MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Foundations of Bayesian Inference for Complex Statistical Models
(hybrid meeting)

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ABSTRACT. In this virtual workshop a variety of recent developments in Bayesian high-dimensional and nonparametric statistics were discussed in depth. There were 12 in depth talks delivered via zoom in the afternoons (to allow for US attendance), and several informal evening time meetings on wonder.me, where follow up discussions of the most important mathematical developments took place.

Introduction by the Organizers

All 12 talks were of the highest quality, summarising and highlighting fundamental recent developments in the field, triggering lively discussions even despite the virtual format on zoom. The material presented in the talks covered a wide range of aspects of Bayesian nonparametric statistics and its mathematical foundations. Loosely speaking there were 3 main clusters of topics, on *i) Asymptotic behaviour of Bayes methods, ii) Bayesian inverse problems,* and *iii) Sampling methods for complex posterior distributions*. We now summarise the contributions in somewhat more detail.

i) Asymptotic behaviour of Bayes methods

There were two talks on the recently emerged area of Bayesian multiple testing, and Ismael Castillo and Elisabeth Gassiat presented an overview of recent progress on the asymptotic behaviour of such methods in a variety of settings, including

Hidden Markov models. Chao Gao presented his work on a unified convergence rate analysis of variational Bayes methods, which are often relevant in complex settings where standard computation of posteriors is impossible. Aretha Teckentrup reviewed recent work of hers on convergence properties of Gaussian process regression in a 'noise-less' regression setting. Johannes Schmidt-Hieber talked about recent results establishing contraction rates for posterior distribution arising from 'deep' Gaussian processes (where multiple layers are generated by conditioning steps). Botond Szabo reviewed recent work of himself and collaborators on Gaussian process regression in 'distributed' settings with computational 'communication constraints'.

ii) Bayesian inverse problems

Another cluster of the workshop was concerned with recent progress in the understanding of Bayesian methodology applied in inverse problems (arising with PDEs or otherwise). Martin Burger presented recent work on the variational interpretation and computation of MAP estimators (posterior modes) arising from log-concave priors. Nik Kovachki presented his work with Andrew Stuart and Bamdad Hosseini on learning operators in Bayesian inverse problems. Hanne Kekkonen presented her consistency results for nonparametric Bayesian inference in a nonlinear inverse problem arising with a parabolic Schrödinger equation. Tapio Helin discussed results about the use of the Laplace approximation to approximately compute posterior distributions by 'Gaussian surrogates'.

ii) Sampling methods for complex posterior distributions

Eric Moulines discussed new MCMC/importance sampling type algorithms based on non-equilibrium sampling ideas, and described recent progress on the theoretical understanding of such methods. Sven Wang presented results on poly-nomial time computational guarantees for Langevin MCMC samplers for high-dimensional posterior measures arising in non-log-concave PDE settings with a Schrödinger equation.

Workshop (hybrid meeting): Foundations of Bayesian Inference for Complex Statistical Models

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Abstracts

Bayesian multiple testing: overview and sharp boundary for sparse sequences

Ismaël Castillo

(joint work with Kweku Abraham & Étienne Roquain)

Bayesian posterior distributions that allow for variable selection are often used in practice to address multiple testing questions. Besides their empirical success, they have been advocated among others by Bradley Efron for use in combination with empirical Bayes estimators of unknown prior parameters.

We consider three popular multiple testing procedures based on spike and slab priors. The first simply selects coordinates based on low posterior probabilities of coming from the null distribution, so-called ℓ–values (also known as 'local FDR' values). The second procedure is based on cumulative ℓ–values and the third on thresholding of so-called q–values (Storey 2003). While simple decision-theoretic arguments show that these procedures have optimality properties in the Bayesian setting assuming the prior is correct, it is natural to wonder whether their excellent behaviour in practice can be backed-up by theoretical guarantees if the true parameter is a fixed sparse (but otherwise arbitrary) vector.

In a sparse normal means setting, we demonstrate that the procedures behave optimally in a number of ways, if the spike-and-slab weight is calibrated using marginal maximum likelihood in an Empirical Bayes fashion. On the one hand, we prove that the frequentist FDR (False Discovery Rate) of these procedures is uniformly controlled: it goes to zero slowly for the ℓ–value procedure, and stays close to a user-specified nominal level for the q–value procedure. On the other hand, we study the power through the FNR (False Negative Rate). We investigate multiple testing minimax rates and prove that sharp adaptive minimaxity for the multiple testing risk is achieved by Empirical Bayes-calibrated ℓ–value procedures.

