

Improved Iterative Schemes for
REML Estimation of Variance Parameters
in Linear Mixed Models

Emma Knight

School of Agriculture, Food and Wine
The University of Adelaide

13 October 2008

Contents

Abstract	vii
Declaration	ix
Acknowledgements	xi
1 Introduction	1
1.1 Review of comparisons of algorithms used to compute REML estimates of variance parameters	3
1.2 Methods used to calculate estimates of variance parameters in common statistical software	4
1.3 Improved Iterative Schemes	6
1.4 Outline	7
2 Mixed Models	9
2.1 Model	9
2.2 Estimation	11
2.2.1 Best Linear Unbiased Prediction	11
2.2.2 REML Estimation of Variance Parameters	17
2.3 Iterative Schemes	27
3 AI Algorithm	29
3.1 Introduction	29
3.2 AI Algorithm	33
3.3 Absorption, Backsubstitution and Inversion	35
4 EM Algorithm	41
4.1 Introduction	41
4.2 Definition of the EM Algorithm	45
4.3 Monotonicity of the EM Algorithm	45
4.4 Self-Consistency of the EM Algorithm	47

4.5	REML EM Algorithm for Mixed Models	48
5	PXEM Algorithm	55
5.1	Introduction	55
5.2	REML PXEM Algorithm for Mixed Models	56
6	Rates of Convergence	67
6.1	Introduction	67
6.2	Convergence Criterion	67
6.3	Order of Convergence	68
6.3.1	Newton-Raphson Algorithm	69
6.3.2	Fisher Scoring Algorithm	70
6.3.3	Average Information Algorithm	71
6.3.4	EM Algorithm	71
6.3.5	PXEM Algorithm	76
6.3.6	Measuring the Linear Rate of Convergence	78
7	Improved Iterative Schemes	81
7.1	Introduction	81
7.2	Hybrid Schemes	81
7.3	Local Schemes	83
7.3.1	Local EM Algorithm	87
7.3.2	Local PXEM Algorithm	88
7.3.3	Implementation of Local Schemes	94
7.4	Starting Values	95
8	Variance Components Model	97
8.1	Introduction	97
8.2	Variance Components Model and Results	97
8.2.1	AI Algorithm	98
8.2.2	EM Algorithm	99
8.2.3	PXEM Algorithm	101
8.2.4	Local EM Scheme	106
8.2.5	Local PXEM Scheme	107
8.2.6	Starting Values	108
8.3	Lamb Weight Data	111
8.4	Simulated Incomplete Block Design Data	118

8.4.1	Incomplete Block Design with 9 replicates	119
8.4.2	Incomplete Block Design with 3 replicates	135
8.5	Robust Iterative Scheme	150
9	Unstructured G Model	157
9.1	Introduction	157
9.2	Unstructured G Model and Results	158
9.2.1	AI Algorithm	161
9.2.2	EM Algorithm	162
9.2.3	Computing EM updates	167
9.2.4	PXEM Algorithm	169
9.2.5	Local EM Scheme	175
9.2.6	Local PXEM Scheme	177
9.2.7	Starting Values	178
9.2.7.1	Multivariate Data	178
9.2.7.2	Random Coefficient Data	184
9.3	Random Coefficient Data Sets	186
9.3.1	Orthodontic Data	186
9.3.2	Ultrafiltration Data	196
9.3.3	Simulated Random Coefficient Data	206
9.4	Multi-Environment Plant Variety Data	229
9.4.1	Simulated Multi-Environment Plant Variety Data	229
9.5	Robust Iterative Scheme	260
10	Conclusion	267
	Appendix	273
	Bibliography	283

Abstract

Residual maximum likelihood (REML) estimation is a popular method of estimation for variance parameters in linear mixed models, which typically requires an iterative scheme. The aim of this thesis is to review several popular iterative schemes and to develop an improved iterative strategy that will work for a wide class of models.

The average information (AI) algorithm is a computationally convenient and efficient algorithm to use when starting values are in the neighbourhood of the REML solution. However when reasonable starting values are not available, the algorithm can fail to converge. The expectation-maximisation (EM) algorithm and the parameter expanded EM (PXEM) algorithm are good alternatives in these situations but they can be very slow to converge. The formulation of these algorithms for a general linear mixed model is presented, along with their convergence properties.

A series of hybrid algorithms are presented. EM or PXEM iterations are used initially to obtain variance parameter estimates that are in the neighbourhood of the REML solution, and then AI iterations are used to ensure rapid convergence. Composite local EM/AI and local PXEM/AI schemes are also developed; the local EM and local PXEM algorithms update only the random effect variance parameters, with the estimates of the residual error variance parameters held fixed. Techniques for determining when to use EM-type iterations and when to switch to AI iterations are investigated. Methods for obtaining starting values for the iterative schemes are also presented.

The performance of these various schemes is investigated for several different linear mixed models. A number of data sets are used, including published data sets and simulated data. The performance of the basic algorithms is compared to that of the various hybrid algorithms, using both uninformed and informed starting values. The theoretical and empirical convergence rates are calculated and compared for the basic algorithms.

The direct comparison of the AI and PXEM algorithms shows that the PXEM algorithm, although an improvement over the EM algorithm, still falls well short of the AI algorithm in terms of speed of convergence. However, when the starting values are too far from the REML solution, the AI algorithm can be unstable. Instability is most likely to arise in models with a more complex variance structure. The hybrid schemes use EM-type iterations to move close enough to the REML solution to enable the AI algorithm to successfully converge. They are shown to be robust to choice of starting values like the EM and PXEM algorithms, while demonstrating fast convergence like the AI algorithm.

Declaration

This work contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text.

I consent to this copy of my thesis, when deposited in the University Library, being made available for loan and photocopying, subject to the provisions of the Copyright Act 1968.

Emma Knight

Acknowledgements

Thankyou to my supervisors Professor Ari Verbyla, Professor Brian Cullis and Professor Robin Thompson for their guidance, support and encouragement.

I thank my colleagues at the Australian National University for their continual support and encouragement; Jeff Wood for providing a sounding board and for reading and commenting on sections of my thesis, Ross Cunningham for letting me know that the tough days towards the end were not unusual, Christine Donnelly for the pep talks that helped to motivate and focus me, David Lindenmayer for his patience and understanding, and to Rachel Muntz, Sam Banks, Adam Felton and Diane Jakobasch for listening when I just needed someone to listen.

To those friends who were brave enough to enquire about the progress I was or was not making, I thank them for their best wishes and for putting up with my sometimes unfriendly responses. And to those friends who knew not to ask, thankyou. In particular I would like to thank Sheridan Price, Luke Cartwright, Bec Darbyshire, Jen and Sean Moran and Damien Brown for their friendship, support and encouragement.

I am grateful to my family for their continual love and support, and for their belief that I would eventually get there. Finally I thank my husband Paul for his endless patience, understanding and love, and for not only providing, but also hiding and rationing chocolate supplies.