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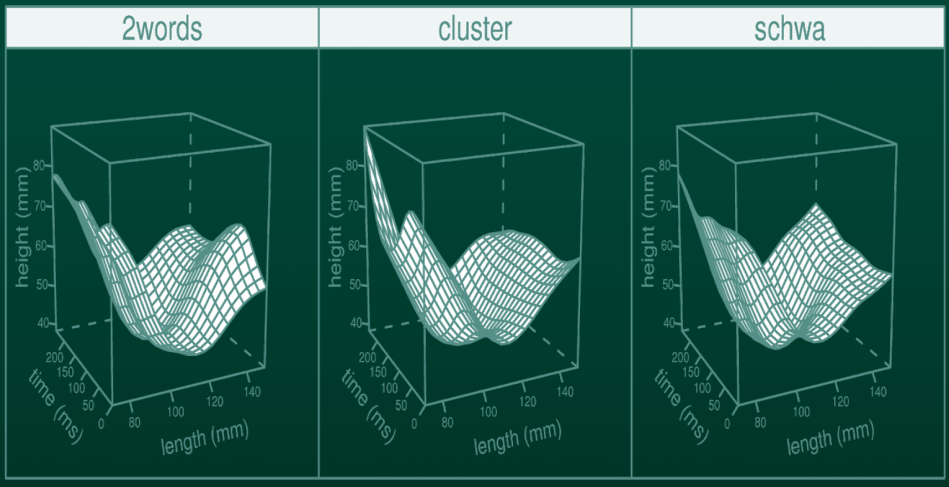
Smoothing Splines

Methods and Applications



Yuedong Wang

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Smoothing Splines

Methods and Applications

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Smoothing Splines

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TO

YAN, CATHERINE, AND KEVIN

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Symbol Description

$(x)_+$	$\max\{x, 0\}$
$x \wedge z$	$\min\{x, z\}$
$x \vee z$	$\max\{x, z\}$
$\det^+$	Product of the nonzero eigenvalues
$k_r(x)$	Scaled Bernoulli polynomials
$(\cdot, \cdot)$	Inner product
$\|\cdot\|$:	Norm
$\mathcal{X}$	Domain of a function
$\mathcal{S}$	Unit sphere
$\mathcal{H}$	Function space
$\mathcal{L}$	Linear functional
$\mathcal{N}$	Nonlinear functional
P	Projection
$\mathcal{A}$	Averaging operator
$\mathcal{M}$	Model space
$R(x, z)$	Reproducing kernel
$\mathbb{R}^d$	Euclidean d-space
$NS^{2m}(t_1, \cdots, t_k)$	Natural polynomial spline space
$W_2^m[a, b]$	Sobolev space on $[a, b]$
$W_2^m(per)$	Sobolev space on unit circle
$W_2^m(\mathbb{R}^d)$	Thin-plate spline model space
$W_2^m(\mathcal{S})$	Sobolev space on unit sphere
$\oplus$	Direct sum of function spaces
$\otimes$	Tensor product of function spaces

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Preface

Statistical analysis often involves building mathematical models that examine the relationship between dependent and independent variables. This book is about a general class of powerful and flexible modeling techniques, namely, *spline smoothing*.

Research on smoothing spline models has attracted a great deal of attention in recent years, and the methodology has been widely used in many areas. This book provides an introduction to some basic smoothing spline models, including polynomial, periodic, spherical, thin-plate, L-, and partial splines, as well as an overview of more advanced models, including smoothing spline ANOVA, extended and generalized smoothing spline ANOVA, vector spline, nonparametric nonlinear regression, semiparametric regression, and semiparametric mixed-effects models. Methods for model selection and inference are also presented.

The general forms of nonparametric/semiparametric linear/nonlinear fixed/mixed smoothing spline models in this book provide unified frameworks for estimation, inference, and software implementation. This book draws on the theory of reproducing kernel Hilbert space (RKHS) to present various smoothing spline models in a unified fashion. On the other hand, the subject of smoothing spline in the context of RKHS and regularization is often regarded as technical and difficult. One of my main goals is to make the advanced smoothing spline methodology based on RKHS more accessible to practitioners and students. With this in mind, the book focuses on methodology, computation, implementation, software, and application. It provides a gentle introduction to the RKHS, keeps theory at the minimum level, and provides details on how the RKHS can be used to construct spline models.

