Workshop: Imaging With Uncertainty Quantification (IUQ), September 2022

A 3-day workshop on computational uncertainty quantification for inverse problems, preceded by a 1-day training course on our software CUQIpy

Training course: Sept. 26

Workshop: Sept. 27-29, 2022

Held at conference center Konventum in Helsingør (Elsinore), north of Copenhagen.

Arranged by the research project CUQI.

Tuesday, Sept. 27

09:00	- 09:15	*Introduction*	
09:15	- 10:15	Marcelo Pereyra	An introduction to Bayesian imaging with data-driven priors encoded by neural networks
10:15	- 10:45	Rémi Laumont	Bayesian imaging using Plug & Play priors: when Langevin meets Tweedie
10:45	- 11:15	*Coffee break*	
11:15	- 12:15	Hanne Kekkonen	Random tree Besov priors
12:15	- 12:45	Yiqiu Dong	The horseshoe prior for edge-preserving Bayesian inversion
13:00	- 14:00	*LUNCH*	
14:00	- 15:00	Thomas Mejer Hansen	Probabilistic integration of (geo)-information
15:00	- 15:30	*Coffee break*	
15:30	- 16:00	Jakob S. Jørgensen	CUQIpy: A new Pyhthon platform for computational uncertainty quantifiation for inverse problems
16:00	- 16:30	Johannes Hertrich	The ower of Patches for Training Normalizing Flows
16:30	- 17:30	POSTER SESSION	
17:30	- 18:30	Guided tour at Konventum	
19:00		*DINNER*	

Wednesday, Sept.28

09:00	- 10:00	Aku Seppänen	Recovery from modelling errors in non-stationary inverse problems
10:00	- 10:30	Fabian Parzer	Uncertainty-aware blob detection in astronomical imaging
10:30	- 11:00	*Coffee break*	
11:00	- 12:00	Faouzi Triki	Inverse moving point source problem for the wave equation
12:00	- 12:30	Remo Kretschmann	Optimal and Bayesian hypothesis testing in statistical inverse problems
12:30	- 13:00	Mirza Karamehmedović	Forward Uncertainty Quantification for the Helmholtz Equation
13:00	- 14:00	*LUNCH*	
14:00		Bus departure for excursion to Kronborg (open till 17:00) (No bus back to Konventum!)	
19:00		*CONFERENCE DINNER at Konventum*	

Thursday, Sept. 29

09:00	- 10:00	Bangti Jin	Deep Image Prior of Inverse Problems: Acceleration and Probability Treatment
10:00	- 10:30	Babak Maboudi Afkham	Uncertainty quantification of inclusion boundaries in the context of X-ray tomography
10:30	- 11:00	*Coffee break*	
11:00	- 12:00	Alexander Litvinenko	Weakly Supervised Regression on Uncertain Datasets
12:00	- 12:30	Kim Knudsen	Sound speed uncertainty in Acousto-Electric Tomography
12:30	- 13:00	Jasper Everink	Sparse Bayesian Inference with Regularized Gaussians
13:00	- 14:00	*LUNCH*	
14:00	- 15:00	Tanja Tarvainen	Bayesian Approach to Quantitative Photoacoustic Tomography
15:00	- 15:30	*Coffee break*	
15:30	- 16:00	Charlesquin Mbakam	Empirical Bayesian estimation for semi-blind inverse problems: Application to image deblurring with total variation regularization
16:00		*End of workshop*	

An introduction to Bayesian imaging with data-driven priors encoded by neural networks*

Marcelo Pereyra[1]

[1] *Maxwell Institute for Mathematical Sciences & School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, United Kingdom.*
email: `m.pereyra@hw.ac.uk`

Abstract

This talk presents methodology for Bayesian analysis and computation in imaging inverse problems where the prior knowledge is available in the form of training data. We consider this data to be a sample from the marginal distribution of the unknown image we seek to reconstruct. We discuss two main approaches to encode this prior knowledge by a deep neural network in a way that is amenable to rigorous and computationally efficient Bayesian inference.

