Multivariate spatial smoothing using additive regression splines

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Abstract

We describe additive regression spline models as tools for smooth interpolation of fields that depend on several variables in a spatially varying way. Additive regression models can bypass the usual technical difficulties associated with the curse of dimension. We formulate the additive regression spline minimisation problem and prove that this problem is uniquely solvable under suitable conditions on the data. The resulting additive regression spline may be seen as a special case of general additive tensor product splines. Moreover, we show that additive regression splines may be implemented by a relatively straightforward extension of the methods used in the implementation of standard thin plate splines. The performance of additive regression splines is demonstrated on a simulated noisy data set.

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1 Introduction

In many physical situations of interest there arises a need to interpolate data using multiple predictors. In many cases the interpolated surface required for application is two or three dimensional. This is often the case in the environmental sciences, for example, where measured point data are used to estimate information about the spatial distribution of some environmental variable. It can also be appropriate to discern how the effects of certain predictors vary across the spatial extent of the region under consideration. For example, precipitation is known to be influenced by the shape of the underlying topography. Thus when smoothing precipitation data it is desirable to include predictors such as elevation and topographic slope and aspect, in addition to those quantifying the data point locations, to achieve accurate precipitation surfaces. However, Hutchinson and Sharples [8, 9, 11] showed that interpolation accuracy is critically dependent on the incorporation of a spatially varying dependence on these topographic variables.

A common problem that arises when fitting multivariate data is that smoothing methods are limited by the fact that estimating a d-variate function with no constraints on its structure, apart from smoothness, requires data sets of impractical size for larger values of d, a problem referred to as the *curse of dimension*. Given the technical difficulties associated with the curse of dimension and the fact that the required output is a two or three dimensional surface, interpolation based on higher dimensional data can be numerically expensive (if not completely impractical) while aiming to produce more elaborate dependencies on the predictor variables than actually needed. It is therefore natural to employ a data fitting method that bypasses the curse of dimension by identifying only the underlying two or three dimensional (spatial) dependencies on multiple predictors.

In this paper we describe a data model that satisfies this requirement and demonstrate how to solve the associated spline optimisation problem. The resulting additive regression spline is a special case of the more general tensor product splines [3, 4, 6, 14]. However, unlike tensor product splines, additive regression splines can be implemented via a relatively simple extension of the methods used to derive standard thin-plate smoothing splines. This can be done without appeal to the underpinning reproducing kernel structure that is usually associated with tensor product splines.

In Section 2 we introduce the additive regression spline model. We also show that the associated spline optimisation problem is uniquely solvable under mild assumptions about the data, and that the functional components of additive regression splines are ordinary thin-plate splines. In Section 3 we use standard methods to reduce the variational problem to that of solving a simple linear system and show how the procedure used to derive ordinary thin-plate splines may be extended to allow the derivation of additive regression splines. We give an example of the use of additive regression splines in Section 4.

2 Additive regression splines

We consider data sets of the form $\{z_i, \mathbf{x}_i, h_{i1}, \ldots, h_{iN}\}_{i=1}^n$. Here z_i refers to the dependent variable, $\mathbf{x}_i$ denotes the spatial location at which z_i is recorded and $h_{i1}, \ldots, h_{iN}$ denote the N additional predictors that are to be included in the data fitting process. We assume that $z_i, h_{i1}, \ldots, h_{iN} \in \mathbb{R}$ and $\mathbf{x}_i \in \mathbb{R}^d$. Typically applications will call for $d = 2$ or 3, but we do not assume this to be the case in what follows.

We propose the data model

$$z_i = f_0(\mathbf{x}_i) + \sum_{j=1}^{N} h_{ij} f_j(\mathbf{x}_i) + \epsilon_i \,, \quad i = 1, \ldots, n \,, \tag{1}$$

that is seen to be a special case of the more general additive tensor product spline models [6, 14, 15]. The data model can also be simply thought of as spatially varying linear regression with the constant parameters found in linear regression models replaced by the multivariate functions $f_0, \ldots, f_N$. The functions $f_0, \ldots, f_N$ that accompany the additional predictor variables will be referred to as the additive components of the model.

