Mixtures of $g$-Priors for Generalised Additive Model Selection with Penalised Splines

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We propose an objective Bayesian approach to the selection of covariates and their penalised splines transformations in generalised additive models. Specification of a reasonable default prior for the model parameters and combination with a multiplicity-correction prior for the models themselves is crucial for this task. Here we use well-studied and well-behaved continuous mixtures of $g$-priors as default priors. We introduce the methodology in the normal model and extend it to non-normal exponential families. A simulation study and an application from the literature illustrate the proposed approach. An efficient implementation is available in the R-package “hypergsplines”.

Keywords: penalised splines, Bayesian variable selection, $g$-prior, shrinkage, objective Bayes.

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1. Introduction

Semiparametric regression has achieved an impressive dissemination over the last years. Its central idea is to replace parametric regression functions by smooth, semi-parametric components. Following Hastie and Tibshirani (1990), suppose we have $p$ continuous covariates $x_1, \ldots, x_p$ and use the additive model

$$
y = \beta_0 + \sum_{j=1}^{p} m_j(x_j) + \epsilon, \quad (1)$$

where $m_j$ are smooth but otherwise unspecified functions and $\epsilon \sim N(0, \sigma^2)$. For identifiability purposes we further assume that $\mathbb{E}\{m_j(X_j)\} = 0$ with respect to the marginal distribution of covariate $X_j$. Estimation of the smooth terms in (1) can be carried out in different ways, where we here make use of penalised splines, see e.g. Eilers and Marx (2010) or Wood (2006). A general introduction to penalised spline smoothing has been provided by Ruppert, Wand, and Carroll (2003) and the approach has become a popular smoothing technique since then, see Ruppert, Wand, and Carroll (2009). The general idea is to decompose the function $m_j$ into a linear and a nonlinear part, where the latter is represented through a spline basis, that is

$$
m_j(x_j) = x_j \beta_j + Z_j(x_j)^T u_j. \quad (2)$$

Here $Z_j(x_j)$ is a $K \times 1$ spline basis vector at position $x_j$ and $u_j$ is the corresponding coefficient vector. Conveniently one may choose a truncated polynomial basis for $Z_j(\cdot)$ but representation (2) holds in general as well, see Wand and Ormerod (2008). To achieve a smooth fit one imposes a (quadratic) penalty on the spline coefficient vector $u_j$ which is formulated as the normal prior

$$
u_j \sim N_K(0_K, \sigma^2 \rho_j I_K), \quad (3)$$

where $0_K$ is the all-zeros vector and $I_K$ is the identity matrix of dimension $K$. Here the variance factor $\rho_j$ steers the amount of penalisation (relative to the regression variance $\sigma^2$). A larger $\rho_j$ leads to a higher prior variance of the spline coefficients and hence a more wiggly function $m_j$, while a smaller $\rho_j$ leads to a stronger penalty on $\|u_j\|$ and thus a smoother function $m_j$. Setting $\rho_j$ to zero imposes $u_j \equiv 0_K$ so that $m_j(x_j)$ collapses to a linear term $m_j(x_j) = x_j \beta_j$. Hence the role of $\rho_j$ ($j = 1, \ldots, p$) extends to
the selection of (generalised) additive models, which will be the focus of this paper. Variable selection will be treated by allowing the alternative \( m_j(x_j) \equiv 0 \).

Variable selection in generalised additive models is important to reduce the variance of effect estimates due to uninformative covariates. The field is wide and many different approaches have been proposed in the last years. Friedman (2001) and Tutz and Binder (2006) describe boosting algorithms, which are extended by Kneib, Hothorn, and Tutz (2009) to geoadditve regression models (Fahrmeir, Kneib, and Lang, 2004). For the same model class, Belitz and Lang (2008) propose to use information-criteria or cross-validation, while Fahrmeir, Kneib, and Konrath (2010) and Panagiotelis and Smith (2008) use spike-and-slab priors for variable and function selection. Brezger and Lang (2008) adopt the concept of Bayesian contour probabilities (Held, 2004) to decide on the inclusion and form of covariate effects. Cottet, Kohn, and Nott (2008) generalise earlier work by Yau, Kohn, and Wood (2003) to Bayesian double-exponential regression models, which comprise generalised additive models as a special case. Shrinkage approaches are proposed by Wood (2011) and Marra and Wood (2011). Zhang and Lin (2006) use a lasso-type penalised likelihood approach, and Ravikumar, Liu, Lafferty, and Wasserman (2008) and Meier, van de Geer, and Bühlmann (2009) use penalties favouring both sparsity and smoothness of high-dimensional models. Likelihood-ratio testing methods are described by Kauermann and Tutz (2001) and Cantoni and Hastie (2002). This list mirrors the multitude as well as the variety of the different approaches and the enumeration is, of course, in no way exhaustive.

In this paper we propose a novel Bayesian variable and function selection approach based on mixtures of (generalised) \( g \)-priors. This type of prior for the parameters in the generalised additive model traces back to the \( g \)-prior in the linear model (Zellner, 1986). Its hyper-parameter \( g \) acts as an inverse relative prior sample size, and assigning it a hyper-prior solves the information paradox (Liang, Paulo, Molina, Clyde, and Berger, 2008, section 4.1) of the fixed-\( g \) case (Berger and Pericchi, 2001, p. 148) in the linear model. We will subsequently refer to such mixtures of \( g \)-priors generically as hyper-\( g \) priors. One specific example are the hyper-\( g \) priors of Liang et al. (2008, section 3.2), which enjoy a closed form for the marginal likelihood and lead to consistent model selection and model-averaged prediction. We will proceed to use these, because they have been well studied and have shown good frequentist properties in the Gaussian linear model, and have already been extended to generalised linear mod-
els by Sabanés Bové and Held (2011a). We follow the conventional prior approach (Berger and Pericchi, 2001, section 2.1) by using non-informative improper priors for parameters which are common to all models, and default proper hyper-$g$ priors for model-specific parameters.

While hyper-$g$ priors have been discussed extensively in the Bayesian variable selection literature, e.g. by Cui and George (2008), Liang et al. (2008), Forte (2011) and Celeux, Anbari, Marin, and Robert (2012), this is the first paper to our knowledge that applies hyper-$g$ priors to generalised additive models. The general idea of applying default priors (as hyper-$g$ priors) which have originally been developed for linear models to generalised additive models is new. The methodology presented here is straightforward to use with other default priors. The rationale is that default priors have carefully and exhaustively been constructed for the linear model, so their advantages should be used when inferring about generalised additive models. Moreover, this paper is one of the few Bayesian papers considering automatic and simultaneous variable selection and transformation.

