}_{j=1}^J$ denotes the ensemble of particles at time t, $\bar{u} = \frac{1}{J}\sum_{j=1}^J u^{(j)}$ and $\overline{G(u)} = \frac{1}{J}\sum_{j=1}^J u^{(j)}$ are the empirical means, $C^{up}(u) = \frac{1}{J}\sum_{k=1}^J (u^{(k)} - \bar{u}) \otimes (G(u^{(k)}) - \overline{G(u)})$ and $C^{pp}(u) = \frac{1}{J}\sum_{k=1}^J (G(u^{(k)}) - \overline{G(u)}) \otimes (G(u^{(k)}) - \overline{G(u)})$ empirical covariances and $W^{(1)}, \ldots, W^{(J)}$ are pairwise independent cylindrical Wiener processes. We refer to [1, 2, 3, 9, 10, 11, 12] for more details on the derivation of the limit and the analysis.

Our aim in this work is to extend the current results of Tikhonov regularization for EKI (abbreviated to TEKI, [6]) for a fixed regularization parameter to an adaptive choice. Assuming that the prior is Gaussian with zero mean and covariance C_0, the ensemble can be shown to converge (under suitable assumptions for an extended forward problem) to the minimizer of the Tikhonov regularized functional

$$\mathcal{L}(u; y) := \frac{1}{2}\|y - G(u)\|_\Gamma^2 + \frac{\lambda}{2}\|u\|_{C_0}^2.$$

for fixed regularization $\lambda > 0$. We develop adaptive strategies for TEKI, where we consider the task of choosing the regularization parameter within the iterative method of finding the underlying unknown parameter. To have some theoretical understanding of our new algorithms, we extend the EKI analysis to the noisy regime of data [5]. We consider the stochastic formulation of EKI viewed as coupled system of stochastic differential equations resulting from the continuous time limit (2) and present well-posedness and convergence results for fixed and time-varying regularization parameter. For the learning process of the regularization

parameter, three strategies are proposed: the first is based on a bilevel optimization approach, the second and third adaptive methods take motivation from Bayesian methodologies, namely through the the maximum a-posteriori (MAP) and that of hierarchical EKI. The hierarchical approach is appealing in this setting as it allows to learn a parametrized covariance matrix as regularization or even the full covariance matrix through its eigen-decomposition. Numerical experiments demonstrate that the adaptive regularization methods for TEKI outperform that of both fixed regularization and the vanilla EKI, cp. [5]. Even though the theory is so far limited to the linear case, the experiments show promising results also for the nonlinear setting. The generalization to nonlinear forward operators as well as to other forms of regularization will be subject to future work.

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On polynomial-time guarantees for Bayesian computation in PDE models

Sven Wang

(joint work with Richard Nickl)

The problem of generating random samples of high-dimensional posterior distributions is considered. The main results consist of non-asymptotic computational guarantees for Langevin-type MCMC algorithms which scale polynomially in key quantities such as the dimension of the model, the desired precision level, and the

number of available statistical measurements. As a direct consequence, it is shown that posterior mean vectors as well as optimisation based maximum a posteriori (MAP) estimates are computable in polynomial time, with high probability under the distribution of the data. These results are complemented by statistical guarantees for recovery of the ground truth parameter generating the data. A key intermediate result is that the posterior distribution, which itself is not necessarily log-concave, can be approximated by a globally log-concave distribution in Wasserstein distance, up to an exponentially small error.

Our results are derived in a general high-dimensional non-linear regression setting (with Gaussian process priors), employing a set of local 'geometric' assumptions on the parameter space, and assuming that a good initialiser of the algorithm is available. The main example which the theory is applied to is a representative non-linear model from PDEs involving a steady-state Schrödinger equation.

