Regression modelling using priors with Fisher information covariance kernels (I-priors)

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To my parents.

Abstract

I-priors are a class of objective priors on regression functions which makes use of its Fisher information in a function space framework. We present firstly some methodology and computational work on estimating regression functions by working in the appropriate reproducing kernel Hilbert space of functions and assuming an I-prior on the function of interest. Secondly, work on extending the I-prior methodology to categorical responses for classification is presented, in which estimation is performed using a variational approximation to the likelihood. Finally, a fully Bayes approach is considered where we use I-priors for variable selection. http://phd.haziqj.ml and http://myphdcode.haziqj.ml

Keywords: Gaussian process, regression, binary, multinomial, variational, Bayes, empirical Bayes, expectation maximisation, EM algorithm

Declaration

I certify that the thesis I have presented for examination for the MPhil/PhD degree of the London School of Economics and Political Science is solely my own work other than where I have clearly indicated that it is the work of others (in which case the extent of any work carried out jointly by me and any other person is clearly identified in it).

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I declare that my thesis consists of XX,XXX words.

I confirm that Chapters 2 and 3 were jointly co-authored with Dr. Wicher Bergsma, and I contributed 60% of these works.

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Chapter 1

Introduction

Regression analysis is undoubtedly one of the most important tools available at a practitioner's disposal to understand the relationship between one or more explanatory variables x, and the independent variable of interest, y. This relationship is usually expressed as $y \approx f(x;\theta)$, where f is called the *regression function*, and this is dependent on one or more parameters denoted by θ. Regression analysis concerns the estimation of said regression function, and once a suitable estimate $\hat f$ has been found, post-estimation procedures such as prediction, and inference surrounding f or θ, may be performed.

Estimation of the regression function may be done in many ways. This thesis concerns the use of *I-priors* (Bergsma, 2017), in a semi-Bayesian manner, for regression modelling. The I-prior is an objective, entropy-maximising prior for the regression function which makes use of its Fisher information. The essence of regression modelling using I-priors is introduced briefly below, but as the development of I-priors is fairly recent, we dedicate two full chapters (Chapters 2 and 3) to describe the concept fully.

This thesis has three main chapters which we hope to present as methodological innovations surrounding the use of I-priors for regression modelling. Chapter 4 describes computational methods relating to the estimation of I-prior models. Chapter 5 extends the I-prior methodology to fit discrete outcome models. Chapter 6 discusses the use of I-priors for model selection. This short chapter ultimately provides an outline of the thesis, in addition to introducing the statistical model of interest.

1.1 Regression models

sec:introregmod

For subject $i \in \{1, \ldots, n\}$, assume a real-valued response y_i has been observed, as well as a row vector of p covariates $x_i = (x_{i1}, \ldots, x_{ip})$, where each x_{ik} belongs to some set $\mathcal{X}_k$, for $k = 1, \ldots, p$. Let $\mathcal{S} = \{(y_1, x_1), \ldots, (y_n, x_n)\}$ denote this observed sample of size n. Consider then the following regression model, which stipulates the dependence of the y_i on the x_i:

$$y_i = \alpha + f(x_i) + \epsilon_i, \tag{1.1}$$

{eq:model1}

where f is some regression function to be estimated, and α is an intercept. Additionally, it is assumed that the errors ϵ_i are normally distributed according to

$$(\epsilon_1, \ldots, \epsilon_n)^\top \sim \mathrm{N}_n(0, \mathbf{\Psi}^{-1}). \tag{1.2}$$

{eq:model1ass}

where $\mathbf{\Psi} = (\psi_{ij})_{i,j=1}^n$ is the precision matrix. We shall often refer to model (1.1) subject to (1.2) as the *normal regression model*. The choice of multivariate normal errors is not only a convenient one (as far as distributional assumptions go), but one that is motivated by the principle of maximum entropy.

Interestingly, a wide variety of statistical models can be captured by the seemingly humble normal regression model, simply by varying the form of the regression function f. For instance, when f can be parameterised linearly as $f(x_i) = x_i^\top \beta$, $\beta \in \mathbb{R}^p$, we then have the ordinary linear regression—a staple problem in statistics and other quantitative fields.

We might also have that the data is separated naturally into groups or levels by design, for example, data from stratified sampling, students within schools, or longitudinal measurements over time. In such a case, we might want to consider a regression function with additive components

$$f(x_i^{(j)}, j) = f_1(x_i^{(j)}) + f_2(j) + f_{12}(x_i^{(j)}, j)$$

where $x_i^{(j)}$ denotes the p-dimensional ith observation for group $j \in \{1, \ldots, m\}$. Again, assuming a linear parameterisation, this is recognisable as the multilevel or random-effects linear model, with f_2 representing the varying intercept via $f_2(j) = \alpha_j$, f_{12} representing the varying slopes via $f_{12}(x_{ij}, j) = x_i^\top \beta_j$, with $\beta_j \in \mathbb{R}^p$, and f_1 representing the fixed-effects linear component $x_i^\top \beta$ as above.

Moving on from linear models, smoothing models may be of interest as well. A myriad of models exist for this type of problem, with most classed as nonparametric regression, and the more popular ones include LOcal regrESSion (LOESS), kernel regression, and smoothing splines. Semiparametric regression models, on the other hand, combines the linear component of a regression model with a non-parameteric component.

Further, the regression problem is made more intriguing when the set of covariates $\mathcal{X}$ is functional—in which case the linear regression model aims to estimate coefficient functions $\beta : \mathcal{T} \to \mathbb{R}$ from the model

$$y_i = \int_{\mathcal{T}} x_i(t)\beta(t) \, \mathrm{d}t + \epsilon_i.$$

Nonparametric and semiparametric regression with functional covariates have also been widely explored. Models of this nature still fall under the remit of the normal regression model by selecting a regression functional with domain over the functional covariates.

1.2 Vector space of functions

It would be beneficial to prescribe some sort of structure for which 1) we may choose a regression function appropriately, and 2) this function will generalise well to unseen data (prediction). This needed structure is given to us by assuming that our regression function for the normal model lies in some reproducing kernel Hilbert space (RKHS) $\mathcal{F}$ equipped with the reproducing kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. Often, the reproducing kernel (or simply kernel, for short) is indexed by one or more parameters which we shall denote as η. Correspondingly, the kernel is rightfully denoted as h_η to indicate the dependence of the parameters on the kernels, though where this is seemingly obvious, might be omitted. Throughout this thesis we shall make the assumption that our regression function lies in a reproducing kernel Hilbert space $\mathcal{F}$.

RKHSs provides a geometrical advantage to learning algorithms: Projections of the inputs to a richer and more informative (and higher dimensional) feature space, where learning is more likely to be successful, need not be figured out explicitly. Instead, the feature maps are implicitly calculated by the use of kernel functions. This is known as the "kernel trick" in the machine learning literature, and it has facilitated the success of kernel methods for learning, particularly in algorithms with inner products involving the transformed inputs.

Due to the one-to-one mapping between the set of kernel functions and the set of RKHSs, choosing a regression function is equivalent to choosing a kernel function, and this is chosen according to the desired effects of the covariates on the regression function. An in-depth discussion on kernels and RKHSs will be provided later in Chapter 2, but for now, it suffices to say that kernels which invoke a linear, smooth and categorical dependence, are of interest. This would allow us to fit the various models described earlier within this RKHS framework.

1.3 Estimating the regression function

Having decided on a functional structure for f, we now turn to the task of choosing the best $f \in \mathcal{F}$ that fits the data sample $\mathcal{S}$. 'Best' here could mean a great deal of things, such as choosing f which minimises an empirical risk measure[1] defined by

$$\text{ER}[f] = \frac{1}{n}\sum_{i=1}^n \Lambda\big(y_i, f(x_i)\big)$$

for some loss function $\Lambda : \mathbb{R}^2 \to [0,\infty)$. A common choice for the loss function is the *squared loss function*

$$\Lambda\big(y_i, f(x_i)\big) = \sum_{j=1}^n \psi_{ij}\big(y_i - f(x_i)\big)\big(y_j - f(x_j)\big),$$

and when used, defines the *least squares regression*. For the normal model, the minimiser of the empirical risk measure under the squared loss function is also the maximum likelihood (ML) estimate of f, since $\text{ER}[f]$ would be twice the negative log-likelihood of f, up to a constant.

The ML estimator of f interpolates the data if the dimension of $\mathcal{F}$ is at least n, so is of little use. The most common method to overcome this issue is *Tikhonov regularisation*, whereby a regularisation term is added to the risk function, with the aim of imposing a penalty on the complexity of f. In particular, smoothness assumptions on f can be represented by using its RKHS norm $\|\cdot\|_\mathcal{F} : \mathcal{F} \to \mathbb{R}$ as the regularisation term[2]. Therefore, the solution to the regularised least squares problem—call this f_{reg}—is the

[1] More appropriately, the risk functional $\text{R}[f] = \int \Lambda(y, f(x)) \, \text{dP}(y,x)$, i.e., the expectation of the loss function under some probability measure of the observed sample, should be used. Often the true probability measure is not known, so the empirical risk measure is used instead.

minimiser of the function from $\mathcal{F}$ to $\mathbb{R}$ defined by the mapping

$$f \mapsto \frac{1}{n}\sum_{i=1}^n \sum_{j=1}^n \psi_{ij}\big(y_i - f(x_i)\big)\big(y_j - f(x_j)\big) + \lambda^{-1}\Vert f - f_0 \Vert_{\mathcal{F}}^2, \tag{1.3}$$

{eq:penfunctional}

which also happens to be the *penalised maximum likelihood* solution. Here $f_0 \in \mathcal{F}$ can be thought of a prior 'best guess' for the function f. The $\lambda^{-1} > 0$ parameter—known as the regularisation parameter—controls the trade-off between the data-fit term and the penalty term, and is not usually known a priori and must be estimated from the data.

An attractive consequence of the representer theorem (Kimeldorf and Wahba, 1970) for Tikhonov regularisation implies that f_{reg} admits the form

$$f_{\text{reg}} = f_0 + \sum_{i=1}^n h(\cdot, x_i) w_i, \qquad w_i \in \mathbb{R}, \ \forall i = 1, \dots, n, \tag{1.4}$$

{eq:repform}

even if $\mathcal{F}$ is infinite-dimensional. This simplifies the original minimisation problem from a search for f over a possibly infinite-dimensional domain to a search for the optimal coefficients w_i in n dimensions.

Tikhonov regularisation also has a well-known Bayesian interpretation, whereby the regularisation term encodes prior information about the function f. For the normal regression model with $f \in \mathcal{F}$, an RKHS, it can be shown that f_{reg} is the posterior mean of f given a *Gaussian process prior* with mean f_0 and covariance kernel $\operatorname{Cov}\big(f(x_i), f(x_j)\big) = \lambda h(x_i, x_j)$. The exact solution for the coefficients $\mathbf{w} = (w_1, \dots, w_n)^\top$ are in fact $\mathbf{w} = \big(\mathbf{H} + \mathbf{\Psi}^{-1}\big)^{-1}(\mathbf{y} - \mathbf{f}_0)$, where $\mathbf{H} = \big(h(x_i, x_j)\big)_{i,j=1}^n$ (often referred to as the Gram matrix or kernel matrix) and $(\mathbf{y} - \mathbf{f}_0) = (y_1 - f_0(x_1), \dots, y_n - f_0(x_n))^\top$.

1.4 Regression using I-priors

sec:introregiprior

Building upon the Bayesian interpretation of regularisation, Bergsma (2017) proposes a prior distribution for the regression function such that its realisations admit the form for the solution given in the representer theorem. The *I-prior* for the regression function f in (1.1) subject to (1.2) is defined as the distribution of a random function of the form

[2] Concrete notions of complexity penalties can be introduced if $\mathcal{F}$ is a normed space, though RKHSs are typically used as it gives great conveniences (see Chapter 2).

(1.4) when the w_i are distributed according to

$$(w_1, \dots, w_n)^\top \sim \mathrm{N}_n(\mathbf{0}, \mathbf{\Psi}),$$

where $\mathbf{0}$ is a length n vector of zeroes. As a result, we may view the I-prior for f as having the Gaussian process distribution

$$\mathbf{f} := \big(f(x_1), \dots, f(x_n)\big)^\top \sim \mathrm{N}_n(\mathbf{f}_0, \mathbf{H}_\eta \mathbf{\Psi} \mathbf{H}_\eta) \tag{1.5}$$

{eq:iprior}

with $\mathbf{H}_\eta$ an $n \times n$ matrix with (i,j) entries equal to $h_\eta(x_i, x_j)$, and $\mathbf{f}_0$ a vector containing the $f_0(x_i)$'s. The covariance matrix of this multivariate normal prior is related to the Fisher information for f, and hence the name I-prior—the 'I' stands for information. Furthermore, the I-prior happens to be an entropy-maximising prior, subject to certain constraints. More on the I-prior in Chapter 2.

As with Gaussian process regression (GPR), the function f is estimated by its posterior mean. For the normal model, the posterior distribution for the regression function conditional on the responses $\mathbf{y} = (y_1, \dots, y_n)$,

$$p(\mathbf{f}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{f})}{\int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}) \, \mathrm{d}\mathbf{f}}, \tag{1.6}$$

can easily be found, and it is in fact normally distributed. The posterior mean for f evaluated at a point $x \in \mathcal{X}$ is given by

$$\mathrm{E}\left[f(x)\big|\mathbf{y}\right] = f_0(x) + \mathbf{h}_\eta^\top(x) \cdot \overbrace{\mathbf{\Psi}\mathbf{H}_\eta \big(\mathbf{H}_\eta \mathbf{\Psi} \mathbf{H}_\eta + \mathbf{\Psi}^{-1}\big)^{-1}(\mathbf{y} - \mathbf{f}_0)}^{\tilde{\mathbf{w}}} \tag{1.7}$$

{eq:postmean}

where we have defined $\mathbf{h}_\eta(x)$ to be the vector of length n with entries $h_\eta(x, x_i)$ for $i = 1, \dots, n$. Incidentally, the elements of the n-vector $\tilde{\mathbf{w}}$ defined in (1.7) are the posterior means of the random variables w_i in the formulation (1.4). The point-evaluation posterior variance for f is given by

$$\mathrm{Var}\left[f(x)\big|\mathbf{y}\right] = \mathbf{h}_\eta^\top(x) \big(\mathbf{H}_\eta \mathbf{\Psi} \mathbf{H}_\eta + \mathbf{\Psi}^{-1}\big)^{-1} \mathbf{h}_\eta^\top(x). \tag{1.8}$$

{eq:postvar}

Prediction for a new data point $x_{\text{new}} \in \mathcal{X}$ then concerns obtaining the *posterior predictive distribution*

$$p(y_{\text{new}}|\mathbf{y}) = \int p(y_{\text{new}}|f_{\text{new}}, \mathbf{y}) p(f_{\text{new}}|\mathbf{y}) \, \mathrm{d}f_{\text{new}},$$

where we had defined $f_{\text{new}} := f(x_{\text{new}})$. This is again a normal distribution in the case of the normal model, with the same mean[3] as in (1.7), but a slightly different variance. These are of course well-known results in Gaussian process literature—see, for example, Rasmussen and Williams (2006) for details.

There is also the matter of optimising model parameters θ, which in our case, collectively refers to the kernel parameters η and the precision matrix of the errors $\mathbf{\Psi}$. θ may be estimated in several ways, either by likelihood-based methods or fully Bayesian methods. The former includes methods such as direct maximisation of the (marginal) likelihood, $L(\theta) = \int p(\mathbf{y}|\theta, \mathbf{f})p(\mathbf{f}) \mathrm{d}\mathbf{f}$, and the expectation-maximisation (EM) algorithm. Both are seen as a form of *empirical Bayes* estimation. In a fully Bayesian setting on the other hand, Markov chain Monte Carlo methods may be employed, assuming prior distributions on the model parameters.

1.5 Advantages and limitations of I-priors

The I-prior methodology has the following advantages:

1. **A unifying methodology for various regression models.**

   The I-prior methodology has the ability to fit a multitude of regression models simply by choosing the RKHS to which the regression function belongs. As such, it can be seen as a unifying methodology for various regression models.

2. **Simple estimation procedure.**

   Estimation of model parameters using the aforementioned methods are very simple to implement, barring any computational and numerical hurdles, which will be discussed. This encourages parsimony, as the I-prior allows complex models to be specified by just a handful of model parameters.

3. **Prevents over-fitting and under-smoothing.**

   As alluded to earlier, the process of inferring f from data is an "ill-posed" problem. In fact, any function f that passes through the data points is a solution. Regularising the problem with the use of I-priors prevents over-fitting, with the

[3] The fact that it is the same is inconsequential. It happens to be that the mean of the predictive distribution $\mathrm{E}[y_{\text{new}}|\mathbf{y}]$ for a normal model is the same as *prediction of the mean at the posterior*, $\mathrm{E}[f(x_{\text{new}})|\mathbf{y}]$. Rasmussen and Williams, 2006 points out that this is due to symmetries in the model and the posterior.

added advantage that the posterior solution under an I-prior does not tend to under-smooth as much as Tikhonov regularisation does (see Chapter 2 for details). Under-smoothing can adversely impact the estimate of f, and in real terms might even show features and artefacts that are not really there.

4. **Better prediction.**

   Empirical studies and real-data examples show that small and large sample predictive performance of I-priors are comparative to, and often better than, other leading state-of-the-art models, including the closely related Gaussian process regression.

5. **Straightforward inference.**

   Marginal likelihoods after integrating out the I-prior are easily obtained, making model selection via comparison of likelihood a viable option. This method of comparing marginal likelihood with maximum likelihood estimate plug-ins of the model parameters, is viewed as comparing empirical Bayes factors in the Bayesian literature.

6. **Proper prior and posterior**

   Both the I-prior for f and the posterior solution lies in $\mathcal{F}$.

2. Is this an advantage?

The main drawback of using I-prior models computational in nature, namely, the requirement of working with an $n \times n$ matrix and its inverse, as seen in Equations (1.7) and (1.8), regardless of estimation method (ML or Bayes). Analysis of data sets that are not more than a few thousand in size can be considered feasible; anything more than this is debilitatingly slow to compute. In addition, care must be taken to avoid numerical instabilities when calculating the marginal log-likelihood during parameter estimation, which can affect gradient based optimisation or the EM algorithm.

Another issue when performing likelihood based methods is that the optimisation objective may be non-convex such that multiple local optima may exist. In such cases, multiple restarts from different initialisation may ultimately lead to a global maximum, although some difficulties may be faced when numerical instabilities occur.

Lastly, a remark on model assumptions, which are twofold: 1) Assumption of $f \in \mathcal{F}$, some RKHS; and 2) normality of errors. Of the two, the latter is more likely to be violated, especially when dealing with discrete responses, e.g. in classification. Deviating from the normality assumption would require approximation techniques to be implemented in order to obtain the posterior distributions of interest.

1.6 Outline of thesis

This thesis is structured as follows:

- Following this introductory chapter, **Chapter 2** provides a brief overview of functional analysis, and in particular, descriptions of interesting function spaces for regression. In **Chapter 3**, the concept of the Fisher information is extended to potentially infinite-dimensional parameters. This allows us to define the Fisher information for the regression function which parameterises the normal regression model, and we explain how this relates to the I-prior.

- The aforementioned computational methods relating to the estimation of I-prior models are explored in **Chapter 4**, namely the direct optimisation of the log-likelihood, the EM algorithm, and MCMC methods. The goal is to describe a stable and efficient algorithm for estimating I-prior models. The R package **iprior** is the culmination of the effort put in towards completing this chapter, which has been made publicly available on the Comprehensive R Archive Network (CRAN). This chapter has also been submitted for publication to Computational Statistics and Data Analysis.

- Many models of interest involve response variables of a categorical nature. A naïve implementation of the I-prior model is certainly possible, but there is a more proper way to account for non-normality of errors. **Chapter 5** extends the I-prior methodology to discrete outcomes. There, the non-Gaussian likelihood that arises in the posteriors are approximated by way of variational inference. The advantages of the I-prior in normal regression models carry over into categorical response models.

- **Chapter 6** attempts to contribute to the area of variable selection. The use of I-priors in the normal model, like Gaussian process priors, allow model comparison to be done easily. Specifically for linear models with p variables to select from, model comparison requires elucidation of 2^p marginal likelihoods, and this becomes infeasible when p is large. We use a stochastic search method to choose models that have high posterior probabilities of occurring, equivalent to choosing models that have large Bayes factors.

Chapters 4–6 contain computer implementations of the statistical methodologies described therein, and the code for replication are made available at `http://myphdcode.haziqj.ml`.

Chapter 2

Vector space of functions

One of the main assumptions for regression modelling with I-priors is that the regression functions lie in some vector space of functions. The purpose of this chapter is to provide a concise review of functional analysis leading up to the theory of reproducing kernel Hilbert and Kreĭn spaces (RKHS/RKKS). The interest with these RKHS and RKKS is that these spaces have well-established mathematical structure and offer desirable topologies. In particular, it allows the possibility of deriving the Fisher information for regression functions—this will be covered in Chapter 3. As we shall see, RKHS are also extremely convenient in that they may be specified completely via their reproducing kernels. Several of these function spaces are of interest to us, for example, spaces of linear functions, smoothing functions, and functions whose inputs are nominal values and even functions themselves. RKHS are widely studied in the applied statistical and machine learning literature, but perhaps RKKS are less so. To provide an early insight, RKKS are simply a generalisation of RKHS, and are defined as the difference between two RKHSs. The flexibility provided by RKKS will prove both useful and necessary, especially when considering the sums and products of scaled function spaces, as is done in I-prior modelling.

It is emphasised that a deep knowledge of functional analysis, including RKHS and RKKS theory, is not at all necessary for I-prior modelling, so perhaps the advanced reader may wish to skip Sections 2.1–2.3. Section 2.4 describes the fundamental RKHS of interest for I-prior regression, which we refer to as the “building block” RKHS/RKKS. The reason for this is that it is possible to construct new RKKS from existing ones, and this is described in Section 2.5.

A remark on notation: Sets and vector spaces are denoted by calligraphic letters, and as much as possible, we shall stick to the convention that $\mathcal{F}$ denotes function spaces, and $\mathcal{X}$ denotes set of covariates or function inputs. Occasionally, we will describe a generic Hilbert space denoted by $\mathcal{H}$. Elements of the vector space of real functions over a set $\mathcal{X}$ are denoted $f(\cdot)$, or simply f. This distinguishes them from the actual evaluation of the function at an input point $x \in \mathcal{X}$, denoted $f(x) \in \mathbb{R}$. For a much cleaner read, we dispense with boldface notation for vectors and matrices when talking about them, without ambiguity, in the abstract sense.

2.1 Some functional analysis

The core study of functional analysis revolves around the treatment of functions as objects in vector spaces over a field[1]. Vector spaces, or linear spaces as they are sometimes known, may be endowed with some kind of structure so as to allow ideas such as closeness and limits to be conceived. Of particular interest to us is the structure brought about by *inner products*, which allow the rigorous mathematical study of various geometrical concepts such as lengths, directions, and orthogonality, among other things. We begin with the definition of an inner product.

def:innerprod

Definition 2.1 (Inner products)**.** Let $\mathcal{F}$ be a vector space over $\mathbb{R}$. A function $\langle \cdot, \cdot \rangle_\mathcal{F} : \mathcal{F} \times \mathcal{F} \to \mathbb{R}$ is said to be an inner product on $\mathcal{F}$ if all of the following are satisfied:

- **Symmetry:** $\langle f, g \rangle_\mathcal{F} = \langle g, f \rangle_\mathcal{F}$, $\forall f, g \in \mathcal{F}$.
- **Linearity:** $\langle af_1 + bf_2, g \rangle_\mathcal{F} = a\langle f_1, g \rangle_\mathcal{F} + b\langle f_2, g \rangle_\mathcal{F}$, $\forall f_1, f_2, g \in \mathcal{F}$ and $\forall a, b \in \mathbb{R}$.
- **Non-degeneracy:** $\langle f, f \rangle_\mathcal{F} = 0 \Leftrightarrow f = 0$.

Additionally, an inner product is said to be *positive definite* if $\langle f, f \rangle_\mathcal{F} \geq 0$, $\forall f \in \mathcal{F}$. Inner products need not necessarily be positive definite, and we shall revisit this fact later when we cover Krein spaces. However, for the purposes of the discussion moving forward, the inner products that are referenced are the positive definite kind, unless otherwise stated.

We can always define a *norm* on $\mathcal{F}$ using the inner product as

$$\|f\|_\mathcal{F} = \sqrt{\langle f, f \rangle_\mathcal{F}}. \tag{2.1}$$

{eq:normip}

[1] In this thesis, this will be $\mathbb{R}$ exclusively.

Norms are another form of structure that specifically captures the notion of length. This is defined below.

Definition 2.2 (Norms)**.** Let $\mathcal{F}$ be a vector space over $\mathbb{R}$. A non-negative function $||\cdot||_\mathcal{F} : \mathcal{F} \times \mathcal{F} \to [0, \infty)$ is said to be a norm on $\mathcal{F}$ if all of the following are satisfied:

- **Absolute homogeneity:** $||\lambda f||_\mathcal{F} = |\lambda| \cdot ||f||_\mathcal{F}$, $\forall \lambda \in \mathbb{R}$, $\forall f \in \mathcal{F}$
- **Subadditivity:** $||f + g||_\mathcal{F} \leq ||f||_\mathcal{F} + ||g||_\mathcal{F}$, $\forall f, g \in \mathcal{F}$
- **Point separating:** $||f||_\mathcal{F} = 0 \Leftrightarrow f = 0$

The subadditivity property is also known as the *triangle inequality.* Also note that since $\|-f\|_\mathcal{F} = \|f\|_\mathcal{F}$, and by the triangle inequality and point separating property, we have that $\|f\|_\mathcal{F} = \frac{1}{2}\|f\|_\mathcal{F} + \frac{1}{2}\|-f\|_\mathcal{F} \geq \frac{1}{2}\|f - f\|_\mathcal{F} = 0$, thus implying non-negativity of norms. Several important relationships between norms and inner products hold in linear spaces, namely, the *Cauchy-Schwarz inequality*

$$|\langle f, g \rangle_\mathcal{F}| \leq \|f\|_\mathcal{F} \cdot \|g\|_\mathcal{F};$$

the *parallelogram law*

$$\|f + g\|^2_\mathcal{F} - \|f + g\|^2_\mathcal{F} = 2\|f\|^2_\mathcal{F} + 2\|g\|^2_\mathcal{F};$$

and the *polarisation identity*

$$\|f + g\|^2_\mathcal{F} + \|f + g\|^2_\mathcal{F} = 4\langle f, g \rangle_\mathcal{F},$$

for some $f, g \in \mathcal{F}$.

A vector space endowed with an inner product (c.f. norm) is called an inner product space (c.f. normed vector space). As a remark, inner product spaces can always be equipped with a norm using (2.1), but not always the other way around. A norm needs to satisfy the parallelogram law for an inner product to be properly defined.

The norm $||\cdot||_\mathcal{F}$, in turn, induces a metric (a notion of distance) on $\mathcal{F}$: $D(f, g) = ||f - g||_\mathcal{F}$, for $f, g \in \mathcal{F}$. With these notions of distances, one may talk about sequences of functions in $\mathcal{F}$ which are *convergent*, and sequences whose elements become arbitrarily close to one another as the sequence progresses (*Cauchy*).

Definition 2.3 (Convergent sequence)**.** A sequence $\{f_n\}_{n=1}^{\infty}$ of elements of a normed vector space $(\mathcal{F}, ||\cdot||_{\mathcal{F}})$ is said to *converge* to some $f \in \mathcal{F}$, if for every $\epsilon > 0$, $\exists N = N(\epsilon) \in \mathbb{N}$, such that $\forall n > N$, $||f_n - f||_{\mathcal{F}} < \epsilon$.

Definition 2.4 (Cauchy sequence)**.** A sequence $\{f_n\}_{n=1}^{\infty}$ of elements of a normed vector space $(\mathcal{F}, ||\cdot||_{\mathcal{F}})$ is said to be a Cauchy sequence if for every $\epsilon > 0$, $\exists N = N(\epsilon) \in \mathbb{N}$, such that $\forall n, m > N$, $||f_n - f_m||_{\mathcal{F}} < \epsilon$.

Every convergent sequence is Cauchy (from the triangle inequality), but the converse is not true. If the limit of the Cauchy sequence exists within the vector space, then the sequence converges to it. If the vector space contains the limits of all Cauchy sequences (or in other words, if every Cauchy sequence converges), then it is said to be *complete*.

There are special names given to complete vector spaces. A complete inner product space is known as a *Hilbert space*, while a complete normed space is called a *Banach space*. Out of interest, an inner product space that is not complete is sometimes known as a *pre-Hilbert space*, since its completion with respect to the norm induced by the inner product is a Hilbert space.

A subset $\mathcal{G} \subseteq \mathcal{F}$ is a *closed subspace* of $\mathcal{F}$ if it is closed under addition and multiplication by a scalar. That is, for any $g, g' \in \mathcal{G}$, $\lambda_1 g + \lambda_2 g'$ is also in $\mathcal{G}$. For Hilbert spaces, each closed subspace is also complete, and thus a Hilbert space in its own right. Although, as a remark, not every Hilbert subspace need be closed, and therefore complete.

Being vectors in a vector space, we can discuss mapping the vectors onto a different space, or in essence, having a function acted upon them. To establish terminology, we define linear functionals, bilinear form, and linear operators.

Definition 2.5 (Linear functional)**.** Let $\mathcal{F}$ be a Hilbert space. A *functional* L is a map from $\mathcal{F}$ to $\mathbb{R}$, and we denote its action on a function f as $L(f)$. A functional is called *linear* if it satisfies $L(f + g) = L(f) + L(g)$ and $L(\lambda f) = \lambda L(f)$, for all $f, g \in \mathcal{F}$ and $\lambda \in \mathbb{R}$.

Definition 2.6 (Bilinear form)**.** Let $\mathcal{F}$ be a Hilbert space. A *bilinear form* B takes inputs $f, g \in \mathcal{F}$ and returns a real value. It is linear in each argument separately, i.e.

- $B(\lambda_1 f + \lambda_2 g, h) = \lambda_1 B(f, h) + \lambda_2 B(g, h)$; and
- $B(f, \lambda_1 g + \lambda_2 h) = \alpha B(f, g) + \lambda_2 B(f, h)$,

for all $f, g, h \in \mathcal{F}$ and $\lambda_1, \lambda_2 \in \mathbb{R}$.

Definition 2.7 (Linear operator)**.** Let $\mathcal{F}$ and $\mathcal{G}$ be two Hilbert spaces over $\mathbb{R}$. An operator A is a map from $\mathcal{F}$ to $\mathcal{G}$, and we denote its action on a function $f \in \mathcal{F}$ as $Af \in \mathcal{G}$. A *linear operator* satisfies $A(f+g) = A(f) + A(g)$ and $A(\lambda f) = \lambda A(f)$, for all $f, g \in \mathcal{F}$ and $\lambda \in \mathbb{R}$.

The term 'functional' is classically used in calculus of variations to denote 'a function of a function', i.e. a function having another function as its input, and outputs a real number. Really, from a function space perspective, it is simply a mapping of functions onto another vector space (the reals in this case). More generally, if the output space is another Hilbert space, then it is an operator. An interesting property of these operators to look at, besides linearity, is whether or not they are *continuous*.

def:continuity

Definition 2.8 (Continuity)**.** Let $\mathcal{F}$ and $\mathcal{G}$ be two Hilbert spaces. A function $A : \mathcal{F} \to \mathcal{G}$ is said to be *continuous at* $g \in \mathcal{F}$, if for every $\epsilon > 0$, $\exists \delta = \delta(\epsilon, g) > 0$ such that

$$\|f - g\|_{\mathcal{F}} < \delta \quad \Rightarrow \quad \|Af - Ag\|_{\mathcal{G}} < \epsilon.$$

A is *continuous* on $\mathcal{F}$, if it is continuous at every point $g \in \mathcal{F}$. If, in addition, δ depends on ϵ only, A is said to be *uniformly continuous*.

Continuity in the sense of linear operators here means that a convergent sequence in $\mathcal{F}$ can be mapped to a convergent sequence in $\mathcal{G}$. For a special case of linear operator, the evaluation functional, this means that a function in $\mathcal{F}$ is continuous if the evaluation functional is continuous—more on this later in Section 2.2. There is an even stronger notion of continuity called the *Lipschitz continuity*.

Definition 2.9 (Lipschitz continuity)**.** Let $\mathcal{F}$ and $\mathcal{G}$ be two Hilbert spaces. A function $A : \mathcal{F} \to \mathcal{G}$ is *Lipschitz continuous* if $\exists M > 0$ such that $\forall f, f' \in \mathcal{F}$,

$$\|Af - Af'\|_{\mathcal{G}} \leq M \|f - f'\|_{\mathcal{F}}.$$

Clearly, Lipschitz continuity implies uniform continuity: choose $\delta = \delta(\epsilon) := \epsilon / M$ and replace this in Definition 2.8. A continuous, linear operator is also one that is bounded:

def:boundedop

Definition 2.10 (Bounded operator)**.** The linear operator $A : \mathcal{F} \to \mathcal{G}$ between two Hilbert spaces $\mathcal{F}$ and $\mathcal{G}$ is said to be *bounded* if there exists some $M > 0$ such that

$$\|Af\|_{\mathcal{G}} \leq M \|f\|_{\mathcal{F}}.$$

The smallest such M is defined to be the *operator norm*, denoted $\|A\| := \sup_{f \in \mathcal{F}} \frac{\|Af\|_{\mathcal{G}}}{\|f\|_{\mathcal{F}}}$.

thm:boundcont

Lemma 2.1 (Equivalence of boundedness and continuity)**.** *Let $\mathcal{F}$ and $\mathcal{G}$ be two Hilbert spaces, and $A : \mathcal{F} \to \mathcal{G}$ a linear operator. A is a bounded if and only if it is continuous.*

Proof. Suppose that L is bounded. Then, $\forall f, f' \in \mathcal{F}$, there exists some $M > 0$ such that $\|A(f-g)\|_{\mathcal{G}} \leq M\|f-g\|_{\mathcal{G}}$. Conversely, let A be a continuous linear operator, especially at the zero vector. In other words, $\exists \delta > 0$ such that $\|A(f)\|_{\mathcal{G}} = \|A(f+0-0)\|_{\mathcal{G}} = \|A(f) - A(0)\| \leq 1$, $\forall f \in \mathcal{F}$ whenever $\|f\|_{\mathcal{F}} \leq \delta$. Thus, for all non-zero $f \in \mathcal{F}$,

$$\begin{aligned}
\|A(f)\|_{\mathcal{G}} &= \left\| \frac{\|f\|_{\mathcal{F}}}{\delta} A\left(\frac{\delta}{\|f\|_{\mathcal{F}}} f \right) \right\|_{\mathcal{G}} \\
&= \left| \frac{\|f\|_{\mathcal{F}}}{\delta} \right| \cdot \left\| A\left(\frac{\delta}{\|f\|_{\mathcal{F}}} f \right) \right\|_{\mathcal{G}} \\
&\leq \frac{\|f\|_{\mathcal{F}}}{\delta} \cdot 1,
\end{aligned}$$

and thus A is bounded. □

So important is the concept of linearity and continuity, that there are specially named spaces which contain linear and continuous functionals.

Definition 2.11 (Dual spaces)**.** Let $\mathcal{F}$ be a Hilbert space. The space $\mathcal{F}^*$ of *linear functionals* is called the *algebraic dual space* of $\mathcal{F}$. The space $\mathcal{F}'$ of *continuous linear functionals* is called the *continuous dual space* or alternatively, the *topological dual space*, of $\mathcal{F}$.

As it turns out, the algebraic dual space and continuous dual space coincide in finite-dimensional Hilbert spaces: take any $L \in \mathcal{F}'$; since L is finite-dimensional, it is bounded, and therefore continuous (see Lemma 2.1) so $L \in \mathcal{F}'$ and $\mathcal{F}^* \subseteq \mathcal{F}'$; but $\mathcal{F}' \subseteq \mathcal{F}^*$ trivially, so $\mathcal{F}^* \equiv \mathcal{F}'$. For infinite-dimensional Hilbert spaces, this is not so, but in any case, we will only be considering the continuous dual space in this thesis. The following result is an important one, which states that (continuous) linear functionals of an inner product space are nothing more than just inner products.

Theorem 2.2 (Riesz representation)**.** *Let $\mathcal{F}$ be a Hilbert space. Every element L of the continuous dual space $\mathcal{F}'$, i.e. all continuous linear functionals $L : \mathcal{F} \to \mathbb{R}$, can be uniquely written in the form $L = \langle \cdot, g \rangle_{\mathcal{F}}$, for some $g \in \mathcal{F}$.*

Proof. Omitted—see Rudin (1987, Theorem 4.12) for a proof. □

The notion of isometry (transformation that preserves distance) is usually associated with metric spaces—two metric spaces being isometric means that they identical in as far as their metric properties are concerned. For Hilbert spaces (or normed spaces in general), there is an analogous concept as well in *isometric isomorphism* (a bijective isometry), such that two Hilbert spaces being isometrically isomorphic imply that they have exactly the same geometric structure, but may very well contain fundamentally different objects.

Definition 2.12 (Isometric isomorphism)**.** Two Hilbert spaces $\mathcal{F}$ and $\mathcal{G}$ are said to be *isometrically isomorphic* if there is a linear bijective map $A : \mathcal{F} \to \mathcal{G}$ which preserves the inner product, i.e.

$$\langle f, f' \rangle_{\mathcal{F}} = \langle Af, Af' \rangle_{\mathcal{G}}.$$

A consequence of the Riesz representation theorem is that it gives us a canonical isometric isomorphism $A : f \mapsto \langle \cdot, f \rangle_{\mathcal{F}}$ between $\mathcal{F}$ and its continuous dual $\mathcal{F}'$, whereby $\|Af\|_{\mathcal{F}'} = \|f\|_{\mathcal{F}}$. Implicitly, this means that $\mathcal{F}'$ is a Hilbert space as well.

Another important type of mapping is the mapping P of an element in $\mathcal{F}$ onto a closed subspace $\mathcal{G} \subset \mathcal{F}$, such that $Pf \in \mathcal{G}$ is closest to f. This mapping is called the *orthogonal projection*, due to the fact that such projections yield perpendicularity in the sense that $\langle f - Pf, g \rangle_{\mathcal{G}} = 0$ for any $g \in \mathcal{G}$. The remainder $f - Pf$ belongs to the *orthogonal complement* of $\mathcal{G}$.

Definition 2.13 (Orthogonal complement)**.** Let $\mathcal{F}$ be a Hilbert space and $\mathcal{G} \subset \mathcal{F}$ be a closed subspace. The linear subspace $\mathcal{G}^\perp = \{f \,|\, \langle f, g \rangle_{\mathcal{G}} = 0, \forall g \in \mathcal{G}\}$ is called the orthogonal complement of $\mathcal{G}$.

Theorem 2.3 (Orthogonal decomposition)**.** *Let $\mathcal{F}$ be a Hilbert space and $\mathcal{G} \subset \mathcal{F}$ be a closed subspace. For every $f \in \mathcal{F}$, we can write $f = g + g^c$, where $g \in \mathcal{G}$ and $g^c \in \mathcal{G}^\perp$, and this decomposition is unique.*

Proof. Omitted—see Rudin (1987, Theorem 4.11) for a proof. □

We can write $\mathcal{F} = \mathcal{G} \oplus \mathcal{G}^\perp$, where the $\oplus$ symbol denotes the *direct sum*, and such a decomposition is called a *tensor sum decomposition*. In infinite-dimensional Hilbert spaces, some subspaces are not closed, but all orthogonal complements are closed. In such spaces, the orthogonal complement of the orthogonal complement of $\mathcal{G}$ is the closure of $\mathcal{G}$, i.e. $(\mathcal{G}^\perp)^\perp =: \overline{\mathcal{G}}$, and we say that $\mathcal{G}$ is dense in $\overline{\mathcal{G}}$. Another interesting fact regarding the orthogonal complement is that $\mathcal{G} \cap \mathcal{G}^\perp = \{0\}$, since any $g \in \mathcal{G} \cap \mathcal{G}^\perp$ must be orthogonal to itself, i.e. $\langle g, g \rangle_\mathcal{G} = 0$ implying that $g = 0$.

thm:orthdecomp2

Corollary 2.3.1. *Let $\mathcal{G}$ be a subspace of a Hilbert space $\mathcal{F}$. Then, $\mathcal{G}^\perp = \{0\}$ if and only if $\mathcal{G}$ is dense in $\mathcal{F}$.*

Proof. If $\mathcal{G}^\perp = \{0\}$ then $(\mathcal{G}^\perp)^\perp = \overline{\mathcal{G}} = \mathcal{F}$. Conversely, since $\mathcal{G}$ is dense in $\mathcal{F}$, we have $\mathcal{G}^\perp = \overline{\mathcal{G}}^\perp = \mathcal{F}^\perp = \{0\}$. □

Besides tensor sums, of importance is the concept of *tensor products*, which can be thought of as a generalisation of the outer product in Euclidean space.

Definition 2.14 (Tensor products)**.** Let $x_1 \in \mathcal{H}_1$ and $x_2 \in \mathcal{H}_2$ be two elements of two real Hilbert spaces. Then, the tensor product $x_1 \otimes x_2 : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathbb{R}$, is a bilinear form defined as

$$(x_1 \otimes x_2)(y_1, y_2) = \langle x_1, y_1 \rangle_{\mathcal{H}_1} \langle x_2, y_2 \rangle_{\mathcal{H}_2}$$

for any $(y_1, y_2) \in \mathcal{H}_1 \times \mathcal{H}_2$.

Correspondingly, we may also define the *tensor product space.*

Definition 2.15 (Tensor product space)**.** The tensor product space $\mathcal{H}_1 \otimes \mathcal{H}_2$ is the completion of the space

$$\mathcal{A} = \left\{ \sum_{j=1}^J x_{1j} \otimes x_{2j} \,\middle|\, x_{1j} \in \mathcal{H}_1, x_{2j} \in \mathcal{H}_2, J \in \mathbb{N} \right\}.$$

with respect to the norm induced by the inner product

$$\left\langle \sum_{j=1}^J x_{1j} \otimes x_{2j}, \sum_{k=1}^K y_{1k} \otimes y_{2k} \right\rangle_\mathcal{A} = \sum_{j=1}^J \sum_{k=1}^K \langle x_{1j}, y_{1k} \rangle_{\mathcal{H}_1} \langle x_{2j}, y_{2k} \rangle_{\mathcal{H}_2}.$$

Interestingly, the tensor product can be viewed as an operator between two Hilbert spaces. That is, for each pair of elements $(x_1, x_2) \in \mathcal{H}_1 \times \mathcal{H}_2$, we define the operator $A : \mathcal{H}_1 \to \mathcal{H}_2$ in the following way:

$$\begin{aligned} A_{x_1,x_2} : \mathcal{H}_1 &\to \mathcal{H}_2 \\ y_1 &\mapsto \langle x_1, y_1 \rangle_{\mathcal{H}_1} x_2 \end{aligned}$$

For some $y_1 \in \mathcal{H}_1$ and $y_2 \in \mathcal{H}_2$, we have that

$$\begin{aligned}\langle A_{x_1,x_2}(y_1), y_2\rangle_{\mathcal{H}_2} &= \big\langle \langle x_1, y_1\rangle_{\mathcal{H}_1} x_2, y_2 \big\rangle_{\mathcal{H}_2} \\ &= \langle x_1, y_1\rangle_{\mathcal{H}_1} \langle x_2, y_2\rangle_{\mathcal{H}_2} \\ &= (x_1 \otimes x_2)(y_1, y_2).\end{aligned}$$

It is seen that the tensor product $x_1 \otimes x_2$ is is associated with the rank one operator $B : \mathcal{H}_1' \to \mathcal{H}_2$ defined by $z \mapsto z(x_1)x_2$ with $z = \langle x_1, \cdot \rangle_{\mathcal{H}_1}$. We write $B = x_1 \otimes x_2$. Therefore, this extends a linear identification between $\mathcal{H}_1 \otimes \mathcal{H}_2$ and the space of finite-rank operators from $\mathcal{H}_1'$ to $\mathcal{H}_2$. We now have three distinct interpretations of the tensor product:

4. From Wikipedia. But don't really get it, although it might explain the Fisher information between linear functionals.

- **Bilinear form** (as defined in Definition 3.5).

$$\begin{aligned}x_1 \otimes x_2 : \mathcal{H}_1 \times \mathcal{H}_2 &\to \mathbb{R} \\ (y_1, y_2) &\mapsto \langle x_1, y_1\rangle_{\mathcal{H}_1} \langle x_2, y_2\rangle_{\mathcal{H}_2}\end{aligned}$$

  for $x_1, y_1 \in \mathcal{H}_1$ and $x_2, y_2 \in \mathcal{H}_2$.

- **Operator**.

$$\begin{aligned}x_1 \otimes x_2 : \mathcal{H}_1 &\to \mathcal{H}_2 \\ y_1 &\mapsto \langle x_1, y_1\rangle_{\mathcal{H}_1} x_2\end{aligned}$$

- **General form** (as an element in the tensor space).

$$x_1 \otimes x_2 \in \mathcal{H}_1 \otimes \mathcal{H}_2.$$

For the last part of this introductory section on functional analysis, we discuss measures on Hilbert spaces, and in particular, a probability measure. Let $\mathcal{H}$ be a real Hilbert space. As discussed earlier, we can define a metric on $\mathcal{H}$ using $D(x, x') = \|x - x'\|_{\mathcal{H}}$, where the norm on $\mathcal{H}$ is the norm induced by the inner product. A collection Σ of subsets of $\mathcal{H}$ is called a *σ-algebra* if $\emptyset \in \Sigma$, $S \in \Sigma$ implies its complement $S^c \in \Sigma$, and $S_j \in \Sigma$, $j \geq 1$ implies $\bigcup_{j=1}^\infty S_j \in \Sigma$. The smallest σ-algebra containing all open subsets of $\mathcal{H}$ is called the *Borel σ-algebra*, and its members the Borel sets. Denote by $\mathcal{B}(\mathcal{H})$ the Borel σ-algebra of $\mathcal{H}$.