The current work generalises the hyper-$g$ priors for generalised linear models (Sabanés Bové and Held, 2011a). In the same paper, we showed how fractional polynomials (FPs, Sabanés Bové and Held, 2011b), which extend ordinary polynomials by square roots, reciprocals and the logarithm, can be used to model nonlinear covariate effects. However, FPs have the disadvantage of being not invariant to linear transformations of the covariates. For variable and function selection, Fahrmeir et al. (2010) and Scheipl, Fahrmeir, and Kneib (2011) use a mixture of two inverse-gamma distributions with a very small (”spike”) and a larger mean (”slab”) as a hyper-prior for the variances of the regression coefficients’ independent normal priors. The posterior probability for inclusion of a coefficient is then estimated from the proportion of Markov chain Monte Carlo (MCMC) variance samples in the “slab”. While this prior structure eases the MCMC algorithm, it does not take into account the correlation structure of the covariates, and depends on the specification of the prior means in the two mixture components. Cottet et al. (2008) also use independent normal inverse-gamma priors for the regression coefficients, but they explicitly exclude coefficients from the model. For nonlinear effects they utilise low-rank approximations of smoothing splines, which require the choice of a threshold on the eigenvalue scale.

The paper is organised as follows. We first apply the hyper-$g$ priors of Liang et al.
(2008) to additive models in Section 2. The methodology is extended to generalised additive models in Section 3. A multiplicity-correction prior on the model space and a stochastic search procedure are described in Section 4. We apply our approach to simulated and real data in Section 5 and suggest postprocessing techniques in Section 6. Section 7 closes the paper with a discussion.

2. Hyper-$g$ Priors for Additive Models

Assume we have observed independent responses $y_i$ at covariate values $x_{i1}, \ldots, x_{ip}$, $i = 1, \ldots, n$, from the additive normal model (1). For each covariate $j = 1, \ldots, p$, we stack the covariate values into the $n \times 1$ vector $\tilde{x}_j = (x_{1j}, \ldots, x_{nj})^T$ and the spline basis vectors into the $n \times K$ matrix $\tilde{Z}_j = (Z_j(x_{1j}), \ldots, Z_j(x_{nj}))^T$. The subsequent Gram-Schmidt process (see Björck, 1967)

$$x_j = \tilde{x}_j - \frac{1_n^T \tilde{x}_j}{1_n^T 1_n} = \tilde{x}_j - 1_n \bar{x}_j,$$

$$Z_j = \tilde{Z}_j - \frac{1_n^T \tilde{Z}_j}{1_n^T 1_n} - x_j \frac{x_j^T \tilde{Z}_j}{x_j^T x_j},$$

where $1_n$ denotes the all-ones vector of dimension $n$, ensures that $1_n$, $x_j$ and the columns of $Z_j$ are orthogonal to each other, i.e. $1_n^T x_j = 0$ and $1_n^T Z_j = x_j^T Z_j = 0_K$.

A central measure of model complexity is the degrees of freedom. While in parametric models this is just the number of parameters, for smoothing and mixed models Aerts, Claeskens, and Wand (2002, section 2.2) translate the variance factor $\rho_j$ into the corresponding degrees of freedom

$$d_j(\rho_j) = \text{tr}\{(Z_j^T Z_j + \rho_j^{-1} I)^{-1} Z_j^T Z_j\} + 1 \in (1, K + 1)$$

for a smoothly modelled covariate effect $m_j$. Note that $d_j(\rho_j) = \sum_{k=1}^{K} \lambda_{jk}/(\lambda_{jk} + \rho_j^{-1})$ is easy to calculate via the (positive) eigenvalues $\lambda_{jk}$ of $Z_j^T Z_j$. This also shows that $d_j(\rho_j)$ is strictly increasing with derivative $\sum_{k=1}^{K} \lambda_{jk}/(\rho_j \lambda_{jk} + 1)^2 > 0$, which implies that we may (numerically) invert the function to $\rho_j(d_j)$. In fact, by fixing the degrees of freedom $d_j$ for function $m_j(x_j)$ we define the variance factor $\rho_j$. Subsequently we will restrict the degrees of freedom to take values in a finite set $\mathcal{D} \subset \{0\} \cup [1, K + 1)$, say $\mathcal{D} = \{0, 1, 2, 3, \ldots, K\}$. For $d_j = 0$ we set $m_j(x_j) \equiv 0$ while for $d_j = 1$ we have the
linear model $m_j(x_j) = x_j \beta_j$. In general, model (1) is indexed by $d = (d_1, \ldots, d_p)$ giving the degrees of freedom for each functional component and hence the structure of the model.

After combining the $l = \sum_{j=1}^p \mathbb{1}(d_j \geq 1)$ vectors $x_j$ to the $n \times l$ linear design matrix $X_d = (x_j : d_j \geq 1)$ and the $j = \sum_{j=1}^p \mathbb{1}(d_j > 1)$ matrices $Z_j$ to the $n \times JK$ spline design matrix $Z_d = (Z_j : d_j > 1)$, and analogously constructing the respective coefficient vectors $\beta_d$ and $u_d$, the conditional additive model for the response vector $y = (y_1, \ldots, y_n)^T$ is

$$y | \beta_0, \beta_d, u_d, \sigma^2 \sim N_n(1_n \beta_0 + X_d \beta_d + Z_d u_d, \sigma^2 I_n).$$

Integrating out the the spline coefficient vector $u_d \sim N_{JK}(0_{JK}, \sigma^2 D_d)$, where $D_d$ is block-diagonal with $J$ blocks $\rho_j I_k$ ($d_j > 1$), yields the marginal model

$$y | \beta_0, \beta_d, \sigma^2 \sim N_n(1_n \beta_0 + X_d \beta_d, \sigma^2 V_d)$$

with $V_d = I_n + Z_d D_d Z_d^T$. This general linear model can be decorrelated into a standard linear model by using the Cholesky decomposition $V_d = V_d^{T/2} V_d^{1/2}$: For the transformed response vector $\tilde{y} = V_d^{-T/2} y$ we have

$$\tilde{y} | \beta_0, \beta_d, \sigma^2 \sim N_n(1_n \beta_0 + \tilde{X}_d \beta_d, \sigma^2 I_n)$$

with analogously transformed all-ones vector $\tilde{1}_n = V_d^{-T/2} 1_n$ and design matrix $\tilde{X}_d = V_d^{-T/2} X_d$. Note that now also $\tilde{y}$ and $\tilde{1}_n$ depend on the model $d$, but we suppress this dependence for ease of notation.

We will now show how to use the hyper-$g$ priors of Liang et al. (2008) for the parameters $\beta_0$, $\beta_d$ and $\sigma^2$ in the decorrelated model (9). The hyper-$g$ priors comprise a locally uniform prior $f(\beta_0) \propto 1$ on the intercept, Jeffreys’ prior $f(\sigma^2) \propto (\sigma^2)^{-1}$ on the regression variance and the $g$-prior (Zellner, 1986)

$$\beta_d | g, \sigma^2 \sim N_I \left(0_L, g \sigma^2 (\tilde{X}_d^T \tilde{X}_d)^{-1} \right)$$

on the linear coefficient vector. Note that the prior precision matrix in (10) is proportional to $\sigma^{-2} \tilde{X}_d^T \tilde{X}_d = \sigma^{-2} X_d^T V_d^{-1} X_d$, which is the Fisher information matrix of $\beta_d$ in model (8). The prior construction is completed with either a uniform hyper-prior on the shrinkage coefficient $g/(1 + g)$,

$$\frac{g}{1 + g} \sim U(0, 1),$$
leading to the hyper-$g$ prior, or with

$$\frac{g/n}{1 + g/n} \sim U(0, 1),$$

leading to the hyper-$g/n$ prior. We recommend to use the latter, because it also leads to consistent posterior model probabilities if the true model is the null model (see Table 1 in Section 5.1 for an illustration of this).