The functions $f_0, \ldots, f_N$ may be estimated by minimising

$$\sum_{i=1}^{n} \left[z_i - f_0(\mathbf{x}_i) - \sum_{j=1}^{N} h_{ij} f_j(\mathbf{x}_i) \right]^2 + \sum_{j=0}^{N} \rho_j J_d^m(f_j) \,, \tag{2}$$

where $J_d^m(f)$ denotes the mth order roughness penalty (seminorm):

$$J_d^m(f) = \int_{\mathbb{R}^d} \|D^m f\|^2 \, dx \,.$$

The non-negative smoothing parameters $\rho_1, \ldots, \rho_N$ will be assumed to be known constants. In practice they may be determined by appealing to standard methods such as minimising the generalised cross validation (GCV) or generalised maximum likelihood (GML) [5, 13].

We consider each of the functions f_j, $j = 0, \ldots, N$ as elements of the Hilbert–Sobolev space $H^m(\mathbb{R}^d)$ [1]. The roughness penalty functional then defines a canonical decomposition of this space

$$H^m(\mathbb{R}^d) = \ker(J_d^m) \oplus \ker(J_d^m)^\perp .$$

Using $\{\phi_\nu\}_{\nu=1}^M$ to denote the basis of $\ker(J_d^m)$ we define the $n \times M$ matrix T by $T_{i\nu} = \phi_\nu(\mathbf{x}_i)$. It is also convenient to define the diagonal matrices $H_j = \operatorname{diag}(h_{1j}, h_{2j}, \ldots, h_{nj})$ with $H_0 = I$.

As mentioned in the introduction, establishing the unique existence of a minimiser of (2) will have bearing on the nature of the functions $f_0, \ldots, f_N$. However, before doing so we recast the minimisation problem in a more abstract setting; this will allow us to appeal to the elegant spline existence theorems of Atteia [2].

The natural space in which $\mathbf{f} = (f_0, \ldots, f_N)$ resides is the Hilbert–Sobolev space $X = H^m(\mathbb{R}^d) \times \cdots \times H^m(\mathbb{R}^d) = H^m(\mathbb{R}^d)^{N+1}$. We will also make use of the Hilbert space $Y = L^2(\mathbb{R}^d)^{N+1}$.

Furthermore, we define the continuous, linear surjections $u : X \to Y$ and $v : X \to \mathbb{R}^n$ by

$$u : \mathbf{f} \mapsto (D^m f_0, \ldots, D^m f_N) \quad \text{and} \quad v : \mathbf{f} \mapsto (v_1(\mathbf{f}), \ldots, v_n(\mathbf{f})) ,$$

where

$$v_i(\mathbf{f}) = f_0(\mathbf{x}_i) + \sum_{j=1}^{N} h_{ij} f_j(\mathbf{x}_i)$$

for each $i = 1, \ldots, n$.

We also define the auxiliary Hilbert space $W = Y \times \mathbb{R}^n$ and mapping $\ell : X \to W$ by

$$\ell : \mathbf{f} \mapsto (u(\mathbf{f}), v(\mathbf{f})) .$$

Since each $\rho_j \geq 0$, Y inherits a natural inner product from $L^2(\mathbb{R}^d)$ by

$$\langle (f_0, \ldots, f_N), (g_0, \ldots, g_N) \rangle_Y = \sum_{j=0}^{N} \rho_j \langle f_j, g_j \rangle_{L^2(\mathbb{R}^d)} .$$

W then inherits an inner product from Y and $\mathbb{R}^n$

$$\langle (\mathbf{f}_1, \mathbf{z}_1), (\mathbf{f}_2, \mathbf{z}_2) \rangle_W = \langle \mathbf{f}_1, \mathbf{f}_2 \rangle_Y + \langle \mathbf{z}_1, \mathbf{z}_2 \rangle_{\mathbb{R}^n} .$$

It follows that finding functions f_j that minimise (2) amounts to finding $\mathbf{f} \in X$ such that

$$\|\ell(\mathbf{f}) - (\boldsymbol{\theta}_Y, \mathbf{z})\|_W = \min\{\|\ell(\mathbf{g}) - (\boldsymbol{\theta}_Y, \mathbf{z})\|_W : \mathbf{g} \in X\} , \tag{3}$$

where $\mathbf{z} = (z_1, \ldots, z_n)$ describes the dependent data values and $\boldsymbol{\theta}_Y$ denotes the zero element in Y.