Recall that a function $\nu : \Sigma \to [0, \infty]$ is called a *measure* if it satisfies

- **Non-negativity:** $\nu(S) \geq 0$ for all S in Σ;
- **Null empty set:** $\nu(\emptyset) = 0$; and
- **σ-additivity:** for all countable, mutually disjoint sets $\{S_i\}_{i=1}^\infty$,

$$\nu\left(\bigcup_{i=1}^\infty S_i\right) = \sum_{i=1}^\infty \nu(S_i).$$

A measure ν on $\big(\mathcal{H}, \mathcal{B}(\mathcal{H})\big)$ is called a *Borel measure* on $\mathcal{H}$. We shall only concern ourselves with finite Borel measures. In addition, if $\nu(\mathcal{H}) = 1$ then ν is a *(Borel) probability measure* and the measure space $\big(\mathcal{H}, \mathcal{B}(\mathcal{H}), \nu\big)$ is a *(Borel) probability space.*

Let $(\Omega, \mathcal{E}, \mathrm{P})$ be a probability space. We say that a mapping $X : \Omega \to \mathcal{H}$ is a *random element* in $\mathcal{H}$ if $X^{-1}(B) \in \mathcal{E}$ for every Borel set, i.e., X is a function such that for every $B \in \mathcal{B}(\mathcal{H})$, its preimage $X^{-1}(B) = \{\omega \in \Omega \,|\, X(\omega) \in B\}$ lies in Σ. This is simply a generalisation of the definition of random variables in regular Euclidean space. From this definition, we can also properly define random functions f in a Hilbert space of functions $\mathcal{F}$. In any case, every random element X induces a probability measure on $\mathcal{H}$ defined by

$$\nu(B) = \mathrm{P}\left(X^{-1}(B)\right) = \mathrm{P}\left(\omega \in \Omega | X(\omega) \in B\right) = \mathrm{P}(X \in B).$$

The measure ν is called the *distribution* of X. The *density* p of X is a measurable function with the property that

$$\mathrm{P}(X \in B) = \int_{X^{-1}(B)} \omega \, \mathrm{dP}(\omega) = \int_B p(x) \, \mathrm{d}\nu(x).$$

Definition 2.16 (Mean vector)**.** Let ν be a Borel probability measure on a real Hilbert space $\mathcal{H}$. Supposing that a random element X of $\mathcal{H}$ is *integrable*, that is to say

$$\mathrm{E}\|X\|_\mathcal{H} = \int_\mathcal{H} \|x\|_\mathcal{H} \, \mathrm{d}\nu(x) < \infty,$$

then the unique element $\mu \in \mathcal{H}$ satisfying

$$\langle \mu, x' \rangle = \int_\mathcal{X} \langle x, x' \rangle_\mathcal{X} \, \mathrm{d}\nu(x) = \mathrm{E}\langle X, x' \rangle_\mathcal{H}$$

for all $x' \in \mathcal{H}$ is called the *mean vector.*

Definition 2.17 (Covariance operator)**.** Let ν be a Borel probability measure on a real Hilbert space $\mathcal{H}$. Suppose that a random element X of $\mathcal{H}$ is *square integrable*, i.e., $\operatorname{E}\|X\|_{\mathcal{H}}^2 < \infty$, and let μ be the mean vector of X. Then the *covariance operator* C is defined by the mapping

$$\begin{aligned} C &: \mathcal{H} \to \mathcal{H} \\ & x \mapsto \operatorname{E}\big[\langle X - \mu, x\rangle_{\mathcal{H}}(X-\mu)\big]. \end{aligned}$$

The covariance operator C is also an element of $\mathcal{H} \otimes \mathcal{H}$ that satisfies

$$\begin{aligned} \langle C, x \otimes x'\rangle_{\mathcal{H}\otimes\mathcal{H}} &= \int_{\mathcal{H}} \langle z - \mu, x\rangle_{\mathcal{H}} \langle z - \mu, x'\rangle_{\mathcal{H}} \,\mathrm{d}\nu(z) \\ &= \operatorname{E}\big[\langle X - \mu, x\rangle_{\mathcal{H}}\langle X - \mu, x'\rangle_{\mathcal{H}}\big] \end{aligned}$$

for all $x, x' \in \mathcal{H}$.

From the definition of the covariance operator, we see that it induces a symmetric, bilinear form, which we shall denote by $\operatorname{Cov} : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$, through

$$\begin{aligned} \langle Cx, x'\rangle_{\mathcal{H}} &= \big\langle \operatorname{E}\big[\langle X - \mu, x\rangle_{\mathcal{H}}(X-\mu)\big], x'\big\rangle_{\mathcal{H}} \\ &= \operatorname{E}\big[\langle X - \mu, x\rangle_{\mathcal{H}}\langle X - \mu, x'\rangle_{\mathcal{H}}\big] \\ &=: \operatorname{Cov}(x, x'). \end{aligned}$$

Definition 2.18 (Gaussian vectors)**.** A random element X is called *Gaussian* if $\langle X, x\rangle_{\mathcal{H}}$ has a normal distribution for all fixed $x \in \mathcal{H}$. A Gaussian vector X is characterised by its mean element $\mu \in \mathcal{H}$ and its covariance $C \in \mathcal{H} \otimes \mathcal{H}$.

2.2 Reproducing kernel Hilbert space theory

sec:rkhstheory

The introductory section sets us up nicely to discuss the coveted reproducing kernel Hilbert space. This is a subset of Hilbert spaces for which its evaluation functionals are continuous (by definition, in fact). The majority of this section, apart from defining RKHS, is to convince ourselves that each and every RKHS of functions can be specified solely through its reproducing kernel. To begin, we consider a fundamental linear functional on a Hilbert space of functions $\mathcal{F}$, that assigns a value to $f \in \mathcal{F}$ for each $x \in \mathcal{X}$.

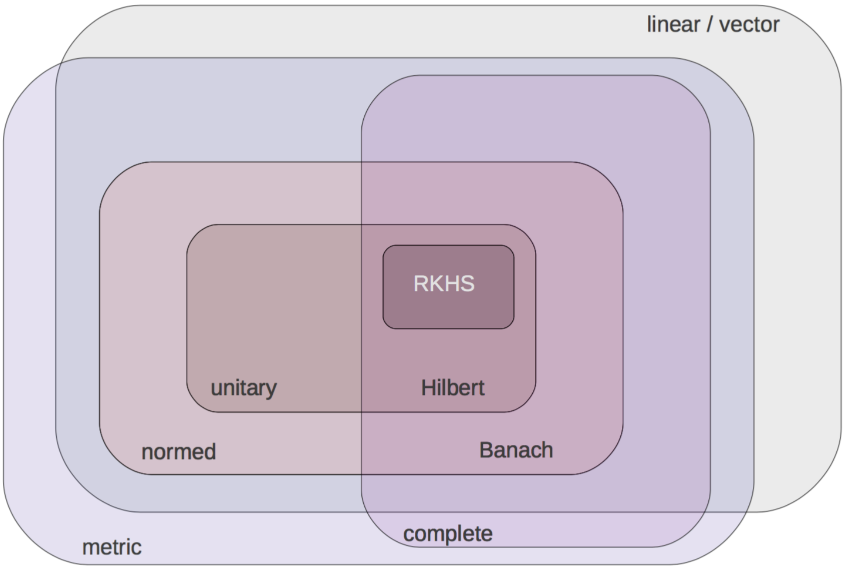


Figure 2.1: A hierarchy of vector spaces[2].

Definition 2.19 (Evaluation functional)**.** Let $\mathcal{F}$ be a vector space of functions $f : \mathcal{X} \to \mathbb{R}$, defined on a non-empty set $\mathcal{X}$. For a fixed $x \in \mathcal{X}$, the functional $\delta_x : \mathcal{F} \to \mathbb{R}$ as defined by $\delta_x(f) = f(x)$ is called the (Dirac) evaluation functional at x.

It is easy to see that evaluation functionals are always linear: $\delta_x(\lambda f + g) = (\lambda f + g)(x) = \lambda f(x) + g(x) = \lambda\delta_x(f) + \delta_x(g)$. This is in fact the linearity that was implied earlier on at the beginning of Chapter 2 when introducing the notion of functions behaving like vectors. As a remark, the calculation of the (penalised) likelihood functional involves evaluations. It is therefore important for the evaluation functional to be continuous. It turns out, this is exactly what RKHS provide.

def:rkhs **Definition 2.20** (Reproducing kernel Hilbert space)**.** A Hilbert space $\mathcal{F}$ of real-valued functions $f : \mathcal{X} \to \mathbb{R}$ on a non-empty set $\mathcal{X}$ is called a *reproducing kernel Hilbert space* if the evaluation functional $\delta_x : f \mapsto f(x)$ is continuous (equivalently, bounded) on $\mathcal{F}$, $\forall x \in \mathcal{X}$.

Continuity of evaluation functionals in an RKHS means that functions that are close in RKHS norm imply that they are also close pointwise, but the converse is not neces-

[2] Reproduced from the lecture slides of Dino Sejdinovic and Arthur Gretton entitled ‘Foundations of Reproducing Kernel Hilbert Spaces: Advanced Topics in Machine Learning’, 2014. URL: http://www.stats.ox.ac.uk/~sejdinov/teaching/atml14/Theory_slides2_2014.pdf.

sarily true. This gives some reassurance when trying to estimate f from $\mathcal{F}$ using the norm of $\mathcal{F}$ as a criterion for selection. More formally,

thm:normpointconv

Corollary 2.3.2 (Norm convergence implies pointwise convergence in RKHS)**.** *Let $\mathcal{F}$ be an RKHS of real functions over $\mathcal{X}$, and let f_n be a sequence of points in $\mathcal{F}$. Then, for some $f \in \mathcal{F}$,*

$$\lim_{n\to\infty} \|f_n - f\|_\mathcal{F} = 0 \quad \Rightarrow \quad \lim_{n\to\infty} |f_n(x) - f(x)| = 0.$$

Proof. Suppose $\mathcal{F}$ is an RKHS with reproducing kernel h. Then,

$$\begin{aligned}
|\delta_x(f) - \delta_x(g)| &= |\delta_x(f-g)| \\
&= |(f-g)(x)| \\
&= |\langle f-g, h(\cdot,x)\rangle_\mathcal{F}| \quad \text{(reproducing property)} \\
&\leq \|h(\cdot,x)\|_\mathcal{F} \cdot \|f-g\|_\mathcal{F} \quad \text{(by Cauchy-Schwarz)} \\
&= \sqrt{h(x,x)} \cdot \|f-g\|_\mathcal{F}.
\end{aligned}$$

□

Insert figure squiggly line and smooth line.

While the continuity condition by definition is what makes an RKHS, it is neither easy to check this condition in practice, nor is it intuitive as to the meaning of its name. In fact, there isn't even any mention of what a reproducing kernel actually is. In order to benefit from the desirable continuity property of RKHS, we should look at this from another, more intuitive, perspective. By invoking the Riesz representation theorem, we see that for all $x \in \mathcal{X}$, there exists a unique element $h_x \in \mathcal{F}$ such that

$$f(x) = \delta_x(f) = \langle f, h_x\rangle_\mathcal{F}, \forall f \in \mathcal{F}$$

holds. Since h_x itself is a function in $\mathcal{F}$, it holds that for every $x' \in \mathcal{X}$ there exists a $h_{x'} \in \mathcal{F}$ such that

$$h_x(x') = \delta_{x'}(h_x) = \langle h_x, h_{x'}\rangle_\mathcal{F}.$$

This leads us to the definition of a *reproducing kernel* of an RKHS—the very notion that inspired its name.

def:repkern

Definition 2.21 (Reproducing kernels)**.** Let $\mathcal{F}$ be a Hilbert space of functions over a non-empty set $\mathcal{X}$. A symmetric, bivariate function $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a *kernel*, and it is a *reproducing kernel* of $\mathcal{F}$ if h satisfies

- $\forall x \in \mathcal{X}$, $h(\cdot, x) \in \mathcal{F}$; and
- $\forall x \in \mathcal{X}$, $f \in \mathcal{F}$, $\langle f, h(\cdot, x) \rangle_{\mathcal{F}} = f(x)$ (the reproducing property).

In particular, for any $x, x' \in \mathcal{X}$,

$$h(x, x') = \langle h(\cdot, x), h(\cdot, x') \rangle_{\mathcal{F}}.$$

An important property for reproducing kernels of a RKHS is that they are positive-definite functions. That is, $\forall \lambda_1, \dots, \lambda_n \in \mathbb{R}$ and $\forall x_1, \dots, x_n \in \mathcal{X}$,

$$\sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j h(x_i, x_j) \geq 0.$$

thm:posdef

Claim 2.4 (Reproducing kernels of RKHS are positive-definite)**.** *Let $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a reproducing kernel for a Hilbert space $\mathcal{F}$. Then h is a symmetric and positive definite function.*

Proof.

$$\begin{aligned}
\sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j h(x_i, x_j) &= \sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j \langle h(\cdot, x_i), h(\cdot, x_j) \rangle_{\mathcal{F}} \\
&= \left\langle \sum_{i=1}^n \lambda_i h(\cdot, x_i), \sum_{j=1}^n \lambda_j h(\cdot, x_j) \right\rangle_{\mathcal{F}} \\
&= \left\| \sum_{i=1}^n \lambda_i h(\cdot, x_i) \right\|_{\mathcal{F}}^2 \\
&\geq 0
\end{aligned}$$

□

Remark 2.1. In the kernel method literature, a *kernel* $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is usually defined as the inner product between inputs in feature space. That is, take $\phi : \mathcal{X} \to \mathcal{V}$, $x \mapsto \phi(x)$, where $\mathcal{V}$ is a Hilbert space. Then the kernel is defined as $h(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{V}}$, for any $x, x' \in \mathcal{X}$. $\mathcal{V}$ is known as the *feature space* and ϕ the *feature map*. In many mathematical models involving feature space mappings, elucidation of the feature map and feature space is not necessary, and computation is made simpler by the use of kernels (known as the *kernel trick*). Note that kernels defined in this manner are positive definite, while in this thesis, we opt for a more general definition allowing for non-positive kernels.

Introducing the following definition of the *kernel matrix* (also known as the *Gram matrix*) is useful at this point.

Definition 2.22 (Kernel matrix)**.** Let $\{x_1, \dots, x_n\}$ be a sample of points, where each $x_i \in \mathcal{X}$, and h a kernel over $\mathcal{X}$. Define the *kernel matrix* $\mathbf{H}$ for h as the $n \times n$ matrix with (i,j) entries equal to $h(x_i, x_j)$.

Now, one might ask what the relationship between a reproducing kernel and a RKHS is. We assert the following:

- **RKHS $\Leftrightarrow$ reproducing kernel**. For every RKHS $\mathcal{F}$ of functions over a set $\mathcal{X}$, there corresponds a unique, positive-definite reproducing kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, and vice-versa.
- **P.d. function $\Rightarrow$ RKHS**. For every positive-definite function $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, there corresponds a unique RKHS $\mathcal{F}$ that has h as its reproducing kernel.

In essence, there is a bijection between the set of positive-definite kernels and the set of reproducing kernel Hilbert spaces. The rest of this subsection is a discussion of this assertion, which is proven by the two theorems that follow.

thm:rkhsunique

Theorem 2.5 (RKHS uniqueness)**.** *Let $\mathcal{F}$ be a Hilbert space of functions over $\mathcal{X}$. $\mathcal{F}$ is a RKHS if and only if $\mathcal{F}$ has a reproducing kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, and that h is unique to $\mathcal{F}$.*

Proof. First we tackle existence, i.e., we prove that $\mathcal{F}$ is a RKHS if and only if $\mathcal{F}$ has a reproducing kernel. Suppose $\mathcal{F}$ is a Hilbert space of functions, and $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a reproducing kernel for $\mathcal{F}$. Then, choosing $\delta = \epsilon / \|h(\cdot, x)\|_\mathcal{F}$, for any $f \in \mathcal{F}$ such that $\|f - g\|_\mathcal{F} < \delta$, we have

$$\begin{aligned}
|\delta_x(f) - \delta_x(g)| &= |(f-g)(x)| \\
&= |\langle f - g, h(\cdot, x) \rangle_\mathcal{F}| \quad \text{(reproducing property)} \\
&\leq \|h(\cdot, x)\|_\mathcal{F} \cdot \|f - g\|_\mathcal{F} \quad \text{(by Cauchy-Schwarz)} \\
&= \epsilon.
\end{aligned}$$

Thus, the evaluation functional is (uniformly) continuous on $\mathcal{F}$, and by definition, $\mathcal{F}$ is a RKHS. Now suppose that $\mathcal{F}$ is a RKHS, and h is a kernel function over $\mathcal{X} \times \mathcal{X}$. The reproducing property of h is had by following the argument preceding Definition 2.21.

As for uniqueness, assume that the RKHS $\mathcal{F}$ has two reproducing kernels h_1 and h_2. Then, $\forall f \in \mathcal{F}$ and $\forall x \in \mathcal{X}$,

$$\langle f, h_1(\cdot, x) - h_2(\cdot, x) \rangle_{\mathcal{F}} = f(x) - f(x) = 0.$$

In particular, if we take $f = h_1(\cdot, x) - h_2(\cdot, x)$, we obtain $\|h_1(\cdot, x) - h_2(\cdot, x)\|^2_{\mathcal{F}} = 0$. Thus, $h_1 = h_2$. □

thm:moorea

Theorem 2.6 (Moore-Aronszajn)**.** *If $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a positive-definite function then there exists a unique RKHS whose reproducing kernel is h.*

Sketch proof. Most of the details here have been omitted, except for the parts which we feel are revealing as to the properties of an RKHS. For a complete proof, see Berlinet and Thomas-Agnan (2011). Start with the linear space

$$\mathcal{F}_0 = \left\{ f_n : \mathcal{X} \to \mathbb{R} \,\middle|\, f_n = \sum_{i=1}^n w_i h(\cdot, x_i), x_i \in \mathcal{X}, w_i \in \mathbb{R}, n \in \mathbb{N} \right\}$$

and endow this linear space with the following inner product:

$$\left\langle \sum_{i=1}^n w_i h(\cdot, x_i), \sum_{j=1}^m w'_j h(\cdot, x'_j) \right\rangle_{\mathcal{F}_0} = \sum_{i=1}^n \sum_{j=1}^m w_i w'_j h(x_i, x'_j).$$

It may be shown that this indeed a valid inner-product satisfying the conditions laid in Definition 2.1. At this point, the reproducing property is already had:

$$\begin{aligned}
\langle f_n, h(\cdot, x) \rangle_{\mathcal{F}_0} &= \left\langle \sum_{i=1}^n w_i h(\cdot, x_i), h(\cdot, x) \right\rangle_{\mathcal{F}_0} \\
&= \sum_{i=1}^n w_i h(x_i, x) \\
&= f_n(x),
\end{aligned}$$

for any $f_n \in \mathcal{F}_0$.

Let $\mathcal{F}$ be the completion of $\mathcal{F}_0$ with respect to this inner product. In other words, define $\mathcal{F}$ to be the set of functions $f : \mathcal{X} \to \mathbb{R}$ for which there exists a Cauchy sequence $\{f_n\}_{n=1}^\infty$ in $\mathcal{F}_0$ converging pointwise to $f \in \mathcal{F}$. The inner product for $\mathcal{F}$ is defined to be

$$\langle f, f' \rangle_\mathcal{F} = \lim_{n\to\infty} \langle f_n, f'_n \rangle_{\mathcal{F}_0}.$$

The sequence $\{\langle f_n, f'_n \rangle_{\mathcal{F}_0}\}_{n=1}^\infty$ is convergent and does not depend on the sequence chosen, but only on the limits f and f' (Berlinet and Thomas-Agnan, 2011, Lemma 5). We may check that this indeeds defines a valid inner product. The reproducing property carries over to the completion:

$$\begin{aligned}
\langle f, h(\cdot,x) \rangle_\mathcal{F} &= \lim_{n\to\infty} \langle f_n, h(\cdot,x) \rangle_{\mathcal{F}_0} \\
&= \lim_{n\to\infty} f_n(x) \\
&= f(x).
\end{aligned}$$

To prove uniqueness, let $\mathcal{G}$ be another RKHS with reproducing kernel h. $\mathcal{F}$ has to be a closed subspace of $\mathcal{G}$, since $h(\cdot,x) \in \mathcal{G}$ for all $x \in \mathcal{X}$, and because $\mathcal{G}$ is complete and contains $\mathcal{F}_0$ and hence its completion. Using the orthogonal decomposition theorem, we have $\mathcal{G} = \mathcal{F} \oplus \mathcal{F}^\perp$, i.e. any $g \in \mathcal{G}$ can be decomposed as $g = f + f^c$, $f \in \mathcal{F}$ and $f^c \in \mathcal{F}^\perp$. For each element $g \in \mathcal{G}$ we have that, for all $x \in \mathcal{X}$,

$$\begin{aligned}
g(x) &= \langle g, h(\cdot,x) \rangle_\mathcal{G} \\
&= \big\langle f + f^c, h(\cdot,x) \big\rangle_\mathcal{G} \\
&= \big\langle f, h(\cdot,x) \big\rangle_\mathcal{G} + \cancelto{0}{\big\langle f^c, h(\cdot,x) \big\rangle_\mathcal{G}} \\
&= f(x)
\end{aligned}$$

so therefore $g \in \mathcal{F}$ too. It must be that $\mathcal{F} \equiv \mathcal{G}$. □

A consequence of the above proof is that we can show that any function f in a RKHS $\mathcal{F}$ with kernel h can be written in the form $f(x) = \sum_{i=1}^n h(x, x_i) w_i$, with some $(w_1, \dots, w_n) \in \mathbb{R}^n$, $n \in \mathbb{N}$. More precisely, $\mathcal{F}$ is the completion of the space $\mathcal{G} = \operatorname{span}\{h(\cdot,x) \,|\, x \in \mathcal{X}\}$ endowed with the inner product as stated in Section 2.2.

2.3 Reproducing kernel Kreĭn space theory

In this section, we shall review basic Kreĭn and reproducing kernel Kreĭn space theory, and comment on the similarity and differences between it and RKHS. Kreĭn spaces are spaces endowed with a Hilbertian topology, characterised by an inner product which is non-positive.

Definition 2.23 (Negative and indefinite inner products)**.** Let $\langle \cdot, \cdot \rangle_{\mathcal{F}}$ be an inner product of a vector space $\mathcal{F}$, as per Definition 2.1. An inner product is said to be *negative-definite* if for all $f \in \mathcal{F}$, $\langle f, f \rangle_{\mathcal{F}} \leq 0$. It is *indefinite* if it is neither positive- nor negative-definite.

Definition 2.24 (Kreĭn space)**.** An inner product space $\big(\mathcal{F}, \langle \cdot, \cdot \rangle_{\mathcal{F}}\big)$ is a *Krein space* if there exists two Hilbert spaces $\big(\mathcal{F}_+, \langle \cdot, \cdot \rangle_{\mathcal{F}_+}\big)$ and $\big(\mathcal{F}_-, \langle \cdot, \cdot \rangle_{\mathcal{F}_-}\big)$ spanning $\mathcal{F}$ such that

- All $f \in \mathcal{F}$ can be decomposed into $f = f_+ + f_-$, where $f_+ \in \mathcal{F}_+$ and $f_- \in \mathcal{F}_-$.
- This decomposition is orthogonal, i.e. $\mathcal{F}_+ \cup \mathcal{F}_- = \{0\}$, and $\langle f_+, f_- \rangle_{\mathcal{F}} = 0$ for all $f_+ \in \mathcal{F}_+$ and $f_- \in \mathcal{F}_-$, with the inner product on $\mathcal{F}$ defined below.
- $\forall f, f' \in \mathcal{F}$, $\langle f, f' \rangle_{\mathcal{F}} = \langle f_+, f'_+ \rangle_{\mathcal{F}_+} - \langle f_-, f'_- \rangle_{\mathcal{F}_-}$.

Let P be the projection of the Kreĭn space $\mathcal{F}$ onto $\mathcal{F}_+$, and $Q = I - P$ the projection onto $\mathcal{F}_-$. These are caleld the *fundamental projections* of $\mathcal{F}$. We shall refer to $\mathcal{F}_+$ as the *positive subspace*, and $\mathcal{F}_-$ as the *negative subspace*. These monikers stem from the fact that for all $f, f' \in \mathcal{F}$, $\langle Pf, Pf' \rangle_{\mathcal{F}_+} \geq 0$ while $\langle Qf, Qf' \rangle_{\mathcal{F}_-} \leq 0$. We introduce the notation $\ominus$ to refer to the Kreĭn space decomposition: $\mathcal{F} = \mathcal{F}_+ \ominus \mathcal{F}_-$. There is then a notion of an *associated Hilbert space*.

Definition 2.25 (Associated Hilbert space)**.** Let $\mathcal{F}$ be a Kreĭn space with decomposition into Hilbert spaces $\mathcal{F}_+$ and $\mathcal{F}_-$. Denote by $\mathcal{F}_{\mathcal{H}}$ the associated Hilbert space defined by $\mathcal{F}_{\mathcal{H}} = \mathcal{F}_+ \oplus \mathcal{F}_-$, with inner product

$$\langle f, f' \rangle_{\mathcal{F}_{\mathcal{H}}} = \langle f_+, f'_+ \rangle_{\mathcal{F}_+} + \langle f_-, f'_- \rangle_{\mathcal{F}_-},$$

for all $f, f' \in \mathcal{F}$.

The associated Hilbert space can be found via the linear operator $J = P - Q$ called the *fundamental symmetry*. That is, a Kreĭn space $\mathcal{F}$ can be turned into its associated Hilbert space by using the positive-definite inner product of the associated Hilbert space as $\langle f, f' \rangle_{\mathcal{F}_{\mathcal{H}}} = \langle f, Jf' \rangle_{\mathcal{F}}$, for all $f, f' \in \mathcal{F}$. The converse is true too: Starting from a

Hilbert space $\mathcal{F}_\mathcal{H}$ and an operator J, the vector space endowed with the inner product $\langle f, f' \rangle_\mathcal{F} = \langle f, Jf' \rangle_{\mathcal{F}_\mathcal{H}}$, for all $f, f' \in \mathcal{F}$, is a Kreĭn space.

We realise that for a Kreĭn space $\mathcal{F}$, $|\langle f, f \rangle_\mathcal{F}| \leq \|f\|^2_{\mathcal{F}_\mathcal{H}}|$ for all $f \in \mathcal{F}$, and we say that $\mathcal{F}_\mathcal{H}$ majorises the $\mathcal{F}$, and in fact it is the smallest Hilbert space to do so. The strong topology on $\mathcal{F}$ is defined to be the topology arising from the norm of $\mathcal{F}_\mathcal{H}$, and this does not depend on the decomposition chosen (Ong et al., 2004).

Definition 2.26 (Reproducing kernel Krein space)**.** A Krein space $\mathcal{F}$ of real-valued functions $f : \mathcal{X} \to \mathbb{R}$ on a non-empty set $\mathcal{X}$ is called a *reproducing kernel Krein space* if the evaluation functional $\delta_x : f \mapsto f(x)$ is continuous on $\mathcal{F}$, $\forall x \in \mathcal{X}$, endowed with its strong topology (i.e. the topology of its associated Hilbert space $\mathcal{F}_\mathcal{H}$).

One might wonder whether the uniqueness theorem (Theorem 2.5) holds for RKKS. Indeed, for every RKKS $\mathcal{F}$ of functions over a set $\mathcal{X}$, there corresponds a unique reproducing kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.

Lemma 2.7 (Uniqueness of kernel for RKKS)**.** *Let $\mathcal{F}$ be a RKKS of functions over a set $\mathcal{X}$, with $\mathcal{F} = \mathcal{F}_+ \ominus \mathcal{F}_-$. Then, $\mathcal{F}_+$ and $\mathcal{F}_-$ are both RKHS with kernel h_+ and h_-, and the kernel $h = h_+ - h_-$ is a unique, symmetric, reproducing kernel for $\mathcal{F}$.*

Proof. Since $\mathcal{F}$ is a RKKS, evaluation functionals are continuous on $\mathcal{F}$ with respect to topology of the associated Hilbert space $\mathcal{F}_\mathcal{H} = \mathcal{F}_+ \oplus \mathcal{F}_-$. Therefore, $\mathcal{F}_\mathcal{H}$ is a RKHS, and so too are $\mathcal{F}_+$ and $\mathcal{F}_-$ with respective kernels h_+ and h_-.

Furthermore, $h(\cdot, x) \in \mathcal{F}$ since $h_+(\cdot, x) \in \mathcal{F}_+$ and $h_-(\cdot, x) \in \mathcal{F}_-$ for some $x \in \mathcal{X}$. Then, for any $f \in \mathcal{F}$,

$$\begin{aligned}
\langle f, h(\cdot, x) \rangle_\mathcal{F} &= \langle f, h_+(\cdot, x) \rangle_\mathcal{F} - \langle f, h_-(\cdot, x) \rangle_\mathcal{F} \\
&= \langle f_+, h_+(\cdot, x) \rangle_{\mathcal{F}_+} - \cancelto{0}{\langle f_-, h_+(\cdot, x) \rangle_{\mathcal{F}_-}} \\
&\qquad - \cancelto{0}{\langle f_+, h_-(\cdot, x) \rangle_{\mathcal{F}_+}} + \langle f_-, h_-(\cdot, x) \rangle_{\mathcal{F}_-} \\
&= f_+(x) + f_-(x) \\
&= f(x)
\end{aligned}$$

The last two lines are achieved by linearity of evaluation functionals ($\delta_x(f_+) + \delta_x(f_-) = \delta_x(f_+ + f_-)$), and the fact that $f = f_+ + f_-$ (by the Kreĭn space decomposition). We have that $h = h_+ - h_-$ is a reproducing kernel for $\mathcal{F}$. Uniqueness follows as a consequence of the non-degeneracy condition of the respective inner products for $\mathcal{F}_+$ and $\mathcal{F}_-$. □

Remark 2.2. Unlike reproducing kernels of RKHSs, reproducing kernels of RKKSs may not be positive-definite.

The analogue of the Moore-Aronszajn theorem holds partially for RKKS, up to uniqueness. That is, there is *at least* one associated RKKS with kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ if and only if h can be decomposed as the difference between two positive kernels h_+ and h_- over $\mathcal{X}$, i.e., $h = h_+ - h_-$. The proof of this statement is rather involved, so is omitted in the interest of maintaining coherence to the discussion at hand. This subject has been studied by various authors, one may refer to works by Alpay (1991, Theorem 2 & Example in Section 4), and Mary (2003, Theorem 2.28).

The take-away message as we close this section is that there is no bijection, but a surjection, between the set of RKKS and the set of bivariate, symmetric functions over $\mathcal{X} \times \mathcal{X}$. In any case, Hilbertian topology applies to Kreĭn spaces via the associated Hilbert space, and in particular, RKKS provide a functional space for which evaluation functionals are continuous. The motivation for the use of Kreĭn spaces will become clear when constructing function spaces out of (scaled) building block RKHS later in Section 2.5.

2.4 RKHS building blocks

This section describes what we refer to as the "building block" RKHS of functions. In the context of regression modelling, we may assume that the regression function lies in any one of these single RKHS, although it may be more appropriate to consider function spaces built upon these RKHS for more complex models. Construction of new function spaces from these building block RKHS will be discussed in the next section.

6. Update graphics.

2.4.1 The RKHS of constant functions

The vector space of constant functions $\mathcal{F}$ over a set $\mathcal{X}$ contains the functions $f : \mathcal{X} \to \mathbb{R}$ such that $f(x) = c_f \in \mathbb{R}, \forall x \in \mathcal{X}$. These functions would be useful to model an overall average, i.e. an "intercept effect". The space $\mathcal{F}$ can be equipped with a norm to form an RKHS, as shown in the following lemma.

Proposition 2.8 (RKHS of constant functions)**.** *The space $\mathcal{F}$ as described above endowed with the norm $\|f\|_{\mathcal{F}} = |c_f|$ forms an RKHS with the reproducing kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ as defined, rather simply by,*

$$h(x, x') = 1,$$

known as the constant kernel.

Proof. If $\mathcal{F}$ is an RKHS with kernel h as described, then $\mathcal{F}$ is spanned by the functions $h(\cdot, x) = 1$, so it is clear that $\mathcal{F}$ consists of constant functions over $\mathcal{X}$. On the other hand, if the space $\mathcal{F}$ is equipped with the inner product $\langle f, f' \rangle_{\mathcal{F}} = c_f c_{f'}$, then the reproducing property follows, since $\langle f, h(\cdot, x) \rangle_{\mathcal{F}} = c_f = f(x)$. Hence, $\|f\|_{\mathcal{F}} = \sqrt{\langle f, f \rangle_{\mathcal{F}}} = |c_f|$. □

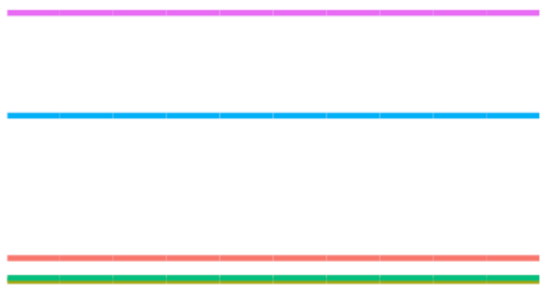


Figure 2.2: Sample paths from the RKHS of constant functions.

2.4.2 The canonical (linear) RKHS

Consider a function space $\mathcal{F}$ over $\mathcal{X}$ which consists of functions of the form $f_\beta : \mathcal{X} \to \mathbb{R}$, $f_\beta : x \mapsto \langle x, \beta \rangle_{\mathcal{X}}$ for some $\beta \in \mathbb{R}$. Suppose that $\mathcal{X} \equiv \mathbb{R}^p$, then $\mathcal{F}$ consists of the linear functions $f_\beta(x) = x^\top \beta$. More generally, if $\mathcal{X}$ is a Hilbert space, then its continuous dual consists of elements of the form $f_\beta = \langle \cdot, \beta \rangle_{\mathcal{X}}$ by the Riesz representation theorem. We can show that the continuous dual space of $\mathcal{X}$ is a RKHS which consists of these linear functions.

Proposition 2.9 (The canonical RKHS)**.** *The continuous dual space a Hilbert space $\mathcal{X}$, denoted by $\mathcal{X}'$, is a RKHS of linear functions over $\mathcal{X}$ of the form $\langle \cdot, \beta \rangle_{\mathcal{X}}$, $\beta \in \mathcal{X}$. Its* *reproducing kernel* $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ *is defined by*

$$h(x, x') = \langle x, x' \rangle_{\mathcal{X}}.$$

Proof. Define $f_\beta := \langle \cdot, \beta \rangle_{\mathcal{X}}$ for some $\beta \in \mathcal{X}$. Clearly this is linear and continuous, so $f_\beta \in \mathcal{X}'$, and so $\mathcal{X}'$ is a Hilbert space containing functions $f : \mathcal{X} \to \mathbb{R}$ of the form $f_\beta(x) = \langle x, \beta \rangle_{\mathcal{X}}$. By the Riesz representation theorem, every element of $\mathcal{X}'$ has the form f_β. It also gives us a natural isometric isomorphism such that the following is true:

$$\langle \beta, \beta' \rangle_{\mathcal{X}} = \langle f_\beta, f_{\beta'} \rangle_{\mathcal{X}'}.$$

Hence, for any $f_\beta \in \mathcal{X}'$,

$$\begin{aligned} f_\beta(x) &= \langle x, \beta \rangle_{\mathcal{X}} \\ &= \langle f_x, f_\beta \rangle_{\mathcal{X}'} \\ &= \big\langle \langle \cdot, x \rangle_{\mathcal{X}}, f_\beta \big\rangle_{\mathcal{X}'}. \end{aligned}$$

Thus, $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ as defined by $h(x, x') = \langle x, x' \rangle_{\mathcal{X}}$ is the reproducing kernel of $\mathcal{X}'$. □

In many other literature, the kernel $h(x, x') = \langle x, x' \rangle_{\mathcal{X}}$ is also known as the *linear kernel*. The use of the term 'canonical' is fitting not just due to the relation between a Hilbert space and its continuous dual space. Let $\phi : \mathcal{X} \to \mathcal{V}$ be the feature map from the space of covariates (inputs) to some feature space $\mathcal{V}$. Suppose both $\mathcal{X}$ and $\mathcal{V}$ are Hilbert spaces, then a kernel is defined as

$$h(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{V}}.$$

Taking the feature map to be $\phi(x) = \langle \cdot, x \rangle_{\mathcal{X}}$, we can prove the reproducing property to obtain $h(x, x') = \langle x, x' \rangle_{\mathcal{X}}$, which implies $\phi(x) = h(\cdot, x)$, and thus ϕ is the *canonical feature map* (Steinwart and Christmann, 2008, Lemma 4.19).

The origin of a Hilbert space may be arbitrary, in which case a centring may be appropriate. We define the centred canonical RKHS as follows.

Definition 2.27 (Centred canonical RKHS)**.** Let $\mathcal{X}$ be a Hilbert space, P be a probability measure over $\mathcal{X}$, and $\mu \in \mathcal{X}$ be the mean of a random element $X \in \mathcal{X}$. Define $(\mathcal{X} - \mu)'$, the continuous dual space of $\mathcal{X} - \mu$, to be the *centred canonical RKHS*. $(\mathcal{X} - \mu)'$ consists of the centred linear functions $f_\beta(x) = \langle x - \mu, \beta \rangle_{\mathcal{X}}$, for $\beta \in \mathcal{X}$, such that $\operatorname{E} f_\beta(X) = 0$. The reproducing kernel of $(\mathcal{X} - \mu)'$ is

$$h(x, x') = \langle x - \mu, x' - \mu \rangle_{\mathcal{X}}.$$

Proof. That the centred canonical RKHS consists of zero mean function, $\operatorname{E} f_\beta(X) = 0$, consider the following argument:

$$\begin{aligned} \operatorname{E} f_\beta(X) &= \operatorname{E}\langle X - \mu, \beta \rangle_{\mathcal{X}} \\ &= \operatorname{E}\langle X, \beta \rangle_{\mathcal{X}} - \langle \mu, \beta \rangle_{\mathcal{X}}, \end{aligned}$$

and since $\operatorname{E}\langle X, \beta \rangle_{\mathcal{X}} = \langle \mu, \beta \rangle_{\mathcal{X}}$ for any $\beta \in \mathcal{X}$, the results follows. □

Remark 2.3. In practice, the probability measure P over $\mathcal{X}$ is unknown, so we find it useful to use the empirical distribution over $\mathcal{X}$ instead, so that $\mathcal{X}$ is centred by the sample mean $\hat\mu = \frac{1}{n}\sum_{i=1}^n x_i$.

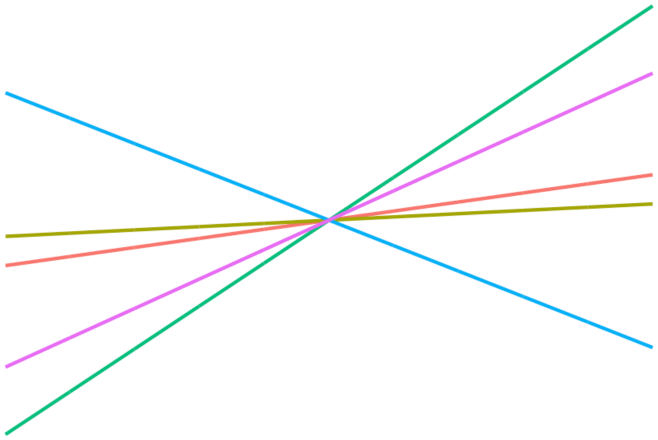


Figure 2.3: Sample paths from the canonical RKHS.

2.4.3 The fractional Brownian motion RKHS

Brownian motion, which also goes by the name Wiener process, has been an inquisitive subject in the mathematical sciences, and here, we describe a function space influenced by a generalised version of Brownian motion paths.

Suppose $B_\gamma(t)$ is a continuous-time Gaussian process on $[0,T]$, i.e. for any finite set of indices $t_1,\dots,t_k$, where each $t_j \in [0,T]$, $\big(B_\gamma(t_1),\dots,B_\gamma(t_k)\big)$ is a multivariate normal random variable. $B_\gamma(t)$ is said to be a *fractional Brownian motion* (fBm) if $\operatorname{E} B_\gamma(t) = 0$ for all $t \in [0,T]$ and

$$\operatorname{Cov}\big(B_\gamma(t), B_\gamma(s)\big) = \frac{1}{2}\big(|t|^{2\gamma} + |s|^{2\gamma} - |t-s|^{2\gamma}\big) \qquad \forall t,s \in [0,T],$$

where $\gamma \in (0,1)$ is called the *Hurst index*, *Hurst parameter* or even *Hurst coefficient*. Introduced by Mandelbrot and Van Ness (1968), fBms are a generalisation of Brownian motion. The Hurst parameter plays two roles: 1) It describes the raggedness of the resultant motion, with higher values leading to smoother motion; and 2) it determines the type of process the fBm is, as past increments of $B_\gamma(t)$ are weighted by $(t-s)^{\gamma-1/2}$. When $\gamma = 1/2$ exactly, then the fBm is a standard Brownian motion and its increments are independent; when $\gamma > 1/2$ (resp. $\gamma < 1/2$) its increments are positively (resp. negatively) correlated.

Now let $\mathcal{X}$ be a Hilbert space. Schoenberg, 1937 has shown that, for $0 < \gamma \le 1$, there exists a Hilbert space $\mathcal{V}$ and a function $\phi_\gamma : \mathcal{X} \to \mathcal{V}$ such that $\forall x, x' \in \mathcal{X}$,

$$\big\|\phi_\gamma(x) - \phi_\gamma(x')\big\|_\mathcal{V} = \|x - x'\|_\mathcal{X}^\gamma.$$

Using the polarisation identity, we find that the kernel of the RKHS with feature space $\mathcal{V}$ and feature map ϕ_γ defines a kernel function $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ identical to the fBm covariance kernel.

def:fbmrkhs

Definition 2.28 (Fractional Brownian motion RKHS)**.** The fractional Brownian motion (fBm) RKHS $\mathcal{F}$ is the space of functions on the Hilbert space $\mathcal{X}$ possessing the reproducing kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ defined by

$$h_\gamma(x,x') = \big\langle \phi_\gamma(x), \phi_\gamma(x') \big\rangle_\mathcal{V} = \frac{1}{2}\big(\|x\|_\mathcal{X}^{2\gamma} + \|x'\|_\mathcal{X}^{2\gamma} - \|x - x'\|_\mathcal{X}^{2\gamma}\big),$$

which depends on the Hurst coefficient $\gamma \in (0,1)$. We shall reference this space as the fBm-γ RKHS.

Remark 2.4. When $\gamma = 1$, by the polarisation identity we get $h(x,x') = \langle x, x' \rangle_\mathcal{X}$, which is the (reproducing) kernel of the canonical RKHS.

From its construction, it is clear that the fBm kernel is positive definite, and thus defines an RKHS. That the fBm RKHS describes a space of functions is proved in Cohen

(2002), who studied this space in depth. It is also noted in the collection of examples of Berlinet and Thomas-Agnan (2011, pp.71 & 319).

The Hurst coefficient γ controls the "smoothness" of the functions in the RKHS. We can talk about smoothness in the context of Hölder continuity of functions.

Definition 2.29 (Hölder condition)**.** A function f over a set $(\mathcal{X}, \|\cdot\|_\mathcal{X})$ is said to be *Hölder continuous* of order $0 < \gamma \leq 1$ if there exists a $C > 0$ such that $\forall x, x' \in \mathcal{X}$,

$$|f(x) - f(x')| \leq C\|x - x'\|^\gamma.$$

Functions in the Hölder space $\mathrm{C}^{k,\gamma}(\mathcal{X})$, where $k \geq 0$ is an integer, consists of those functions over $\mathcal{X}$ having continuous derivatives up to order k and such that the kth partial derivatives are Hölder continuous of order γ. Unlike realisations of actual fBm paths with Hurst index γ, which are well-known to be almost surely Hölder continuous of order less than γ (Embrechts and Maejima, 2002, Theorem 4.1.1), functions in its namesake RKHS are strictly smoother.

Claim 2.10. *The fBm-γ RKHS $\mathcal{F}$ of functions over $(\mathcal{X}, \|\cdot\|_\mathcal{X})$ are Hölder continuous of order γ.*

Proof. For some $f \in \mathcal{F}$ we have $f(x) = \langle f, h(\cdot, x)\rangle_\mathcal{F}$ by the reproducing property of the kernel h of $\mathcal{F}$. It follows from the Cauchy-Schwarz inequality that for any $x, x' \in \mathcal{X}$,

$$\begin{aligned}|f(x) - f(x')| &= |\langle f, h(\cdot,x) - h(\cdot,x')\rangle_\mathcal{F}| \\ &\leq \|f\|_\mathcal{F} \cdot \big\|h(\cdot,x) - h(\cdot,x')\big\|_\mathcal{F} \\ &= \|f\|_\mathcal{F} \cdot \|x - x'\|_\mathcal{X}^\gamma,\end{aligned}$$

since

$$\begin{aligned}\big\|h(\cdot,x) - h(\cdot,x')\big\|_\mathcal{F}^2 &= \big\|h(\cdot,x)\big\|_\mathcal{F}^2 + \big\|h(\cdot,x')\big\|_\mathcal{F}^2 - 2\langle h(\cdot,x), h(\cdot,x')\rangle_\mathcal{F} \\ &= h(x,x) + h(x',x') - 2h(x,x') \\ &= \|x - x'\|_\mathcal{X}^{2\gamma},\end{aligned}$$

and thus proving the claim. □

The fBm-γ RKHS is spanned by the functions $h(\cdot, x)$, which means that $f(0) = 0$ for all $f \in \mathcal{F}$, which may be undesirable. We define the centred fBm RKHS as follows.

7. This is the same for any RKHS?

Definition 2.30 (Centred fBm RKHS)**.** Let $\mathcal{X}$ be a Hilbert space, P be a probability measure over $\mathcal{X}$, and $\mu \in \mathcal{X}$ be the mean with respect to this probability measure. The kernel $\bar{h} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ defined by

$$\bar{h}(x, x') = \frac{1}{2} \operatorname{E} \left[\|x - X\|_{\mathcal{X}}^{2\gamma} + \|x' - X'\|_{\mathcal{X}}^{2\gamma} - \|x - x'\|_{\mathcal{X}}^{2\gamma} - \|X - X'\|_{\mathcal{X}}^{2\gamma} \right]$$

is the reproducing kernel of the *centred* fBm-γ RKHS, which consists of functions f in the fBm-γ RKHS such that $\operatorname{E} f(X) = 0$. In the above definition, $X, X' \sim \mathrm{P}$ are two independent copies of a random vector $X \in \mathcal{X}$.

Remark 2.5. Again, when $\gamma = 1$, we get the reduction

$$\begin{aligned}
\bar{h}(x, x') &= \frac{1}{2} \operatorname{E} \left[\|x - X\|_{\mathcal{X}}^{2} + \|x' - X'\|_{\mathcal{X}}^{2} - \|x - x'\|_{\mathcal{X}}^{2} - \|X - X'\|_{\mathcal{X}}^{2} \right] \\
&= \frac{1}{2} \operatorname{E} \left[\langle X, X \rangle_{\mathcal{X}} + \langle X', X' \rangle_{\mathcal{X}} + 2\langle x, x' \rangle_{\mathcal{X}} - 2\langle x, X \rangle_{\mathcal{X}} - 2\langle x', X' \rangle_{\mathcal{X}} \right] \\
&= \langle \mu, \mu \rangle_{\mathcal{X}} + \langle x, x' \rangle_{\mathcal{X}} - \langle x, \mu \rangle_{\mathcal{X}} - \langle \mu, x' \rangle_{\mathcal{X}} \\
&= \langle x - \mu, x' - \mu \rangle_{\mathcal{X}},
\end{aligned}$$

which is the (reproducing) kernel of the centred canonical RKHS.

2.4.4 The squared exponential RKHS

The squared exponential (SE) kernel function is indeed known to be the default kernel used for Gaussian process regression in machine learning. It is a positive definite function, and hence defines an RKHS. The definition of the SE RKHS is as follows.