Basically all formulae given by Liang et al. (2008) carry over to our setting, since inner products of the response vector $y$, the all-ones vector $1_n$ and the design matrix $X_d$ in model (8) carry over to their transformed counterparts $\tilde{y}$, $\tilde{1}_n$ and $\tilde{X}_d$ in model (9). This is due to

$$V_d^{-1} = (I_n + Z_d D_d Z_d^T)^{-1} = I_n - Z_d (Z_d^T Z_d + D_d^{-1})^{-1} Z_d^T,$$

which follows from the matrix inversion lemma (see Henderson and Searle, 1981) and leads to $\tilde{1}_n^T 1_n = 1_n^T 1_n = n$, $\tilde{1}_n^T X_d = 1_n^T X_d = 0_I$, and $\tilde{1}_n^T \tilde{y} = 1_n^T y$ by straightforward calculations. A most convenient property of the hyper-$g$ priors is that they yield closed form marginal likelihoods, which need to be computed on the original response scale via the change of variables formula:

$$f(y \mid d) \propto f(\tilde{y} \mid d) \left| V_d^{1/2} \right|^{-1},$$

where $f(\tilde{y} \mid d)$ is the marginal likelihood of the transformed response vector $\tilde{y}$ in the standard linear model (9). The closed forms for $f(\tilde{y} \mid d)$ under the hyper-$g$ priors are given in Appendix A, along with other implementation details.

Other hyper-priors could be assigned to $g$, but will typically not lead to a closed form of the marginal likelihood. Examples are the incomplete inverse-gamma prior on $1 + g$ (Cui and George, 2008, p. 891), which generalises the above uniform prior on $g/(1 + g)$, and an inverse-gamma prior on $g$, which corresponds to the Cauchy prior of Zellner and Siow (1980). The hyper-$g/n$ prior is a special case of the conventional robust prior proposed by Forte (2011), for which a closed form of the marginal likelihood exists. An overview of mixtures of $g$-priors is given by Ley and Steel (2011).

It is not clear that the good properties of hyper-$g$ priors (or other default priors in the Gaussian linear model) would be retained if we based them on the conditional model (7) without integrating out the random effects. We followed the natural idea
of transforming the mixed model into a standard model, where default priors have already been studied extensively. Moreover, computation would be harder if we proceeded otherwise. Hence we prefer to keep the good properties of the default priors by integrating out the random effects.

Posterior inference in a given model \( d \) is based on Monte Carlo estimation of the parameters in model (7), using the factorisation

\[
f(\beta_0, \beta_d, u_d, \sigma^2, g \mid y) = f(u_d \mid \beta_0, \beta_d, \sigma^2, y) f(\beta_0, \beta_d \mid \sigma^2, g, y) f(\sigma^2 \mid y) f(g \mid y).
\] (13)

Sampling of \( g, \sigma^2 \) and subsequently \( \beta_0, \beta_d \) can be done along the lines of Sabanés Bové and Held (2011b, section 2.3), by adapting their algorithm to the transformations in model (9).

Finally, the spline coefficient vector \( u_d \) is sampled from

\[
f(u_d \mid \beta_0, \beta_d, \sigma^2, y) \propto f(u_d \mid \sigma^2) f(y \mid \beta_0, \beta_d, u_d, \sigma^2)
\]
\[
\propto \exp \left\{ -\frac{1}{2\sigma^2} \left[ u_d^T D_d^{-1} u_d + \| y - 1_n \beta_0 - X_d \beta_d - Z_d u_d \|^2 \right] \right\}
\]
\[
\propto N_{JK} \left( u_d \mid \Sigma_d Z_d^T (y - X_d \beta_d), \sigma^2 \Sigma_d \right),
\] (14)

where \( \Sigma_d = (Z_d^T Z_d + D_d^{-1})^{-1} \) and \( \beta_0 \) disappears because \( Z_d^T 1_n = 0_{JK} \).

Given posterior samples for the linear coefficient \( \beta_j \) and the spline coefficient vector \( u_j \) for covariate \( j \) (\( d_j > 1 \)), we would like to transform these into samples for the function \( m_j(x_j) \), along a grid vector \( \tilde{x}_j^* \) of \( n^* \) points (on the same scale as the original \( \tilde{x}_j \) used for the model fitting). This is in principle straightforward, but one has to carefully apply analogous transformations as in (4) and (5) to \( \tilde{x}_j^* \) and the corresponding spline basis matrix \( Z_j^* \):

\[
x_j^* = \tilde{x}_j^* - 1_n \frac{1_n^T \tilde{x}_j}{1_n^T 1_n},
\] (15)
\[
Z_j^* = \tilde{Z}_j^* - 1_n \frac{1_n^T \tilde{Z}_j}{1_n^T 1_n} - x_j^* \frac{x_j^T \tilde{Z}_j}{x_j^T x_j}.
\] (16)

Afterwards, for each coefficient sample one can compute the corresponding vector of function values \( m_j(\tilde{x}_j^*) = x_j^* \beta_j + Z_j^* u_j \). Similarly, prediction samples for the corresponding response vector \( y^* \) can be extracted from the sampling output.
3. Hyper-$g$ Priors for Generalised Additive Models

Now we extend the above setting and assume that the covariate effects $m_j(x_j)$ enter additively into the linear predictor

$$\eta = \beta_0 + \sum_{j=1}^{p} m_j(x_j)$$  \hspace{1cm} (17)

of an exponential family distribution with canonical parameter $\theta$, mean $\mathbb{E}(y) = h(\eta) = db(\theta) / d\theta$ and variance $\text{Var}(y) = \phi / w \cdot d^2 b(\theta) / d\theta^2$ (see McCullagh and Nelder, 1989). We restrict our attention to non-normal distributions with fixed dispersion $\phi$ (as $\phi = 1$ for the Bernoulli and Poisson distribution) and known weight $w$. For $n$ observations, the linear predictor vector $\eta = (\eta_1, \ldots, \eta_n)^T$ is

$$\eta = 1_n \beta_0 + X_d \beta_d + Z_d u_d$$  \hspace{1cm} (18)

and the likelihood is

$$f(y | \beta_0, \beta_d, u_d) \propto \exp \left\{ \sum_{i=1}^{n} \frac{y_i \theta_i - b(\theta_i)}{\phi / w_i} \right\}. \hspace{1cm} (19)$$

The main challenge for the derivation of a generalised $g$-prior is that the marginal density $f(y | \beta_0, \beta_d)$, which results from integrating out the spline coefficient vector

$$u_d \sim N_{JK}(0_{JK}, D_d) \hspace{1cm} (20)$$

from (19), has no closed form. In particular, it is not Gaussian, in contrast to (8).

