Regression modelling with I-priors
With applications to functional, multilevel, and longitudinal data

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Abstract

We introduce the I-prior methodology as a unifying framework for estimating a variety of regression models, including varying coefficient, multilevel, or longitudinal models, and models with functional covariates and responses. It can also be used for multi-class classification, with low or high dimensional covariates. Predictive performance for real data sets is competitive.

The I-prior is generally defined as a maximum entropy prior. For a regression function, the I-prior is Gaussian with covariance kernel proportional to the Fisher information on the regression function, which is estimated by its posterior distribution under the I-prior. The I-prior has the intuitively appealing property that the more information is available on a linear functional of the regression function, the larger the prior variance, and the smaller the influence of the prior mean on the posterior distribution.

Advantages compared to competing methods, such as Gaussian process regression or Tikhonov regularization, are ease of estimation and model comparison. In particular, we develop an EM algorithm with a simple E and M step for estimating hyperparameters, facilitating estimation for complex models. We also propose a novel parsimonious model formulation, requiring a single scale parameter for each (possibly multidimensional) covariate and no further parameters for interaction effects. This simplifies estimation because fewer hyperparameters need to be estimated, and also simplifies model comparison of models with the same covariates but different interaction effects; in this case, the model with the highest estimated likelihood can be selected.

As we show, natural spaces for the regression functions used for I-prior modelling are reproducing kernel Krein spaces (RKKs). These spaces do not have the positive definiteness restriction of reproducing kernel Hilbert spaces, which yields a computational advantage. An R-package implementing our methodology is available (Jamil, 2019).

Keywords: reproducing kernel, RKHS, RKK, Fisher information, objective prior, empirical Bayes, regression, supervised learning, statistical learning, longitudinal data analysis, nonparametric regression, functional data analysis, multilevel models, classification.

1 Introduction

Consider a sample \((x_1, y_1), \ldots, (x_n, y_n)\), where \(y_i\) is a real-valued measurement on unit \(i\), and \(x_i = (x_{i1}, \ldots, x_{ip})\) is a row vector of \(p\) covariates, where each each \(x_{ik}\) belongs to some set \(\mathcal{X}_k\) and may for example be real, categorical, multidimensional, or functional. To describe the dependence of the \(y_i\) on the \(x_i\), we consider the regression model

\[
y_i = f(x_i) + \varepsilon_i, \quad f \in \mathcal{F}
\]

(1)
where $\mathcal{F}$ is a space of functions. We assume the errors have a multivariate normal distribution, i.e.,
\[
(\varepsilon_1, \ldots, \varepsilon_n) \sim \text{MVN}(0, \Psi^{-1}),
\]
where $\Psi = (\psi_{ij})$ is an $n \times n$ positive definite precision matrix. Here, $\Psi$ is taken to be known up to a low dimensional parameter, e.g., $\Psi = \psi I_n$ ($\psi > 0$, $I_n$ the $n \times n$ identity matrix), reflecting i.i.d. errors.

The function $f$ is assumed to be partitioned into a sum of main effects and possible interactions. An example for $p = 2$ is
\[
f(x) = f(x_1, x_2) = \alpha + f_1(x_1) + f_2(x_2) + f_{12}(x_1, x_2),
\]
and for $p = 3$,
\[
f(x) = f(x_1, x_2, x_3) = \alpha + f_1(x_1) + f_2(x_2) + f_3(x_3) + f_{12}(x_1, x_2) + f_{23}(x_2, x_3).
\]
Here, each of the $x_k$ may be, for example, scalar, categorical, Euclidean, or functional. As we outline in Section 3, this setup can be used to formulate a wide variety of parametric and nonparametric models, including multilevel, varying coefficient, functional, longitudinal, and multi-class classification models.

To give a simple example, if $f_1(x_1) = x_1 \beta_1$ for some constant $\beta_1$, and $f_{12}(x_1, x_2) = x_1 \beta_{12}(x_2)$ for some function $\beta_{12}$, we can rewrite (3) as
\[
f(x_1, x_2) = \alpha + x_1 \beta_1 + f_2(x_2) + x_1 \beta_{12}(x_2) = (\alpha + f_2(x_2)) + x_1 (\beta_1 + \beta_{12}(x_2))
\]
(5)
If $x_2$ is categorical, this yields the familiar parametric two-level linear model, where $\alpha + f_2(x_2)$ and $\beta_1 + \beta_{12}(x_2)$ are the intercept and slope for “group” $x_2$. If on the other hand $x_2$ is Euclidean, the model is more usually referred to as the nonparametric varying coefficient model (Hastie & Tibshirani, 1993), where $\alpha + f_2(x_2)$ and $\beta_1 + \beta_{12}(x_2)$ are the intercept and slope of the model, both of which are assumed to vary smoothly with $x_2$. More simply, if $x_2$ in (5) is real and $f_2(x_2) = x_2 \beta_2$ and $\beta_{12}(x_2) = x_2 \beta_{12}$ for some constants $\beta_2$ and $\beta_{12}$, we obtain the multiple regression model with an interaction,
\[
f(x_1, x_2) = \alpha + x_1 \beta_1 + x_2 \beta_2 + x_1 x_2 \beta_{12}
\]
These three models are usually estimated with different methods. For the two-level model, a typical assumption might be that the pairs $\{(\beta_1, \beta_{12}(x_2))|x_2 \in \mathcal{X}_2\}$ are i.i.d. bivariate normal, so that $f$ can be estimated by its posterior mean. For the varying coefficient model, typically a penalized least squares procedure is used, with a penalty such as $\int_{\mathcal{X}_2} \beta_{12}(t)^2 dt$, where $\beta_{12}$ is the second derivative of $\beta_{12}$. For the multiple regression model, $f$ is typically estimated using the maximum likelihood method. In this paper, we propose instead to use a single methodology, which can also be used for a wide range of extensions to these models.

### 1.1 Estimation

The aforementioned examples illustrate the three most popular existing techniques for estimating $f$ in (1) subject to (2), namely maximum likelihood (ML – equivalent to generalized least squares), Tikhonov regularization and Gaussian process (GP) regression (note a random coefficient model is not usually thought of as a GP regression, but since $f$ is assumed Gaussian,
it can be considered as such). Maximum likelihood estimation is equivalent to minimizing the generalized least squares criterion

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{ij}(y_i - f(x_i))(y_j - f(x_j))
\]

in terms of \( f \in \mathcal{F} \). It is only suitable if the dimension of \( \mathcal{F} \) is small compared to the sample size \( n \), and Tikhonov regularization and GP regression are much more generally applicable. The Tikhonov regularizer minimizes the penalized generalized least squares functional

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{ij}(y_i - f(x_i))(y_j - f(x_j)) + \tau \|f\|_F^2
\]  

(6)

where \( \|f\|_F \) is the norm of \( f \) and \( \tau \) a positive smoothing parameter. In GP regression, a Gaussian prior is assumed for \( f \), which is estimated by its posterior distribution, which is also Gaussian. The latter two methods are closely connected, in that Tikhonov regularizers have an interpretation as posterior means in GP regression (Kimeldorf & Wahba, 1970, Rasmussen & Williams, 2006, Section 6.2). Nevertheless, they differ in that Tikhonov regularization is based on a function space view of regression, while Gaussian process regression is probabilistic model-based, in that the user chooses a probabilistic model for the regression function.

This paper introduces the I-prior methodology for estimating \( f \) in (1) subject to (2) as an alternative to the aforementioned methods. Hence, like Tikhonov regularization, it is based on a function space view of regression. We derive the I-prior as a maximum entropy prior subject to a constraint based on the Fisher information. The I-prior for \( f \) is Gaussian, with mean chosen a priori (e.g., zero), and covariance kernel proportional to the Fisher information on \( f \). The regression function is estimated by its posterior distribution under the I-prior, with the posterior mean as a suitable point estimator. An intuitively attractive property of the I-prior is that the more information is available on a linear functional of the regression function (e.g., a regression coefficient), the larger the prior variance, and the smaller the influence of the prior mean on the posterior mean. The I-prior methodology can be viewed as contributing to the field of statistical supervised learning (Hastie, Tibshirani, & Friedman, 2009), where prediction, estimation and inference are some of the key aims.

1.2 ANOVA RKKS and its (hyper)parameters

To specify the space of regression functions \( \mathcal{F} \), we adopt the so-called ANOVA kernel construction (Wahba, 1990a; Gu, 2013), which can suitably encode interaction effects. A kernel provides a set of basis functions for a function space. Each covariate is assigned a positive definite kernel, and an ANOVA kernel representing main and interaction effects is obtained by taking a sum of tensor products of these kernels. Each kernel is multiplied by a scale parameter, to take into account the arbitrary measurement scale of any covariate. An ANOVA kernel with non-negative scale parameters is positive definite, and hence defines a reproducing kernel Hilbert space (RKHS). This allows, for example, the RKHS norm to be used in (6). Alternatively, a positive definite kernel can be used as a covariance kernel in GP regression. In the present paper we allow negative scale parameters, so that the ANOVA kernel may become indefinite, and defines a reproducing kernel Krein space (RKKS) of regression functions. Even if some scale parameters are negative, the Fisher information on the regression remains positive definite, so that the I-prior is well-defined. In the present context, restricting the scale parameters to be positive would be arbitrary and unnecessary.
A key challenge is estimating these scale parameters and any other possible hyperparameters of the kernels and of the error covariance matrix. In Tikhonov regularization, the hyperparameters are typically obtained by minimizing some cross-validation criterion, such as the generalized cross-validation criterion of Craven and Wahba (1979). In GP regression, they can be estimated by empirical or hierarchical Bayes methods (Rasmussen & Williams, 2006). In this paper we take an empirical Bayes approach, and estimate any hyperparameters of the I-prior and of the error distribution using the maximum marginal likelihood method. Of course, a fully Bayes approach is also possible in the I-prior setting, but it seems difficult to choose suitable priors for the scale parameters. Empirical Bayes has the advantage of being “automatic”, in the sense that the user need not choose hyperpriors. Furthermore, we found it leads to good predictive performance for various data sets.

Especially if there are a large number of hyperparameters, it can become very difficult to estimate these by directly minimizing a cross-validation criterion or maximizing the marginal likelihood using a gradient method, because these objective functions can be highly non-convex or non-concave (see Figure 2 in Bergsma (2020) illustrating that this can be so for the marginal likelihood even when there are only two hyperparameters). A major computational advantage of the I-prior methodology is that, as we show, it is possible to construct an EM algorithm with simple E and M steps for estimating the scale parameters of the ANOVA kernel and any parameters of the error covariance matrix. In contrast, for GP regression, the M step is computationally as complex as maximizing the marginal likelihood directly, making EM an unattractive option. Because of the small radius of convergence of Fisher scoring and Newton-Raphson, we often found it impossible with these methods to find the global maximum of the marginal likelihood. Even when starting with EM and switching to Fisher scoring, we found it to be numerically less stable than EM (see Bergsma, 2020, Section 6.1, for an explanation of the numerical problems evaluating the marginal likelihood).

A brief remark may be worthwhile to clarify the types of parameters involved in this paper. For model (1), the main parameters of interest are \( f \) and/or linear functionals of \( f \), such as regression coefficients or components of \( f \) such as in (3) or (4). The error precision matrix \( \Psi \) (assumed to have a low-dimensional parameterization) is treated as a nuisance parameter in this paper. The aforementioned scale parameters and any possible kernel parameters are hyperparameters of \( F \), and determine its topology. The I-prior for \( f \) is a function of the model, and has as hyperparameters the scale parameters, any kernel parameters, and \( \Psi \).