Using machine learning in geophysical data assimilation – Some of the issues and some ideas

Alberto Carrassi

(joint work with Javier Amezcua, Daniel Ayers, Laurent Bertino, Marc Bocquet, Julien Brajard, Yumeng Chen, Simon Driscoll, Charlotte Durand, Alban Farchi, Tobias Finn, Chris Jones, Varun Ohija, Einar Olason, Ivo Pasmans)

In recent years, data assimilation, and more generally the climate science modelling enterprise have been influenced by the rapid advent of artificial intelligence, in particular machine learning (ML), opening the path to various form of ML-based methodology. In this talk we will schematically show how ML can be included in the prediction and DA workflow in three different ways. First, in a so-called "non-intrusive" ML, we will show the use of supervised learning to estimate the local Lyapunov exponents (LLEs) based exclusively on the system's state [1]. In this approach, ML is used as a supplementary tool, added to the given physical model. Our results prove ML is successful in retrieving the correct LLEs, although the skill is itself dependent on the degree of local homogeneity of the LLEs on the system's attractor. In the second and third approach, ML is used to substitute fully [4] or partly [5] a physical model with a surrogate one reconstructed from data. Nevertheless, for high-dimensional chaotic dynamics such as geophysical flows this reconstruction is hampered by (i) the partial and noisy observations that can realistically be gathered, (ii) the need to learn from long time series of data, and (iii) the unstable nature of the dynamics. To achieve such inference successfully we have suggested to combine DA and ML in several ways. We will show how to unify these approaches from a Bayesian perspective, together with a description of the numerous similarities between them [2, 3]. We will show that the use of DA in the combined approach is pivotal to extract much information from the sparse, noisy, data. The full surrogate model achieves prediction skill up to 4 to 5 Lyapunov time, and its power spectra density is almost identical to that of the original data, except for the high-frequency modes which are not well captured [4].

The ML-based parametrization of the unresolved scales in the third approach [5] is also extremely skilful. This has been studied using a coupled atmosphere-ocean model and again the use of coupled DA [6] in the combined DA-ML method makes possible to exploit the data information from one model compartment (e.g., the ocean) to the other (e.g., the atmosphere).

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Approximation of triangular transport maps

Jakob Zech

(joint work with Youssef Marzouk, Dinh Dũng, Van Kien Nguyen, Christoph Schwab)

One of the main challenges in Bayesian inference is to efficiently sample from high-dimensional "target" distributions, which are known only through their unnormalized densities. A possible approach is to couple a tractible "reference" distribution ρ with the target π via a transport map T, that pushes forward ρ to π, i.e.

$$T_\sharp \rho = \pi. \tag{1}$$

Given such T, sampling from π is achieved via $T(X) \sim \pi$ where $X \sim \rho$.

In this talk we discuss regularity and approximability of triangular transports. Specifically, as a reference ρ we consider the uniform probability measure on $[-1,1]^d$, and we assume the target π to be supported on $[-1,1]^d$ with analytic and strictly positive Lebesgue density. It is well-known, that there then exists a unique map $T : [-1,1]^d \to [-1,1]^d$ satisfying (1) such that the jth component T_j of T depends only on $(x_1, \dots, x_j) \in [-1,1]^j$ and is strictly monotonically increasing as a function of $x_j \in [-1,1]$. This "triangular" transport is known in the literature as the Knothe-Rosenblatt (KR) map. We show that under the present assumptions, the KR map $T : [-1,1]^d \to [-1,1]^d$ is itself an analytic function,

and we investigate its domain of holomorphic extension. Using classical polynomial approximation theory for analytic functions, as well as recent findings in the approximation theory for neural networks, we prove that T can be approximated at an exponential rate with sparse polynomials or rectified linear unit (ReLU) neural networks, see [1, Sections 4 and 5].