User-friendly software is key to the routine use of any statistical method. The `assist` library in R implements methods presented in this book for fitting various nonparametric/semiparametric linear/nonlinear fixed/mixed smoothing spline models. The `assist` library can be obtained at

`http://www.r-project.org`

Much of the exposition is based on the analysis of real examples. Rather than formal analysis, these examples are intended to illustrate the power and versatility of the spline smoothing methodology. All data analyses are performed in R, and most of them use functions in the

`assist` library. Codes for all examples and further developments related to this book will be posted on the web page

`http://www.pstat.ucsb.edu/faculty/yuedong/book.html`

This book is intended for those wanting to learn about smoothing splines. It can be a reference book for statisticians and scientists who need advanced and flexible modeling techniques. It can also serve as a text for an advanced-level graduate course on the subject. In fact, topics in Chapters 1–4 were covered in a quarter class at the University of California — Santa Barbara, and the University of Science and Technology of China.

I was fortunate indeed to have learned the smoothing spline from Grace Wahba, whose pioneering work has paved the way for much ongoing research and made this book possible. I am grateful to Chunlei Ke, my former student and collaborator, for developing the `assist` package. Special thanks goes to Anna Liu for reading the draft carefully and correcting many mistakes. Several people have helped me over various phases of writing this book: Chong Gu, Wensheng Guo, David Hinkley, Ping Ma, and Wendy Meiring. I must thank my editor, David Grubbes, for his patience and encouragement. Finally, I would like to thank several researchers who kindly shared their data sets for inclusion in this book; they are cited where their data are introduced.

Yuedong Wang
Santa Barbara
December 2010

Chapter 1

Introduction

1.1 Parametric and Nonparametric Regression

Regression analysis builds mathematical models that examine the relationship of a dependent variable to one or more independent variables. These models may be used to predict responses at unobserved and/or future values of the independent variables. In the simple case when both the dependent variable y and the independent variable x are scalar variables, given observations (x_i, y_i) for $i = 1, \ldots, n$, a *regression model* relates dependent and independent variables as follows:

$$y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n, \tag{1.1}$$

where f is the *regression function* and ϵ_i are zero-mean independent random errors with a common variance σ^2. The goal of regression analysis is to construct a model for f and estimate it based on noisy data.

For example, for the Old Faithful geyser in Yellowstone National Park, consider the problem of predicting the waiting time to the next eruption using the length of the previous eruption. Figure 1.1(a) shows the scatter plot of waiting time to the next eruption ($y =$ `waiting`) against duration of the previous eruption ($x =$ `duration`) for 272 observations from the Old Faithful geyser. The goal is to build a mathematical model that relates the waiting time to the duration of the previous eruption. A first attempt might be to approximate the regression function f by a straight line

$$f(x) = \beta_0 + \beta_1 x. \tag{1.2}$$

The least squares straight line fit is shown in Figure 1.1(a). There is no apparent sign of lack-of-fit. Furthermore, there is no clear visible trend in the plot of residuals in Figure 1.1(b).

Often f is nonlinear in x. A common approach to dealing with nonlinear relationship is to approximate f by a *polynomial of order m*

$$f(x) = \beta_0 + \beta_1 x + \cdots + \beta_{m-1} x^{m-1}. \tag{1.3}$$

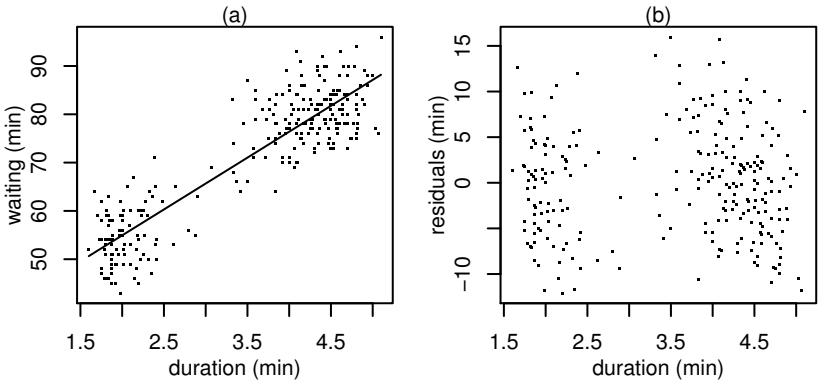

FIGURE 1.1 Geyser data, plots of (a) observations and the least squares straight line fit, and (b) residuals.