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[3] Kweku Abraham, Ismaël Castillo, Étienne Roquain, *Sharp multiple testing boundary for sparse sequences*, manuscript in preparation.

Distance measures for Learning and Bayesian Inversion

Martin Burger

(joint work with Felix Lucka, Tapio Helin, Martin Benning)

Common distance measures in statistics are based on variances or covariances, which corresponds to Hilbert space norms. In recent high-dimensional applications such as Bayesian inverse problems or machine learning one often chooses to work with priors very far from Gaussians, which implies that the geometric structure is very far from a Hilbertian one. Thus, quantification in terms of a Hilbert space norm can be far from optimal.

In the case of log-concave priors we investigate distance measures such as Bregman distances and (scaled) Jensen distances, which turn out to be efficient for analyzing the variational problems related to maximum a-posteriori error estimates. Our results show that for appropriate choice of the distances, the maximum a-posteriori probablity estimate or the conditional mean estimate can be obtained as minimizers. This directly yields contraction estimates in a corresponding transport distances. The latter can be generalized to estimates between posterior distributions in the transport distances. In the infinite-dimensional setting a similar analysis can be applied, but the distances have to modified if the negative logarithm of the prior is not one-homogeneous.

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Convergence Rates of Variational and Empirical Bayes: A Unified Analysis

Chao Gao

(joint work with Fengshuo Zhang)

We study the convergence rates of empirical Bayes posterior distributions for non-parametric and high-dimensional inference. We show that as long as the hyperparameter set is discrete, the empirical Bayes posterior distribution induced by the maximum marginal likelihood estimator can be regarded as a variational approximation to a hierarchical Bayes posterior distribution. This connection between empirical Bayes and variational Bayes allows us to leverage the recent results in the variational Bayes literature, and directly obtains the convergence rates of empirical Bayes posterior distributions from a variational perspective. For a more general hyperparameter set that is not necessarily discrete, we introduce a new technique called "prior decomposition" to deal with prior distributions that can be written as convex combinations of probability measures whose supports are low-dimensional subspaces. This leads to generalized versions of the classical "prior

mass and testing" conditions for the convergence rates of empirical Bayes. Our theory is applied to a number of statistical estimation problems including non-parametric density estimation and sparse linear regression.

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Non-Equilibrium Sampling

Eric Moulines

(joint work with Achille Thin, Yazid Janati, Sylvain Le Corff, Charles Ollion, Arnaud Doucet, Alain Durmus, Christian Robert)

Sampling from a complex distribution π and approximating its intractable normalizing constant Z are challenging problems. In this paper, a novel family of importance samplers (IS) and Markov chain Monte Carlo (MCMC) samplers is derived. Given an invertible map T, these schemes combine (with weights) elements from the forward and backward Orbits through points sampled from a proposal distribution ρ. The map T does not leave the target π invariant, hence the name NEO, standing for Non-Equilibrium Orbits.cNEO-IS provides unbiased estimators of the normalizing constant and self-normalized IS estimators of expectations under π while NEO-MCMC combines multiple NEO-IS estimates of the normalizing constant and an iterated sampling-importance resampling mechanism to sample from π. For T chosen as a discrete-time integrator of a conformal Hamiltonian system, NEO-IS achieves state-of-the art performance on difficult benchmarks and NEO-MCMC is able to explore highly multimodal targets. Additionally, we provide detailed theoretical results for both methods. In particular, we show that NEO-MCMC is uniformly geometrically ergodic and establish explicit mixing time estimates under mild conditions.

Convergence, Robustness and Flexibility of Gaussian Process Regression

Aretha Teckentrup

(joint work with Matt Dunlop, Mark Girolami, Andrew Stuart)

We are interested in the task of estimating an unknown, deterministic function from a set of point evaluations. In this context, Gaussian process regression is often used as a Bayesian inference procedure. However, hyper-parameters appearing in the mean and covariance structure of the Gaussian process prior, such as smoothness of the function and typical length scales, are often unknown and learnt from the data, along with the posterior mean and covariance.

In the first part of the talk, we study the robustness of Gaussian process regression with respect to mis-specification of the hyper-parameters. We work in the framework of empirical Bayes', where a point estimate of the hyper-parameters is

computed, using the data, and then used within the standard Gaussian process prior to posterior update. Using results from scattered data approximation, we provide a convergence analysis of the method applied to a fixed, unknown function of interest. We show convergence of the mean of the Gaussian process posterior to the true function f, and the convergence of the variance of the Gaussian process posterior to zero.