As an application we focus on parameter estimation problems in engineering, where the forward model is described by a partial differential equation (PDE) depending on an unknown PDE coefficient $a \in L^\infty(D)$ on some bounded Lipschitz domain $D \subseteq \mathbb{R}^s$, $s \in \{2, 3\}$. One example is the elliptic equation

$$-\nabla \cdot (a \cdot \nabla u) = f, \qquad u|_{\partial D} = 0, \tag{2}$$

with $f \in H^{-1}(D)$ and for $a \in L^\infty(D)$ satisfying $\operatorname{esssinf}_{x \in D} a(x) > 0$. The unknown a is modelled as an $L^\infty(D)$-valued random variable

$$a(\boldsymbol{x}, \cdot) = 1 + \sum_{j=1}^{d} x_j r_j \psi_j(\cdot) \in L^\infty(D), \tag{3}$$

for certain fixed $\psi_j(\cdot) \in L^\infty(D)$, $r_j > 0$ and where $x_j \sim \text{uniform}(-1, 1)$ denote iid uniformly distributed random variables on $[-1, 1]$. Given observations of the PDE solution u corrupted by additive Gaussian noise, we verify that the posterior distribution of the unknown coefficients $(x_j)_{j=1}^d$ has an analytic density on $[-1, 1]^d$. As a corollary, the KR map T that pushes forward ρ to the posterior can be approximated at an exponential rate [1, Section 7], which in turn allows efficient sampling from the posterior.

Assuming $\sup_j \|\psi_j(\cdot)\|_{L^\infty(D)} \leq 1$ and polynomial decay $r_j \leq C j^{-\alpha}$ for some fixed constants $C > 0$, $\alpha > 1$, we extend these results to the infinite dimensional case $d = \infty$ and prove that the curse of dimension can be overcome in the approximation of $T : [-1, 1]^\infty \to [-1, 1]^\infty$. Moreover, our results imply the existence of transformations $\Phi_N : [-1, 1]^N \to L^\infty(D)$, such that for a latent variable $X_N \sim \text{uniform}([-1, 1]^N)$, the distribution of its image $\Phi_N(X_N) \in L^\infty(D)$ converges to the posterior distribution of a on $L^\infty(D)$ as $N \to \infty$. Here $\Phi_N(\boldsymbol{x}) = \sum_{j=1}^N \tilde{T}_j(x_1, \ldots, x_{j-1}) r_j \psi_j(\cdot)$, where each $\tilde{T}_j : [-1, 1]^j \to [-1, 1]$ is a rational function, and the total number of learnable coefficients in all $\tilde{T}_j$, $j = 1, \ldots, N$, is of size $O(N)$. In this setting we prove the upper bound $O(N^{-\alpha+1+\varepsilon})$ for the q-Wasserstein distance between the posterior and the distribution of $\Phi_N(X_N)$ as $N \to \infty$. Here $q \in [1, \infty)$ and $\varepsilon > 0$ are fixed but arbitrary. Details can be found in [2, Section 6].

Finally, for the purpose of computing posterior expectations, we present a different approach based on sparse-grids. In this case we let

$$a(\boldsymbol{x}, \cdot) = 1 + \exp\left(\sum_{j \in \mathbb{N}} x_j r_j \psi_j(\cdot) \right) \in L^\infty(D)$$

with $x_j \sim \mathcal{N}(0, 1)$ iid standard Gaussian, i.e. we assume a lognormal prior. For bounded polygonal Lipschitz domains $D \subseteq \mathbb{R}^2$, and with the forward operator

described by the PDE (2), we prove that the posterior expectation of certain quantities of interest can be approximated with a multilevel-sparse grid Gauss-Hermite quadrature. The multilevel quadrature requires approximate evaluations of the likelihood at each quadrature point. This is achieved by using (higher order) finite elements (FEM) on graded meshes to approximate the forward model. In this setting we show an algebraic convergence rate, that depends in particular on the decay of the functions $r_j\psi_j(\cdot)$ in certain corner weighted Kondratiev spaces on D. The convergence rate is proven w.r.t. the total number of degrees of freedom of all required FEM solutions. Further details and precise statements are given in [3, Section 7].