Figure 1.2 shows the scatter plot of acceleration ($y =$ `acceleration`) against time after impact ($x =$ `time`) from a simulated motorcycle crash experiment on the efficacy of crash helmets. It is clear that a straight line cannot explain the relationship between acceleration and time. Polynomials with $m = 1, \ldots, 20$ are fitted to the data, and Figure 1.2 shows the best fit selected by *Akaike's information criterion* (AIC). There are waves in the fitted curve at both ends of the range. The fit is still not completely satisfactory even when polynomials up to order 20 are considered. Unlike the linear regression model (1.2), except for small m, coefficients in model (1.3) no longer have nice interpretations.

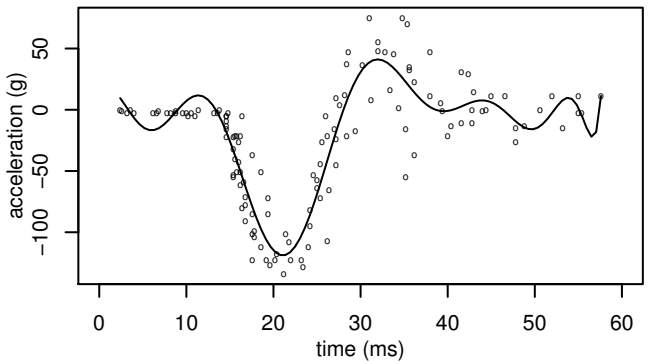

FIGURE 1.2 Motorcycle data, plot of observations, and a polynomial fit.

In general, a *parametric regression* model assumes that the form of f is known except for finitely many unknown parameters. The specific form of f may come from scientific theories and/or approximations to mechanics under some simplified assumptions. The assumptions may be too restrictive and the approximations may be too crude for some applications. An inappropriate model can lead to systematic bias and misleading conclusions. In practice, one should always check the assumed form for the function f.

It is often difficult, if not impossible, to obtain a specific functional form for f. A *nonparametric regression* model does not assume a predetermined form. Instead, it makes assumptions on qualitative properties of f. For example, one may be willing to assume that f is "smooth", which does not reduce to a specific form with finite number of parameters. Rather, it usually leads to some infinite dimensional collections of functions. The basic idea of nonparametric regression is to let the data speak for themselves. That is to let the data decide which function fits the best without imposing any specific form on f. Consequently, nonparametric methods are in general more flexible. They can uncover structure in the data that might otherwise be missed.

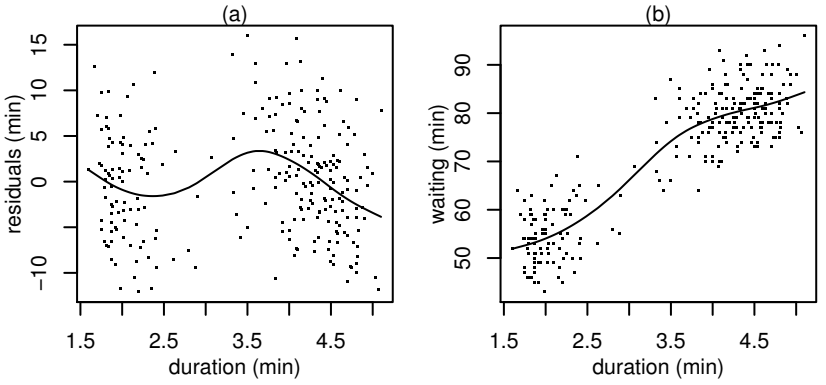

FIGURE 1.3 Geyser data, plots of (a) residuals from the straight line fit and the cubic spline fit to the residuals, and (b) the cubic spline fit to the original data.

