

Variational Bayesian Inference: Message Passing Schemes and Streamlined Multilevel Data Analysis

Tui Hiraka Nolan

*Submitted to the School of Mathematical and Physical
Sciences, Faculty of Science in partial fulfilment of the
requirements for the degree of*

Doctor of Philosophy (Mathematics)

at the

UNIVERSITY OF TECHNOLOGY SYDNEY

April, 2020

Certificate of Original Authorship

I, Tui Hiraka Nolan, declare that this thesis is submitted in fulfilment of the requirements for the award of Doctor of Philosophy (Mathematics), in the School of Mathematical and Physical Sciences, Faculty of Science at the University of Technology Sydney.

This thesis is wholly my own work, unless otherwise referenced or acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis. This document has not been submitted for qualifications at any other academic institution.

This research is supported by the Australian Government Research Training Program.

Production Note:

Signature: Signature removed prior to publication.

Date: 24 April 2020

Acknowledgements

I wish to extend my deepest thanks to my supervisor, Professor Matt Wand, for his guidance and mentorship. His support has provided opportunities and career pathways that were otherwise inaccessible, and I am truly grateful. I am extremely fortunate to have him as a role model and a friend.

My doctoral studies were supported by a Research Training Program Scholarship and a Jumbunna Postgraduate Research Scholarship, which I very much appreciate.

I would like to extend my gratitude to UTS: Jumbunna Institute for Indigenous Education and Research and the Aurora Education Foundation. Both of these organisations have influenced my passion for promoting education within the Indigenous Australian community. My selection in the 2016 Aurora Indigenous Scholars International Study Tour opened my eyes to the international opportunities that are available through my doctoral studies.

Sincere thanks are due to my family, who have provided continual support and encouragement. A special thanks to my late father, John Nolan. Although he did not witness this academic journey, his legacy of hard work and dedication has motivated and guided me in the success of this research endeavour.

To my wife, Cassandra Nolan, thank you for your love and encouragement. Your companionship has been my most valued source of support, which has inspired me during the most difficult periods of this doctoral program.

Publications

Nolan, T., & Wand, M. (2019). *Solutions to sparse multilevel matrix problems*. (Submitted to Statistics and Probability Letters and available on arXiv at arXiv:1903.03089)

Nolan, T., Menictas, M., & Wand, M. (2019). *Streamlined computing for variational inference with higher level random effects*. (Submitted to the Journal of Machine Learning Research and available on arXiv at arXiv:1903.06616)

Menictas, M., Nolan, T., Simpson, D., & Wand, M. (2019). *Streamlined variational inference for higher level group-specific curve models*. (Submitted to Statistical Modelling and currently available on arXiv at arXiv:1903.04043)

Nolan, T., & Wand, M. (2017). Accurate logistic variational message passing: algebraic and numerical details. *Stat*, 6, 102–112.

Awards and Honours from my Doctoral Candidature

Fulbright Postdoctoral Scholarship (The Kinghorn Foundation and Western Sydney University, 2019)

Aboriginal and Torres Strait Islander Scientist Travelling Research Award (Australian Academy of Science and the Alan Turing Institute, 2019)

STEM Professional Early Career Award (CSIRO, 2019)

Research Training Program Scholarship (University of Technology Sydney and the Australian Government, 2016–2019)

Jumbunna Postgraduate Research Scholarship (UTS: Jumbunna Institute for Indigenous Education and Research, 2016–2019)

Aurora Indigenous Scholars International Study Tour (Aurora Education Foundation and the Aspiration Initiative, 2016)

Abstract

Mean-field variational Bayes (MFVB) is a deterministic technique for approximating intractable integrals arising in Bayesian inference. They are typically used for making approximate inference for parameters in complex statistical models. Most of its foundational literature and applications are in Machine Learning. However, in the age of “Big Data”, and by extension large sample sizes, MFVB has become an important tool in Statistics.

The approximating schemes afforded by MFVB rely on heavy algebraic derivations across the model. The emergence of Big Data has resulted in more complex statistical models, making the process of formulating an MFVB algorithm cumbersome. Fortunately, the MFVB updating scheme can be simplified by representing the parameters of the statistical model in a probabilistic graph. The derivations are made more efficient by decomposing the required computations into calculations that are local to each node in the graph.