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Localization for EnKF and inverse problems

Xin Tong

(joint work with Jana de Wiljes, Matthias Morzfeld and Youssef Marzouk)

The curse of dimension can be found in both data assimilation (DA) and inverse problem (IP). In DA, algorithms like ensemble Kalman filter (EnKF) uses sample covariance to estimate the underlying uncertainty. But such estimation tends to be erroneous if the sample size is smaller than the problem dimension. The localization technique exploits the sparse structure which can be commonly found in many geophysical DA problems, and removes the possible spurious correlation in sample covariance estimation. It can be rigorously proved that localized EnKF can work well if 1) the underlying process is linear or 2) there is complete and accurate observation. But the general discussion will be difficult since forward maps in DA problem tend to be chaotic. In IP, there is no forward map involved. So more general results can be derived. First, if we use localized ensemble Kalman inversion (EKI) to solve IP through the variational approach, we can show the ensemble converges to the global solution even if the ensemble size is much smaller than the problem dimension. And if we try to solve IP using the Bayesian approach, localization technique can be used to design efficient Markov Chain Monte Carlo (MCMC), of which the acceptance rate and convergence rate are both independent of problem dimension.

Duality between Estimation and Control

Prashant G. Mehta
(joint work with Jin W. Kim and Sean Meyn)

My talk is concerned with variational (optimal control type) formulations for the problems of nonlinear filtering/smoothing. Such formulations are referred to as duality between optimal estimation and optimal control. Recent interest in duality comes from its potential to obtain control-oriented algorithms for data assimilation and simulation problems.

My talk is in four parts: In part I, I review the two types of duality, viz., the minimum-variance duality and the minimum-energy duality, for the classical linear Gaussian filtering and smoothing problems. In part II, I review a dual formulation, originally due to Newton-Mitter, which generalizes the minimum energy duality to the nonlinear non-Gaussian case. The formulation can be used to derive the nonlinear smoothing equation. In part III, I describe a recent generalization of the minimum-variance duality theory to nonlinear filtering. This generalization is an exact extension, in the sense that the dual optimal control problem has the same minimum variance structure for linear and nonlinear filtering problems. In part IV, I will conclude with some pointers to the numerical algorithms for data assimilation based upon the dual approaches.

McKean-Vlasov SDEs in nonlinear filtering

Sahani Pathiraja
(joint work with Sebastian Reich and Wilhelm Stannat)

In the realm of monte carlo based filtering, ensemble Kalman type methods have arguably been the method of choice for high dimensional non-linear applications due to their desirable stability properties. However, such approaches are not consistent with Bayes theorem even as the ensemble size goes to infinity. Over the last few decades, a range of so-called particle flow type filters have been developed which show strong potential for providing consistent estimates in high dimensional nonlinear applications.

I will discuss some recent work that develops a framework through which to derive various forms of such filters, demonstrating how different assumptions on the form of the control or "gain function" lead to different filters proposed in the literature and their links. Additional results related to well-posedness of a filter and its diffusion map based approximation will be discussed.

Nonparametric estimation for stochastic partial differential equations via localisation

Markus Reiss

(joint work with Randolf Altmeyer)

We first discuss differences for parametric drift estimation between stochastic ordinary and partial differential equations (SODEs/SPDEs). We review the spectral estimation approach for SPDEs, which gives structural insights into estimation problems for SPDEs. For nonparametric problems (functional parameters), however, the eigensystem of the generator is generally unknown and the spectral approach is no longer feasible.

We therefore consider the specific problem of estimating the space-dependent diffusivity of a stochastic heat equation from time-continuous observations with local space resolution h, as proposed in [1]. The rather counterintuitive result and its efficiency as $h \to 0$ are discussed in detail.

The methodology extends to cover stochastic reaction-diffusion and more general semilinear SPDEs. These robustness results require regularity results for the nonlinear part in semi-linear SPDEs. An application to experimental data from cell repolarisation and the stochastic Meinhard model for pattern formation shows the relevance for applications, compare [2].