### 1.3 Parsimonious model specification

Apart from the I-prior estimation method, a second main innovation in this paper is a parsimonious specification of models with interaction effects (see Section 2.3.2). This idea is very simple but as far as we are aware has not been adopted before, and can also be applied in the context of Tikhonov regularization or Gaussian process regression. In particular, we only use a single scale parameter for each covariate, and no further parameters for any interaction effects. This is in contrast with the usual approach, where separate scale parameters are assigned to each interaction effect. The main role of the scale parameters is to ensure invariance to the measurement units of to covariates, and this is achieved without having separate parameters for interaction effects. Our parsimonious approach greatly simplifies the estimation of models with interaction effects, in particular because we found that the number of possible local maxima of the marginal likelihood increases rapidly with the number of scale parameters. This can make it extremely difficult to find the global maximum if there are many scale parameters. A second advantage of our parsimonious approach is that it allows a semi-Bayes approach to the selection of interaction effects, potentially able to detect effects with smaller sample sizes than with existing approaches. That is, model selection among models with the same main effects can be
done simply be choosing the model with the highest estimated marginal likelihood (examples are given in Sections 6.3 and 6.4).

1.4 Unifying methodology for regression

A third contribution of this paper is that we show that a wide variety of models, including multilevel, longitudinal, varying coefficient, and models with functional covariates and/or responses, can be formulated within the ANOVA framework and estimated with a single method. An advantage is that this makes it potentially easier to formulate models in software, for example, all models in this paper can be fitted using similar code in the R-package `iprior` (Jamil, 2019). Furthermore, the unified approach immediately suggests models not previously considered, such as models with interactions between functional, Euclidean, and qualitative covariates. The practical feasibility of this is enhanced because estimation of models is greatly simplified by the EM algorithm and the parsimonious use of scale parameters.

1.5 Overview of paper and relation to previous work

In Section 2, a summary of existing theory of RKHSs and RKKSs including ANOVA RKKSs is given as needed for this paper. To illustrate their use in regression modelling, we describe in Section 3 how a number of well-known models can be described using the ANOVA RKKS framework. In Section 4, the I-prior is defined for model (1) with multivariate normal errors. In Section 5, the posterior distribution of the regression function under the I-prior is given and an EM algorithm for estimating scale parameters is described. In Section 6, we apply the I-prior methodology to a number of data examples in the respective areas of functional data analysis, classification, multilevel modelling, and longitudinal data analysis, illustrating some possible advantages over existing techniques, and showing competitive predictive performance. In Section 7 we briefly compare the I-prior methodology with competing methods, and the paper concludes with a discussion in Section 8.

The present paper complements Bergsma (2020), which covers the case of a single, possibly multidimensional covariate. In this case there is a single scale parameter, and the RKHS framework suffices, whereas in the present paper we require the possibly indefinite reproducing kernel Krein spaces. In that paper, more details are given on the I-prior derivation, and a generalization of I-priors to a broad class of statistical models is given in the appendix. The relation with competing methods is outlined, including $g$-priors, Jeffreys and reference priors, and Fisher kernels. A detailed comparison with Tikhonov regularization is given, with particular detail on the relation with cubic spline smoothing. It is explained how I-priors work when the regression functions are linear, or when they are assumed to lie in the fractional Brownian motion RKHS, and it is explained in some detail why this is a particularly attractive RKHS for I-prior modelling.

Jamil (2018) provides a number of extensions to the present methodology, including probit and logit models using a fully Bayes approach, Bayesian variable selection using I-priors, and Nyström approximations for speeding up the I-prior methodology. Furthermore, he contributed a user friendly R package `iprior` (Jamil, 2019), further described in Jamil and Bergsma (2019).

2 Function spaces with reproducing kernels

This section summarizes existing theory as needed for this paper. In Section 2.1 we give the definition and some well-known basic properties of RKHSs and RKKSs. Section 2.2 briefly lists the RKHSs used in this paper. These RKHSs are used as building blocks to construct RKKSs
over product spaces, called ANOVA RKKSs, which is the topic of the next Section 2.3. The RKHSs we use in this paper will be centered, i.e., the functions in the RKHS have zero mean, which is described in Section 2.4. The reason for centering is that it ensures identification of components of a regression function such as in (3) and (4).

2.1 Definitions and basic properties

The first comprehensive treatment of RKHSs was given by Aronszajn (1950), and their usefulness for statistics was initially demonstrated by Parzen (1961) and further developed by Kimeldorf and Wahba (1970). Some more recent overviews of RKHS theory with a view to application in statistics and machine learning are Wahba (1990b), Berlinet and Thomas-Agnan (2004), Steinwart and Christmann (2008, Chapter 4) and Hofmann, Schölkopf, and Smola (2008). Schwartz (1964) developed a general theory of Hilbertian subspaces of topological vector spaces which includes the theory of RKKSs. The first applications to statistics and machine learning of RKKSs were given by Ong, Mary, Canu, and Smola (2004) and Canu, Ong, and Mary (2009). A recent technical survey of the theory of RKKSs is given by Gheondea (2013). Below, we give a very brief overview of the theory as needed for this paper, more details can be found in the aforementioned literature.

We begin with the definition of the (possibly indefinite or negative definite) inner product.

**Definition 1.** Let \( \mathcal{F} \) be a vector space over the reals. A function \( \langle \cdot, \cdot \rangle_{\mathcal{F}} : \mathcal{F} \times \mathcal{F} \to \mathbb{R} \) is called an inner product on \( \mathcal{F} \) if, for all \( f, f', f'' \in \mathcal{F} \),

- (symmetry) \( \langle f, f' \rangle_{\mathcal{F}} = \langle f', f \rangle_{\mathcal{F}} \)
- (linearity) \( \langle \alpha f + f', f'' \rangle_{\mathcal{F}} = \alpha \langle f, f'' \rangle_{\mathcal{F}} + \langle f', f'' \rangle_{\mathcal{F}} \)
- (nondegeneracy) \( (\forall g \in \mathcal{F} : \langle f, g \rangle_{\mathcal{F}} = 0) \Rightarrow f = 0 \)

If \( \langle f, f \rangle_{\mathcal{F}} \geq 0 \) for all \( f \in \mathcal{F} \), the inner product is called positive definite and \( \|f\|_{\mathcal{F}} := \langle f, f \rangle_{\mathcal{F}} \) is called a norm on \( \mathcal{F} \). If \( \langle f, f \rangle_{\mathcal{F}} \leq 0 \) for all \( f \in \mathcal{F} \), the inner product is called negative definite. An inner product which is neither positive definite nor negative definite is called indefinite.

Recall that a Hilbert space is a complete inner product space with a positive definite inner product. The more general notion of Krein space is defined as follows.

**Definition 2.** A vector space \( \mathcal{F} \) equipped with the inner product \( \langle \cdot, \cdot \rangle_{\mathcal{F}} \) is called a Krein space if there are two Hilbert spaces \( \mathcal{F}_+ \) and \( \mathcal{F}_- \) spanning \( \mathcal{F} \) such that

- All \( f \in \mathcal{F} \) can be decomposed as \( f = f_+ + f_- \) where \( f_+ \in \mathcal{F}_+ \) and \( f_- \in \mathcal{F}_- \).
- For all \( f, f' \in \mathcal{F} \), \( \langle f, f' \rangle_{\mathcal{F}} = \langle f_+, f'_+ \rangle_{\mathcal{F}_+} - \langle f_-, f'_- \rangle_{\mathcal{F}_-} \)

Note that any Hilbert space is a Krein space, which can be seen by taking \( \mathcal{F}_- = \{0\} \).

We next define the notion of a reproducing kernel:

**Definition 3.** Let \( \mathcal{F} \) be a Krein space of functions over a set \( \mathcal{X} \). A symmetric function \( h : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) is a reproducing kernel of \( \mathcal{F} \) if and only if

1. \( h(x, \cdot) \in \mathcal{F} \) for all \( x \in \mathcal{X} \)
2. \( f(x) = \langle f, h(x, \cdot) \rangle_{\mathcal{F}} \) for all \( f \in \mathcal{F} \) and \( x \in \mathcal{X} \).
A Hilbert space resp. Krein space is called a reproducing kernel Hilbert space (RKHS) resp. reproducing kernel Krein space (RKKS) if it possesses a reproducing kernel. Sometimes in this paper we will use the shorthand ‘kernel’ to refer to ‘reproducing kernel’.

A function \( h : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) is said to be positive definite on \( \mathcal{X} \) if \( \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j h(x_i, x_j) \geq 0 \) for all scalars \( \alpha_1, \ldots, \alpha_n \) and all \( x_1, \ldots, x_n \in \mathcal{X} \). From the definition of positive definite inner products it follows that the reproducing kernel of an RKHS is symmetric and positive definite. The reproducing kernel of an RKKS can be shown to be the difference of two positive definite kernels so need not be positive definite. It follows that an inner product in an RKKS (\( \mathcal{F}(\cdot, \cdot)_{\mathcal{F}} \)) is the difference of two positive definite inner products

\[
     \langle f, f' \rangle_{\mathcal{F}} = \langle f, f' \rangle_{\mathcal{F}^+} - \langle f, f' \rangle_{\mathcal{F}^-}
\]

We define the norm of \( f \in \mathcal{F} \) as the norm in the corresponding RKHS, i.e.,

\[
     \|f\|_{\mathcal{F}}^2 = \|f\|_{\mathcal{F}^+}^2 + \|f\|_{\mathcal{F}^-}^2
\]

The Moore-Aronszajn theorem states that every symmetric positive definite function defines a unique RKHS. Every RKKS also has a unique kernel, but a given kernel may have more than one RKKS associated with it (e.g., Alpay, 1991).

### 2.2 Some useful RKHSs

Below we describe some RKHSs that we will use in this paper. A summary is given in Table 1.

#### 2.2.1 RKHS of constant functions

The RKHS of constant functions with reproducing kernel given by \( h(x, x') = 1 \). For a constant function \( f \) with \( f(x) = c \), \( \|f\|_{\mathcal{F}} = |c| \). (The RKHS of constant functions will be an essential component in the construction of RKKSs over product spaces in Section 2.3.1.)

#### 2.2.2 RKHSs over finite sets

Let \( \mathcal{X} \) be a finite set. The canonical RKHS over \( \mathcal{X} \) is the RKHS whose kernel is the Kronecker delta function, i.e., \( h(x, x') = \delta_{x,x'} \) consists of the set of all functions \( f : \mathcal{X} \to \mathbb{R} \), with squared norm

\[
     \|f\|_{\mathcal{F}}^2 = \sum_{x \in \mathcal{X}} f(x)^2.
\]

Table 1: List of RKHSs. Here, \( \delta \) is the Kronecker delta, \( p(x) \) is the proportion of the sample equal to \( x \), and \( S \) is the sample covariance matrix. Note that only the kernel for the FBM-\( \gamma \) RKHS has a hyperparameter.

| \( \mathcal{X} \)          | RKHS                  | Functions \( f(x) \) | Kernel \( h(x, x') \)          | Centered kernel                                      |
|---------------------------|-----------------------|-----------------------|--------------------------------|------------------------------------------------------|
| Any set                   | Constant              | Constant functions    | 1                              | -                                                   |
| Finite set                | Canonical             | All functions         | \( \delta_{x,x'} \)             | \( \delta_{x,x'} - p(x) - p(x') + \sum_{t \in \mathcal{X}} p(t)^2 \) |
| Finite set                | Pearson               | All zero mean functions | \( \delta_{x,x'}/p(x) - 1 \) | \( \delta_{x,x'}/p(x) - 1 \) |
| Hilbert space             | Canonical             | \( \langle x, \beta \rangle_{\mathcal{X}} \) | \( \langle x, x' \rangle_{\mathcal{X}} \) | (\( x - \bar{x}, x' - \bar{x} \))_{\mathcal{X}} |
| \( \mathbb{R}^p \)       | Mahalanobis           | \( x^\top \beta \)   | \( x^\top S^{-1}x' \)          | (\( x - \bar{x} \))^\top S^{-1}(x' - \bar{x}) |
| \( \mathbb{R} \)         | Brownian motion       | \( f_x \sim \beta(t)dt \) | \( \frac{1}{2}(|x| + |x'| - |x - x'|) \) | Eq. (13) (\( \gamma = 1/2 \)) |
| Hilbert space             | Brownian motion       | Hölder \( \geq 1/2 \) | \( \frac{1}{2}(|x| + \|x'\| - \|x - x'\|) \) | Eq. (13) (\( \gamma = 1/2 \)) |
| Hilbert space             | FBM-\( \gamma \)      | Hölder \( \geq \gamma \) | \( \frac{1}{2}(\|x\|^2 + \|x'\|^2 - \|x - x'\|^2) \) | Eq. (13) |


Note that, viewing $f$ as a $|\mathcal{X}|$-dimensional vector, the canonical RKHS over $\mathcal{X}$ is just standard Euclidean space.

