AFRL-AFOSR-VA-TR-2020-0088

HIERARCHICAL METHODOLOGY FOR INVERSE PROBLEMS

Andrew Stuart
CALIFORNIA INSTITUTE OF TECHNOLOGY

06/16/2020
Final Report

Air Force Research Laboratory
AF Office Of Scientific Research (AFOSR)/ RTA2
Arlington, Virginia 22203
Air Force Materiel Command

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
06-07-2020

2. REPORT TYPE
Final Performance

3. DATES COVERED *(From - To)*
01 Apr 2017 to 31 Mar 2020

4. TITLE AND SUBTITLE
HIERARCHICAL METHODOLOGY FOR INVERSE PROBLEMS

5a. CONTRACT NUMBER

5b. GRANT NUMBER
FA9550-17-1-0185

5c. PROGRAM ELEMENT NUMBER
61102F

6. AUTHOR(S)
Andrew Stuart

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
CALIFORNIA INSTITUTE OF TECHNOLOGY
1200 E. CALIFORNIA BLDV
PASADENA, CA 91125 US

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AF Office of Scientific Research
875 N. Randolph St. Room 3112
Arlington, VA 22203

10. SPONSOR/MONITOR'S ACRONYM(S)
AFRL/AFOSR RTA2

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-AFOSR-VA-TR-2020-0088

12. DISTRIBUTION/AVAILABILITY STATEMENT
A DISTRIBUTION UNLIMITED: PB Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT
Predictive mechanistic models have a long and rich history, stretching back through centuries of human knowledge development. The wealth of data now available presents an opportunity to leverage these models to new levels of predictive capability,through careful calibration, and also presents new ways of thinking about modelling, which are data-driven, and which have emerged over the last two decades in the machine learning community. Calibration of models to data is often refered to in the mathematics literature as an inverse problem.
The goal of the funded work was to marry the best features of mechanistic modelling and data-driven modelling via the development of novel hierarchical algorithms for inverse problems. Hierarchical methods are attractive because, at the cost of relatively cheap outer optimization loop, typically for a small number of parameters, greater predictive capability is achieved. The result of the work is new computational methodologies for inverse problems, both classical and statistical, founded on theoretical understanding and with demonstrable applicability to important inverse problems in the physical sciences.

15. SUBJECT TERMS
inverse problem, hierarchical Bayesian

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			FAHROO, FARIBA

Unclassified	Unclassified	Unclassified	UU	**PAGES**	**19b. TELEPHONE NUMBER** *(Include area code)* 703-696-8429

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18

AFOSR Report Submission Form

Report Type: Final Report
Primary Contact Email: astuart@caltech.edu
Primary Contact Phone Number: (626)893-4526
Organization/Institution Name: California Institute Of Technology

Award Information

Grant/Contract Title: Hierarchical Methodology for Inverse Problems

Grant/Contract Number: FA9550-17-1-0185

Principal Investigator Name: Andrew Stuart

Program Officer: Fariba Farhoo

Report Information - Final Report

Reporting Period Start Date: 1st April 2017

Reporting Period End Date: 31st March 2020

Abstract:
Predictive mechanistic models have a long and rich history, stretching back through centuries of human knowledge development. The wealth of data now available presents an opportunity to leverage these models to new levels of predictive capability, through careful calibration, and also presents new ways of thinking about modelling, which are data-driven, and which have emerged over the last two decades in the machine learning community. Calbibration of models to data is often refered to in the mathematics literature as an inverse problem.

The goal of the funded work was to marry the best features of mechanistic modelling and data-driven modelling via the development of novel hierarchical algorithms for inverse problems. Hierarchical methods are attractive because, at the cost of relatively cheap outer optimization loop, typically for a small number of parameters, greater predictive capability is achieved. The result of the work is new computational methodologies for inverse problems, both classical and statistical, founded on theoretical understanding and with demonstrable applicability to important inverse problems in the physical sciences.

Distribution Statement:
All the research undertaken is publicably available in the form of archival journal publications, or on the arXiv, whilst waiting evaluation by a journal.