A function $\mathbf{f} \in X$ satisfying (3) will be called an additive regression spline.

The existence and uniqueness of additive regression splines may now be established as a special case of the abstract results found in [2].

Theorem 1 *If the matrix* $[H_0T : H_1T : \cdots : H_NT]$ *is of full rank then for each* $\mathbf{z} \in \mathbb{R}^n$ *there is a unique* $\mathbf{f} \in X$ *such that*

$$\|\ell(\mathbf{f}) - (\boldsymbol{\theta}_Y, \mathbf{z})\|_W = \min\{\|\ell(\mathbf{g}) - (\boldsymbol{\theta}_Y, \mathbf{z})\|_W : \mathbf{g} \in X\} .$$

Proof: Using the definitions of u and v it is possible to show that $v(\ker(u))$ is closed in $\mathbb{R}^n$. Atteia [2, Lemma 1.1] proves that this is the case if and only if $u(\ker(v))$ is closed in Y. If $\mathbf{g} \in X \cap \ker(u)$, then

$$g_j = \sum_{\nu=1}^{M} d_{j\nu} \phi_\nu ,$$

whereas if $\mathbf{g} \in \ker(v)$, then

$$g_0(\mathbf{x}_i) + \sum_{j=1}^{N} h_{ij} g_j(\mathbf{x}_i) = 0\,, \quad \text{for each} \quad i = 1, \ldots, n\,.$$

Hence $\mathbf{g} \in \ker(u) \cap \ker(v)$ if and only if, for all $i = 1, \ldots, n$,

$$g_j = \sum_{\nu=1}^{M} d_{j\nu}\phi_\nu \quad \text{and} \quad \sum_{\nu=1}^{M} \left(d_{0\nu} + \sum_{j=1}^{N} h_{ij} d_{j\nu} \right) \phi_\nu(\mathbf{x}_i) = 0\,.$$

However,

$$\sum_{\nu=1}^{M} \left(d_{0\nu} + \sum_{j=1}^{N} h_{ij} d_{j\nu} \right) \phi_\nu(\mathbf{x}_i) = \sum_{\nu=1}^{M} \sum_{j=0}^{N} d_{j\nu} [H_j T]_{i\nu}\,,$$

and so if $[H_0T : H_1T : \cdots : H_NT]$ is of full rank we conclude that each $d_{j\nu} = 0$, which is to say that $\ker(u) \cap \ker(v) = \{\boldsymbol{\theta}_X\}$ where $\boldsymbol{\theta}_X$ denotes the zero element of X .

The theorem now follows as a consequence of [2, Theorem 2.1]. ♠

Having established the unique existence of additive regression splines we have the following important corollary.

Corollary 2 *If $\mathbf{f} = (f_0, \ldots, f_N)$ is the minimiser of (2) then each f_j is an ordinary thin-plate smoothing spline and thus has representation*

$$f_j(\mathbf{x}) = \sum_{\nu=1}^{M} a_{\nu j}\phi_\nu(\mathbf{x}) + \sum_{i=1}^{n} b_{ij} E_m(\mathbf{x}, \mathbf{x}_i)\,, \quad j = 0, \ldots, N\,,$$

where $\{\phi_\nu\}$ is a basis for $\ker(J_d^m)$, the polynomials of total degree less than m, and E_m is the reproducing kernel function for the space $\ker(J_d^m)^\perp$.

