An Introduction to (Smoothing Spline) ANOVA Models in RKHS, With Examples in Geographical Data, Medicine, Atmospheric Science and Machine Learning.

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1 Introduction

Smoothing Spline ANOVA (SS-ANOVA) models in reproducing kernel Hilbert spaces (RKHS) provide a very general framework for data analysis, modeling and learning in a variety of fields. Discrete, noisy scattered, direct and indirect observations can be accommodated with multiple inputs and multiple possibly correlated outputs and a variety of meaningful structures. The purpose of this paper is to give a brief overview of the approach and describe and contrast a series of applications, while noting some recent results.

2 The general SS-ANOVA model

The SS-ANOVA model with Gaussian data has the form

\[ y_i = f(t_1(i), \ldots, t_d(i)) + \epsilon_i, \quad i = 1, \ldots, n, \]  

where \( \epsilon = (\epsilon_1, \ldots, \epsilon_n)' \sim N(0, \sigma^2 I_{n \times n}) \), \( t_\alpha \in T^{(\alpha)} \), where \( T^{(\alpha)} \) is a measurable space, \( \alpha = 1, \ldots, d \); \( (t_1, \ldots, t_d) = t \in T = T^{(1)} \otimes \cdots \otimes T^{(d)} \), and \( \sigma^2 \) may be unknown. For \( f \) satisfying some measurability conditions a unique ANOVA decomposition of \( f \) of the form

\[ f(t_1, \ldots, t_d) = \mu + \sum_\alpha f_\alpha(t_\alpha) + \sum_{\alpha \beta} f_{\alpha \beta}(t_{\alpha \beta}) + \cdots \]  

can always be defined as follows: Let \( d\mu_\alpha \) be a probability measure on \( T^{(\alpha)} \) and define the averaging operator \( E_\alpha \) on \( T \) by

\[ (E_\alpha f)(t) = \int_{T^{(\alpha)}} f(t_1, \ldots, t_d)d\mu_\alpha(t_\alpha). \]

Then the identity is decomposed as

\[ I = \prod_\alpha (E_\alpha + (I - E_\alpha)) = \prod_\alpha E_\alpha + \sum_\alpha (I - E_\alpha) \prod_{\beta \neq \alpha} E_\beta \]

\[ + \sum_{\alpha < \beta} (I - E_\alpha)(I - E_\beta) \prod_{\gamma \neq \alpha, \beta} E_\gamma + \cdots + \prod_\alpha (I - E_\alpha). \]

The components of this decomposition generate the ANOVA decomposition of \( f \) of the form (2) by \( C = (\prod_\alpha E_\alpha)f, f_\alpha = ((I - E_\alpha)\prod_{\beta \neq \alpha} E_\beta)f, f_{\alpha \beta} = ((I - E_\alpha)(I - E_\beta)\prod_{\gamma \neq \alpha, \beta} E_\gamma)f, \) and so forth.
Further details in the RKHS context may be found in Wahba (1990) Gu & Wahba (1993) Wahba, Wang, Gu, Klein, & Klein (1995)

The idea behind SS-ANOVA is to construct an RKHS $\mathcal{H}$ of functions on $\mathcal{T}$ so that the components of the SS-ANOVA decomposition represent an orthogonal decomposition of $f$ in $\mathcal{H}$. Then RKHS methods can be used to explicitly impose smoothness penalties of the form $\sum_{\alpha} \lambda_{\alpha} J_{\alpha}(f_{\alpha}) + \sum_{\alpha<\beta} \lambda_{\alpha\beta} J_{\alpha\beta}(f_{\alpha\beta}) + \cdots$, where, however, the series will be truncated at some point. This is done as follows: Let $\mathcal{H}^{(\alpha)}$ be an RKHS of functions on $\mathcal{T}^{(\alpha)}$ with $\int_{\mathcal{T}^{(\alpha)}} f_{\alpha}(t_{\alpha})d\mu_{\alpha} = 0$ for $f_{\alpha}(t_{\alpha}) \in \mathcal{H}^{(\alpha)}$, and let $[1^{(\alpha)}]$ be the one dimensional space of constant functions on $\mathcal{T}^{(\alpha)}$. Construct $\mathcal{H}$ as