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Stochastic gradient in continuous time: discrete and continuous data

Jonas Latz

(joint work with Kexin Jin, Chenguang Liu, Carola-Bibiane Schönlieb)

We study two optimisation problems on $X := \mathbb{R}^n$. The first one considers the minimisation of a sample mean:

$$\min_{\theta \in X} \frac{1}{N} \sum_{i=1}^{N} \Phi_i(\theta), \tag{1}$$

where $(\Phi_i)_{i=1}^N$ is a family of continuously differentiable functions and we assume that the optimisation problem is well-defined. The second problem concerns the minimisation of an expected value:

$$\min_{\theta \in X} \int_S \phi(\theta, y) \mathrm{d}\pi(y), \tag{2}$$

where S is a compact set, ϕ is integrable with respect to y and continuously differentiable with respect to θ, π is a probability measure on $(S, \mathcal{B}S)$, and we assume

again that the optimisation problem is well-defined. We refer to the problems (1) and (2) as the discrete data case [2] and continuous data case [1], respectively. Of course, the discrete data case is contained in the second case, by choosing $S := \{1, \dots, N\}$, $\phi(\cdot, y) := \Phi_y$, and $\pi := N^{-1}\#$. Thus, we now concentrate on the second case.

Optimisation problems of form (2) can be solved using the stochastic gradient descent method [3]. Here, we iterate:

$$\theta_k \leftarrow \theta_{k-1} - \eta_k \nabla_\theta \phi(\theta_{k-1}, y_k), \qquad (k \geq 1),$$

where $y_1, y_2, \dots \sim \pi$ i.i.d. and $\theta_0 \in X$ is an appropriate initial value. This method converges to a minimiser of $\theta \mapsto \int_S \phi(\theta, y) \mathrm{d}\pi(y)$, if $\theta \mapsto \phi(\theta, \cdot)$ is strongly convex and if the *learning rate* $\eta_k \to 0$ sufficiently slowly, as $k \to \infty$. The method is also popular in non-convex optimisation, especially in deep learning.

In the works [1, 2], we study a continuous-time version of the stochastic gradient descent method given through the following dynamical system:

$$\frac{\mathrm{d}\theta(t)}{\mathrm{d}t} = -\nabla_\theta \phi(\theta(t), y(t)) \qquad (t \geq 0), \qquad \theta(0) = \theta_0,$$

where $(y(t))_{t \geq 0}$ is a certain homogeneous-in-time Feller process on S that attains π as its unique stationary measure to which it converges exponentially.

Under certain smoothness and convexity assumptions, we can show that the process $(\theta(t))_{t \geq 0}$ has a unique stationary measure to which it converges exponentially in a certain Wasserstein distance. This case mimics the case of a constant sequence $(\eta_k)_{k=1}^\infty$. To represent a decreasing learning rate, we rescale the time in $(y(t))_{t \geq 0}$, i.e., we replace $y(t)$ by $y(\beta(t))$ for an appropriate super linear function β. In this case, we can show convergence to the minimiser of the target function, retrieving the result for the discrete time algorithm in our more general continuous setting.

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Reduced basis neural network surrogates for Bayesian inversion and optimal experimental design

Omar Ghattas

(joint work with Thomas O'Leary-Roseberry, Keyi Wu, Peng Chen)

Solution of Bayesian inverse problems (BIPs) governed by large-scale complex models in high parameter dimensions (such as PDEs with discretized infinite-dimensional parameter fields) quickly becomes prohibitive, since the forward model must be solved numerous times—as many as millions—to characterize the uncertainty in the parameters.