Definition 2.31 (Squared exponential RKHS)**.** The squared exponential (SE) RKHS $\mathcal{F}$ of functions over some set $\mathcal{X} \subseteq \mathbb{R}^p$ equipped with the 2-norm $\|\cdot\|_2$ is defined by the positive definite kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$

$$h(x, x') = \exp \left(- \frac{\|x - x'\|_2^2}{2l^2} \right).$$

The real-valued parameter $l > 0$ is called the *lengthscale* parameter, and is a smoothing parameter for the functions in the RKHS.

It is known by many other names, including the Gaussian kernel, due to its semblance to the kernel of the Gaussian pdf. Especially in the machine learning literature, the term

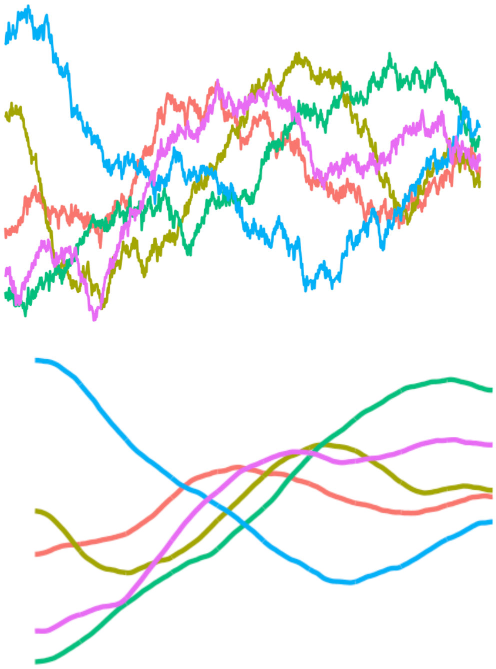


Figure 2.4: Sample paths from the fBm RKHS with varying Hurst coefficients.

Gaussian radial basis functions (RBF) is used, and commonly the simpler parameterisation $\gamma = 1/2l^2$ is utilised. Duvenaud (2014) remarks that "exponentiated quadratic" is a better fitting and descriptive name for this kernel.

Despite being used extensively for learning algorithms using kernels, an explicit study of the RKHS defined by the SE kernel was not done until recently by Steinwart, Hush, et al. (2006). In that work, the authors describe the nature of real-valued functions in the SE RKHS by considering a a real restriction on the SE RKHS of functions over complex values. Their derivation of an orthonormal basis of such an RKHS proved the SE kernel to be the reproducing kernel for the SE RKHS.

SE kernels are known to be "universal". That is, it satisfies the following definition of universal kernels due to Micchelli et al. (2006).

Definition 2.32 (Universal kernel)**.** Let $\text{C}(\mathcal{X})$ is the space of all continuous, complex-valued functions $f : \mathcal{X} \to \mathbb{C}$ equipped with the maximum norm $\|\cdot\|_\infty$, and denote $\mathcal{K}(\mathcal{X})$ as the space of *kernel sections* $\overline{\text{span}}\{h(\cdot,x) | x \in \mathcal{X}\}$, where here, h is a complex-valued kernel function. A kernel h is said to be *universal* if given any compact subset $\mathcal{Z} \subset \mathcal{X}$, any positive number ϵ and any function $f \in \mathrm{C}(\mathcal{Z})$, there is a function $g \in \mathcal{K}(\mathcal{Z})$ such that $\|f - g\|_{\mathcal{Z}} \leq \epsilon$.

The consequence of this universal property vis-à-vis regression modelling is that any (continuous) regression function f may be approximated very well by a function $\hat{f}$ belonging to the SE RKHS, and these two functions can get arbitrarily close to each other in the max norm sense. This, together with some very convenient computational advantages that the SE kernel brings (more on this in a later chapter), is a testament to the popularity of SE kernels.

In a similar manner to the two previous subsections, we may also derive the *centred* SE RKHS.

Definition 2.33 (Centred SE RKHS)**.** Let $\mathcal{X} \subseteq \mathbb{R}^p$ be equipped with the 2-norm $\|\cdot\|_2$, and let P denote the distribution over $\mathcal{X}$. Assuming integrability of $h(x, X)$, for any $x \in \mathcal{X}$ and a random element $X \in \mathcal{X}$, the *centred* squared exponential (SE) RKHS (with lengthscale l) of functions over $\mathcal{X}$ is defined by the positive definite kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$

$$h(x, x') = e^{-\frac{\|x-x'\|_2^2}{2l^2}} - \mathrm{E}\, e^{-\frac{\|x-X'\|_2^2}{2l^2}} - \mathrm{E}\, e^{-\frac{\|X-x'\|_2^2}{2l^2}} + \mathrm{E}\, e^{-\frac{\|X-X'\|_2^2}{2l^2}},$$

where $X, X' \sim \mathrm{P}$ are two independent random elements of $\mathcal{X}$. This ensures that $\mathrm{E}\, f(X) = 0$ for any f in this RKHS.

2.4.5 The Pearson RKHS

In all of the previous RKHS of functions, the domain $\mathcal{X}$ was taken to be some Euclidean space. The Pearson RKHS is a vector space of functions whose domain $\mathcal{X}$ is a finite set. Let P be a probability measure over the finite set $\mathcal{X}$. The Pearson RKHS is defined as follows.

Definition 2.34 (Pearson RKHS)**.** The *Pearson RKHS* is the RKHS of functions over a finite set $\mathcal{X}$ defined by the reproducing kernel

$$h(x, x') = \frac{\delta_{xx'}}{\mathrm{P}(X = x)} - 1,$$

where $X \sim \mathrm{P}$ and δ is the Kronecker delta.

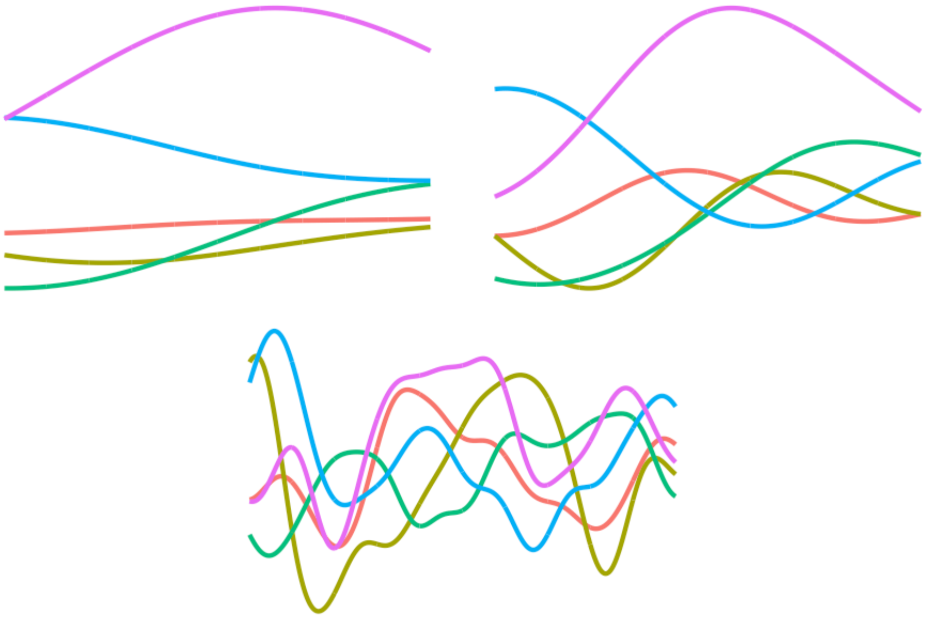


Figure 2.5: Sample paths from the SE RKHS with varying values for the lengthscale.

The Pearson RKHS contains functions which are centred, and has the desirable property that the contribution of $f(x)^2$ to the squared norm of f is proportional to $\operatorname{P}(X = x)$.

Claim 2.11. *Let $\mathcal{F}$ be the Pearson RKHS of functions over a finite set $\mathcal{X}$. Then,*

$$\mathcal{F} = \{f : \mathcal{X} \to \mathbb{R} | \operatorname{E} f(X) = 0\}$$

with

$$\|f\|_{\mathcal{F}}^2 = \operatorname{Var} f(X) = \sum_{x \in \mathcal{X}} \operatorname{P}(X = x) f(x)^2, \ \forall f \in \mathcal{F}.$$

Proof. Write $p_x = \operatorname{P}(X = x)$. The set of functions $\{h(\cdot, x) | x \in \mathcal{X}\}$ form a basis for $\mathcal{F}$, and thus each $f \in \mathcal{F}$ can be written as $f(x) = \sum_{x' \in \mathcal{X}} w_{x'} h(x, x')$ for some scalars $w_i \in \mathbb{R}$, $i \in \mathcal{X}$. But $\operatorname{E} h(X, x') = \operatorname{E}[\delta_{Xx'}]/p_{x'} - 1 = p_{x'}/p_{x'} - 1 = 0$, and thus $\operatorname{E} f(X) = 0$. Conversely, suppose $f : \mathcal{X} \to \mathbb{R}$ is such that $\operatorname{E} f(X) = 0$. Taking $w_x = p_x f(x)$, we see that

$$\begin{aligned}\sum_{x'\in\mathcal{X}} w_{x'}h(x,x') &= \frac{w_x}{p_x} - \sum_{x'\in\mathcal{X}} w_{x'} \\ &= \frac{f(x)\cancel{p_x}}{\cancel{p_x}} - \overset{\mathrm{E}\, f(X) = 0}{\cancel{\sum_{x'\in\mathcal{X}} p_{x'}f(x')}} \qquad = f(x)\end{aligned}$$

and thus $h(\cdot,x)$ spans $\mathcal{F}$ so $f \in \mathcal{F}$. To provide the second part, noting that with the choice $w_x = p_x f(x)$ and due to the reproducing property of h for the RKHS $\mathcal{F}$, the squared norm is

$$\begin{aligned}\langle f, f\rangle_\mathcal{F} &= \left\langle \sum_{x\in\mathcal{X}} w_x h(\cdot,x), \sum_{x'\in\mathcal{X}} w_{x'}h(\cdot,x') \right\rangle_\mathcal{F} \\ &= \sum_{x\in\mathcal{X}}\sum_{x'\in\mathcal{X}} w_x w_{x'} \left\langle h(\cdot,x), h(\cdot,x')\right\rangle_\mathcal{F} \\ &= \sum_{x\in\mathcal{X}}\sum_{x'\in\mathcal{X}} w_x w_{x'} h(x,x') \\ &= \sum_{x\in\mathcal{X}} w_x f(x) \\ &= \sum_{x\in\mathcal{X}} \mathrm{P}(X = x) f(x)^2,\end{aligned}$$

which is also the variance of $f(X)$. □

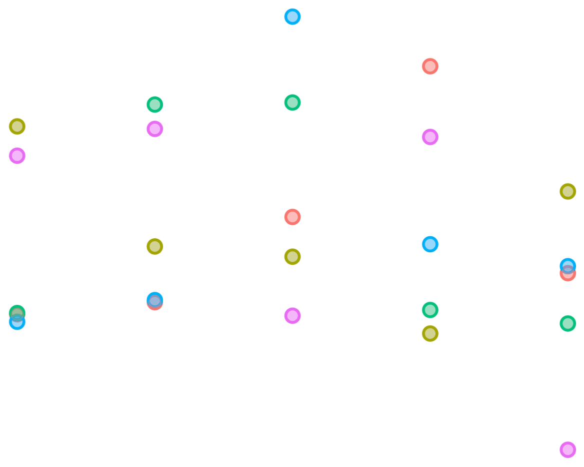


Figure 2.6: Sample "paths" from the Pearson RKHS. These are represented as points over a finite set.

sec:constructrkks

2.5 Constructing RKKS from existing RKHS

The previous section outlined all of the basic RKHSs of functions that will form the building blocks when constructing more complex function spaces. As previously mentioned in the preliminaries, sums of kernels are kernels and products of kernels are also kernels. This provides us a platform for constructing new RKHS from existing ones. To be more flexible in the specification of these new function spaces, we do not restrict ourselves to positive definite kernels only, thereby necessitating us to use the theory of RKKS.

2.5.1 Sums, products and scaling of RKHS

Sums of positive definite kernels are also positive definite kernels, and the product of positive definite kernel is a positive definite kernel. They each, in turn, are associated with a RKHS that is defined by the sum of kernels and product of kernels, respectively. The two lemmas below formalise these two facts.

thm:sumkernels

Lemma 2.12 (Sum of kernels)**.** *If h_1 and h_2 are kernels on $\mathcal{X}_1$ and $\mathcal{X}_2$ respectively, then $h = h_1 + h_2$ is a kernel on $\mathcal{X}_1 \times \mathcal{X}_2$. Moreover, denote $\mathcal{F}_1$ and $\mathcal{F}_2$ the RKHS defined by h_1 and h_2 respectively. Then $\mathcal{F} = \mathcal{F}_1 \oplus \mathcal{F}_2$ is an RKHS defined by $h = h_1 + h_2$, where*

$$\mathcal{F}_1 \oplus \mathcal{F}_2 = \{ f : \mathcal{X}_1 \times \mathcal{X}_2 \to \mathbb{R} \,|\, f = f_1 + f_2, f_1 \in \mathcal{F}_1 \textit{ and } f_2 \in \mathcal{F}_2 \}.$$

For all $f \in \mathcal{F}$,

$$\|f\|^2_{\mathcal{F}} = \min_{f_1+f_2=f} \left\{ \|f_1\|^2_{\mathcal{F}_1} + \|f_2\|^2_{\mathcal{F}_2} \right\}.$$

Proof. That $h_1 + h_2$ is a kernel should be obvious, as the sum of two positive definite functions is also positive definite. For a proof of the remaining statements, see Berlinet and Thomas-Agnan (2011, Theorem 5). □

thm:prodkernels

Lemma 2.13 (Products of kernels)**.** *Let $\mathcal{F}_1$ and $\mathcal{F}_2$ be two RKHS of functions over $\mathcal{X}_1$ and $\mathcal{X}_2$, with respective reproducing kernels h_1 and h_2. Then, $h = h_1 h_2$ is a kernel on $\mathcal{X}_1 \times \mathcal{X}_2$. Moreover, the tensor product space $\mathcal{F}_1 \otimes \mathcal{F}_2$ is an RKHS with reproducing kernel h.*

Proof. Fix $n \in \mathbb{N}$, and let $\mathbf{H}_1$ and $\mathbf{H}_2$ be the kernel matrices for h_1 and h_2 respectively. Since these kernel matrices are symmetric and positive-definite by virtue of h_1 and h_2

being symmetric and positive-definite functions, we can write $\mathbf{H}_1 = \mathbf{A}^\top\mathbf{A}$ and $\mathbf{H}_1 = \mathbf{B}^\top\mathbf{B}$ for some matrices $\mathbf{A}$ and $\mathbf{B}$: perform an (orthogonal) eigendecomposition of each of the kernel matrices, and take square roots of the eigenvalues. Let $\mathbf{H}$ be the kernel matrix for $h = h_1h_2$. With $x_i = (x_{i1}, x_{i2})$, its (i,j) entries are

$$\begin{aligned}
h(x_i, x_j) &= h_1(x_{i1}, x_{i2})h_2(x_{j1}, x_{j2}) \\
&= (\mathbf{A}^\top\mathbf{A})_{ij} \cdot (\mathbf{B}^\top\mathbf{B})_{ij} \\
&= \sum_{k=1}^n a_{ik}a_{jk} \sum_{l=1}^n b_{il}b_{jl},
\end{aligned}$$

where we have denoted b_{ij} and c_{ij} to be the (i,j)th entries of $\mathbf{B}$ and $\mathbf{C}$ respectively. Then,

$$\begin{aligned}
\sum_{i=1}^n\sum_{j=1}^n h(x_i, x_j) &= \sum_{k=1}^n\sum_{l=1}^n\sum_{i=1}^n\sum_{j=1}^n \lambda_i\lambda_j a_{ik}a_{jk}b_{il}b_{jl} \\
&= \sum_{k=1}^n\sum_{l=1}^n \left(\sum_{i=1}^n \lambda_i a_{ik}b_{il}\right)\left(\sum_{j=1}^n \lambda_j a_{jk}b_{jl}\right) \\
&= \sum_{k=1}^n\sum_{l=1}^n \left(\sum_{i=1}^n \lambda_i a_{ik}b_{il}\right)^2 \\
&\geq 0
\end{aligned}$$

Again, for the remainder of the statement in the lemma, we refer to Berlinet and Thomas-Agnan (2011, Theorem 13). □

A familiar fact from linear algebra is realised here from Lemmas 2.12 and 2.13: 1) the addition of positive definite matrices is a positive definite matrix; and 2) the *Hadamard product*[3] of two positive definite matrices is a positive definite matrix.

The scale of an RKHS of functions $\mathcal{F}$ over a set $\mathcal{X}$ with kernel h may be arbitrary. To resolve this issue, a scale parameter $\lambda \in \mathbb{R}$ for the kernel h may be introduced, which will typically need to be estimated from the data. If h is a positive definite kernel on $\mathcal{X} \times \mathcal{X}$, and $\lambda \geq 0$ a scalar, then this yields a scaled RKHS $\mathcal{F}_\lambda = \{\lambda f \,|\, f \in \mathcal{F}\}$ with reproducing kernel λh, where $\mathcal{F}$ is the RKHS defined by h.

[3] The Hadamard product is an element-wise multiplication of two matrices $\mathbf{A}$ and $\mathbf{B}$ of identical dimensions, denoted $\mathbf{A} \circ \mathbf{B}$. That is, $(\mathbf{A} \circ \mathbf{B})_{ij} = \mathbf{A}_{ij}\mathbf{B}_{ij}$.

Restricting λ to the positive reals is arbitrary and unnecessarily restrictive. Especially when considering sums and products of scaled RKHSs, having negative scale parameters also give additional flexibility. The resulting kernels from summation and/or multiplication with negative kernels may no longer be positive-definite, and in such cases, they give rise to RKKS instead.

Remark 2.6. Recall that a RKKS $\mathcal{F}$ of functions over $\mathcal{X}$ can be uniquely decomposed as the difference between two RKHSs $\mathcal{F}_+$ and $\mathcal{F}_-$, and its associated Hilbert space $\mathcal{F}_\mathcal{H}$ is the RKHS $\mathcal{F}_+ \oplus \mathcal{F}_-$. If it is important to note that both $\mathcal{F}$ and $\mathcal{F}_\mathcal{H}$ contain identical functions over $\mathcal{X}$, but their topologies are different. That is to say, functions that are close with respect to the norm of $\mathcal{F}$ may not be close to each other in the norm of $\mathcal{F}_\mathcal{H}$.

2.5.2 The polynomial RKKS

A polynomial construction based on a particular RKHS building block is considered here. For example, using the canonical RKHS in the polynomial construction would allow us to easily add higher order effects of the covariates $x \in \mathcal{X}$. In particular, we only require a single scale parameter in polynomial kernel construction.

Definition 2.35 (The polynomial RKKS)**.** Let $\mathcal{X}$ be a Hilbert space. The kernel function $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ obtained through the d-degree polynomial construction of linear kernels is

$$h_\lambda(x,x') = \big(\lambda \cdot \langle x,x'\rangle_\mathcal{X} + c\big)^d,$$

where $\lambda \in \mathbb{R}$ is a scale parameter for the linear kernel, and $c \in \mathbb{R}$ is a real constant called the *offset*. This kernel defined the *polynomial RKKS* of degree d.

Write

$$h_\lambda(x,x')_\mathcal{F} = \sum_{k=0}^{d} \frac{d!}{k!(d-k)!} c^{k-d} \lambda^k \langle x,x'\rangle_\mathcal{X}^k.$$

Evidently, as the name suggests, this is a polynomial involving the canonical kernel. In particular, each of the k-powered kernels (i.e., $\langle x,x'\rangle_\mathcal{X}^k$) defines an RKHS of their own (since these are merely products of kernels), and therefore the sum of these k-powered kernels define the polynomial RKHS.

The offset parameter influences trade-off between the higher-order versus lower-order terms in the polynomial. It is sometimes known as the bias term.

Claim 2.14. *The polynomial RKKS of functions over $\mathbb{R}$, denoted $\mathcal{F}$, contains polynomial functions of the form $f(x) = \sum_{k=0}^d \beta_k x^k$.*

Proof. By construction, $\mathcal{F} = \mathcal{F}_0 \oplus \bigoplus_{i=1}^d \bigotimes_{j=1}^i \mathcal{F}_j$, where each $\mathcal{F}_j, j \neq 0$ is the canonical RKHS, and $\mathcal{F}_0$ is the RKHS of constant functions. Each $g \in \mathcal{F}$ can therefore be written as $g = \beta_0 + \sum_{i=1}^d \prod_{j=1}^i f_j$, and $f_j(x) = b_j x$ from before, where b_j is a constant. Therefore, $g(x) = \sum_{k=0}^d \beta_k x^k$. □

Remark 2.7. We may opt to use other RKHSs as the building blocks of the polynomial RKHS. In particular, using the centred canonical kernel seems natural, so that each of the functions in the constituents of the direct sum of spaces is centred. However, the polynomial RKKS itself will not be centred.

2.5.3 The ANOVA RKKS

We find it useful to begin this subsection by spending some time to elaborate on the classical analysis of variance (ANOVA) decomposition, and the associated notions of main effects and interactions. This will go a long way in understanding the thinking behind constructing an ANOVA-like RKKS of functions.

The classical ANOVA decomposition

The standard one-way ANOVA is essentially a linear regression model which allows comparison of means from two or more samples. Given sets of observations $y_j = \{y_{1j}, \dots, y_{n_j j}\}$, $j = 1, \dots, m$, we consider the linear model $y_{ij} = \mu_j + \epsilon_{ij}$, where ϵ_{ij} are independent, univariate normal random variables with a common variance. This covariate-less model is used to make inferences about the *treatment means* μ_j. Often, the model is written in the *overparameterised* form by substituting $\mu_j = \mu + \tau_j$. This gives a different, arguably better, interpretability to the model: The τ_j's, referred to as the *treatment effects*, now represent the amount of deviation from the grand, *overall mean* μ. Estimating all τ_j's and μ separately is not possible because there is one degree of freedom that needs to be addressed in the model: There are $p+1$ mean parameters to estimate but only information from p means. A common fix to the identifiability issue is to set one of the μ_j's, say the first one μ_1, to zero, or impose the restriction $\sum_{j=1}^m \mu_j = 0$. The former treats one of the m levels as the control, while the latter treats all treatment effects symmetrically.

Now write the ANOVA model slightly differently, as $y_i = f(x_i) + \epsilon_i$, where f is defined on the discrete domain $\mathcal{X} = \{1, \dots, m\}$, and i indexes all of the $n := \sum_{j=1}^m n_j$ observations. Here, f represents the group-level mean, returning μ_j for some $j \in \mathcal{X}$. In a similar manner, we can perform the ANOVA decomposition on f as

$$f = Af + (I - A)f = f_o + f_t,$$

where A is an averaging operator that "averages out" its argument x and returns a constant, and I is the identity operator. $f_o = Af$ is a constant function representing the *$\underline{o}$verall mean*, whereas $f_t = (I - A)f$ is a function representing the *$\underline{t}$reatment effects* τ_j. Here are two choices of A:

- $Af(x) = f(1) = \mu_1$. This implies $f(x) = f(1) + \big(f(x) - f(1)\big)$. The overall mean μ is the group mean μ_1, which corresponds to setting the restriction $\mu_1 = 0$.
- $Af(x) = \sum_{x=1}^m f(x)/m =: \bar\alpha$. This implies $f(x) = \bar\alpha + \big(f(x) - \bar\alpha\big)$. The overall mean is $\mu = \sum_{j=1}^m \alpha_j/m$, which corresponds to the restriction $\sum_{j=1}^m \mu_j = 0$.

By definition, $AAf = A^2 f = Af$, because averaging a constant returns that constant [Side note: This idempotent property of the linear operator A on f speaks to the possibility of it being an *orthogonal projection*, and indeed this is so—we shall return to this point later when we describe functional ANOVA decomposition]. We must have that $Af_t = A(I - A)f = Af - A^2 f = 0$. The choice of A is arbitrary, as is the choice of restriction, so long as it satisfies the condition that $Af_c = 0$.

The multiway ANOVA can be motivated in a similar fashion. Let $x = (x_1, \dots, x_p) \in \prod_{k=1}^p \mathcal{X}_k$, and consider functions that map $\prod_{k=1}^p \mathcal{X}_j$ to $\mathbb{R}$. Let A_j be an averaging operator on $\mathcal{X}_k$ that averages the kth component of x from the active argument list, i.e. $A_k f$ is constant on the $\mathcal{X}_k$ axis but not necessarily an overall constant function. An ANOVA decomposition of f is

$$f = \left(\prod_{k=1}^p (A_k + I - A_k) \right) f = \sum_{\mathcal{K} \in \mathcal{P}_p} \left(\prod_{k \in \mathcal{K}} (I - A_k) \prod_{k \notin \mathcal{K}} A_k \right) f = \sum_{\mathcal{K} \in \mathcal{P}_p} f_{\mathcal{K}}$$

where we had denoted $\mathcal{P}_p = \mathcal{P}(\{1, \dots, p\})$ to be the power set of $\{1, \dots, p\}$ whose cardinality is 2^p. The summands $f_{\mathcal{K}}$ will compose of the overall effect, main effects, two-way interaction terms, and so on. Each of the terms will satisfy the condition $A_k f_{\mathcal{K}} = 0, \forall k \in \mathcal{K} \in \mathcal{P}_p$.

Example 2.1 (Two-way ANOVA decomposition)**.** Let $p = 2$, $\mathcal{X}_1 = \{1, \dots, m_1\}$, and $\mathcal{X}_2 = \{1, \dots, m_2\}$. The power set $\mathcal{P}_2$ is $\big\{\{\}, \{1\}, \{2\}, \{1, 2\}\big\}$. The ANOVA decomposition of f is

$$f = f_0 + f_1 + f_2 + f_{12}.$$

Here are two choices for the averaging operator A_k analogous to the previous illustration in the one-way ANOVA.

- Let $A_1 f(x) = f(1, x_2)$ and $A_2 f(x) = f(x_1, 1)$. Then,

$$\begin{aligned} f_0 &= A_1 A_2 f &&= f(1,1) \\ f_1 &= (I - A_1) A_2 f &&= f(x_1, 1) - f(1,1) \\ f_2 &= A_1 (I - A2) f &&= f(1, x_2) - f(1,1) \\ f_{12} &= (I - A_1)(I - A2) f &&= f(x_1, x_2) - f(x_1, 1) - f(1, x_2) + f(1,1). \end{aligned}$$

- Let $A_k f(x) = \sum_{x_k=1}^{m_k} f(x_1, x_2)/m_k, k = 1, 2$. Then,

$$\begin{aligned} f_0 &= A_1 A_2 f &&= f_{\cdot\cdot} \\ f_1 &= (I - A_1) A_2 f &&= f_{x_1\cdot} - f_{\cdot\cdot} \\ f_2 &= A_1 (I - A_2) f &&= f_{\cdot x_2} - f_{\cdot\cdot} \\ f_{12} &= (I - A_1)(I - A_2) f &&= f - f_{x_1\cdot} - f_{\cdot x_2} + f_{\cdot\cdot}, \end{aligned}$$

  where $f_{\cdot\cdot} = \sum_{x_1, x_2} f(x_1, x_2)/m_1 m_2$, $f_{x_1\cdot} = \sum_{x_2} f(x_1, x_2)/m_2$, and $f_{\cdot x_1} = \sum_{x_1} f(x_1, x_2)/m_1$.

Functional ANOVA decomposition

Let us now extend the ANOVA decomposition idea to a general function $f : \mathcal{X} \to \mathbb{R}$ in some vector space $\mathcal{F}$. Specifically, we shall consider the (Hilbert) space of square integrable functions over $\mathcal{X}$ with measure ν, $\mathcal{F} \equiv \mathrm{L}^2(\mathcal{X}, \nu)$. We shall jump straight into the multiway ANOVA analogue for functional decomposition, and to that end, consider $x = (x_1, \dots, x_p) \in \prod_{k=1}^p \mathcal{X}_k =: \mathcal{X}$ a measurable space, where each of the spaces $\mathcal{X}_k$ has measure ν_k, and $\nu = \nu_1 \times \cdots \times \nu_d$ is the product measure on $\mathcal{X}$. As $\mathcal{X}$ need not necessarily be a collection of finite sets, we need to figure out a suitable linear operator that performs an "averaging" of some sort.

Consider the linear operator $A_k : \mathcal{F} \to \mathcal{F}_{-k}$, where $\mathcal{F}_{-k}$ is a vector space of functions for which the kth component is constant over $\mathcal{X}$, defined by

$$A_k f = \int_{\mathcal{X}_k} f(x_1, \dots, x_p) \, \mathrm{d}\nu(x_k). \tag{2.2}$$

{eq:avgoper}

Thus, for the one-way ANOVA ($p = 1$), we get

$$f = \overbrace{\int_{\mathcal{X}} f(x) \mathrm{d}\nu(x)}^{f_0} + \overbrace{\left(f - \int_{\mathcal{X}} f(x) \mathrm{d}\nu(x) \right)}^{f_1} \tag{2.3}$$

{eq:functionalanova1}

and for the two-way ANOVA ($p = 2$), we have $f = f_0 + f_1 + f_2 + f_{12}$, with

$$\begin{aligned}
f_0 &= \int_{\mathcal{X}_1} \int_{\mathcal{X}_2} f(x_1, x_2) \, \mathrm{d}\nu(x_1) \, \mathrm{d}\nu(x_2) \\
f_1 &= \int_{\mathcal{X}_2} \left(f(x_1, x_2) - \int_{\mathcal{X}_1} f(x_1, x_2) \, \mathrm{d}\nu(x_1) \right) \mathrm{d}\nu(x_2) \\
f_2 &= \int_{\mathcal{X}_1} \left(f(x_1, x_2) - \int_{\mathcal{X}_2} f(x_1, x_2) \, \mathrm{d}\nu(x_2) \right) \mathrm{d}\nu(x_1) \\
f_{12} &= f(x_1, x_2) - \int_{\mathcal{X}_1} f(x_1, x_2) \mathrm{d}\nu(x_1) - \int_{\mathcal{X}_2} f(x_1, x_2) \, \mathrm{d}\nu(x_2) \\
&\quad + \int_{\mathcal{X}_1} \int_{\mathcal{X}_2} f(x_1, x_2) \mathrm{d}\nu(x_1) \, \mathrm{d}\nu(x_2).
\end{aligned}$$

As a remark, the averaging operator A_k defined in (2.2) is indeed true to its name, in that it calculates the mean function of f over the kth coordinate. For comparison, this is identical to the second type of restriction we considered in the classical ANOVA previously (i.e., setting $\sum_j \mu_j = 0$). We must also have, as before, that $A_k f_{\mathcal{K}} = 0, \forall k \in \mathcal{K} \in \mathcal{P}_p$. For the one-way functional ANOVA decomposition in (2.3), it must be that f_1 is a zero-mean function. As for the two-way ANOVA, it is the case that $\int_{\mathcal{X}_k} f_1(x_1, x_2) \mathrm{d}\nu(x_k) = 0, k = 1, 2$, and $\int_{\mathcal{X}_1} \int_{\mathcal{X}_2} f_{12}(x_1, x_2) \mathrm{d}\nu(x_1) \mathrm{d}\nu(x_1) = 0$.

We notice that the decomposition in (2.3) is orthogonal:

Claim 2.15. *For the ANOVA decomposition in* (2.3)*, f_0 and f_1 are orthogonal for the usual L^2 inner product.*

Proof. Note that f_0 is a constant function, and that $f_1 = f - f_0$. Thus,

$$\begin{aligned}\langle f_0, f_1 \rangle &= \int f_0 f_1 \mathrm{d}\nu \\ &= f_0 \int (f - f_0) \, \mathrm{d}\nu \\ &= f_0 (f_0 - f_0) = 0.\end{aligned}$$

□

In fact, for $k = 1$, any $f \in \mathcal{F}$ can be decomposed as a sum of a constant plus a zero mean function, so we have the geometric decomposition of the vector space $\mathcal{F} = \mathcal{F}_0 \overset{\perp}{\oplus} \bar{\mathcal{F}}_1$, where $\mathcal{F}_0$ is a vector space of constant functions, and $\bar{\mathcal{F}}_1$ a vector space of zero-mean functions over $\mathcal{X}_1$. For $k \geq 2$ we can argue something similar. The space $\mathcal{F}$ has the tensor product structure[4] $\mathcal{F} = \mathcal{F}_1 \otimes \cdots \otimes \mathcal{F}_p$, and considered individually, each $\mathcal{F}_k$ can be decomposed orthogonally $\mathcal{F}_k = \mathcal{F}_0 \overset{\perp}{\oplus} \bar{\mathcal{F}}_k$. Note that $\mathcal{F}_k$ consists of functions $f : \mathcal{X}_k \to \mathbb{R}$. Expanding out under the distributivity rule of tensor products and rearranging slightly, we obtain

$$\begin{aligned}\mathcal{F} &= \big(\mathcal{F}_0 \overset{\perp}{\oplus} \bar{\mathcal{F}}_1\big) \otimes \cdots \otimes \big(\mathcal{F}_0 \overset{\perp}{\oplus} \bar{\mathcal{F}}_1\big) \\ &= \mathcal{F}_0^{\otimes p} \overset{\perp}{\oplus} \bigoplus_{j=1}^{p}{}^{\perp} \left(\mathcal{F}_0^{\otimes (p-1)} \otimes \bar{\mathcal{F}}_j \right) \overset{\perp}{\oplus} \bigoplus_{\substack{j,k=1 \\ j<k}}^{p}{}^{\perp} \left(\mathcal{F}_0^{\otimes (p-2)} \otimes \bar{\mathcal{F}}_j \otimes \bar{\mathcal{F}}_k \right) \qquad (2.4) \\ &\qquad \overset{\perp}{\oplus} \cdots \overset{\perp}{\oplus} \left(\bar{\mathcal{F}}_1 \otimes \cdots \otimes \bar{\mathcal{F}}_p \right).\end{aligned}$$

{eq:funcanovaspace}

To clarify,

- $\mathcal{F}_0^{\otimes p}$ is the space of constant functions $f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_p \to \mathbb{R}$.
- $\left(\mathcal{F}_0^{\otimes (p-1)} \otimes \bar{\mathcal{F}}_j \right)$ is the space of functions that are constant on all coordinates except the jth coordinate of x. Further, the functions are centred on the jth coordinate.
- $\left(\mathcal{F}_0^{\otimes (p-2)} \otimes \bar{\mathcal{F}}_j \otimes \bar{\mathcal{F}}_k \right)$ is the space of functions that are constant on all coordinates except the jth and kth coordinate of x. Further, the functions are centred on these two coordinates.
- $\bar{\mathcal{F}}_1 \otimes \cdots \otimes \bar{\mathcal{F}}_p$ is the space of zero-mean functions $f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_p \to \mathbb{R}$.
- Similarly for the rest of the spaces in the summand, of which there are 2^p members all together.

Therefore, given an arbitrary function $f \in \mathcal{F}$, the projection of f onto the above respective orthogonal spaces in (2.4) leads to the *functional ANOVA representation*

$$f(x) = \mu + \sum_{j=1}^{p} f_j(x_j) + \sum_{\substack{j,k=1 \\ j<k}}^{p} f_{jk}(x_j, x_k) + \cdots + f_{1\cdots p}(x). \tag{2.5}$$

{eq:functionalanova2}

Definition 2.36 (Functional ANOVA representation)**.** Let $\mathcal{P}_d = \mathcal{P}(\{1, \dots, d\})$, the power set of $\{1, \dots, d\}$. For any function $f \in \mathcal{F} \equiv \mathrm{L}^2(\mathcal{X}_1 \times \cdots \times \mathcal{X}_d, \nu_1 \otimes \cdots \otimes \nu_d)$, the formula for f in (2.5) is known as the *functional ANOVA representation* of f if $\forall k \in \mathcal{K} \in \mathcal{P}_p$,

$$A_k f_\mathcal{K} = \int_{\mathcal{X}_\mathcal{K}} f_\mathcal{K}(x_\mathcal{K}) \mathrm{d}\nu_k(x_k) = 0, \tag{2.6}$$

{eq:funcanovaorth}

where $\mathcal{X}_\mathcal{K} = \prod_{k \in \mathcal{K}} \mathcal{X}_k$, and $x_\mathcal{K} = \{x_k, k \in \mathcal{K}\}$ is an element of this space. In other words, the integral of $f_\mathcal{K}$ with respect to any of the variables indexed by the elements in $\mathcal{K}$ (itself an element of the power set), is zero. The requirement (2.6) ensures orthogonality of the summands in (2.5).

For the constant term, main effects, and two-way interaction terms, the familiar classical expressions are obtained:

$$\begin{aligned}
f_0 &= \int f \mathrm{d}\nu \\
f_j &= \int f \textstyle\prod_{i \neq j} \mathrm{d}\nu_i - f_0 \\
f_{jk} &= \int f \textstyle\prod_{i \neq j,k} \mathrm{d}\nu_i - f_j - f_k - f_0.
\end{aligned}$$

Remark 2.8. Not all of the higher order terms need to be included. There may even be a model motivated reason for dropping certain main effects or interaction effects.

The ANOVA kernel

At last, we come to the section of deriving the ANOVA RKKS, and, rest assured, the preceding long build-up will prove to be not in vain. The main idea is to construct an

[4] There is an isomorphism $\mathrm{L}^2(\mathcal{X}_1 \times \cdots \times \mathcal{X}_d, \nu_1 \otimes \cdots \otimes \nu_d) \cong \mathrm{L}^2(\mathcal{X}_1, \nu_1) \otimes \cdots \otimes \mathrm{L}^2(\mathcal{X}_d, \nu_d)$. See, for example, Reed and Simon (1972) and Krée (1974).

RKKS such that the functions that lie in them will have the ANOVA representation in (2.5). The bulk of the work has been done, and in fact we know exactly how this ANOVA RKKS should be structured—it is the space as specified in (2.4). The ANOVA RKKS will be constructed by a similar manipulation of the individual kernels representing the RKHS building blocks.

Definition 2.37 (The ANOVA RKKS)**.** For $k = 1, \dots, p$, let $\mathcal{F}_k$ be a centred RKHS of functions over the set $\mathcal{X}_k$ with kernel $h_k : \mathcal{X}_k \times \mathcal{X}_k \to \mathbb{R}$. Let $\lambda_k, k = 1, \dots, p$ be real-valued scale parameters. The ANOVA RKKS of functions $f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_p \to \mathbb{R}$ is specified by the ANOVA kernel, defined by

$$h_\lambda(x, x') = \prod_{k=1}^{p} \big(1 + \lambda_k h_k(x_k, x'_k)\big). \tag{2.7}$$

{eq:anovarkks}

The construction an ANOVA RKKS is very very simple in through multiplication of univariate kernels. Expanding out equations (2.7), we see that it is in fact a sum of products of kernels with increasing orders of interaction:

$$\begin{aligned} h_\lambda(x, x') = 1 + \sum_{j=1}^{p} \lambda_j h_j(x_j, x'_j) + \sum_{\substack{j,k=1 \\ j<k}}^{p} \lambda_j \lambda_k h_j(x_j, x'_j) h_k(x_k, x'_k) \\ + \cdots + \prod_{j=1}^{p} \lambda_j h_j(x_j, x'_j). \end{aligned}$$

It is now clear from the expansion that the ANOVA RKKS yields functions that resemble those with the ANOVA representation in (2.5): The mean value of the function stems from the '1', i.e. it lies in an RKHS of constant functions; the main effects are represented by the sum of the individual kernels; the two-way interaction terms are represented by the second-order kernel interactions; and so on.

Example 2.2. Consider two RKKSs $\mathcal{F}_k$ with kernel $\lambda_k h_k$, $k = 1, 2$. The ANOVA kernel defining the ANOVA RKKS $\mathcal{F}$ is

$$h_\lambda\big((x_1, x_2), (x'_1, x'_2)\big) = 1 + \lambda_1 h_1(x_1, x'_1) + \lambda_2 h_2(x_2, x'_2) + \lambda_1 \lambda_2 h_1(x_1, x'_1) h_2(x_2, x'_2).$$

Suppose that $\mathcal{F}_1$ and $\mathcal{F}_2$ are the centred canonical RKKS of functions over $\mathbb{R}$. Then, functions in $\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus (\mathcal{F}_1 \otimes \mathcal{F}_2)$ are of the form

$$f(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2.$$

As remarked in the previous subsection, not all of the components of the ANOVA RKKS need to be included in the construction. The selective exclusion of certain interactions characterises many interesting statistical models. Excluding certain terms of the ANOVA RKKS is equivalent to setting the scale parameter for those relevant components to be zero, i.e., they play no role in the decomposition of the function. With this in mind, the ANOVA RKKS then gives us an objective way of model-building, from linear regression, to multilevel models, longitudinal models, and so on.

2.6 Summary

The brief notes on functional analysis allow us to describe the theory of reproducing kernel Hilbert and Kreĭn spaces. These are of great interest to us because the topology endowed on such spaces gives great assurances—in particular, all evaluation functionals are continuous in these spaces. Moreover, RKHS and RKKS can be specified completely through kernel functions, with new and complex function spaces built simply by manipulation of these kernel functions. Of particular importance is the ANOVA functional decomposition, for which we realise provides an objective way of constructing various statistical models (such models will be described later on in detail in Chapter 4).

An annotated collection of bibliographical references used for this chapter is as follows.

- **Functional analysis**. On the introductory material relating to functional analysis in Section 2.1, the lecture notes by Sejdinovic and Gretton (2012) is recommended, and forms the basis for most of the material described. Additionally, Rudin (1987) provides a complementary reading.
- **RKHS theory**. There are certainly no shortages of introductory texts relating to the theory of RKHS: Steinwart and Christmann (2008), Berlinet and Thomas-Agnan (2011), and Gu (2013) to name a few. The concise sketch proof for the Moore-Aronszajn theorem was mostly inspired by Hein and Bousquet (2004, Theorem 4)

- **RKKS theory**. The innovation of indefinite inner product spaces perhaps started in mathematical physics literature, for which the theory of special relativity depends. Four-dimensional space-time is an often cited example. In any case, we referred to mainly Ong et al. (2004), which gives an overview in the context of learning using indefinite kernels. Alpay (1991) and Zafeiriou (2012) were also useful for understanding the fundamental concepts of RKKS.

- **RKHS building blocks**. The main building block RKHS, i.e. the canonical RKHS, the fBm RKHS and the Pearson RKHS are described in the manuscript of Bergsma (2017).

- **ANOVA and functional ANOVA**. Classical ANOVA is pretty much existent in every fundamental statistical textbook. These texts have extremely well written introductions to this very important concept: Casella and R. L. Berger (2002, Ch. 11), Dean and Voss (1999, Ch. 3). On the relation between classical ANOVA and functional ANOVA decomposition, Gu (2013) offers novel insights. There is diverse literature concerning functional ANOVA, namely from the fields of statistical learning (e.g. Wahba, 1990), applied mathematics (e.g. Kuo et al., 2010), and sensitivity analysis (e.g. Sobol, 2001; Durrande et al., 2013). What is interesting is that several authors who simply set out to obtain a suitable functional decomposition, all ended up somewhat independently recovering the ANOVA decomposition as being "optimal" in some sense. This speaks largely to this classical idea that is ANOVA.

2.7 Miscellanea

2.7.1 A vector space... of 'functions'?

At first glance, this may seem strange, that the notion of functions (as mappings from input to output space) and vector spaces are somehow equatable. Upon further thought, one realises that firstly, two functions of a similar, particular form may be added together (in some meaningful way) resulting in a function in that same form. Secondly, multiplication of a function by a scalar c can be thought of as c times the output of that function. Indeed, running through the checklist of what constitutes a vector space, we find that a "space of functions" satisfies them all. In modern linear algebra texts, this checklist is the eight axioms of vector spaces over a field $\mathbb{F}$: The vectors forms an abelian group under addition, and this group has an $\mathbb{F}$-module structure.

Chapter 3

Fisher information and the I-prior

Traditionally, Fisher information is calculated for unknown parameters θ of probability distribution from observable random variables. In a similar light, we can treat the regression function f in the model stated in (1.1), subject to (1.2), as the unknown "parameter" for which we would like information regarding. In this chapter, we extend the notion of Fisher information to abstract objects in Hilbert spaces, and also to linear functionals of these objects. This will allow us to achieve our aim of deriving the Fisher information for our regression function.

Following this, we shall discuss the notion of prior distributions for regression functions, and how one might assign a suitable prior. In our case, we choose an objective prior following (Jaynes, 1957a; Jaynes, 1957b)—in the absence of any prior knowledge, a prior distribution which maximises entropy should be used. It turns out, the entropy maximising prior for f is Gaussian with mean chosen a priori and covariance kernel proportional to the Fisher information. Such a distribution on f is called the I-prior distribution.

3.1 The traditional Fisher information

It was Fisher (1922) who introduced the method of maximum likelihood as an objective way of conducting statistical inference. This method of inference is distinguished from the Bayesian school of thought in that only the data may inform deductive reasoning, but not any sort of prior probabilities. Towards the later stages of his career[1], his work reflected the view that the likelihood is to be more than simply a device to obtain parameter estimates; it is also a vessel that carries uncertainty about estimation. In this light and in the absence of the possibility of making probabilistic statements, one should look to the likelihood in order to make rational conclusions about an inference problem. Specifically, we may ask two things of the likelihood function: where is the maxima and what does the graph around the maxima look like? The first of these two problems is maximum likelihood estimation, while the second concerns the Fisher information.

In simple terms, the Fisher information measures the amount of information that an observable random variable Y carries about an unknown parameter θ of the statistical model that models Y. To make this concrete, Y has the density function $p(\cdot|\theta)$ which depends on θ. Write the log-likelihood function of θ as $L(\theta) = \log p(Y|\theta)$, and the gradient function of the log-likelihood (the *score function*) with respect to θ as $S(\theta) = \partial L(\theta)/\partial\theta$. The *Fisher information* about the parameter θ is defined to be expectation of the second moment of the score function,

$$\mathcal{I}(\theta) = \operatorname{E}\left[\left(\frac{\partial}{\partial\theta}\log p(Y|\theta)\right)^2\right].$$

Here, expectation is taken with respect to the random variable Y under its true distribution. Under certain regularity conditions, it can be shown that $\operatorname{E}[S(\theta)] = 0$, and thus the Fisher information is in fact the variance of the score function, since $\operatorname{Var}[S(\theta)] = \operatorname{E}[S(\theta)^2] - \operatorname{E}^2[S(\theta)]$. Further, if $\log p(Y|\theta)$ is twice differentiable with respect to θ, then it can be shown that under certain regularity conditions,

$$\mathcal{I}(\theta) = \operatorname{E}\left[-\frac{\partial^2}{\partial\theta^2}\log p(Y|\theta)\right].$$

Many textbooks provides a proof of this fact—see, for example, Wasserman (2013, Section 9.7).

From the last equation above, we see that the Fisher information is related to the curvature or concavity of the graph of the log-likelihood function, averaged over the random variable Y. The curvature, defined as the second derivative on the graph[2] of a function, measures how quickly the function changes with changes in its input values.