$$\mathcal{H} = \prod_{j=1}^{d} ([1^{(\alpha)}] \oplus \{\mathcal{H}^{(\alpha)}\})$$

$$= [1] \oplus \sum_j \mathcal{H}^{(\alpha)} \oplus \sum_{\alpha<\beta} \mathcal{H}^{(\alpha)} \otimes \mathcal{H}^{(\beta)} \oplus \cdots,$$

where $[1]$ denotes the constant functions on $\mathcal{T}$. With some abuse of notation, factors of the form $[1^{(\alpha)}]$ are omitted whenever they multiply a term of a different form. Thus $\mathcal{H}^{(\alpha)}$ is a shorthand for $[1^{(1)}] \otimes \cdots \otimes [1^{(\alpha-1)}] \otimes \mathcal{H}^{(\alpha)} \otimes [1^{(\alpha+1)}] \otimes \cdots \otimes [1^{(d)}]$ (which is a subspace of $\mathcal{H}$). The components of the ANOVA decomposition are now in mutually orthogonal subspaces of $\mathcal{H}$. Note that the components will depend on the measures $d\mu_{\alpha}$ and these should be chosen in a specific application so that the fitted mean, main effects, two factor interactions, etc. have reasonable interpretations.

Next, $\mathcal{H}^{(\alpha)}$ is decomposed into a parametric part and a smooth part, by letting $\mathcal{H}^{(\alpha)} = \mathcal{H}^{(\alpha)}_{\pi} \oplus \mathcal{H}^{(\alpha)}_{s}$, where $\mathcal{H}^{(\alpha)}_{\pi}$ is finite dimensional (the “parametric” part) and $\mathcal{H}^{(\alpha)}_{s}$ (the “smooth” part) is the orthocomplement of $\mathcal{H}^{(\alpha)}_{\pi}$ in $\mathcal{H}^{(\alpha)}$. Elements of $\mathcal{H}^{(\alpha)}_{\pi}$ are not penalized through the device of letting $J_{\alpha}(f_{\alpha}) = \|P^{(\alpha)} f_{\alpha}\|^2$ where $P^{(\alpha)}$ is the orthogonal projector onto $\mathcal{H}^{(\alpha)}_{\pi}$. $[\mathcal{H}^{(\alpha)} \otimes \mathcal{H}^{(\beta)}]$ is now a direct sum of four orthogonal subspaces: $[\mathcal{H}^{(\alpha)} \otimes \mathcal{H}^{(\beta)}] = [\mathcal{H}^{(\alpha)}_{\pi} \otimes \mathcal{H}^{(\beta)}_{\pi}] \oplus [\mathcal{H}^{(\alpha)}_{\pi} \otimes \mathcal{H}^{(\beta)}_{s}] \oplus [\mathcal{H}^{(\alpha)}_{s} \otimes \mathcal{H}^{(\beta)}_{\pi}] \oplus [\mathcal{H}^{(\alpha)}_{s} \otimes \mathcal{H}^{(\beta)}_{s}]$. By convention the elements of the finite dimensional space $[\mathcal{H}^{(\alpha)}_{\pi} \otimes \mathcal{H}^{(\beta)}_{\pi}]$ will not be penalized. Continuing this way results in an orthogonal decomposition of $\mathcal{H}$ into sums of products of unpenalized finite dimensional subspaces, plus main effects ‘smooth’ subspaces, plus two factor interaction spaces of the form parametric $\otimes$ smooth $[\mathcal{H}^{(\alpha)}_{\pi} \otimes \mathcal{H}^{(\beta)}_{s}]$, smooth $\otimes$ parametric $[\mathcal{H}^{(\alpha)}_{s} \otimes \mathcal{H}^{(\beta)}_{\pi}]$ and smooth $\otimes$ smooth $[\mathcal{H}^{(\alpha)}_{s} \otimes \mathcal{H}^{(\beta)}_{s}]$ and similarly for the three and higher factor subspaces.