Alternatively, the Pearson RKHS over a finite probability space $(\mathcal{X},p)$ is defined as the RKHS with reproducing kernel
\[ h(x, x') = \left\{ \begin{array}{ll} \frac{\delta_{xx'}}{p(x)} - 1 & p(x) > 0 \text{ and } p(x') > 0 \\ 0 & \text{otherwise} \end{array} \right. , \]
and consists of all functions with $\sum_{x \in \mathcal{X}} p(x) f(x) = 0$ and
\[ \|f\|_F^2 = \sum_{x \in \mathcal{X}} p(x) f(x)^2 \tag{8} \]
See Jamil (2018) for a proof. Potential advantages of the Pearson RKHS compared to the canonical RKHS is that, due to the weighting with $p(x)$, the norm of $f$ is less sensitive to collapsing of categories, and $f(x)$ for $x$ with zero probability mass do not contribute to the norm.

### 2.2.3 RKHSs over Hilbert spaces

Let $\mathcal{X}$ be a Hilbert space with inner product $\langle \cdot, \cdot \rangle_{\mathcal{X}}$. The canonical RKHS over $\mathcal{X}$ is defined as its continuous dual space whose reproducing kernel is given by
\[ h(x, x') = \langle x, x' \rangle_{\mathcal{X}}. \]
Functions in this space are of the form $f(x) = \langle x, \beta \rangle_{\mathcal{X}}$, with norm $\|f\|_{\mathcal{X}} = \|\beta\|_{\mathcal{X}}$.

A special case is the Mahalanobis RKHS, defined as the canonical RKHS over $\mathcal{X} = \mathbb{R}^p$ equipped with the Mahalanobis inner product; for a covariance matrix $S$, it is defined as
\[ \langle x, x' \rangle_{\text{Mah}} = x^\top S^{-1} x' \]

The Brownian motion RKHS is defined as the RKHS over $\mathcal{X}$ whose reproducing kernel is the generalized Brownian motion covariance kernel
\[ h(x, x') = -\frac{1}{2} \left( \|x - x'\|^2_{\mathcal{X}} - \|x\|^2_{\mathcal{X}} - \|x'\|^2_{\mathcal{X}} \right) \]
Functions in the Brownian motion RKHS are Hölder of degree at least $1/2$ (see Bergsma (2020) for a proof). In the simplest nontrivial case, $\mathcal{X} = \mathbb{R}$, and the RKHS consists of functions with a square integrable derivative, whose norm is the $L^2$ norm of the derivative, i.e., every $f \in \mathcal{F}$ can be written as $f(x) = \int_{-\infty}^{x} \beta(t)dt$ for some square integrable $\beta$, and has norm $\int_{\mathbb{R}} \beta(t)^2dt$.

The fractional Brownian motion (FBM) RKHS is the RKHS whose reproducing kernel is the generalized FBM covariance kernel
\[ h(x, x') = -\frac{1}{2} \left( \|x - x'\|^2_{\mathcal{X}} - \|x\|^2_{\mathcal{X}} - \|x'\|^2_{\mathcal{X}} \right) \]
Functions in the FBM-\(\gamma\) RKHS are Hölder of degree at least $\gamma$ (see Bergsma (2020) for a proof).

### 2.3 Construction of RKKSs over product spaces

ANOVA constructions of RKKSs over product spaces are a natural tool for formulating regression models, and generalize ANOVA RKHSs which were introduced for this purpose by Wahba (1990a) and Gu and Wahba (1993). In Section 2.3.1 we describe ANOVA RKKSs, an immediate extension of ANOVA RKHSs which are needed in this paper. In Section 2.3.2, we describe what as far as we are aware is a novel approach to use scale parameters parsimoniously in the ANOVA construction.
2.3.1 ANOVA RKKSs

An ANOVA decomposition of a function \( f \) over product space \( \mathcal{X}_1 \times \mathcal{X}_2 \) is given by (3) where the components are orthogonal in some way. To formalize this, let us first define the tensor product of RKHSs. Let \( \mathcal{F}_1 \) and \( \mathcal{F}_2 \) by two RKHSs over \( \mathcal{X}_1 \) resp. \( \mathcal{X}_2 \). For \( f_1 \in \mathcal{F}_1 \) and \( f_2 \in \mathcal{F}_2 \), the tensor product \( f_{12} = f_1 \otimes f_2 \) is defined by \( f_{12}(x_1, x_2) = f_1(x_1)f_2(x_2) \). The tensor product of \( \mathcal{F}_1 \) and \( \mathcal{F}_2 \) is denoted as \( \mathcal{F}_1 \otimes \mathcal{F}_2 \) and is defined as the closure of the set of functions \( \{f_1 \otimes f_2 | f_1 \in \mathcal{F}_1, f_2 \in \mathcal{F}_2\} \) equipped with the inner product

\[
\langle f_1 \otimes f_2, f_1' \otimes f_2' \rangle_{\mathcal{F}_1 \otimes \mathcal{F}_2} = \langle f_1, f_1' \rangle_{\mathcal{F}_1} \langle f_2, f_2' \rangle_{\mathcal{F}_2}.
\]

The tensor product of RKKSs is defined analogously, the closure being defined with respect to the corresponding positive definite inner product.

Let \( \mathcal{C}_k \) be the RKHS of constant functions over \( \mathcal{X}_k \) with kernel \( c_k(x, x') = 1 \) and let \( \mathcal{F}_k \) be an RKKS over \( \mathcal{X}_k \) with kernel \( h_k \) \((k = 1, 2)\). An ANOVA RKKS over \( \mathcal{X}_1 \times \mathcal{X}_2 \) is given as

\[
\mathcal{F} = \mathcal{C}_1 \otimes \mathcal{C}_2 + \mathcal{F}_1 \otimes \mathcal{C}_2 + \mathcal{C}_1 \otimes \mathcal{F}_2 + \mathcal{F}_1 \otimes \mathcal{F}_2
\]

with kernel \( h \) given by

\[
h((x_1, x_2), (x_1', x_2')) = 1 + h_1(x_1, x_1') + h_2(x_2, x_2') + h_1(x_1, x_1')h_2(x_2, x_2')
\]

In this paper we assume the components \( h_k \) are centered relative to data \( \{x_{1k}, \ldots, x_{nk}\} \subset \mathcal{X}_k \) (Section 2.4). Hence, the \( \mathcal{C}_k \) and \( \mathcal{F}_k \) are orthogonal in the sense that

\[
\sum_{i=1}^{n} c_k(x_{1k})f_k(x_{1k}) = \sum_{i=1}^{n} f_k(x_{1k}) = 0
\]

for any \( c_k \in \mathcal{C}_k \) and \( f_k \in \mathcal{F}_k \).

With \( p \) covariates, the ANOVA model with all interactions can be written succinctly as

\[
\mathcal{F} = \bigoplus_{k=1}^{p} (\mathcal{C}_k \otimes \mathcal{F}_k)
\]

with reproducing kernel

\[
h(x, x') = \prod_{k=1}^{p} (1 + h_k(x_k, x_k'))
\]

More general ANOVA kernels are described in Appendix A.

2.3.2 Scale parameters for kernels

In practice, the length of a vector in an RKHSs is measured on an arbitrary scale, and this can be taken into account by multiplying the kernel by a real-valued scale parameter which is to be estimated. In the ANOVA case, we can multiply kernel \( h_k \) by \( \mu_k \in \mathbb{R} \) and kernel \( c_k \) by \( \tau_k \in \mathbb{R} \) \((k = 1, \ldots, p)\). Then the ANOVA kernel for \( p = 2 \) is given by

\[
h_{\mu, \tau}((x_1, x_2), (x_1', x_2')) = \tau_1 \tau_2 + \mu_1 \tau_2 h_1(x_1, x_1') + \tau_1 \mu_2 h_2(x_2, x_2') + \mu_1 \mu_2 h_1(x_1, x_1')h_2(x_2, x_2')
\]

This expression is overparameterized, and setting \( \lambda_0 = \tau_1 \tau_2 \) and \( \lambda_k = \mu_k / \tau_k \) (assuming \( \tau_k \neq 0 \)), we obtain the identified parameterization

\[
h_\lambda((x_1, x_2), (x_1', x_2')) = \lambda_0 \{1 + \lambda_1 h_1(x_1, x_1') + \lambda_2 h_2(x_2, x_2') + \lambda_1 \lambda_2 h_1(x_1, x_1')h_2(x_2, x_2')\} \quad (11)
\]
Typically, the kernels \( h_k \) will be positive definite, so that the corresponding \( F_k \) are RKHSs. Then if at least one of the lambda parameters is negative, a function space with \( h_\lambda \) as its kernel will be an RKKS.

In the literature, a less parsimonious construction than (11) has been used, namely

\[
h_v((x_1, x_2), (x'_1, x'_2)) = v_0 + v_1 h_1(x_1, x'_1) + v_2 h_2(x_2, x'_2) + v_{12} h_1(x_1, x'_1) h_2(x_2, x'_2)
\]  

(e.g., Wahba, 1990b, Section 10.2, Berlinet & Thomas-Agnan, 2004, Section 10.2, Gu, 2013, Section 2.4.5). We refer to the corresponding RKKS as the extended ANOVA RKKS. Here, each of the four terms has a separate scale parameter, and is thus less parsimonious than our approach which only requires three scale parameters. For models with all interactions, our approach has \( p + 1 \) scale parameters, while in the extended ANOVA RKKS \( 2^p \) scale parameters are required if every interaction is assigned a separate parameter.

Note that ANOVA and corresponding extended ANOVA RKKSs contain exactly the same set of functions. Thus our parsimonious approach is not restrictive in this sense.

We have not seen our parsimonious construction of ANOVA kernels explicitly in the literature. However, if we view the role of the scale parameters as ensuring kernels are independent of the measurement units of the covariates, it is immediately justified for the most commonly used kernels. For example, if \( h(x, x') = \lambda(x, x') \), and \( x \) and \( x' \) are measured in \( kg \), then the unit of \( \lambda \) should be \( kg^{-2} \) in order to make the kernel unitless. This property then immediately extends to tensor product kernels and sums of these. Note that only those kernels for which \( h(cx, cx') = gh(c)h(x, x') \) for any \( c \) and some function \( gh(c) \) can be made unitless. However, this property is satisfied for most of the commonly used kernels, including all used in this paper, and including for example all stationary kernels. For kernels not satisfying this property, the extended ANOVA construction might be used.

### 2.4 Centering of RKKSs

To identify models such as (3) and (4), in this paper we use centered kernels/function spaces, where the centering is relative to the sample. For model (3), this leads to the identifying restrictions

\[
\sum_{i=1}^{n} f_1(x_{1i}) = \sum_{i=1}^{n} f_2(x_{2i}) = \sum_{i=1}^{n} f_{12}(x_{1i}, x'_{2i}) = \sum_{i=1}^{n} f_{12}(x'_1, x_{2i}) = 0 \quad \text{for any } x'_1 \in X_1 \text{ and } x'_{2i} \in X_2.
\]

Analogous identifying restrictions then apply to model (4).