Before addressing this problem we first consider appropriate construction of the design matrices $X_d$ and $Z_d$ and calculation of the degrees of freedom $d_j(d)$ for a smoothly modelled term $m_j$. Starting with the latter, a reasonable generalisation of (6) is (see Ruppert et al., 2003, section 11.4)

$$d_j(d) = \text{tr}\{(Z_j^T \hat{W} Z_j + \rho_j^{-1} I)^{-1} Z_j^T \hat{W} Z_j\} + 1, \hspace{1cm} (21)$$

which uses a fixed weight matrix $\hat{W} = W(1_n \hat{\beta}_0)$, where $W(\eta) = \text{diag}\{(dh(\eta_i) / d\eta)^2 / \text{Var}(y_i)\}_{i=1}^{n}$ is the usual generalised linear model weight matrix and $\hat{\beta}_0$ is the intercept estimate from the null model $d = 0_p$. This definition avoids dependence of $\rho_j(d_j)$ on the model
under consideration. As a consequence, we need to generalise the orthogonalisation of the original covariate vector $\tilde{x}_j$ and spline basis matrix $\tilde{Z}_j$ from (4) and (5) to

$$x_j = \tilde{x}_j - \frac{1_n^T W \tilde{x}_j}{1_n^T W 1_n}$$

and

$$Z_j = Z_j - \frac{1_n^T W \tilde{Z}_j}{1_n^T W 1_n} - \frac{x_j^T W \tilde{Z}_j}{x_j^T W x_j}$$

implying that $1_n, x_j$ and the columns of $Z_j$ are orthogonal to each other with respect to the inner product in terms of $W$. This ensures that (21) correctly captures only the degrees of freedom associated with the nonlinear part of $m_j$. Note that (15) and (16) are adapted analogously.

We will now derive a generalised $g$-prior analogous to (10) for the linear coefficient vector $\beta_d$ in the generalised additive model. The idea is to use the iterative weighted least squares (IWLS) approximation to (19) to obtain an approximate normal model of the form (7) and then derive the resulting $g$-prior (10). With a slight abuse of notation, e.g. $h(\eta) = (h(\eta_1), \ldots, h(\eta_n))^T$, let

$$z_0 = \eta_0 + \text{diag}(dh(\eta_0)/d\eta)^{-1}(y - h(\eta_0))$$

be the adjusted response vector resulting from a first-order approximation to $h^{-1}(y)$ around $y = h(\eta_0)$. Then

$$z_0 | \beta_0, \beta_d, u_d \sim N(1_n \beta_0 + X_d \beta_d + Z_d u_d, W_0^{-1})$$

with $W_0 = W(\eta_0)$ is the working normal model (see e.g. McCullagh and Nelder, 1989, p. 40). Remember that the IWLS algorithm iteratively updates $\eta_0$ by weighted least squares estimation of the coefficients in (25). Here, we fix $\eta_0 = 0_n$, which is the value expected a priori. Then we rewrite (25) using $z_0 = W_0^{1/2} \tilde{z}_0$ etc. as

$$\tilde{z}_0 | \beta_0, \beta_d, u_d \sim N(\tilde{1}_n \beta_0 + \tilde{X}_d \beta_d + \tilde{Z}_d u_d, I_n),$$

which brings us back to a normal model of the form in (7). By computing the corresponding $g$-prior (10), we arrive at the generalised $g$-prior

$$\beta_d | g \sim N_1(0_n, gI_0^{-1})$$

(27)
with prior precision matrix proportional to

\[
J_0 = \tilde{X}_d^T (I_n + \tilde{Z}_d D_d \tilde{Z}_d^T)^{-1} \tilde{X}_d
= X_d^T W_0^{1/2} (I_n + W_0^{1/2} Z_d D_d Z_d^T W_0^{1/2})^{-1} W_0^{1/2} X_d.
\] (28)

An appealing feature of this prior is that it directly generalises the $g$-prior proposed by Sabanés Bové and Held (2011a) for generalised linear models, to which it reduces when there are no spline effects in the model, i.e. $J_0 = X_d^T W_0 X_d$. An alternative and more rigorous derivation of (28) as the Fisher information obtained from a Laplace approximation to the marginal model $f(y \mid \beta_0, \beta_d)$ is presented in the supplementary material available at Biometrika online.

The generalised hyper-$g$ prior

\[
f(\beta_0, \beta_d, u_d, g) = f(\beta_0) f(\beta_d \mid g) f(g) f(u_d)
\] (29)

is defined to comprise the locally uniform prior $f(\beta_0) \propto 1$ on the intercept $\beta_0$, the generalised $g$-prior (27) on the linear coefficient vector $\beta_d$, the penalty prior (20) on the spline coefficient vector $u_d$, and some proper hyper-prior $f(g)$ on the hyper-parameter $g$. Posterior inference under this prior can be implemented by a straightforward extension of the approach of Sabanés Bové and Held (2011a, section 3), which is outlined in the following. The efficient R-package “hypergsplines” for this and all other computations in this paper is available from R-Forge.\(^1\)

Let $X_a = (1_n, X_d, Z_d)$ and $\beta_a = (\beta_0, \beta_d^T, u_d^T)^T$ denote the grand design matrix and regression coefficient vector, respectively, such that $\eta = X_a \beta_a$. The prior for $\beta_a$ conditional on $g$ has a Gaussian form with mean zero and singular precision matrix $\text{diag} \{0, g^{-1} J_0, D_d^{-1}\}$. Thus, the Gaussian approximation of $f(\beta_a \mid y, g, d)$, which is necessary for the Laplace approximation of $f(y \mid g, d)$, can be obtained by the Bayesian IWLS algorithm (West, 1985). Afterwards, an approximation of the marginal likelihood of model $d$,

\[
f(y \mid d) = \int_0^\infty f(y \mid g, d) f(g) \, dg,
\] (30)

\(^1\)The website is \url{http://hypergsplines.r-forge.r-project.org/}. To install the R-package, just type \texttt{install.packages("hypergsplines",repos="http://r-forge.r-project.org")} into R.
is obtained by numerical integration of the Laplace approximation $\tilde{f}(y \mid g, d)$. Note that recently integrated Laplace approximations have successfully been applied in a more general context (Rue, Martino, and Chopin, 2009). Finally, we can use a tuning-free Metropolis-Hastings algorithm to sample from the joint posterior of $\beta_a$ and $g$ in a specific model $d$.