Now suppose that we have selected the model $\mathcal{M}$, that is, we have decided which subspaces will be included. Collect all of the included unpenalized subspaces into a subspace, call it $\mathcal{H}^0$, of dimension $M$, and relabel the other subspaces as $\mathcal{H}^{\beta}, \beta = 1, 2, \cdots, p$. $\mathcal{H}^\beta$ may stand for a subspace $\mathcal{H}^{(\alpha)}_{\pi}$, or one of the three subspaces in the decomposition of $[\mathcal{H}^{(\alpha)} \otimes \mathcal{H}^{(\beta)}]$ which contains at least one ‘smooth’ component, or, a higher order subspace with at least one ‘smooth’ component. Collecting these subspaces as $\mathcal{M} = \mathcal{H}^0 \oplus \sum_\beta \mathcal{H}^{\beta}$, the estimation problem in the Gaussian case becomes: Find $f$ in $\mathcal{M} = \mathcal{H}^0 \oplus \sum_\beta \mathcal{H}^{\beta}$ to minimize

$$\frac{1}{n} \sum_{i=1}^{n} (y_i - f(t(i)))^2 + \lambda \sum_{\beta} \theta_{\beta}^{-1} \|P^{\beta} f\|^2,$$

where $P^{\beta}$ is the orthogonal projector in $\mathcal{M}$ onto $\mathcal{H}^{\beta}$, and choose the (overparameterized) tuning parameters $\lambda, \theta_{\beta}$. Bayesian confidence intervals, with the so-called ‘across the function’ property, are available for these models.
The residual sum of squares (RSS) in (8) is replaced by the log likelihood

\[ \mathcal{L}(y, f) = -\sum_{i=1}^{n} [y_i f(t(i)) - b(f(t(i)))] \]  

(9)

for data from exponential families. Some of the examples below will involve Bernoulli (0, 1) data, in which case \( b(f) = \log(1 + e^f) \). Software for computing and tuning SS-ANOVA models may be found in the codes GRKPACK, RKPACK and gss and elsewhere, links to these and other spline related codes can be found via http://www.stat.wisc.edu/~wahba

goto ”SOFTWARE”. Tuning methods are discussed in the first talk in this session. RSS may be replaced by robust functionals, or any convex functionals satisfying some mild conditions insuring uniqueness, and, in recent work on classification by support vector machines, RSS is replaced by so-called hinge functions.

3 Applications in Environmental Data

Gu & Wahba (1993) considered data from the Eastern Lake Survey of 1984 which gave water acidity measurements and geographic locations, and other measurements of lakes in the Blue Ridge Mountains area. Of interest is the pH as it depends on the geographic location and calcium concentration in the lakes. Model diagnostics were proposed there, and the model

\[ y_i = f_1(t_1(i)) + f_2(t_2(i)) + f_{1,2}(t_1(i), t_2(i)) + \epsilon_i \]  

(10)

was chosen, where \( t_1 \) is calcium content and \( t_2 \) is the pair (latitude, longitude). The thin plate spline penalty was imposed on the spatial variable. The calcium content and geography main effects models were plotted, and it can be seen that geography is a near proxy for elevation along the Blue Ridge mountains.

4 Risk factor estimation

Wahba et al. (1995) considered the risk of progression of diabetic retinopathy in a subpopulation of the Wisconsin Epidemiological Study of Diabetic Retinopathy, whose baseline retinopathy score was below (i. e. good) a prespecified level. The observations were \( y_i = 1 \) if the \( i \)th person’s retinopathy progressed at the first followup, and 0 if it had not. Here \( f \) is the log odds ratio, \( f = \log[p/(1 - p)] \). Three important variables were identified by informal means (see Section 9) and were \( t_1 = \) duration of diabetes, \( t_2 = \) glycosylated hemoglobin, and \( t_3 = \) body mass index, and was modeled as

\[ f(t) = \mu + f_1(t_1) + a_2 t_2 + f_3(t_3) + f_{13}(t_1, t_3). \]

(11)

An interesting scientific result was found, that, persons in the study group with the longest duration of diabetes were at a lower risk, possibly because they had survived longest without exceeding the prespecified threshold.