We say a function space \( F \) over \( \mathcal{X} \) is centered with respect to a data set \( \{x_1, \ldots, x_n\} \subset \mathcal{X} \) if

\[
\sum_{i=1}^{n} f(x_i) = 0 \quad \forall f \in F
\]

It can be verified that an RKKS \( F \) is centered if and only if its kernel \( h \) is centered, in the sense that \( \sum_{i=1}^{n} h(x, x_i) = 0 \) for all \( x \in \mathcal{X} \). If \( h \) is a kernel, then \( h_{\text{cent}} \) defined as follows is centered:

\[
h_{\text{cent}}(x, x') = h(x, x') - \frac{1}{n} \sum_{i=1}^{n} h(x, x_i) - \frac{1}{n} \sum_{i=1}^{n} h(x_i, x') + \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} h(x_i, x_j)
\]

Table 1 gives a list of kernels discussed in Section 2.2 and their centered versions (see Appendix B for the derivation of the centered canonical kernel over a finite set). The centered FBM RKKS has kernel

\[
h_{\text{cent}}(x, x') = \frac{1}{n} \sum_{j=1}^{n} (\|x - x_j\|_{\mathcal{X}}^2 - \frac{1}{n} \sum_{j=1}^{n} \|x - x_j\|_{\mathcal{X}}^2 - \frac{1}{n} \sum_{i=1}^{n} \|x_i - x_j\|_{\mathcal{X}}^2 + \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \|x_i - x_j\|_{\mathcal{X}}^2)
\]  

(13)
Model: \( y_i = \alpha + f_1(x_i) + \varepsilon_i, \ x_i \in X_1, \ f_1 \in \mathcal{F}_1 \)

| \( X_1 \) | RKHS | \( \mathcal{F}_1 \) | Model name | Usual notation |
|---|---|---|---|---|
| A finite set | Pearson/Canonical | One-way ANOVA/Varying intercept model | \( y_{ij} = \alpha + \beta_j + \varepsilon_{ij} \) |
| \( \mathbb{R} \) | Canonical | Simple regression | \( y_i = \alpha + x_i \beta + \varepsilon_i \) |
| An RKHS | Canonical | Functional linear regression | \( y_i = \alpha + \int x_i(t) \beta(t) d\mu(t) + \varepsilon_i \) |
| An RKHS | FBM | Smooth functional regression | \( y_i = \alpha + f(x_i) + \varepsilon_i \) |

Table 2: Some models with one, possibly multidimensional covariate

### 3 Regression models

We show how some well-known models can be written in the form (1) and how they can be formulated using the ANOVA function space construction. As explanatory or response variables, we focus on the following in this paper:

1. Nominal categorical or qualitative; e.g., *type of cancer* (14 types) and *vowel* (11 types) (Section 6.2), *school index* (65 schools) (Section 6.3) and *cow index* (60 cows) and *treatment* (2 treatments) (Section 6.4).

2. Euclidean; e.g., 16,063 *gene expressions* and a 10-dimensional vector of *voice features* (Section 6.2).

3. Functional; e.g., a *spectrometric curve* (Section 6.1) and the *growth curve* of a cow (Section 6.4).

We model nominal categorical variables using the Pearson kernel, and Euclidean and functional variables using either the canonical or the FBM kernel.

In Sections 3.1 and 3.2 we consider models with one and two covariates respectively (see also Tables 2 and 3). In Section 3.3 we consider multidimensional or functional responses, and in Section 3.4 we consider multi-class classification models.

#### 3.1 Models with one covariate

If \( p = 1 \), the ANOVA construction with a centered kernel over \( X_1 \) yields

\[
y_i = \alpha + f_1(x_i) + \varepsilon_i, \quad f_1 \in \mathcal{F}_1, x_i \in X_1, \sum_{i=1}^{n} f_1(x_i) = 0 \tag{14}
\]

where \( \mathcal{F}_1 \) is in a centered function space over a set \( X_1 \). Recall that the centering gives the identifying restriction \( \sum_{i=1}^{n} f(x_i) = 0 \) for all \( f \in \mathcal{F}_1 \).

If \( X_1 \) is a finite set, then (14) is known as a one-way ANOVA model or varying intercept model, which can be reformulated as

\[
y_{jk} = \alpha + \alpha_k + \varepsilon_{jk}, \quad f_1 \in \mathcal{F}_1, k \in X_1 \tag{15}
\]

where index \( i \) has been recoded into \( (j, k) \) if observation \( i \) is the \( k \)th observation in group \( j \in X \), i.e., if \( i \) is the \( k \)th observation for which \( x_i = j \). Here, \( \alpha_j = f(j) \) is called the intercept for group \( j \in X \). The identifying restriction becomes \( \sum_{j \in X} p_j \alpha_j = 0 \), where \( p_j \) is the number of subjects in group \( j \). (Some may prefer other identifying restrictions such as \( \sum \alpha_j = 0 \); for consistency, we use identification based on centered kernels for all variables in this paper).
we obtain the functional linear model (e.g., Yao, M"uller, and Wang (2005))

\[
X = \mathcal{F}_1 \times \mathcal{F}_2
\]

tered function spaces, we obtain the identifying restrictions

\[
\sum f = \mathcal{F}_1 \times \mathcal{F}_2
\]

We now consider examples of regression models (1) where

\[3.2 \text{ Models with two covariates}\]

Models with two, possibly multidimensional covariates

| $\mathcal{X}_1$ | RKHS $\mathcal{F}_1$ | $\mathcal{X}_2$ | RKHS $\mathcal{F}_2$ | Model name | Usual notation |
|-----------------|----------------------|-----------------|----------------------|-------------|----------------|
| Finite set      | Pearson              | $\mathbb{R}$    | Canonical            | Varying slope model | $y_{ij} = \alpha + \alpha_j + x_{ij}\beta + x_{ij}\beta_j + \epsilon_{ij}$ |
| $\mathbb{R}^p$  | FBM                  | $\mathbb{R}^p$  | Canonical            | Varying coefficient model | $y_i = \alpha + x_{2i}\beta(x_{1i}) + \epsilon_i$ |
| $\mathbb{R}^p$  | FBM                  | $\mathbb{R}^p$  | Canonical            | Multivariate regression | $y_{ij} = \alpha + x_i\beta_j + \epsilon_{ij}$ |
| $\mathbb{R}^p$  | FBM                  | $\mathbb{R}^p$  | Canonical            | Functional response model | $y_i(t) = f(x_i, t) + \epsilon_i$ |

Table 3: Some models with two, possibly multidimensional covariates

If $\mathcal{X}_1$ is a Euclidean space and $\mathcal{F}_1$ a space of linear functions, we can reformulate (14) as

\[
y_i = \alpha + x_i^\top \beta + \epsilon_i. \tag{16}
\]

If $\mathcal{X}_1 = L^2(\mathcal{T}, \mu)$ for some measurable space $(\mathcal{T}, \mu)$ and $\mathcal{F}_1$ a set of linear functionals over $\mathcal{X}_1$, we obtain the functional linear model (e.g., Yao, Müller, and Wang (2005))

\[
y_i = \alpha + \int_{\mathcal{T}} x_i(t)\beta(t)d\mu(t) + \epsilon_i
\]

3.2 Models with two covariates

We now consider examples of regression models (1) where $f$ is of the form (3). Using centered function spaces, we obtain the identifying restrictions $\sum_{i=1}^n f_1(x_{1i}) = \sum_{i=1}^n f_2(x_{2i}) = \sum_{i=1}^n f_{12}(x_{1i}, x_{2i}) = 0$ for any $x_1 \in \mathcal{X}_1$ and $x_2 \in \mathcal{X}_2$.

If $\mathcal{X}_1 = \mathcal{X}_2 = \mathbb{R}$ and $\mathcal{F}_1$ and $\mathcal{F}_2$ are the set of linear functions over $\mathbb{R}$, we obtain the standard multiple regression model with an interaction,

\[
y_i = \alpha + x_{1i}\beta_1 + x_{2i}\beta_2 + x_{1i}x_{2i}\beta_{12} + \epsilon_i \tag{17}
\]

Note that generally this is a different model from (16) with an interaction term added, because (17) is based on two function spaces, with possibly different properties, and (16) is based on only one. In particular, (16) is suitable if the $x_{1i}$ and the $x_{2i}$ are, say, repeated measurements of a characteristic such as height, while (17) is suitable if the $x_{1i}$ and $x_{2i}$ are measured on different scales, such as height and weight.

Alternatively, if $\mathcal{F}_1$ is the set of linear functions over $\mathcal{X}_1 = \mathbb{R}$ and $\mathcal{F}_2$ is a set of smooth functions over some set $\mathcal{X}_2$, we obtain

\[
y_i = \alpha + x_{1i}\beta_1 + f_2(x_{2i}) + x_{1i}\beta(x_{2i}) + \epsilon_i
\]

where $\beta$ is a smooth function over $\mathcal{X}_2$. This is called a varying coefficient model (Hastie & Tibshirani, 1993), with $\beta(x_{2i})$ the varying coefficient of $x_{1i}$. If on the other hand $\mathcal{X}_2$ is finite set and $\mathcal{F}_2$ the set of all functions over $\mathcal{X}_2$, we can rephrase (1) subject to (3) as a varying slope model,

\[
y_{jk} = \alpha + x_{jk}\beta + \alpha_k + x_{jk}\beta_k + \epsilon_{jk} \tag{18}
\]
3.3 Multidimensional response models

If the $x_{jk} \in \mathcal{X}_1$ and $f_1(x_{jk}) = x_{jk} \beta$, $f_2(k) = \alpha_k$, and $f_{12}(x_{jk}, k) = x_{jk} \beta_k$. Thus, we treat group as a nominal categorical variable. We have a multilevel model with two levels, involving a linear regression for each group $k \in \mathcal{X}_2$. The intercept and slope for group $k$ are $\alpha + \alpha_k$ and $\beta + \beta_k$. Using centered function spaces, the identifying restrictions are $\sum_k p_k \alpha_k = \sum_k \pi_k \beta_k = 0$, where $\pi_k = (np_k)^{-1} \sum_k x_{jk}$ is the $k$th group mean. As for the varying intercept model, we take these identifying restrictions in order to treat all variables identically, but of course other identifying restrictions can be used as well. More generally, if $\mathcal{F}_i$ is a set of not necessarily linear functions, we obtain the general two-level model

$$y_{jk} = \alpha + f_1(x_{jk}) + \alpha_k + f_{1,k}(x_{jk}) + \varepsilon_{jk}$$

where $f_1, f_{1,k} \in \mathcal{F}_1$.

3.4 Multi-class classification

Consider a multi-class classification problem where, with $\mathcal{C}$ a finite set of classes, we have observations $(x_1, c_1), \ldots, (x_n, c_n)$ for $x_j \in \mathcal{X}$ and $c_j \in \mathcal{C}$. The aim is to find a prediction function to predict the class $c \in \mathcal{C}$ for a future observation $x \in \mathcal{X}$. We can use the present framework as follows. Let $y_{jk} = 1$ if $c_j = k$ and let $y_{jk} = 0$ otherwise. We can then use the multidimensional response model (20), or more generally (21). We naively assume the errors are i.i.d. normal conditional on $\sum_{k \in \mathcal{C}} \varepsilon_{jk} = 0$. Though this is unrealistic, the real data examples in Section 6 show competitive performance of this approach.

Since by assumption $\sum_{k \in \mathcal{C}} y_{jk} = 1$ and $\sum_{k \in \mathcal{C}} \varepsilon_{jk} = 0$ for $j = 1, \ldots, n$, the model is not identified with the usual restrictions we need to add some extra ones. Summing the left and right hand sides of (21) over $k$, we obtain $1 = |\mathcal{C}|(\alpha + f_1(x_j))$ for $j = 1, \ldots, n$, giving the model

$$y_{jk} = |\mathcal{C}|^{-1} + \alpha_k + f_{1,k}(x_j) + \varepsilon_{jk}$$

subject to the identifying restrictions $\sum_{k \in \mathcal{C}} \alpha_k = 0$, $\sum_{k \in \mathcal{C}} f_{1,k}(x_j) = 0$ for all $j$, and $\sum_{j=1}^n f_{1,k}(x_j) = 0$ for all $k$. Note that a main effect for $x_i$ is not needed in (22).

3.5 Other models

Above we just gave some examples of the models that are possible. Other models are easily obtained by changing the kernels or adding more covariates. For example, in Section 6.4 we consider a functional response model with two categorical covariates.
4 The I-prior

Consider model (1) subject to (2), where $F$ is an RKKS with reproducing kernel $h$. In this section we derive a prior for the regression function $f$ based on the Fisher information on $f$.