First, following the manifold hypothesis, we construct a data-driven prior which can be learnt from the training data by using modern deep generative modelling techniques, such as variational auto-encoders, generative adversarial networks and normalising flows. We study theoretical aspects of the resulting posterior distribution (e.g., existence and well-posedness), as well as scalable sampling algorithms to perform inference with these models.

The second approach seeks to represent the prior by using a Gaussian image denoising algorithm, usually a neural network designed to perform strongly in the sense of the estimation mean-squared error. Once trained, the denoiser is used in a plug-and-play manner within an unadjusted Langevin algorithm, in lieu of the gradient or the proximal operator of the log-prior density. This allows using the denoiser to perform inference for any imaging problem, not only denoising. Again, we study theoretical aspects of the resulting posterior distribution (e.g., existence and well-posedness), as well as scalable sampling algorithms.

The proposed approaches are demonstrated with a range of challenging imaging problems and comparisons with alternative approaches from the state of the art. This talk is based on work presented in [1, 2, 3, 4, 5].

References

[1] A. F. Vidal, V. De Bortoli, M. Pereyra, A. Durmus, "Maximum Likelihood Estimation of Regularization Parameters in High-Dimensional Inverse Problems: An Empirical Bayesian Approach Part I: Methodology and Experiments", SIAM Journal on Imaging Sciences, vol. 13, no. 4, 2020.

[2] R. Laumont, V. de Bortoli, A. Almansa, J. Delon, A. Durmus, and M. Pereyra, "Bayesian imaging using Plug and Play priors: when Langevin meets Tweedie", SIAM Journal on Imaging Sciences, vol. 15, no. 2, 2022.

[3] R. Laumont, V. de Bortoli, A. Almansa, J. Delon, A. Durmus, and M. Pereyra, "On Maximum-a-Posteriori estimation with Plug & Play priors and stochastic gradient descent", arXiv:2201.06133.

[4] M. Holden, M. Pereyra, K. Zygalakis, "Bayesian Imaging With Data-Driven Priors Encoded by Neural Networks", SIAM Journal on Imaging Sciences, vol. 15, no. 2, 2022.

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*The work of MP is supported by UKRI EPSRC (EP/T007346/1, EP/V006134/1, EP/W007681/1).

Bayesian imaging using Plug & Play priors: when Langevin meets Tweedie

Rémi Laumont, Valentin De Bortoli, Julie Delon, Andrés Almansa, Alain Durmus, Marcelo Pereyra
Université de Paris, Ecole Normale Supérieure, Université de Paris, Ecole Normale Supérieure Paris-Saclay, Heriot-Watt University

Email : remi.laumont@parisdescartes.fr

Key-words : Bayesian inferences, Inverse problems, Deblurring, Inpainting, Langevin Algorithm, Markov Chain Monte-Carlo

Remark : This work has been accepted for publication in SIAM Journal Imaging Sciences (preprint available at `https://arxiv.org/pdf/2103.04715.pdf`). Readers might also be interested in [1].

Abstract :

This talk presents theory for Bayesian analysis and computation with Plug-and-Play priors that are implicitly defined by an image denoising algorithm. We study Plug-and-Play Unadjusted Langevin Algorithms for Monte Carlo sampling and minimum mean squared error estimation. We establish detailed convergence guarantees for these algorithms under realistic assumptions on the denoising operators used, with special attention to denoisers based on deep neural networks. We also show that these algorithms approximately target a decision-theoretically optimal Bayesian model that is well-posed and meaningful also from a frequentist viewpoint. This is demonstrated on several canonical imaging problems.

References

[1] Rémi Laumont, Valentin De Bortoli, Andrés Almansa, Julie Delon, Alain Durmus, and Marcelo Pereyra. On Maximum-a-Posteriori estimation with Plug & Play priors and stochastic gradient descent. working paper or preprint, 2021.