[1] The introductory chapter of Pawitan (2001) and the citations therein give a delightful account of the evolution of the Fisherian view regarding statistical inference.

[2] Formally, the graph of a function g is the set of all ordered pairs $(x, g(x))$.

This then gives an intuition regarding the uncertainty surrounding θ at its maximal value; high Fisher information is indicative of a sharp peak at the maxima and therefore small variance, while low Fisher information is indicative of a shallow maxima for which many θ share similar log-likelihood values. Fisher information may be added much in the same way as log-likelihood may be added—the *total Fisher information* from n independent and identically distributed random variables $Y_1, \dots, Y_n$ is simply the sum of the n *unit Fisher information*, i.e. $\mathcal{I}_n(\theta) = n\mathcal{I}(\theta)$.

8. Check if total Fisher information is relevant.

3.2 Fisher information for Hilbert space objects

We extend the idea beyond thinking about parameters as merely numbers in the usual sense, to abstract objects in Hilbert spaces. This generalisation allows us to extend the concept of Fisher information to regression functions in RKHSs later. The score and Fisher information is derived in a familiar manner, but extra care is required when taking derivatives with respect to Hilbert space objects. We discuss a generalisation of the concept of differentiability from real-valued functions of a single, real variable, as is common in calculus, to functions between Hilbert spaces.

def:frechet

Definition 3.1 (Fréchet derivative)**.** Let $\mathcal{V}$ and $\mathcal{W}$ be two Hilbert spaces, and $\mathcal{U} \subseteq \mathcal{V}$ be an open subset. A function $f : \mathcal{U} \to \mathcal{W}$ is called *Fréchet differentiable* at $x \in \mathcal{U}$ if there exists a bounded, linear operator $T : \mathcal{V} \to \mathcal{W}$ such that

$$\lim_{v \to 0} \frac{\big\|f(x+v) - f(x) - Tv\big\|_{\mathcal{W}}}{\|v\|_{\mathcal{V}}} = 0$$

If this relation holds, then the operator T is unique, and we write $\mathrm{d}f(x) := T$ and call it the *Fréchet derivative* or *Fréchet differential* of f at x. If f is differentiable at every point $\mathcal{U}$, then f is said to be *(Fréchet) differentiable* on $\mathcal{U}$.

Remark 3.1. Since $\mathrm{d}f(x)$ is a bounded, linear operator, by Lemma 2.1, it is also continuous.

Remark 3.2. While the Fréchet derivative is most commonly defined as derivatives of functions between Banach spaces, the definition itself also applies to Hilbert spaces. Since our main focus are RKHSs, it is presented as such, and we follow the definitions supplied in Balakrishnan (1981, Definition 3.6.5) and Bouboulis and Theodoridis (2011, Section 6).

Remark 3.3. The use of the open subset $\mathcal{U}$ in the definition above for the domain of the function f is so that the notion of f being differentiable is possible even without having it defined on the entire space $\mathcal{V}$.

The intuition here is similar to that of regular differentiability, in that the linear operator T well approximates the change in f at x (the numerator), relative to the change in x (the denominator)—the fact that the limit exists and is zero, it must mean that the numerator converges faster to zero than the denominator does. In Landau notation, we have the familiar expression $f(x+v) = f(v) + \mathrm{d}f(x)(v) + o(v)$, that is, the derivative of f at x gives the best linear approximation to f near x. Note that the limit in the definition is meant in the usual sense of convergence of functions with respect to the norms of $\mathcal{V}$ and $\mathcal{W}$.

For the avoidance of doubt, $\mathrm{d}f(x)$ is not a vector in $\mathcal{W}$, but is an element of the set of bounded, linear operators from $\mathcal{V}$ to $\mathcal{W}$, denoted $\mathrm{L}(\mathcal{V};\mathcal{W})$. That is, if $f : \mathcal{U} \to \mathcal{W}$ is a differentiable function at all points in $\mathcal{U} \subseteq \mathcal{V}$, then its derivative is a linear map

$$\begin{gathered}\mathrm{d}f : \mathcal{U} \to \mathrm{L}(\mathcal{V};\mathcal{W}) \\ x \mapsto \mathrm{d}f(x).\end{gathered}$$

It follows that this function may also have a derivative, which by definition will be a linear map as well. This is the *second Fréchet derivative* of f, defined by

$$\begin{gathered}\mathrm{d}^2 f : \mathcal{U} \to \mathrm{L}\big(\mathcal{V};\mathrm{L}(\mathcal{V};\mathcal{W})\big) \\ x \mapsto \mathrm{d}^2 f(x).\end{gathered}$$

To make sense of the space on the right-hand side, consider the following argument.

- Take any $\phi(\cdot) \in \mathrm{L}\big(\mathcal{V};\mathrm{L}(\mathcal{V};\mathcal{W})\big)$. For all $v \in \mathcal{V}$, $\phi(v) \in \mathrm{L}(\mathcal{V};\mathcal{W})$, and $\phi(v)$ is linear in v.

- Since $\phi(v) \in \mathrm{L}(\mathcal{V};\mathcal{W})$, it is itself a linear operator taking elements from $\mathcal{V}$ to $\mathcal{W}$. We can write it as $\phi(v)(\cdot)$ for clarity.

- So, for any $v' \in \mathcal{V}$, $\phi(v)(v') \in \mathcal{W}$, and it depends linearly on v' too. Thus, given any two $v, v' \in \mathcal{V}$, we obtain an element $\phi(v)(v') \in \mathcal{W}$ which depends linearly on both v and v'.

- It is therefore possible to identify $\phi \in \mathrm{L}\big(\mathcal{V};\mathrm{L}(\mathcal{V};\mathcal{W})\big)$ with an element $\psi \in \mathrm{L}(\mathcal{V} \times \mathcal{V}, \mathcal{W})$ such that for all $v, v' \in \mathcal{V}$, $\phi(v)(v') = \psi(v, v')$.

To summarise, there is an isomorphism between the space on the right-hand side and the space $\mathrm{L}(\mathcal{V} \times \mathcal{V}, \mathcal{W})$ of all continuous bilinear maps from $\mathcal{V}$ to $\mathcal{W}$. The second derivative $\mathrm{d}^2 f(x)$ is therefore a bounded, bilinear operator from $\mathcal{V} \times \mathcal{V}$ to $\mathcal{W}$.

Another closely related type of differentiability is the concept of *Gâteaux differentials*, which is the formalism of the functional derivative in calculus of variations. Let $\mathcal{V}$, $\mathcal{W}$ and $\mathcal{U}$ be as before, and consider the function $f : \mathcal{U} \to \mathcal{W}$.

Definition 3.2 (Gâteaux derivative)**.** The *Gâteaux differential* or the *Gâteaux derivative* $\partial_v f(x)$ of f at $x \in \mathcal{U}$ in the direction $v \in \mathcal{V}$ is defined as

$$\partial_v f(x) = \lim_{t \to 0} \frac{f(x + tv) - f(x)}{t},$$

for which this limit is taken relative to the topology of $\mathcal{W}$. The function f is said to be *Gâteaux differentiable* at $x \in \mathcal{U}$ if f has a directional derivative along all directions at x. We name the operator $\partial f(x) : \mathcal{V} \to \mathcal{W}$ which assigns $v \mapsto \partial_v f(x) \in \mathcal{W}$ the *Gâteaux derivative* of f at x, and the operator $\partial f : \mathcal{U} \to (\mathcal{V};\mathcal{W}) = \{A \,|\, A : \mathcal{V} \to \mathcal{W}\}$ which assigns $x \mapsto \partial f(x)$ simply the *Gâteaux derivative* of f.

Remark 3.4. For Gâteaux derivatives, $\mathcal{V}$ need only be a vector space, while $\mathcal{W}$ a topological space. Tapia (1971, p. 55) wrote that for quite some time analysis was simply done using the topology of the real line when dealing with functionals. As a result, important concepts such as convergence could not be adequately discussed.

Remark 3.5 (Tapia, 1971, p. 52). The space $(\mathcal{V};\mathcal{W})$ of operators from $\mathcal{V}$ to $\mathcal{W}$ is not a topological space, and there is no obvious way to define a topology on it. Consequently, we cannot consider the Gâteaux derivative of the Gâteaux derivative.

Unlike the Fréchet derivative, which is by definition a linear operator, the Gâteaux derivative may fail to satisfy the additive condition of linearity[3]. Even if it is linear, it may fail to depend continuously on some $v' \in \mathcal{V}$ if $\mathcal{V}$ and $\mathcal{W}$ are infinite dimensional. In this sense, Fréchet derivatives are more demanding than Gâteaux derivatives. Nevertheless, the reasons we bring up Gâteaux derivatives is because it is usually simpler to calculate Gâteaux derivatives than Fréchet derivatives, and the two concepts are connected by the lemma below.

[3] Although, for all scalars $\lambda \in \mathbb{R}$, the Gâteaux derivative is homogenous: $\partial_{\lambda v} f(x) = \lambda \partial_v f(x)$.

Lemma 3.1 (Fréchet differentiability implies Gâteaux differentiability)**.** *If f is Fréchet differentiable at $x \in \mathcal{U}$, then $f : \mathcal{U} \to \mathcal{W}$ is Gâteaux differentiable at that point too, and $df(x) = \partial f(x)$.*

Proof. Since f is Fréchet differentiable at $x \in \mathcal{U}$, we can write $f(x+v) \approx f(x) + \mathrm{d}f(x)(v)$ for some $v \in \mathcal{V}$. Then,

$$\begin{aligned}
&\lim_{t\to 0} \left\| \frac{f(x+tv) - f(x)}{t} - \mathrm{d}f(x)(v) \right\|_{\mathcal{W}} \qquad (3.1) \\
&\qquad = \lim_{t\to 0} \frac{1}{t} \big\| f(x+tv) - f(x) - \mathrm{d}f(x)(tv) \big\|_{\mathcal{W}} \\
&\qquad = \lim_{t\to 0} \frac{\big\| f(x+tv) - f(x) - \mathrm{d}f(x)(tv) \big\|_{\mathcal{W}}}{\|tv\|_{\mathcal{V}}} \cdot \|v\|_{\mathcal{V}}
\end{aligned}$$

{eq:frecimplygat}

converges to 0 since f is Fréchet differentiable at x, and $t \to 0$ if and only if $\|tv\|_{\mathcal{V}} \to 0$. Thus, f is Gâteaux differentiable at x, and the Gâteaux derivative $\partial_v f(x)$ of f at x in the direction v coincides with the Fréchet derivatiave of f at x evaluated at v. □

On the other hand, Gâteaux differentiability does not necessarily imply Fréchet differentiability. A sufficient condition for Fréchet differentiability is that the Gâteaux derivative is continuous at the point of differentiation, i.e., the map $\partial f : \mathcal{U} \to (\mathcal{V};\mathcal{W})$ is continuous at $x \in \mathcal{U}$. In other words, if $\partial f(x)$ is a bounded linear operator and the convergence in (3.1) is uniform with respect to all v such that $\|v\|_{\mathcal{V}} = 1$, then $\mathrm{d}f(x)$ exists and $\mathrm{d}f(x) = \partial f(x)$ (Tapia, 1971, p. 57 & 66).

Consider now the function $\mathrm{d}f(x) : \mathcal{V} \to \mathcal{W}$ and suppose that f is twice Fréchet differentiable at $x \in \mathcal{U}$, i.e. $\mathrm{d}f(x)$ is Fréchet differentiable at $x \in \mathcal{U}$ with derivative $\mathrm{d}^2 f(x) : \mathcal{V} \times \mathcal{V} \to \mathcal{W}$. Then, $\mathrm{d}f(x)$ is also Gâteaux differentiable at the point x and the two differentials coincide. In particular, we have

$$\left\| \frac{\mathrm{d}f(x+tv)(v') - \mathrm{d}f(x)(v')}{t} - \mathrm{d}^2 f(x)(v,v') \right\|_{\mathcal{W}} \to 0 \text{ as } t \to 0, \qquad (3.2)$$

{eq:frech2gat}

by a similar argument in the proof above. We will use this fact when we describe the Hessian in a little while.

There is also the concept of *gradients* in Hilbert space. Recall that the Riesz representation theorem says that the mapping $A : \mathcal{V} \to \mathcal{V}'$ from the Hilbert space $\mathcal{V}$ to its continuous dual space $\mathcal{V}'$ defined by $A = \langle \cdot, v \rangle_{\mathcal{V}}$ for some $v \in \mathcal{V}$ is an isometric isomorphism. Again, let $\mathcal{U} \subseteq \mathcal{V}$ be an open subset, and let $f : \mathcal{U} \to \mathbb{R}$ be a (Fréchet) differentiable function with derivative $\mathrm{d}f : \mathcal{U} \to \mathrm{L}(\mathcal{V}, \mathbb{R}) \equiv \mathcal{V}'$. We define the gradient as follows.

Definition 3.3 (Gradients in Hilbert space)**.** The *gradient* of f is the operator $\nabla f : \mathcal{U} \to \mathcal{V}$ defined by $\nabla f = A^{-1} \circ \mathrm{d}f$. Thus, for $x \in \mathcal{U}$, the gradient of f at x, denoted $\nabla f(x)$, is the unique element of $\mathcal{V}$ satisfying

$$\langle \nabla f(x), v \rangle_{\mathcal{V}} = \mathrm{d}f(x)(v)$$

for any $v \in \mathcal{V}$. Note that ∇f being a composition of two continuous functions, is itself continuous.

Remark 3.6. Alternatively, the gradient can be motivated using the Riesz representation theorem in Definition 3.1 of the Fréchet derivative. Since $\mathcal{V}' \ni T : \mathcal{V} \to \mathbb{R}$, there is a unique element $v^* \in \mathcal{V}$ such that $T(v) = \langle v^*, v \rangle_{\mathcal{V}}$ for any $v \in \mathcal{V}$. The element $v^* \in \mathcal{V}$ is called the gradient of f at x.

Since the gradient of f is an operator on $\mathcal{U}$ to $\mathcal{V}$, it may itself have a (Fréchet) derivative. Assuming existence, i.e., f is twice Fréchet differentiable at $x \in \mathcal{U}$, we call this derivative the *Hessian* of f. From (3.2), it must be that

$$\begin{aligned}
\mathrm{d}^2 f(x)(v, v') &= \lim_{t \to 0} \frac{\mathrm{d}f(x + tv)(v') - \mathrm{d}f(x)(v')}{t} \\
&= \lim_{t \to 0} \frac{\langle \nabla f(x + tv), v' \rangle_{\mathcal{V}} - \langle \nabla f(x), v' \rangle_{\mathcal{V}}}{t} \\
&= \left\langle \lim_{t \to 0} \frac{\nabla f(x + tv) - \nabla f(x)}{t}, v' \right\rangle_{\mathcal{V}} \\
&= \left\langle \partial_v \nabla f(x), v' \right\rangle_{\mathcal{V}} .
\end{aligned}$$

The second line follows from the definition of gradients, and the third line follows by linearity of inner products. Note that since the Fréchet and Gâteaux differentials coincide, we have that $\partial_v \nabla f(x) = \mathrm{d}\nabla f(x)(v)$. Letting $\mathcal{V}$, $\mathcal{W}$ and $\mathcal{U}$ be as before, we now define the Hessian for the function $f : \mathcal{U} \to \mathcal{W}$.

Definition 3.4 (Hessian)**.** The Fréchet derivative of the gradient of f is known as the *Hessian* of f. Denoted $\nabla^2 f$, it is the mapping $\nabla^2 f : \mathcal{U} \to \mathrm{L}(\mathcal{V}, \mathcal{V})$ defined by $\nabla^2 f = \mathrm{d}\nabla f$, and it satisfies

$$\left\langle \nabla^2 f(x)(v), v' \right\rangle_{\mathcal{V}} = \mathrm{d}^2 f(x)(v, v').$$

for $x \in \mathcal{U}$ and $v, v' \in \mathcal{V}$.

Remark 3.7. Since $\mathrm{d}^2 f(x)$ is a bilinear form in $\mathcal{V}$, we can equivalently write

$$\mathrm{d}^2 f(x)(v, v') = \langle \mathrm{d}^2 f(x), v \otimes v' \rangle_{\mathcal{V}\otimes\mathcal{V}}$$

following the correspondence between bilinear forms and tensor product spaces.

With the differentiation tools above, we can now derive the Fisher information that we set out to derive at the beginning of this section. Let Y be a random variable with density in the parametric family $\{p(\cdot|\theta) \,|\, \theta \in \Theta\}$, where Θ is now assumed to be a Hilbert space with inner product $\langle \cdot, \cdot \rangle_\Theta$. If $p(Y|\theta) > 0$, the log-likelihood function of θ is the real-valued function $L(\cdot|Y) : \Theta \to \mathbb{R}$ defined by $\theta \mapsto \log p(Y|\theta)$. The score S, assuming existence, is defined to be the (Fréchet) derivative of $L(\cdot|Y)$ at θ, i.e. $S : \Theta \to \mathrm{L}(\Theta, \mathbb{R}) \equiv \Theta'$ defined by $S = \mathrm{d}L(\cdot|Y)$. The second (Fréchet) derivative of $L(\cdot|Y)$ at θ is then $\mathrm{d}^2 L(\cdot|Y) : \Theta \to \mathrm{L}(\Theta \times \Theta, \mathbb{R})$. We now prove the following proposition.

thm:fisherinfohilbert

Proposition 3.2 (Fisher information in Hilbert space)**.** *Assume that* $p(Y|\cdot)$ *and* $\log p(Y|\cdot)$ *are both Fréchet differentiable at* θ*. Then, the Fisher information for* $\theta \in \Theta$ *is the element in the tensor product space* $\Theta \otimes \Theta$ *defined by*

$$\mathcal{I}(\theta) = \mathrm{E}[\nabla L(\theta|Y) \otimes \nabla L(\theta|Y)].$$

Equivalently, assuming further that $\log p(Y|\cdot)$ *is twice Fréchet differentiable at* θ*, the Fisher information can be written as*

$$\mathcal{I}(\theta) = \mathrm{E}[-\nabla^2 L(\theta|Y)].$$

Note that both expectations are taken under the true distribution of random variable Y*.*

Proof. The Gâteaux derivative of $L(\cdot|Y) = \log p(Y|\cdot)$ at $\theta \in \Theta$ in the direction $b \in \Theta$, which is also its Fréchet derivative, is

$$\begin{aligned}
\partial_b L(\theta|Y) &= \frac{\mathrm{d}}{\mathrm{d}t} \log p(Y|\theta + tb) \bigg|_{t=0} \\
&= \frac{\frac{\mathrm{d}}{\mathrm{d}t} p(Y|\theta + tb)\big|_{t=0}}{p(Y|\theta)} \\
&= \frac{\partial_b p(Y|\theta)}{p(Y|\theta)}.
\end{aligned}$$

Since it assumed that $p(Y|\cdot)$ is Fréchet differentiable at θ, $\mathrm{d}p(Y|\theta)(b) = \partial_b p(Y|\theta)$. The expectation of the score for any $b \in \Theta$ is shown to be

$$
\begin{aligned}
\mathrm{E}[\mathrm{d}L(\theta|Y)(b)] &= \mathrm{E}\left[\frac{\mathrm{d}p(Y|\theta)(b)}{p(Y|\theta)}\right] \\
&= \int \frac{\mathrm{d}p(Y|\theta)(b)}{\cancel{p(Y|\theta)}} \cancel{p(Y|\theta)} \,\mathrm{d}Y \\
&= \left(\mathrm{d}\int p(Y|\cdot)\,\mathrm{d}Y\right)(\theta)(b) \\
&= \left\langle \left(\nabla \int p(Y|\cdot)\,\mathrm{d}Y\right)(\theta), b \right\rangle_\Theta \\
&= 0.
\end{aligned}
$$

The interchange of Lebesgue integrals and Fréchet differentials is allowed under certain conditions[4] (Kammar, 2016). The derivative of $\int p(Y|\cdot)\,\mathrm{d}Y$ at any value of $\theta \in \Theta$ is the zero vector as it is the derivative of a constant (i.e., 1).

Using the classical notion that the Fisher information is the variance of the score function, then, for fixed $b, b' \in \Theta$, combined with the fact that $\mathrm{E}[\mathrm{d}L(\theta|Y)]$ is a zero mean function, we have that

$$
\begin{aligned}
\mathcal{I}(\theta)(b,b') &= \mathrm{E}[\mathrm{d}L(\theta|Y)(b) \cdot \mathrm{d}L(\theta|Y)(b')] \\
&= \mathrm{E}\left[\langle \nabla L(\theta|Y), b\rangle_\Theta \langle \nabla L(\theta|Y), b'\rangle_\Theta\right] \\
&= \left\langle \mathrm{E}[\nabla L(\theta|Y) \otimes \nabla L(\theta|Y)], b \otimes b'\right\rangle_{\Theta\otimes\Theta}.
\end{aligned}
$$

Hence, $\mathcal{I}(\theta)$ as a bilinear form corresponds to the element $\mathrm{E}[\nabla L(\theta|Y) \otimes \nabla L(\theta|Y)] \in \Theta\otimes\Theta$.

[4] The conditions are:

1. $L(\cdot|Y)$ is Frechét differentiable on $\mathcal{U} \subseteq \Theta$ for almost every $Y \in \mathbb{R}$.
2. $L(\theta|Y)$ and $\mathrm{d}L(\theta|Y)(b)$ are both integrable with respect to Y, for any $\theta \in \mathcal{U} \subseteq \Theta$ and $b \in \Theta$.
3. There is an integrable function $g(Y)$ such that $L(\theta|Y) \leq g(Y)$ for all $\theta \in \Theta$ and almost every $Y \in \mathbb{R}$.

These conditions as stated are analogous to the measure theoretic requirements for Leibniz's integral rule to hold (differentiation under the integral sign). For nice and well-behaved probability densities, like the normal density that we will be working with, this isn't an issue.

The Gâteaux derivative of the Fréchet differential is the second Fréchet derivative, since $L(\cdot|Y)$ is assumed to be twice differentiable at $\theta \in \Theta$:

$$\begin{aligned}
\mathrm{d}^2 L(\theta|Y)(b,b') &= \partial_{b'} \mathrm{d}L(\theta|Y)(b) \\
&= \partial_{b'} \left(\frac{\mathrm{d}p(Y|\theta)(b)}{p(Y|\theta)} \right) \\
&= \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\mathrm{d}p(Y|\theta + tb')(b)}{p(Y|\theta + tb')} \right) \Bigg|_{t=0} \\
&= \frac{p(Y|\theta)\mathrm{d}^2 p(Y|\theta)(b,b') - \mathrm{d}p(Y|\theta)(b)\mathrm{d}p(Y|\theta)(b')}{p(Y|\theta)^2} \\
&= \frac{\mathrm{d}^2 p(Y|\theta)(b,b')}{p(Y|\theta)} - \mathrm{d}L(\theta|Y)(b)\mathrm{d}L(\theta|Y)(b').
\end{aligned}$$

Taking expectations of the first term in the right-hand side, we get that

$$\begin{aligned}
\mathrm{E}\left[\frac{\mathrm{d}^2 p(Y|\theta)(b,b')}{p(Y|\theta)} \right] &= \int \frac{\mathrm{d}\big(\mathrm{d}p(Y|\theta)\big)(b,b')}{\cancel{p(Y|\theta)}} \cancel{p(Y|\theta)} \, \mathrm{d}Y \\
&= \left(\mathrm{d}^2 \int p(Y|\cdot) \, \mathrm{d}Y \right) (\theta)(b,b') \\
&= \left\langle \left(\nabla^2 \int p(Y|\cdot) \, \mathrm{d}Y \right) (\theta)(b), b' \right\rangle_\Theta \\
&= 0.
\end{aligned}$$

Thus, we see that from the first result obtained,

$$\begin{aligned}
\mathrm{E}[-\mathrm{d}^2 L(\theta|Y)(b,b')] &= \mathrm{E}[\mathrm{d}L(\theta|Y)(b)\mathrm{d}L(\theta|Y)(b')] \\
&= \mathcal{I}(\theta)(b,b'),
\end{aligned}$$

while

$$\begin{aligned}
\mathrm{E}[-\mathrm{d}^2 L(\theta|Y)(b,b')] &= -\,\mathrm{E}\langle \nabla^2 L(\theta|Y)(b), b' \rangle_\Theta \\
&= \langle -\,\mathrm{E}\,\nabla^2 L(\theta|Y)(b), b' \rangle_\Theta.
\end{aligned}$$

It would seem that $\mathrm{E}[-\nabla^2 L(\theta|Y)(b)]$ is an operator from Θ onto itself which also induces a bilinear form equivalent to $\mathrm{E}[-\mathrm{d}^2 L(\theta|Y)]$. Therefore, $\mathcal{I}(\theta) = \mathrm{E}[-\nabla^2 L(\theta|Y)]$. □

The Fisher information $\mathcal{I}(\theta)$ for θ, much like the covariance operator, can be viewed in one of three ways:

1. As its general form, i.e. an element in $\Theta \otimes \Theta$;
2. As an operator $\mathcal{I}(\theta) : \Theta \to \Theta$ defined by $\mathcal{I}(\theta)(b) = \operatorname{E}[-\nabla^2 L(\theta|Y)](b)$; and finally
3. As a bilinear form $\mathcal{I}(\theta) : \Theta \times \Theta \to \mathbb{R}$ defined by $\mathcal{I}(\theta)(b, b') = \langle - \operatorname{E} \nabla^2 L(\theta|Y)(b), b' \rangle_\Theta$ $= \operatorname{E}[-\mathrm{d}^2 L(\theta|Y)(b, b')]$.

In particular, viewed as a bilinear form, the evaluation of the Fisher information for θ at two points b and b' in Θ is seen as the Fisher information between two continuous, linear functionals of θ. For brevity, we denote this $\mathcal{I}(\theta_b, \theta_{b'})$, where $\theta_b = \langle \theta, b \rangle_\theta$ for some $b \in \Theta$. The natural isometry between Θ and Θ' then allows us to write

$$\mathcal{I}(\theta_b, \theta_{b'}) = \langle \mathcal{I}(\theta), b \otimes b' \rangle_{\Theta \otimes \Theta} = \big\langle \mathcal{I}(\theta), \langle \cdot, b \rangle_\Theta \otimes \langle \cdot, b' \rangle_\Theta \big\rangle_{\Theta' \otimes \Theta'}. \tag{3.3}$$

{eq:fisher-linear-functional}

3.3 Fisher information for regression functions

We are now equipped to derive the Fisher information for our regression function. For convenience, we restate the regression model and its assumptions. The regression model relating response variables $y_i \in \mathbb{R}$ and the covariates $x_i \in \mathcal{X}$, for $i = 1, \dots, n$ is

$$y_i = \alpha + f(x_i) + \epsilon_i \tag{1.1}$$

$$(\epsilon_1, \dots, \epsilon_n)^\top \sim \mathrm{N}_n(0, \mathbf{\Psi}^{-1}) \tag{1.2}$$

where $\alpha \in \mathbb{R}$ is an intercept and f is in an RKHS $\mathcal{F}$ with kernel $h_\eta : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.

thm:fisherregf

Lemma 3.3 (Fisher information for regression function)**.** *For the regression model (1.1) subject to (1.2) and $f \in \mathcal{F}$ where $\mathcal{F}$ is an RKHS with kernel h, the Fisher information for f is given by*

$$\mathcal{I}(f) = \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} h(\cdot, x_i) \otimes h(\cdot, x_j)$$

where ψ_{ij} are the (i,j)-th entries of the precision matrix $\mathbf{\Psi}$ of the normally distributed model errors. More generally, suppose that $\mathcal{F}$ has a feature space $\mathcal{V}$ such that the mapping $\phi : \mathcal{X} \to \mathcal{V}$ is its feature map, and if $f(x) = \langle \phi(x), v \rangle_\mathcal{V}$, then the Fisher information $I(v) \in \mathcal{V} \otimes \mathcal{V}$ for v is

$$\mathcal{I}(v) = \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} \phi(x_i) \otimes \phi(x_j).$$

Proof. For $x \in \mathcal{X}$, let $k_x : \mathcal{V} \to \mathbb{R}$ be defined by $k_x(v) = \langle \phi(x), v \rangle_{\mathcal{V}}$. Clearly, k_x is linear and continuous. Hence, the Gâteaux derivative of $k_x(v)$ in the direction u is

$$\begin{aligned}
\partial_u k_x(v) &= \lim_{t \to 0} \frac{k(v+tu) - k(v)}{t} \\
&= \lim_{t \to 0} \frac{\langle \phi(x), v + tu \rangle_{\mathcal{V}} - \langle \phi(x), v \rangle_{\mathcal{V}}}{t} \\
&= \lim_{t \to 0} \frac{t \langle \phi(x), u \rangle_{\mathcal{V}}}{t} \\
&= \langle \phi(x), u \rangle_{\mathcal{V}}.
\end{aligned}$$

Since clearly $\partial_u k_x(v)$ is a continuous linear operator for any $u \in \mathcal{V}$, it is bounded, so the Fréchet derivative exists and $\mathrm{d}k_x(v) = \partial k_x(v)$. Let $\mathbf{y} = \{y_1, \dots, y_n\}$, and denote the hyperparameters of the regression model by $\boldsymbol{\theta} = \{\alpha, \boldsymbol{\Psi}, \eta\}$. Without loss of generality, assume $\alpha = 0$; even if not, we can always add back α to the y_i's later. Regardless, both α and $\mathbf{y}$ are constant in the differential of $L(v|\mathbf{y}, \boldsymbol{\theta})$. The log-likelihood of v is given by

$$L(v|\mathbf{y}, \boldsymbol{\theta}) = \text{const.} - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} \big(y_i - k_{x_i}(v)\big)\big(y_j - k_{x_j}(v)\big)$$

and the score by

$$\begin{aligned}
\mathrm{d}L(\cdot|\mathbf{y}, \boldsymbol{\theta}) &= -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} \cdot \mathrm{d}(k_{x_i} k_{x_j} - y_j k_{x_i} - y_i k_{x_j} + y_i y_j) \\
&= -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} (k_{x_j} \mathrm{d}k_{x_i} + k_{x_i} \mathrm{d}k_{x_j} - y_j \mathrm{d}k_{x_i} - y_i \mathrm{d}k_{x_j}).
\end{aligned}$$

Differentiating again gives

$$\begin{aligned}
\mathrm{d}^2 L(\cdot|\mathbf{y}, \boldsymbol{\theta}) &= -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} (\mathrm{d}k_{x_j} \mathrm{d}k_{x_i} + \mathrm{d}k_{x_i} \mathrm{d}k_{x_j}) \\
&= - \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} \cdot \mathrm{d}k_{x_i} \mathrm{d}k_{x_j}
\end{aligned}$$

since the derivative of $\mathrm{d}k_x$ is zero (it is the derivative of a constant). We can then calculate the Fisher information to be

$$\begin{aligned}\mathcal{I}(v) = -\operatorname{E}\left[\mathrm{d}^2 L(v|\mathbf{y},\boldsymbol{\theta})\right] &= \operatorname{E}\left[\sum_{i=1}^n\sum_{j=1}^n \psi_{ij}\langle\phi(x_i),\cdot\rangle_{\mathcal{V}}\langle\phi(x_j),\cdot\rangle_{\mathcal{V}}\right] \\ &= \sum_{i=1}^n\sum_{j=1}^n \psi_{ij}\langle\phi(x_i)\otimes\phi(x_j),\cdot\rangle_{\mathcal{V}\otimes\mathcal{V}} \\ &= \sum_{i=1}^n\sum_{j=1}^n \psi_{ij}\cdot\phi(x_i)\otimes\phi(x_j).\end{aligned}$$

Here, we had treated $\phi(x_i)\otimes\phi(x_j)$ as a bilinear operator, since $\mathcal{I}(v)\in\mathcal{V}\otimes\mathcal{V}$ as well. Also, the expectation is free of the random variable under expectation (i.e., $\mathbf{y}$), which makes the second line possible.

By taking the canonical feature $\phi(x) = h(\cdot,x)$, we have that $\phi \equiv h(\cdot,x) : \mathcal{X}\to\mathcal{F}\equiv\mathcal{V}$ and therefore for $f\in\mathcal{F}$, the reproducing property gives us $f(x) = \langle h(\cdot,x), f\rangle_{\mathcal{F}}$, so the formula for $\mathcal{I}(f)\in\mathcal{F}\otimes\mathcal{F}$ follows. □

The above lemma gives the form of the Fisher information for f in a rather abstract fashion. Consider the following example of applying Lemma Lemma 3.3 to obtain the Fisher information for a standard linear regression model.

Example 3.1 (Fisher information for linear regression)**.** As before, suppose model (1.1) subject to (1.2) and $f\in\mathcal{F}$, an RKHS. For simplicity, we assume iid errors, i.e. $\boldsymbol{\Psi} = \psi\mathbf{I}_n$. Let $\mathcal{X} = \mathbb{R}^p$, and the feature space $\mathcal{V} = \mathbb{R}^p$ be equipped with the usual dot product $\langle\cdot,\cdot\rangle_{\mathcal{V}} : \mathcal{V}\otimes\mathcal{V}\to\mathbb{R}$ defined by $v^\top v$. Consider also the identity feature map $\phi : \mathcal{X}\to\mathcal{V}$ defined by $\phi(\mathbf{x}) = \mathbf{x}$. For some $\boldsymbol{\beta}\in\mathcal{V}$, the linear regression model is such that $f(\mathbf{x}) = \mathbf{x}^\top\boldsymbol{\beta} = \langle\phi(\mathbf{x}),\boldsymbol{\beta}\rangle_{\mathcal{V}}$. Therefore, according to Lemma Lemma 3.3, the Fisher information for β is

$$\begin{aligned}\mathcal{I}(\boldsymbol{\beta}) &= \sum_{i=1}^n\sum_{j=1}^n \psi\cdot\phi(\mathbf{x}_i)\otimes\phi(\mathbf{x}_j) \\ &= \psi\sum_{i=1}^n\sum_{j=1}^n \mathbf{x}_i\otimes\mathbf{x}_j \\ &= \psi\mathbf{X}^\top\mathbf{X}.\end{aligned}$$

Note that the operation '⊗' on two vectors in Euclidean space is simply their outer product. The resulting $\mathbf{X}$ is a $n \times p$ matrix containing the entries $\mathbf{x}_1^\top, \dots, \mathbf{x}_n^\top$ row-wise. This is of course recognised as the Fisher information for the regression coefficients in the standard linear regression model.

We can also compute the Fisher information for linear functionals of f, and in particular, for point evaluation functionals of f, thereby allowing us to compute the Fisher information at two points $f(x)$ and $f(x')$.

thm:fisherreglinfunc

Corollary 3.3.1 (Fisher information between two linear functionals of f)**.** *For our regression model as defined in (1.1) subject to (1.2) and f belonging to a RKHS $\mathcal{F}$ with kernel h, the Fisher information at two points $f(x)$ and $f(x')$ is given by*

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

Proof. In a RKHS $\mathcal{F}$, the reproducing property gives $f(x) = \langle f, h(\cdot, x) \rangle_\mathcal{F}$ and in particular, $\langle h(\cdot, x), h(\cdot, x') \rangle_\mathcal{F} = h(x, x')$. By (3.3), we have that

$$\begin{aligned}
\mathcal{I}(f)\big(h(\cdot,x), h(\cdot,x')\big) &= \big\langle \mathcal{I}(f), h(\cdot,x) \otimes h(\cdot,x') \big\rangle_{\mathcal{F}\otimes\mathcal{F}} \\
&= \left\langle \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} h(\cdot,x_i) \otimes h(\cdot,x_j) \ , \ h(\cdot,x) \otimes h(\cdot,x') \right\rangle_{\mathcal{F}\otimes\mathcal{F}} \\
&= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} \big\langle h(\cdot,x_i), h(\cdot,x) \big\rangle_\mathcal{F} \big\langle h(\cdot,x_j), h(\cdot,x') \big\rangle_\mathcal{F} \\
&= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} h(x,x_i) h(x',x_j).
\end{aligned}$$

The second to last line follows from the definition of the usual inner product for tensor spaces, and the last line follows by the reproducing property. □

An inspection of the formula in Corollary 3.3.1 reveals the fact that the Fisher information for $f(x)$, $\mathcal{I}\big(f(x), f(x)\big)$, is positive if and only if $h(x, x_i) \neq 0$ for at least one $i \in \{1, \dots, n\}$. In practice, this condition is often satisfied for all x, so this result might be considered both remarkable and reassuring, because it suggests we can estimate f over its entire domain, no matter how big, even though we only have a finite amount of data points.

3.4 The induced Fisher information RKHS

sec:induced FisherRKHS

From Lemma 3.3, the formula for the Fisher information uses n points of the observed data $x_i \in \mathcal{X}$. This seems to suggest that the Fisher information only exists for a finite subspace of the RKHS $\mathcal{F}$. Indeed, this is the case, and we will be specific about the subspace for which there is Fisher information. Consider the following set, a similar one considered in the proof of the Moore-Aronszajn theorem (Theorem 2.6):

$$\mathcal{F}_n = \left\{ f : \mathcal{X} \to \mathbb{R} \,\middle|\, f(x) = \sum_{i=1}^n h(x,x_i)w_i, \ w_i \in \mathbb{R}, \ i = 1,\dots,n \right\}. \tag{3.4}$$

{eq:subspaceFn}

Since $h(\cdot,x_i) \in \mathcal{F}$, then any $f \in \mathcal{F}_n$ is also in $\mathcal{F}$ by linearity, and thus $\mathcal{F}_n$ is a subset of $\mathcal{F}$. Further, $\mathcal{F}_n$ is closed under addition and multiplication by a scalar, and is therefore a subspace of $\mathcal{F}$. Unlike in Theorem 2.6, this is a finite subspace with dimension n.

Let $\mathcal{F}_n^\perp$ be the orthogonal complement of $\mathcal{F}_n$ in $\mathcal{F}$. By the orthogonal decomposition theorem, any regression function $f \in \mathcal{F}$ can be uniquely decomposed as $f = f_n + r$, with $f_n \in \mathcal{F}_n$ and $r \in \mathcal{F}_n^\perp$, where $\mathcal{F} = \mathcal{F}_n \oplus \mathcal{F}_n^\perp$. We saw earlier in Theorem 2.6 that $\mathcal{F}$ is the closure of $\mathcal{F}_n$, so therefore $\mathcal{F}$ is dense in $\mathcal{F}_n$, and hence by Corollary 2.3.1 we have that $\mathcal{F}_n^\perp = \{0\}$. Alternatively, we could have argued the following: any $r \in \mathcal{F}_n^\perp$ is orthogonal to each of the $h(\cdot,x_i) \in \mathcal{F}$, so by the reproducing property of h, $r(x_i) = \langle r, h(\cdot,x_i)\rangle_\mathcal{F} = 0$. This seems to suggest the statement in the following corollary.

Corollary 3.3.2. *With $g \in \mathcal{F}$, the Fisher information for g is zero if and only if $g \in \mathcal{F}_n^\perp$, i.e. if and only if $g(x_1) = \cdots = g(x_n) = 0$.*

Proof. Let $\mathcal{I}(f)$ be the Fisher information for f. The Fisher information for $\langle f, r\rangle_\mathcal{F}$ is

$$\begin{aligned}
\mathcal{I}(f)(r,r) &= \langle \mathcal{I}(f), r \otimes r \rangle_{\mathcal{F}\otimes\mathcal{F}} \\
&= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} \langle h(\cdot,x_i), r\rangle_\mathcal{F} \langle h(\cdot,x_j), r\rangle_\mathcal{F} \\
&= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} r(x_i) r(x_j).
\end{aligned}$$

So if $r \in \mathcal{F}_n^\perp$, then $r(x_1) = \cdots = r(x_n) = 0$, and thus the Fisher information at $r \in \mathcal{F}_n^\perp$ is zero. Conversely, if the Fisher information is zero, it must necessarily mean that $r(x_1) = \cdots = r(x_n) = 0$ since $\psi_{ij} > 0$, and thus $r \in \mathcal{F}_n^\perp$. □

The above corollary implies that the Fisher information for our regression function $f \in \mathcal{F}$ exists only on the n-dimensional subspace $\mathcal{F}_n$. More subtly, as there is no Fisher information for $r \in \mathcal{F}_n^\perp$, r cannot be estimated from the data. Thus, in estimating f, we will only ever consider the finite subspace $\mathcal{F}_n \subset \mathcal{F}$ where there is Fisher information about f.

As it turns out, $\mathcal{F}_n$ can be identified as a RKHS with reproducing kernel equal to the Fisher information for f. That is, the real, symmetric, and positive-definite function h_n over $\mathcal{X} \times \mathcal{X}$ defined by $h_n(x, x') = \mathcal{I}\big(f(x), f(x')\big)$ is associated to the RKHS which is $\mathcal{F}_n$, equipped with the squared norm $\|f\|^2_{\mathcal{F}_n} = \sum_{i,j=1}^n w_i(\mathbf{\Psi}^{-1})_{ij} w_j$. This is stated in the next lemma.

Lemma 3.4. *Let $\mathcal{F}_n$ as in (3.4) be equipped with the inner product*

$$\langle f, f' \rangle_{\mathcal{F}_n} = \sum_{i=1}^n \sum_{j=1}^n w_i(\mathbf{\Psi}^{-1})_{ij} w'_j = \mathbf{w}^\top \mathbf{\Psi} \mathbf{w}' \tag{3.5}$$

{eq:Fninnerprod}

for any two $f = \sum_{i=1}^n h(\cdot, x_i) w_i$ and $f' = \sum_{j=1}^n h(\cdot, x_j) w'_j$ in $\mathcal{F}_n$. Then, $h_n : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ as defined by

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

is the reproducing kernel of $\mathcal{F}_n$.

Proof. Since $\mathcal{F}_n$ is a finite subspace of $\mathcal{F}$, it is complete, and thus a Hilbert space. What remains to be proven is the reproducing property of h_n for $\mathcal{F}_n$. First note that by defining $w_j(x) = \sum_{k=1}^n \psi_{jk} h(x, x_k)$, we see that

$$h_n(x, \cdot) = \sum_{j=1}^n \sum_{k=1}^n \psi_{jk} h(x, x_j) h(\cdot, x_k) = \sum_{j=1}^n w_j(x) h(\cdot, x_j)$$

Furthermore, writing $h(\cdot, x_j) = \sum_{k=1}^n \delta_{jk} h(\cdot, x_k)$, we see that $h(\cdot, x_j)$ is also an element of $\mathcal{F}_n$, and in particular,

$$\big\langle h(\cdot, x_i), h(\cdot, x_k) \big\rangle_{\mathcal{F}_n} = \sum_{j=1}^n \sum_{l=1}^n \delta_{ij} (\mathbf{\Psi}^{-1})_{jl} \delta_{lk} = (\mathbf{\Psi}^{-1})_{ik}$$

where δ is the Kronecker delta. Denote by ψ_{ij}^{-} the (i,j)th element of $\mathbf{\Psi}^{-1}$. A fact we will use later is $\sum_{k=1}^n \psi_{jk}\psi_{ik}^{-} = (\mathbf{\Psi}\mathbf{\Psi}^{-1})_{ji} = (\mathbf{I}_n)_{ji} = \delta_{ji}$. Then,

$$\begin{aligned}
\langle f, h_n(x,\cdot)\rangle_{\mathcal{F}_n} &= \left\langle \sum_{i=1}^n h(\cdot,x_i)w_i, \sum_{j=1}^n\sum_{k=1}^n \psi_{jk}h(x,x_j)h(\cdot,x_k) \right\rangle_{\mathcal{F}_n} \\
&= \sum_{i=1}^n w_i \sum_{j=1}^n\sum_{k=1}^n \psi_{jk}h(x,x_j)\big\langle h(\cdot,x_i), h(\cdot,x_k)\big\rangle_{\mathcal{F}_n} \\
&= \sum_{i=1}^n w_i \sum_{j=1}^n\sum_{k=1}^n \psi_{jk}h(x,x_j)\psi_{ik}^{-} \\
&= \sum_{i=1}^n w_i \sum_{j=1}^n \delta_{ji}h(x,x_j) \\
&= \sum_{i=1}^n w_i h(x,x_i) \\
&= f(x).
\end{aligned}$$

Therefore, h_n is a reproducing kernel for $\mathcal{F}_n$. □

3.5 The I-prior

In the introductory chapter, we discussed that unless the regression function f is regularised (for instance, using some prior information), the ML estimator of f is likely to be inadequate. In choosing a prior distribution for f, we appeal to the principle of maximum entropy, which states that the probability distribution which best represents the current state of knowledge is the one with largest entropy. In this section, we aim to show the relationship between the Fisher information for f and its maximum entropy prior distribution. Before doing this, we recall the definition of entropy and derive the maximum entropy prior distribution for a parameter which has unrestricted support. Let (Θ, D) be a metric space and let $\nu = \nu_D$ be a volume measure induced by D (e.g. Hausdorff measure). In addition, assume ν is a probability measure over Θ so that $(\Theta, \mathcal{B}(\Theta), \nu)$ is a Borel probability space.

Definition 3.5 (Entropy)**.** Denote by p a probability density over Θ relative to ν. Suppose that $\int p \log p \, \mathrm{d}\nu < \infty$, i.e., $p \log p$ is Lebesgue integrable and belongs to the space

$\mathrm{L}^1(\Theta,\nu)$. The entropy of a distribution p over Θ relative to a measure ν is defined as

$$H(p) = -\int_\Theta p(\theta)\log p(\theta)\,\mathrm{d}\nu(\theta).$$

In deriving the maximum entropy distribution, we will need to maximise the functional H with respect to p. Typically this is done using calculus of variations techniques of functional derivatives. Since we have already introduced concepts of Fréchet and Gâteaux derivatives earlier, we shall use those instead. Assume that the entropy H is Fréchet differentiable at p, and that the probability densities p under consideration belong to the Hilbert space of square integrable functions $\mathrm{L}^2(\Theta,\nu)$ with inner product $\langle p,p'\rangle_{L^2(\Theta,\nu)} = \int pp'\,\mathrm{d}\nu$. Now since the Fréchet derivative of H at p is assumed to exist, it is equal to the Gâteaux derivative, which can be computed as follows:

$$\begin{aligned}
\partial_q H(p) &= \frac{\mathrm{d}}{\mathrm{d}t} H(p+tq)\bigg|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left\{ -\int_\Theta \big(p(\theta)+tq(\theta)\big)\log\big(p(\theta)+tq(\theta)\big)\,\mathrm{d}\nu(\theta) \right\}\bigg|_{t=0} \\
&= -\int_\Theta \left\{ \frac{\mathrm{d}}{\mathrm{d}t}\big(p(\theta)+tq(\theta)\big)\log\big(p(\theta)+tq(\theta)\big)\bigg|_{t=0} \right\}\mathrm{d}\nu(\theta) \\
&= -\int_\Theta \left(\frac{p(\theta)q(\theta)}{p(\theta)+tq(\theta)} + \frac{tq(\theta)^2}{p(\theta)+tq(\theta)} + q(\theta)\log\big(p(\theta)+tq(\theta)\big) \right)\bigg|_{t=0}\mathrm{d}\nu(\theta) \\
&= -\int_\Theta q(\theta)\big(1+\log p(\theta)\big)\,\mathrm{d}\nu(\theta) \\
&= \big\langle -\big(1+\log p\big), q \big\rangle_\Theta \\
&= \mathrm{d}H(p)(q).
\end{aligned}$$

By definition, the gradient of H at p, denoted $\nabla H(p)$, is equal to $-1-\log p$. This agrees with the usual functional derivative of the entropy obtained via standard calculus of variations, which is typically denoted $\partial H/\partial p$. We now present another well known result from information theory, regarding the form of the maximum entropy distribution.

thm:maxentr

Lemma 3.5 (Maximum entropy distribution). *Let (Θ, D) be a metric space, $\nu = \nu_D$ be a volume measure induced by D, and p be a probability density function on Θ. The entropy maximising density $\tilde p$, which satisfies*

$$\operatorname*{arg\,max}_{p\in L^2(\Theta,\nu)} H(p) = -\int_\Theta \tilde p(\theta)\log\tilde p(\theta)\,\mathrm{d}\nu(\theta),$$

subject to the constraints

$$\operatorname{E}\left[D(\theta,\theta_0)^2\right] = \int_\Theta D(\theta,\theta_0)^2 p(\theta)\,\mathrm{d}\nu(\theta) = const., \qquad \int_\Theta p(\theta)\,\mathrm{d}\nu(\theta) = 1,$$

$$\textit{and} \quad p(\theta) \geq 0, \forall\theta\in\Theta,$$

is the density given by

$$\tilde p(\theta) \propto \exp\left(-\frac{1}{2}D(\theta,\theta_0)^2\right),$$

for some fixed $\theta_0 \in \Theta$. If (Θ, D) is a Euclidean space and ν a flat (Lebesgue) measure then $\tilde p$ represents a (multivariate) normal density.