Explanation for Distribution Statement: A -- Approved for Public Release

SF298 Form: Attached

*** Additional Information ***

The research was organized around four work packages. The first, WP1, was devoted to the development of Vector-Valued Bayesian Level Sets. These have proven useful for the reconstruction of functions with unknown interfaces, since work of Santosa; developing them as a methodology for Bayesian inversion, and hence to quantify uncertainty in the determination of the interface, has been an outstanding problem until recently. Aspects of the problem have been addressed in this work by drawing links with classification problems in machine learning -- boundaries between different classes are analogous to interfaces in PDE based physical inverae problems. WP2 is concerned with Hierarchical Length and Amplitude Scales; a clear message from Gaussian process regression is that the use of hierarchical parameters can increase expressive power in approximation theory immesurably, often with only a small increase in cost. The work in WP2 has shown how this idea can be developed systematically within the context of inverse problems more general than the regression problem tackled via Gaussian processes, leading to wide applicability. WP3 takes this idea further to the setting in which the hierarchical parameter is itself a field: Deep Gaussian Processess. This idea emerged in the machine learning literature and once again has resonance with analogous ideas rising in PDE-based physical inverse problems; this resonance has been developed as part of WP3. WP4 is concerned with Hierarchical Classical Regularization: typically hierarchical methods are develoed in the Bayesian setting, but the link with MAP estimators (the most likely point in the Bayesian posterior) enables the drawing of conclusions concerning classical optimization based methodologies for inversion; in particular hierarchical Bayesian methods lead to hierarchical optimization approachs. Substantial progress has been made in all four of the work packages and, additionally, cross-cutting research has been published.

In WP1 we completed and submitted a paper demonstrating application of the Bayesian level set methodology to the classification of videos of human motion, including uncertainty quantification and human-in-the-loop learning [4]; we also worked on application of the method to inverse problems arising from the eikonal equation, with potential application in aircraft vehicle planning design, and travel time tomography, [11]. In WP2 we published a paper in which the methodology is applied to ensemble Kalman inversion (EKI, a derivative free optimization methodology with wide applicability) [3]; we submitted a paper in which the methodology is applied to Monte Carlo Markov Chain methods which are dimension robust – the number of iterations is independent of the level of mesh resolution [9]; and, together with AFOSR-funded researcher and Caltech colleague Houman Owhadi, we developed a theory for hierarchical learning in the solution of regression problems [10]; and we studied similar questions for other linear inverse problems in [7]. Regarding WP3 we published a paper which provides a foundational theory for this subject area [2]. In WP4 we submitted a paper demonstrating how Tikhonov regularization can be included within EKI, a form of hierarchical inversion since the EKI already regularizes through the subspace property [6]. In addition to these papers directly addressing the four work packages, papers [1,5,8] address various inverse problems using methodologies that cut across the workpackages, tackling new applications (optical tomography and inverse optimal transport) and introducing new methodologies (linear approximations within Bayesian iterative approaches).

Awards and Honors: In spring 2020 the PI was elected a Fellow Of The Royal Society, the UK's national academy for sciences and engineering. During the course of the award the PI was invited to deliver plenary lectures, related in part to AFOSR funded research, in the following fora:

• Strathclyde Numerical Analysis Meeting. Glasgow, Scotland, June 27th–30th 2017.

• FOCM 2017. Barcelona, Spain, July 10th–14th 2017.

• 14th US National Congress on Computational Mechanics. Montreal, Canada, July 17th–20th 2017.

• BayesComp Inaugural Conference. Barcelona, Spain, March 25th–28th 2018.

• Big Data and Data Science for Learning in the Digital World. Madrid, Spain, June 4th–6th 2018.

• The 20th European Conference on Mathematics for Industry. Budapest, Hungary, June18th–22nd 2018.

• 7th International Symposium on Data Assimilation (ISDA2019). Kobe, Japan, January 21st–25th 2019.