5 Time and Space Models on the Globe

In Wahba & Luo (1997) Luo, Wahba & Johnson (1997) thirty years (1961-90) of Dec. Jan. Feb. average temperature measurements at 1000 stations around the globe (with missing data) was
analyzed for spatial trends, as well as a global trend. Here $t = (t_1, t_2) = (x, P)$ where $x$ is year, and $P$ is (latitude, longitude). The RKHS of historical global temperature functions is $H = \{[1^{(1)}] \oplus [\phi] \oplus H_s^{(1)} \oplus [1^{(2)}] \oplus H_s^{(2)}\}$, a collection of functions $f(x, P)$, on $\{1, 2, ..., 30\} \otimes S$, where $S$ is the sphere, and $H$ and $f$ have corresponding decompositions given below:

$$
\mathcal{H} = \{1\} \oplus [\phi] \oplus H_s^{(1)} \oplus [1^{(2)}] \oplus H_s^{(2)} \oplus [\phi] \otimes H_s^{(2)} \oplus H_s^{(1)} \otimes H_s^{(2)}
$$

$$
f(x, P) = C + d\phi(x) + f_1(x) + f_2(P) + \phi(x)f_{\phi,2}(P) + f_{12}(x, P) = \text{mean} + \text{global} + \text{time} + \text{space} + \text{main} \text{ by space} + \text{space-time} + \text{trend} \text{ effect} + \text{time effect} + \text{interaction}
$$

Here $\phi$ is a linear function which averages to 0. A sum of squares of second differences was applied to the time variable, and a spline on the sphere penalty (Wahba (1981)Wahba (1982)) was applied to the space variable. For a cross country skier in the midwest, as this author is, the results were very disappointing, in that they clearly showed a warming trend stretching from the midwest towards Alaska (trend by space term) which was stronger than the global mean trend.

6 Multiple correlated Bernoulli outcomes

Gao, Wahba, Klein & Klein (2001) were motivated by a demographic study involving a population with a variety of observed risk factors for several particular eye diseases, the outcomes were the incidence of one or more of several diseases or conditions in either or both of two eyes. Outcomes of the two eyes in a particular subject are presumed to be correlated, and incidences of the various outcomes may also be correlated. The amount of correlation may be of particular interest. The risk factors could be person specific or eye-specific. The "two-eye" methods are a special case of what might be called "k-eye" methods where one person (unit) has several component outcomes which might have correlated outcomes, depending on unit-specific and component specific risk factors.

The general log-linear model for multivariate Bernoulli data goes as follows: Assuming there are $J$ different endpoints, and $K_j$ repeated measurements for the $j$th endpoint, let $Y_{jk}$ denote the $k$th measurement of the $j$th endpoint. For example, in ophthalmological studies, we have two repeated measurements for each disease: left eye and right eye. In a typical longitudinal study, we have repeated measurements over the time. $Y = (Y_{jk}, j = 1, ..., J, k = 1, ..., K_j)$ is a multivariate Bernoulli outcome variable. Let $X_{jk} = (X_{jkd,1}, X_{jkd,2}, ..., X_{jkd,D})$ be a vector of predictor variables ranging over the subset $\mathcal{X}$ of $\mathbb{R}^D$, where $X_{jkd}$ denotes the $d$th predictor variable for the $k$th measurement of the $j$th endpoint. Some predictor variables may take different values for different measurements while others may be the same for all $Y_{jk}$’s. For example, in ophthalmology studies, there may be present both person-specific predictors and eye-specific predictors. The person-specific predictors are the same for each person. For the eye-specific predictors, the set of predictor variables is the same, but they may take different values for the left and right eyes. We can treat observations from both eyes as correlated repeated measurements in our model. Let $X = (X_{jk}, j = 1, ..., J, k = 1, ..., K_j)$. Then $(X, Y)$ is a pair of random vectors. For a response vector $y = (y_{jk}, j = 1, ..., J, k = 1, ..., K_j)$, its joint probability distribution conditioning on the predictor variables $X$ can be written as