### 4. Model Prior and Stochastic Search

We propose a prior $f(d)$ on the model space $D^p$ which explicitly corrects for the multiplicity of testing inherent in the simultaneous analysis of the $p$ covariates (see Scott and Berger, 2010): *A priori*, the number of covariates included in the model ($I$) is uniformly distributed on $\{0, 1, \ldots, p\}$. The choice of the $I$ covariates is then uniformly distributed on all possible configurations, and their degrees of freedom are independent and uniformly distributed on $D \setminus \{0\} = \{1, 2, 3, \ldots, K\}$. Altogether, this gives

$$1/f(d) = (p + 1) \binom{p}{I} K^I. \quad (31)$$

A nice property of this prior is that it leads to marginal prior probabilities $P(d_j = 0) = P(d_j > 0) = 1/2$. Elsewhere this is often achieved by assigning independent priors to the $p$ covariates, which implies that averaged over all models, $I \sim \text{Bin}(p, 1/2)$. It is clear that our uniform prior on $I$ allows the data $y$ to have a maximum effect on the posterior of $I$ because it is the reference prior (Bernardo, 1979). Note that this prior actually favours models with high or low numbers of covariates, as there are fewer such models. This or similar model priors have been used in a number of previous papers, including e.g. George and McCulloch (1993), Panagiotelis and Smith (2008) and Ley and Steel (2009).

Alternatively, one might also use a fixed (independent of $K$) prior probability for a linear effect ($d_j = 1$). This is appropriate for the situation where one explicitly wants to test linearity versus nonlinearity of each effect. Furthermore, a multiplicity correction for these tests can be implemented by assuming that the number of smoothly included covariates ($J$) is uniformly distributed on $\{0, 1, \ldots, I\}$ and their choice is uniform on all possible choices. This would add one level to the prior hierarchy.
As the model space $\mathcal{D}^p$ grows exponentially in the number of covariates $p$, only for small values of $p$ all possible models can be evaluated. Otherwise the marginal likelihoods $f(y \mid d)$ and posterior model probabilities $f(d \mid y) \propto f(y \mid d) f(d)$ can be computed only for a subset of the model space. Usually this subset is determined by stochastic search procedures. Here we propose to use a simple Metropolis-Hastings algorithm with two possible move types in the proposal kernel:

**Move** Sample a covariate index $j \sim U\{1, 2, \ldots, p\}$ and decrease or increase $d_j$ to the next adjacent value in $D$ (with probability 1/2 each, or deterministically if $d_j = 0$ or $d_j = K$, respectively).

**Swap** Sample a pair $(i, j) \sim U\{(1,1), (1,2), \ldots, (p,p)\}$ of covariate indices ($i \leq j$) and swap $d_i$ and $d_j$.

The ‘Swap’ move is designed to efficiently trace models with high posterior probability even in situations where covariates are almost collinear. For each Metropolis-Hastings iteration, a ‘Move’ is chosen with some fixed probability (we use 3/4), and otherwise a ‘Swap’. Denote the current model by $d$, then the proposed model $d'$ is accepted with probability

$$
\alpha(d' \mid d) = 1 \wedge \frac{f(y \mid d') f(d') q(d' \mid d)}{f(y \mid d) f(d) q(d \mid d')}
$$

where the calculation of the proposal probability ratio $q(d' \mid d) / q(d \mid d')$ is straightforward, see Appendix B.

The advantage of such an MCMC based model exploration compared to more elaborate stochastic search algorithms (e.g. Hans, Dobra, and West, 2007; Clyde, Ghosh, and Littman, 2011) is that it does not preclude estimation of posterior model probabilities via sampling frequencies, as it was originally proposed for MCMC model composition by Madigan and York (1995). Recently reported problems with renormalized probability estimates (Clyde and Ghosh, 2010; García-Donato and Martínez-Beneito, 2011) can be avoided by using the model sampling frequencies instead. Nevertheless, other search procedures might be beneficial when only the maximum a posteriori (MAP) model and not e.g. the marginal posterior inclusion probabilities for the covariates are of interest.
5. Applications

We examine the performance of the proposed additive model selection methodology with a simulation study in Section 5.1, and illustrate logistic regression using the Pima Indian data set in Section 5.2.

5.1. Simulation Study in Additive Models

In order to study the frequentist properties of our approach, we performed a simulation study. The full details are provided as supplementary material which is available at Biometrika online. Here we summarise the main results.

Three different true models were simulated: The first model (“null”) was the null model with \( p = 20 \) nuisance covariates. The second model (“small”) also had \( p = 20 \) covariates of which 3 had a linear effect and 3 had a nonlinear (quadratic, sine, and skew-normal density) effect. Correlations of different strength were generated between some of the covariates. The third model (“large”) was identical to the second model, but included additional 80 nuisance covariates, which were independent of the first 20 covariates. For the “small” and “large” model, one covariate was chosen to be a surrogate for the true, quadratic, effect of another covariate. It masks the quadratic effect if only linear effects can be fitted by a variable selection algorithm. For three different sample sizes \( n = 50, 100, 1000 \), and for the three different true models, we simulated \( n \) observations from the Gaussian additive model (1) with \( \beta_0 = 0 \) and \( \sigma^2 = 0.2^2 \). This was repeated 50 times for each combination of model and sample size, in order to assess the sampling variability.

We applied the proposed additive model selection approaches to each data set, using the hyper-\( g \) and hyper-\( g/n \) priors. As the computational complexity of the marginal likelihood (12) is cubic in the spline basis dimension \( K \) (see Appendix A), we want to use splines with few, quantile-based knots. Therefore, we choose cubic O’Sullivan splines (Wand and Ormerod, 2008). Here, we got basis matrices \( Z_j \) with \( K = 8 \) columns from 6 inner knots at the septiles. We applied the stochastic search algorithm described in Section 4 with \( 10^6 \) iterations.

We compared the results with those from pure variable selection including only linear functions, Bayesian FPs (Sabanés Bové and Held, 2011b), spike-and-slab function
Concerning discovery of the true set of influential covariates, the additive model selection procedures introduced in this paper were very competitive with the considered alternative methods, as is illustrated in Table 1. In particular, they showed clear advantages in the case of small and moderate sample sizes. Using splines instead of only linear functions proved essential for the discovery of the masked quadratic effect and hence convergence to the true model.

Variable inclusion performance did not differ substantively with respect to sensitivity, specificity and area under the ROC curve between the considered methods, with the exception of a slightly worse performance of the two linear methods. However, as shown in Table 2, the hyper-\(g\) and hyper-\(g/n\) spline methods were clearly better in distinguishing truly effective covariates from highly correlated nuisance covariates. Moreover, for small sample sizes, they outperformed the other nonlinear methodologies concerning discovery of the masked quadratic effect. In this task the merely linear methods obviously failed.

