

**An anisotropic Matérn
spatial covariance model:
REML estimation and properties**

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Contents

1	Introduction	1
1.1	Background	1
1.2	Advances	1
1.3	Structure of the thesis	3
1.4	Principal contributions	4
2	Classical geostatistics	5
2.1	What is geostatistics?	5
2.2	Aims of spatial data analysis	6
2.3	Notation for geostatistical spatial data	6
2.4	Approaches to spatial data analysis	6
2.5	Stationarity	8
2.6	Isotropy	9
2.7	The spatial covariance function	10
2.8	Separability	12
2.9	The variogram	13
2.10	The empirical variogram	18
2.11	Estimating the variogram	19
2.12	Kriging, assuming a known variogram	19
2.13	The nugget effect	24
2.14	Kriging using covariance	27
2.15	Classical and Gaussian geostatistics	28
3	Model-based geostatistics	29
3.1	Gaussian spatial processes	29
3.2	Linear models for spatial data	29
3.3	Gaussian linear mixed models	31
3.4	Residual maximum likelihood (REML)	32
3.5	Prediction in the linear mixed models context	34
3.6	Kriging using linear mixed models	36
3.7	Plug-in predictions	38
3.8	Modelling a nugget effect	39

3.9	A general prediction result	40
3.10	Application to model-based spatial prediction	41
3.11	Kriging using linear mixed models — Summary	43
4	The Matérn class of spatial covariance models	45
4.1	Matérn correlation	45
4.2	Alternative parameterisations	48
4.3	Derivatives	49
4.4	Numerical difficulties	55
4.5	REML Implementation	65
4.6	Initial values	66
5	Geometric anisotropy and the Matérn Class	69
5.1	Geometric anisotropy	69
5.2	Derivatives for geometric anisotropy	71
5.3	Matérn correlation with geometric anisotropy	71
5.4	Minkowski metric	75
5.5	Initial values	76
5.6	Separable $AR(1) \times AR(1)$	77
5.7	A test for anisotropy	78
5.8	ASReml implementation	85
5.9	Extended Matérn class	86
6	Three examples	89
6.1	Soil salinity ECa data for rice growing	89
6.1.1	Obtaining initial values	93
6.1.2	Results	94
6.1.3	Implications for predictions	98
6.1.4	Predictions for the study region	99
6.2	Fine-scale soil pH	102
6.3	Cashmore soil water data	106
6.4	Concluding remarks	118
7	Simulations	121
7.1	Motivation	121
7.2	Parameter combinations	123
7.3	Sampling schemes	124
7.4	Convergence criteria and measures of performance	125
7.5	Results	130
7.5.1	Isotropic simulations without nugget	130
7.5.2	Isotropic simulations with nugget	137

7.5.3	Anisotropic simulations without nugget	141
7.5.4	Anisotropic simulations with nugget	144
7.6	Approximate standard errors	144
7.7	Comparing simulation results	149
7.8	Discussion and Conclusions	155
8	Model misspecification and PEV	161
8.1	Motivation	161
8.2	Method	161
8.3	Results	164
9	Overview and Concluding Remarks	169
9.1	Background	169
9.2	Anisotropic Matérn covariance	169
9.3	Application to examples	170
9.4	Simulation results	171
9.5	Model misspecification and mean squared error of prediction	171
9.6	Further work	172
	Appendices	174
A	Matrix Results	175
A.1	Partitioned matrix inverses	175
A.2	Matrix differentiation	178
B	Results for modified Bessel functions	181
C	Conditional Gaussian distribution	183
D	Angular function results	185
E	Exit codes from ASReml	187
F	Standard errors based on expected information	191
G	Reprint of paper	193

Abstract

This thesis concerns the development, estimation and investigation of a general anisotropic spatial correlation function, within model-based geostatistics, expressed as a Gaussian linear mixed model, and estimated using residual maximum likelihood (REML).

The Matérn correlation function is attractive because of its parameter which controls smoothness of the spatial process, and which can be estimated from the data. This function is combined with geometric anisotropy, with an extension permitting different distance metrics, forming a flexible spatial covariance model which incorporates as special cases many infinite-range spatial covariance functions in common use.

Derivatives of the residual log-likelihood with respect to the four correlation-model parameters are derived, and the REML algorithm coded in Splus for testing and refinement as a precursor to its implementation into the software ASReml, with additional generality of linear mixed models. Suggestions are given regarding initial values for the estimation. A residual likelihood ratio test for anisotropy is also developed and investigated.

Application to three soil-based examples reveals that anisotropy does occur in practice, and that this technique is able to fit covariance models previously unavailable or inaccessible.

Simulations of isotropic and anisotropic data with and without a nugget effect reveal the following principal points. Inclusion of some closely-spaced locations greatly improves estimation, particularly of the Matérn smoothness parameter, and of the nugget variance when present. The presence of geometric anisotropy does not adversely affect parameter estimation. Presence of a nugget effect introduces greater uncertainty into the parameter estimates, most dramatically for the smoothness parameter, and also increases the chance of non-convergence and decreases the power of the test for anisotropy. Estimation is more difficult with very “unsmooth” processes (Matérn smoothness parameter 0.1 or 0.25) — non-convergence is more likely and estimates are less precise and/or more biased. However it is still often possible to fit the full model including both anisotropy and nugget effect using REML with as few as 100 observations.

Additional simulations involving model misspecification reveal that ignoring anisotropy when it is present can substantially increase the mean squared error of prediction, but overfitting by attempting to model anisotropy when it is absent is less damaging. Further, plug-in estimates of prediction error variance are reasonable estimates of the actual mean squared error of prediction, regardless of the model fitted, weakening the argument requiring Bayesian approaches to properly allow for uncertainty in the parameter estimates when estimating prediction error variance.

The most valuable outcome of this research is the implementation of an anisotropic Matérn correlation function in ASReml, including the full generality of Gaussian linear

mixed models which permits additional fixed and random effects, making publicly available the facility to fit, via REML estimation, a much wider range of variance models than has previously been readily accessible. This greatly increases the probability and ease with which a well-fitting covariance model can be found for a spatial data set, thus contributing to improved geostatistical spatial analysis.

Declaration

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