As shown by Bergsma (2020), the Fisher information on $f$ is given by

$$ I[f](x, x') = \sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{ij} h(x, x_i) h(x, x_j) $$

$I[f]$ is positive definite and hence induces an RKHS over $X$, which we denote by $F_n$. $F_n$ is a finite dimensional subspace of $F$, consisting of functions of the form $f(x) = \sum_{i=1}^{n} h(x, x_i) w_i$, with squared norm $\|f\|_{F_n}^2 = \sum w_i w_j \psi_{ij}$, where $\psi_{ij}$ is the $(i,j)$th element of the error covariance matrix $\Psi^{-1}$ (Bergsma, 2020, Lemma 2). With $\hat{f}$ an unbiased estimator of the true regression function $f$, the Crámer-Rao inequality implies that for any $g \in F$

$$ \text{var}((g, \hat{f})_X) \geq \|g\|_{F_n}^2 $$

By standard weighted least squares theory, equality is achieved if $\hat{f}$ is a maximum likelihood estimator of $f$.

We can write any $f \in F$ as $f = f_n + r_n$, where $f_n \in F_n$ and $r_n(x_1) = \ldots = r_n(x_n) = 0$. Then $r_n \in F_n^\perp$, where $F_n^\perp$ is the orthogonal complement of $F_n$ in $F$. The likelihood for $f$ does not depend on $r_n$, i.e., the data contain no information on $r_n$, and we can replace $r_n$ by a `best guess'. In this paper, we set $r_n = 0$.

We define the I-prior as a maximum entropy prior as follows. Let $\nu$ be volume measure induced by $\|\cdot\|_{F_n}$. The entropy of a prior $\pi$ over $F_n$ relative to $\nu$ is

$$ \mathcal{E}(\pi) = -\int_{F_n} \pi(f) \log \pi(f) \nu(df). $$

We define the I-prior for $f$ as the prior $\pi$ maximizing entropy subject to the constraint

$$ E_{g \sim \pi} \|g\|_{F_n}^2 = \text{constant} $$

Variational calculus shows that an I-prior for $f$ is the Gaussian variable with mean $r_0 = 0$ and covariance kernel proportional to the Fisher information on $f$, i.e.,

$$ \text{cov}_\pi(f(x), f(x')) = \tau^2 \sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{ij} h(x, x_i) h(x', x_j) $$

for some $\tau > 0$. Equivalently, under the I-prior, $f$ can be written in the form

$$ f(x) = \tau \sum_{i=1}^{n} h(x, x_i) w_i, \quad (w_1, \ldots, w_n) \sim \text{MVN}(0, \Psi), \quad (23) $$

Note that the ANOVA kernel described in Section 2.3 has a scale parameter $\lambda_0$ which makes the parameter $\tau$ superfluous, and we will omit $\tau$ in further developments.

Let us consider some examples, described in more detail in Bergsma (2020). Firstly, if $F$ consists of functions $f(x) = x^\top \beta$ ($x, \beta \in \mathbb{R}^p$) with norm $\|f\|_F = \|\beta\|_{\mathbb{R}^p}$, then under the I-prior, $\beta \sim \text{MVN}(0, \lambda XX^\top \Psi X)$, where $X$ is the $n \times p$ matrix with ith row $x_i$. If instead of with the Euclidean norm we equip $\mathbb{R}^p$ with the Mahalanobis norm, $\beta \sim \text{MVN}(0, \lambda(X^\top \Psi X)^{-1})$, which is the $g$-prior (Zellner, 1986) with $g = \lambda$. 


Secondly, if $F$ is the Brownian motion RKHS, $f \in F$ are of the form

\[ f(x) = \int_{-\infty}^{x} \beta(t) dt, \]

and $\|f\|_{F}^{2} = \int_{R} \beta(t)^{2} dt$. If $f \in F_{n} \subset F$, then it can be shown that

\[ \beta(t) = \sum_{i: x_{i} \leq t} w_{i} = \frac{f(x_{i+1}) - f(x_{i})}{x_{i+1} - x_{i}}, \]

with $i_{t} = \max_{x_{i} \leq t} i$. Note that $\sum w_{i} = 0$ and hence $\lim_{t \to \pm \infty} \beta(t) = 0$. Under the I-prior, the $w_{i}$ are distributed as in (23), hence the I-prior for $f$ is an generalized integrated discrete Brownian bridge (generalized as the normal increments need not be independent). If the errors are i.i.d., $\beta$ is an ordinary Brownian bridge. The posterior mean is therefore similar to a cubic spline smoother, which is the posterior mean based on an integrated Brownian motion. Note however that the I-prior assumes the true regression function has only a single derivative, while the cubic spline smoother, based on a penalty $\int \hat{f}(t)^{2} dt$, assumes it has two.

4.1 Motivation for use of FBM RKHS with I-priors

As explained in more detail in Bergsma (2020), the use of the I-prior methodology is particularly attractive if $F$ is a fractional Brownian motion (FBM) RKHS over a Euclidean space. FBM process paths are non-differentiable and, having Hölder smoothness ranging between 0 and 1, an FBM process prior for the regression function may be too rough for many applications. In contrast, functions in the FBM RKHS with Hurst coefficient $\gamma$ are (weakly) differentiable if the Hurst $\gamma \geq 1/2$ and have minimum Hölder smoothness $2\gamma$. This wide range of smoothnesses make it an attractive general purpose function space for nonparametric regression. Another advantage is that it allows us to do multivariate smoothing with just one or two parameters to be estimated: either only the scale parameter $\lambda$, while using a default setting of, say, $1/2$ for the Hurst coefficient, or both the scale parameter and the Hurst coefficient. This is in contrast with standard kernel based smoothing methods, which require a scale parameter and at least one kernel hyperparameter to be estimated. For example, if we use the exponential kernel

\[ r(x, x') = \lambda \exp \left(-\frac{\|x - x\|^2}{2\sigma^2}\right), \quad (24) \]

the scale parameter $\lambda$, the smoothness parameter $\xi$ (somewhat analogous to the Hurst coefficient), and a ‘variance’ parameter $\sigma^2$ need to be estimated. Default settings $\xi = 1$ or $\xi = 2$ could be used to reduce the number of free parameters to two. Furthermore, the functions in the squared exponential RKHS are analytical, which is too smooth for many applications.

5 Estimation of I-prior models

In this section we describe how to estimate $f \in F$ in (1) subject to (2) by its posterior distribution under the I-prior, when $F$ is an ANOVA RKKS. The posterior distribution of $f$ is multivariate normal and given in Lemma 1. The posterior mean can be used as a point estimator, and (estimated) credible sets can be obtained from the posterior covariance matrix. In practice, estimators and credible sets of linear functionals of $f$ will be of interest, for example, the components of (3), or so-called features of $f$ such as regression coefficients. These can be
obtained by standard linear transformations of the posterior mean and covariance matrix of \( f \),
the details of which are not in the scope of this paper.

The most difficult part of the estimation of \( f \in \mathcal{F} \) is the estimation of the scale parameters
of the ANOVA kernel of \( \mathcal{F} \) and the parameters of the error covariance matrix. As mentioned,
the error covariance matrix is assumed to have only a small number of parameters, for example,
if the errors are i.i.d. there is only the common error variance to estimate, or if the errors
are AR(1) two real-valued parameters need to be estimated. In Gaussian process regression,
the scale and error parameters are typically estimated by directly maximizing the marginal
likelihood, which can be numerically difficult if there are multiple scale parameters. Instead,
we propose an EM algorithm with simple E and M steps. In contrast, for Gaussian process
regression it is well-known that the M step is as complex as maximizing the marginal likelihood
directly.

In this section, for readability, we switch to boldface notation for finite-dimensional vectors
and matrices. Hence the matrix \( \Psi \) in (2) will be denoted by the boldface \( \mathbf{\Psi} \).

5.1 Marginal likelihood and posterior distribution of parameter estimates

Denote \( y = (y_1, \ldots, y_n)^\top, f = (f(x_1), \ldots, f(x_n))^\top, f_0 = (f_0(x_1), \ldots, f_0(x_n))^\top, \varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)^\top,\)
\( \mathbf{w} = (w_1, \ldots, w_n)^\top \). Then (1) implies \( y = f + \varepsilon \). Let \( H_\lambda \) be the \( n \times n \) matrix with \((i, j)\)th
coordinate \( h_\lambda(x_i, x_j) \), where \( h_\lambda \) is an ANOVA reproducing kernel with scale parameter vector \( \lambda \) (see Section 2.3).

Under the I-prior, \( f \sim \text{MVN}(f_0, H_\lambda \mathbf{\Psi} H_\lambda) \), so the marginal distribution of \( y \) is
\[
y \sim \text{MVN}(f_0, V_y)
\] where the marginal covariance is given as
\[
V_y = H_\lambda \mathbf{\Psi} H_\lambda + \mathbf{\Psi}^{-1}
\] Thus, the marginal log likelihood of \((\lambda, \mathbf{\Psi})\) is
\[
L(\lambda, \mathbf{\Psi} | y) = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |V_y| - \frac{1}{2} (y - f_0)^\top V_y^{-1} (y - f_0).
\] The maximum likelihood (ML) estimate \((\hat{\lambda}, \hat{\mathbf{\Psi}})\) of \((\lambda, \mathbf{\Psi})\) maximizes \( L(\lambda, \mathbf{\Psi} | y) \), and can be obtained using the EM algorithm described below. Having obtained \((\hat{\lambda}, \hat{\mathbf{\Psi}})\), \( f \) can be estimated
by its posterior distribution under the I-prior:

Lemma 1. The posterior distribution of \( f \) in (1) subject to (2) given \( y \) under the I-prior \( \pi \) is
Gaussian with mean given by
\[
E_\pi[f(x) | y] = f_0(x) + \sum_{i=1}^n h(x, x_i) \hat{w}_i
\]
where
\[
\hat{\mathbf{w}} = \mathbf{\Psi} H_\lambda V_y^{-1} (y - f_0)
\] and covariance kernel given by
\[
\text{cov}_\pi(f(x), f(x') | y_1, \ldots, y_n) = \sum_{i=1}^n \sum_{j=1}^n h(x, x_i) h(x', x_j) (V_y^{-1})_{ij}
\]
The proof is standard and given in Bergsma (2020).
5.2 Estimation of parameters using the EM algorithm

We now describe the EM algorithm for estimating the scale parameter $\lambda$ of $H_\lambda$, as well as parameters of the precision matrix $\Psi$ (often it is just assumed the errors are i.i.d. $N(0, \psi^{-1})$, i.e., $\Psi = \psi I_n$). For estimating these parameters, EM turns out to be particularly efficient. There can be other unknown parameters as well, e.g., the Hurst coefficient for the FBM RKHS, but for this parameter EM is computationally much less attractive, and we will not go into this.

The EM algorithm has, as is well-known, guaranteed convergence under conditions often satisfied in practice. In the present case, the E-step is in closed form while the M-step is typically not, but in practice the M-step is computationally easy to carry out.