Concerning the average mean squared errors of the model-averaged posterior mean function estimates \(\hat{m}_j(x_j)\), the proposed additive model selection procedures were very competitive. They performed well or better than the best compared method each, as is shown in Table 3. It is interesting that the hyper-\(g\) splines were slightly but

|                                | null \(n = 50, 100, 1000\) | small \(n = 50, 100, 1000\) | large \(n = 50, 100, 1000\) |
|--------------------------------|-----------------------------|-----------------------------|-----------------------------|
| Hyper-\(g\) splines            | 83                          | 49                          | 2                           |
| Hyper-\(g/n\) splines          | 86                          | 47                          | 0                           |
| Hyper-\(g\) linear             | 20                          | 0                           | 0                           |
| Hyper-\(g/n\) linear           | 50                          | 0                           | 0                           |
| Bayesian FPs                   | 37                          | 2                           | 0                           |
| Spike-and-slab                 | 89                          | 3                           | 0                           |
| Knot selection                 | 92                          | 0                           | 0                           |

*Table 1 – Median posterior probability of the true model in percentage, when the true model is defined by correct variable inclusion.*
consistently better than the hyper-g/n splines. We also investigated the coverage rates of pointwise 95% credible intervals for the functions, and found that the two proposed methods were slightly conservative.

Finally, the average computational effort of the two proposed additive model selection procedures ranged between one minute for \( n = 100 \) in a “null” data set to about 50 minutes for \( n = 50 \) in a “large” data set.

### 5.2. Pima Indian Diabetes Data

We now apply the generalised additive model selection approach to the logistic regression of \( p = 7 \) potential risk factors on the presence of diabetes in \( n = 532 \) women of Pima Indian heritage (Frank and Asuncion, 2010; Ripley, 1996), see Table 4 for details. We use cubic O’Sullivan splines with 4 inner knots at the quintiles and the generalised hyper-g/n prior, and explore the model space of dimension \( 7^7 = 823543 \) with \( 10^6 \) iterations of the stochastic search algorithm. The computational complexity is higher than for the normal response case, with 95 minutes required for the evaluation of 39 081 models. We validated the results with an exhaustive evaluation of all models, requiring 33 hours. Indeed, the stochastic search found 99% of the posterior probability mass and the 733 top models.

| Method           | small n = 50, 100, 1000 | large n = 50, 100, 1000 |
|------------------|-------------------------|-------------------------|
| Hyper-g splines  | 75 97 98                | 26 100 100 |
| Hyper-g/n splines| 79 97 98                | 20 100 100 |
| Hyper-g linear   | 18 44 87                | 6 26 98     |
| Hyper-g/n linear | 22 48 90                | 17 26 98     |
| Bayesian FPs     | 41 89 68                | 9 92 81     |
| Spike-and-slab   | 30 88 97                | 1 60 97     |
| Knot selection   | 9 78 99                 | 4 13 99     |

*Table 2 – Average difference \( \frac{1}{2}(P_{16} + P_{17}) - \frac{3}{4}(P_{18} + P_{19} + P_{20}) \) of inclusion probabilities \( P_j = P\{m_j(x_j) \neq 0 | y\} \) (in percentage points) between the truly effective covariates \( x_{16} \) and \( x_{17} \) and the nuisance covariates \( x_{18}, x_{19}, x_{20}, \) which had correlation 0.8 with \( x_{16} \) and \( x_{17} \). (The optimal value is 100, the worst value is −100.)*
Table 3 – Average mean squared errors (in $10^{-4}$ units) of function estimates. Numbers are averaged over all covariates and the 50 replications.

| Variable Description | Small $n = 50$, 100, 1000 | Medium $n = 50$, 100, 1000 | Large $n = 50$, 100, 1000 |
|----------------------|--------------------------|---------------------------|---------------------------|
| Hyper-$g$ splines     | 0.03 0.01 0.00           | 39.15 10.32 1.68          | 30.42 1.88 0.33           |
| Hyper-$g/n$ splines   | 0.05 0.01 0.00           | 47.82 18.33 3.20          | 784.44 2.78 0.61          |
| Hyper-$g$ linear      | 0.76 0.14 0.01           | 158.10 133.55 121.97      | 45.11 32.26 24.36         |
| Hyper-$g/n$ linear    | 0.22 0.02 0.00           | 189.57 169.00 120.96      | 378.07 36.23 26.09        |
| Bayesian FPs          | 0.14 0.03 0.00           | 16837.92 3026.61 29.51    | 76.78 356.30 5.80         |
| Spike-and-slab        | 1.90 1.82 0.57           | 80.94 14.00 2.09          | 45.45 8.71 0.81           |
| Knot selection        | 0.03 0.00 0.00           | 180.03 35.29 2.07         | 47.23 29.33 0.78          |

Table 4 – Description of the variables in the Pima Indian diabetes data set.

| Variable $x$ | Description |
|--------------|-------------|
| $y$          | Signs of diabetes according to WHO criteria (Yes = 1, No = 0) |
| $x_1$        | Number of pregnancies |
| $x_2$        | Plasma glucose concentration in an oral glucose tolerance test [mg/dl] |
| $x_3$        | Diastolic blood pressure [mm Hg] |
| $x_4$        | Triceps skin fold thickness [mm] |
| $x_5$        | Body mass index (BMI) [kg/m$^2$] |
| $x_6$        | Diabetes pedigree function |
| $x_7$        | Age [years] |
Table 5 – Marginal posterior inclusion probabilities in the Pima Indian diabetes data set.

|                  | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ | $x_7$ |
|------------------|-------|-------|-------|-------|-------|-------|-------|
| not included ($d_j = 0$) | 0.74  | 0.00  | 0.88  | 0.91  | 0.00  | 0.04  | 0.01  |
| linear ($d_j = 1$)    | 0.07  | 0.48  | 0.06  | 0.04  | 0.11  | 0.26  | 0.00  |
| smooth ($d_j > 1$)    | 0.19  | 0.52  | 0.06  | 0.05  | 0.89  | 0.70  | 0.99  |

In Table 5 the marginal posterior probabilities for linear and smooth inclusion of the covariates are shown. There is clear evidence for inclusion of the covariates $x_2$, $x_5$, $x_6$ and $x_7$, which have posterior inclusion probabilities over 96%. For the other three covariates, the inclusion probability is below 30%. Smooth modelling of the effects of $x_5$, $x_6$ and $x_7$ seems to be necessary, while this is not so clear for $x_2$.

In order to examine the mixing properties of the stochastic search algorithm proposed in Section 4, we compared the results based on starting the MCMC chain from the full model with $d_j = 4$ instead of the previously used null model with $d_j = 0$ ($j = 1, \ldots, p$). The results are very close: for example, the entries in Table 5 differ by at most $2.28 \cdot 10^{-4}$, and the top 500 models which were visited by the chains are identical. These results are an indication that slow mixing is not a problem for the presented stochastic search algorithm.

Figure 1 shows the estimated covariate effects in the MAP model which features a linear term for $x_2$ and smooth terms for $x_5$, $x_6$ and $x_7$. The estimates are obtained from 10 000 MCMC samples. Note that for linear functions $m_j$, the pointwise credible intervals coincide with the simultaneous credible intervals (Besag, Green, Higdon, and Mengersen, 1995, p. 30). This is because all straight lines samples intersect in one point, which is due to the centring of the covariates in (22). Furthermore, we observe that the Chib and Jeliazkov (2001) estimate ($-240.924$, MCMC standard error 0.008) of the log marginal likelihood of the MAP model, which was also computed, is quite close to the integrated Laplace approximation ($-241.01$). This indicates that the integrated Laplace approximation is fairly accurate.