For illustration, we fit cubic splines to the geyser data. The cubic spline is a special nonparametric regression model that will be introduced in Section 1.2. A cubic spline fit to residuals from the linear model (1.2) reveals a nonzero trend in Figure 1.3(a). This raises the question of

whether a simple linear regression model is appropriate for the geyser data. A cubic spline fit to the original data is shown in Figure 1.3(b). It reveals that there are two clusters in the independent variable, and a different linear model may be required for each cluster. Sections 2.10, 3.8, and 3.9 contain more analysis of the geyser data. A cubic spline fit to the motorcycle data is shown in Figure 1.4. It fits data much better than the polynomial model. Sections 2.10, 3.8, 5.4.1, and 6.4 contain more analysis of the motorcycle data.

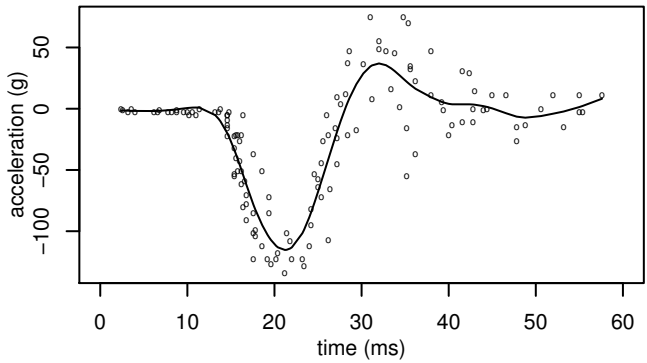

FIGURE 1.4 Motorcycle data, plot of observations, and the cubic spline fit.

The above simple exposition indicates that the nonparametric regression technique can be applied to different steps in regression analysis: data exploration, model building, testing parametric models, and diagnosis. In fact, as illustrated throughout the book, *spline smoothing* is a powerful and versatile tool for building statistical models to exploit structures in data.

1.2 Polynomial Splines

The polynomial (1.3) is a global model which makes it less adaptive to local variations. Individual observations can have undue influence on the fit in remote regions. For example, in the motorcycle data, the behavior of the mean function varies drastically from one region to another.

These local variations led to oscillations at both ends of the range in the polynomial fit. A natural solution to overcome this limitation is to use piecewise polynomials, the basic idea behind *polynomial splines*.

Let $a < t_1 < \cdots < t_k < b$ be fixed points called *knots*. Let $t_0 = a$ and $t_{k+1} = b$. Roughly speaking, polynomial splines are piecewise polynomials joined together smoothly at knots. Formally, a *polynomial spline* of order r is a real-valued function on $[a, b]$, $f(t)$, such that

(i) f is a piecewise polynomial of order r on $[t_i, t_{i+1})$, $i = 0, 1, \ldots, k$;

(ii) f has $r - 2$ continuous derivatives and the $(r-1)$st derivative is a step function with jumps at knots.

Now consider even orders represented as $r = 2m$. The function f is a *natural polynomial spline* of order $2m$ if, in addition to (i) and (ii), it satisfies the *natural boundary conditions*

(iii) $f^{(j)}(a) = f^{(j)}(b) = 0,\ j = m, \ldots, 2m-1.$

The natural boundary conditions imply that f is a polynomial of order m on the two outside subintervals $[a, t_1]$ and $[t_k, b]$. Denote the function space of natural polynomial splines of order $2m$ with knots $t_1, \ldots, t_k$ as $NS^{2m}(t_1, \ldots, t_k)$.

One approach, known as *regression spline*, is to approximate f using a polynomial spline or natural polynomial spline. To get a good approximation, one needs to decide the number and locations of knots. This book covers a different approach known as *smoothing spline*. It starts with a well-defined model space for f and introduces a penalty to prevent overfitting. We now describe this approach for polynomial splines.