Random tree Besov priors

Hanne Kekkonen[1], Matti Lassas[2], Eero Saksman[3], Samuli Siltanen[4]

[1] *Delft University of Technology*
email: `h.n.kekkonen@tudelft.nl`
[2] *University of Helsinki*
email: `matti.lassas@helsinki.fi`
[3] *University of Helsinki*
email: `eero.saksman@helsinki.fi`
[4] *University of Helsinki*
email: `samuli.siltanen@helsinki.fi`

Abstract

We propose alternatives for Bayesian a priori distributions that are frequently used in the study of inverse problems. The aim is to construct priors that have same kind of good edge-preserving properties than total variation or Mumford-Shah but correspond to well defined infinite dimensional random variables and can be approximated with finite dimensional random variables. This is done by introducing a new random variable T that takes values in the space of 'trees', and which is chosen so that the realisations of the unknown have singularities only on a small set.

The horseshoe prior for edge-preserving Bayesian inversion*

Yiqiu Dong[1]

[1] *DTU Compute*
email: `yido@dtu.dk`

Abstract

In many large-scale inverse problems characterization of sharp edges in the solution is desired. In the Bayesian approach to inverse problems, edge-preservation is often achieved using Markov random field priors based on heavy-tailed distributions. Another strategy, popular in sparse statistics, is the application of hierarchical shrinkage priors. An advantage of this formulation lies in expressing the prior as a conditionally Gaussian distribution depending on heavy-tailed distributed hyperparameters. In this presentation, we revisit the shrinkage horseshoe prior and introduce its formulation for edge-preserving settings. We discuss a Gibbs sampling framework to solve the Bayesian inverse problem. Applications from imaging science show that our computational procedure is able to compute sharp edge-preserving posterior point estimates with reduced uncertainty.

*This work was supported by a Villum Investigator grant (no. 25893) from The Villum Foundation.

Probabilistic integration of (geo)-information

Thomas Mejer Hansen[1]

[1] *Department of Geoscience, Aarhus University*
email: `tmeha@geo.au.dk`

Abstract

A general probabilistic formulation of inverse problem theory was provided almost 40 years ago in the seminal work by Tarantola and Valette (1982) [1]. In their work, the solution to an inverse problem is a posterior probability distribution $\sigma(\mathbf{m})$ which reflects the conjunction of direct (the prior) and indirect (the likelihood) information about the model parameters $\mathbf{m}$. Direct information is quantified directly through the prior probability distribution $\rho(\mathbf{m})$. Indirect information refers to information from data $\mathbf{d}$ that is related to the model parameters through some operator g as $\mathbf{d}) = g(\sigma(\mathbf{m}))$, and quantified through the likelihood function $L(\mathbf{m})$ that measure how well some observed data fit experimental computed as $\mathbf{d} = g(\mathbf{m})$. The posterior distribution is simply given by $\sigma(\mathbf{m}) = k\rho(\mathbf{m})L(\mathbf{m})$.

Early on applications of the probabilistic inverse method relied on quite simple prior and noise models. In the specific case where g refers to a linear operator and both $\sigma(\mathbf{m})$ and $L(\mathbf{m})$ can be described by Gaussian statistics, the posterior is also Gaussian, and can be computed analytically [2].

But, the original formulation in Tarantola and Valette (1982a) allows the use of, in principle, arbitrarily complex prior, forward, and noise models. In 1995 Mosegaard and Tarantola proposed the extended Metropolis algorithm [3], which in principle allows using any prior, that can be sampled using an algorithm. Later was demonstrated how in principle, most any (combination of) geostatistical simulation methods can be used to quantify, and relatively efficiently sample, quite complex prior models [4]. This presentation will focus on the use of informed prior models and correlated noise models, that allow quantifying both quite realistic prior information and noise on geophysical data. First, some examples will be given on how to quantify geological prior information and correlated noise in geophysical data. Then a number of algorithms will be discussed that all can account for the same information, but that differ in generalizability and computational efficiency.