---

2Every 2nd sample was saved after burning the first 1000 iterations, with acceptance rate 67% using two IWLS steps per proposal.
Figure 1 – Estimated covariate effects in the MAP model for the Pima Indian diabetes data set, based on 10 000 MCMC samples: Posterior means (solid lines), pointwise (dashed lines) and simultaneous (dotted lines) 95%-credible intervals are shown.
The results are qualitatively similar to those obtained with a FP modelling approach by Sabanés Bové and Held (2011a, section 5) and with a cubic smoothing spline approach by Cottet et al. (2008, section 3.2). It is interesting that in the earlier work by Yau et al. (2003, section 5.2), a very low posterior inclusion probability (0.07) for $x_6$ was reported for a different subset of the original Pima Indian diabetes data set. If pure variable selection without covariate transformation is considered, as in Holmes and Held (2006, section 2.6) and Sabanés Bové and Held (2011a, section 4), the strong nonlinear effect of $x_7$ is missed completely, and instead $x_1$ gets a higher posterior inclusion probability. This may be a case of a masked nonlinear effect, as was simulated in Section 5.1, and highlights the importance of allowing for nonlinear covariate effects.

6. Postprocessing

Given the list of all possible models $d \in D^p$, or a subset found by the stochastic search procedure described in Section 4, one may consider postprocessing the results.

First, when the main interest lies in variable selection, the models which feature the same covariates can be summarised into a meta-model as follows: The posterior probabilities of the sub-models are summed up to give the posterior probability of the meta-model, and estimates in the meta-model are obtained by averaging the sub-models with weights proportional to their posterior probabilities (see e.g. Hoeting, Madigan, Raftery, and vol. 1999, for model averaging). For example, the best meta-model for the Pima Indian diabetes data includes $x_2$, $x_5$, $x_6$ and $x_7$ and has posterior probability 0.598. The corresponding estimates of the covariate effects are shown in Figure 2. This best meta-model happens to be identical with the median probability meta-model, which features all covariates having marginal posterior inclusion probability greater than 50% (Barbieri and Berger, 2004), cp. Table 5. Similarly, it could be interesting to summarise models which only differ in the degrees of freedom for smooth terms. This would correspond to the situation of testing linearity versus nonlinearity of covariate effects (cp. Section 4).

Second, in order to allow for continuous degrees of freedom, one can optimise the marginal likelihood of the MAP model with respect to the degrees of freedom of the covariates included. That is, an optimisation of $f(y \mid d)$ over the continuous range
Figure 2 – Estimated covariate effects in the best meta-model (and median probability meta-model) for the Pima Indian diabetes data, based on 20,000 samples: Posterior means (solid lines), point-wise (dashed lines) and simultaneous (dotted lines) 95%-credible intervals are shown.
1 < d_i < K + 1 is performed for all covariates included in the MAP model. For example, the MAP configuration for the Pima Indian diabetes data is (0, 1, 0, 0, 3, 2, 4) and the resulting optimised configuration is (0, 1, 0, 0, 3.42, 2.1, 3.74), which increases the log marginal likelihood from −241.01 to −240.86. Although d_5 and d_7 changed considerably in the optimisation, the resulting function estimates are very similar to those from the MAP model in Figure 1 and are hence omitted.

7. Discussion

Our Bayesian approach to simultaneous variable and function selection in generalised regression is based on fixed-dimensional spline bases and penalty-parameter smoothness control. In this respect, it differs from knot-selection approaches such as Smith and Kohn (1996) and Denison et al. (1998). We found that fixed-dimensional spline bases are flexible enough to capture the functional forms we expect (see e.g. Abrahamowicz, MacKenzie, and Esdaile, 1996). Moreover, by using fixed-dimensional smooth components we can constrain a covariate effect to be exactly linear. This enables us to look at posterior probabilities of linear versus smooth inclusion of covariates. Approaches which use variable-dimensional smooth components and select knots, as Denison et al. (1998), cannot fit linear functions.

We are only considering roughness penalties on a fixed grid of values, which scales automatically for each covariate via the degrees of freedom transformation. We found that it is a very useful approximation of a continuous scale, and postprocessing is possible to remove the restriction to the grid values. In the examples we have looked at, the resulting optimised models yielded very similar results compared to the MAP model. In this regard, our approach is close to many popular Lasso-type proposals, which optimise the tuning-parameters on a fixed grid via cross-validation (e.g. Zou and Hastie, 2005). Cantoni and Hastie (2002) propose a likelihood-ratio-type test statistic to compare additive models with different degrees of freedom. Fong, Rue, and Wakefield (2010) use a similar scaling to examine the prior on the degrees of freedom implied by the prior on the variance component in a generalised linear mixed model. They also use O'Sullivan spline bases as we did in our applications, but they do not consider variable selection.
In a frequentist setting, Marra and Wood (2011, section 2.1) propose to use an additional penalty on the linear part of the spline function in order to shrink it adaptively to zero. To include variable selection, a lower threshold for the effective degrees of freedom must be chosen. Our generalised $g$-prior (27) also shrinks the linear parts of the spline functions to zero, where the prior covariance matrix takes the correlations between the covariates into account. Incorporating the covariates correlation in the coefficients prior allows for better discrimination between influential and correlated nuisance covariates. Empirical results from our simulation study in Section 5.1 support this. Furthermore, we explicitly ex- or include covariates and then compare the resulting models based on their posterior probabilities.

We propose a conventional prior for the intercept and the linear coefficients, which directly generalises the hyper-$g$ priors in the linear model (Liang et al., 2008) and in the generalised linear model (Sabanés Bové and Held, 2011a). Pauler (1998) proposes a related unit-information prior for the fixed effects in linear mixed models, but fixes $g = n$ in (10). Overstall and Forster (2010) propose a unit-information prior for the fixed effects in generalised linear mixed models, but the information matrix is based on the first-stage likelihood and not on the integrated likelihood as in our approach. Also, no hyper-prior on the parameter $g$ is considered, because it is fixed at $g = n$. As they use an inverse-Wishart prior on the covariance matrix of the random effects, their approach is perhaps better suited to generic random effects models. Forster, Gill, and Overstall (2012) propose a novel reversible-jump MCMC algorithm to infer the corresponding posterior model probabilities.

In future work, we would like to combine the semiparametric splines with the parametric FPs (Sabanés Bové and Held, 2011b). The idea is that a smooth term $m_j(x_j)$ could also be modelled by a FP instead of a spline. This extension could be implemented coherently, because the prior formulations are compatible. With such a general framework, the important question whether a parsimonious FP (e.g. $m_7 = x_7\beta_7 + x_7^2\beta_7$ in the Pima Indian diabetes data example) is sufficient could be answered via posterior probabilities (see Strasak, Umlauf, Pfeiffer, and Lang (2011) for a simulation study comparing the stepwise FP approach by Royston and Sauerbrei (2008) with penalised spline approaches). Moreover we will apply mixtures of $g$-priors to additive Cox-type survival models.
Appendix

Section A gives details on the computation of the marginal likelihood (12) for normal additive models. Section B derives the proposal probabilities for the stochastic search described in Section 4.