Consider the regression model (1.1). Suppose f is "smooth". Specifically, assume that $f \in W_2^m[a, b]$ where the *Sobolev space*

$$W_2^m[a,b] = \big\{ f :\ f, f', \ldots, f^{(m-1)} \text{ are absolutely continuous,} \int_a^b (f^{(m)})^2 dx < \infty \big\}. \tag{1.4}$$

For any $a \le x \le b$, Taylor's theorem states that

$$f(x) = \underbrace{\sum_{\nu=0}^{m-1} \frac{f^{(\nu)}(a)}{\nu!}(x-a)^\nu}_{\text{polynomial of order } m} + \underbrace{\int_a^x \frac{(x-u)^{m-1}}{(m-1)!} f^{(m)}(u)du}_{\text{Rem}(x)}. \tag{1.5}$$

It is clear that the polynomial regression model (1.3) ignores the remainder term $\text{Rem}(x)$ in the hope that it is negligible. It is often difficult

to verify this assumption in practice. The idea behind the spline smoothing is to let data decide how large $\text{Rem}(x)$ should be. Since $W_2^m[a,b]$ is an infinite dimensional space, a direct fit to f by minimizing the *least squares* (LS)

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2 \tag{1.6}$$

leads to interpolation. Therefore, certain control over $\text{Rem}(x)$ is necessary. One natural approach is to control how far f is allowed to depart from the polynomial model. Under appropriate norms defined later in Sections 2.2 and 2.6, one measure of distance between f and polynomials is $\int_a^b (f^{(m)})^2 dx$. It is then reasonable to estimate f by minimizing the LS (1.6) under the constraint

$$\int_a^b (f^{(m)})^2 dx \le \rho \tag{1.7}$$

for a constant ρ. By introducing a Lagrange multiplier, the constrained minimization problem (1.6) and (1.7) is equivalent to minimizing the *penalized least squares* (PLS):

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2 + \lambda \int_a^b (f^{(m)})^2 dx. \tag{1.8}$$

In the remainder of this book, a polynomial spline refers to the solution of the PLS (1.8) in the model space $W_2^m[a,b]$. A *cubic spline* is a special case of the polynomial spline with $m = 2$. Since it measures the roughness of the function f, $\int_a^b (f^{(m)})^2 dx$ is often referred to as a *roughness penalty*. It is obvious that there is no penalty for polynomials of order less than or equal to m. The *smoothing parameter* λ balances the trade-off between goodness-of-fit measured by the LS and roughness of the estimate measured by $\int_a^b (f^{(m)})^2 dx$.

Suppose that $n \ge m$ and $a \le x_1 < x_2 < \cdots < x_n \le b$. Then, for fixed $0 < \lambda < \infty$, (1.8) has a unique minimizer $\hat{f}$ and $\hat{f} \in NS^{2m}(x_1, \ldots, x_n)$ (Eubank 1988). This result indicates that even though we started with the infinite dimensional space $W_2^m[a,b]$ as the model space for f, the solution to the PLS (1.8) belongs to a finite dimensional space. Specifically, the solution is a natural polynomial spline with knots at distinct design points. One approach to computing the polynomial spline estimate is to represent $\hat{f}$ as a linear combination of a basis of $NS^{2m}(x_1, \ldots, x_n)$. Several basis constructions were provided in Section 3.3.3 of Eubank (1988). In particular, the R function `smooth.spline` implements this approach for the cubic spline using the B-spline basis. For example, the cubic spline fit in Figure 1.4 is derived by the following statements:

```
> library(MASS); attach(mcycle)
> smooth.spline(times, accel, all.knots=T)
```

This book presents a different approach. Instead of basis functions, representers of reproducing kernel Hilbert spaces will be used to represent the spline estimate. This approach allows us to deal with many different spline models in a unified fashion. Details of this approach for polynomial splines will be presented in Sections 2.2 and 2.6.

When $\lambda = 0$, there is no penalty, and the natural spline that interpolates observations is the unique minimizer. When $\lambda = \infty$, the unique minimizer is the mth order polynomial. As λ varies from ∞ to 0, we have a family of models ranging from the parametric polynomial model to interpolation. The value of λ decides how far f is allowed to depart from the polynomial model. Thus the choice of λ holds the key to the success of a spline estimate. We discuss how to choose λ based on data in Chapter 3.