It is suggested that probabilistic methods are becoming increasingly practical, not least due to the developments in machine learning, to a point where the main problem is no longer to solve the data integration problem, but instead, the focus should be on the important aspects of quantifying the available information in a probabilistic form.

References

[1] Tarantola A and Valette B. Inverse problems= quest for information. *Journal of geophysics*. 1982;50(1):159-70.

[2] Tarantola A and Valette B. Generalized nonlinear inverse problems solved using the least squares criterion. *Reviews* of Geophysics. 1982 May;20(2):219-32.

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CUQIpy: A new Python platform for computational uncertainty quantification in inverse problems*

Nicolai A. B. Riis[1], Amal M. A. Alghamdi[2], Felipe Uribe[3], Silja L. Christensen[4], Babak M. Afkham[5], Per Christian Hansen[6], Jakob S. Jørgensen[7]

[1] *Department of Applied Mathematics and Computer Science*
Technical University of Denmark
email: `nabr@dtu.dk`

[2] *Department of Applied Mathematics and Computer Science*
Technical University of Denmark
email: `amaal@dtu.dk`

[3] *Department of Applied Mathematics and Computer Science*
Technical University of Denmark
email: `furca@dtu.dk`

[4] *Department of Applied Mathematics and Computer Science*
Technical University of Denmark
email: `swech@dtu.dk`

[5] *Department of Applied Mathematics and Computer Science*
Technical University of Denmark
email: `bmaaf@dtu.dk`

[6] *Department of Applied Mathematics and Computer Science*
Technical University of Denmark
email: `pcha@dtu.dk`

[7] *Department of Applied Mathematics and Computer Science*
Technical University of Denmark
email: `jakj@dtu.dk`

Abstract

In this talk we present CUQIpy (pronounced ”cookie pie”) – a new computational modelling environment in Python that uses uncertainty quantification (UQ) to access and quantify the uncertainties in solutions to inverse problems. The overall goal of the software package is to allow both expert and non-expert (without deep knowledge of statistics and UQ) users to perform UQ related analysis of their inverse problem while focusing on the modelling aspects. To achieve this goal the package utilizes state-of-the-art tools and methods in statistics and scientific computing specifically tuned to the ill-posed and often large-scale nature of inverse problems to make UQ feasible.

We showcase the software on problems relevant to imaging science such as computed tomography and partial differential equation-based inverse problems.

CUQIpy is developed as part of the CUQI project at the Technical University of Denmark and is available at `https://github.com/CUQI-DTU/CUQIpy`.

*This work was supported by a Villum Investigator grant (no. 25893) from The Villum Foundation.

The Power of Patches for Training Normalizing Flows

Fabian Altekrüger[1,3], Alexander Denker[2], Paul Hagemann[1], Johannes Hertrich[1], Peter Maass[2], Gabriele Steidl[1]

[1] *Technical University Berlin*
email: `j.hertrich@math.tu-berlin.de`
[3] *Humboldt University Berlin*
[2] *University of Bremen*

Abstract

In this talk we introduce two kinds of data-driven patch priors learned from very few images: First, the Wasserstein patch prior penalizes the Wasserstein-2 distance between the patch distribution of the reconstruction and a possibly small reference image. Such a reference image is available for instance when working with materials' microstructures or textures. The second regularizer learns the patch distribution using a normalizing flow. Since already a small image contains a large number of patches, this enables us to train the regularizer based on very few training images.

For both regularizers, we show that they induce indeed a probability distribution such that they can be used within a Bayesian setting. We demonstrate the performance of patch priors for MAP estimation and posterior sampling within Bayesian inverse problems. For both approaches, we observe numerically that only very few clean reference images are required to achieve high-quality results and to obtain stability with respect to small pertubations of the problem.

This talk is based on the papers [1, 2, 3].