Sketch proof. This follows from standard calculus of variations, though we provide a sketch proof here. Set up the Langrangian

$$\begin{aligned}\mathcal{L}(p,\gamma_1,\gamma_2) = -\int_\Theta p(\theta)\log p(\theta)\,\mathrm{d}\nu(\theta) + \gamma_1\left(\int_\Theta D(\theta,\theta_0)^2 p(\theta)\,\mathrm{d}\nu(\theta) - \text{const.}\right) \\ + \gamma_2\left(\int_\Theta p(\theta)\,\mathrm{d}\nu(\theta) - 1\right).\end{aligned}$$

From the above illustration preceding the lemma, taking derivatives with respect to p yields

$$\frac{\partial}{\partial p}\mathcal{L}(p,\gamma_1,\gamma_2)(\theta) = -1 - \log p(\theta) + \gamma_1 D(\theta,\theta_0)^2 + \gamma_2.$$

Set this to zero, and solve for $p(\theta)$:

$$\begin{aligned}p(\theta) &= \exp\left(\gamma_1 D(\theta,\theta_0)^2 + \gamma_2 - 1\right) \\ &\propto \exp\left(\gamma_1 D(\theta,\theta_0)^2\right).\end{aligned}$$

This density is positive for any values of γ_1 (and γ_2), and it normalises to one if $\gamma_1 < 0$. As γ_1 can take any value less than zero, we choose $\gamma_1 = -1/2$.

Now, if $\Theta \equiv \mathbb{R}^m$ and ν is the Lebesgue measure, then $D(\theta,\theta_0)^2 = \|\theta-\theta_0\|^2_{\mathbb{R}^m}$, so $\tilde p$ is recognised as a multivariate normal density centred at θ_0 with identity covariance matrix. □

Returning to the normal regression model of (1.1) subject to (1.2), we shall now derive the maximum entropy prior for f in some RKHS $\mathcal{F}$. One issue that we have is that the set $\mathcal{F}$ is potentially "too big" for the purpose of estimating f, that is, for certain pairs of functions $\mathcal{F}$, the data do not allow an assessment of whether one is closer to the truth than the other. In particular, the data do not contain information to distinguish between two functions f and g in $\mathcal{F}$ for which $f(x_i) = g(x_i), i = 1, \dots, n$. Since the Fisher information for a linear functional of a non-zero $f \in \mathcal{F}_n$ is non-zero, there is information to allow a comparison between any pair of functions in $f_0 + \mathcal{F}_n := \{f_0 + f \,|\, f_0 \in \mathcal{F}, f \in \mathcal{F}_n\}$. A prior for f therefore need not have support $\mathcal{F}$, instead it is sufficient to consider priors with support $f_0 + \mathcal{F}_n$, where $f_0 \in \mathcal{F}$ is fixed and chosen a priori as a "best guess" of f. We now state and prove the I-prior theorem.

Theorem 3.6 (The I-prior)**.** *Let $\mathcal{F}$ be an RKHS with kernel h, and consider the finite dimensional subspace $\mathcal{F}_n$ of $\mathcal{F}$ equipped with an inner product as in Lemma 2.5. Let ν be a volume measure induced by the norm $\|\cdot\|_{\mathcal{F}_n} = \sqrt{\langle \cdot, \cdot \rangle_{\mathcal{F}_n}}$. With $f_0 \in \mathcal{F}$, let $\mathcal{P}_0$ be the class of distributions p such that*

$$\operatorname{E}\left[\|f - f_0\|^2_{\mathcal{F}_n}\right] = \int_{\mathcal{F}_n} \|f - f_0\|^2_{\mathcal{F}_n} \, p(f) \, \mathrm{d}\nu(f) = const.$$

Denote by $\tilde{p}$ the density of the entropy maximising distribution among the class of distributions within $\mathcal{P}_0$. Then, $\tilde{p}$ is Gaussian over $\mathcal{F}$ with mean f_0 and covariance function equal to the reproducing kernel of $\mathcal{F}_n$, i.e.

$$\operatorname{Cov}\big(f(x), f(x')\big) = h_n(x, x').$$

We call $\tilde{p}$ the I-prior *for f.*

Proof. Recall the fact that any $f \in \mathcal{F}$ can be decomposed into $f = f_n + r$, with $f_n \in \mathcal{F}_n$ and $r \in \mathcal{F}_n^\perp$. Also recall that there is no Fisher information about any $r \in \mathcal{R}_n$, and therefore it is not possible to estimate r from the data. Therefore, $p(r) = 0$, and one needs only consider distributions over $\mathcal{F}_n$ when building distributions over $\mathcal{F}$.

The norm on $\mathcal{F}_n$ induces the metric $D(f, f') = \|f - f'\|_{\mathcal{F}_n}$. For $f, f_0 \in \mathcal{F}$, take the orthogonal projections of these vectors onto $\mathcal{F}_n$

9. Double check this proof.

$$f = \sum_{i=1}^n h(\cdot, x_i) w_i + r_f \quad \text{and} \quad f_0 = \sum_{i=1}^n h(\cdot, x_i) w_{i0} + r_0$$

and compute the squared distance between them:

$$
\begin{aligned}
D(f, f_0)^2 &= \|f - f_0\|^2_{\mathcal{F}_n} \\
&= \left\| \sum_{i=1}^n h(\cdot, x_i) w_i - \sum_{i=1}^n h(\cdot, x_i) w_{i0} \right\|^2_{\mathcal{F}_n} \\
&= \left\| \sum_{i=1}^n h(\cdot, x_i)(w_i - w_{i0}) \right\|^2_{\mathcal{F}_n} \\
&= (\mathbf{w} - \mathbf{w}_0)^\top \boldsymbol{\Psi}^{-1} (\mathbf{w} - \mathbf{w}_0).
\end{aligned}
$$

Thus, by Lemma 3.5, the maximum entropy distribution for $f = \sum_{i=1}^n h(\cdot, x_i) w_i$ is

$$
(w_1, \dots, w_n)^\top \sim \mathrm{N}_n(\mathbf{w}_0, \boldsymbol{\Psi}).
$$

This implies that f is Gaussian, since

$$
\langle f, f' \rangle_{\mathcal{F}} = \left\langle \sum_{i=1}^n h(\cdot, x_i) w_i, f' \right\rangle_{\mathcal{F}} = \sum_{i=1}^n w_i \left\langle h(\cdot, x_i), f' \right\rangle_{\mathcal{F}}
$$

is a sum of normal random variables, and therefore $\langle f, f' \rangle_{\mathcal{F}}$ is normally distributed for any $f' \in \mathcal{F}$. The mean $\mu \in \mathcal{F}$ of this random vector f satisfies $\mathrm{E}\langle f, f' \rangle_{\mathcal{F}} = \langle \mu, f' \rangle_{\mathcal{F}}$ for all $f' \in \mathcal{F}_n$, but

$$
\begin{aligned}
\mathrm{E}\langle f, f' \rangle_{\mathcal{F}} &= \mathrm{E} \left\langle \sum_{i=1}^n h(\cdot, x_i) w_i, f' \right\rangle_{\mathcal{F}} \\
&= \mathrm{E} \left[\sum_{i=1}^n w_i \left\langle h(\cdot, x_i), f' \right\rangle_{\mathcal{F}} \right] \\
&= \sum_{i=1}^n w_{i0} \left\langle h(\cdot, x_i), f' \right\rangle_{\mathcal{F}} \\
&= \left\langle \sum_{i=1}^n h(\cdot, x_i) w_{i0}, f' \right\rangle_{\mathcal{F}} \\
&= \langle f_0, f' \rangle_{\mathcal{F}},
\end{aligned}
$$

so $\mu \equiv f_0 = \sum_{i=1}^n h(\cdot, x_i) w_{i0}$.

The covariance between two evaluation functionals of f is shown to satisfy

$$\begin{aligned}
\operatorname{Cov}\big(f(x), f(x')\big) &= \operatorname{Cov}\big(\langle f, h(\cdot,x)\rangle_{\mathcal{F}}, \langle f, h(\cdot,x')\rangle_{\mathcal{F}}\big) \\
&= \operatorname{E}\big(\langle f - f_0, h(\cdot,x)\rangle_{\mathcal{F}} \langle f - f_0, h(\cdot,x')\rangle_{\mathcal{F}}\big) \\
&= \big\langle C, h(\cdot,x) \otimes h(\cdot,x')\big\rangle_{\mathcal{F}\otimes\mathcal{F}},
\end{aligned}$$

where $C \in \mathcal{F} \otimes \mathcal{F}$ is the covariance element of f. Write $h_x := \langle h(\cdot,x), f\rangle_{\mathcal{F}}$. Then, by the usual definition of covariances, we have that

$$\operatorname{Cov}(h_x, h_{x'}) = \operatorname{E}[h_x h_{x'}] - \operatorname{E}[h_x]\operatorname{E}[h_{x'}],$$

where, making use of the reproducing property of h for $\mathcal{F}$, the first term on the right-hand side is

$$\begin{aligned}
\operatorname{E}[h_x h_{x'}] &= \operatorname{E}\left[\left\langle h(\cdot,x), \sum_{i=1}^n h(\cdot,x_i)w_i \right\rangle_{\mathcal{F}} \left\langle h(\cdot,x'), \sum_{j=1}^n h(\cdot,x_j)w_j \right\rangle_{\mathcal{F}}\right] \\
&= \operatorname{E}\left[\sum_{i=1}^n\sum_{j=1}^n w_i w_j \left\langle h(\cdot,x), h(\cdot,x_i)\right\rangle_{\mathcal{F}} \left\langle h(\cdot,x'), h(\cdot,x_j)\right\rangle_{\mathcal{F}}\right] \\
&= \sum_{i=1}^n\sum_{j=1}^n (\psi_{ij} + w_{i0}w_{j0}) h(x,x_i)h(x',x_j),
\end{aligned}$$

while the second term on the right-hand side is

$$\begin{aligned}
\operatorname{E}[h_x]\operatorname{E}[h_{x'}] &= \left(\sum_{i=1}^n w_{i0} \left\langle h(\cdot,x), h(\cdot,x_i)\right\rangle_{\mathcal{F}}\right) \left(\sum_{j=1}^n w_{j0} \left\langle h(\cdot,x'), h(\cdot,x_j)\right\rangle_{\mathcal{F}}\right) \\
&= \sum_{i=1}^n\sum_{j=1}^n w_{i0}w_{j0} h(x,x_i)h(x',x_j).
\end{aligned}$$

Thus,

$$\operatorname{Cov}\big(f(x), f(x')\big) = \sum_{i=1}^n\sum_{j=1}^n \psi_{ij} h(x,x_i)h(x',x_j),$$

the reproducing kernel for $\mathcal{F}_n$. □

In closing, we reiterate the fact that the I-prior for f in the normal regression model subject to f belonging to some RKHS $\mathcal{F}$ has the simple representation

$$
\begin{gathered}
f(x_i) = f_0(x_i) + \sum_{k=1}^n h(x_i, x_k) w_k \\
(w_1, \dots, w_n)^\top \sim \text{N}_n(\mathbf{0}, \boldsymbol{\Psi}).
\end{gathered}
$$

Equivalently, this may be written as a Gaussian process-like prior

$$
\big(f(x_1), \dots, f(x_n)\big)^\top \sim \text{N}(\mathbf{f}_0, \mathbf{H}\boldsymbol{\Psi}\mathbf{H}),
$$

where $\mathbf{f}_0 = \big(f_0(x_1), \dots, f_0(x_n)\big)^\top$ is the vector of prior mean functional evaluations, and $\mathbf{H}$ is the kernel matrix.

3.6 Conclusion

In estimating the regression function f of the normal model in (1.1) subject to (1.2), and f belonging to an RKHS $\mathcal{F}$, we established that the entropy maximising prior distribution for f is Gaussian with some prior mean f_0 that needs to be chosen, and covariance function equal to the Fisher information for f. We call this the I-prior for f.

The dimension of the function space $\mathcal{F}$ could be huge, infinite-dimensional even, while the task of estimating $f \in \mathcal{F}$ only relies on a finite amount of data point. However, we are certain that the Fisher information for f exists only for the finite subspace $\mathcal{F}_n$ as defined in (3.4), and it is zero everywhere else. This suggests that the data only allows us to provide an estimation to the function $f \in \mathcal{F}$ by considering functions in an (at most) n-dimensional subspace instead. In other words, it would be futile to consider functions in a space larger than this, and hence there is an element of dimension reduction here, especially when $\dim(\mathcal{F}) \gg n$.

By equipping the subspace $\mathcal{F}_n$ with the inner product (3.5), $\mathcal{F}_n$ is revealed to be a RKHS with reproducing kernel equal to the Fisher information for f. Importantly, functions in the subspace $\mathcal{F}_n$ are structurally similar to the functions in the parent space $\mathcal{F}$. The problem at hand then boils down to a Gaussian process regression using the kernel of the RKHS $\mathcal{F}_n$, which is the Fisher information for f.

3.7 Miscellanea

3.7.1 Expected versus observed Fisher information

For many applications, it is of interest to evaluate the (total) Fisher information at the maximum likelihood estimate under a sampling scenario. However, the expectation required to calculate the Fisher information above cannot be done without knowing the true value of θ. As a point of clarification, we ought to make the distinction between the *expected* Fisher information and the *observed* Fisher information under a sampling scenario. There are two quantities that are typically used as an approximation, and these are explained below. Let $y = \{y_1, \dots, y_n\}$ represent an independent and identically distributed observed sample from $p(\cdot|\theta)$. The maximum likelihood (ML) estimator $\hat\theta = \arg\max_\theta L(\theta)$ for θ satisfies the first order conditions $S(\hat\theta) = 0$, where the log-likelihood function and the score function makes use of all of the observed samples, i.e. $L(\theta) = \sum_{i=1}^n \log p(y_i|\theta)$. In a sampling experiment, the total Fisher information (denoted $\mathcal{I}_n(\theta)$) is just n times the unit Fisher information, i.e. $\mathcal{I}_n(\theta) = n\mathcal{I}(\theta)$. Following Efron and Hinkley (1978), the expected Fisher information is defined to be $\mathcal{I}_n(\hat\theta)$, while the observed Fisher information is

$$\hat{\mathcal{I}}_n = -\sum_{i=1}^n \frac{\partial^2}{\partial\theta^2} \log p(y_i|\theta) \bigg|_{\theta=\hat\theta}.$$

which is also by definition the negative Hessian. Note that

$$\mathcal{J}(\theta) = -\frac{1}{n}\sum_{i=1}^n \frac{\partial^2}{\partial\theta^2} \log p(y_i|\theta)$$

$\frac{1}{n}\hat{\mathcal{I}}_n \to \mathcal{I}(\hat\theta)$ in probability as $n \to \infty$ by the weak law of large numbers. Both of these quantities are used as replacements of the actual Fisher information about the "true" parameter. In the context of measuring curvatures, the expected Fisher information would be used (Pawitan, 2001), but in the context of efficient variance for ML estimates, the observed Fisher information is favoured (Efron and Hinkley, 1978). which by the law of large numbers, converges in probability to the expected Fisher information $\mathcal{I}(\theta)$ as defined above. In practice, one would not be able to calculate $\mathcal{I}$ without knowing the true value for θ, so replacing occurrences of θ with (the MLE)

In particular, near the MLE, low Fisher information indicates a shallow maxima, while high observed information indicates a "sharp" maxima. A shallow maxima is an indication that many nearby values have similar log-likelihood, but a sharp maxima is indicative of a high confidence surrounding the MLE.

We used the true Fisher information. Efron and Hinkley (1978) say favour the observed information instead. Does this change if we use MLE $\hat{f}$ instead? Probably not... we don't use MLE anyway!

https://stats.stackexchange.com/questions/179130/gaussian-process-proofs-and-results

https://stats.stackexchange.com/questions/268429/do-gaussian-process-regression-have-t

3.7.2 Functional derivatives

Definition 3.6 (Directional derivative and gradient)**.** Let $(\mathcal{H}, \langle\cdot,\cdot\rangle_\mathcal{H})$ be an inner product space, and consider a function $g : \mathcal{H} \to \mathbb{R}$. Denote the directional derivate of g in the direction z by $\nabla_z g$, that is,

$$\nabla_z g(x) = \lim_{\delta \to 0} \frac{g(x + \delta z) - g(x)}{\delta}.$$

The gradient of g, denoted by ∇g, is the unique vector field satisfying

$$\langle \nabla g(x), z \rangle_\mathcal{H} = \nabla_z g(x), \quad \forall x, z \in \mathcal{H}.$$

Definition 3.7 (Functional derivative)**.** Given a manifold M representing continuous/smooth functions ρ with certain boundary conditions, and a functional $F : M \to \mathbb{R}$, the functional derivative of $F[\rho]$ with respect to ρ, denoted $\partial F / \partial \rho$, is defined by

$$\begin{aligned} \int \frac{\partial F}{\partial \rho}(x)\phi(x) \mathrm{d}x &= \lim_{\epsilon \to 0} \frac{F[\rho + \epsilon\phi] - F[\rho]}{\epsilon} \\ &= \left[\frac{\mathrm{d}}{\mathrm{d}\epsilon} F[\rho + \epsilon\phi] \right]_{\epsilon=0}, \end{aligned}$$

where ϕ is an arbitrary function. The function $\partial F / \partial \rho$ as the gradient of F at the point ρ, and

$$\partial F(\rho, \phi) = \int \frac{\partial F}{\partial \rho}(x)\phi(x) \mathrm{d}x$$

as the directional derivative at point ρ in the direction of ϕ. Analogous to vector calculus, the inner product with the gradient gives the directional derivative.

Example 3.2 (Functional derivative of entropy)**.** Let X be a discrete random variable with probability mass function $p(x) \geq 0$, for $\forall x \in \Omega$, a finite set. The entropy is a functional of p, namely

$$\mathcal{E}[p] = -\sum_{x \in \Omega} p(x) \log p(x).$$

Equivalently, using the counting measure ν on Ω, we can write

$$\mathcal{E}[p] = -\int_\Omega p(x) \log p(x) \mathrm{d}\nu(x).$$

$$\begin{aligned}
\int_\Omega \frac{\partial \mathcal{E}}{\partial p}(x)\phi(x)\,\mathrm{d}x &= \left[\frac{\mathrm{d}}{\mathrm{d}\epsilon} \mathcal{E}[p + \epsilon\phi] \right]_{\epsilon=0} \\
&= \left[-\frac{\mathrm{d}}{\mathrm{d}\epsilon} \big(p(x) + \epsilon\phi(x)\big) \log \big(p(x) + \epsilon\phi(x)\big) \right]_{\epsilon=0} \\
&= -\int_\Omega \left(\frac{p(x)\phi(x)}{p(x) + \epsilon\phi(x)} + \frac{\epsilon\phi(x)}{p(x) + \epsilon\phi(x)} + \phi(x) \log \big(p(x) + \epsilon\phi(x)\big) \right) \mathrm{d}x \\
&= -\int_\Omega \left(1 + \log p(x)\right) \phi(x)\,\mathrm{d}x.
\end{aligned}$$

Thus, $(\partial \mathcal{E} / \partial p)(x) = -1 - \log p(x)$.

3.7.3 Data dependent priors

Here we consider data dependent priors—seemingly data dependent (i.e. dependent on X) but the whole model is conditional on X implicitly, so there is no issue. If prior depended on y then there is a problem, at least, violates Bayesian first principles (using the data twice such that a priori and a posteriori same amount of information).

Chapter 4

Modelling with I-priors

In the previous chapter, we defined an I-prior for the normal regression model (1.1) subject to (1.2) and f belonging to a reproducing kernel Hilbert or Krein space of functions $\mathcal{F}$, as a Gaussian distribution on f with covariance function equal to the Fisher information for f. We also saw how new function spaces can be constructed via the polynomial and ANOVA RKKS. In this chapter, we shall describe various regression models, and identify them with appropriate RKKSs, so that an I-prior may be defined on it.

Methods for estimating I-prior models are described in Section 4.2. Estimation here refers to obtaining the posterior distribution of the regression function under an I-prior, while optimising the kernel parameters of $\mathcal{F}$ and the error precision $\boldsymbol{\Psi}$. Likelihood based methods, namely direct optimisation of the likelihood and the expectation-maximisation (EM) algorithm, are the preferred estimation methods of choice. Having said this, it is also possible to estimate I-prior models under a full Bayesian paradigm by employing Markov chain Monte Carlo methods to sample from the relevant posterior densities.

Careful considerations of the computational aspects are required to ensure efficient estimation of I-prior models, and these are discussed in Section 4.3. The culmination of the computational work on I-prior estimation is the **iprior** package (Jamil and Bergsma, 2017), which is a publicly available R package that has been published to CRAN.

Finally, several examples of I-prior modelling are presented in Section 4.5: in particular, a multilevel data set, a longitudinal data set, and a data set involving a functional covariate, are analysed using the I-prior methodology.

4.1 Various regression models

sec:various-regression

In the introductory chapter (Section 1.1), we described several interesting regression models. The goal of this section is to formulate the I-prior model that describes each of these models. This is done by carefully choosing the RKHS/RKKS $\mathcal{F}$ of real functions over a set $\mathcal{X}$ to which the regression function f belongs. Without loss of generality and for simplicity, assume a prior mean of zero for the I-prior distribution.

4.1.1 Multiple linear regression

Let $\mathcal{X} \equiv \mathbb{R}^p$ be equipped with the regular Euclidean dot product, and $\mathcal{F}_\lambda$ be the scaled canonical RKHS of functions over $\mathcal{X}$ with kernel $h_\lambda(\mathbf{x}, \mathbf{x}') = \lambda \mathbf{x}^\top \mathbf{x}'$, for any two $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^p$. Then, an I-prior on f implies that

$$
\begin{aligned}
f(\mathbf{x}_i) &= \sum_{j=1}^n \lambda \mathbf{x}_i^\top \mathbf{x}_j w_j \\
&= \sum_{j=1}^n \lambda \left(\sum_{k=1}^p x_{ik} x_{jk} \right) w_j \\
&= \beta_1 x_{i1} + \cdots + \beta_p x_{ip},
\end{aligned}
$$

where each $\beta_k := \lambda \sum_{j=1}^n x_{jk} w_j$. This implies a multivariate normal prior distribution for the regression coefficients

$$
\boldsymbol{\beta} := (\beta_1, \dots, \beta_p) \sim \mathrm{N}_p(\mathbf{0}, \lambda^2 \mathbf{X}^\top \boldsymbol{\Psi} \mathbf{X}), \tag{4.1}
$$

{eq:ipriorcanonical}

where $\mathbf{X}$ is the $n \times p$ design matrix for the covariates, excluding the column of ones at the beginning typically reserved for the intercept. As expected, the covariance matrix for $\boldsymbol{\beta}$ is recognised as the scaled Fisher information matrix for the regression coefficients.

If the covariates are not scaled similarly, then the values of f are incoherent—if x_1 measures weight in kilograms and x_2 height in centimetres, what measurement does $\beta_1 x_1 + \beta_2 x_2$ represent? To overcome this, one could decompose the regression function into

10. Can't I just standardise x?

$$
f(\mathbf{x}_i) = f_1(x_{i1}) + \cdots + f_p(x_{ip})
$$

for which $f \in \mathcal{F}_\lambda \equiv \mathcal{F}_{\lambda_1} \oplus \cdots \oplus \mathcal{F}_{\lambda_p}$, and $\mathcal{F}_{\lambda_k}$, $k = 1, \dots, p$ are unidimensional canonical RKHSs with kernels $h_{\lambda_k}(x_{ik}, x_{jk}) = \lambda_k x_{ik} x_{jk}$. In effect, we now have p scale parameters, one for each of the RKKSs associated with the p covariates. The RKKS $\mathcal{F}_\lambda$ therefore has kernel

$$h(\mathbf{x}_i, \mathbf{x}_j) = \sum_{k=1}^{p} \lambda_k x_{ik} x_{jk},$$

and hence each regression coefficient can now be written as $\beta_k = \sum_{j=1}^n \lambda_k x_{jk} w_j$, for which we see the λ_k's scaling role on the x_{jk}'s. Thus, the corresponding I-prior for $\boldsymbol\beta$ is

$$\boldsymbol\beta \sim \text{N}_p(\mathbf{0}, \lambda^2 \mathbf{X}^\top \boldsymbol\Lambda \boldsymbol\Psi \boldsymbol\Lambda \mathbf{X}),$$

with $\boldsymbol\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$. Note that $\mathcal{F}_\lambda$ can be seen as a special case of the ANOVA RKKS, in which only the main effects are considered, in which case the *centred canonical RKHSs* should be considered instead. This approach is disadvantageous when p is large, in which case there would be numerous scale parameters to estimate.

Remark 4.1. The I-prior for $\boldsymbol\beta$ in (4.1) bears resemblance to the g-prior (Zellner, 1986), and in fact, the g-prior can be interpreted as an I-prior if the inner product of $\mathcal{X}$ is the Mahalonobis inner product. See Miscellanea 4.7.1 for a discussion.

4.1.2 Multilevel linear modelling

sec:multilevelmodels

Let $\mathcal{X} \equiv \mathbb{R}^p$, and suppose that alongside the covariates, there is information on group levels $\mathcal{M} = \{1, \dots, m\}$ for each unit i. That is, every observation for unit i is known to belong to a specific group j, and we write $\mathbf{x}_i^{(j)}$ to indicate this. Let n_j denote the sample size for cluster j, and the overall sample size be $n = \sum_{j=1}^m n_j$. When modelled linearly with the responses $y_i^{(j)}$, the model is known as a multilevel (linear) model, although it is known by many other names: random-effects models, random coefficient models, hierarchical models, and so on. As this model is seen as an extension of linear models, applications are plenty, especially in research designs for which the data varies at more than one level.

Consider a functional ANOVA decomposition of the regression function as follows:

$$f(\mathbf{x}_i^{(j)}, j) = \alpha + f_1(\mathbf{x}_i^{(j)}) + f_2(j) + f_{12}(\mathbf{x}_i^{(j)}, j). \tag{4.2}$$

{eq:anovamultilevel}

To mimic the multilevel model, assume $f_1 \in \mathcal{F}_1$ the Pearson RKHS, $f_2 \in \mathcal{F}_2$ the centred canonical RKHS, and $f_{12} \in \mathcal{F}_{12} = \mathcal{F}_1 \otimes \mathcal{F}_2$, the tensor product space of $\mathcal{F}_1$ and $\mathcal{F}_2$. As we know, α is the overall intercept, and the varying intercepts are given by the function

f_2. While f_1 is the (main) linear effect of the covariates, f_{12} provides the varying linear effect of the covariates by each group. The I-prior for $f - \alpha$ is assumed to lie in the function space $\mathcal{F} - \alpha$, which is an ANOVA RKKS with kernel

$$h_\lambda\big((\mathbf{x}_i^{(j)}, j), (\mathbf{x}_i^{(j')}, j')\big) = \lambda_1 h_1(\mathbf{x}_i^{(j)}, \mathbf{x}_{i'}^{(j')}) + \lambda_2 h_2(j, j') + \lambda_1\lambda_2 h_1(\mathbf{x}_i^{(j)}, \mathbf{x}_{i'}^{(j')}) h_2(j, j'),$$

with h_1 the centred canonical kernel and h_2 the Pearson kernel. The reason for not including an RKHS of constant functions in $\mathcal{F}$ is because the overall intercept is usually simpler to estimate as an external parameter (see Section 4.2.1).

We can show that the regression function (4.2) corresponds to the standard way of writing the multilevel model,

$$f(\mathbf{x}_i^{(j)}, j) = \beta_0 + \mathbf{x}_i^{(j)\top}\boldsymbol{\beta}_1 + \beta_{0j} + \mathbf{x}_i^{(j)\top}\boldsymbol{\beta}_{1j}.$$

and determine the prior distributions on $(\beta_{0j}, \boldsymbol{\beta}_{1j}^\top)^\top \in \mathbb{R}^{p+1}$. For the interested reader, the details are in Miscellanea 4.7.2. The standard multilevel random effects assumption is that $(\beta_{0j}, \boldsymbol{\beta}_{1j}^\top)^\top$ is normally distributed with mean zero and covariance matrix $\boldsymbol{\Phi}$. In total, there are $p+1$ regression coefficients and $(p+1)(p+2)/2$ covariance parameters in Φ to be estimated. In contrast, the I-prior model is parameterised by only two RKKS scale parameters—one for $\mathcal{F}_1$ and one for $\mathcal{F}_2$—and the error precision ψ. While the estimation procedure for $\boldsymbol{\Phi}$ in the standard multilevel model can result in non-positive covariance matrices, the I-prior model has the advantage that positive definiteness is taken care of automatically[1].

As a remark, the following regression functions are nested

- $f(\mathbf{x}_i^{(j)}, j) = f_0 + f_1(\mathbf{x}_i^{(j)}) + f_2(j)$ (random intercept model);
- $f(\mathbf{x}_i^{(j)}, j) = f_0 + f_1(\mathbf{x}_i^{(j)})$ (linear regression model);
- $f(\mathbf{x}_i^{(j)}, j) = f_0 + f_2(j)$ (ANOVA model);
- $f(\mathbf{x}_i^{(j)}, j) = f_0$ (intercept only model),

and thus one may compare likelihoods to ascertain the best fitting model. In addition, one may add flexibility to the model in two possible ways:

[1] By virtue of the estimate of the regression function belonging to $\mathcal{F}_n$, an RKHS with a positive definite kernel equal to the Fisher information for f.

1. **More than two levels**. The model can be easily adjusted to reflect the fact that that the data is structured in a hierarchy containing three or more levels. For the three level case, let the indices $j \in \{1, \dots, m_1\}$ and $k \in \{1, \dots, m_2\}$ denote the two levels, and simply decompose the regression function accordingly:

$$f(\mathbf{x}_i^{(j,k)}, j, k) = f_0 + f_1(\mathbf{x}_i^{(j,k)}) + f_2(j) + f_3(k) + f_{12}(\mathbf{x}_i^{(j,k)}, j) + f_{13}(\mathbf{x}_i^{(j,k)}, k) \\ + f_{23}(j,k) + f_{123}(\mathbf{x}_i^{(j,k)}, j, k).$$

2. **Covariates not varying with levels**. Suppose now we would like to add covariates with a fixed effect to the model, i.e., covariates $\mathbf{z}_i^{(j)}$ which are not assumed to affect the responses differently in each group. The regression function would be:

$$f(\mathbf{x}_i^{(j)}, j, \mathbf{z}_j) = f_0 + f_1(\mathbf{x}_i^{(j)}) + f_2(j) + f_3(\mathbf{z}_i^{(j)}) + f_{12}(\mathbf{x}_i^{(j)}, j).$$

   This can be seen as a limited functional ANOVA decomposition of f.

Remark 4.2. Indexing can be tricky, but we find the following helpful. Supposing $m = 2$, and $n_1 = n_2 = 3$, then a typical panel data set looks like this:

y	x	z	i	j	k
y_{11}	x_{11}	z_1	1	1	1
y_{21}	x_{21}	z_1	2	1	2
y_{31}	x_{31}	z_1	3	1	3
y_{12}	x_{12}	z_2	1	2	4
y_{22}	x_{22}	z_2	2	2	5
y_{32}	x_{32}	z_2	3	2	6

The y's are the responses, x's covariates, and z's group-level covariates. If $\iota : (i,j) \mapsto k$ is a function which maps the dual index set (i,j) to the single index set $k \in \{1, \dots, n\}$, then the multilevel regression function can be expressed as the regression function in model (1.1).

4.1.3 Longitudinal modelling

Longitudinal or panel data observes covariate measurements $x_i \in \mathcal{X}$ and responses $y_i(t) \in \mathbb{R}$ for individuals $i = 1, \dots, n$ across a time period $t \in \{1, \dots, T\} =: \mathcal{T}$. Often, the time indexing set $\mathcal{T}$ may be unique to each individual i, so measurements for unit i happens across a time period $\{t_{i1}, \dots, t_{iT_i}\} =: \mathcal{T}_i$—this is known as an unbalanced panel. It is also possible that covariate measurements vary across time too, so appropriately they are denoted $x_i(t)$. For example, $x_i(t)$ could be repeated measurements of the variable x_i at time point $t \in \mathcal{T}_i$. The relationship between the response variables $y_i(t)$ at time $t \in \mathcal{T}_i$ is captured through the equation

$$y_i(t) = f\big(x_i, t\big) + \epsilon_i(t)$$

where the distribution of $\boldsymbol{\epsilon}_i = \big(\epsilon_i(t_{i1}), \dots, \epsilon_i(t_{iT_i})\big)^\top$ is Gaussian with mean zero and covariance matrix $\boldsymbol{\Psi}_i$. Assuming $\boldsymbol{\Psi}_i = \psi_i \mathbf{I}_{T_i}$ or even $\boldsymbol{\Psi}_i = \psi \mathbf{I}_{T_i}$ are perfectly valid choices, even though this seemingly ignores any time dependence between the observations. In reality, the I-prior induces time dependence of the observations via the kernels in the prior covariance matrix for f. Additionally, the random vectors $\boldsymbol{\epsilon}_i$ and $\boldsymbol{\epsilon}_{i'}$ are assumed to be independent for any two distinct $i, i' \in \{1, \dots, n\}$.

Using the functional ANOVA decomposition on the regression function, we obtain

$$f(x_i, t) = f_0 + f_1(x_i) + f_2(t) + f_{12}(x_i, t), \tag{4.3}$$

{eq:longitudinalanova}

where f_0 is an overall constant, $f_1 \in \mathcal{F}_1$, $f_2 \in \mathcal{F}_2$, and $f_{12} \in \mathcal{F}_1 \otimes \mathcal{F}_2$. Choices for $\mathcal{F}_1$ and $\mathcal{F}_2$ are plentiful. In fact, any of the RKHS/RKKS described in Chapter 3 can be used to either model a linear dependence (canonical RKHS), nominal dependence (Pearson RKHS), polynomial dependence (polynomial RKKS) or smooth dependence (fBm or SE RKHS) on the x_i's and t's on f.

Remark 4.3. Although (4.3) is a special case of the multilevel model decomposition (4.2) for which $x_i = x_i(t)$ (time-varying covariates), it is different to how longitudinal models are normally treated using a mixed effects model. As a multilevel model, longitudinal models treat the individuals as the groups or clusters (level two), and the time points as the various measurements within the clusters (level one).

4.1.4 Smoothing models

Single- and multi-variable smoothing models can be fitted under the I-prior methodology using the fBm RKHS. In standard kernel based smoothing methods, the squared exponential kernel is often used, and the corresponding RKHS contains analytic functions. There are several attractive properties of using the fBm RKHS, and for one-dimensional smoothing, these are discussed below.

Assume that, up to a constant, the regression function lies in the scaled, centred fBm RKHS $\mathcal{F}$ of functions over $\mathcal{X} \equiv \mathbb{R}$ with Hurst index $1/2$. Thus, with a centring with respect to the empirical distribution P_n of $\{x_1, \dots, x_n\}$ and using the absolute norm on $\mathbb{R}$, $\mathcal{F}$ has kernel

$$h_\lambda(x,x') = \frac{\lambda}{2n^2} \sum_{i=1}^n \sum_{j=1}^n \big(|x - x_i| + |x' - x_j| - |x - x'| - |x_i - x_j| \big).$$

According to van der Vaart and van Zanten (2008, Section 10), $\mathcal{F}$ contains absolutely continuous functions possessing a square integrable weak derivative satisfying $f(0) = 0$. The norm is given by $\|f\|_{\mathcal{F}}^2 = \int \dot f^2 \mathrm{d}x$. The posterior mean of f based on an I-prior is then a (one-dimensional) smoother for the data. For f of the form $f = \sum_{i=1}^n h(\cdot, x_i) w_i$, i.e., $f \in \mathcal{F}_n$, the finite subspace of $\mathcal{F}$ as in Section 3.4, then Bergsma (2017) shows that f can be represented as

$$f(x) = \int_{-\infty}^x \beta(t) \, \mathrm{d}t \tag{4.4}$$

{eq:ipriorbrownianbridge}

where

$$\beta(t) = \sum_{i:x_i \le t} w_i = \frac{f(x_{i_t+1}) - f(x_{i_t})}{x_{i_t+1} - x_{i_t}} \tag{4.5}$$

with $i_t = \max_{x_i \le t} i$. Under the I-prior with an iid assumption on the errors, the w_i's are zero mean normal random variables with variance ψ, so that β as defined above is an ordinary Brownian bridge with respect to the empirical distribution P_n. The I-prior for f is piecewise linear with knots at $x_1, \dots, x_n$, and the same holds true for the posterior mean. The implication is that the I-prior automatically adapts to irregularly spaced x_i: in any region where there are no observations, the resulting smoother is linear. This is explained by the reduced Fisher information about the derivative of the regression curve in regions with no observation.

In Bergsma (2017), it is stated that the covariance function for β is

$$\operatorname{Cov}\big(\beta(x), \beta(x')\big) = n\Big(\min\{\mathrm{P}_n(X < x), \mathrm{P}_n(X_n < x')\} - \mathrm{P}_n(X < x)\,\mathrm{P}_n(X_n < x') \Big)$$

From this, notice that $\operatorname{Var}\beta(x) = \mathrm{P}_n(X_n < x)\big(1 - \mathrm{P}_n(X_n < x)\big)$, which shows an automatic boundary correction: close to the boundary there is little Fisher information on the derivative of the regression function $\beta(x)$, so the prior variance is small. This will lead to more shrinkage of the posterior derivative of f towards the derivative of the prior mean f_0.

Another advantage of the I-prior methodology is the ability to fit single or multi-dimensional smoothing models with just two parameters to be estimated: the RKHS scale parameter λ and the error precision $\mathbf{\Psi}$. The Hurst parameter $\gamma \in (0,1)$ of the fBm RKHS can also be treated as a free parameter for added flexibility, but for most practical applications, we find that the default setting of $\gamma = 1/2$ performs sufficiently well.

Remark 4.4. From (4.4), the prior process for f is thus an integrated Brownian bridge. This shows a close relation with cubic spline smoothers, which can be interpreted as the posterior mean when the prior is an integrated Wiener process (Wahba, 1990). Unlike I-priors however, cubic spline smoothers do not have automatic boundary corrections, and typically the additional assumption is made that the smoothing curve is linear at the boundary knots.

4.1.5 Regression with functional covariates

sec:regfunctionalcov

Suppose that we have functional covariates x in the real domain, and that $\mathcal{X}$ is a set of differentiable functions. If so, it is reasonable to assume that $\mathcal{X}$ is a Hilbert-Sobolev space with inner product

$$\langle x, x' \rangle_{\mathcal{X}} = \int \dot x(t) \dot x'(t) \, \mathrm{d}t,$$

so that we may apply the linear, fBm or any other kernels which make use of inner products by making use of the polarisation identity. Furthermore, let $z \in \mathbb{R}^T$ be the discretised realisation of the function $x \in \mathcal{X}$ at regular intervals $t = 1, \dots, T$. Then

$$\langle x, x' \rangle_{\mathcal{X}} \approx \sum_{t=1}^{T-1} (z_{t+1} - z_t)(z'_{t+1} - z'_t).$$

For discretised observations at non-regular intervals $\{t_1, \dots, t_T\}$ then a more general formula to the above one might be used, for instance,

$$\langle x, x' \rangle_{\mathcal{X}} \approx \sum_{i=1}^{T-1} \frac{(z_{t_{i+1}} - z_{t_i})(z'_{t_{i+1}} - z'_{t_i})}{t_{i+1} - t_i}.$$

4.2 Estimation

sec:ipriorestimation

After selecting a RKHS/RKKS $\mathcal{F}$ of functions over $\mathcal{X}$ suitable for the regression problem at hand, one then proceeds to estimate the posterior distribution of the regression function. The I-prior model (1.1) subject to (1.2) and $f \in \mathcal{F}$ has the simple and convenient representation

$$\begin{gathered} y_i = \alpha + f_0(x_i) + \overbrace{\sum_{k=1}^n h_\eta(x_i, x_k) w_k}^{f(x_i)} + \epsilon_i \\ (\epsilon_1, \dots, \epsilon_n)^\top \sim \mathrm{N}_n(\mathbf{0}, \boldsymbol{\Psi}^{-1}) \\ (w_1, \dots, w_n)^\top \sim \mathrm{N}_n(\mathbf{0}, \boldsymbol{\Psi}), \end{gathered} \tag{4.6}$$

{eq:model2}

where $f_0 : \mathcal{X} \to \mathbb{R}$ is a function chosen a priori representing the 'best guess' of f, and the dependence of the kernel of $\mathcal{F}$ on parameters η is emphasised through the subscript in $h_\eta : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.

The parameters of the I-prior model are collectively denoted by $\theta = \{\alpha, \eta, \boldsymbol{\Psi}\}$. Given θ and a prior choice for f_0, the posterior regression function is determined solely by the posterior distribution of the w_i's. Using standard multivariate normal results, one finds that the posterior distribution for $\mathbf{w} := (w_1, \dots, w_n)^\top$ is $\mathbf{w}|\mathbf{y} \sim \mathrm{N}_n(\tilde{\mathbf{w}}, \tilde{\mathbf{V}}_w)$, where

$$\tilde{\mathbf{w}} = \boldsymbol{\Psi}\mathbf{H}_\eta\mathbf{V}_y^{-1}(\mathbf{y} - \alpha\mathbf{1}_n - \mathbf{f}_0) \quad \text{and} \quad \tilde{\mathbf{V}}_w = \big(\mathbf{H}_\eta\boldsymbol{\Psi}\mathbf{H}_\eta + \boldsymbol{\Psi}^{-1}\big)^{-1} = \mathbf{V}_y^{-1}, \tag{4.7}$$

{eq:posteriorw}

using the familiar notation that we introduced in Section 1.4. For a derivation, see Appendix A.1. By linearity, the posterior distribution for f is also normal.

In each modelling scenario, there are a number of kernel parameters η that need to be estimated from the data. Assuming that the covariate space is $\mathcal{X} = \mathcal{X}_1 \times \cdots \times \mathcal{X}_p$, and there is an ANOVA like decomposition of the function space $\mathcal{F}$ into its constituents spaces $\mathcal{F}_1, \dots, \mathcal{F}_p$, then at the very least, there are p scale parameters $\lambda_1, \dots, \lambda_p$ for each of the RKHSs. Depending on the RKHS used, there could be more kernel parameters that need to be optimised, for instance, the Hurst index for the fBm RKHS, the lengthscale for the SE RKHS, and/or the offset for the polynomial RKKS. However, these may be treated as fixed parameters as well.

The following subsections describe possible estimation procedures for the hyperparameters of the model. Henceforth, for simplicity, the following additional standing assumptions are imposed on the I-prior model (4.6):

A1 **Centred responses**. Set $\alpha = 0$ and replace the responses by their centred versions $y_i \mapsto \tilde y_i = y_i - \frac{1}{n}\sum_{i=1}^n$. ass:A1

A2 **Zero prior mean**. Assume a zero prior mean $f_0(x) = 0$ for all $x \in \mathcal{X}$. ass:A2

A3 **Iid errors**. Assume identical and independent (iid) errors random variables, i.e., $\boldsymbol\Psi = \psi \mathbf{I}_n$. ass:A3

Assumptions A1 and A2 are motivated by the discussion in Section 4.2.1. Although assumption A3 is not strictly necessary, it is often a reasonable one and one that simplifies the estimation procedure greatly.

4.2.1 The intercept and the prior mean

sec:intercept

In most statistical models, an intercept is a necessary inclusion which aids interpretation. In the context of the I-prior model (4.6), a lack of an intercept would fail to account for the correct locational shift of the regression function along the y-axis. Further, when zero-mean functions are considered, the intercept serves as being the 'grand mean' value of the responses.

The addition of an intercept to the regression model may be viewed in one of two ways. The first is to view it as a function belonging to the RKHS of constant functions $\mathcal{F}_0$, and thereby tensor summing this space to $\mathcal{F}$. In the polynomial and ANOVA RKKSs, we saw that an intercept is naturally induced by the inclusion of a RKHS of constant functions in their construction. The second is to simply treat the intercept as a parameter of the model to be estimated. In any of the other RKHSs described in Chapter 2, an intercept would need to be added separately.

These two methods convey the same mathematical model, and there is very little difference in the way of interpretation, although estimation is entirely different. In the first method, the intercept-less RKHS/RKKS $\mathcal{F}$ with kernel h is made to include an intercept by modifying the kernel to be $h + 1$. The intercept will then be implicitly taken care of without having dealt with it explicitly. However, it can be obtained by realising that for $\alpha \in \mathcal{F}_0$ the RKHS of constant functions, then $\alpha = \sum_{i=1}^n w_i$.