Proof: Consider the problem of finding g_j minimising $\|\ell(\mathbf{g}) - (\boldsymbol{\theta}_Y, \mathbf{z})\|_W$ with $g_0, g_1, \ldots, g_{j-1}, g_{j+1}, \ldots, g_N$ arbitrary fixed functions. This amounts to finding g_j minimising $\|\bar{\mathbf{z}} - g_j(\mathbf{x})\|^2_{\mathbb{R}^n} + \rho_j J^m_d(g_j)$ where $\bar{\mathbf{z}}$ describes the appropriately amended data. From this it is clear, following the usual arguments [15], that g_j is a standard thin-plate smoothing spline with corresponding representation. Now since the functions g_l, $l \neq j$, are arbitrary, it follows from the uniqueness of additive regression splines that $g_j = f_j$. ♠

3 Implementation

Since the component functions f_j are ordinary thin-plate splines we may write the model (1) in vector form as

$$\mathbf{z} = \sum_{j=0}^{N} H_j T \mathbf{a}_j + H_j K \mathbf{b}_j + \boldsymbol{\epsilon}\,,$$

where $\mathbf{z} = (z_1, \ldots, z_n)'$ and $\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_n)'$. Here K is a conditionally positive definite, symmetric $n \times n$ matrix with entries $K_{ik} = E_m(\mathbf{x}_i, \mathbf{x}_k)$. The matrix K is conditionally positive definite if $\mathbf{b}'K\mathbf{b} > 0$ for all nonzero $\mathbf{b}$, satisfying $T'\mathbf{b} = \mathbf{0}$, [15]. The vectors $\mathbf{a}_j$ and $\mathbf{b}_j$ are $(a_{1j}, \ldots, a_{Mj})'$ and $(b_{1j}, \ldots, b_{nj})'$, respectively. Moreover, we have $T'\mathbf{b}_j = \mathbf{0}$ for all $j = 0, \ldots, N$ [15].

Rewriting (2) the functions $f_0, \ldots, f_N$ are estimated by minimising

$$\left\| \mathbf{z} - \sum_{j=0}^{N} (H_j T \mathbf{a}_j + H_j K \mathbf{b}_j) \right\|^2 + \sum_{j=0}^{N} \rho_j \mathbf{b}_j^T K \mathbf{b}_j \qquad (4)$$

with respect to $\mathbf{a}_j$ and $\mathbf{b}_j$, with each ρ_j held constant.

We suppose for the moment that each H_j is invertible. We will see in what follows that this assumption may be removed, though we will require that at least one H_j is invertible. However, this requirement can be fulfilled without any loss of generality; in particular, $H_0 = I$ is invertible. Following our assumption then, we define

$$\mathbf{d}_j = H_j^{-1}\mathbf{b}_j\,, \quad j = 0, \ldots, N\,.$$

Defining the auxiliary matrices $S_j = H_j T$ and $M_j = H_j K H_j$ for $j = 1, \ldots, N$, we may write (4) as

$$\left\|\mathbf{z} - \sum_{j=0}^{N}(S_j\mathbf{a}_j + M_j\mathbf{d}_j)\right\|^2 + \sum_{j=0}^{N}\rho_j\mathbf{d}_j^T M_j\mathbf{d}_j\,. \tag{5}$$

Note also that since $T'\mathbf{b}_j = \mathbf{0}$ for all $j = 0, \ldots, N$,

$$S_j'\mathbf{d}_j = T'H_jH_j^{-1}\mathbf{b}_j = \mathbf{0}\,.$$

Lemma 3 *Suppose T has full rank, $T'\mathbf{d} = \mathbf{0}$ and K is conditionally positive definite as defined above. If*

$$\|\mathbf{v} - T\mathbf{a} - S\mathbf{b} - K\mathbf{d}\|^2 + \rho\mathbf{d}'K\mathbf{d}$$

is a minimum with respect to the vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{d}$ then $S'\mathbf{d} = \mathbf{0}$.

Proof: The matrix T admits a QR-decomposition,

$$T = [Q_1 : Q_2]\begin{bmatrix} R \\ 0 \end{bmatrix}.$$

It follows from the orthogonality of $[Q_1 : Q_2]$ that, for the expression in question to be a minimum, $\mathbf{a}$ must satisfy

$$R\mathbf{a} = Q_1'(\mathbf{v} + S\mathbf{b} + K\mathbf{d})\,,$$

where $\mathbf{b}$ and $\mathbf{d}$ are the minimisers of

$$\|Q_2'\mathbf{v} - Q_2'S\mathbf{b} - Q_2^T K\mathbf{d}\|^2 + \rho\mathbf{d}'K\mathbf{d}\,.$$