In the second part of the talk, we discuss deep Gaussian processes as a class of flexible non-stationary prior distributions. We provide a general framework in which deep Gaussian processes can be constructed and analysed, and we demonstrate the power of deep Gaussian processes in a regression problem where we wish to recover a multi-scale function from noisy point evaluations.

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Learning Operators for Forward and Inverse Problems

Nikola Kovachki

A general framework for data-driven approximation of input-output maps between infinite-dimensional spaces is developed. Motivated by the recent successes of neural networks, the proposed approach uses a combination of ideas from deep learning and model reduction. This combination results in a neural network approximation which, in principle, is defined on infinite-dimensional spaces and, in practice, is robust to the dimension of the finite-dimensional approximations of these spaces required for computation. For large classes of input-output maps, and suitably chosen probability measures on the inputs, convergence of the proposed approximation methodology is proved. Numerically, the effectiveness of the method is demonstrated on classes of parametric PDE problems with applications in reservoir modeling, the deformation of plastic materials, and the turbulent flow of fluids. Convergence and robustness of the approximation scheme with respect to the size of the discretization is established. The method is shown to be faster and more accurate than many existing algorithms in the literature.

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Posterior contraction for deep Gaussian process priors

JOHANNES SCHMIDT-HIEBER

(joint work with Gianluca Finocchio)

Deep neural networks are now state of the art for many complex learning tasks and, in particular, outperform shallow neural networks. While the role of depth in neural networks is not yet completely understood, an interesting follow-up question is whether other methods can be enhanced my making them deep. Nonparametric Bayes with Gaussian process priors is a popular method in machine learning and closely related to Bayesian neural networks. By composing Gaussian processes, we easily can create deep processes. Little is, however, known regarding the theoretical properties of deep Gaussian processes. We fill this gap by studying deep Gaussian process priors from the frequentist Bayes perspective, assuming that the data are generated from the nonparametric regression model and that the underlying regression function itself has a composition structure. Conditions are derived that guarantee a posterior contraction rate close to the minimax estimation rate. These conditions can be verified if the deep Gaussian process prior construction is based on standard families of Gaussian processes.

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On polynomial-time computation of high-dimensional posterior measures by Langevin-type algorithms

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.

The results are derived in a general high-dimensional non-linear regression setting (with Gaussian process priors) where posterior measures are not necessarily log-concave, employing a set of local 'geometric' assumptions on the parameter space, and assuming that a good initialiser of the algorithm is available. The theory is applied to a representative non-linear example from PDEs involving a steady-state Schrödinger equation.

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Consistency of Bayesian inference with Gaussian process priors for a parabolic inverse problem

HANNE KEKKONEN

We consider the statistical nonlinear inverse problem of recovering the absorption term $f > 0$ in the heat equation

$$\begin{cases} \partial_t u - \frac{1}{2}\Delta_x u + fu = 0 & \text{on } \mathcal{O} \times (0, \mathbf{T}) \\ u = g & \text{on } \partial\mathcal{O} \times (0, \mathbf{T}) \\ u(\cdot, 0) = u_0 & \text{on } \mathcal{O}, \end{cases}$$

where $\mathcal{O} \in \mathbb{R}^d$ is a bounded domain, $\mathbf{T} < \infty$ is a fixed time, and g, u_0 are given sufficiently smooth functions describing boundary and initial values respectively. The data is assumed to consist of N discrete noisy point evaluations of the solution u_f on $\mathcal{O} \times (0, \mathbf{T})$. We study the statistical performance of Bayesian nonparametric procedures based on a large class of Gaussian process priors. We show that, as the number of measurements increases, the resulting posterior distributions concentrate around the true parameter generating the data, and derive a convergence rate for the reconstruction error of the associated posterior means. We also consider the optimality of the contraction rates and prove a lower bound for the minimax convergence rate for inferring f from the data, and show that optimal rates can be achieved with truncated Gaussian priors.

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Laplace approximation in Bayesian inverse problems

TAPIO HELIN

(joint work with Remo Kretschmann)

The Laplace approximation is a popular approximative numerical scheme in large-scale non-linear Bayesian inverse problems. In addition to the large-scale problems, it is frequently applied in Bayesian optimal experimental design and has recently been considered as a reference measure for numerical quadrature and importance sampling. We quantify approximative properties of the Laplace method applied to the posterior distribution arising in non-linear Bayesian inverse problems. Our work is motivated by Schillings et al. (2020), where it is shown that in such a setting the Laplace approximation error in Hellinger distance converges to zero in the order of the noise level.