On the other hand, consider the intercept as a parameter α to be estimated. Obtaining an estimate α using a likelihood-based argument is rather simple. From (4.6), $\operatorname{E} y_i = \alpha + f_0(x_i)$ for all $i = 1, \dots, n$, so the maximum likelihood estimate for $\operatorname{E} y$ is its sample mean $\bar y = \frac{1}{n}\sum_{i=1} y_i$, and hence the ML estimate for α is $\hat\alpha = \bar y - \frac{1}{n}\sum_{i=1}^n f_0(x_i)$. Alternatively, the estimation of α under a fully Bayesian treatment is possible by assuming an appropriate hyperprior on it, such as a conjugate normal prior $\operatorname{N}(a, A^{-1})$. If so, the conditional posterior of α given $\mathbf{w}$, η, $\boldsymbol\Psi$ and f_0 is also normal with mean $\tilde a$ and variance $\tilde A$, where

$$\tilde A = \sum_{i,j=1}^n \psi_{ij} + A \quad \text{and} \quad \tilde a = \tilde A^{-1} \left(\sum_{i=1}^n [(\mathbf{y} - \mathbf{f}_0 - \mathbf{H}_\eta \mathbf{w})\boldsymbol\Psi]_i + Aa \right).$$

This fact can be used, say, in conjunction with a Gibbs sampling procedure treating the rest of the unknowns as random. Note that the posterior mean for α is

$$\operatorname{E}[\alpha|\mathbf{y}] = \operatorname{E}_{\mathbf{w}}\big[\operatorname{E}[\alpha|\mathbf{y},\mathbf{w}]\big] = \frac{\sum_{i,j=1}^n \psi_{ij}(y_i - f_0(x_i)) + Aa}{\sum_{i,j=1}^n \psi_{ij} + A},$$

which, in the iid errors case, is seen to be a weighted sum of the ML estimate $\hat\alpha$ and the prior mean a. Unless there is a strong reason to add prior information to the intercept, the ML estimate seems to be the simplest approach. Assumption A1 implies a ML estimation of the intercept parameter.

Now, a note on the prior mean f_0. For kernels with the property that $h(x, x^*) \to 0$ as $D(x, x^*) \to \infty$ for $x \in \mathcal{X}_{\text{train}}$ and $x^* \in \mathcal{X}_{\text{new}}$ such as the SE kernel, this means that predictions outside the training set will be zero and thus rely on the prior mean f_0. However, all of the other kernels in this thesis, namely the fBm, canonical, and polynomial kernels, do not have this property—they instead use information provided by the training data to extrapolate predictions far away from the data set. A prior mean of zero seems reasonable and safe in the absence of any prior information, so long as the global and local properties of the regression function are understood with respect to the kernel chosen. $f_0 = 0$ also implies a complete reliance on the data rather than subjective prior belief of a suitable choice for f.

Of course, should it be felt appropriate, a non-zero function f_0 may be imposed as the prior mean. If $f_0(x) = \mu_0 \in \mathbb{R}$ for all $x \in \mathcal{X}$, then this basically implies another intercept in the model, if it is not already present. Note that when treating μ_0 as a hyperparameter to be estimated, then this does not yield a fully identified model, and only $\alpha + \mu_0$ may be estimated.

4.2.2 Direct optimisation

Under assumptions A1 and A2, a direct optimisation of the parameters $\theta = \{\eta, \boldsymbol{\Psi}\}$ using the log-likelihood of θ is straightforward to implement. Denote $\boldsymbol{\Sigma}_\theta := \mathbf{H}_\eta \boldsymbol{\Psi} \mathbf{H}_\eta + \boldsymbol{\Psi}^{-1} = \mathbf{V}_y$. From (4.6), the (marginal) log-likelihood of θ is given by

$$\begin{aligned} L(\theta) &= \log \int p(\mathbf{y}|\mathbf{w}) p(\mathbf{w}) \, \mathrm{d}\mathbf{w} \\ &= -\frac{n}{2} \log 2\pi - \frac{1}{2} \log |\boldsymbol{\Sigma}_\theta| - \frac{1}{2} \tilde{\mathbf{y}}^\top \boldsymbol{\Sigma}_\theta^{-1} \tilde{\mathbf{y}}. \end{aligned} \tag{4.8}$$

{eq:marglogliky}

The term marginal refers to the fact that we are averaging out the random function represented by $\mathbf{w}$. Direct optimisation is typically done using conjugate gradients with a Cholesky decomposition on the covariance kernel to maintain stability, but we opt for an eigendecomposition of the kernel matrix $\mathbf{H}_\eta = \mathbf{V} \cdot \operatorname{diag}(u_1, \dots, u_n) \cdot \mathbf{V}^\top$ instead. Further, under assumption A3 and since $\mathbf{H}_\eta$ is a symmetric matrix, we have that $\mathbf{V}\mathbf{V}^\top = \mathbf{I}_n$, and thus

$$\mathbf{V}_y = \mathbf{V} \cdot \operatorname{diag}(\psi u_1^2 + \psi^{-1}, \dots, \psi u_n^2 + \psi^{-1}) \cdot \mathbf{V}^\top$$

for which the inverse and log-determinant is easily obtainable. This method is relatively robust to numerical instabilities and is better at ensuring positive definiteness of the covariance kernel. The eigendecomposition is performed using the **Eigen** C++ template library and linked to **iprior** using **Rcpp** (Eddelbuettel and Francois, 2011). The hyperparameters are transformed by the **iprior** package so that an unrestricted optimisation using the quasi-Newton L-BFGS algorithm provided by `optim()` in R. Note that minimisation is done on the deviance scale, i.e., minus twice the log-likelihood. The direct optimisation method can be prone to local optima, in which case repeating the optimisation at different starting points and choosing the one which yields the highest likelihood is one way around this.

11. Show ridge in the log-likelihood plot.

Let $\mathbf{U}$ be the Fisher information matrix for $\theta \in \mathbb{R}^q$. Standard calculations (Appendix A.3) show that under the marginal distribution $\tilde{\mathbf{y}} \sim \mathrm{N}_n\left(\mathbf{0}, \boldsymbol{\Sigma}_\theta\right)$, the (i,j)th coordinate of $\mathbf{U}$ is

$$u_{ij} = \frac{1}{2} \operatorname{tr} \left(\boldsymbol{\Sigma}_\theta^{-1} \frac{\partial \boldsymbol{\Sigma}_\theta}{\partial \theta_i} \boldsymbol{\Sigma}_\theta^{-1} \frac{\partial \boldsymbol{\Sigma}_\theta}{\partial \theta_j} \right)$$

where the derivative of a matrix with respect to a scalar is the element-wise derivative of the matrix. With $\hat\theta$ denoting the ML estimate for θ, under suitable conditions, $\sqrt{n}(\hat\theta - \theta)$ has an asymptotic multivariate normal distribution with mean zero and covariance matrix $\mathbf{U}^{-1}$ (Casella and R. L. Berger, 2002). In particular, the standard errors for θ_k are the diagonal elements of $\mathbf{U}^{-1/2}$.

4.2.3 Expectation-maximisation algorithm

Evidently, (4.6) lends itself to resembling a random-effects model, for which the EM algorithm can easily be employed to estimate its hyperparameters. Assume A1 and A2 holds. By treating the complete data as $\{\mathbf{y}, \mathbf{w}\}$ and the w_i's as "missing", the tth iteration of the E-step entails computing

$$\begin{aligned}
Q(\theta) &= \mathrm{E}_{\mathbf{w}} \left[\log p(\mathbf{y}, \mathbf{w} | \theta) \,\middle|\, \mathbf{y}, \theta^{(t)} \right] \\
&= \mathrm{E}_{\mathbf{w}} \left[\text{const.} - \frac{1}{2} (\tilde{\mathbf{y}} - \mathbf{H}_\eta \mathbf{w})^\top \mathbf{\Psi} (\tilde{\mathbf{y}} - \mathbf{H}_\eta \mathbf{w}) - \frac{1}{2} \mathbf{w}^\top \mathbf{\Psi}^{-1} \mathbf{w} \,\middle|\, \mathbf{y}, \theta^{(t)} \right] \qquad (4.9) \\
&= \text{const.} - \frac{1}{2} \tilde{\mathbf{y}}^\top \mathbf{\Psi} \tilde{\mathbf{y}} - \frac{1}{2} \operatorname{tr} \Big(\overbrace{(\mathbf{H}_\eta \mathbf{\Psi} \mathbf{H}_\eta + \mathbf{\Psi}^{-1})}^{\Sigma_\theta} \tilde{\mathbf{W}}^{(t)} \Big) + \tilde{\mathbf{y}}^\top \mathbf{\Psi} \mathbf{H}_\eta \tilde{\mathbf{w}}^{(t)},
\end{aligned}$$

{eq:QfnEstep}

where $\tilde{\mathbf{w}}^{(t)} = \mathrm{E}[\mathbf{w} | \mathbf{y}, \theta^{(t)}]$ and $\tilde{\mathbf{W}}^{(t)} = \mathrm{E}[\mathbf{w}\mathbf{w}^\top | \mathbf{y}, \theta^{(t)}]$ are the first and second posterior moments of $\mathbf{w}$ calculated at the tth EM iteration. These can be computed directly from (4.7), substituting for $\theta^{(t)} = \{\eta^{(t)}, \mathbf{\Psi}^{(t)}\}$ as appropriate. Note that (4.9) follows as a direct consequence of the results in Appendix A.1.

Now, assume that A3 holds. The M-step then assigns $\theta^{(t+1)}$ the value of θ which maximises the Q function above. This boils down to solving the first order conditions

$$\frac{\partial Q}{\partial \eta} = -\frac{1}{2} \operatorname{tr} \left(\frac{\partial \mathbf{\Sigma}_\theta}{\partial \eta} \tilde{\mathbf{W}}^{(t)} \right) + \psi \cdot \tilde{\mathbf{y}}^\top \frac{\partial \mathbf{H}_\eta}{\partial \eta} \tilde{\mathbf{w}}^{(t)} \qquad (4.10)$$

{eq:emtheta}

$$\frac{\partial Q}{\partial \psi} = -\frac{1}{2} \tilde{\mathbf{y}}^\top \tilde{\mathbf{y}} - \operatorname{tr} \left(\frac{\partial \mathbf{\Sigma}_\theta}{\partial \psi} \tilde{\mathbf{W}}^{(t)} \right) + \tilde{\mathbf{y}}^\top \mathbf{H}_\eta \tilde{\mathbf{w}}^{(t)} \qquad (4.11)$$

{eq:empsi}

equated to zero. As $\partial \mathbf{\Sigma}_\theta / \partial \psi = \mathbf{H}_\eta^2 - \psi^{-2} \mathbf{I}_n$, the solution to (4.11) for ψ is separable in η. Meaning, given values for η, the solution $\psi^{(t+1)}$ emits a closed form

$$\psi^{(t+1)} = \left\{ \frac{\operatorname{tr} \tilde{\mathbf{W}}^{(t)}}{\tilde{\mathbf{y}}^\top \tilde{\mathbf{y}} + \operatorname{tr}(\mathbf{H}_\eta^2 \tilde{\mathbf{W}}^{(t)}) - 2 \tilde{\mathbf{y}}^\top \mathbf{H}_\eta \tilde{\mathbf{w}}^{(t)}} \right\}^{1/2}. \qquad (4.12)$$

{eq:closedformpsi}

We use this fact to form a sequential updating scheme $\eta^{(t)} \to \psi^{(t+1)} \to \eta^{(t+1)} \to \cdots$, and this form of the EM algorithm is known as the *expectation conditional maximisation* algorithm (Meng and Rubin, 1993). The solution to (4.10) can also be found in closed-form given values ψ, for many models, but in general, this is not the case. In cases where closed-form solutions do exist for η, then it is just a matter of iterating the update equations until a suitable convergence criterion is met (e.g. no more sizeable increase in successive log-likelihood values). In cases where closed-form solutions do not exist for η, the Q function is again optimised with respect to η using the L-BFGS algorithm.

In our experience, the EM algorithm is more stable than direct maximisation, in the sense that the EM steps increase the likelihood in a gentle manner that prevents sudden explosions of the likelihood. The reason for this is that the Q function is generally convex in the parameters (at the very least, it is convex in each coordinate of θ, in most cases anyway). As such, the EM is especially suitable if there are many scale parameters to estimate, but on the flip side, it is typically slow to converge. The **iprior** package provides a method to automatically switch to the direct optimisation method after running several EM iterations. This then combines the stability of the EM with the speed of direct optimisation.

4.2.4 Markov chain Monte Carlo methods

For completeness, it should be mentioned that a full Bayesian treatment of the model is possible, with additional priors on the set of hyperparameters. Markov chain Monte Carlo (MCMC) methods can then be employed to sample from the posteriors of the hyperparameters, with point estimates obtained using the posterior mean or mode, for instance. Additionally, the posterior distribution encapsulates the uncertainty about the parameter, for which inference can be made. Posterior sampling can be done using Gibbs-based methods in **WinBUGS** (Lunn et al., 2000) or **JAGS** (Plummer, 2003), and both have interfaces to R via **R2WinBUGS** (Sturtz et al., 2005) and **runjags** (Denwood, 2016) respectively. Hamiltonian Monte Carlo (HMC) sampling is also a possibility, and the Stan project (Carpenter et al., 2017) together with the package **rstan** (Stan Development Team, 2016) makes this possible in R.

On the software side, all of these MCMC packages require the user to code the model individually, and we are not aware of the existence of MCMC-based packages which are able to estimate GPR models. This makes it inconvenient for GPR and I-prior models, because in addition to the model itself, the kernel functions need to be coded as well and ensuring computational efficiency would be a difficult task.

Speaking of efficiency, it is more advantageous to marginalise the I-prior and work with the marginal model (4.8), rather than the hierarchical specification (4.6). The reason for this is that the latter model has a parameter space whose dimension is $O(n)$, while the former only samples the hyperparameters. The posterior sampling for the w_i's in (equivalently, the posterior Gaussian process $f(x) = \sum_{i=1}^n h_\lambda(x, x_i)w_i$) is performed using the normal posterior distribution in (4.7).

4.2.5 Comparison of estimation methods

sec:compare estimation

Consider a one-dimensional smoothing example. $n = 150$ data pairs (y_i, x_i) have been randomly sampled according to the true relationship

$$r_i = \text{const.} + \overbrace{0.35 \cdot \phi(x_i|1, 0.8^2) + 0.65 \cdot \phi(x_i|4, 1.5^2) + \mathbb{1}(x_i > 4.5) \cdot e^{1.25(x_i - 4.5)}}^{f_{\text{true}}(x_i)}, \tag{4.13}$$

{eq:example smoothingdata}

where $\phi(\cdot|\mu, \sigma^2)$ is the probability density function of the normal distribution with mean μ and variance σ^2. The observed y_i's are thought to be noisy versions of the true points, i.e. $y_i = r_i + \epsilon_i$, with ϵ_i following an indescript, not necessarily normal, distribution. The predictors $x_1, \dots, x_n$ have been sampled roughly from the interval $(-1, 6)$, and the sampling was intentionally not uniform so that there is slight sparsity in the middle. Figure 4.1 plots the sampled points and the true regression function.

We attempt to estimate f_{true} by a function f belonging to the fBm-0.5 RKHS $\mathcal{F}_\lambda$, with an I-prior on f. There are two parameters that need to be estimated: the scale parameter λ for the fBm-0.5 RKHS, and the error precision ψ. These can be estimated using the maximum likelihood methods described above, namely by direct optimisation and the EM algorithm. These two methods are implemented in the **iprior** package. A full Bayesian treatment is possible, and we use the **rstan** implementation of Stan to perform Hamiltonian Monte Carlo sampling of the posterior densities. A vague prior choice for λ and ψ are prescribed, namely

$$\lambda, \psi \overset{\text{iid}}{\sim} \text{N}_+(0, 100),$$

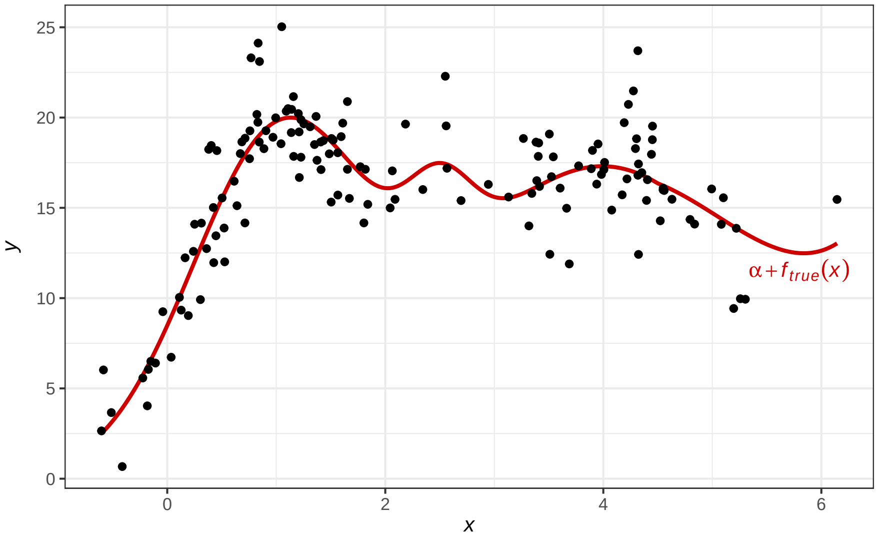


Figure 4.1: A plot of the sampled data points according to equation (4.13), with the true regression function superimposed.

fig:examplesmoothingdata

where $\text{N}_+(\mu, \sigma^2)$ represents the *half-normal* distribution[2]. We have also set an improper prior density $p(\alpha) \propto$ const. for the intercept. The advantage of HMC is that efficiency is not dictated by conjugacy, so there is freedom to choose any appropriate prior choice on the parameters.

Table 4.1: Table comparing the estimated parameter values, (marginal) log-likelihood values, and also time taken for the three estimation methods.

tab:comparemethodsestimate

	Direct optimisation	EM algorithm	Hamiltonian MC
Intercept (α)	16.1 (NA)	16.1 (NA)	16.1 (0.17)
Scale (λ)	5.01 (1.23)	5.01 (1.26)	5.61 (1.42)
Precision (ψ)	0.236 (0.03)	0.236 (0.03)	0.237 (0.03)
Log density	-339.7	-339.7	-341.1
Predictive RMSE	0.574	0.575	0.582
Iterations	12	266	2000
Time taken (s)	0.96	3.65	232

Table 4.1 tabulates the estimated parameter values, (marginal) log-likelihood values, and also time taken for the three estimation methods. The three methods concur on the estimated parameter values, although the scale parameter has been estimated slightly

[2] The random variable $X \sim \text{N}_+(\mu, \sigma^2)$ has the density $p(x) = \phi(x|\mu, \sigma^2)\,\mathbb{1}(x \geq 0)$.

differently, which is possibly attributed to the effect of the prior for λ. The resulting log-likelihood value for the Bayesian method is lower than the ML methods, which also took the longest to compute. Although the EM algorithm took longer than the direct optimisation method to compute, the time taken per iteration is significantly shorter than one Newton iteration.

4.3 Computational considerations

sec:ipriorcompcons

Computational complexity for estimating I-prior models (and in fact, for GPR in general) is dominated by the inversion (by way of eigendecomposition in our case) of the $n \times n$ matrix $\mathbf{\Sigma}_\theta = \mathbf{H}_\eta \mathbf{\Psi} \mathbf{H}_\eta + \mathbf{\Psi}^{-1}$, which scales as $O(n^3)$ in time. For the direct optimisation method, this matrix inversion is called when computing the log-likelihood, and thus must be computed at each Newton step. For the EM algorithm, this matrix inversion appears when calculating $\tilde{\mathbf{w}}$ and $\tilde{\mathbf{W}}$, the first and second posterior moments of the I-prior random effects. Furthermore, storage requirements for I-priors models are similar to that of GPR models, which is $O(n^2)$. In what follows, assumptions A1–A3 hold.

4.3.1 The Nyström approximation

The shared computational issues of I-prior and GPR models allow us to delve into machine learning literature, which is rich in ways to resolve these issue, as summarised by Quiñonero-Candela and Rasmussen (2005). One such method is to exploit low rank structures of kernel matrices. The idea is as follows. Let $\mathbf{Q}$ be a matrix with rank $q < n$, and suppose that $\mathbf{Q}\mathbf{Q}^\top$ can be used sufficiently well to represent the kernel matrix $\mathbf{H}_\eta$. Then

$$(\psi \mathbf{H}_\eta^2 + \psi^{-1}\mathbf{I}_n)^{-1} \approx \psi \left[\mathbf{I}_n - \mathbf{Q} \left((\psi^2 \mathbf{Q}^\top \mathbf{Q})^{-1} + \mathbf{Q}^\top \mathbf{Q} \right)^{-1} \mathbf{Q}^\top \right],$$

obtained via the Woodbury matrix identity, is potentially a much cheaper operation which scales $O(nq^2)$: $O(q^3)$ to do the inversion, and $O(nq)$ to do the multiplication (because typically the inverse is premultiplied to a vector). When using the linear kernel for a low-dimensional covariate then the above method is exact. This fact is clearly demonstrated by the equivalence of the p-dimensional linear model implied by (4.1) with the n-dimensional I-prior model using the canonical RKHS. If $p \ll n$ then certainly using the linear representation is much more efficient.

However, other interesting kernels such as the fractional Brownian motion (fBm) kernel or the squared exponential kernel results in kernel matrices which are full rank. An approximation to the kernel matrix using a low-rank matrix is the Nyström method (Williams and Seeger, 2001). The theory has its roots in approximating eigenfunctions, but this has since been adopted to speed up kernel machines. The main idea is to obtain an (approximation to the true) eigendecomposition of $\mathbf{H}_\eta$ based on a small subset $m \ll n$ of the data points.

Let $\mathbf{H}_\eta = \mathbf{V}\mathbf{U}\mathbf{V}^\top = \sum_{i=1}^n u_i \mathbf{v}_i \mathbf{v}_i^\top$ be the (orthogonal) decomposition of the symmetric matrix $\mathbf{H}_\eta$. As mentioned, avoiding this expensive $O(n^3)$ eigendecomposition is desired, and this is achieved by selecting a subset $\mathcal{M}$ of size m of the n data points $\{1, \dots, n\}$, so that $\mathbf{H}_\eta$ may be approximated using the rank m matrix $\mathbf{H}_\eta \approx \sum_{i \in \mathcal{M}} \tilde u_i \tilde{\mathbf{v}}_i \tilde{\mathbf{v}}_i^\top$. Without loss of generality, reorder the rows and columns of $\mathbf{H}_\eta$ so that the data points indexed by $\mathcal{M}$ are used first:

$$\mathbf{H}_\eta = \begin{pmatrix} \mathbf{A}_{m \times m} & \mathbf{B}_{m \times (n-m)} \\ \mathbf{B}^\top_{m \times (n-m)} & \mathbf{C}_{(n-m)\times(n-m)} \end{pmatrix}.$$

In other words, the data points indexed by $\mathcal{M}$ forms the smaller $m \times m$ kernel matrix $\mathbf{A}$. Let $\mathbf{A} = \mathbf{V}_m \mathbf{U}_m \mathbf{V}_m^\top = \sum_{i=1}^m u_i^{(m)} \mathbf{v}_i^{(m)} \mathbf{v}_i^{(m)\top}$ be the eigendeceomposition of $\mathbf{A}$. The Nyström method provides the formulae for $\tilde u_i$ and $\tilde{\mathbf{v}}_i$ (Rasmussen and Williams, 2006, §8.1, equations 8.2 and 8.3) as

$$\begin{aligned} \tilde u_i &:= \frac{n}{m} u_i^{(m)} \in \mathbb{R} \\ \tilde{\mathbf{v}}_i &:= \sqrt{\frac{m}{n}} \frac{1}{u_i^{(m)}} \begin{pmatrix} \mathbf{A} & \mathbf{B} \end{pmatrix}^\top \mathbf{v}_i^{(m)} \in \mathbb{R}^n. \end{aligned}$$

Denoting $\mathbf{U}_m$ as the diagonal matrix of eigenvalues $u_1^{(m)}, \dots, u_m^{(m)}$, and $\mathbf{V}_m$ the corresponding matrix of eigenvectors $\mathbf{v}_i^{(m)}$, we have

$$\mathbf{H}_\eta \approx \overbrace{\begin{pmatrix} \mathbf{V}_m \\ \mathbf{B}^\top \mathbf{V}_m \mathbf{U}_m^{-1} \end{pmatrix}}^{\bar{\mathbf{V}}} \mathbf{U}_m \overbrace{\begin{pmatrix} \mathbf{V}_m^\top & \mathbf{U}_m^{-1} \mathbf{V}_m^\top \mathbf{B} \end{pmatrix}}^{\bar{\mathbf{V}}^\top}.$$

Unfortunately, it may be the case that $\bar{\mathbf{V}}\bar{\mathbf{V}}^\top \neq \mathbf{I}_n$, while orthogonality is crucial in order to easily calculate the inverse of $\mathbf{\Sigma}_\theta$. An additional step is required to obtain an orthogonal version of the Nyström decomposition, as studied by Fowlkes et al. (2001).

Let $\mathbf{K} = \mathbf{A} + \mathbf{A}^{-\frac{1}{2}}\mathbf{B}^\top\mathbf{B}\mathbf{A}^{-\frac{1}{2}}$, where $\mathbf{A}^{-\frac{1}{2}} = \mathbf{V}_m\mathbf{U}_m^{-\frac{1}{2}}\mathbf{V}_m$, and obtain the eigendecomposition of this $m \times m$ matrix $\mathbf{K} = \mathbf{R}\hat{\mathbf{U}}\mathbf{R}^\top$. Defining

$$\hat{\mathbf{V}} = \begin{pmatrix} \mathbf{A} \\ \mathbf{B}^\top \end{pmatrix} \mathbf{A}^{-\frac{1}{2}}\mathbf{R}\hat{\mathbf{U}}^{-\frac{1}{2}} \in \mathbb{R}^n \times \mathbb{R}^m,$$

then we have that $\mathbf{H}_\eta \approx \hat{\mathbf{V}}\hat{\mathbf{U}}\hat{\mathbf{V}}^\top$ such that $\hat{\mathbf{V}}\hat{\mathbf{V}}^\top = \mathbf{I}_n$. Estimating I-prior models with the Nyström method including the orthogonalisation step takes roughly $O(nm^2)$ time and $O(nm)$ storage.

12. Attempt to prove this.

The issue of selecting the subset $\mathcal{M}$ remains. The simplest method, and that which is implemented in the **iprior** package, would be to uniformly sample a subset of size m from the n points. Although this works well in practice, the quality of approximation might suffer if the points do not sufficiently represent the training set. In this light, greedy approximations have been suggested to select the m points, so as to reduce some error criterion relating to the quality of approximation. For a brief review of more sophisticated methods of selecting $\mathcal{M}$, see Rasmussen and Williams (2006, §8.1, pp. 173–174).

4.3.2 An efficient EM algorithm

sec:efficientEM1

The evaluation of the Q function in (4.9) is $O(n^3)$, because a change in the values of θ requires evaluating $\mathbf{\Sigma}_\theta = \psi\mathbf{H}_\eta^2 + \psi^{-1}\mathbf{I}_n$, for which squaring $\mathbf{H}_\eta$ takes the bulk of the computational time. In this section, we describe an efficient method of evaluating Q if the I-prior model only involves estimating the RKHS scale parameters and the error precision under assumptions A1–A3.

Corresponding to p building block RKHSs $\mathcal{F}_1, \dots, \mathcal{F}_p$ of functions over $\mathcal{X}_1, \dots, \mathcal{X}_p$, there are p scale parameters $\lambda_1, \dots, \lambda_p$ and reproducing kernels $h_1, \dots, h_p$. Write $\theta = \{\lambda_1, \dots, \lambda_p, \psi\}$. The most common modelling scenarios that will be encountered are listed below:

1. **Single scale parameter**. With $p = 1$, $f \in \mathcal{F} \equiv \lambda_1\mathcal{F}_1$ of functions over a set $\mathcal{X}$. $\mathcal{F}$ may be any of the building block RKHSs. Note that $\mathcal{X}_1$ itself may be more than one-dimensional. The kernel over $\mathcal{X}_1 \times \mathcal{X}_1$ is therefore

$$h_\lambda = \lambda_1 h_1.$$

2. **Multiple scale parameters**. Here, $\mathcal{F}$ is a RKKS of functions $f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_p \to \mathbb{R}$, and thus $\mathcal{F} \equiv \lambda_1\mathcal{F}_1 \oplus \cdots \oplus \lambda_p\mathcal{F}_p$, where each $\mathcal{F}_k$ is one of the building block RKHSs. The kernel is
$$h_\lambda = \lambda_1 h_1 + \cdots + \lambda_p h_p.$$

3. **Multiple scale parameters with level-2 interactions**. This occurs commonly with multilevel and longitudinal models. Suppose that $\mathcal{X}_1$ is the set of 'levels' and there are $p-1$ covariate sets $\mathcal{X}_k$, $k = 2, \cdots, p$. The function space $\mathcal{F}$ is a special case of the ANOVA RKKS containing only main and two-way interaction effects, and its kernel is
$$h_\lambda = \sum_{j=1}^p \lambda_j h_j + \sum_{j<k} \lambda_j\lambda_k h_j h_k,$$
where $\mathcal{F}_1$ is the Pearson RKHS, and the remaining are any of the building block RKHSs.

4. **Polynomial RKKS**. When using the polynomial RKKS of degree d to incite a polynomial relationship of the covariate set $\mathcal{X}_1$ on the function $f \in \mathcal{F}$ (excluding an intercept), then the kernel of $\mathcal{F}$ is
$$h_\lambda = \sum_{k=1}^d b_k \lambda_1^k h_1^k.$$
where $b_k = \frac{d!}{k!(d-k)!}$, $k = 1, \dots, d$ are constants.

Of course, many other models are possible, such as the ANOVA RKKS with all p levels of interactions. What we realise is that any of these scenarios are simply a sum-product of a manipulation of the set of scale parameters $\lambda = \{\lambda_1, \dots, \lambda_p\}$ and the set of kernel functions $h = \{h_1, \dots, h_p\}$.

Let us be more concrete about what we mean by 'manipulation' of the sets λ and h. Define an 'instruction operator' which expands out both sets identically as required by the modelling scenario. Computationally speaking, this instruction could be as simple as a list containing the indices to multiply out. For the four scenarios above, the list $\mathcal{Q}$ is

1. $\mathcal{Q} = \big\{\{1\}\big\}$.
2. $\mathcal{Q} = \big\{\{1\}, \dots, \{p\}\big\}$.
3. $\mathcal{Q} = \big\{\{1\}, \dots, \{p\}, \{1,2\}, \dots, \{p-1, p\}\big\}$.

4. $\mathcal{Q} = \big\{\{1\}, \{1,1\}, \dots, \{\overbrace{1,\dots,1}^{d}\}\big\}$.

For the polynomial RKKS in the fourth example, one must also multiply the constants b_k to the λ's as appropriate. Let q be the cardinality of the set $\mathcal{Q}$, which is the number of summands required to construct the kernel for $\mathcal{F}$. Denote the instructed sets as $\xi = \{\xi_1, \dots, \xi_q\}$ for λ and $a = \{a_1, \dots, a_q\}$ for h. We can write the kernel h_λ as a linear combination of ξ and a,

$$h_\lambda = \xi_1 a_1 + \cdots + \xi_q a_q.$$

The reason this is important is because changes in λ for h_λ only changes the ξ_k's, but not the a_k's. This allows us to compute and store all of the required $n \times n$ kernel matrices $\mathbf{A}_1, \dots, \mathbf{A}_q$ from the application of instruction set on h evaluated at all pairs of data points $(x_i, x_j) \in \mathcal{X} \times \mathcal{X}$. This process of initialisation need only be done once prior to commencing the EM algorithm—a step we refer to as 'kernel loading'. In the **iprior** package, kernel loading is performed using the `kernL()` command.

Notice that

$$\begin{aligned}
\operatorname{tr}\big(\mathbf{\Sigma}_\theta \tilde{\mathbf{W}}^{(t)}\big) &= \operatorname{tr}\big((\psi \mathbf{H}_\eta^2 + \psi^{-1}\mathbf{I}_n)\tilde{\mathbf{W}}^{(t)}\big) \\
&= \psi \operatorname{tr}(\mathbf{H}_\eta^2 \tilde{\mathbf{W}}^{(t)}) + \psi^{-1} \operatorname{tr} \tilde{\mathbf{W}}^{(t)} \\
&= \psi \operatorname{tr}\left(\sum_{j,k=1}^q \xi_j \xi_k \big(\mathbf{A}_j\mathbf{A}_k + (\mathbf{A}_j\mathbf{A}_k)^\top\big)\tilde{\mathbf{W}}^{(t)} \right) + \psi^{-1} \operatorname{tr} \tilde{\mathbf{W}}^{(t)} \\
&= 2\psi \sum_{j,k=1}^q \xi_j \xi_k \operatorname{tr}\Big(\mathbf{A}_j\mathbf{A}_k \tilde{\mathbf{W}}^{(t)}\Big) + \psi^{-1} \operatorname{tr} \tilde{\mathbf{W}}^{(t)}.
\end{aligned}$$

Provided that we have the matrices $\mathbf{A}_{jk} = \mathbf{A}_j\mathbf{A}_k$, $j,k = 1,\dots,q$ in addition to $\mathbf{A}_1, \dots, \mathbf{A}_q$ pre-calculated and stored, then evaluating $\operatorname{tr}\big(\mathbf{A}_{jk}\tilde{\mathbf{W}}^{(t)}\big) = \operatorname{vec}(\mathbf{A}_{jk})^\top \operatorname{vec}(\tilde{\mathbf{W}}^{(t)})$ is $O(n^2)$, although this only need to be done once per EM iteration. Thus, with the kernels loaded, the overall time complexity to evaluate Q is $O(n^2)$ at the beginning of each iteration, but roughly linear in ξ thereafter.

As a remark, we have achieved efficiency at the expense of storage and a potentially long initialisation phase of kernel loading. The storing of the kernel matrices a can be very expensive, especially if the sample size is very large. On the bright side, once the kernel matrices are stored in memory, the **iprior** package allows them to be reused again and again. A practical situation where this might be useful is when we would like to repeat the EM at various initial values.

4.3.3 The exponential family EM algorithm

In the original EM paper by Dempster et al. (1977), the EM algorithm was demonstrated to be easily administered to complete data likelihoods belonging to the exponential family for which the maximum likelihood estimates are easily computed. If this is the case, then the M-step simply involves replacing the unknown sufficient statistics in the ML estimates with their *conditional expectations* (see Section 4.7.3 for details). Certain I-prior models emit this property, namely regression functions belonging to the full or limited ANOVA RKKS, and we describe its estimation below.

Assume A1–A3 applies, and that only the error precision ψ and the RKHS scale parameters $\lambda_1, \dots, \lambda_p$ need to be estimated, i.e. all other kernel parameters are fixed—a similar situation was described in the previous subsection. For the full ANOVA RKKS, the kernel is

$$\begin{aligned} h_\lambda &= \sum_{i=1}^p \lambda_i h_i + \sum_{i<j} \lambda_i \lambda_j h_i h_j + \cdots + \prod_{i=1}^p \lambda_i h_i \\ &= \overbrace{\lambda_k \left(h_k + \sum_i \lambda_i h_i h_k + \cdots + h_k \prod_{i \neq k} \lambda_i h_i \right)}^{\text{terms of } \lambda_k} + \overbrace{\sum_{i\neq k} \lambda_i h_i + \sum_{i,j \neq k} \lambda_i \lambda_j h_i h_j + \cdots + 0}^{\text{no } \lambda_k \text{ here}} \\ &= \lambda_k r_k + s_k \end{aligned}$$

where r_k and s_k are both functions over $\mathcal{X} \times \mathcal{X}$, defined respectively as the terms of the ANOVA kernel involving λ_k, and the terms not involving λ_k. The reason for splitting h_λ like this will become apparently momentarily.

Programmatically this looks complicated to implement in software, but in fact it is not. Consider again the instruction list $\mathcal{Q}$ for the ANOVA RKKS (Example 3, Section 4.3.2). We can split this list into two: $\mathcal{R}_k$ as those elements of $\mathcal{Q}$ which involve the index k, and $\mathcal{S}_k$ as those elements of $\mathcal{Q}$ which do not involve the index k. Let ζ_k, e_k be the sets of λ and h after applying the instructions of $\mathcal{R}_k$, and let ξ_k and a_k be the sets of λ and h after applying the instructions of $\mathcal{S}_k$. Now, we have

$$r_k = \frac{1}{\lambda_k} \sum_{i=1}^{|\mathcal{R}_k|} \zeta_{ik} e_{ik} \quad \text{and} \quad s_k = \sum_{i=1}^{|\mathcal{S}_k|} \xi_{ik} a_{ik}.$$

Defining $\mathbf{R}_k$ and $\mathbf{S}_k$ as the kernel matrices with (i,j) entries $r_k(x_i, x_j)$ and $s_k(x_i, x_j)$ respectively, we have that

$$\mathbf{H}_\eta^2 = \lambda_k^2 \mathbf{R}_k^2 + \lambda_k \overbrace{\big(\mathbf{R}_k\mathbf{S}_k + (\mathbf{R}_k\mathbf{S}_k)^\top\big)}^{\mathbf{U}_k} + \mathbf{S}_k^2.$$

Consider now the full data log-likelihood for λ_k, $k = 1, \dots, p$, conditionally dependent on the rest of the unknown parameters ψ and $\lambda_{-k} = \{\lambda_1, \dots, \lambda_p\} \backslash \{\lambda_k\}$:

$$\begin{aligned} L(\lambda_k|\mathbf{y}, \mathbf{w}, \lambda_{-k}, \psi) &= \text{const.} - \frac{1}{2}\operatorname{tr}\Big((\psi\mathbf{H}_\eta^2 + \psi^{-1}\mathbf{I}_n)\mathbf{w}\mathbf{w}^\top\Big) + \psi\tilde{\mathbf{y}}^\top\mathbf{H}_\eta\mathbf{w} \qquad (4.14) \\ &= \text{const.} - \lambda_k^2 \cdot \frac{\psi}{2}\operatorname{tr}(\mathbf{R}_k^2\mathbf{w}\mathbf{w}^\top) + \lambda_k \cdot \Big(\psi\tilde{\mathbf{y}}^\top\mathbf{R}_k\mathbf{w} - \frac{\psi}{2}\operatorname{tr}(\mathbf{U}_k\mathbf{w}\mathbf{w}^\top)\Big). \end{aligned}$$

{eq:loglikl ambdak}

Notice that the above likelihood is an exponential family distribution with the natural parameterisation $\beta = (-\lambda_k^2, \lambda_k)$ and sufficient statistics T_1 and T_2 defined by

$$T_1 = \frac{\psi}{2}\operatorname{tr}(\mathbf{R}_k^2\mathbf{w}\mathbf{w}^\top) \quad \text{and} \quad T_2 = \psi\tilde{\mathbf{y}}^\top\mathbf{R}_k\mathbf{w} - \frac{\psi}{2}\operatorname{tr}(\mathbf{U}_k^2\mathbf{w}\mathbf{w}^\top).$$

This likelihood is maximised at $\hat{\lambda}_k = T_2/2T_1$, but of course, the variables $w_1, \dots, w_n$ are never observed. As per the exponential family EM routine, replace occurrences of $\mathbf{w}$ and $\mathbf{w}\mathbf{w}^\top$ with their respective conditional expectations, i.e. $\mathbf{w} \mapsto \operatorname{E}[\mathbf{w}|\mathbf{y}] = \tilde{\mathbf{w}}$ and $\mathbf{w}\mathbf{w}^\top \mapsto \operatorname{E}[\mathbf{w}\mathbf{w}^\top|\mathbf{y}] = \tilde{\mathbf{V}}_w + \tilde{\mathbf{w}}\tilde{\mathbf{w}}^\top$ as defined in (4.7). That the λ_k's have closed-form expressions, together with the closed-form expression for ψ in (4.12), greatly simplifies the EM algorithm. At the M-step, one simply updates the parameters in turn, and as such, there is no maximisation per se.

The algorithm is summarised in Algorithm 1. The exponential family EM for ANOVA-type I-prior models require $O(n^3)$ computational time at each step, which is spent on computing the matrix inverse in the E-step. The M-step takes at most $O(n^2)$ time to compute. As a remark, it is not necessary that h_λ is the full ANOVA RKKS; any of the examples 1–3 in Section 4.3.2 can be estimated using this method, since they are seen as special cases of the ANOVA decomposition.

While the exponential family EM algorithm takes similar computational time as the efficient EM algorithm described in Section 4.3.2, there is one compelling reason to consider Algorithm 1: conjugacy of the exponential family of distributions. Realise that $\lambda_k|(\mathbf{y}, \mathbf{w}, \lambda_{-k}, \psi)$ is in fact normally distributed, with mean and variance given by $T_2/2T_1$ and $1/2T_1$ respectively. If we were so compelled to assign a normal prior on each alg:EM2

Algorithm 1 Exponential family EM for ANOVA-type I-prior models

```
procedure INITIALISATION
    Initialise $\lambda_1^{(0)}, \dots, \lambda_p^{(0)}, \psi^{(0)}$
    Compute and store matrices as per $\mathcal{R}_k$ and $\mathcal{S}_k$.
    $t \leftarrow 0$
end procedure

while not converged do
    procedure E-STEP
        $\tilde{\mathbf{w}} \leftarrow \psi^{(t)}\mathbf{H}_{\eta^{(t)}}\big(\psi^{(t)}\mathbf{H}^2_{\eta^{(t)}} + \psi^{-(t)}\mathbf{I}_n\big)^{-1}\tilde{\mathbf{y}}$
        $\tilde{\mathbf{W}} \leftarrow \big(\psi^{(t)}\mathbf{H}^2_{\eta^{(t)}} + \psi^{-(t)}\mathbf{I}_n\big)^{-1} + \tilde{\mathbf{w}}\tilde{\mathbf{w}}^\top$
    end procedure

    procedure M-STEP
        for $k = 1, \dots, p$ do
            $T_{1k} \leftarrow \frac{1}{2}\operatorname{tr}(\mathbf{R}_k^2\tilde{\mathbf{W}})$
            $T_{2k} \leftarrow \tilde{\mathbf{y}}^\top\mathbf{R}_k\tilde{\mathbf{w}} - \frac{1}{2}\operatorname{tr}(\mathbf{U}_k^2\tilde{\mathbf{W}}^\top)$
            $\lambda_k^{(t+1)} \leftarrow T_{2k}/2T_{1k}$
        end for
        $T_3 \leftarrow \tilde{\mathbf{y}}^\top\tilde{\mathbf{y}} + \operatorname{tr}(\mathbf{H}^2_{\eta^{(t)}}\tilde{\mathbf{W}}^{(t)}) - 2\tilde{\mathbf{y}}^\top\mathbf{H}_{\eta^{(t)}}\tilde{\mathbf{w}}^{(t)}$
        $\psi^{(t+1)} \leftarrow \operatorname{tr}\tilde{\mathbf{W}}^{(t)}/T_3$
    end procedure
    $t \leftarrow t + 1$
end while
```

of the λ_k's, then the conditionally dependent log-likelihood of λ_k, $L(\lambda_k|\mathbf{y}, \mathbf{w}, \lambda_{-k}, \psi)$, would have a normal log-likelihood prior involving λ_k added on. Importantly, viewed as a posterior log-density for λ_k, the posterior density for λ_k would also be a normal distribution. The EM as a whole would then generate maximum a posteriori (MAP) estimates for the parameters. Although not shown here, similar conjugacy benefits for the ψ parameter can be argues, whereby the gamma distribution is the density in question. The usual EM algorithm without using any priors can be viewed as using improper priors for the parameters, i.e. $p(\lambda_k) \propto \text{const.}$ and $p(\psi) \propto \text{const.}$.

In the next chapter on binary and multinomial regression using I-priors, the exponential family EM algorithm described here is especially relevant, as it is connected to the variational Bayesian algorithm (Bernardo et al., 2003) that will be used for estimating the models described therein.

Remark 4.5. Earlier, we restricted attention to ANOVA RKKS. Hopefully, it is now apparent that ANOVA kernels are a requirement for Algorithm 1 to work easily. As soon as higher degrees of the λ_k's come into play, e.g. using the polynomial kernel, then the ML estimate for λ_k involve solving a polynomial of degree $2d-1$ the FOC equations. Although this is not in itself hard to do, the elegance of the algorithm, especially viewed as having the normal conjugacy property for the $\lambda_k' s$, is lost.

4.3.4 Accelerating the EM algorithm

A criticism of the EM algorithm is that it may take many iterations to converge. Several novel ideas have been looked at in a bid to 'accelerate the EM algorithm', as it were. One such approach, which does not require any amendment to the particular EM algorithm at hand, is called the *monotonically over-relaxed EM algorithm* (MOEM) by Yu (2012).

The idea of MOEM is as follows. At every iteration of the MOEM, perform as usual the E-step and M-step to obtain an updated parameter value $\theta_{\text{EM}}^{(t+1)}$. Instead of using this update value of the parameter, modify it instead, and use

$$\theta^{(t+1)} = (1+\omega)\theta_{\text{EM}}^{(t+1)} - \omega\theta^{(t)},$$

where ω is an *over-relaxation* parameter. Under mild conditions, among them that $Q(\theta^{(t+1)}) > Q(\theta^{(t)})$, the MOEM estimate does not decrease the log-likelihood at each step. This condition is a slight inconvenience to check under the usual EM algorithm, but is a great companion to exponential family EM algorithm. From (4.14), we see that $Q(\lambda_k) = \text{E}_{\mathbf{w}}\left[L(\lambda_k|\theta\backslash\{\lambda_k\})|\mathbf{y},\theta^{(t)}\right]$ is quadratic in λ_k, therefore any $\omega \in [0,1]$ will maintain monotonicity of the EM algorithm.

4.4 Post-estimation

One of the perks of a (semi-)Bayesian approach to regression modelling is that we are able to use Bayesian post-estimation machinery involving the relevant posterior distributions. With the normal I-prior model, there is the added benefit that posterior distributions are easily obtained in closed form. The plots that are shown in this subsection is a continuation of the example from subsection 4.2.5.

Recall that for the I-prior model (4.6), the regression function $f(x) = \sum_{i=1}^n h_{\hat\eta}(x, x_i)\tilde w_i$ has the posterior Gaussian distribution specified by the multivariate-normal mean and variance of the $\tilde w_i$'s given in (4.7). Denote by $\mathbf{h}_{\hat\eta}(x)$ the n-vector with entries equal to $h_{\hat\eta}(x, x_i)$. Precisely, the posterior density for the regression function is

$$p\big(f(x)|\mathbf{y}\big) \sim \mathrm{N}\left(\mathbf{h}_{\hat\eta}(x)\hat{\mathbf{w}}, \mathbf{h}_{\hat\eta}(x)^\top \big(\mathbf{H}_{\hat\eta}\hat{\boldsymbol\Psi}\mathbf{H}_{\hat\eta} + \hat{\boldsymbol\Psi}^{-1}\big)^{-1}\mathbf{h}_{\hat\eta}(x)\right) \tag{4.15}$$

for any x in the domain of the regression function. Here, the hats on the parameters indicate the use of the optimised model parameters, i.e. the ML or MAP estimates.