1.3 Scope of This Book

Driven by many sophisticated applications and fueled by modern computing power, many flexible nonparametric and semiparametric modeling techniques have been developed to relax parametric assumptions and to exploit possible hidden structure. There are many different nonparametric methods. This book concentrates on one of them, *smoothing spline*. Existing books on this topic include Eubank (1988), Wahba (1990), Green and Silverman (1994), Eubank (1999), Gu (2002), and Ruppert, Wand and Carroll (2003). The goals of this book are to (a) make the advanced smoothing spline methodology based on reproducing kernel Hilbert spaces more accessible to practitioners and students; (b) provide software and examples so that the spline smoothing methods can be routinely used in practice; and (c) provide a comprehensive coverage of recently developed smoothing spline nonparametric/semiparametric linear/nonlinear fixed/mixed models. We concentrate on the methodology, implementation, software, and application. Theoretical results are stated without proofs. All methods will be demonstrated using real data sets and R functions.

The polynomial spline in Section 1.2 concerns the functions defined on the domain $[a, b]$. In many applications, the domain of the regression function is not a continuous interval. Furthermore, the regression function may only be observed indirectly. **Chapter 2** introduces gen-

eral smoothing spline regression models with reproducing kernel Hilbert spaces on general domains as model spaces. Penalized LS estimation, Kimeldorf–Wahba representer theorem, computation, and the R function `ssr` will be covered. Explicit constructions of model spaces will be discussed in detail for some popular smoothing spline models including polynomial, periodic, thin-plate, spherical, and L-splines.

Chapter 3 introduces methods for selecting the smoothing parameter and making inferences about the regression function. The impact of the smoothing parameter and basic concepts for model selection will be discussed and illustrated using an example. Connections between smoothing spline models and Bayes/mixed-effects models will be established. The unbiased risk, generalized cross-validation, and generalized maximum likelihood methods will be introduced for selecting the smoothing parameter. Bayesian and bootstrap confidence intervals will be introduced for the regression function and its components. The locally most powerful, generalized maximum likelihood and generalized cross-validation tests will also be introduced to test the hypothesis of a parametric model versus a nonparametric alternative.

Analogous to multiple regression, **Chapter 4** constructs models for multivariate regression functions based on smoothing spline analysis of variance (ANOVA) decompositions. The resulting models have hierarchical structures that facilitate model selection and interpretation. Smoothing spline ANOVA decompositions for tensor products of some commonly used smoothing spline models will be illustrated. Penalized LS estimation involving multiple smoothing parameters and componentwise Bayesian confidence intervals will be covered.

Chapter 5 presents spline smoothing methods for heterogeneous and correlated observations. Presence of heterogeneity and correlation may lead to wrong choice of the smoothing parameters and erroneous inference. Penalized weighted LS will be used for estimation. Unbiased risk, generalized cross-validation, and generalized maximum likelihood methods will be extended for selecting the smoothing parameters. Variance and correlation structures will also be discussed.

Analogous to generalized linear models, **Chapter 6** introduces smoothing spline ANOVA models for observations generated from a particular distribution in the exponential family including binomial, Poisson, and gamma distributions. Penalized likelihood will be used for estimation, and methods for selecting the smoothing parameters will be discussed. Nonparametric estimation of variance and spectral density functions will be presented.

Analogous to nonlinear regression, **Chapter 7** introduces spline smoothing methods for nonparametric nonlinear regression models where some unknown functions are observed indirectly through nonlinear function-

als. In addition to fitting theoretical and empirical nonlinear nonparametric regression models, methods in this chapter may also be used to deal with constraints on the nonparametric function such as positivity or monotonicity. Several algorithms based on Gauss–Newton, Newton–Raphson, extended Gauss–Newton and Gauss–Seidel methods will be presented for different situations. Computation and the R function `nnr` will be covered.

Chapter 8 introduces semiparametric regression models that involve both parameters and nonparametric functions. The mean function may depend on the parameters and the nonparametric functions linearly or nonlinearly. The semiparametric regression models include many well-known models such as the partial spline, varying coefficients, projection pursuit, single index, multiple index, functional linear, and shape invariant models as special cases. Estimation, inference, computation, and the R function `snr` will also be covered.