Our main results introduce novel error estimates for a given noise level that additionally quantify the effect due to the non-linearity of the forward mapping and the dimension of the problem. In particular, we are interested in inverse problems, where a linear forward mapping is perturbed by a small non-linear mapping. Our results provide insight into Bayesian inference in non-linear inverse problems, where linearization of the forward mapping has suitable approximation properties.

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Bayesian multiple testing for dependent data and hidden Markov models
Elisabeth Gassiat

Given a nonparametric Hidden Markov Model (HMM) with two states, the question of constructing efficient multiple testing procedures is considered, treating one of the states as an unknown null hypothesis. A procedure is introduced, based on nonparametric empirical Bayes ideas, that controls the False Discovery Rate (FDR) at a user–specified level. Guarantees on power are also provided, in the form of a control of the true positive rate. One of the key steps in the construction requires supremum–norm convergence of preliminary estimators of the emission densities of the HMM. We provide the existence of such estimators, with convergence at the optimal minimax rate, for the case of a HMM with $J \geq 2$ states, which is of independent interest. Then, we are interested in the procedures for strutured sequences of hypothesis. The behaviour of the HMM prior is investigated when it approaches the limit case of independent variables, where phase transitions may appear. In such cases, rates of estimation of the parameters is shown to depend on quantities related to the distance to the limit cases.

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Product vs mixture of experts: On distributed Gaussian Process regression

BOTOND SZABO

(joint work with Amine Hadji, Aad van der Vaart, Harry van Zanten)

Gaussian Process (GP) are arguably one of the most popular choices of priors in Bayesian nonparametrics, with applications including predicting the spread of malaria, medical imaging, artificial intelligence, and modeling the rate of cell growth. However, the computation of the posteriors coming from GP priors typically scale poorly with the data size n even in the standard nonparametric regression model, i.e. the computational complexity of training and predicting are $O(n^3)$ and $O(n^2)$, respectively. This considerably limits their practical applicability for big data sets.

In practice various approximation methods were proposed to speed up the computations, including distributed Bayes, variational Bayes, coreset methods, banded or reduced rank approximation of the posterior covariance matrix, just to mention a few. In the presentation we focus on distributed Bayesian techniques, where the data is divided over local machines/cores and the posteriors are computed locally in parallel to each other based on the partial data sets. Then in the final step the local posteriors are aggregated into a global approximation of the original posterior distribution. The distributed architecture, beside speeding up the computations, also helps in reducing the memory requirement and in protecting privacy. We investigate the statistical properties of distributed Bayesian methods, i.e. whether the resulting approximate posteriors contract around the true functional parameter of interest with the optimal minimax rate and if the corresponding approximate credible sets are asymptotically valid confidence sets.

Depending on how the data are divided over the local machines we distinguish two main classes of approaches, the product and mixture of GP experts. In the product of experts the data are divided randomly, each local machine receiving observations over the whole domain of the regression function. In the mixture of experts the data are divided spatially, each local machine receiving all the observations corresponding to a given small region or bin. Various techniques were proposed in the literature for both cases, typically with very limited, if any, theoretical underpinning. In our work we compare these methods and provide theoretical guarantees and limitations for them.

We start our analysis with the product of experts methods, including naive averaging, Consensus Monte Carlo [7], WASP [6], (generalized) Gaussian Product of Experts [1], Bayesian Committee Machine [10],... etc. First we derive contraction rates and frequentist coverage results in a non-adaptive framework where the regularity of the functional parameter is assumed to be known. We show that although several of the proposed approaches provide bad estimation and unreliable uncertainty quantification, appropriately tunned methods can achieve the minimax contraction rate and provide asymptotically valid confidence sets, see

[8, 2]. However, typically the regularity of the regression function is not available in practice. To deal with these problem several approaches were proposed in the distributed setting, including maximizing the sum of local marginal likelihood functions or providing cross validated estimator for the regularity based on local data sets. However, these standard approaches do not achieve adaptation due to the insufficient information content available locally.

In the second part of the talk we consider the mixture of expert methods where the local posteriors are computed over small regions and then "glued" together. We derive optimal minimax contraction rates both in the non-adaptive and adaptive setting in the nonparametric regression model for rescaled integrated Brownian motion priors, [3]. However, the resulting approximation has discontinuities at the boundary of the local regions. To deal with this problem various methods were proposed for optimally combining the local posteriors, including the patched GP method [4] or a two step mixture approach [9, 5]. In our numerical analysis we take the weighted average of the local posteriors (extended to the whole domain), with weights proportional to the inverse of the posterior variance times the exponentiated and rescaled distance to the local bins/regions. We show empirically that our approach deals with the discontinuities and provides good estimations and reliable uncertainty quantification.

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