A. Marginal likelihood computation

Under the hyper-$g$ prior, which assumes a uniform prior on the shrinkage coefficient $g/(g + 1)$, the marginal likelihood of the transformed response vector is (Liang et al., 2008)

$$f(\tilde{y} \mid d) \propto \left| V_d^{-T/2}(y - \mathbf{1}_n \bar{y}) \right|^{-(n-1)} (I + 2)^{-1} _2F_1 \left( \frac{n-1}{2}; 1; \frac{I + 4}{2}; \bar{R}_d^2 \right)$$  \hspace{1cm} (32)

where $\bar{y} = \frac{1}{n-1} \sum_{i=1}^n y_i$ is the Gaussian hypergeometric function (Abramowitz and Stegun, 1964, p. 558) and $\bar{R}_d^2$ is the classical coefficient of determination in model (8). Under the hyper-$g/n$ prior, which assumes a uniform prior on the term $(g/n)/(g/n + 1)$, the marginal likelihood in the standard linear model is (Forte, 2011, p. 155)

$$f(\tilde{y} \mid d) \propto n^{-1/2}(1 - \bar{R}_d^2)^{-(n-1)/2} \frac{2}{I+2} \times A_{F_1} \left( \frac{I}{2} + 1; \frac{I + 1 - n}{2}; \frac{n - 1}{2}; \frac{I}{2} + 2; \frac{n - 1}{n}, \frac{n - (1 - \bar{R}_d^2)^{-1}}{n} \right),$$  \hspace{1cm} (33)

where $A_{F_1}$ is the Appell hypergeometric function of the first kind (Appell, 1925). Colavecchia and Gasaneo (2004) provide Fortran code for computing this special function, which is accessible in R via the package “appell” (Sabanés Bové, 2012). For large sample sizes $n > 100$ or when the numerical computations of the special functions in (32) or (33) fail, we instead use Laplace approximations as described by Liang et al. (2008, appendix A).

For the coefficient of determination $\bar{R}_d^2 = SSM_d / SST_d$ required in (32) or (33), we need to compute the sum of squares in total ($SST_d$) and the sum of squares explained
by the model (\(SS_{M_d}\)). For \(SS_{T_d}\), we have

\[
SS_{T_d} = (y - 1_n\bar{y})^T V_{d}^{-1} (y - 1_n\bar{y}) = \|y - 1_n\bar{y}\|^2 - \|W_{d}^T (y - 1_n\bar{y})\|^2.
\]

Note that the first term in (12) can be written as

\[
\|V_{d}^{-T/2} (y - 1_n\bar{y})\|^{-(n-1)} = SS_{T_d}^{-(n-1)/2}.
\]

For \(SS_{M_d}\), note that the fit of the general linear model is \(\hat{y}_{d} = 1_n\bar{y} + X_d\hat{\beta}_d\), where

\[
\hat{\beta}_d = (X_d^T V_{d}^{-1} X_d)^{-1} X_d^T V_{d}^{-1} y
\]

is the weighted least squares estimate of \(\beta_d\). Therefore

\[
SS_{M_d} = (\hat{y}_d - 1_n\bar{y})^T V_{d}^{-1} (\hat{y}_d - 1_n\bar{y}) = \hat{\beta}_d^T X_d^T V_{d}^{-1} X_d \hat{\beta}_d
\]

can be computed by Cholesky factorising \(X_d^T V_{d}^{-1} X_d = C_d^T C_d\), solving the triangular system \(C_d^T v_d = X_d^T V_{d}^{-1} y\) and setting \(SS_{M_d} = \|v_d\|^2\).

For the computations above, we need the inverse of the covariance matrix \(V_{d} \in \mathbb{R}^{n \times n}\). While usually a Cholesky factorisation would be done, here it is advisable to avoid it because it has complexity \(O(n^3)\) and is therefore computationally expensive. Therefore, we instead work with the formula

\[
V_{d}^{-1} = I_n - Z_d M_{d}^{-1} Z_d^T
\]

for the precision matrix, where \(M_d = Z_d^T Z_d + D_d^{-1}\). The latter matrix has dimension \(JK\), which is usually smaller than \(n\), provided the spline basis dimension \(K\) is small. Thus, the Cholesky factorisation \(M_d = M_d^{1/2} M_d^{1/2}\) is relatively fast, and we compute \(W_d = Z_d M_d^{-1/2}\) such that \(V_{d}^{-1} = I_n - W_d W_d^T\).

Finally, to compute the determinant term in (12), we can again avoid factorising \(V_d\), because we have

\[
\left|V_{d}^{1/2}\right|^{-1} = \left|V_{d}^{-1}\right|^{1/2} = \left|I_n - W_d W_d^T\right|^{1/2} = \left|I_{JK} - W_d^T W_d\right|^{1/2},
\]

see Harville (1997, p. 416) for the last equality. So again only a matrix of dimension \(JK\), namely \(I_{JK} - W_d^T W_d\), needs to be factorised. Here, a LU factorisation can be used.
B. Proposal probabilities

First note that the two proposal types 'Move' and 'Swap' do not overlap, because a 'Move' always changes exactly one \( d_j \), while a 'Swap' either changes none or two \( d_j \)'s. Denote with \( p_m \) the probability to choose a 'Move'.

Suppose a 'Move' was proposed for covariate \( j \in \{0, 1, \ldots, p\} \). We then have

\[
q(d' \mid d) = p_m \cdot \frac{1}{p} \begin{cases} 
1, & d_j \in \{0, K\}, \\
\frac{1}{2}, & \text{else}
\end{cases}
\]

and analogously

\[
q(d \mid d') = p_m \cdot \frac{1}{p} \begin{cases} 
1, & d'_j \in \{0, K\}, \\
\frac{1}{2}, & \text{else}
\end{cases}
\]

with proposal ratio

\[
\frac{q(d' \mid d)}{q(d \mid d')} = \begin{cases} 
\frac{1}{2}, & d'_j \in \{0, K\}, \\
2, & d_j \in \{0, K\}, \\
1, & \text{else}.
\end{cases}
\]

For the 'Swap' proposal, suppose covariates \( i \) and \( j \) are proposed to interchange their model parameters \( d_i \) and \( d_j \). Of course, if \( d_i = d_j \), then the proposal ratio equals unity because \( d' = d \). In the other case, both model parameters are changed, and

\[
q(d' \mid d) = q(d \mid d') = (1 - p_m) \cdot \left( \frac{p}{2} \right)^{-1},
\]

so that for a 'Swap' we always have \( q(d' \mid d) / q(d \mid d') = 1 \).

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