$$P(Y = y|X) =$$
\[
\exp \left( \sum_{j=1}^{J} \sum_{k=1}^{K_j} f_{j,k} y_{j,k} + \sum_{j=1}^{J} \sum_{k_1 < k_2} \alpha_{j,k_1,k_2} y_{j,k_1} y_{j,k_2} \right) \\
+ \sum_{j_1 < j_2} \sum_{k_1,k_2} \alpha_{j_1,k_1,j_2,k_2} y_{j_1,k_1} y_{j_2,k_2} + \ldots + \alpha_{11,12,\ldots,JK_J} y_{11} y_{12} \ldots y_{JK_J} \\
- b(f, \alpha) \}
\]

where

\[
b(f, \alpha) = \log(1 + \sum_{j,k} e^{f_{j,k}} + \sum_{j_1,k_1,j_2,k_2} e^{(f_{j_1,k_1} + f_{j_2,k_2} + \alpha_{j_1,k_1,j_2,k_2})} + \ldots + e^{(\sum_{a=1}^{M} f + \sum_{a=1}^{M} \alpha_a)})
\]

Let \( M = \sum_{j=1}^{J} K_j \) be the length of the vector \( Y \). There are in total \( 2^M - 1 \) parameters: \( (f, \alpha) = (f_{11}, f_{12}, \ldots, f_{JK_J}, \alpha_{11,12,\ldots,JK_J}) \), which may depend on \( X \). The parameter space is unconstrained. They have straightforward interpretations in terms of conditional probabilities. For example,

\[
f_{jk} = \logit(P(Y_{jk} = 1|Y(-j,k) = 0, X))
\]

is the conditional logit function;

\[
\alpha_{j_1,k_1,j_2,k_2} = \log OR(Y_{j_1,k_1}, Y_{j_2,k_2}|Y(-j_1,k_1,-j_2,k_2) = 0, X)
\]

is the conditional log odds ratio, which is a meaningful way to measure pairwise association; interpretations of other terms are given in the paper.

\( n \) independent observations \( (x_i, y_i), i = 1, \ldots, n, \) are given, where \( y_i = (y_{i1}, y_{i2}, \ldots, y_{iJK_J}) \) and \( x_i = (x_{i11}, x_{i12}, \ldots, x_{iJK_J}) \). Here \( y_{ijk} \) and \( x_{ijk} = (x_{ijk1}, x_{ijk2}, \ldots, x_{ijkD}) \) are the outcome variable and predictor vector for the \( k \)th measurement of the \( j \)th endpoint of the \( i \)th subject. Let \( f_{jk}(i) \) be the conditional logit function for the \( k \)th measurement of the \( j \)th endpoint of the \( i \)th subject. There is little reason to believe the \( f_{jk} \) will take different functional forms for the same endpoint. Hence we can assume \( f_{ijk} = f_j(x_{ijk}) \). The same reasoning applies to the association terms. The \( f_{jk} \) were modeled via SS-ANOVA in the paper, and a leaving-out-one-person based generalized cross validation for the smoothing parameters was obtained.

### 7 Multichotomous responses

Lin (1998) considered multichotomous outcomes, the data is \( (y_i, t(i)) \) where \( y_i \) is coded to show that the \( i \) subject, with attribute vector \( t(i) \) is in one of \( k + 1 \) categories, \( k > 1 \). Let \( p_j(t), j = 0, 1, \ldots, k \) be the probability that a subject with attribute vector \( t \) is in category \( k \), \( \sum_{j=0}^{k} p_j(t) = 1 \). Let \( f^j(t) = \log[p_j(t)/p_0(t)], j = 1, \ldots, k \). Then

\[
p_j(t) = \frac{e^{f^j(t)}}{1 + \sum_{j=1}^{k} e^{f^j(t)}}, j = 1, \ldots, k \tag{15}
\]

\[
p_0(t) = \frac{1}{1 + \sum_{j=1}^{k} e^{f^j(t)}} \tag{16}
\]
The class label for the $i$th subject is coded as $y_i = (y_{i1}, \ldots, y_{ik})$ where $y_{ij} = 1$ if the $i$th subject is in class $j$ and 0 otherwise. Letting $f = (f^1, \ldots, f^k)$ the negative log likelihood can be written as

$$\mathcal{L}(y, f) = \sum_{i=1}^{n} \{-\sum_{j=1}^{k} y_{ij} f^j(t_i) + \log\left(\sum_{j=1}^{k} 1 + e^{f^j(t_i)}\right)\}.$$ 