References

[1] F. Altekrüger, A. Denker, P. Hagemann, J. Hertrich, P. Maass and G. Steidl, *PatchNR: Learning from Small Data by Patch Normalizing Flow Regularization*, Arxiv Preprint 2205.12021, 2022. Code available at: `https://github.com/FabianAltekrueger/patchNR`

[2] F. Altekrüger and J. Hertrich, *WPPNets and WPPFlows: The Power of Wasserstein Patch Priors for Superresolution*, Arxiv Preprint 2201.08157, 2022. Code available at: `https://github.com/FabianAltekrueger/WPPNets`

[3] J. Hertrich, A. Houdard and C. Redenbach, *Wasserstein Patch Prior for Image Superresolution*, IEEE Transactions on Computational Imaging, vol. 8, pp. 693-704, 2022. Code available at: `https://github.com/johertrich/Wasserstein_Patch_Prior`

Recovery from modelling errors in non-stationary inverse problems

Aku Seppänen[1], Elias Vänskä[1], Outi Kurri[1], Jari P. Kaipio[1]

[1] *University of Eastern Finland, Department of Applied Physics, Kuopio, Finland*
email: `Aku.Seppanen@uef.fi`

Abstract

This talk considers non-stationary inverse problems in imaging, i.e., problems of imaging temporally evolving targets on the basis of sequentially measured indirect data of the target. As example applications we consider imaging of moving fluids in industrial process tomography [1], and estimation of fugitive greenhouse gas emissions in environmental monitoring [2]. We formulate both of the associated reconstruction problems in the framework of Bayesian state estimation, which bases upon modelling of both the measurements (observation model) and the temporal evolution of the model unknown (evolution model). In the aforementioned applications, the evolution of the target is modelled with a stochastic convection-diffusion equation. In the industrial imaging case, the imaging modality is electrical impedance tomography and in the environmental monitoring example, the open-path laser dispersion spectroscopy. In both cases, the estimates of the time-varying targets are computed using recursive methods, such as extended Kalman filters and smoothers.

The special focus of this talk is in handling modelling errors in non-stationary inverse problems. Those errors can arise from various uncertainties associated with both the evolution and observation models – such as unknown flow fields in convection-diffusion problems [3, 4, 5] and unknown contact impedances of electrodes in electrical impedance tomography [1]. Another source of modelling errors is the model reduction which is often needed in order to reduce the computational burden in these four-dimensional (4D) imaging applications [1, 2]. We demonstrate how the state estimates can often be made tolerant with respect to above types of modelling errors by using so-called Bayesian approximation error methods [6].

References

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[2] E. Vanskä, Proper orthogonal decomposition based model reduction in Bayesian estimation of gas emissions, *MSc thesis. University of Eastern Finland*, 2021.

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Uncertainty-aware blob detection in astronomical imaging*

Prashin Jethwa[1], Fabian Parzer[2], Otmar Scherzer[3], Glenn van de Ven[4]

[1] *Department of Astrophysics, University of Vienna*
[2] *Faculty of Mathematics, University of Vienna*
email: fabian.kai.parzer@univie.ac.at
[3] *Faculty of Mathematics, University of Vienna*
[4] *Department of Astrophysics, University of Vienna*

Abstract

Blob detection, i. e. detection of blob-like shapes in an image, is a common problem in astronomy. A difficulty arises when the image of interest has to be recovered from noisy measurements, and thus comes with uncertainties. Formulating the reconstruction of the image as a Bayesian inverse problem, we propose an uncertainty-aware version of the classic Laplacian-of-Gaussians method for blob detection [1]. It combines ideas from scale-space theory, statistics and variational regularization to identify salient blobs in uncertain images. The proposed method is illustrated on a problem from stellar dynamics: the identification of components in a stellar distribution recovered from integrated-light spectra.

This talk is based on our recent preprint [2].

References

[1] T. Lindeberg, *Feature Detection with Automatic Scale Selection*, Int. J. Comput. Vis., 1998.

[2] P. Jethwa, F. Parzer, O. Scherzer and G. van de Ven, *Uncertainty-Aware Blob Detection with an Application to Integrated-Light Stellar Population Recoveries*, arXiv:2208.05881, 2022.