Now since $T'\mathbf{d} = \mathbf{0}$ we must have $\mathbf{d} = Q_2\boldsymbol{\gamma}$ for some $\boldsymbol{\gamma}$ and since K is conditionally positive definite $B = Q_2'KQ_2$ is positive definite. Letting $\mathbf{w} = Q_2'\mathbf{v}$, differentiating with respect to $\mathbf{b}$ and $\boldsymbol{\gamma}$ and using the non-singularity of B we have

$$\begin{aligned} S'Q_2(B\boldsymbol{\gamma} + Q_2'S\mathbf{b} - \mathbf{w}) &= 0\,, & (6)\\ (B+\rho I)\boldsymbol{\gamma} + Q_2'S\mathbf{b} - \mathbf{w} &= 0\,. & (7)\end{aligned}$$

Multiplying (7) on the left by $S'Q_2$ and subtracting the resulting equation from (6) we find that $S'Q_2\boldsymbol{\gamma} = \mathbf{0}$, which is to say that $S'\mathbf{d} = \mathbf{0}$. ♠

For each $l, m = 1, \ldots, N$ with $l \neq m$ let

$$\mathbf{v} = \mathbf{z} - \sum_{j\neq l, j\neq m} S_j\mathbf{a}_j - \sum_{j\neq l} M_j\mathbf{d}_j\,.$$

Then we may write (5) as

$$\|\mathbf{v} - S_l\mathbf{a}_l - M_l\mathbf{d}_l - S_m\mathbf{a}_m\|^2 + \sum_{j=0}^{N} \rho_j\mathbf{d}_j' M_j\mathbf{d}^j\,.$$

To infer the unique existence of additive regression splines we assumed that T is of full rank, hence minimising (5) with respect to $\mathbf{a}_l, \mathbf{d}_l, \mathbf{a}_m$ and invoking Lemma 3, we have

$$S_m'\mathbf{d}_l = \mathbf{0}\,, \quad \text{for all} \quad 0 \le m, l \le N\,.$$

Therefore, if $\mathcal{S} = [S_0 : S_1 : \cdots : S_N]$ then $\mathcal{S}'\mathbf{d}_l = \mathbf{0}$ for all $0 \le l \le N$. Moreover, if

$$\mathcal{S} = [Q_1 : Q_2]\begin{bmatrix} R \\ 0 \end{bmatrix}$$

is the QR-decomposition of $\mathcal{S}$, we have for all $0 \le l \le N$ that $\mathbf{d}_l = Q_2\boldsymbol{\xi}_l$ for some $\boldsymbol{\xi}_l$.

Utilising the QR-decomposition further, minimising (5) is seen to be equivalent to minimising

$$\left\| Q_1'\mathbf{z} - R\boldsymbol{\alpha} - \sum_{j=0}^{N} Q_1' M_j Q_2 \boldsymbol{\xi}_j \right\|^2 + \left\| Q_2'\mathbf{z} - \sum_{j=0}^{N} Q_2' M_j Q_2 \boldsymbol{\xi}_j \right\|^2 + \sum_{j=0}^{N} \rho_j \boldsymbol{\xi}_j' Q_2' M_j Q_2 \boldsymbol{\xi}_j \,,$$

where we have set $\boldsymbol{\alpha} = (\mathbf{a}_0, \ldots, \mathbf{a}_N)'$. Letting $\mathbf{w} = Q_2'\mathbf{z}$ and $B_j = Q_2' M_j Q_2$ we are therefore required to minimise

$$\left\| \mathbf{w} - \sum_{j=0}^{N} B_j \boldsymbol{\xi}_j \right\|^2 + \sum_{j=0}^{N} \rho_j \boldsymbol{\xi}_j' B_j \boldsymbol{\xi}_j \,, \tag{8}$$

with $\boldsymbol{\alpha}$ given by

$$R\boldsymbol{\alpha} = Q_1'\mathbf{z} - \sum_{j=0}^{N} Q_1' M_j Q_2 \boldsymbol{\xi}_j \,.$$