Efficient evaluation of the parameter-to-observable (p2o) map, which involves solution of the forward model, is key to making BIPs tractable. Surrogate approximations of p2o maps [4] have the potential to greatly accelerate BIPs, provided the p2o map can be accurately approximated using (far) fewer forward model solves than would be required for solving the BIP using the full p2o map. Unfortunately, constructing such surrogates presents significant challenges when the parameter dimension is high and the forward model is expensive.

Deep neural networks (DNNs) have emerged as leading contenders for overcoming these challenges. We demonstrate that black box application of DNNs for problems with infinite dimensional parameter fields leads to poor generalization, particularly in the common situation where training data are limited in number due to the expense of executing the model. However, by constructing a network architecture that is adapted to the geometry and intrinsic low-dimensionality of the p2o map as revealed by adjoint-based Hessian actions, one can construct a parsimonious reduced basis DNN surrogate with superior approximation properties using only limited training data [5, 6]. We employ this reduced basis DNN surrogate to make tractable the solution of Bayesian optimal experimental design (OED) problems [7, 8], in particular for finding sensor locations that maximize the expected information gain [1, 9]. Application to inverse wave scattering [2, 3] is presented.

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Dynamical mean field theory for the analysis of message passing algorithms

Manfred Opper
(joint work with Burak Çakmak)

Message passing algorithms are computational tools for approximating posterior marginal densities or moments for probabilistic data models (for an overview see e.g. [1]). While in applications, their predictions are often found to be surprisingly accurate and convergence is often fast, they are in general not well understood theoretically. This talk discusses simplified data models for which such algorithms can be analysed in an asymptotic limit. We will specialise on the dynamical properties of the algorithms.

As a toy model for a posterior probability distribution (without any 'real data'), we consider the joint probability of N Ising 'spins' $\mathbf{s} = (s_1, \ldots, s_N)$, with $s_i = \pm 1$, and with pairwise interactions of the form

$$\pi(\mathbf{s}) = \frac{1}{Z} \exp\left[\sum_{i<j} s_i J_{ij} s_j + h \sum_i s_i\right] \tag{1}$$

The goal of statistical 'inference' would be to compute the magnetisations $m_i = E[s_i]$. Approximations to such computations can often be derived from generalised mean field methods, which were developed in statistical physics of disordered systems. One can model the effect of the 'frozen' randomness defined by data in the posterior by assuming that the matrices $\mathbf{J}$ are random e.g. belonging to a spherically invariant ensemble $\mathbf{J} \doteq \mathbf{O}^\top \mathbf{\Lambda} \mathbf{O}$ with $\mathbf{\Lambda}$ diagonal and $\mathbf{O}$ a random orthogonal matrix. For such a scenario, G. Parisi & M Potters [2], generalising earlier work of D. J. Thouless and P. W. Anderson and R. G. Palmer (TAP) proposed so–called 'TAP' coupled mean field equations of the form

$$m_i = \tanh\left(\sum_j J_{ij} m_j - \mathrm{R}_{\mathbf{J}}(\chi) m_i + h\right)$$

for $i = 1, \ldots, N$ with $\chi \doteq 1 - \frac{1}{N}\sum_j m_j^2$. The random matrix ensemble enters via the term $\mathrm{R}_{\mathbf{J}}(\chi)$, the so–called R–transform of the spectrum. These equations are assumed to become exact in the high temperature phase (sufficiently small β) in the limit $N \to \infty$.

The task of a message passing algorithm would be to provide an iterative and fast computation of the fixed points of these equations. A so–called AMP (approximate message passing) [3] style algorithm adapted to this toy problem [4] would iterate

$$\gamma_i(t+1) = \sum_{j=1}^{N} A_{ij} g(\gamma_j(t))$$

in parallel for $i = 1, \ldots, N$, where $\mathbf{A} \doteq \frac{1}{\hat{\chi}}(\lambda \mathbf{I} - \mathbf{J})^{-1} - \mathbf{I}$ and $g(x) \doteq \frac{1}{\chi} \tanh(x+h) - x$ for $t = 0, 1, 2, 3, \ldots$, given specific random initialisations. The parameters λ and $\hat{\chi}$ are solutions of (pre–computed) scalar equations. Finally, at convergence, one has to set $m_i = \chi(\gamma_i + g(\gamma_i))$.

