Nonparametric Regression and Generalized Linear Models

A ROUGHNESS PENALTY APPROACH

P.J. GREEN

and

B.W. SILVERMAN

School of Mathematics
University of Bristol
UK

CHAPMAN & HALL/CRC

Boca Raton London New York Washington, D.C.

Contents

Preface **xi**

1 Introduction **1**
1.1 Approaches to regression 1
1.1.1 Linear regression 1
1.1.2 Polynomial regression 2
1.2 Roughness penalties 2
1.2.1 The aims of curve fitting 2
1.2.2 Quantifying the roughness of a curve 4
1.2.3 Penalized least squares regression 5
1.3 Extensions of the roughness penalty approach 7
1.4 Computing the estimates 9
1.5 Further reading **9**

2 Interpolating and smoothing splines **11**
2.1 Cubic splines 11
2.1.1 What is a cubic spline? 11
2.1.2 The value-second derivative representation 12
2.2 Interpolating splines 13
2.2.1 Constructing the interpolating natural cubic spline 15
2.2.2 Optimality properties of the natural cubic spline interpolant 16
2.3 Smoothing splines 17
2.3.1 Restricting the class of functions to be considered 18
2.3.2 Existence and uniqueness of the minimizing spline curve 18
2.3.3 The Reinsch algorithm 19
2.3.4 Some concluding remarks 21
2.4 Plotting a natural cubic spline 22

2.4.1 Constructing a cubic given values and second derivatives at the ends of an interval 22
2.4.2 Plotting the entire cubic spline 23
2.5 Some background technical properties 24
2.5.1 The key property for g to be a natural cubic spline 24
2.5.2 Expressions for the roughness penalty 24
2.6 Band matrix manipulations 25
2.6.1 The Cholesky decomposition 26
2.6.2 Solving linear equations **26**

One-dimensional case: further topics 29
3.1 Choosing the smoothing parameter 29
3.2 Cross-validation - 3©,
3.2.1 Efficient calculation of the cross-validation score 31
3.2.2 Finding the diagonal elements of the hat matrix 33
3.3 Generalized cross-validation 35
3.3.1 The basic idea 35
3.3.2 Computational aspects 35
3.3.3 Leverage values 36
3.3.4 Degrees of freedom $7
3.4 Estimating the residual variance . 38
3.4.1 Local differencing 38
3.4.2 Residual sum of squares about a fitted curve 39
3.4.3 Some comparisons 40
3.5 Weighted smoothing 40
3.5.1 Basic properties of the weighted formulation 41
3.5.2 The Reinsch algorithm for weighted smoothing 41
3.5.3 Cross-validation for weighted smoothing 42
3.5.4 Tied design points 43
3.6 The basis functions approach 44
3.6.1 Details of the calculations 46
3.7 The equivalent kernel 47
3.7.1 Roughness penalty and kernel methods 47
3.7.2 Approximating the weight function 47
3.8 The philosophical basis of roughness penalties 49
3.8.1 Penalized likelihood SO
3.8.2 The bounded roughness approach 51
3.8.3 The Bayesian approach 51
3.8.4 A finite-dimensional Bayesian formulation 54
3.8.5 Bayesian inference for functional of the curve 55
3.9 Nonparametric Bayesian calibration 57
3.9.1 The monotonicity constraint 58

3.9.2 Accounting for the error in the prediction observation 59
3.9.3 Considerations of efficiency 59
3.9.4 An application in forensic odontology **60**

4 Partial splines 63
4.1 Introduction **63**
4.2 The semiparametric formulation **64**
4.3 Penalized least squares for semiparametric models **65**
4.3.1 Incidence matrices **65**
4.3.2 Characterizing the minimum **65**
4.3.3 Uniqueness of the solution **66**
4.3.4 Finding the solution in practice **68**
4.3.5 A direct method **69**
4.4 Cross-validation for partial spline models **70**
4.5 A marketing example **71**
4.5.1 A partial spline approach **72**
4.5.2 Comparison with a parametric model **73**
4.6 Application to agricultural field trials **75**
4.6.1 A discrete roughness penalty approach **75**
4.6.2 Two spring barley trials **77**
4.7 The relation between weather and electricity sales **79**
4.7.1 The observed data and the model assumed **79**
4.7.2 Estimating the temperature response **81**
4.8 Additive models **83**
4.9 An alternative approach to partial spline fitting **85**
4.9.1 Speckman's algorithm **85**
4.9.2 Application: the marketing data **86**
4.9.3 Comparison with the penalized least squares method **86**

5 Generalized linear models 89
5.1 Introduction **89**
5.1.1 Unifying regression models **89**
5.1.2 Extending the model **90**
5.2 Generalized linear models **91**
5.2.1 Exponential families **91**
5.2.2 Maximum likelihood estimation **93**
5.2.3 Fisher scoring **94**
5.2.4 Iteratively reweighted least squares **95**
5.2.5 Inference in GLMs 95
5.3 A first look at nonDarametric GLMs **98**

5.3.1 Relaxing parametric assumptions 98
5.3.2 Penalizing the log-likelihood **98**
5.3.3 Finding the solution by Fisher scoring **99**
5.3.4 Application: estimating actuarial death rates 101
5.4 Semiparametric generalized linear models 104
5.4.1 Maximum penalized likelihood estimation 105
5.4.2 Finding maximum penalized likelihoodestimates by Fisher scoring 105
5.4.3 Cross-validation for GLMs **107**
5.4.4 Inference in semiparametric GLMs **110**
5.5 Application: tumour prevalence data **111**
5.6 Generalized additive models **112**

***6* Extending the model** **115**
6.1 Introduction **115**
6.2 The estimation of branching curves **115**
6.2.1 An experiment on sunflowers **116**
6.2.2 The estimation method **116**
6.2.3 Some results **118**
6.3 Correlated responses and non-diagonal weights **120**
6.4 Nonparametric link functions **121**
6.4.1 Application to the tumour prevalence data 124
6.5 Composite likelihood function regression models 125
6.6 A varying coefficient model with censoring **126**
6.7 Nonparametric quantile regression **129**
6.7.1 The LMS method **129**
6.7.2 Estimating the curves **130**
6.8 Quasi-likelihood **134**

7 Thin plate splines **137**
7.1 Introduction **137**
7.2 Basic definitions and properties **137**
7.2.1 Quantifying the smoothness of a surface **138**
7.3 Natural cubic splines revisited **139**
7.4 Definition of thin plate splines **142**
7.5 Interpolation **143**
7.5.1 Constructing the interpolant **143**
7.5.2 An optimality property **144**
7.5.3 An example **144**
7.6 Smoothing **147**
7.6.1 Constructing the thin plate spline smoother 147
7.6.2 An example **148**

7.6.3 Non-singularity of the defining linear system 148
7.7 Finite window thin plate splines 150
7.7.1 Formulation of the finite window problem 150
7.7.2 An example of finite window interpolation and smoothing 151
7.7.3 Some mathematical details 153
7.8 Tensor product splines 155
7.8.1 Constructing tensor products of one-dimensional families 155
7.8.2 A basis function approach to finite window roughness penalties 156
7.9 Higher order roughness functionals 159
7.9.1 Higher order thin plate splines 160

8 Available software 163
8.1 Routines within the S language 163
8.1.1 The S routine `smooth, spline` 163
8.1.2 The new S modelling functions 164
8.2 The GCVPACK routines 165
8.2.1 Details of the algorithm 166

References 169

Author index 175

Subject index 177