Differentiating (8) with respect to $\boldsymbol{\xi}_m$ gives

$$B_m' B_m \boldsymbol{\xi}_m + \rho_m B_m \boldsymbol{\xi}_m - B_m' \mathbf{w} + \sum_{j \neq m} B_m' B_j \boldsymbol{\xi}_j = \mathbf{0} \,.$$

Since B_m is symmetric and invertible, this reduces to

$$\rho_m \boldsymbol{\xi}_m + \sum_{j=0}^{N} B_j \boldsymbol{\xi}_j = \mathbf{w}$$

for any $0 \le m \le N$. Subtracting the equation with $m = l$ from the equation with $m = 0$ gives

$$\rho_0 \boldsymbol{\xi}_0 = \rho_l \boldsymbol{\xi}_l \,, \quad \text{for all} \quad 0 \le l \le N \,.$$

If we let $\theta_j = \rho_0/\rho_j$ then we have reduced the problem to solving the system

$$\left(\rho_0 I + \sum_{j=0}^{N} \theta_j B_j\right) \boldsymbol{\xi}_0 = \mathbf{w} \,, \tag{9}$$

$$\boldsymbol{\xi}_j = \theta_j \boldsymbol{\xi}_0 \,, \quad j = 1, 2, \ldots, N \,. \tag{10}$$

Moreover, $\boldsymbol{\xi}_j = \theta_j \boldsymbol{\xi}_0$ implies $\mathbf{d}_j = \theta_j \mathbf{d}_0$, and $\mathbf{b}_j = H_j \mathbf{d}_j$ implies $\mathbf{b}_j = \theta_j H_j \mathbf{d}_0$, $j = 1, \ldots, N$, and so we may have equivalently endeavoured to minimise

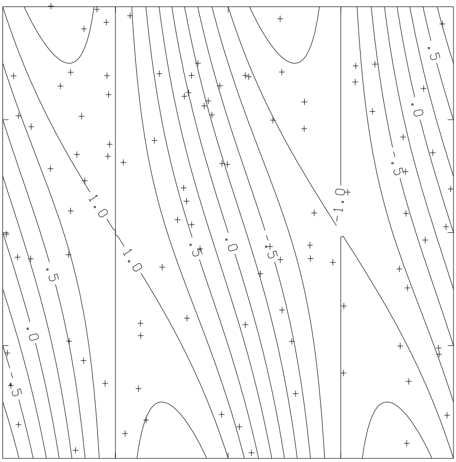
$$\left\| \mathbf{z} - \sum_{j=0}^{N} (H_j T \mathbf{a}_j + \theta_j H_j K H_j \mathbf{d}_0) \right\|^2 + \rho_0 \sum_{j=0}^{N} \theta_j \mathbf{d}_0' H_j K H_j \mathbf{d}_0 \,.$$

Equivalently, we should minimise

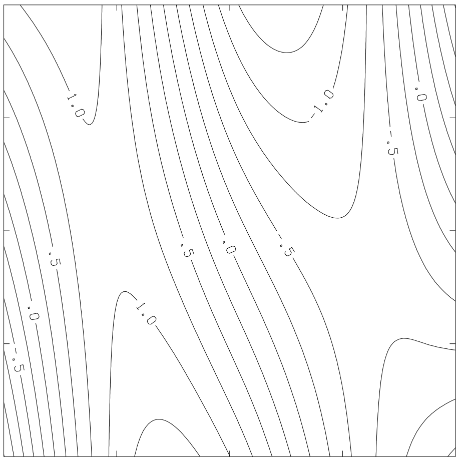
$$\|\mathbf{z} - \mathcal{S}\boldsymbol{\alpha} - \mathcal{K}\mathbf{d}_0\|^2 + \rho_0 \mathbf{d}_0 \mathcal{K} \mathbf{d}_0 \tag{11}$$

where $\mathcal{S} = [H_0 T : H_1 T : \cdots : H_N T]$ and $\mathcal{K} = \sum_{j=0}^{N} \theta_j H_j K H_j$.