• Jacques Morgenstern Colloqium, INRIA. Nice, France, March 28th 2019.

• Jacques Louis Lions Laboratory 50th Anniversary. Paris, France, November 27th–29th 2019.

Students and Postdocs Funded: In addition to funding for the PI, AFOSR funds also supported PhD student Nikola Kovachki; he is curretly in his fourth year of study. AFOSR funds additionally supported four postdoctoral researchers: Matthew Dunlop, Franca Hoffmann, Bamdad Hosseini and Shiwei Lan. Hoffmann and Lan now have permanent faculty positions at Caltech (from 2022) and ASU, respectively. Dunlop and Hosseini are postdoctoral researchers at NYU and at Caltech respectively.

Archival Publications (published) during reporting period:

[1] D.Calvetti, M.M.Dunlop, E.Somersalo, A.M.Stuart, Iterative Updating of Model Error for Bayesian Inversion.

Inverse Problems, 34 (2018) 025008.
http://stuart.caltech.edu/publications/pdf/stuart140.pdf

[2] MM. Dunlop, MA. Girolami, AM. Stuart, AL. Teckentrup; How Deep Are Deep Gaussian Processes?, Journal of Machine Learning Research 19(54):1−46, 2018.
http://stuart.caltech.edu/publications/pdf/stuart144.pdf

[3] N.K.Chada, M.A.Iglesias, L.Roininen, A.M.Stuart, Parameterizations for Ensemble Kalman Inversion. Inverse Problems, 34 (2018) 055009.
http://stuart.caltech.edu/publications/pdf/stuart142.pdf

[4] Y. Qiao, C. Shi, C. Wang, H. Li, M. Haberland, X. Luo, AM. Stuart, AL. Bertozzi; Uncertainty Quantification for Semi-supervised Multi-class Classification in Image Processing and Ego-Motion Analysis of Body-Worn Videos.
http://stuart.caltech.edu/publications/pdf/stuart146.pdf

[5] A. M. Stuart and M.-T. Wolfram; Inverse Optimal Transport. SIAM J. Appl. Math. 80-1 (2020), pp. 599-619.
http://stuart.caltech.edu/publications/pdf/stuart153.pdf

[6] NK. Chada, AM. Stuart, XT. Tong; Tikhonov Regularization Within Ensemble Kalman Inversion. SIAM J. Numer. Anal., 58(2), 1263–1294.
http://stuart.caltech.edu/publications/pdf/stuart154.pdf

[7] M. M. Dunlop, T. Helin, A. M. Stuart; Hyperparameter Estimation in Bayesian MAP Estimation: Parameterizations and Consistency. SMAI J. of Computational Mathematics 6(2020), 69--100.
http://stuart.caltech.edu/publications/pdf/stuart156.pdf

[8] K. Newton, Q. Li, and A. M. Stuart; Diffusive Optical Tomography in the Bayesian Framework, SIAM Multiscale Model. Simul. Vol. 18, No. 2, pp. 589-611.
http://stuart.caltech.edu/publications/pdf/stuart157.pdf

[9] V.Chen, M.M.Dunlop, O.Papaspiliopoulos, A.M.Stuart; Robust MCMC Sampling with Non-Gaussian and Hierarchical Priors in High Dimensions.
https://arxiv.org/abs/1803.03344

[10] Y. Chen, H. Owhadi, A. M. Stuart; Consistency of Empirical Bayes And Kernel Flow For Hierarchical Parameter Estimation. arXiv:2005.11375

[11] O.R.A. Dunbar, M. M. Dunlop, C. M. Elliott, V. H. Hoang, A. M. Stuart; Reconciling Bayesian and Perimeter Regularization for Binary Inversion SIAM Journal on Scientific Computing (SISC), To Appear. arXiv:1706.01960

New discoveries, inventions, or patent disclosures: None

Changes in research objectives, if any: None.

Change in AFOSR Program Officer, if any: Jean-Luc Cambier was replaced by Fariba Farhoo

Extensions granted or milestones slipped, if any: None