With $g$ denoting the density function related to its argument and using (23) with $\tau = 1$, the complete data log likelihood is

$$L(\lambda, \Psi | y, w) = \log g(y | w, \lambda, \Psi) + \log g(w | \Psi)$$

$$= c + \frac{1}{2} \log |\Psi| - \frac{1}{2} (y - f)^\top \Psi (y - f) - \frac{1}{2} \log |\Psi| - \frac{1}{2} w^\top \Psi^{-1} w$$

$$= c - \frac{1}{2} (y - f)^\top \Psi (y - f) - \frac{1}{2} w^\top \Psi^{-1} w$$

$$= c - \frac{1}{2} (y - f_0 - H_\lambda w)^\top \Psi (y - f_0 - H_\lambda w) - \frac{1}{2} w^\top \Psi^{-1} w$$

$$= c - \frac{1}{2} (y - f_0)^\top \Psi (y - f_0) - \frac{1}{2} w^\top \Psi H_\lambda \Psi H_\lambda w + (y - f_0)^\top \Psi H_\lambda w - \frac{1}{2} w^\top \Psi^{-1} w$$

$$= c - \frac{1}{2} (y - f_0)^\top \Psi (y - f_0) - \frac{1}{2} \text{tr} \left[V_y w w^\top \right] + (y - f_0)^\top \Psi H_\lambda w,$$

where $c$ is a constant. Write

$$\tilde{W} = E(ww^\top | y, \lambda, \Psi) = \tilde{V}_w + \bar{w} \bar{w}^\top,$$

where $\bar{w}$ and $\tilde{V}_w$ are given by (28) and (26). Let $\bar{w}^{(0)}$ and $\tilde{W}^{(0)}$ be $\bar{w}$ and $\tilde{W}$ with $\Psi$ and $\lambda$ replaced by $\Psi^{(0)}$ and $\lambda^{(0)}$. The E-step consists of computing

$$Q(\lambda, \Psi) = E \left\{ L(\lambda, \Psi | y, w) | y, \lambda^{(0)}, \Psi^{(0)} \right\}$$

$$= c - \frac{1}{2} (y - f_0)^\top \Psi (y - f_0) - \frac{1}{2} \text{tr} \left[V_y \tilde{W}^{(0)} \right] + (y - f_0)^\top \Psi H_\lambda \bar{w}^{(0)}. \quad (29)$$

The M-step entails maximizing $Q(\lambda, \Psi)$. We assume the global maximum can be found by differentiating, equating to zero, and solving. Supposing $\Psi$ but not $H_\lambda$ depends on a parameter $\psi$ and $H_\lambda$ but not $\Psi$ depends on a parameter $\lambda$, the derivatives are given by

$$\frac{\partial Q(\lambda, \Psi)}{\partial \lambda} = - \text{tr} \left[ \frac{\partial H_\lambda}{\partial \lambda} \Psi H_\lambda \tilde{W}^{(0)} \right] + (y - f_0)^\top \Psi \frac{\partial H_\lambda}{\partial \lambda} \bar{w}^{(0)}$$

$$\frac{\partial Q(\lambda, \Psi)}{\partial \psi} = - \frac{1}{2} (y - f_0)^\top \frac{\partial \Psi}{\partial \psi} (y - f_0) - \frac{1}{2} \text{tr} \left[ \frac{\partial V_y}{\partial \psi} \tilde{W}^{(0)} \right] + (y - f_0)^\top \frac{\partial \Psi}{\partial \psi} H_\lambda \bar{w}^{(0)}.$$

For the examples in Section 6, the errors are i.i.d., so $\Psi = \psi I_n$ for a scalar $\psi$, and $H_\lambda$ represents an ANOVA kernel as described in Section 2.3, so it is of the form $H_\lambda = \sum_{s=1}^k g_s(\lambda) H_s$, where $g_s$ is a polynomial function. Then

$$\frac{\partial \Psi}{\partial \psi} = I_n, \quad \frac{\partial H_\lambda}{\partial \lambda} = \sum_{s=1}^k \frac{\partial g_s(\lambda)}{\partial \lambda} H_s.$$
The partial derivatives of $Q$ set to zero can then normally be solved very quickly numerically for the purposes of this paper. For example, if $g_s(\lambda) = \lambda_s$ (which is the case, e.g., if there are no interactions in the model) then the equations have a closed form solution. In general, with i.i.d. errors, and $\mathcal{V}$ the set of (possibly multidimensional) variables involved, $2|\mathcal{V}| + 1$ polynomial equations in $2|\mathcal{V}| + 1$ unknowns need to be solved, which we found can be done very rapidly using built in solvers in R and Mathematica. The computational bottleneck is not the M step, but the E step which is $O(n^3)$.

We did sometimes encounter accuracy problems, making it impossible to obtain full convergence of the EM algorithm (this problem was encountered and mentioned in Section 6.2). This is not a problem just for EM, as the marginal likelihood is difficult to estimate as well, see Bergsma (2020) for a visualization of this problem. For prediction purposes, the lack of convergence did not seem to matter, but the lack of an accurate maximal value of the marginal likelihood can make model comparison difficult.

6 Application to data

We reanalyze some well-known data sets in the respective areas of multilevel modelling, functional data analysis, classification, and longitudinal data analysis. Whereas in the literature different methods are typically used in different areas, and often more than method per area, we fit all models using the single method introduced in this paper. In all cases we obtain a performance competitive with existing techniques in terms of mean squared prediction error for test data. Furthermore, since estimation can be done using the EM algorithm described in Section 5, our methodology is flexible in that it is easy to incorporate extra covariates and interaction effects using the parsimonious ANOVA framework given in Section 2.3.

Sections 6.1 and 6.2 focus on prediction, while Sections 6.3 and 6.4 focus on model selection and estimation of effects of interest. In Section 6.1, we analyze a data set with a real response and a functional covariate. In Section 6.2 we look at multi-class classification, both with high and low dimensional covariates. The latter two sections illustrate the potentially good predictive performance of the I-prior methodology compared to other methods. Furthermore, they illustrate the ease with which high-dimensional smoothing can be done using the I-prior. In Section 6.3 we fit the standard multilevel varying intercept and varying slope models using the I-prior, and illustrate the differences between the I-prior approach and the standard random effects approach. Here, the I-prior method has an estimation advantage in that there is no positive definite latent covariance matrix to be estimated, and a simple EM algorithm can be used for estimating the hyperparameters. In Section 6.4 we do a longitudinal data analysis with I-priors. Here, we treat the longitudinal response curves as ‘functional’ responses. In contrast to standard approaches, we do not need to specify a covariance structure for the longitudinal responses, instead we merely need to specify an appropriate class of functions, e.g., a class of smooth functions.

Throughout this section, we will use the parsimonious ANOVA approach described in Section 2.3.2 for which interaction effects do not require extra scale parameters. In Section 6.4, we will compare this approach with the ‘classical’ non-parsimonious extended ANOVA one (also under the I-prior) where each interaction effect does take an extra scale parameter. As mentioned before, the scale parameters’ purpose is to ensure independence of measurement units, and hence there is no need to have additional scale parameters for interaction effects. This does not restrict for example the range of possible covariance matrices for the estimated intercepts and slopes in a multilevel model.
6.1 Regression with a functional covariate

We illustrate the prediction of a real valued response when one of the covariates is a function using a widely analysed data set used for quality control in the food industry. The data consist of measurements on a sample of 215 pieces of finely chopped meat. The response variable is fat content, and the covariate is light absorbance for 100 different wavelengths. The absorbance curve can be considered a ‘functional’ variable (see a sample of such curves plotted in Figure 1). For more details see http://lib.stat.cmu.edu/datasets/tecator and Thodberg (1996). Our aim is to predict fat content from the 100 measurements of absorbance. The first 172 observations in the data set are used as a training sample, and the remaining 43 observations are used as a test sample (following Thodberg’s original recommendation).

Many different methods have been applied in the literature to the data set, estimating a model using the training sample and evaluating its performance using the test sample. One of the best results was achieved early on by Thodberg (1996), who used neural networks on the first 10 principal components and achieved a test mean squared error of 0.36. The best test error performance we found was by Vila, Wagner, and Neveu (2000) who achieved an error rate of 0.34, also using neural networks on the principal components. More recently various other statistical models have been tried on the data set, see Table 4 for a summary. In spite of their lesser performance compared to neural networks, the interest of these methods is that they do not rely on an a priori data reduction in terms of the main principal components.

The $i$th spectral curve is denoted $x_i$, with $x_i(t)$ denoting the absorbance for wavelength $t$. We assume $x_i \in \mathcal{X}$, where $\mathcal{X}$ is a set of functions over $\mathbb{R}$ and is equipped with an appropriate inner product. From Figure 1 it appears the curves are differentiable, so it seems reasonable to assume the $\mathcal{X}$ is the Brownian motion RKHS over $\mathbb{R}$ with squared norm

$$\|x\|_{\mathcal{X}}^2 = \int_{\mathbb{R}} \dot{x}(t)^2 dt.$$

Since $\mathcal{X}$ is a Hilbert space, a linear effect of the spectral curve on fat content can now be modelled using the canonical RKHS over $\mathcal{X}$. We see in Table 4 that both Tikhonov regularization and the I-prior give a poor performance, with test RMSEs of 3.54 and 2.89, respectively. Next we fitted a smooth dependence of fat content on spectrometric curve using the FBM RKHS over $\mathcal{X}$. As seen in the table, Tikhonov regularization performs very poorly. We tried various values of the Hurst coefficient, but all give worse results than the linear model. On the other hand, the I-prior performs rather well for different RKHSs, including the FBM and the squared exponential ones. We had some convergence problems so could not get the ML estimator of $\gamma$, the Hurst coefficient for the FBM RKHS, so instead estimated it by minimizing the cross-validation error (10-fold cross-validation gave $\hat{\gamma} = 0.98$). For the squared exponential RKHS we did manage to find the ML estimator $\hat{\sigma}$ of $\sigma$, and it is given in Table 4.
### Table 4: RMSEs for predicting fat content from spectrometric functional covariate (see Figure 1): previously published results, Tikhonov regularization, and I-prior methodology.

| Method                                           | RMSE Training | RMSE Test  |
|-------------------------------------------------|---------------|------------|
| Global constant model                           | 12.50         | 13.3       |
| Neural network (Vila et al., 2000)              | 0.34          |            |
| Kernel smoothing (Ferraty & Vieu, 2006, Section 7.2) | 1.85          |            |
| Double index model (Chen, Hall, & Müller, 2011) | 1.58          |            |
| Single index model (Goia & Vieu, 2014)          | 1.18          |            |
| Sliced inverse regression (Lian & Li, 2014)     | 0.90          |            |
| MARS (Zhu, Yao, & Zhang, 2014)                  | 0.88          |            |
| Partial least squares (Zhu et al., 2014)        | 1.01          |            |
| CSEFAM (Zhu et al., 2014)                       | 0.85          |            |
| Tikhonov regularization (linear)                | 3.32          | 3.54       |
| Tikhonov regularization (FBM-1/2 kernel)        | 4.32          | 4.54       |
| I-prior (linear)                                | 2.82          | 3.15       |
| I-prior (FBM RKHS with $\gamma = 0.5$)         | 0.00          | 0.67       |
| I-prior (FBM RKHS with $\tilde{\gamma} = 0.98$)| 0.00          | 0.57       |
| I-prior (squared exponential RKHS, $\tilde{\sigma} = 0.0079$) | 0.35          | 0.58       |

Instead of fat content, protein content can be predicted from the spectral curve. With the I-prior based on a smooth dependence of protein content on the spectral curve we obtained an RMSE of 0.52, using a local (non-global) maximum likelihood estimate of the Hurst coefficient, $\tilde{\gamma} = 0.997$. This improves on Zhu et al. (2014) who obtained an RMSE of 0.85.

### 6.2 Multi-class classification

We apply the model described in Section 3.4 to two data sets that have received widespread attention in the literature, one for which the most important covariate is low dimensional and one for which it is high dimensional. In both cases, the classes $1, \ldots, T$ are unordered. The effect of $x$ is first assumed to be linear, then smooth, and the results are compared. We show that the classifier obtained from the I-prior is competitive with the other classifiers that we were able to find in the literature. Bergsma (2020) previously considered I-prior modelling for two-class classification.

The first problem was originally presented by Ramaswamy et al. (2001), and concerns the prediction of cancer type based on 16,063 gene expression measurements (see Figure 2). A training set of 144 patients with 14 different types of cancer is available, as well as a test set.
| Method                               | Training errors | Test errors |
|--------------------------------------|-----------------|-------------|
| Nearest neighbors                    | 41              | 26          |
| $L^2$-penalized discriminant analysis | 25              | 12          |
| Support vector classifier            | 26              | 14          |
| Lasso                                | 30.7            | 12.5        |
| $L^1$ penalized multinomial          | 17              | 13          |
| Elastic net penalized multinomial    | 22              | 11.8        |
| SCRDA (Guo, Hastie, & Tibshirani, 2007) | 24              | 8           |
| Scout (Witten & Tibshirani, 2011)    | 21              | 8           |
| I-prior (linear)                     | 0               | 12          |
| I-prior (smooth, $\gamma = 0.8$)    | 0               | 10          |

Table 5: Comparison of classifier performance for the 14 cancer classification problem. The covariate is high-dimensional, consisting of a vector of 16,063 gene expressions. The top six lines are taken from Hastie et al. (2009), Table 18.1. With the I-prior, high-dimensional smoothing is as straightforward as fitting a linear effect, while giving slightly better test performance. We did have some numerical problems with maximum likelihood estimation of the Hurst coefficient $\gamma$, which we took to be 0.8.

of 54 patients which can be used to assess the performance of a classifier. Assuming a linear dependence on class of the covariate vector of 16,063 gene expressions, we obtained 0 training errors and test 12 errors, which competes well with other methods (see Table 5). In particular our training error rate far outperforms competing methods. Modelling a smooth dependence of class on the covariate vector gave some numerical problems and we were unable to obtain full convergence of the EM algorithm. Fortunately, the classification errors did not seem to be affected by this, so we are confident these are accurate (the maximum of the likelihood we obtained, not given here, was inaccurate). For $0.72 < \gamma < 0.86$ the training/test errors were 0/10, which was the best we could achieve.