(17)

$f^j = \sum_{\nu=1}^{M} \phi_{\nu} + h^j$ where the $h^j$ can have an ANOVA decomposition. Then $\lambda\|h\|^2_{\mathcal{H}_K}$ in (8) is replaced by

$$\sum_{j=1}^{k} \sum_{\alpha} \lambda_{j\alpha} J_{j\alpha}(h^j_{\alpha}) + \sum_{\alpha<\beta} \lambda_{j\alpha\beta} J_{j\alpha\beta}(h^j_{\alpha\beta}) + \cdots.$$ 

(18)

Ten year mortality data of a group of $n = 646$ subjects with the risk factors age ($x_1$), glycosylated hemoglobin ($x_2$) and systolic blood pressure ($x_3$) were (among other things) recorded at baseline and they were divided into four categories with respect to their status after ten years, as 0 = alive, 1 = died of diabetes, 2 = died of heart disease, and 3 = died of other causes. Each of the $f^j$, $j = 1, 2, 3$ was modeled as $f^j(x_1, x_2, x_3) = \mu^j + f^2_1(x_1) + f_2^3(x_2) + f_3^3(x_3) + f_2^3(x_2, x_3)$. The $p_{ij}, j = 0, \ldots, 3$ were estimated by minimizing $\mathcal{I}(y, f) = (17) + (18)$ and the multiple smoothing parameters estimated by a generalized cross validation method for polychotomous data given in Lin (1998). The plots graphically convey the suggestion that the younger deaths are disproportionately diabetic, thus quickly raising further questions to confront the database.

8 The multicategory support vector machine

The multicategory support vector machine (MSV) proposed in Lee, Lin & Wahba (2002). Lee, Lin & Wahba (2001) considers the case where each subject is in one of $k$ categories labeled as $j = 1, \ldots, k$, as in the preceding section, except for notational convenience there are $k$ instead of $k + 1$ categories. The support vector machine is an efficient method for classification - it is not estimating the probability of membership in a particular category as before, but its target is an indicator as to which category as subject is in (or most likely to be in) (see Lin (2002). The class label $y_i$ is now coded as a $k$ dimensional vector with 1 in the $j$th position if example $i$ is in category $j$ and $-\frac{1}{k-1}$ otherwise. For example $y_i = (1, \frac{1}{k-1}, \ldots, \frac{1}{k-1})$ indicates that the $i$th example is in category 1. We define a $k$-tuple of separating functions $f(t) = (f^1(t), \ldots, f^k(t))$, with each $f^j = d^j + h^j$ with $h^j \in \mathcal{H}_K$, and which will be required to satisfy a sum-to-zero constraint, \[ \sum_{j=1}^{k} f^j(t) = 0, \] for all $t \in \mathcal{T}$. Note that, unlike the estimate of Section 7, all categories are treated symmetrically.

Let $L_{jr} = 1, r \neq j, L_{jj} = 0, j, r = 1, \cdots, k$. Let $\text{cat}(y_i) = j$ if $y_i$ is from category $j$. Then, if $y_i$ is from category $j$, $L_{\text{cat}(y_i)r} = 0$ if $r = j$ and 1 otherwise. Then the MSVM is defined as the vector of functions $f_{\lambda} = (f^{j_1}_{\lambda}, \ldots, f^{j_k}_{\lambda})$, with each $h^k \in \mathcal{H}_K$ satisfying the sum-to-zero constraint, which minimizes

$$\frac{1}{n} \sum_{i=1}^{n} \sum_{r=1}^{k} L_{\text{cat}(y_i)r} (f^{r}(t_i) - y_{ir}) + \lambda \sum_{j=1}^{k} \|h^j\|^2_{\mathcal{H}_K}.$$ 

(19)

Generalizations of the penalty term are possible, if necessary. It can be shown that the $k = 2$ case reduces to the usual 2-category SVM just discussed, and it is shown in Lee et al. (2001) that the target for the MSVM is $f(t) = (f^1(t), \ldots, f^k(t))$ with $f^j(t) = 1$ if $p_j(t)$ is bigger than the other $p_t(t)$ and $f^j(t) = -\frac{1}{k-1}$ otherwise. See also Wahba (2002).
9 Summary