*PJ and GvdV acknowledge funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme under grant agreement No 724857 (Consolidator Grant ArcheoDyn). PJ and GvdV also acknowledge support by the Austrian Science Fund (FWF): F6811-N36. FP and OS were funded by the Austrian Science Fund (FWF): F6807-N36. The financial support by the Austrian Federal Ministry for Digital and Economic Affairs, the National Foundation for Research, Technology and Development and the Christian Doppler Research Association is gratefully acknowledged.

Inverse moving point source problem for the wave equation

Faouzi Triki[1]

[1] *Université Grenoble Alpes*
email: `faouzi.triki@univ-grenoble-alpes.fr`

Abstract

In the talk I will present recent results on the inverse problem of identifying moving point sources for a three-dimensional wave equation from boundary measurements [1, 2]. Precisely, I will show that the knowledge of the field generated by the source at six different points of the boundary over a finite time interval is sufficient to determine uniquely its trajectory. I will also present Lipschitz stability estimate for the inversion under additional assumptions on the point sources.

References

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Optimal and Bayesian hypothesis testing in statistical inverse problems*

Remo Kretschmann[1], Daniel Wachsmuth[1], Frank Werner[1]

[1] *Institute of Mathematics, University of Würzburg*
email: remo.kretschmann@mathematik.uni-wuerzburg.de
email: daniel.wachsmuth@mathematik.uni-wuerzburg.de
email: frank.werner@mathematik.uni-wuerzburg.de

Abstract

In many inverse problems, one is not primarily interested in the whole solution $u^\dagger \in \mathcal{X}$, but in specific features of it that can be described by a family of linear functionals of $u^\dagger$. We perform statistical inference for such features by means of hypothesis testing.

This problem has recently been treated by multiscale methods based upon unbiased estimates of those functionals [1]. Constructing hypothesis tests using unbiased estimators, however, has two severe drawbacks: Firstly, unbiased estimators only exist for sufficiently smooth linear functionals, and secondly, they suffer from a huge variance due to the ill-posedness of the problem, so that the corresponding tests have bad detection properties.

One way to overcome both of these issues is by considering hypothesis tests with maximal power among all tests based upon linear estimators that have a given level of significance. While the construction of such optimal tests requires knowledge of the true solution $u^\dagger$, we present a way to compute hypothesis tests adaptively that maintain almost optimal power with high probability.

Another way to overcome aforementioned issues is by considering the problem from a Bayesian point of view, assigning a prior distribution to $u^\dagger$, and using the resulting posterior distribution to define regularized hypothesis tests. We study both of these approaches analytically and numerically for linear inverse problems and compare them with unregularized hypothesis testing.

References

[1] K. Proksch; F. Werner; A. Munk (2018). Multiscale scanning in inverse problems. Ann. Statist., 46(6B), p.3569–3602, doi:10.1214/17-AOS1669.

*The work of the authors was supported by DFG, Project WE 6204/2-1.

Forward Uncertainty Quantification for the Helmholtz Equation

Mirza Karamehmedović[1]

[1] *Department of Applied Mathematics and Computer Science*
Technical University of Denmark
email: `mika@dtu.dk`

Abstract

We consider the inhomogeneous Helmholtz equation in the plane with a Gaussian random field coefficient, and derive and characterize a singular system of the associated forward (source-to-near field measurement) operator. To this end we incorporate stochastic integrals (in the L2 sense) into a classical representation of the solution of the Helmholtz equation. Our work is applicable in the uncertainty quantification and robustness analysis of solution of acoustic and 2D electromagnetic inverse source problems in the presence of random media.

Deep Image Prior of Inverse Problems: Acceleration and Probabilistic Treatment

Bangti Jin[1]

[1] *Department of Mathematics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong*
email: `btjin@math.cuhk.edu.hk, bangti.jin@gmail.com`

Abstract

Since its first proposal in 2018, deep image prior has emerged as a very powerful unsupervised deep learning technique for solving inverse problems. The approach has demonstrated very encouraging empirical success in image denoising, deblurring, super-resolution etc. However, there are also several known drawbacks of the approach, notably high computational expense. In this talk, we describe some our efforts: we propose to accelerate the training process by pretraining on synthetic dataset and further we propose a novel probabilistic treatment of deep image prior to facilitate uncertainty quantification.