We focus on constructing variational Bayesian inference algorithms based on a modularised format known as variational message passing (VMP), which is founded upon the notion of messages passed between fragments on a factor graph. Primitive functions, which represent the localised messages over factor graph fragments, are derived and can be called upon for direct implementation into arbitrarily large statistical models. The MFVB and VMP approaches result in superficially different algorithms, but converge to identical posterior density function approximations because they are founded upon the same optimisation problem. For complex statistical models, VMP has the advantage that the iterative updates are adjusted into a modularised format by taking advantage of the localised computations afforded by variational Bayesian methods. The resulting algorithm is a sequence of fragment-based functions that represent a compartmentalisation of the required algebra and computer coding.

Despite the computational convenience of VMP algorithms over their MFVB counterparts, the speed of both classes is limited for multilevel data models, such as Gaussian response linear mixed models. Statistical inference on such models requires standard matrix operations, such as inversion and matrix-vector multiplication, on sparse matrices, which are difficult to achieve efficiently. Furthermore, computational storage issues restrict the size of such models. Streamlined matrix algebraic results are necessary for implementing fast frequentist and variational Bayesian inference, which is not inhibited by storage-greedy sparse matrix operations, on multilevel data models.

This thesis develops factor graph fragment functions that can be used to build complex statistical models and achieves streamlined matrix algebraic derivations for multilevel data analysis.

Contents

1	Introduction	2
1.1	Notational Guide	3
1.1.1	Logic and Set Notation	3
1.1.2	Matrix Notation	3
1.1.3	Functional Notation	4
1.1.4	Algorithmic Notation	5
1.2	Vector Differential Calculus	7
1.2.1	Vector and Matrix Operations	7
1.2.2	A Primer on Vector Differential Calculus	8
1.3	Probabilistic Graph Theory	10
1.3.1	Directed Acyclic Graphs	11
1.3.2	Undirected Graphs	12
1.3.3	Conditional Independence	14
1.3.4	Applications of Graphical Models	15
1.4	Exponential Families	16
1.4.1	Basics of Exponential Families	16
1.4.2	Graphical Models in Exponential Form	17
1.5	Semiparametric Regression	18
1.5.1	Mixed Model Representation	21
1.6	Bayesian Inference	22
1.6.1	Bayesian Statistics	22
1.6.2	Markov Chain Monte Carlo	22
2	Variational Bayesian Inference	24
2.1	Mean Field Variational Bayes	25
2.2	Variational Message Passing	26
2.3	Exponential Family Special Case	29
2.3.1	Normal Distribution Special Case	30
2.4	Fundamental Fragments for Arbitrarily Large Regression Models	31
2.4.1	Gaussian Prior Fragment	32
2.4.2	Inverse G-Wishart Prior Fragment	32
2.4.3	Iterated Inverse G-Wishart Fragment	33
2.4.4	Dirichlet Prior Fragment	34

2.4.5	Gaussian Penalisation Fragment	35
2.4.6	Gaussian Likelihood Fragment	37
2.4.7	A Note on Fragment Inputs	37
2.5	A Motivating Example	38
2.5.1	The MFVB Approach	39
2.5.2	The VMP Approach	41
2.5.3	Arbitrarily Large Model Viewpoint	42
2.5.4	Heuristic Justification of the Mean Field Approximation	44
2.6	Assessment of Accuracy for Variational Bayesian Approximations	46
2.7	Consequences of the Mean Field Approximation	47
2.A	Exponential Family Results	47
2.A.1	Normal Distribution	48
2.A.2	Inverse G-Wishart Distribution	49
2.A.3	Beta and Dirichlet Distributions	51
2.A.4	Binomial and Multinomial Distributions	52
3	Normal Mixture Models	53
3.1	Univariate Normal Mixture Model	54
3.2	Multivariate Normal Mixture Model	57
3.3	Extension to Regression Models with Missing Data	59
3.4	Simulations of the Univariate Normal Mixture Model	64
3.4.1	Assessment of Accuracy	64
3.4.2	Speed Comparisons	65
3.5	Discussion	65
3.A	Derivation of Algorithm 20	66
3.B	Derivation of Algorithm 21	68
3.C	Derivation of Algorithm 22	69
3.D	Derivation of Algorithm 23	71
3.E	Derivation of Algorithm 24	73
4	Variational Approximations for Probit Regression Models	76
4.1	Approximation Techniques for the Probit Likelihood Fragment	77
4.1.1	Albert-Chib	77
4.1.2	Ormerod-Wand	78
4.2	Simulations of Probit-Based Regression Models	80
4.2.1	Linear Bayesian Probit Regression Model	80
4.2.2	Semiparametric Bayesian Probit Regression Model	82
4.3	Discussion	85
4.A	Details for the Ormerod-Wand Fragment	86
4.A.1	Adaptive Gauss Hermite Quadrature	86
4.A.2	Derivation of Algorithm 26	87