In order to analyse the coupled nonlinear dynamics in the large N limit, we have applied dynamical mean field theory [5] of statistical physics to the problem. In contrast to previous work on similar problems (see e.g. [3]), this method allows us to construct an effective stochastic process for a single variable $\hat{\gamma}(t)$, which reproduces the entire marginal joint statistics of the path of an arbitrary node i: $\{\gamma_i(0), \gamma_i(1), \ldots, \gamma_i(T)\}$ for $N \to \infty$ over a finite time window $t = 0, 1, 2, \ldots, T$. For the current algorithm [4], we obtain the surprisingly simple result that $\{\hat{\gamma}(t)\}_0^T$ is a Gaussian process over time with a covariance matrix that can be computed recursively over time. Analytical results show an excellent agreement with simulations of the algorithm for large N on single instances of the random matrix. One obtains a necessary condition on model parameters for global convergence as well as exact results for the asymptotic convergence speed. For recent work on putting the statistical physics results on mathematically rigorous basisi, see [6].

The analysis can be extended [7] to other, somewhat more realistic data problems defined by latent Gaussian variable models which are used in machine learning and signal processing. Current work considers the derivation of static properties of MAP estimators from the dynamics of an algorithm.

It is an open problem how well real data can be modelled by the simple random matrix ensembles. It would also be interesting to see if similar models and analysis would be of relevance for large scale data assimilation problems.

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A variational approach to nonlinear and interacting diffusions

Pierre del Moral

This talk presents a novel variational calculus to analyze the stability and the propagation of chaos properties of nonlinear and interacting diffusions. This differential methodology combines gradient flow estimates with backward stochastic interpolations, Lyapunov linearization techniques as well as spectral theory. This framework applies to a large class of stochastic models including non homogeneous diffusions, as well as stochastic processes evolving on differentiable manifolds, such as constraint-type embedded manifolds on Euclidian spaces and manifolds equipped with some Riemannian metric. We present uniform as well as almost sure exponential contraction inequalities at the level of the nonlinear diffusion flow, as well as. uniform propagation of chaos properties w.r.t. the time parameter are also provided. Illustrations are provided in the context of a class of gradient flow diffusions arising in fluid mechanics and granular media literature.

Data Assimilation of Nowcasted Observations

Roland Potthast

The talk first explains the ensemble data assimilation systems employed by Deutscher Wetterdienst on the global and regional scale for its operational systems for Numerical Weather Prediction (NWP). DWD works on the integration of classical nowcasting, i.e. the extrapolation of observations, with classical forecasting, i.e. the use of dynamical systems to predict the further behaviour of the atmosphere. One basic question linked to this integration asks: is it possible and useful to assimilate nowcasted observations into the numerical model for atmospheric prediction.

We investigate the assimilation of nowcasted information into a classical data assimilation cycle. As a reference setup we employ the assimilation of standard observations such as direct observations of particular variables into a forecasting system. The pure advective movement extrapolation of observations as a simple nowcasting (NWC) is usually much better for the first minutes to hours, until outperformed by numerical weather prediction (NWP) based on data assimilation. Can nowcasted information be used in the data assimilation cycle? We study both an oscillator model and the Lorenz 63 model with assimilation based on the Localized Ensemble Transform Kalman Filter (LETKF). We investigate and provide

a mathematical framework for the assimilation of nowcasted information, approximated as a local tendency, into the LETKF in each assimilation step. In particular, we derive and discuss adequate observation error and background uncertainty covariance matrices and interprete the assimilation of nowcasted information as assimilation with an L1-type metric in observation space. Further, we show numerical results which prove that nowcasted information in data assimilation has the potential to significantly improve model based forecasting.

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