References

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Uncertainty quantification of inclusion boundaries in the context of X-ray tomography*

Babak Maboudi Afkham[1]

[1] *DTU Compute*
email: `bmaaf@dtu.dk`

Abstract

Inclusion detection arises in many applications of X-ray tomography, e.g., in medical imaging applications. In such applications, the boundaries of inclusions contain valuable information. The standard approach in extracting the boundaries of inclusions comprises the reconstruction of the inclusions and then post-processing for boundary extraction. This approach can result in undesirable artifacts and inaccuracies in the final results.

We propose a goal-oriented Bayesian approach for detecting boundaries of inclusions. Our method directly infers the boundary of inclusions, hence avoiding post-processing steps. Numerical results suggest this is a robust approach, even in a challenging imaging setup, e.g., limited angle imaging. In addition to estimating the boundaries, we also quantify the uncertainty in estimation. Moreover, our method provides a natural framework for quantifying the regularity (smoothness vs. spikiness), of the boundaries. In medical imaging applications, the regularity parameter provides cruicial information on identifying benign tumors from cancerous ones.

*This work was supported by a Villum Investigator grant (no. 25893) from The Villum Foundation.

Weakly Supervised Regression on Uncertain Datasets*

Alexander Litvinenko[1], Vladimir Berikov[2]

[1] *RWTH Aachen, Aachen, Germany*
email: `litvinenko@uq.rwth-aachen.de`

[2] *Sobolev Institute of Mathematics and Novosibirsk State University, Novosibirsk, Russia*
email: `berikov@math.nsc.ru`

Abstract

We solve a weakly supervised regression problem. Under "weakly" we understand that for some training points the labels are known, for some unknown, and for others uncertain due to the presence of random noise or other reasons such as lack of resources. The solution process requires to optimize a certain objective function (the loss function), which combines manifold regularization and low-rank matrix decomposition techniques. These low-rank approximations allow us to speed up all matrix calculations and reduce storage requirements. This is especially crucial for large datasets. Ensemble clustering is used for obtaining the co-association matrix, which we consider as the similarity matrix. The utilization of these techniques allows us to increase the quality and stability of the solution. In the numerical section, we applied the suggested method to artificial and real datasets using Monte-Carlo modeling [1, 2].

References

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*A. Litvinenko was supported by funding from the Alexander von Humboldt Foundation and V. Berikov by the state contract of the Sobolev Institute of Mathematics (project no 0314-2019-0015) and RFBR grants 19-29-01175 and 18-29-09041.

Sound speed uncertainty in Acousto-Electric Tomography

Kim Knudsen[1], Bjørn Christian Skov Jensen[2]

[1] *Technical University of Denmark*
email: kiknu@dtu.dk
[2] *University of Jyväskylä*
email:

Abstract

Acousto-electric tomography (AET) aims to reconstruct an image of the un- known electric conductivity in an object from exterior measurements of electrostatic currents and voltages while the object is penetrated by ultrasound waves. This is a coupled-physics inverse problem. Knowledge of the ultrasound wave is usually assumed to be accurate, but in reality the object's interior acoustic wave speed and transducer position is quite uncertain. In this work, we model uncertainty in the wave speed, and formulate a conductivity reconstruction method. We also establish theoretical error bounds, and show that the suggested approach can be understood as a regularization scheme for the inverse problem. Finally, we simulate the uncertain wave speed, and computationally explore the severity of the error in the reconstructions. Our results show that even with with reasonable sound speed uncertainty, reliable reconstruction is possible.