The SS-ANOVA models have proved to be useful in a variety of modeling situations, only a few described here. In each case a tuning method which governs the bias-variance tradeoff must be employed, and, for very large sample sizes, efficient approximate methods need to be devised. Model selection, that is, the determination of which variables and/or terms to include in the model is an important issue. Zhang, Wahba, Lin, Voelker, Ferris, Klein & Klein (2001) have recently proposed likelihood basis pursuit, a nonparametric form of the LASSO, for the model selection problem associated with SS-ANOVA. Although a number of tuning methods for the various situations have been proposed, along with numerical methods for large data sets, a variety of problems remain to be investigated, including optimum nonlinear transformations of the variables, efficient computational methods, methods for covariates not missing at random, and public software for very large sample sizes and for some of the more complex structures.

References

Gao, F., Wahba, G., Klein, R. & Klein, B. (2001), ‘Smoothing spline ANOVA for multivariate Bernoulli observations, with applications to ophthalmology data, with discussion’, J. Amer. Statist. Assoc. 96, 127–160.

Gu, C. & Wahba, G. (1993), ‘Smoothing spline ANOVA with component-wise Bayesian “confidence intervals”’, J. Computational and Graphical Statistics 2, 97–117.

Lee, Y., Lin, Y. & Wahba, G. (2001), Multicategory support vector machines, Technical Report 1043, Department of Statistics, University of Wisconsin, Madison WI. To appear, Computing Science and Statistics, 33.

Lee, Y., Lin, Y. & Wahba, G. (2002), Multicategory support vector machines, theory, and application to the classification of microarray data and satellite radiance data, Technical Report 1063, Department of Statistics, University of Wisconsin, Madison WI.

Lin, X. (1998), Smoothing spline analysis of variance for polychotomous response data, Technical Report 1003, PhD thesis, Department of Statistics, University of Wisconsin, Madison WI. Available via G. Wahba’s website.

Lin, Y. (2002), ‘Support vector machines and the Bayes rule in classification’, Data Mining and Knowledge Discovery 6, 259–275.

Luo, Z., Wahba, G. & Johnson, D. (1997), Spatial-temporal analysis of temperature using smoothing spline ANOVA, Technical Report 97-01, Pennsylvania State University Statistics Dept., State College PA.

Wahba, G. (1981), ‘Spline interpolation and smoothing on the sphere’, SIAM J. Sci. Stat. Comput. 2, 5–16.

Wahba, G. (1982), ‘Erratum: Spline interpolation and smoothing on the sphere’, SIAM J. Sci. Stat. Comput. 3, 385–386.
Wahba, G. (1990), *Spline Models for Observational Data*, SIAM. CBMS-NSF Regional Conference Series in Applied Mathematics, v. 59.

Wahba, G. (2002), Soft and hard classification by reproducing kernel hilbert space methods, Technical Report 1067, Department of Statistics, University of Wisconsin, Madison WI. to appear, Proceedings of the National Academy of Sciences.

Wahba, G. & Luo, Z. (1997), ‘Smoothing spline ANOVA fits for very large, nearly regular data sets, with application to historical global climate data’, *Ann. Numer. Math.* 4, 579–597.

Wahba, G., Wang, Y., Gu, C., Klein, R. & Klein, B. (1995), ‘Smoothing spline ANOVA for exponential families, with application to the Wisconsin Epidemiological Study of Diabetic Retinopathy’, *Ann. Statist.* 23, 1865–1895. Neyman Lecture.

Zhang, H., Wahba, G., Lin, Y., Voelker, M., Ferris, M., Klein, R. & Klein, B. (2001), Variable selection via basis pursuit for non-Gaussian data, Technical Report 1042, Statistics Department University of Wisconsin, Madison WI. In Proceedings of the ASA Joint Statistical Meetings 2001 (CDROM), available from the American Statistical Association.

Zhang, H., Wahba, G., Lin, Y., Voelker, M., Ferris, M., Klein, R. & Klein, B. (2002), Variable selection and model building via likelihood basis pursuit, Technical Report 1059, Statistics Department University of Wisconsin, Madison WI.