Prediction of a new data point is also of interest. A priori, assume that $y_{\text{new}} = \hat\alpha + f(x_{\text{new}}) + \epsilon_{\text{new}}$, where $\epsilon_{\text{new}} \sim \mathrm{N}(0, \psi_{\text{new}}^{-1})$, and $f \sim$ I-prior. Denote the covariance between ϵ_{new} and $\boldsymbol\epsilon = (\epsilon_1, \dots, \epsilon_n)^\top$ by $\boldsymbol\sigma_{\text{new}}^\top \in \mathbb{R}^n$. Under an iid model (assumption A3), then $\psi_{\text{new}} = \psi = \operatorname{Var}\epsilon_i$ for any $i \in \{1, \dots, n\}$, and $\boldsymbol\sigma_{\text{new}}^\top = \mathbf{0}$, but otherwise, these extra parameters need to be dealt with somehow, either by specifying them a priori or estimating them again, which seems excessive. In any case, using a linearity argument, the posterior distribution for y_{new} is normal, with mean and variance given by

$$\mathrm{E}[y_{\text{new}}|\mathbf{y}] = \hat\alpha + \mathrm{E}\big[f(x_{\text{new}})|\mathbf{y}\big] + \text{correction term} \tag{4.16}$$

and

$$\operatorname{Var}[y_{\text{new}}|\mathbf{y}] = \operatorname{Var}\big[f(x_{\text{new}})|\mathbf{y}\big] + \psi_{\text{new}}^{-1} + \text{correction term}. \tag{4.17}$$

A derivation is presented in section A.2. Note, that the mean and variance correction term vanishes under an iid assumption A3. The posterior distribution for y_{new} can be used in several ways. Among them, is to construct a $100(1-\alpha)\%$ credibility interval for the (mean) predicted value y_{new} using

$$\mathrm{E}[y_{\text{new}}|\mathbf{y}] \pm \Phi^{-1}(1-\alpha/2) \cdot \operatorname{Var}[y_{\text{new}}|\mathbf{y}]^{\frac12},$$

where $\Phi(\cdot)$ is the standard normal cumulative distribution function. One could also perform a posterior predictive density check of the data $\mathbf{y}$, by repeatedly sampling n points from its posterior distribution. This provides a visual check of whether there are any systematic deviances between what the model predicts, and what is observed from the data.

Lastly, we discuss model comparison. Recall that the marginal distribution for $\mathbf{y}$ after integrating out the I-prior for f in model (4.6) is a normal distribution. Suppose that we are interested in comparing two candidate models M_1 and M_2, each with the parameter

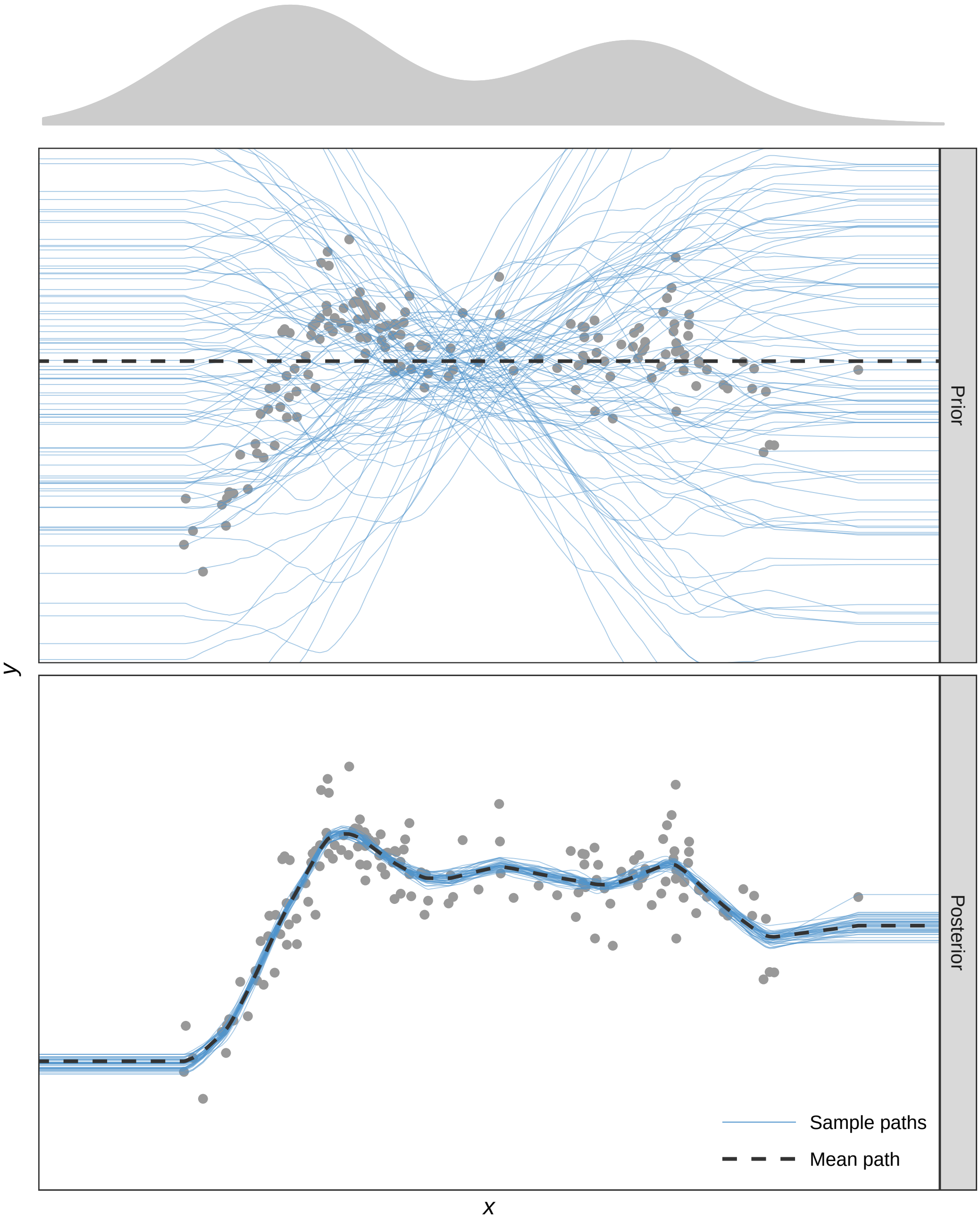


Figure 4.2: Prior (top) and posterior (bottom) sample path realisations of regression functions drawn from their respective distributions when $\mathcal{F}$ is a fBm-0.5 RKHS. At the very top of the figure, a smoothed density estimate of the x's is overlaid. In regions with few data points (near the centre), there is little Fisher information, and hence a conservative prior closer to zero, the prior mean, for this region.

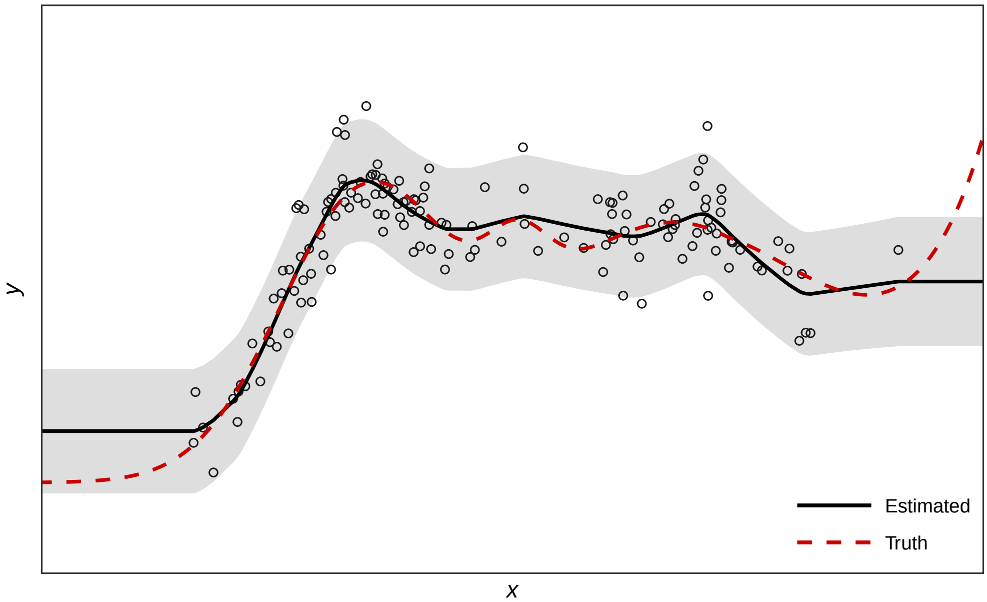


Figure 4.3: The estimated regression line (solid black) is the posterior mean estimate of the regression function (shifted by the intercept), which also gives the posterior mean estimate for the responses y. The shaded region is the 95% credibility interval for predictions. The true regression line (dashed red) is shown for comparison.

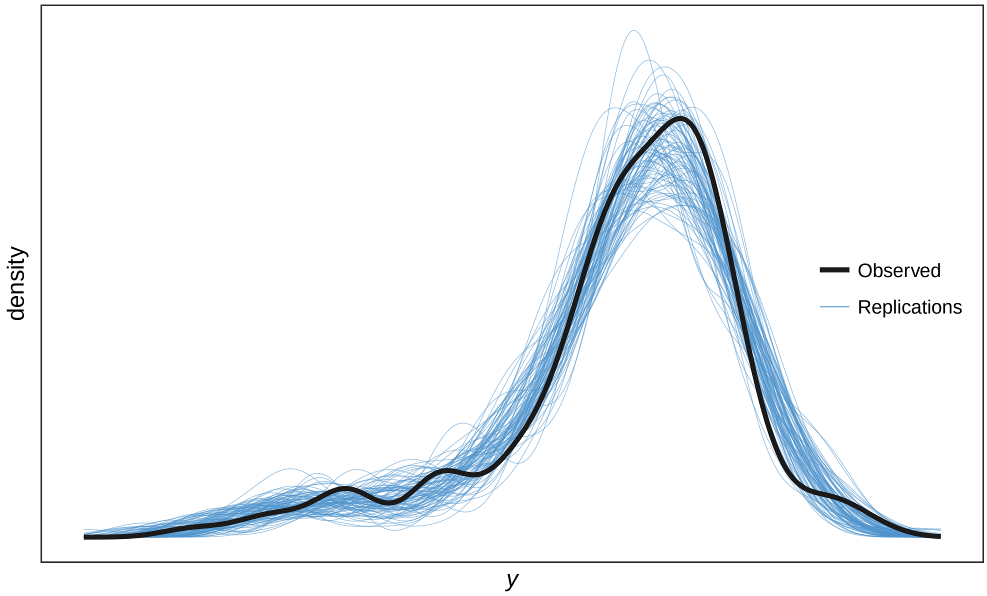


Figure 4.4: Posterior predictive density checks of the responses: repeated sampling from the posterior density of the y_i's and plotting their densities allows us to compare model predictions against observed samples.

set θ_1 and θ_2. Commonly, we would like to test whether or not particular terms in the ANOVA RKKS are significant contributors in explaining the relationship between the responses and predictors. A log-likelihood comparison is possible using an asymptotic chi-squared distribution, with degrees of freedom equal to the difference between the number of parameters in θ_2 and θ_1. This is assuming model M_1 is nested within M_2, which is the case for ANOVA-type constructions. Note that if two models have the same number of parameters, then the model with the higher likelihood is preferred.

Remark 4.6. This method of comparing marginal likelihoods can be seen as Bayesian model selection using *empirical Bayes factors*, where the Bayes factor of comparing model M_1 to model M_2 is defined as

$$\text{BF}(M_1, M_2) = \frac{\int p(\mathbf{y}|\theta_1, \mathbf{f}) p(\mathbf{f}) \, \text{d}\mathbf{f}}{\int p(\mathbf{y}|\theta_2, \mathbf{f}) p(\mathbf{f}) \, \text{d}\mathbf{f}}.$$

The word 'empirical' stems from the fact that the parameters are estimated via an empirical Bayes approach (maximum marginal likelihood). This approach is fine when the number of comparisons to be made is small, but can be computationally unfeasible when many marginal likelihoods need to be pairwise compared. In Chapter 6, we explore a fully Bayesian approach to explore the entire model space for the special case of linear models.

4.5 Examples

sec:ipriorexamples

We demonstrate I-prior modelling on a toy data set to illustrate the Nyström method, as well as three other real-data examples. All of the analyses were conducted in R, and I-prior model estimation was done using the **iprior** package. In all of these examples, A1–A3 were assumed.

4.5.1 Using the Nyström method

We investigate the use of the Nyström method of approximating the kernel matrix in estimating I-prior models. Let us revisit the data set generated by (4.13) described in Section 4.2.5. The features of this regression function are two large bumps at the centres of the mixed Gaussian PDFs, and also a small bump right after $x > 4.5$ caused by the additional exponential function. The true regression function goes to positive infinity as

x increases, and to zero as x decreases. Samples of (x_i, y_i), $i = 1, \dots, 2000$ have been generated by the built-in `gen_smooth()` function, of which the first few lines of the data are shown below.

```
R> dat <- gen_smooth(n = 2000, xlim = c(-1, 5.5), seed = 1)
R> head(dat)

##             y         X
## 1  0.6803514 -2.608953
## 2  3.6747031 -2.554039
## 3 -1.1563508 -2.381275
## 4  2.2657657 -2.280259
## 5  2.5398243 -2.214122
## 6  1.2929592 -2.170532
```

One could fit the regression model using all available data points, with an I-prior from the fBm-0.5 RKHS of functions as follows (note that the `silent` option is used to suppress the output from the `iprior()` function):

```
R> (mod.full <- iprior(y ~ X, dat, kernel = "fbm",
+                      control = list(silent = TRUE)))

## Log-likelihood value: -4355.075
##
##  lambda     psi
## 2.30244 0.23306
```

To implement the Nyström method, the option `nystrom = 50` was added to the above function call, which uses 50 randomly selected data points for the Nyström approximation.

```
R> (mod.nys <- iprior(y ~ X, dat, kernel = "fbm", nystrom = 50,
+                     control = list(silent = TRUE)))

## Log-likelihood value: -1945.33
##
##  lambda     psi
## 1.64833 0.13538
```

The hyperparameters estimated for both models are slightly different. The log-likelihood is also different, but this is attributed to information loss due to the approx-

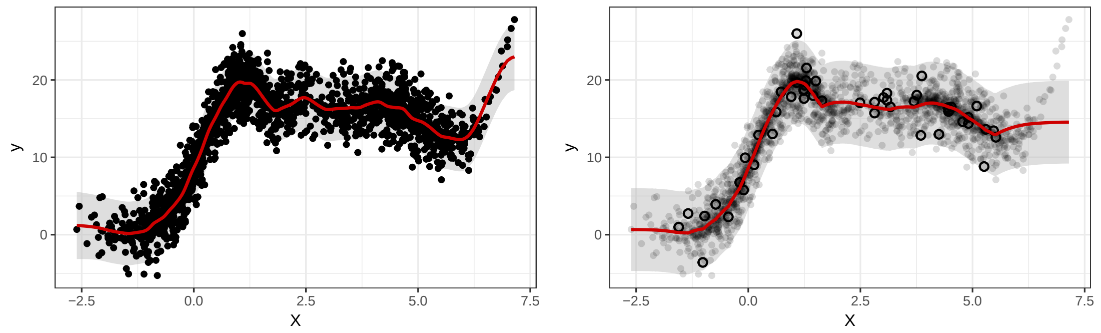


Figure 4.5: Plot of predicted regression function for the full model (left) and the Nyström approximated method (right). For the Nyström plot, the data points that were active are shown by circles with bold outlines.

fig:nystrom.plot

imation procedure. Nevertheless, we see from Figure 4.5 that the estimated regression functions are quite similar in both the full model and the approximated model. The main difference is that the the Nyström method was not able to extrapolate the right hand side of the plot well, because it turns out that there were no data points used from this region. This can certainly be improved by using a more intelligent sampling scheme. The full model took a little under 15 minutes to converge, while the Nyström method took just seconds. Storage savings is significantly higher with the Nyström method as well.

```
R> get_time(mod.full); get_size(mod.full, units = "MB")

## 14.63474 mins
## 128.2 MB

R> get_time(mod.nys); get_size(mod.nys)

## 1.324355 secs
## 965.2 kB
```

4.5.2 Random effects models

In this section, a comparison between a standard random effects model and the I-prior approach for estimating varying intercept and slopes model is illustrated. The example concerns control data[3] from several runs of radioimmunoassays (RIA) for the protein insulin-like growth factor (IGF-I) (explained in further detail in Davidian and Giltinan, 1995, §3.2.1). RIA is a in vitro assay technique which is used to measure concentration of antigens—in our case, the IGF-I proteins. When an RIA is run, control samples at known concentrations obtained from a particular lot are included for the purpose of assay quality control. It is expected that the concentration of the control material remains stable as the machine is used, up to a maximum of about 50 days, at which point control samples from a new batch is used to avoid degradation in assay performance.

```
R> data(IGF, package = "nlme")
R> head(IGF)
```

```
## Grouped Data: conc ~ age | Lot
##   Lot age conc
## 1   1   7 4.90
## 2   1   7 5.68
## 3   1   8 5.32
## 4   1   8 5.50
## 5   1  13 4.94
## 6   1  13 5.19
```

The data consists of IGF-I concentrations (`conc`) from control samples from 10 different lots measured at differing `age`s of the lot. The data were collected with the aim of identifying possible trends in control values `conc` with `age`, ultimately investigating whether or not the usage protocol of maximum sample age of 50 days is justified. J. C. Pinheiro and Bates (2000) remarks that this is not considered a longitudinal problem because different samples were used at each measurement.

We shall model the IGF data set using the I-prior methodology using the ANOVA-decomposed regression function

$$f(\texttt{age}, \texttt{Lot}) = f_1(\texttt{age}) + f_2(\texttt{Lot}) + f_{12}(\texttt{age}, \texttt{Lot})$$

where f_1 lies in the linear RKHS $\mathcal{F}_1$, f_2 in the Pearson RKHS $\mathcal{F}_2$ and f_{12} in the tensor product space $\mathcal{F}_{12} = \mathcal{F}_1 \otimes \mathcal{F}_2$. The regression function f then lies in the RKHS $\mathcal{F} = \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \mathcal{F}_{12}$ with kernel equal to the sum of the kernels from each of the RKHSs. The explanation here is that the `conc` levels are assumed to be related to both `age` and `Lot`, and in particular, the contribution of `age` on `conc` varies with each individual `Lot`. This gives the intended effect of a linear mixed-effects model, which is thought to be suitable

[3] This data is available in the R package **nlme** (J. Pinheiro et al., 2017).

in this case, in order to account for within-lot and between-lot variability. We first fit the model using the **iprior** package, and then compare the results with the standard random effects model using `lme4::lmer()`. The command to fit the I-prior model using the EM algorithm is

```
R> mod.iprior <- iprior(conc ~ age * Lot, IGF, method = "em")

## ========================================
## Converged after 57 iterations.

R> summary(mod.iprior)

## Call:
## iprior(formula = conc ~ age * Lot, data = IGF, method = "em")
##
## RKHS used:
## Linear (age)
## Pearson (Lot)
##
## Residuals:
##    Min. 1st Qu.  Median 3rd Qu.    Max.
## -4.4889 -0.3798 -0.0090  0.2563  4.3973
##
## Hyperparameters:
##           Estimate   S.E.      z P[|Z>z|]
## lambda[1]   0.0000 0.0002 -0.004    0.997
## lambda[2]   0.0007 0.0030  0.238    0.812
## psi         1.4576 0.1366 10.672   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Closed-form EM algorithm. Iterations: 57/100
## Converged to within 1e-08 tolerance. Time taken: 3.043089 secs
## Log-likelihood value: -291.9033
## RMSE of prediction: 0.8273639 (Training)
```

To make inference on the covariates, we look at the scale parameters `lambda`. We see that both scale parameters for `age` and `Lot` are close to zero, and a test of significance is not able to reject the hypothesis that these parameters are indeed null. We conclude that neither `age` nor `Lot` has a linear effect on the `conc` levels. The plot of the fitted regression line in Figure 4.6 does show an almost horizontal line for each `Lot`.

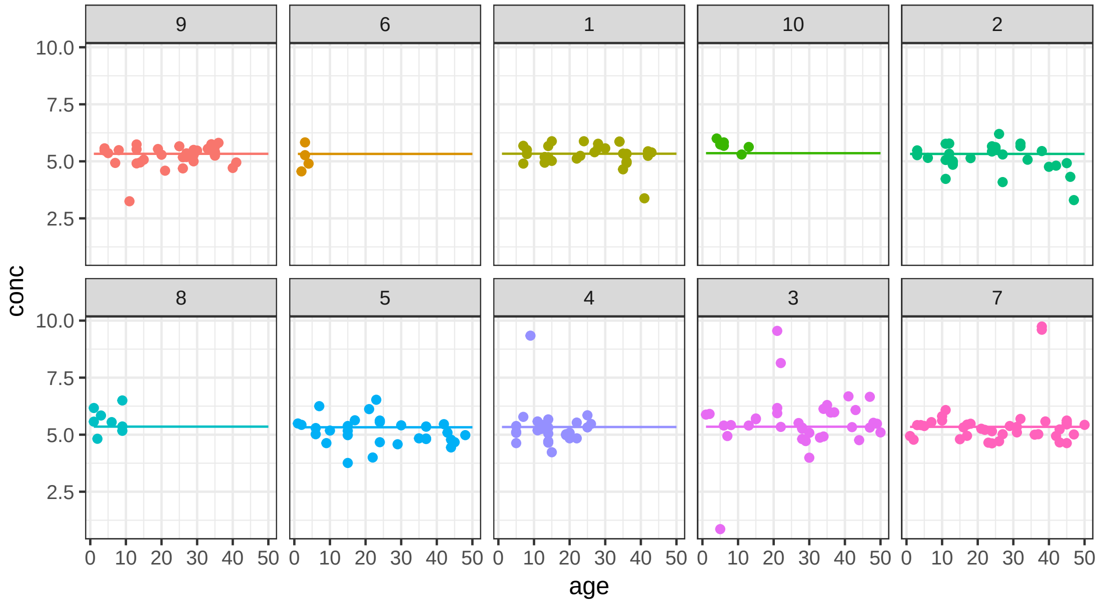


Figure 4.6: Plot of fitted regression line for the I-prior model on the IGF data set, separated into each of the 10 lots.

fig:IGF.mod.iprior.plot

The standard random effects model, as explored by Davidian and Giltinan (1995) and J. C. Pinheiro and Bates (2000), is

$$\begin{gathered}
\texttt{conc}_{ij} = \beta_{0j} + \beta_{1j}\texttt{age}_{ij} + \epsilon_{ij} \\
\begin{pmatrix} \beta_{0j} \\ \beta_{1j} \end{pmatrix} \sim \mathrm{N}\left(\begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}, \begin{pmatrix} \sigma_0^2 & \sigma_{01} \\ \sigma_{01} & \sigma_1^2 \end{pmatrix} \right) \\
\epsilon_{ij} \sim \mathrm{N}(0, \sigma^2)
\end{gathered}$$

for $i = 1, \dots, n_j$ and the index j representing the 10 `Lots`. Fitting this model using `lmer`, we can test for the significance of the fixed effect β_0, for which we find that it is not (p-value = 0.616), and arrive at the same conclusion as in the I-prior model. However, we notice that the package reports a perfect negative correlation between the random effects, σ_{01}. This indicates a potential numerical issue when fitting the model—a value of exactly -1, 0 or 1 is typically imposed by the package to force through estimation in the event of non-positive definite covariance matrices arising. We can inspect the eigenvalues of the covariance matrix for the random effects to check that they are indeed non-positive definite.

```
R> (mod.lmer <- lmer(conc ~ age + (age | Lot), IGF))

## Linear mixed model fit by REML ['lmerMod']
## Formula: conc ~ age + (age | Lot)
##    Data: IGF
## REML criterion at convergence: 594.3662
## Random effects:
##  Groups   Name        Std.Dev. Corr
##  Lot      (Intercept) 0.082507
##           age         0.008092 -1.00
##  Residual             0.820628
## Number of obs: 237, groups:  Lot, 10
## Fixed Effects:
## (Intercept)          age
##    5.374974    -0.002535

R> eigen(VarCorr(mod.lmer)$Lot)

## eigen() decomposition
## $values
## [1]  6.872939e-03 -1.355253e-20
##
## $vectors
##              [,1]        [,2]
## [1,] -0.99522490 -0.09760839
## [2,]  0.09760839 -0.99522490
```

Degenerate covariance matrices often occur in models with a large number of random coefficients. These are typically solved by setting restrictions which then avoids overparameterising the model. One advantage of the I-prior method for varying intercept/slopes model is that the positive-definiteness is automatically taken care of. Furthermore, I-prior models typically require less number of parameters to fit a simi-

Table 4.2: A comparison of the estimates for the covariance matrix of the random effects using the I-prior model and the standard random effects model.

tab:igf

Parameter	iprior	lmer
σ_0	0.012	0.083
σ_1	0.000	0.008
ρ_{01}	0.690	-1.000

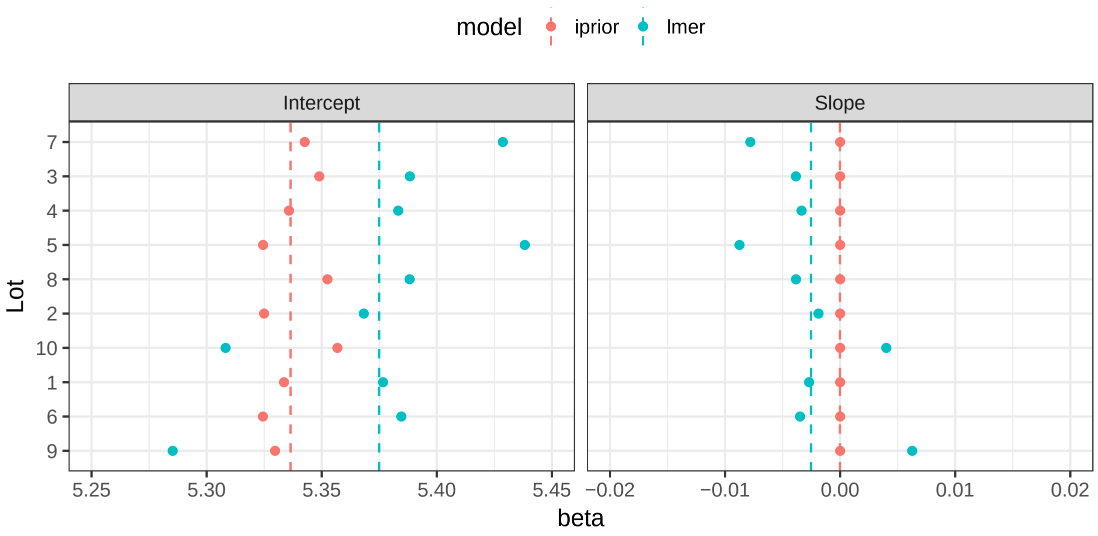


Figure 4.7: A comparison of the estimates for random intercepts and slopes (denoted as points) using the I-prior model and the standard random effects model. The dashed vertical lines indicate the fixed effect values.

fig:IGF.plot.beta

lar varying intercept/slopes model – in the above example, the I-prior model estimated only three parameters, while the standard random effects model estimated a total of six parameters.

It is also possible to "recover" the estimates of the standard random effects model from the I-prior model, albeit in a slighly manual fashion (refer to subsection 4.1.2). Denote by f^j the individual linear regression lines for each of the $j = 1, \dots, 10$ `Lots`. Then, each of these f^j has a slope and intercept for which we can estimate from the fitted values $\hat f^j(x_{ij})$, $i = 1, \dots, n_j$. This would give us the estimate of the posterior mean of the random intercepts and slopes; these would typically be obtained using empirical-Bayes methods in the case of the standard random effects model.

Furthermore, σ_0^2 and σ_1^2 gives a measure of variability of the intercepts and slopes of the different groups, and this can be calculated from the estimates of the random intercepts and slopes. In the same spirit, $\rho_{01} = \sigma_{01}/(\sigma_0\sigma_1)$, which is the correlation between the random intercept and slope, can be similarly calculated. Finally, the fixed effects can be estimated from the intercept and slope of the best fit line running through the I-prior estimated `conc` values. The intuition for this is that the fixed effects are essentially the ordinary least squares (OLS) of a linear model if the groupings are disregarded. Figure 4.7 illustrates the differences in the estimates for the random coefficients, while

Table 4.2 illustrates the differences in the estimates for the covariance matrix. Minor differences do exist, with the most noticeable one being that the slopes in the I-prior model are categorically estimated as zero, and the sign of the correlation ρ_{01} being opposite in both models. Even so, the conclusions from both models are similar.

4.5.3 Longitudinal data analysis

sec:cows

We consider a balanced longitudinal data set consisting of weights in kilograms of 60 cows, 30 of which were randomly assigned to treatment group A, and the remaining 30 to treatment group B. The animals were weighed 11 times over a 133-day period; the first 10 measurements for each animal were made at two-week intervals and the last measurement was made one week later. This experiment was reported by Kenward (1987), and the data set is included as part of the package **jmcm** (J. Pan and Y. Pan, 2016) in R. The variable names have been renamed for convenience.

```
R> data(cattle, package = "jmcm")
R> names(cattle) <- c("id", "time", "group", "weight")
R> cattle$id <- as.factor(cattle$id)  # convert to factors
R> str(cattle)
```

```
## 'data.frame': 660 obs. of  4 variables:
##  $ id    : Factor w/ 60 levels "1","2","3","4",..: 1 1 1 1 1 1 1 1 1..
##  $ time  : num  0 14 28 42 56 70 84 98 112 126 ...
##  $ group : Factor w/ 2 levels "A","B": 1 1 1 1 1 1 1 1 1 1 ...
##  $ weight: int  233 224 245 258 271 287 287 287 290 293 ...
```

The response variable of interest are the `weight` growth curves, and the aim is to investigate whether a treatment effect is present. The usual approach to analyse 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 preceeding observations.

Using the I-prior, it is not necessary to assume the growth curves were drawn randomly. Instead, it suffices to assume that they lie in an appropriate function class. For this example, we assume that the function class is the fBm RKHS, i.e., we assume a smooth effect of time on weight. The growth curves form a multidimensional (or functional) response equivalent to a “wide” format of representing repeated measures data.

tab:cowmodel

Table 4.3: A brief description of the five models fitted using I-priors.

Model	Explanation	Formula (`weight ~ ...`)
1	Growth does not vary with treatment nor among cows	`time`
2	Growth varies among cows only	`id * time`
3	Growth varies with treatment only	`group * time`
4	Growth varies with treatment and among cows	`id * time + group * time`
5	Growth varies with treatment and among cows, with an interaction effect between treatment and cows	`id * group * time`

In our analysis using the **iprior** package, we used the "long" format and thus our (unidimensional) sample size n is equal to 60 cows × 11 repeated measurements. We also have two covariates potentially influencing growth, namely the cow subject `id` and also treatment `group`. The regression model can then be thought of as

$$\texttt{weight} = \alpha + f(\texttt{id}, \texttt{group}, \texttt{time}) + \epsilon$$
$$\epsilon \sim \text{N}(0, \psi^{-1}).$$

We assume iid errors, and in addition to a smooth effect of `time`, we further assume a nominal effect of both cow `id` and treatment `group` using the Pearson RKHS. In the **iprior** package, factor type objects are treated with the Pearson kernel automatically, and the only `model` option we need to specify is the `kernel = "fbm"` option for the `time` variable. We have opted not to estimate the Hurst coefficient in the interest of computational time, and instead left it at the default value of 0.5. Table 4.3 explains the five models we have fitted.

The simplest model fitted was one in which the growth curves do not depend on the treatment effect or individual cows. We then added treatment effect and the cow `id` as covariates, separately first and then together at once. We also assumed that both of these covariates are time-varying, and hence added also the interaction between these covariates and the `time` variable. The final model was one in which an interaction between treatment effect and individual cows was assumed, which varied over time.

All models were fitted using the `mixed` estimation method. Compared to the EM algorithm alone, we found that the combination of direct optimisation with the EM tab:cowresults

Table 4.4: Summary of the five I-prior models fitted to the cow data set.

Model	Formula (weight ~ ...)	Log-likelihood	Error S.D.	Number of parameters
1	time	-2789.23	16.33	1
2	id * time	-2789.60	16.35	2
3	group * time	-2295.16	3.68	2
4	id * time + group * time	-2270.85	3.39	3
5	id * group * time	-2249.26	3.90	3

algorithm in the `mixed` routine fits the model about six times faster for this data set due to slow convergence of EM algorithm. Here is the code and output for fitting the first model:

```
R> # Model 1: weight ~ f(time)
R> set.seed(456)
R> (mod1 <- iprior(weight ~ time, cattle, kernel = "fbm", method = "mixed"))

## Running 5 initial EM iterations
## ======================================================================
## Now switching to direct optimisation
## final  value 1394.615062
## converged
## Log-likelihood value: -2789.231
##
##  lambda     psi
## 0.83592 0.00375
```

The results of the model fit are summarised in Table 4.4. We can test for a treatment effect by testing Model 4 against the alternative that Model 2 is true. The log-likelihood ratio test statistic is $D = -2(-2789.60 - (-2270.85)) = 1037.49$ which has an asymptotic chi-squared distribution with $3 - 2 = 1$ degree of freedom. The p-value for this likelihood ratio test is less than 10^{-6}, so we conclude that Model 4 is significantly better than Model 2.

We can next investigate whether the treatment effect differs among cows by comparing Model 5 against Model 4. As these models have the same number of parameters, we can simply choose the one with the higher likelihood, which is Model 5. We conclude that

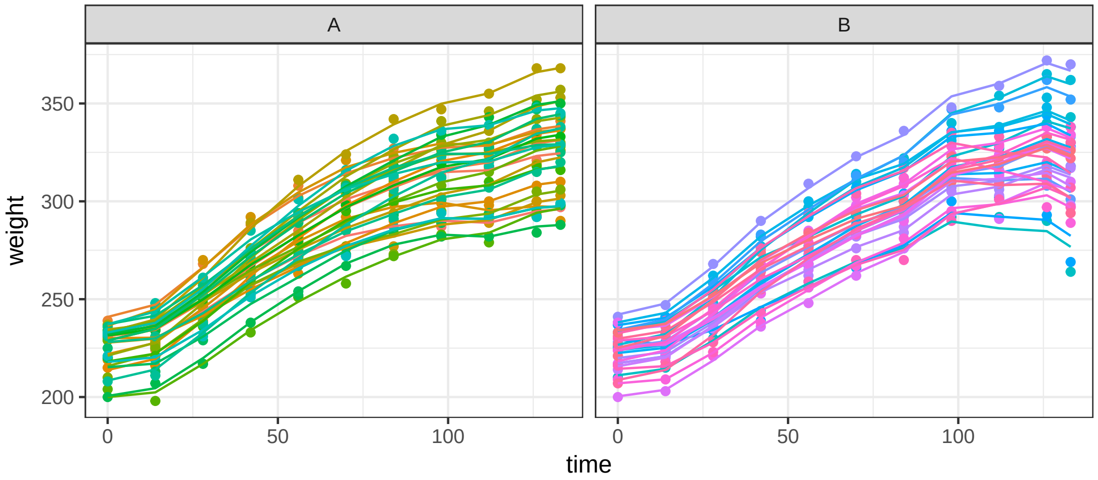


Figure 4.8: A plot of the I-prior fitted regression curves from Model 5. In this model, growth curves differ among cows and by treatment effect (with an interaction between cows and treatment effect), thus producing these 60 individual lines, one for each cow, split between their respective treatment groups (A or B).

fig:cows.plot

treatment does indeed have an effect on growth, and that the treatment effect differs among cows. A plot of the fitted regression curves onto the cow data set is shown in Figure 4.8.

4.5.4 Regression with a functional covariate

We illustrate the prediction of a real valued response with a functional covariate using a widely analysed data set for quality control in the food industry. The data[4] contain samples of spectrometric curve of absorbances of 215 pieces of finely chopped meat, along with their water, fat and protein content. These data are recorded on a Tecator Infratec Food and Feed Analyzer working in the wavelength range 850–1050 nm by the Near Infrared Transmission (NIT) principle. Absorption data has not been measured continuously, but instead 100 distinct wavelengths were obtained. Figure 4.9 shows a sample of 10 such spectrometric curves.

For our analyses and many others' in the literature, the first 172 observations in the data set are used as a training sample for model fitting, and the remaining 43

[4] Obtained from Tecator (see `http://lib.stat.cmu.edu/datasets/tecator` for details). We used the version made available in the dataframe `tecator` from the R package **caret** (Kuhn et al., 2017).

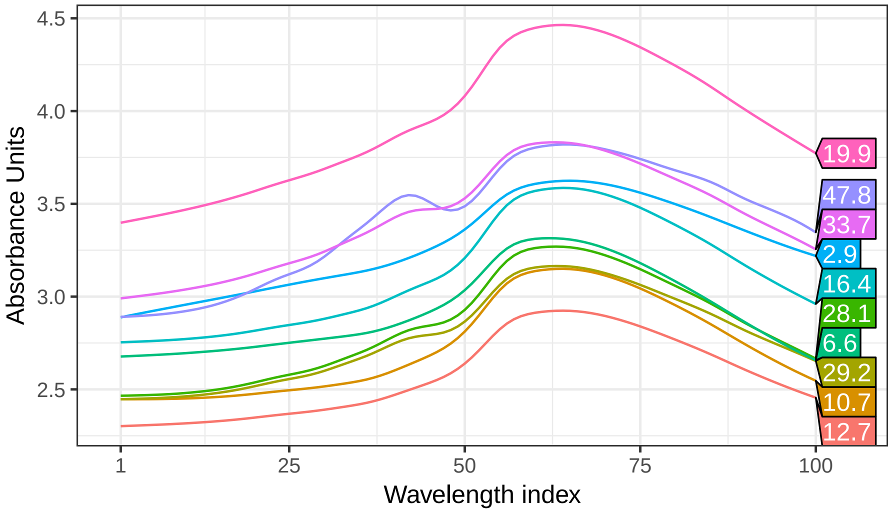


Figure 4.9: Sample of spectrometric curves used to predict fat content of meat. For each meat sample the data consists of a 100 channel spectrum of absorbances and the contents of moisture, fat (numbers shown in boxes) and protein measured in percent. The absorbance is $-\log 10$ of the transmittance measured by the spectrometer. The three contents, measured in percent, are determined by analytic chemistry.

fig:tecator.data

observations as a test sample to evaluate the predictive performance of the fitted model. The focus here is to use the **iprior** package to fit several I-prior models to the Tecator data set, and calculate out-of-sample predictive error rates. We compare the predictive performance of I-prior models against Gaussian process regression and the many other different methods applied on this data set. These methods include neural networks (Thodberg, 1996), kernel smoothing (Ferraty and Vieu, 2006), single and multiple index functional regression models (Chen et al., 2011), sliced inverse regression (SIR) and sliced average variance estimation (SAVE), multivariate adaptive regression splines (MARS), partial least squares (PLS), and functional additive model with and without component selection (FAM & CSEFAM). An analysis of this data set using the SIR and SAVE methods were conducted by Lian and Li (2014), while the MARS, PLS and (CSE)FAM methods were studied by Zhu et al. (2014). Table 4.5 tabulates the results of all of these methods from the various references.

Assuming a regression model as in (4.6), we would like to model the `fat` content y_i using the spectral curves x_i. Let $x_i(t)$ denote the absorbance for wavelength $t = 1, \dots, 100$. From Figure 4.9, it appears that the curves are smooth enough to be differentiable, and therefore it is reasonable to assume that they lie in the Sobolev-Hilbert space as discussed in Section Section 4.1.5. We take first differences of the 100-dimensional matrix, which leaves us with the 99-dimensional covariate saved in the object named absorp. The fat and absorp data have been split into *.train and *.test samples, as mentioned earlier. Our first modelling attempt is to fit a linear effect by regressing the responses fat.train against a single high-dimensional covariate absorp.train using the linear RKHS and the direct optimisation method.

```
R> # Model 1: Canonical RKHS (linear)
R> (mod1 <- iprior(y = fat.train, absorp.train))

## iter   10 value 222.653144
## final  value 222.642108
## converged
## Log-likelihood value: -445.2844
##
##     lambda        psi
## 4576.86595    0.11576
```

Our second and third model uses polynomial RKHSs of degrees two and three, which allows us to model quadratic and cubic terms of the spectral curves respectively. We also opted to estimate a suitable offset parameter, and this is called to iprior() with the option est.offset = TRUE. Each of the two models has a single scale parameter, an offset parameter, and an error precision to be estimated. The direct optimisation method has been used, and while both models converged regularly, it was noticed that there were multiple local optima that hindered the estimation (output omitted).

```
R> # Model 2: Polynomial RKHS (quadratic)
R> mod2 <- iprior(y = fat.train, absorp.train, kernel = "poly2",
+                est.offset = TRUE)
R> # Model 3: Polynomial RKHS (cubic)
R> mod3 <- iprior(y = fat.train, absorp.train, kernel = "poly3",
+                est.offset = TRUE)
```

Next, we attempt to fit a smooth dependence of fat content on the spectrometric curves using the fBm RKHS. By default, the Hurst coefficient for the fBm RKHS is set to be 0.5. However, with the option est.hurst = TRUE, the Hurst coefficient is included in the estimation procedure. We fit models with both a fixed value for Hurst (at 0.5) and an estimated value for Hurst. For both of these models, we encountered numerical issues when using the direct optimisation method. The L-BFGS algorithm kept on pulling the hyperparameter towards extremely high values, which in turn made the log-likelihood value greater than the machine's largest normalised floating-point number (`.Machine$double.xmax = 1.797693e+308`). Investigating further, it seems that estimates at these large values give poor training and test error rates, though likelihood values here are high (local optima). To get around this issue, we used the EM algorithm to estimate the fixed Hurst model, and the `mixed` method for the estimated Hurst model. For both models, the `stop.crit` was relaxed and set to `1e-3` for quicker convergence, though this did not affect the predictive abilities compared to a more stringent `stop.crit`.

```
R> # Model 4: fBm RKHS (default Hurst = 0.5)
R> (mod4 <- iprior(y = fat.train, absorp.train, kernel = "fbm",
+                   method = "em", control = list(stop.crit = 1e-3)))
```

```
## ==============================================
## Converged after 65 iterations.
## Log-likelihood value: -204.4592
##
##     lambda        psi
##    3.24112 1869.32897
```

```
R> # Model 5: fBm RKHS (estimate Hurst)
R> (mod5 <- iprior(fat.train, absorp.train, kernel = "fbm", method = "mixed",
+                   est.hurst = TRUE, control = list(stop.crit = 1e-3)))
```

```
## Running 5 initial EM iterations
## ======================================================================
## Now switching to direct optimisation
## iter   10 value 115.648462
## final  value 115.645800
## converged
## Log-likelihood value: -231.2923
##
##    lambda     hurst       psi
## 204.97184   0.70382   9.96498
```

Finally, we fit an I-prior model using the SE RKHS with lengthscale estimated. Here we illustrate the use of the `restarts` option, in which the model is fitted repeatedly from different starting points. In this case, eight random initial parameter values were used and these jobs were parallelised across the eight available cores of the machine. The additional `par.maxit` option in the `control` list is an option for the maximum number of iterations that each parallel job should do. We have set it to 100, which is the same number for `maxit`, but if `par.maxit` is less than `maxit`, the estimation procedure continues from the model with the best likelihood value. We see that starting from eight different initial values, direct optimisation leads to (at least) two log-likelihood optima sites, −231.5 and −680.5.

```
R> # Model 6: SE kernel
R> (mod6 <- iprior(fat.train, absorp.train, est.lengthscale = TRUE,
+                   kernel = "se", control = list(restarts = TRUE,
+                                                 par.maxit = 100)))

## Performing 8 random restarts on 8 cores
## ======================================================================
## Log-likelihood from random starts:
##     Run 1     Run 2     Run 3     Run 4     Run 5     Run 6     Run 7
## -680.4637 -231.5440 -231.5440 -231.5440 -231.5440 -680.4637 -680.4637
##     Run 8
## -231.5440
## Continuing on Run 3
## final  value 115.771932
## converged
## Log-likelihood value: -231.544
##
##      lambda lengthscale         psi
##    96.10718     0.09269     6.15429
```

Predicted values of the test data set can be obtained using the `predict()` function. An example for obtaining the first model's predicted values is shown below. The `predict()` method for `ipriorMod` objects also return the test MSE if the vector of test data is supplied.

```
R> predict(mod1, newdata = list(absorp.test), y.test = fat.test)

## Test RMSE: 2.890353
##
## Predicted values:
##  [1] 43.607 20.444  7.821  4.491  9.044  8.564  7.935 11.615 13.807
## [10] 17.359
```

Table 4.5: A summary of the root mean squared error (RMSE)of prediction for the I-prior models and various other methods in literature conducted on the Tecator data set. Values for the methods under *Others* were obtained from the corresponding references cited earlier.

tab:tecator

	RMSE	
Model	Train	Test
I-prior		
Linear	2.89	2.89
Quadratic	0.72	0.97
Cubic	0.37	0.58
Smooth (fBm-0.50)	0.00	0.68
Smooth (fBm-0.70)	0.19	0.63
Smooth (SE-0.09)	0.35	1.85
Gaussian process regression		
Linear	0.18	2.36
Smooth (SE-7.04)	0.17	2.10
Others		
Neural network[a]		0.36
Kernel smoothing[b]		1.49
Single/multiple indices model[c]		1.55
Sliced inverse regression		0.90
Sliced average variance estimation		1.70
MARS[d]		0.88
Partial least squares[d]		1.01
CSEFAM[d]		0.85

[a] Neural network best results with automatic relevance determination (ARD) quoted.
[b] Data set used was a 160/55 training/test split.
[c] These are results of a leave-one-out cross-validation scheme.
[d] Data set used was an extended version with $n = 240$, and a random 185/55 training/test split.

```
## # ... with 33 more values
```

These results are summarised in Table 4.5. For the I-prior models, a linear effect of the functional covariate gives a training RMSE of 2.89, which is improved by both the qudratic and cubic model. The training RMSE is improved further by assuming a smooth RKHS of functions for f, i.e. the fBm and SE RKHSs. When it comes to out-of-sample test error rates, the cubic model gives the best RMSE out of the I-prior models for this particular data set, with an RMSE of 0.58. This is followed closely by the fBm RKHS with estimated Hurst coefficient (fBm-0.70) and also the fBm RKHS with default Hurst coefficient (fBm-0.50). The best performing I-prior model is only outclassed by the neural networks of Thodberg (1996), who also performed model selection using automatic relevance determination (ARD). The I-prior models also give much better test RMSE than Gaussian process regression[5].

4.6 Conclusion

The steps for I-prior modelling are essentially three-fold:

1. Select an appropriate function space (equivalently, kernels) for which specific effects are desired on the covariates.
2. Estimate the posterior regression function and optimise the hyperparameters, which include the RKHS scale parameter(s), error precision, and any other kernel parameters such as the Hurst index.
3. Perform post-estimation procedures such as
   - Posterior predictive checks;
   - Model comparison via log-likelihood ratio tests/empirical Bayes factors; and
   - Prediction of new data point.

The main sticking point with the estimation procedure is the involvement of the $n \times n$ kernel matrix, for which its inverse is needed. This requires $O(n^2)$ storage and $O(n^3)$ computational time. The computational issue faced by I-priors are mirrored in Gaussian process regression, so the methods to overcome these computational challenges in GPR can be explored further. However, most efficient computational solutions exploit the nature of the SE kernel structure, which is the most common kernel used in GPR. Nonetheless, we suggest the following as considerations for future work:

1. **Sparse variational approximations**. Variational methods have seen an active development in recent times. By using inducing points (Titsias, 2009) or stochastic variational inference (Hensman et al., 2013), such methods can greatly reduce computational storage and speed requirements. A recent paper by Cheng and

[5] GPR models were fit using `gausspr()` in **kernlab**.