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Sparse Bayesian Inference with Regularized Gaussians*

Jasper M. Everink[1], Yiqiu Dong[2], Martin S. Andersen[3]

[1] *Technical University of Denmark*
email: jmev@dtu.dk
[2] *Technical University of Denmark*
email: yido@dtu.dk
[3] *Technical University of Denmark*
email: mskan@dtu.dk

Abstract

In this talk, we will present a method for Bayesian inference that, unlike many existing Bayesian methods, results in posterior distributions that assign positive probability to sparse vectors. We combine Gaussian distributions with the deterministic effects of sparsity-inducing regularization like l_1 norms, total variation and/or constraints. The resulting posterior distributions assign positive probability to various low-dimensional subspaces and therefore promote sparsity. Samples from this distribution can be generated by solving regularized linear least-squares problems with properly chosen data perturbations. We will discuss some properties of the underlying prior and use this methodology to derive an efficient algorithm for sampling from a Bayesian hierarchical model with sparsity structure.

*This work was supported by The Villum Foundation (grant no. 25893).

Bayesian Approach to Quantitative Photoacoustic Tomography*

Tanja Tarvainen[1]

[1] Department of Applied Physics, University of Eastern Finland, P.O. Box 1627, 70211 Kuopio, Finland
email: tanja.tarvainen@uef.fi

Abstract

Quantitative photoacoustic tomography aims at estimation of concentrations of light absorbing molecules such as oxygenated and deoxyganted haemoglobin [1]. In this inverse problem, two problems are solved [6]. First, in the acoustic inverse problem, an initial pressure caused by absorption of an externally introduced light is estimated from measured photoacoustic waves. Then, in the optical inverse problem, concentrations of light absorbing molecules are estimated from the initial pressure.

We approach the inverse problem of quantitative photoacoustic tomography in the framework of Bayesian inverse problems [3, 6]. We study the posterior distribution of the acoustic inverse problem that, with Gaussian model for noise and prior, is also a Gaussian distribution [7]. For the optical inverse problem, we calculate the *maximum a posteriori* (MAP) estimate and evaluate the reliability utilising a local linearisation [4, 2]. Errors and uncertainties are modelled using Bayesian approximation error modelling [3, 5].

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*The European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 101001417- QUANTOM), the Academy of Finland (projects 336799 Centre of Excellence in Inverse Modeling and Imaging and 320166 the Flagship Program Photonics Research and Innovation).

Empirical Bayesian estimation for semi-blind inverse problems: Application to image deblurring with total variation regularisation

Charlesquin Kemajou Mbakam[1], Marcelo Pereyra[2], Jean-Francois Giovannelli[3]

[1] *Heriot-Watt University*
email: `cmk2000@hw.ac.uk`

[2] *Heriot-Watt University*
email: `mp71@hw.ac.uk`

[3] *University of Bordeaux*
email: `Giova@IMS-Bordeaux.fr`

Abstract

This paper presents the empirical Bayesian methodology for solving inverse problems that are severely ill-posed or ill-conditioned, with a particular focus on the semi-blind deblurring problem in the imaging community. We typically addressed the ill-posed nature of the problem by regularising the estimation problem to make it well-posed. By adopting a Bayesian approach under the assumption the forward operator belongs to a known parametric class, we propose in this paper a novel and highly efficient method to estimate the forward operator's parameters by maximum marginal likelihood estimation, followed by inference on the pseudo posterior to evaluate the empirical Bayesian maximum-a-posteriori (MAP) solution. Since the marginal likelihood is computationally and analytically intractable due to the higher dimensional integral and the non-Gaussian structure of the posterior, our proposed method driven by a Markov kernel adopted a stochastic approximation proximal gradient (SAPG) algorithm, easily deployed in any log-concave and nonsmooth semi-blind problem with fixed model parameters in imaging sciences. The proposed method is demonstrated using three different parametric classes of forward operators (Gaussian, Moffat and Laplace) on semi-blind image deblurring problems with total variation prior. In addition, we conduct model selection in the absence of the ground truth image using a fast heuristic approach. Finally, we show that our method achieves close to the optimal results, which competes with many blind and semi-blind state-of-art convex optimisation method.

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