Chapter 9 introduces semiparametric linear and nonlinear mixed-effects models. Smoothing spline ANOVA decompositions are extended for the construction of semiparametric mixed-effects models that parallel the classical mixed models. Estimation and inference methods, computation, and the R functions `slm` and `snm` will be covered as well.

1.4 The `assist` Package

The `assist` package was developed for fitting various smoothing spline models covered in this book. It contains five main functions, `ssr`, `nnr`, `snr`, `slm`, and `snm` for fitting various smoothing spline models. The function `ssr` fits smoothing spline regression models in Chapter 2, smoothing spline ANOVA models in Chapter 4, extended smoothing spline ANOVA models with heterogeneous and correlated observations in Chapter 5, generalized smoothing spline ANOVA models in Chapter 6, and semiparametric linear regression models in Chapter 8, Section 8.2. The function `nnr` fits nonparametric nonlinear regression models in Chapter 7. The function `snr` fits semiparametric nonlinear regression models in Chapter 8, Section 8.3. The functions `slm` and `snm` fit semiparametric linear and nonlinear mixed-effects models in Chapter 9. The `assist` package is available at

`http://cran.r-project.org`

Figure 1.5 shows how the functions in `assist` generalize some of the existing R functions for regression analysis.

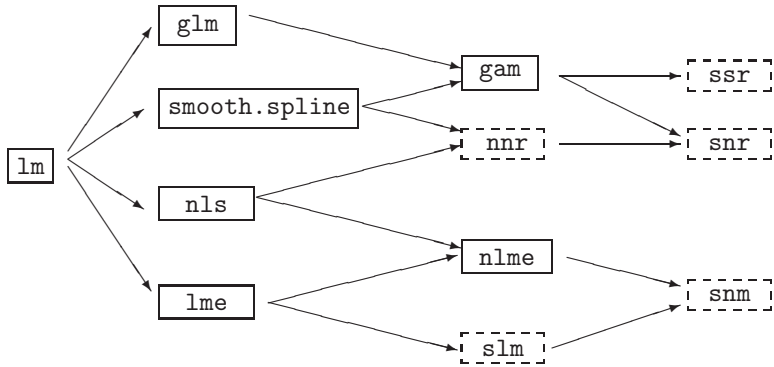

FIGURE 1.5 Functions in `assist` (dashed boxes) and some existing R functions (solid boxes). An arrow represents an extension to a more general model. `lm`: linear models. `glm`: generalized linear models. `smooth.spline`: cubic spline models. `nls`: nonlinear regression models. `lme`: linear mixed-effects models. `gam`: generalized additive models. `nlme`: nonlinear mixed-effects models. `ssr`: smoothing spline regression models. `nnr`: nonparametric nonlinear regression models. `snr`: semiparametric nonlinear regression models. `slm`: semiparametric linear mixed-effects models. `snm`: semiparametric nonlinear mixed-effects models.

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Statistics

A general class of powerful and flexible modeling techniques, spline smoothing has attracted a great deal of research attention in recent years and has been widely used in many application areas, from medicine to economics. **Smoothing Splines: Methods and Applications** covers basic smoothing spline models, including polynomial, periodic, spherical, thin-plate, L-, and partial splines, as well as more advanced models, such as smoothing spline ANOVA, extended and generalized smoothing spline ANOVA, vector spline, nonparametric nonlinear regression, semiparametric regression, and semiparametric mixed-effects models. It also presents methods for model selection and inference.

The book provides unified frameworks for estimation, inference, and software implementation by using the general forms of nonparametric/semiparametric, linear/nonlinear, and fixed/mixed smoothing spline models. The theory of reproducing kernel Hilbert space (RKHS) is used to present various smoothing spline models in a unified fashion. Although this approach can be technical and difficult, the author makes the advanced smoothing spline methodology based on RKHS accessible to practitioners and students. He offers a gentle introduction to RKHS, keeps theory at a minimum level, and explains how RKHS can be used to construct spline models.

Smoothing Splines offers a balanced mix of methodology, computation, implementation, software, and applications. It uses R to perform all data analyses and includes a host of real data examples from astronomy, economics, medicine, and meteorology. The codes for all examples, along with related developments, can be found on the book's web page.

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