The second problem concerns vowel recognition based on a 10-dimensional vector computed from a voice recording. The training and test sets are based on recordings of 8 resp. 7 people, each of whom spoke 11 different vowels 6 times. As seen in Table 6, if a linear effect of the covariates is assumed, the I-prior gives no advantage compared to ordinary least squares. The reason is that there are only a small number of predictors. Again we had some numerical difficulties fitting a smooth model, but the MLE seems to be $\hat{\gamma} = 0.652$ giving training/test error rates 0/0.35, improving on the results given in Hastie et al. (2009).

### 6.3 Multilevel models

The purpose of this section is to show that the I-prior approach for estimating varying intercept and varying slope models is a viable alternative to the standard random effects model. Advantages of the I-prior approach are potentially simpler estimation and testing, while the two methods give broadly similar estimates. We consider a data set which accompanies the MLwiN software (Rasbash, Steele, Browne, & Goldstein, 2012) on school achievement of 4059 pupils at 65 inner-London schools. The response variable is the GCSE score at age 16.

First we consider the varying intercept model (15). The ‘covariate’ is the nominal variable school (ranging from 1 to 65). For the standard random intercept model, the assumption is made
| Method                        | Error rates |
|-------------------------------|-------------|
|                              | Training    | Test        |
| Nearest neighbours           | 0.44        |             |
| OLS regression (linear effects) | 0.48        | 0.67        |
| Linear discriminant analysis | 0.32        | 0.56        |
| Neural network (Gaussian nodes) | 0.45        |             |
| FDA/BRUTO                    | 0.06        | 0.44        |
| FDA/MARS (best reduced dimension) | 0.13        | 0.39        |
| I-prior (linear)             | 0.48        | 0.67        |
| I-prior (smooth, $\hat{\gamma} \approx 0.652$) | 0           | 0.35        |

Table 6: Comparison of classifier performance for the vowel classification problem (first six lines taken from Hastie et al. (2009)). Since the dimension of the covariate is low (equal to 10), the I-prior gives no advantage over ordinary least squares (OLS) if the covariate effect is linear.

![Figure 3: Estimated intercepts and slopes for school achievement data under varying intercept and varying slope model. The numbers are the school indices. In contrast to the I-prior, the standard random effects multilevel model assumes i.i.d. slopes and intercepts across schools. It is seen that I-prior estimated intercepts are bigger in absolute value than the standard ones for small schools (48 and 54; see text).](image-url)
that the intercepts \( f_1(x), x \in X_1 \), are i.i.d. normal with zero mean, i.e., if \( X_1 = \{1, \ldots, m\} \),
\[
(f_1(1), \ldots, f_1(m)) \sim \text{MVN}(0, \sigma^2 I_m)
\]
for some \( \sigma > 0 \).

The I-prior depends on the kernel we assign to \( F_1 \). We choose the Pearson kernel, as the resulting RKHS norm weights school effects proportionally to school size (see (8)). If we assign a Pearson kernel to \( F_1 \), the Fisher information matrix for the intercepts is proportional to \( D_p^{-1} - 11^\top \) where \( D_p \) is the diagonal matrix with \( p \) on the main diagonal, \( p = (p(1), \ldots, p(m))^\top \), \( p(k) \) is the proportion of the sample in group \( k \), and \( 1 \) is the \( m \)-vector of ones (see Appendix B). Hence the intercepts under the I-prior are distributed as
\[
(f_1(1), \ldots, f_1(m)) \sim \text{MVN}(0, \tau^2(D_p^{-1} - 11^\top))
\]
for some \( \tau > 0 \). In this case, the intercepts are independent zero mean normals, conditioned on \( \sum_k p(k)f_1(k) = 0 \), where the \( k \)th intercept has variance \( p(k)^{-1} \).

In Figure 3(a), the posterior means of the intercepts are plotted for the random effects model and the I-prior based on the Pearson RKHS. It can be seen the estimates are in broad agreement, with conspicuously different estimates for schools 48 (−0.11 vs. −0.36) and 54 (−0.38 vs. −0.56), the I-prior giving the largest estimate in absolute value in both cases. The reason for the relatively large I-prior estimates is that the I-prior assigns large prior variance to schools with few pupils, resulting in less shrinkage towards zero than for the standard random effects model. Indeed, schools 48 and 54 have the smallest sample sizes of all schools, namely 2 and 8 (the next smallest school is number 37, with 22 students). Note that if the I-prior was used with the canonical kernel, estimates for small schools would be shrunk more towards zero than under the random effects model.

Next we consider the varying slope model (18), which regresses, for each school, the GCSE score on the result of the London reading test (LRT), taken at age 11. The standard random effects model is based on the assumption that the intercept/slope pairs are i.i.d. bivariate normal with zero mean. To obtain an I-prior, we assume a Pearson RKHS over the set of schools. In Figure 3(b), the posterior means of the slopes obtained using the standard random effects model are plotted against the ones obtained using the I-prior. Again we see broad agreement of the estimates, but much less so than for the varying intercept model.

The I-prior model tends to be more parsimonious than the standard random effects model, in the sense that fewer hyperparameter need to be estimated. For the varying intercept model, there is no difference in this respect, as both models have three hyperparameters. In the random effects model these are the error variance and the mean and variance of the random intercepts. In the I-prior model, these are the error variance, and the two scale parameters for the ANOVA kernel. For the varying slope model, the two models differ in parsimony. The random effects model has six hyperparameters: the error variance and the five parameters of the bivariate normal distribution for the random intercepts and slopes. The I-prior model has only four hyperparameters: the error variance and the three parameters of the ANOVA kernel (see (11)).

A key interest in multilevel modelling is estimation of the joint distribution of the parameters across groups, in the present case the distribution of the slope/intercept pairs across schools. In the random effects approach, a multivariate normal distribution is postulated for these parameters, and the mean and covariance matrix of this distribution are estimated using maximum marginal likelihood. In the I-prior method, there is no assumption of normality of the slope/intercept pairs. Nevertheless, the mean and covariance matrix of the slope/intercept pairs may be estimated from the posterior means of the slopes and intercepts. As seen in Table 8, the I-prior and random effects approaches give similar results.
Table 7: Comparison of I-prior and random effects approaches for the constant slope and varying slope model. In the I-prior approach, the varying slope model is selected because it has the highest likelihood while the two models have the same number of parameters. In the random effects approach, the difference in likelihood has a chi-bar distribution, and the \( p \)-value for testing the constant against the varying slope model is < .0001, so the latter model is selected as well.

| Parameter                  | I-prior estimate | Random effects estimate |
|----------------------------|------------------|-------------------------|
| Mean intercept             | −0.00 (0.01)     | −0.01 (0.04)            |
| Mean slope                 | 0.56 (0.01)      | 0.56 (0.02)             |
| SD intercepts              | 0.29 (0.07)      | 0.30 (0.03)             |
| SD slopes                  | 0.09 (0.03)      | 0.12 (0.00)             |
| Correlation slopes and intercepts | 0.44 (0.01) | 0.50 (0.01)             |
| SD errors                  | 0.74 (0.08)      | 0.74 (0.08)             |

Table 8: Comparing estimated parameters using the I-prior and random effects approaches. In brackets the estimated standard error.

Another advantage of the I-prior model is that estimation of the hyperparameters is easier than for the random effects model, because for the former a simple EM algorithm is available. This advantage is more pronounced for multilevel models with more than two levels and/or more covariates.

Hypothesis testing tends to be simpler for I-prior models. Let us test whether \( \beta_{12,k} = 0 \) in (18) against \( \beta_{12,k} \neq 0 \) for at least one \( k \), i.e., whether the constant slope model

\[
f(k, x_{jk}) = \alpha + \beta_{1,k} + x_{jk}\beta_2
\]

holds against the alternative of a varying slope model (18). Because the number of covariates is the same in the varying and constant slope models (school and LRT), the I-prior approach yields the same number of hyperparameters in both models. This makes comparison of the models particularly easy, as the model with the highest likelihood can simply be chosen, which is the varying slope model (see Table 7). The random effects approach is more complex, and the distribution of the difference in log-likelihoods must be used. In the present case, this difference has an asymptotic chi-bar distribution (e.g., Rabe-Hesketh & Skrondal, 2012, Section 4.6), and a test leads to rejection of the constant slope model. However, for more complex hypotheses, the null distribution has to be simulated.

6.4 Longitudinal data analysis

We consider a balanced longitudinal data set consisting of weights and 60 cows, 30 of which are randomly assigned to a treatment group \( A \) and 30 to a treatment group \( B \). Weight was measured 11 times over a 133-day period, at two-week intervals, except for the last measurement, which was taken one week after the preceding measurement. As the response variable of interest we
take the weight growth curve. In Figure 4 a sample of growth curves is shown. Of interest is investigating whether a treatment effect is present, and if it is, to assess its nature.

The usual approach to analyze a longitudinal data set such as this one is to assume that the observed growth curves are realizations of a Gaussian process. For example, Kenward (1987) assumed a so-called ante-dependence structure of order $k$, which assumes an observation depends on the previous $k$ observations, but given these is independent of any preceding observations. Various other process families have been considered (Núñez-Antón & Zimmerman, 2000; Pourahmadi, 2000; Pan & Mackenzie, 2003; Zhang, Leng, & Tang, 2014), see the latter for an overview. Steele (2008) points out the connections with multilevel and structural equation modelling.

Using the I-prior, it is not necessary to postulate a distribution for the growth curves. Instead, it suffices to assume they lie in an appropriate function class. In this section we assume this function class is the FBM RKHS, i.e., we assume a 'smooth' effect of time on weight (see Table 9). The growth curves form a multidimensional (or functional) response, so we can use the multidimensional/functional response model of Section 3.3. In the present case we have two covariates potentially influencing growth, namely cow index ($C$, indexed by $i$) and treatment ($X$), and we can write the regression model as

$$y_{it} = f(i, x_i, t) + \varepsilon_{it},$$

where $y_{it}$ is weight of cow $i$ at time $t$, and $x_i \in \{A, B\}$ is the treatment group of cow $i$. We assume i.i.d. zero mean normal errors. As discussed in Section 3.3, we can also interpret the model as a unidimensional response model, where the unidimensional response is weight, and covariates are cow index ($C$), treatment ($X$), and time ($T$). A main effect of $C$ on (multidimensional) growth is then equivalent to an interaction effect of $T$ and $C$ on (unidimensional) weight.

| Covariate  | Range               | RKHS         |
|------------|---------------------|--------------|
| Time ($T$) | 0 – 133 days        | Centered FBM ($\gamma = 0.3$) |
| Cow index ($C$) | 1, …, 60   | Pearson     |
| Treatment ($X$) | $\{A, B\}$   | Pearson     |

Table 9: Covariates used for modelling cow data

We can estimate the Hurst coefficient $\gamma$ of the FBM RKHS using the maximum likelihood estimator, but a difficulty is that it varies a lot across models (for the present data set, we found
estimates between 0.2 and 0.4). To make model comparison easier, we took as a compromise a fixed value $\gamma = 0.3$ for all models; we found that substantive conclusions were not greatly affected by the choice of $\gamma$. The model asserting that the growth curve does not vary with treatment or among cows is denoted $\{\}$ (no effect of either $C$ or $X$ on growth), and can be written as

$$y_{it} = \alpha + f(t) + \varepsilon_{it}.$$  

The model asserting that the growth curve depends on cow but without a treatment effect is denoted $\{C\}$, and can be written as

$$y_{it} = \alpha + \beta_i + f(t) + f^C_i(t) + \varepsilon_{it},$$

subject to the identifying constraints $\sum t f(t) = \sum f^C(t) = 0$ and $\sum_{i=1}^{60} f^C_i(t) = 0$ for all $t$. Here $t$ ranges over 0, 14, ..., 133. Further, $f$ and the $f^C_i$ are functions in the centered FBM RKHS. The model which includes a treatment effect on growth, but without an interaction effect of treatment and cow index, is denoted $\{C,X\}$ and can be formulated as

$$y_{it} = \alpha + \beta_i + \xi_{xi} + f(t) + f^C_i(t) + f^X_i(t) + \varepsilon_{it},$$

where $f^X_i$ also lies in the FBM RKHS. Finally, model $\{CX\}$,

$$y_{it} = \alpha + \beta_i + \xi_{xi} + f(t) + f^C_i(t) + f^X_i(t) + f^{CX}_{i,x}(t) + \varepsilon_{it},$$

generalizes $\{C,X\}$ in that it allows the treatment effect to vary among cows.