It is well known that the minimiser of the expression (11) can be derived using the standard methods for deriving ordinary thin plate splines, once the matrices $\mathcal{S}$ and $\mathcal{K}$ have been properly accounted for. It should also be noted that the standard methods for implementing thin-plate splines make no use of the inverses of the matrices involved and so our assumption about the invertibility of the matrices H_j is redundant.



(a)



(b)

Figure 1: (a) Contour plot of $f(x,y) = \sin(\pi x) + y\cos(\pi x)$ and locations of the 100 data points. (b) Contour plot of fitted additive regression spline.

4 Example

We conclude with an example of the use of additive regression splines. We use 100 simulated data points derived from the function

$$f(x,y) = \sin(\pi x) + y\cos(\pi x)\,. \tag{12}$$

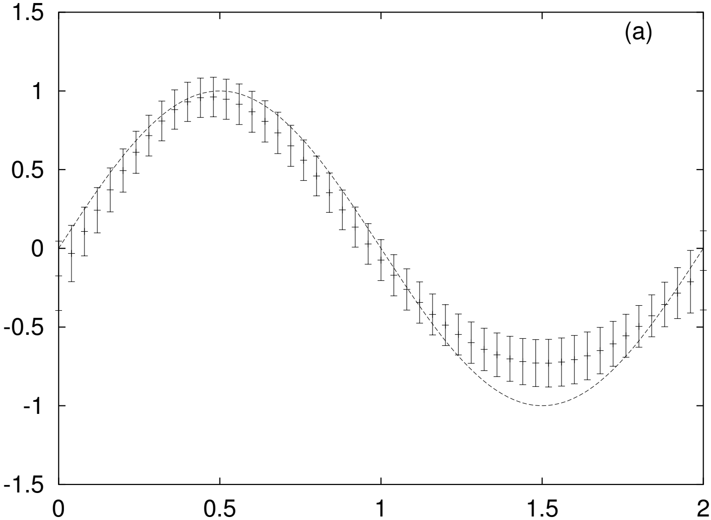
The independent data values $\{x_i, y_i\}$ are chosen at random with $0 \le x_i \le 2$ and $-1 \le y_i \le 1$. The dependent data values are derived by evaluating (12) at each of the independent data locations and perturbing the result by adding a number randomly chosen from $U(-\frac{1}{2}, \frac{1}{2})$. Figure 1a shows a contour plot of the true function defined by (12) as well as the locations of the data points.

The minimum generalised cross validation additive regression spline for the simulated data was derived using appropriate extensions of ANUSPLIN version 4.2 [10]. ANUSPLIN provides summary statistics including an estimate of 0.27 for the standard deviation of the noise associated with the data. This is in good agreement with the theoretical error standard deviation of $1/\sqrt{12} \simeq 0.29$. The additive regression spline contours can be seen in Figure 1b. The component functions of the additive regression spline were calculated on a regular grid and are shown, along with their 95% model confidence intervals and their true counterparts in Figures 2a and 2b.The confidence intervals were derived by ANUSPLIN using the methodology described by [7]. This is based on the Bayesian analysis devised by Wahba [12]. The confidence intervals show reasonable coverage of the true spline component functions, with larger confidence intervals where the actual errors are larger.

5 Conclusion

The additive regression model appears to be a practical option for analysing spatially varying effects of several predictors on observed phenomena. It is attractive from the point of view of overcoming curse of dimension problems associated with the analysis of noisy multivariate data. Moreover its implementation is a straightforward extension of standard thin plate spline methodology. Bayesian standard error estimates associated with minimum GCV additive regression models also appear to be reasonable.

A straightforward extension of the additive regression spline model is to incorporate parametric transformations of the predictor variables. The parameters defining these transformations can be optimised by minimising GCV. A second extension, applied in the precipitation analysis of Hutchinson and Sharples [11], is to permit short range correlation in the noise term in equation (1). This is often a very reasonable assumption for observed physical phenomena. Short range correlation structure can also be specified by one or two parameters that appear to be best optimised by minimising GML rather than GCV [16].