4.B	Approximation of $\text{Corr}(\beta_0, \beta_1 \mathbf{y})$	88
5	Variational Approximations for Logistic Regression Models	89
5.1	Approximation Techniques for the Logistic Likelihood Fragment	90
5.1.1	Jaakkola-Jordan	90
5.1.2	Saul-Jordan	92
5.1.3	Knowles-Minka-Wand	93
5.2	Simulations of Logistic-Based Regression Models	97
5.2.1	Linear Bayesian Logistic Regression Model	97
5.2.2	Semiparametric Bayesian Logistic Regression Model	100
5.3	Other Approximation Techniques	101
5.4	Discussion	102
5.A	Details for the Saul-Jordan Fragment	103
5.A.1	Proof of Lemma 5.1.2	103
5.A.2	Proof of Theorem 5.1.3	103
5.A.3	Derivation of Algorithm 28	104
5.B	Details for the Knowles-Minka-Wand Fragment	104
5.B.1	Proof of Corollary 5.1.4	104
5.B.2	Proof of Theorem 5.1.5	104
5.C	Approximation of $\text{Corr}(\beta_0, \beta_1 \mathbf{y})$	106
6	Solutions to Sparse Multilevel Matrix Problems	107
6.1	Two Level Sparse Matrix Problems	108
6.1.1	Least Squares Form and QR-decomposition Enhancement for Two Level Sparse Matrices	111
6.2	Three Level Sparse Matrix Problems	113
6.2.1	Least Squares Form and QR-decomposition Enhancement for Three Level Sparse Matrices	116
6.3	Discussion	119
6.A	Proofs	120
6.A.1	Proof of Theorem 6.1.1	120
6.A.2	Proof of Theorem 6.1.2	122
6.A.3	Proof of Theorem 6.2.1	124
6.A.4	Proof of Theorem 6.2.2	128
6.B	Algorithms	133
6.B.1	Functions for QR-Decompositions	133
7	Two Level Gaussian Response Models	134
7.1	Two Level Best Linear Unbiased Prediction	135
7.2	Two Level Mean Field Variational Bayes	137
7.3	Two Level Variational Message Passing	141
7.3.1	Streamlined Two Level Gaussian Likelihood Fragment Updates	144

7.3.2	Streamlined Gaussian Penalisation Fragment Updates	145
7.3.3	Computations for the q -Density Functions	146
7.4	Simulations of the Two Level Model	147
7.4.1	Assessment of Accuracy	147
7.4.2	Assessment of Speed and Computational Storage	149
7.5	Discussion	150
7.A	The Lower Bound on the Marginal Log-Likelihood for the Two Level Gaussian Response Model	151
7.B	Proofs	151
7.B.1	Proof of Corollary 7.1.1	151
7.B.2	Proof of Corollary 7.2.1	152
7.B.3	Proof of Corollary 7.3.1	152
7.C	Algorithms	153
7.C.1	TWOLEVELITERATEDINVERSECHISQUARED	153
7.C.2	TWOLEVELITERATEDINVERSEGWISHART	154
7.C.3	Derivation of Algorithm 37	155
7.C.4	Derivation of Algorithm 38	156
7.C.5	Derivation of Algorithm 39	158
8	Three Level Gaussian Response Models	161
8.1	Three Level Best Linear Unbiased Prediction	161
8.2	Three Level Mean Field Variational Bayes	164
8.3	Three Level Variational Message Passing	167
8.3.1	Streamlined Three Level Gaussian Likelihood Fragment	171
8.3.2	Streamlined Three Level Gaussian Penalisation Fragment	173
8.4	Simulations of the Three Level Model	173
8.4.1	Assessment of Accuracy	173
8.4.2	Assessment of Speed and Computational Storage	176
8.5	Discussion	176
8.A	The Lower Bound on the Marginal Log-Likelihood for the Three Level Gaussian Response Model	177
8.B	Proofs	179
8.B.1	Proof of Corollary 8.1.1	179
8.B.2	Proof of Corollary 8.2.1	179
8.B.3	Proof of Corollary 8.3.1	180
8.C	Algorithms	180
8.C.1	THREELEVELITERATEDINVERSECHISQUARED	180
8.C.2	THREELEVELITERATEDINVERSEGWISHART	181
8.C.3	THREELEVELNATURALTOCOMMONPARAMETERS	182
8.C.4	Derivation of Algorithm 44	182
8.C.5	Derivation of Algorithm 45	183

8.C.6	Derivation of Algorithm 46	186
9	Closing Remarks and Future Work	190
9.1	Variational Message Passing Schemes	190
9.2	Sparse Multilevel Data Analysis	191
References		193