In Section 2.3.2, the parsimonious ANOVA RKKS and the less parsimonious extended ANOVA RKKS were described. The former requires a scale parameter for each covariate which has at least a main effect, but no extra parameters for interaction effects, hence models $\{C,X\}$ and $\{CX\}$ have the same number of scale parameters, making comparison of these two models easy, in that simply the one with the highest likelihood can be selected. If the extended ANOVA RKKS is used, one parameter for each main effect and each interaction effect is needed. The two approaches give different likelihoods, as can be seen in the summary in Table 10, but reassuringly yield the same substantive conclusions. In particular, model $\{C,X\}$ is best according to both the AIC and BIC criteria, in both the ANOVA and extended ANOVA approach. Hence, there is evidence for a treatment effect, but there is insufficient evidence that the treatment affects different cows differently. Interestingly, in the extended ANOVA approach, $\{C,X\}$ and $\{CX\}$ give exactly the same fit for this data set.

The extended ANOVA approach resembles classical least squares model selection since there are extra parameters for interaction effects. In this case model $\{C,X\}$ has five parameters, two more than model $\{C\}$, because $X$ has a non-time-varying main effect and a time-varying effect on weight.

Time varying covariates were not available for the present data set but could easily be added. As the data set is balanced (the cows were weighted at the same time points), fitting can be done more efficiently without time varying covariates. However, we have 60 cows and 11 time points, giving $60 \times 11 = 660$ data points, which is easy to handle in any case.

7 Comparison I-priors and existing methods

Bergsma (2020, Section 3) explains the relation with several other priors and methods, including Zellner’s $g$-priors (which can be viewed as I-priors for a linear regression functions when the covariate space is equipped with Mahalanobis distance), Jeffreys priors, and Fisher kernels.
Table 10: Goodness of fit for cow data, see Table 9 for the covariates used. The model consists of the highest order effects on the growth curve, e.g., model \(\{C, X\}\) means the growth curve depends on cow (\(C\)) and treatment (\(X\)), and there is no interaction meaning that the treatment effect is the same for all cows. In the ANOVA models, no extra parameters are needed for interaction effects, and among nested models with the same number of parameters the one with the highest likelihood can be chosen. For the extended ANOVA models, each interaction requires at least one extra parameter.

Below, we explain how RKKSs have previously been used in a regularization context, and we highlight some differences with GP regression and Tikhonov regularization.

Ong et al. (2004) used a regularization framework, where the usual RKHS squared penalty norm \(\|f\|^2_F\) is replaced by the RKKS indefinite inner product \(\langle f, f \rangle_F\). As the latter may be negative, it does not make sense to minimize the “penalized” loss function, and instead they sought a saddle point. Their approach is very different from ours, firstly in that they considered very different RKKSs, and secondly by constructing a Gaussian I-prior over the RKKS the indefiniteness of the inner product becomes irrelevant.

The I-prior methodology has some advantages compared to competing methods, in particular, it has the following properties:

1. Since the support of the I-prior is contained in \(\mathcal{F}\), the posterior distribution of \(f\) under the I-prior is admissible under a broad range of loss functions, that is, there is no other estimator which performs better for any \(f \in \mathcal{F}\).

2. The I-prior is automatic, in the sense that once the kernel for \(\mathcal{F}\) has been chosen, no further user input is needed.

3. An EM algorithm with simple E and M steps for finding the maximum likelihood estimators of the scale parameters of the ANOVA kernel is available (see Section 5).

The main alternatives to I-prior modelling are GP regression and Tikhonov regularization. The first property gives I-prior estimators an advantage over Tikhonov regularizers, which are inadmissible with respect to squared error loss (Chakraborty & Panaretos, 2019). The second property gives the I-prior methodology an advantage over GP regression, which in addition to a metric over \(\mathcal{F}\) requires the user to specify a prior. The third property gives the I-prior methodology an advantage over both Tikhonov regularization and GP regression, for which no simple and generally applicable algorithms are available to estimate scale parameters, which is
potentially problematic if there are multiple covariates. This, in our view, is a major impediment in the broad applicability of these methods.

8 Discussion

The most important reasons for using the I-prior methodology are that, as we aimed to show, it is relatively easy to use, flexible, and yields good predictive power. In particular, I-prior models can be used as a single solution for a wide range of applications where a large variety of methods have been used in the literature. For some well studied data sets we showed that predictive performance is competitive with existing methods. Estimation is greatly facilitated by the availability of a simple EM algorithm, not available for competing methods, as well as the parsimonious ANOVA kernel construction. Comparison of models with the same covariates and different interaction effects (i.e., with the same number of scale parameters in the ANOVA kernel) can straightforwardly be done by comparing likelihoods. The selection of covariates remains not fully solved, but a promising approach is the generalized likelihood ratio test for additive models (Fan & Jiang, 2007).

We used an RKHS/RKKS framework, which may be theoretically motivated as follows. Since prediction is an important aspect of regression analysis, a pointwise consistent estimator of a true regression function $f$ is desirable, i.e., for every $x \in X$, we would like an estimator $\hat{f}_n$ to satisfy $\hat{f}_n(x) \to f(x)$ in probability as $n \to \infty$. RKHSs are precisely those Hilbert spaces of functions in which norm convergence implies pointwise convergence, that is, any normwise consistent estimator $\hat{f}_n$ (i.e., $\|\hat{f}_n - f\|_X \to 0$ in probability) is also pointwise consistent. Hence, the RKHS is a natural choice of Hilbert space for a regression function. Furthermore, due to the availability of a kernel, RKHSs are also convenient for doing computations. For example, in the present context the Fisher information on the regression function exists and has closed form. For the purposes of this present paper, the positive definiteness restriction of the inner product in an RKHS is unnecessarily restrictive, and the extension to the RKKS is natural. Note that for every RKKS there is an RKHS consisting of the same set of functions.

The computational complexity of I-prior modelling is $O(n^3)$, which is the same as for Gaussian process regression and Tikhonov regularization. This becomes prohibitive if, say, $n > 10,000$. The Nyström method can significantly speed computations up and this method is implemented in the package iprior (Jamil, 2019), see Jamil (2018, Section 4.5.3) for details. If all kernels have a particular structure a significant improvement in the computational complexity can be obtained. This is the case for canonical kernels over low dimensional spaces, for Brownian motion kernels over the real line, or for Pearson kernels over a finite set.

Another difficulty with estimation is that the marginal likelihood for the scale parameters may have multiple local maxima, increasing with the number of scale parameters. Our parsimonious approach which has no additional scale parameters for interaction effects reduces this difficulty, but still typically multiple starting points need to be tried with the EM algorithm. Further research is needed to determine good starting values. We do not believe local maxima should be smoothed out in any way, because this would lead to different estimators which we found could lead to a significant deterioration of predictive performance.

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A ANOVA kernel construction

With $\mathcal{V}$ a finite set of variables and any $v \in \mathcal{V}$, let $\mathcal{X}_v$ be nonempty set, let $\mathcal{F}_v$ be the RKKS over $\mathcal{X}_v$ with kernel $h_v$, and let $\mathcal{C}_v$ be the RKHS of constant functions over $\mathcal{X}_v$ with kernel $c_v$ defined by $c_v(x, x') = 1$. Denote the power set of a set $A$ by $\mathcal{P}(A)$, and define the power set of a set of subsets $\mathcal{A}$ as $\mathcal{P}(\mathcal{A}) = \bigcup_{A \in \mathcal{A}} \mathcal{P}(A)$. Let $\mathcal{A}$ be a Sperner family of $\mathcal{V}$, i.e., $\mathcal{A}$ consists of subsets of $\mathcal{V}$ such that no set in $\mathcal{A}$ contains another set in $\mathcal{A}$. Define the RKKS $\mathcal{F}_\mathcal{A}$ over $\times_{v \in \mathcal{V}} \mathcal{X}_v$ as

$$\mathcal{F}_\mathcal{A} = \sum_{A \in \mathcal{P}(\mathcal{A})} \bigotimes_{v \in A} \mathcal{F}_v \bigotimes_{v \in \mathcal{V} \setminus A} \mathcal{C}_v. \quad (30)$$

Then $f \in \mathcal{F}_\mathcal{A}$ are of the form

$$f(x) = \sum_{A \in \mathcal{P}(\mathcal{A})} f_A(x_A)$$

for $x \in \times_{v \in \mathcal{V}} \mathcal{X}_v$, with $x_A$ the subvector of $x$ which retains the coordinates corresponding to $A$. The reproducing kernel of $\mathcal{F}_\mathcal{A}$ is given as

$$h_\mathcal{A} = \sum_{A \in \mathcal{P}(\mathcal{A})} \bigotimes_{v \in A} h_v \bigotimes_{v \in \mathcal{V} \setminus A} c_v.$$
B Kernels over a finite set

Let $\mathcal{X}$ be a finite set and $\{x_1, \ldots, x_n\} \subset \mathcal{X}$ a sample from $\mathcal{X}$. Denote the proportion of the sample equal to $x$ by $p(x) = n^{-1} \sum_{i=1}^{n} \delta_{x, x_i}$, where $\delta$ is the Kronecker delta. The canonical RKHS over $\mathcal{X}$ is defined as the RKHS with reproducing kernel $h_c(x, x') = \delta_{x, x'}$ and the Pearson kernel for $(\mathcal{X}, p)$ is defined as $h_p(x, x') = \delta_{x, x'}/p(x) - 1$ if $p(x) > 0$ and $p(x') > 0$, and $h_p(x, x') = 0$ otherwise. Since $\sum_{i=1}^{n} h_p(x, x_i) = 0$, the Pearson kernel is centered.

We have that $n^{-2} \sum_{i=1}^{n} \sum_{j=1}^{n} \delta_{x_i, x_j} = n^{-1} \sum_{x \in \mathcal{X}} p(x_i)^2$, and the centered canonical kernel is

$$h_c(x, x') = \delta_{x, x'} - p(x) - p(x') + n^{-1} \sum_{t \in \mathcal{X}} p(t)^2$$

Consider model (1) where $\mathcal{F}$ is the RKHS with kernel $h_p$ and the errors are independent $N(0, \psi^{-1})$ random variables. Then the Fisher information $I[f]$ on $f$ evaluated at $(x, x')$ is zero if at least one of $p(x)$ or $p(x')$ is zero, and otherwise

$$I[f](x, x') = \psi \sum_{i=1}^{n} h_p(x, x_i) h_p(x', x_i) = \psi \sum_{i=1}^{n} \left( \delta_{x, x_i}/p(x) - 1 \right) \left( \delta_{x', x_i}/p(x') - 1 \right)$$

$$= \psi \sum_{i=1}^{n} \left( \delta_{x, x_i} \delta_{x', x_i} / p(x) p(x') - \delta_{x, x_i} / p(x) - \delta_{x', x_i} / p(x') + 1 \right) = \psi \left( \delta_{x, x'} / p(x) - 1 \right) = h_p(x, x').$$

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