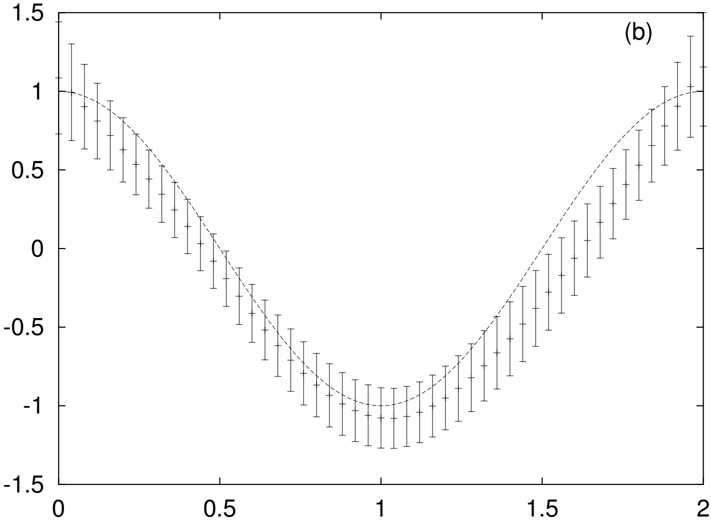


Figure 2: (a) Plot of zeroth additive spline component and 95% model confidence intervals compared with $\sin(\pi x)$. (b) Plot of first additive spline component and 95% model confidence intervals compared with $\cos(\pi x)$.

References

[1] Adams, R. *Sobolev Spaces*. Academic Press, New York (1975). C680

[2] Atteia, M. *Hilbertian Kernels and Spline Functions*. North–Holland, Amsterdam (1992) 145–153. C680, C681, C682

[3] Barry, D. Nonparametric Bayesian regression, *Ann. Statist.* **14** (1986) 934–953. C678

[4] Chen, Z. *Interaction spline models*, Ph.D. Thesis. Department of Statistics, University of Wisconsin, Madison, WI (1989). C678

[5] Gu, C., Wahba, G. Minimizing GCV/GML scores with multiple smoothing parameters via the Newton method, *SIAM J. Sci. Statist. Comput.* **12** (1991) 383–398. C679

[6] Gu, C., Wahba, G. Semiparametric analysis of variance with tensor product thin plate splines, *J. Roy. Statist. Soc. Series B* **55**(2) (1993) 353–368. C678, C679

[7] Hutchinson, M. F. On thin plate splines and kriging, in *Computing and Science in Statistics* **25**, Tarter, M. E., Lock, M. D. (eds.) University of California, Berkeley: Interface Foundation of North America 55–62. C689

[8] Hutchinson, M. F. Interpolation of mean precipitation using thin plate smoothing splines, *International Journal of Geographic Information Systems* **9** (1995) 385–403. C677

[9] Hutchinson, M. F. Interpolation of rainfall data with thin-plate smoothing splines II: Analysis of topographic dependence, *Journal of Geographic Information and Decision Analysis* **2**(2) (1998) 168–185. C677

[10] Hutchinson, M. F. *ANUSPLIN Version 4.2* Centre for Resource and Environmental Studies, Australian National University (2001). http://cres.anu.edu.au/outputs/anusplin.html C688

[11] Hutchinson, M. F., Sharples, J. J. Topographic dependent interpolation of alpine precipitation using additive regression splines, *Journal of Applied Meteorology* (under review). C677, C689

[12] Wahba, G. Bayesian "confidence intervals" for the cross-validated smoothing spline, *J. Roy. Statist. Soc. Series B* **45**(2) (1983) 133–150. C689

[13] Wahba, G. A comparison of GCV and GML for choosing the smoothing parameter in the generalised spline smoothing problem, *Ann. Statist.* **13** (1985) 1378–1402. C679

[14] Wahba, G. Partial and interaction splines for the semiparametric estimation of functions of several variables, in *Computer Science and Statistics: Proceedings of the 18th Symposium*, Boardman, T. (ed.) American Statistical Association, Washington, DC (1986) 75–80. C678, C679

[15] Wahba, G. *Spline Models for Observational Data.* SIAM, Philadelphia (1990). C679, C683

[16] Wang, Y. Smoothing spline models with correlated errors, *Journal of the American Statistical Association* **93** (1998) 341–348 C689