Boots (2017) also suggests a variational algorithm with linear complexity for GPR-type models.

2. **Accelerating the EM algorithm further**. Two methods can be explored. The first is called parameter-expansion EM algorithm (PXEM) by (Liu et al., 1998), which has been shown to be promising for random-effects type models. It involves correcting the M-step by a 'covariance adjustment', so that extra information can be capitalised on to improve convergence rates. The second is a quasi-Newton acceleration of the EM algorithm as proposed by Lange (1995). A slight change to the EM gradient algorithm in the M-step steers the EM algorithm to the Newton-Raphson algorithm, thus exploiting the benefits of the EM algorithm in the early stages (monotonic increase in likelihood) and avoiding the pitfalls of Newton-Raphson (getting stuck in local optima). Both algorithms require an in-depth reassessment of the EM algorithm to be tailored to I-prior models.

4.7 Miscellanea

4.7.1 Similarity to the g-prior

misc:gprior

The I-prior for $\boldsymbol{\beta}$ resembles the objective g-prior (Zellner, 1986) for regression coefficients,

$$\boldsymbol{\beta} \sim \mathrm{N}_p\left(\mathbf{0}, g(\mathbf{X}^\top \boldsymbol{\Psi} \mathbf{X})^{-1}\right),$$

although they are quite different objects. The g-prior for $\boldsymbol{\beta}$ has the *inverse* (scaled) Fisher information matrix as its covariance matrix. This, in itself, has a much different and arguably counterintuitive meaning: large amounts of Fisher information about $\boldsymbol{\beta}$ corresponds to a small prior variance, and hence less deviation away from the prior mean of zero in estimating $\boldsymbol{\beta}$. The choice of the hyperparameter g has been the subject of much debate, with choices ranging from fixing $g = n$ (corresponding to the concept of *unit Fisher information*), to fully Bayesian and empirical Bayesian methods of estimating g from the data.

On the other hand, we note that the g-prior has an I-prior interpretation when argues as follows. Assume that the regression function f lies in the continual dual space of $\mathbb{R}^p$ equipped with the inner product $\langle \mathbf{x}, \mathbf{x}' \rangle_{\mathcal{X}} = \mathbf{x}^\top (\mathbf{X}^\top \boldsymbol{\Psi} \mathbf{X})^{-1} \mathbf{x}$. With this inner product and from (3.3) (p. 79), the Fisher information for $\boldsymbol\beta$ is

$$\begin{aligned}\mathcal{I}_g(\boldsymbol\beta) &= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} (\mathbf{X}^\top \boldsymbol\Psi \mathbf{X})^{-1}\mathbf{x}_i \otimes (\mathbf{X}^\top \boldsymbol\Psi \mathbf{X})^{-1}\mathbf{x}_j \\ &= (\mathbf{X}^\top \boldsymbol\Psi \mathbf{X})^{-1} \cancel{(\mathbf{X}^\top \boldsymbol\Psi \mathbf{X})} \cancel{(\mathbf{X}^\top \boldsymbol\Psi \mathbf{X})^{-1}} \\ &= (\mathbf{X}^\top \boldsymbol\Psi \mathbf{X})^{-1},\end{aligned}$$

and this, rather than the usual $\mathbf{X}^\top \boldsymbol\Psi \mathbf{X}$ as the prior covariance matrix for $\boldsymbol\beta$, means that the I-prior is in fact the standard g-prior.

The metric induced by the inner product is actually the *Mahalanobis distance*, a scale-invariant natural distance if the covariates are measured on different scales. To expand on this idea, circle back to the regression function and write it as $f(\mathbf{x}) = \langle \mathbf{x}, \boldsymbol\beta \rangle_{\mathcal{X}}$. In usual least squares regression, the choice of inner product is irrelevant, so the usual dot product is commonly used (however, as we have seen above, the choice of inner product determines the form of the Fisher information for $\boldsymbol\beta$). In particular, suppose that all the x_{ik}'s, $k = 1,\dots,p$ for each unit $i = 1,\dots,n$ are measured on the same scale; for instance, these could be measurements in centimetres. In this case, the dot product is reasonable, because $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = \sum_{k=1}^p x_{ik}x_{jk}$ and the inner product has a coherent unit, namely the squared unit of the x_{ik}'s. However, if they were a mix of various scaled measurements, then obviously the inner product's unit is incoherent—one would be resorted to adding measurements in different units, for example, cm^2 and kg^2 and so on. In such a case, a unitless inner product is appropriate, like the Mahalonobis inner product, which technically rescales the x_{ik}'s to unity. In summary, if the covariates are all measured on the same scale, then the I-prior is appropriate, and if not, the g-prior is appropriate.

misc:multilevelmodels

4.7.2 Multilevel models

Write $\alpha = \beta_0$, and for simplicity, assume iid errors, i.e., $\boldsymbol\Psi = \psi \mathbf{I}_n$. The form of $f \in \mathcal{F}$ is now $f(\mathbf{x}_i^{(j)}, j) = \sum_{i'=1}^{n_{j'}} \sum_{j'=1}^{m} h_\lambda\big((\mathbf{x}_i^{(j)}, j), (\mathbf{x}_{i'}^{(j')}, j')\big) w_{i'j'}$, where each $w_{i'j'} \sim \mathrm{N}(0, \psi^{-1})$.

Now, functions in the scaled RKHS $\mathcal{F}_2$ have the form

$$\begin{aligned} f_2(j) &= \sum_{i=1}^{n_{j'}} \sum_{j'=1}^{m} \lambda_2 \left(\frac{\delta_{jj'}}{p_j} - 1 \right) w_{ij'} \\ &= \lambda_2 \left(\frac{w_{+j}}{p_j} - w_{++} \right), \end{aligned}$$

where a '+' in the index of w_{ik} indicates a summation over that index, and p_j is the empirical distribution over $\mathcal{M}$, i.e. $p_j = n_j/n$. Clearly $f_2(j)$ is a variable depending on j, so write $f_2(j) = \beta_{0j}$. The distribution of β_{0j} is normal with zero mean and variance

$$\begin{aligned} \operatorname{Var} \beta_{0j} &= \lambda_2^2 \left(\frac{\cancel{n_j}\psi}{n_j^{\cancel{2}}/n^2} + n\psi \right) \\ &= n\psi\lambda_2^2 \left(\frac{1}{p_j} + 1 \right). \end{aligned}$$

The covariance between any two random intercepts β_{0j} and $\beta_{0j'}$ is

$$\begin{aligned} \operatorname{Cov}(\beta_{0j}, \beta_{0j'}) &= \operatorname{Cov}\left(\lambda_2 \left(\frac{w_{+j}}{p_j} - w_{++} \right), \lambda_2 \left(\frac{w_{+j'}}{p_{j'}} - w_{++} \right) \right) \\ &= \frac{\lambda_2^2}{p_j p_{j'}} \cancelto{0}{\operatorname{Cov}(w_{+j}, w_{+j'})} - \frac{\lambda_2^2}{p_j} \operatorname{Cov}(w_{+j}, w_{++}) - \frac{\lambda_2^2}{p_{j'}} \operatorname{Cov}(w_{++}, w_{+j'}) \\ &\quad + \lambda_2^2 \operatorname{Cov}(w_{++}, w_{++}) \\ &= -\frac{\lambda_2^2}{\cancel{n_j}/n} \cancel{n_j}\psi - \frac{\lambda_2^2}{\cancel{n_{j'}}/n} \cancel{n_{j'}}\psi + \lambda_2^2 n\psi \\ &= -n\psi\lambda_2^2. \end{aligned}$$

Functions in $\mathcal{F}_{12}$, on the other hand, have the form

$$\begin{aligned} f_{12}(\mathbf{x}_i, j) &= \sum_{i'=1}^{n_{j'}} \sum_{j'=1}^{m} \lambda_1\lambda_2 \cdot \tilde{\mathbf{x}}_i^{(j)\top} \tilde{\mathbf{x}}_{i'}^{(j')} \cdot \left(\frac{\delta_{jj'}}{p_j} - 1 \right) w_{i'j'} \\ &= \tilde{\mathbf{x}}_i^{(j)\top} \underbrace{\left(\frac{\lambda_1\lambda_2}{p_j} \sum_{i'=1}^{n_j} \tilde{\mathbf{x}}_{i'}^{(j)} w_{i'j} - \lambda_1\lambda_2 \sum_{i'=1}^{n_{j'}} \sum_{j'=1}^{m} \tilde{\mathbf{x}}_{i'}^{(j')} w_{i'j'} \right)}_{\boldsymbol{\beta}_{1j}}, \end{aligned}$$

and this is, as expected, a linear form dependent on cluster j. We can calculate the variance for β_{1j} to be

$$\begin{aligned}
\operatorname{Var}\boldsymbol{\beta}_{1j} &= \lambda_1^2\lambda_2^2 \operatorname{Var}\left(\frac{1}{p_j}\tilde{\mathbf{X}}_j^\top \mathbf{w}_j - \tilde{\mathbf{X}}^\top \mathbf{w}\right) \\
&= \lambda_1^2\lambda_2^2 \left(\frac{\psi}{n_j^2/n^2}\tilde{\mathbf{X}}_j^\top \tilde{\mathbf{X}}_j + \psi \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} - \frac{1}{p_j}\tilde{\mathbf{X}}_j^\top \operatorname{Cov}(\mathbf{w}_j, \mathbf{w})\tilde{\mathbf{X}}^\top\right) \\
&= n\psi\lambda_1^2\lambda_2^2 \left(\frac{1}{p_j}\mathbf{S}_j + \mathbf{S} - \mathbf{S}_j\right) \\
&= n\psi\lambda_1^2\lambda_2^2 \left(\left(\frac{1}{p_j} - 1\right)\mathbf{S}_j + \mathbf{S}\right)
\end{aligned}$$

where $\mathbf{S}_j = \frac{1}{n_j}\sum_{i=1}^{n_j}(\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})^\top(\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})$, $\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n_j}\sum_{j=1}^{m}(\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})^\top(\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})$, and $\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n_j}\sum_{j=1}^{m}\mathbf{x}_i^{(j)}$. The covariance between two vectors of the random slopes is

$$\begin{aligned}
\operatorname{Cov}(\boldsymbol{\beta}_{1j}, \boldsymbol{\beta}_{1j'}) &= \lambda_1^2\lambda_2^2 \operatorname{Cov}\left(\frac{1}{p_j}\tilde{\mathbf{X}}_j^\top \mathbf{w}_j - \tilde{\mathbf{X}}^\top \mathbf{w}, \frac{1}{p_{j'}}\tilde{\mathbf{X}}_{j'}^\top \mathbf{w}_{j'} - \tilde{\mathbf{X}}^\top \mathbf{w}\right) \\
&= \psi\lambda_1^2\lambda_2^2 \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} - \frac{1}{p_j}\tilde{\mathbf{X}}_j^\top \tilde{\mathbf{X}}_j - \frac{1}{p_{j'}}\tilde{\mathbf{X}}_{j'}^\top \tilde{\mathbf{X}}_{j'}\right) \\
&= n\psi\lambda_1^2\lambda_2^2 \left(\mathbf{S} - \mathbf{S}_j - \mathbf{S}_{j'}\right).
\end{aligned}$$

Another quantity of interest is the covariance between the random intercepts and random slopes:

$$\begin{aligned}
\operatorname{Cov}(\beta_{0j}, \boldsymbol{\beta}_{1j}) &= \lambda_1\lambda_2^2 \operatorname{Cov}\left(\frac{1}{p_j}\mathbf{1}_{n_j}^\top \mathbf{w}_j - \mathbf{1}_n^\top \mathbf{w}, \frac{1}{p_j}\tilde{\mathbf{X}}_j^\top \mathbf{w}_j - \tilde{\mathbf{X}}^\top \mathbf{w}\right) \\
&= \psi\lambda_1\lambda_2^2 \left(\cancelto{0}{\mathbf{1}_n^\top \tilde{\mathbf{X}}} + \frac{1}{p_j^2}\mathbf{1}_{n_j}^\top \tilde{\mathbf{X}}_j - \frac{2}{p_j}\mathbf{1}_{n_j}^\top \tilde{\mathbf{X}}_j\right) \\
&= n\psi\lambda_1\lambda_2^2 \left(\left(\frac{1}{p_j} - 2\right)\frac{1}{n_j}\sum_{i=1}^{n_j}(\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})\right) \\
&= n\psi\lambda_1\lambda_2^2 \left(\frac{1}{p_j} - 2\right)(\bar{\mathbf{x}}^{(j)} - \bar{\mathbf{x}})
\end{aligned}$$

and

$$
\begin{aligned}
\operatorname{Cov}(\beta_{0j}, \boldsymbol{\beta}_{1j'}) &= \lambda_1\lambda_2^2 \operatorname{Cov}\left(\frac{1}{p_j}\mathbf{1}_{n_j}^\top \mathbf{w}_j - \mathbf{1}_n^\top \mathbf{w}, \frac{1}{p_{j'}} \tilde{\mathbf{X}}_{j'}^\top \mathbf{w}_{j'} - \tilde{\mathbf{X}}^\top \mathbf{w} \right) \\
&= \psi\lambda_1\lambda_2^2 \left(\cancelto{0}{\mathbf{1}_n^\top \tilde{\mathbf{X}}} + \frac{1}{p_j p_{j'}} \mathbf{1}_{n_j}^\top \cancelto{0}{\operatorname{Cov}(\mathbf{w}_j, \mathbf{w}_{j'})} \tilde{\mathbf{X}}_{j'} - \frac{1}{p_j}\mathbf{1}_{n_j}^\top \tilde{\mathbf{X}}_j - \frac{1}{p_{j'}}\mathbf{1}_{n_{j'}}^\top \tilde{\mathbf{X}}_{j'} \right) \\
&= n\psi\lambda_1\lambda_2^2 \left(-\frac{1}{n_j}\sum_{i=1}^{n_j} (\mathbf{x}_i^{(j)} - \bar{\mathbf{x}}) - \frac{1}{n_{j'}}\sum_{i=1}^{n_{j'}} (\mathbf{x}_i^{(j')} - \bar{\mathbf{x}}) \right) \\
&= n\psi\lambda_1\lambda_2^2 \left(2\bar{\mathbf{x}} - \bar{\mathbf{x}}^{(j)} - \bar{\mathbf{x}}^{(j')} \right).
\end{aligned}
$$

4.7.3 A recap on the exponential family EM algorithm

apx:expem

Consider the density function $p(\cdot|\boldsymbol{\theta})$ of the complete data $\mathbf{z} = \{\mathbf{y}, \mathbf{w}\}$, which depends on parameters $\boldsymbol{\theta} = (\theta_1, \dots, \theta_s)^\top \in \Theta \subseteq \mathbb{R}^s$, belonging to an exponential family of distributions. This density takes the form $p(\mathbf{z}|\boldsymbol{\theta}) = B(\mathbf{z}) \exp\big(\langle \boldsymbol{\eta}(\boldsymbol{\theta}), \mathbf{T}(\mathbf{z}) \rangle - A(\boldsymbol{\theta}) \big)$, where $\boldsymbol{\eta} : \mathbb{R}^s \mapsto \mathbb{R}$ is a link function, $\mathbf{T}(\mathbf{z}) = \big(T_1(\mathbf{z}), \dots, T_s(\mathbf{z}) \big)^\top \in \mathbb{R}^s$ are the sufficient statistics of the distribution, and $\langle \cdot, \cdot \rangle$ is the usual Euclidean dot product. It is often easier to work in the *natural parameterisation* of the exponential family distribution

$$
p(\mathbf{z}|\boldsymbol{\eta}) = B(\mathbf{z}) \exp\big(\langle \boldsymbol{\eta}, \mathbf{T}(\mathbf{z}) \rangle - A^*(\boldsymbol{\eta}) \big) \tag{4.18}
$$

{eq:pdfexpfamnat}

by defining $\boldsymbol{\eta} := \big(\eta_1(\boldsymbol{\theta}), \dots, \eta_r(\boldsymbol{\theta}) \big) \in \mathcal{E}$, and $\exp A^*(\boldsymbol{\eta}) = \int B(\mathbf{z}) \exp \langle \boldsymbol{\eta}, \mathbf{T}(\mathbf{z}) \rangle \, \mathrm{d}\mathbf{z}$ to ensure the density function normalises to one. As an aside, the set $\mathcal{E} := \big\{ \boldsymbol{\eta} = (\eta_1, \dots, \eta_s) \,|\, \int \exp A^*(\boldsymbol{\eta}) < \infty \big\}$ is called the *natural parameter space.* If $\dim \mathcal{E} = r < s = \dim \Theta$, then the the pdf belongs to the *curved exponential family* of distributions. If $\dim \mathcal{E} = r = s = \dim \Theta$, then the family is a *full exponential family.*

Assuming the latent $\mathbf{w}$ variables are observed and working with the natural parameterisation, then the complete maximum likelihood (ML) estimate for $\boldsymbol{\eta}$ is obtained by solving

$$
\frac{\partial}{\partial \boldsymbol{\eta}} \log p(\mathbf{z}|\boldsymbol{\eta}) = \mathbf{T}(\mathbf{z}) - \frac{\partial}{\partial \boldsymbol{\eta}} A^*(\boldsymbol{\eta}) = 0. \tag{4.19}
$$

{eq:expEM1}

Of course, the variable $\mathbf{w}$ are never observed, so the ML estimate for $\boldsymbol{\eta}$ can only be informed from what is observed. Let $p(\mathbf{y}|\boldsymbol{\eta}) = \int p(\mathbf{y}, \mathbf{w}|\boldsymbol{\eta}) \, \mathrm{d}\mathbf{w}$ represent the marginal density of the observations $\mathbf{y}$. Now, the ML estimate for $\boldsymbol\eta$ is obtained by solving

$$\begin{aligned}
\frac{\partial}{\partial\boldsymbol\eta}\log p(\mathbf{y}|\boldsymbol\eta) &= \frac{1}{p(\mathbf{y}|\boldsymbol\eta)} \cdot \frac{\partial}{\partial\boldsymbol\eta} p(\mathbf{y}|\boldsymbol\eta) \\
&= \frac{1}{p(\mathbf{y}|\boldsymbol\eta)} \cdot \frac{\partial}{\partial\boldsymbol\eta} \left(\int p(\mathbf{y},\mathbf{w}|\boldsymbol\eta) \, \mathrm{d}\mathbf{w} \right) \\
&= \frac{1}{p(\mathbf{y}|\boldsymbol\eta)} \cdot \int \left(\frac{\partial}{\partial\boldsymbol\eta} p(\mathbf{y},\mathbf{w}|\boldsymbol\eta) \right) \mathrm{d}\mathbf{w} \\
&= \frac{1}{p(\mathbf{y}|\boldsymbol\eta)} \cdot \int \left(p(\mathbf{y},\mathbf{w}|\boldsymbol\eta) \frac{\partial}{\partial\boldsymbol\eta} \log p(\mathbf{y},\mathbf{w}|\boldsymbol\eta) \right) \mathrm{d}\mathbf{w} \\
&= \int \left(\mathbf{T}(\mathbf{y},\mathbf{w}) - \frac{\partial}{\partial\boldsymbol\eta} A^*(\boldsymbol\eta) \right) p(\mathbf{w}|\mathbf{y},\boldsymbol\eta) \, \mathrm{d}\mathbf{w} \\
&= \mathrm{E}_{\mathbf{w}} \big[\mathbf{T}(\mathbf{y},\mathbf{w}) | \mathbf{y} \big] - \frac{\partial}{\partial\boldsymbol\eta} A^*(\boldsymbol\eta) \qquad (4.20)
\end{aligned}$$

{eq:expEM2}

equated to zero. Note that we are allowed to change the order of integration and differentation provided the integrand is continuously differentiable. So the only difference between the first order condition of (4.19) and that of (4.20) is that the sufficient statistics involving the unknown $\mathbf{w}$ are replaced by their conditional or posterior expectations.

A useful identity to know is that $\frac{\partial}{\partial\boldsymbol\eta} A^*(\boldsymbol\eta) = \mathrm{E}_{\mathbf{z}} \mathbf{T}(\mathbf{z})$ (Casella and R. L. Berger, 2002, Theorem 3.4.2 & Exercise 3.32(a)), which can be expressed in terms of the original parameters $\boldsymbol\theta$. As a consequence, solving for the ML estimate for $\boldsymbol\theta$ from the FOC equations (4.20) is possible without having to deal with the derivative of A^* with respect to the natural parameters. Having said this, an analytical solution in $\boldsymbol\theta$ may not exist, because the relationship of $\boldsymbol\theta$ could be implicit in the set of equations $\mathrm{E}_{\mathbf{w}} \big[\mathbf{T}(\mathbf{w},\mathbf{y}) | \mathbf{y}, \boldsymbol\theta \big] = \mathrm{E}_{\mathbf{y},\mathbf{w}} [\mathbf{T}(\mathbf{y},\mathbf{w})|\boldsymbol\theta]$. One way around this is to employ an iterative procedure, as detailed in Algorithm 2.

alg:EM3

Algorithm 2 Exponential family EM

```
initialise $\boldsymbol\theta^{(0)}$ and $t \leftarrow 0$
while not converged do
    E-step: $\tilde{\mathbf{T}}^{(t+1)}(\mathbf{y},\mathbf{w}) \leftarrow \mathrm{E}_{\mathbf{w}} \big[ \mathbf{T}(\mathbf{w},\mathbf{y}) | \mathbf{y}, \boldsymbol\theta^{(t)} \big]$
    M-step: $\boldsymbol\theta^{(t+1)} \leftarrow$ solution to $\tilde{\mathbf{T}}^{(t+1)}(\mathbf{y},\mathbf{w}) = \mathrm{E}_{\mathbf{y},\mathbf{w}} [\mathbf{T}(\mathbf{y},\mathbf{w})|\boldsymbol\theta]$
    $t \leftarrow t+1$
end while
```

To see how Algorithm 2 motivates the EM algorithm, consider the following argument. Recall that for the EM algorithm, the function $Q_t(\boldsymbol\eta) = \mathrm{E}_{\mathbf{w}}[\log p(\mathbf{y},\mathbf{w}|\boldsymbol\eta)|\mathbf{y},\boldsymbol\eta^{(t)}]$ is maximised at each iteration t. For exponential families of the form (4.18), the Q_t

function turns out to be

$$Q_t(\boldsymbol{\eta}) = \mathrm{E}_{\mathbf{w}} \left[\langle \boldsymbol{\eta}, \mathbf{T}(\mathbf{z}) \rangle | \mathbf{y}, \boldsymbol{\eta}^{(t)} \right] - A^*(\boldsymbol{\eta}) + \log B(\mathbf{z}),$$

and this is maximised at the value of $\boldsymbol{\eta}$ satisfying

$$\frac{\partial}{\partial \boldsymbol{\eta}} Q_t(\boldsymbol{\eta}) = \mathrm{E}_{\mathbf{w}} \left[\mathbf{T}(\mathbf{y}, \mathbf{w}) | \mathbf{y}, \boldsymbol{\eta}^{(t)} \right] - \frac{\partial}{\partial \boldsymbol{\eta}} A^*(\boldsymbol{\eta}) = 0,$$

a similar condition to (4.20) when obtaining ML estimate of $\boldsymbol{\eta}$. Thus, Q_t is maximised by the solution to line 4 in Algorithm Algorithm 2.

4.7.4 A brief introduction to Hamiltonian Monte Carlo

misc:hmc

Hamiltonian Monte Carlo had its beginnings in statistical physics, with the 1987 paper by Duane et al. using what they called 'Hybrid Monte Carlo' in lattice models of quantum theory. Their work merged the approaches of molecular dynamics and Markov chain Monte Carlo methods. As interesting side note, their method abbreviates also to 'HMC', but throughout the statistical literature, it is more commonly referred to by its more descriptive name Hamiltonian Monte Carlo. Incidentally, the use of HMC started with applications to neural networks as early as 1996 (see Neal et al. (2011) for an excellent review of the subject matter). It was not until 2011 when active development of the method, and in particular, software for for statistical applications began. The Stan initiative (Carpenter et al., 2017) began in response to difficulties faced when performing full Bayesian inference on multilevel generalised linear models. These difficulties mainly involved poor efficiency in usual MCMC samplers, particularly high autocorrelations in the posterior chains, which meant that many chains and many iterations were required to get an adequate sample. It was a case of exhausting all possible algorithmic remedies for existing samplers (Gibbs samplers, Metropolis samplers, etc.), and realising that fundamentally not much improvement can be had unless a novel sampling technique was discovered.

The basic idea behind HMC is to use Hamiltonian dynamics to propose new states in the posterior sampling, rather than relying on 'random walks'. If one were to understand and use the geometry of the posterior density to one's benefit, then it should be possible to generate new proposal states with high probabilities of acceptance and move far away from the current state. Hamiltonian dynamics, like classical Newtonian mechanics, provides a framework for modelling the motion of a body in space across time t. Additionally, Hamiltonian dynamics concatenates the position vector x with its momentum z, and the motion of x in d-dimensional space is then described through Hamilton's equations

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial H}{\partial z} \quad \text{and} \quad \frac{\mathrm{d}z}{\mathrm{d}t} = -\frac{\partial H}{\partial x}, \tag{4.21}$$

{eq:hamilton1}

where $H = H(x,z)$ is called the Hamiltonian of the system. The Hamiltonian is an operator which encapsulates the total energy of the system. In a closed system, one can express the sum of operators corresponding to the kinetic energy $K(p)$ and the potential energy $U(z)$ of the system

$$H(x,z) = K(z) + U(x). \tag{4.22}$$

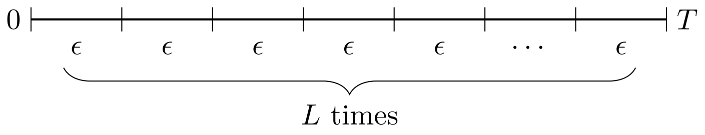
{eq:hamilton2}

Substituing (4.22) into (4.21), we get the system of partial differential equations (PDEs)

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial}{\partial z}K(z) \quad \text{and} \quad \frac{\mathrm{d}z}{\mathrm{d}t} = -\frac{\partial}{\partial x}U(x). \tag{4.23}$$

{eq:hamilton3}

To describe the evolution of $\big(x(t), z(t)\big)$ from time t to $t+T$, it is necessary to discretise time, and split $T = L\epsilon$. The quantity L is known as the number of *leapfrogs*, and ϵ the *step size*.



The system of PDEs is solved using Euler's method, or the more commonly used leapfrog integration, which is a three-step process:

1. **Half-step momentum.** $z(t + \epsilon/2) = z(t) - \frac{\epsilon}{2}\frac{\partial}{\partial x}U\big(x(t)\big)$
2. **Full-step position.** $x(t + \epsilon) = x(t) + \epsilon\frac{\partial}{\partial z}K\big(z(t + \epsilon/2)\big)$
3. **Half-step momentum.** $z(t + \epsilon) = z(t + \epsilon/2) = z(t) - \frac{\epsilon}{2}\frac{\partial}{\partial x}U\big(x(t)\big)$

in which steps 1–3 are repeated L times.

Having knowing the formula for how particles move in space, we can use this information to treat random points drawn from some probability density as 'particles'. Randomness of position and momentum are prescribed through probability densities on each. Given some energy function $E(\theta)$ over states θ, the *canonical distribution* of the states θ (otherwise known as the *canonical ensemble*) is given by the probability density function

$$p(\theta) \propto \exp\left(-\frac{E(\theta)}{k\tau}\right),$$

where k is Boltzmann's constant, τ is the absolute temperature of the system. The Hamiltonian is one such energy function over states (x, z). By replacing $E(\theta)$ by (4.22) in the pdf above, we realise that the distribution for x and z are independent. The system can be manipulated such that $k\tau = 1$—in any case, these are constants which can be absorbed into one of the terms in the pdf anyway.

Using a *quadratic kinetic energy* function $K(z) = z^\top M^{-1} z/2$[6], we find that the probability density function for z is

$$p(z) \propto \exp\left(-\frac{1}{2} z^\top M^{-1} z\right),$$

implying $z \sim \mathrm{N}_d(0, M)$. Here, $M = \operatorname{diag}(m_1, \dots, m_d)$ is called the *mass matrix*, which obviously serves as the variance for the randomly distributed z. As for the potential energy, choose a function such that $U(x) = -\log p(x)$, implying $p(x) \propto \exp\big(-U(x)\big)$. Here, $p(x)$ represents the target density from which we wish to sample, for instance, a posterior density of interest. Thus, to sample variables x from $p(x)$, one artificially introduces momentum variables z and sample jointly instead from $p(x, z) = p(z)p(z)$, and discarding z thereafter. The HMC algorithm is summarised in Algorithm 3.

alg:hmc

Algorithm 3 Hamiltonian Monte Carlo

```
initialise $x^{(0)}$, $z^{(0)}$ and choose values for $L$, $\epsilon$ and $M$
while not converged do
    Draw $z \sim \mathrm{N}_d(0, M)$                                   ▷ Perturb momentum
    Move $(x^{(t)}, z^{(t)}) \mapsto (x^*, z^*)$ using Hamiltonian dynamics   ▷ Proposal state
    Accept/reject proposal state, i.e.                               ▷ Metropolis update
        $$(x^{(t+1)}, z^{(t+1)}) \leftarrow \begin{cases} (x^*, z^*) & \text{w.p. } \min(1, A) \\ (x^{(t)}, z^{(t)}) & \text{otherwise} \end{cases}$$
    where
        $$A = \frac{p(x^*, z^*)}{(x^{(t)}, z^{(t)})} = \exp\Big(H(x, z) - H(x^{(t)}, z^{(t)})\Big)$$
end while
return Samples $\big\{x^{(t)} \,|\, t = 1, 2, \dots\big\}$
```

HMC is often times superior to standard Gibbs sampling, for a variety of reasons. For one, conjugacy does not play any role in the efficiency of the HMC sampler, thus freeing the modeller to choose more appropriate and more intuitive prior densities for the parameters of the model. For another, the HMC sampler is designed to incite little autocorrelations between samples, and thus increasing efficiency.

Several drawbacks do exist with the HMC sampler. Firstly, it is impossible to directly sample from discrete distributions $p(x)$. More concretely, HMC requires that the domain of $p(x)$ is continuous and that $\partial \log p(x)/\partial x$ is inexpensive to compute. To work around this, one must reformulate the model by marginalising out the discrete variables, and obtain them back later by separately sampling from their posteriors. Alternatively, a Gibbs sampler specifically for the discrete variables could be augmented with the HMC sampler. The other drawback of HMC is that there are many tuning parameters (leapfrog L, step-size ϵ, mass matrix M, etc.) that is not immediately easy to perfect, at least not to the novice user.

The implementation of HMC by the programming language Stan, which interfaces many other programming languages including R, Python, MATLAB, Julia, Stata and Mathematica, is a huge step forward in computational Bayesian analysis. Stan takes the liberty of performing all the tuning necessary, and the practitioner is left with simply specifying the model. A vast library of differentiable probability functions are available, with the ability to bring your own code as well. Development is very active and many improvements and optimisations have been made since its inception.

[6] Thinking back to elementary mechanics, this is the familiar $\frac{1}{2}mv^2$ formula for kinetic energy and substituting in the identity $z = mv$, where m is the mass of the object, and v is its velocity.

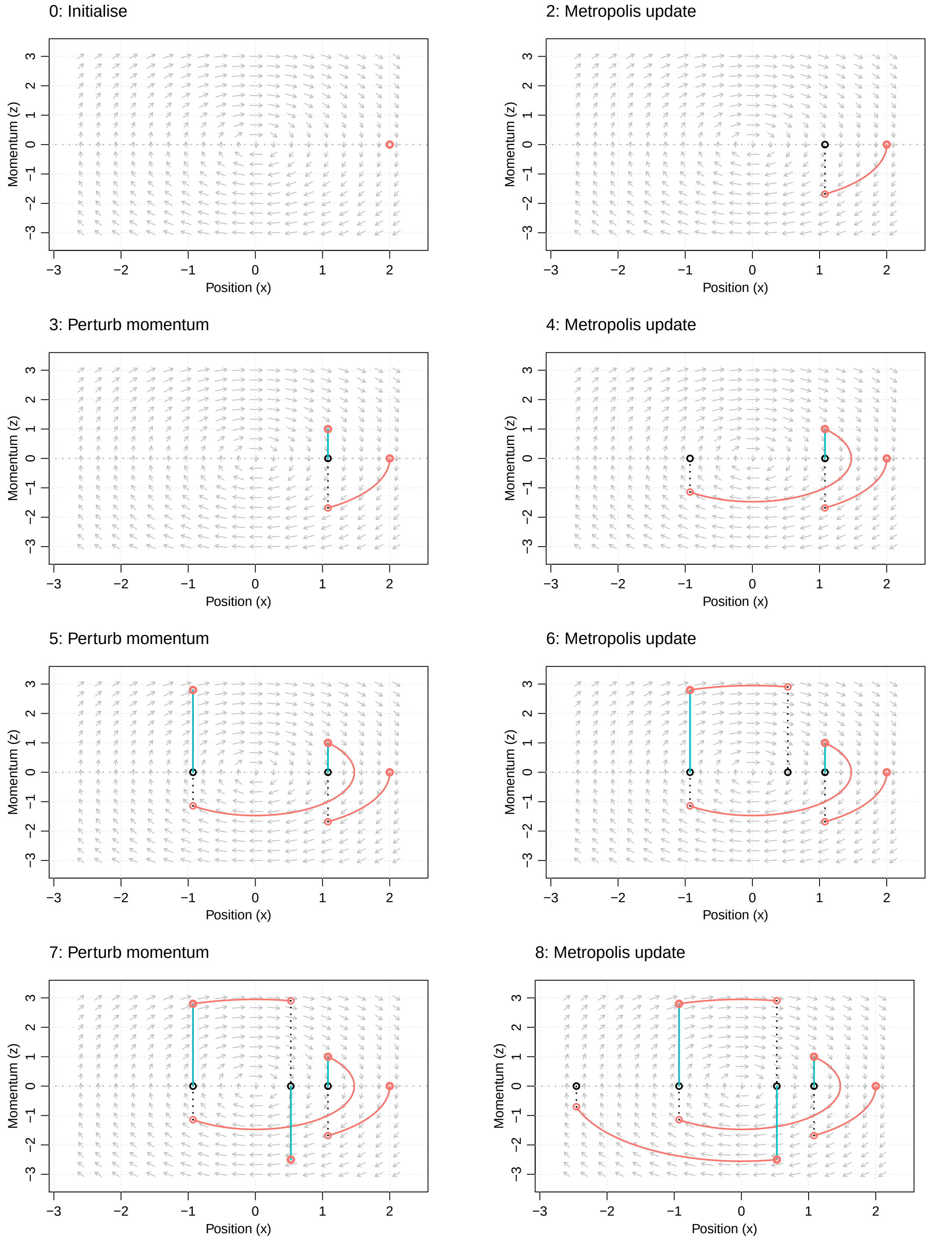


Figure 4.10: A phase diagram schematic of HMC sampling in one-dimension. At step 0, initialise values for momentum and position. At step 1, simulate movement using Hamiltonian dynamics, accept position and discard momentum. At step 2, perturb momentum using a normal density, then repeat.

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Appendix A

Regression modelling using I-priors

A.1 Deriving the posterior distribution for $\mathbf{w}$

apx:posteriorw

In the following derivation, we implicitly assume the dependence on $\mathbf{f}_0$ and θ. The distribution of $\mathbf{y}|\mathbf{w}$ is $\mathrm{N}_n(\boldsymbol{\alpha}+\mathbf{f}_0+\mathbf{H}_\eta\mathbf{w}, \boldsymbol{\Psi}^{-1})$, where $\boldsymbol{\alpha} = \alpha\mathbf{1}_n$, while the prior distribution for $\mathbf{w}$ is $\mathrm{N}_n(\mathbf{0}, \boldsymbol{\Psi})$. Since $p(\mathbf{w}|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{w})p(\mathbf{w})$, we have that

$$\begin{aligned}
\log p(\mathbf{w}|\mathbf{y}) &= \log p(\mathbf{y}|\mathbf{w}) + \log p(\mathbf{w}) \\
&= \text{const.} + \cancel{\frac{1}{2}\log|\boldsymbol{\Psi}|} - \frac{1}{2}(\mathbf{y} - \boldsymbol{\alpha} - \mathbf{f}_0 - \mathbf{H}_\eta\mathbf{w})^\top \boldsymbol{\Psi}(\mathbf{y} - \boldsymbol{\alpha} - \mathbf{f}_0 - \mathbf{H}_\eta\mathbf{w}) \\
&\qquad - \cancel{\frac{1}{2}\log|\boldsymbol{\Psi}|} - \frac{1}{2}\mathbf{w}^\top\boldsymbol{\Psi}^{-1}\mathbf{w} \\
&= \text{const.} - \frac{1}{2}\mathbf{w}^\top(\mathbf{H}_\eta\boldsymbol{\Psi}\mathbf{H}_\eta + \boldsymbol{\Psi}^{-1})\mathbf{w} + (\mathbf{y} - \boldsymbol{\alpha} - \mathbf{f}_0)^\top\boldsymbol{\Psi}\mathbf{H}_\eta\mathbf{w}.
\end{aligned}$$

Setting $\mathbf{A} = \mathbf{H}_\eta\boldsymbol{\Psi}\mathbf{H}_\eta + \boldsymbol{\Psi}^{-1}$, $\mathbf{a}^\top = (\mathbf{y} - \boldsymbol{\alpha} - \mathbf{f}_0)^\top\boldsymbol{\Psi}\mathbf{H}_\eta$, and using the fact that

$$\mathbf{w}^\top\mathbf{A}\mathbf{w} - 2\mathbf{a}^\top\mathbf{w} = (\mathbf{w} - \mathbf{A}^{-1}\mathbf{a})^\top\mathbf{A}(\mathbf{w} - \mathbf{A}^{-1}\mathbf{a}),$$

we have that $\mathbf{w}|\mathbf{y}$ is normally distributed with the required mean and variance.

Alternatively, one could have shown this using standard results of multivariate normal distributions. Noting that the covariance between $\mathbf{y}$ and $\mathbf{w}$ is

$$\begin{aligned}\operatorname{Cov}(\mathbf{y},\mathbf{w}) &= \operatorname{Cov}(\boldsymbol{\alpha}+\mathbf{f}_0+\mathbf{H}_\eta\mathbf{w}+\boldsymbol{\epsilon},\mathbf{w}) \\ &= \mathbf{H}_\eta\operatorname{Cov}(\mathbf{w},\mathbf{w}) \\ &= \mathbf{H}_\eta\boldsymbol{\Psi}\end{aligned}$$

and that $\operatorname{Cov}(\mathbf{w},\mathbf{y}) = \boldsymbol{\Psi}\mathbf{H}_\eta = \mathbf{H}_\eta\boldsymbol{\Psi} = \operatorname{Cov}(\mathbf{y},\mathbf{w})$ by symmetry, the joint distribution $(\mathbf{y},\mathbf{w})$ is

$$\begin{pmatrix}\mathbf{y}\\ \mathbf{w}\end{pmatrix} \sim \mathrm{N}_{n+n}\left(\begin{pmatrix}\boldsymbol{\alpha}+\mathbf{f}_0\\ \mathbf{0}\end{pmatrix}, \begin{pmatrix}\mathbf{V}_y & \mathbf{H}_\eta\boldsymbol{\Psi}\\ \mathbf{H}_\eta\boldsymbol{\Psi} & \boldsymbol{\Psi}\end{pmatrix}\right).$$

Thus,

$$\begin{aligned}\mathrm{E}[\mathbf{w}|\mathbf{y}] &= \mathrm{E}\,\mathbf{w} + \operatorname{Cov}(\mathbf{w},\mathbf{y})(\operatorname{Var}\mathbf{y})^{-1}(\mathbf{y}-\mathrm{E}\,\mathbf{y}) \\ &= \mathbf{H}_\eta\boldsymbol{\Psi}\mathbf{V}_y^{-1}(\mathbf{y}-\boldsymbol{\alpha}-\mathbf{f}_0),\end{aligned}$$

and

$$\begin{aligned}\operatorname{Var}[\mathbf{w}|\mathbf{y}] &= \operatorname{Var}\mathbf{w} - \operatorname{Cov}(\mathbf{w},\mathbf{y})(\operatorname{Var}\mathbf{y})^{-1}\operatorname{Cov}(\mathbf{y},\mathbf{w}) \\ &= \boldsymbol{\Psi} - \mathbf{H}_\eta\boldsymbol{\Psi}\mathbf{V}_y^{-1}\mathbf{H}_\eta\boldsymbol{\Psi} \\ &= \boldsymbol{\Psi} - \boldsymbol{\Psi}\mathbf{H}_\eta\left(\boldsymbol{\Psi}^{-1}+\mathbf{H}_\eta\boldsymbol{\Psi}\mathbf{H}_\eta\right)^{-1}\mathbf{H}_\eta\boldsymbol{\Psi} \\ &= \left(\boldsymbol{\Psi}^{-1}+\mathbf{H}_\eta\boldsymbol{\Psi}\mathbf{H}_\eta\right)^{-1} \\ &= \mathbf{V}_y^{-1}\end{aligned}$$

as a direct consequence of the Woodbury matrix identity.

A.2 Deriving the posterior predictive distribution

apx:postpred

A priori, assume that $y_{\text{new}} \sim \mathrm{N}(\hat\alpha, v_{\text{new}})$, where $v_{\text{new}} = \mathbf{h}_{\hat\eta}(x_{\text{new}})^\top\hat{\boldsymbol{\Psi}}\mathbf{h}_{\hat\eta}(x_{\text{new}}) + \psi_{\text{new}}^{-1}$. Consider the joint distribution of $(y_{\text{new}},\mathbf{y}^\top)^\top$, which is multivariate normal (since both y_{new} and $\mathbf{y}$ are. Write

$$\begin{pmatrix}y_{\text{new}}\\ \mathbf{y}\end{pmatrix} \sim \mathrm{N}_{n+1}\left(\begin{pmatrix}\hat\alpha\\ \hat\alpha\mathbf{1}_n\end{pmatrix}, \begin{pmatrix}v_{\text{new}} & \operatorname{Cov}(y_{\text{new}},\mathbf{y})\\ \operatorname{Cov}(y_{\text{new}},\mathbf{y})^\top & \tilde{\mathbf{V}}_y\end{pmatrix}\right),$$

where

$$
\begin{aligned}
\operatorname{Cov}(y_{\text{new}}, \mathbf{y}) &= \operatorname{Cov}(f_{\text{new}} + \epsilon_{\text{new}}, \mathbf{f} + \boldsymbol{\epsilon}) \\
&= \operatorname{Cov}(f_{\text{new}}, \mathbf{f}) + \operatorname{Cov}(\epsilon_{\text{new}}, \boldsymbol{\epsilon}) \\
&= \operatorname{Cov}\Big(\mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \tilde{\mathbf{w}}, \mathbf{H}_{\tilde\eta}\tilde{\mathbf{w}}\Big) + (\sigma_{\text{new},1}, \dots, \sigma_{\text{new},n}) \\
&= \mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \hat{\boldsymbol{\Psi}} \mathbf{H}_{\tilde\eta} + \boldsymbol{\sigma}_{\text{new}}.
\end{aligned}
$$

The vector of covariances $\boldsymbol{\sigma}_{\text{new}}$ between observations $y_1, \dots, y_n$ and the predicted point y_{new} would need to be prescribed a priori (treated as extra parameters), or estimated again, which seems excessive. Assuming $\boldsymbol{\sigma}_{\text{new}} = \mathbf{0}$ would be acceptable, especially under an iid assumption the error precisions. In any case, using standard multivariate normal results, we get that $y_{\text{new}}|\mathbf{y}$ is also normally distributed with mean

$$
\begin{aligned}
E[y_{\text{new}}|\mathbf{y}] &= \hat\alpha + (\mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \hat{\boldsymbol{\Psi}} \mathbf{H}_{\tilde\eta} + \boldsymbol{\sigma}_{\text{new}}) \tilde{\mathbf{V}}_y^{-1} \tilde{\mathbf{y}} \\
&= \hat\alpha + \mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \overbrace{\mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \hat{\boldsymbol{\Psi}} \mathbf{H}_{\tilde\eta} \tilde{\mathbf{V}}_y^{-1} \tilde{\mathbf{y}}}^{\hat{\mathrm{w}}} + \boldsymbol{\sigma}_{\text{new}} \tilde{\mathbf{V}}_y^{-1} \tilde{\mathbf{y}} \\
&= \hat\alpha + \mathrm{E}\left[f(x_{\text{new}})|\mathbf{y}\right] + \text{mean correction term}
\end{aligned}
$$

and variance

$$
\begin{aligned}
\operatorname{Var}[y_{\text{new}}|\mathbf{y}] &= v_{\text{new}} - (\mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \hat{\boldsymbol{\Psi}} \mathbf{H}_{\tilde\eta} + \boldsymbol{\sigma}_{\text{new}}) \tilde{\mathbf{V}}_y^{-1} (\mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \hat{\boldsymbol{\Psi}} \mathbf{H}_{\tilde\eta} + \boldsymbol{\sigma}_{\text{new}})^\top \\
&= \mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \hat{\boldsymbol{\Psi}} \hat{\mathbf{h}}_{\hat\eta}(x_{\text{new}}) + \psi_{\text{new}}^{-1} - \mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \hat{\boldsymbol{\Psi}} \mathbf{H}_{\tilde\eta} \tilde{\mathbf{V}}_y^{-1} \mathbf{H}_{\tilde\eta} \hat{\boldsymbol{\Psi}} \mathbf{h}_{\hat\eta}(x_{\text{new}}) \\
&\qquad + \text{variance correction term} \\
&= \mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \big(\hat{\boldsymbol{\Psi}} - \hat{\boldsymbol{\Psi}} \mathbf{H}_{\tilde\eta} \tilde{\mathbf{V}}_y^{-1} \mathbf{H}_{\tilde\eta} \hat{\boldsymbol{\Psi}}\big) \mathbf{h}_{\hat\eta}(x_{\text{new}}) + \psi_{\text{new}}^{-1} \\
&\qquad + \text{variance correction term} \\
&= \mathbf{h}_{\hat\eta}(x_{\text{new}})^\top \hat{\mathbf{V}}_y^{-1} \mathbf{h}_{\hat\eta}(x_{\text{new}}) + \psi_{\text{new}}^{-1} + \text{variance correction term} \\
&= \operatorname{Var}\left[f(x_{\text{new}})|\mathbf{y}\right] + \psi_{\text{new}}^{-1} + \text{variance correction term.}
\end{aligned}
$$

A.3 Derivation of the Fisher information for multivariate normal distributions

apx:fishermultinormal

Let $X \sim \mathrm{N}_p(0, \Sigma_\theta)$, that is, the covariance matrix Σ_θ depends on a real, q-dimensional vector θ. Define the derivative of a matrix $\Sigma \in \mathbb{R}^{p \times p}$ with respect to a scalar z, denoted $\partial\Sigma/\partial z \in \mathbb{R}^{p\times p}$, by $(\partial\Sigma/\partial z)_{ij} = \partial\Sigma_{ij}/\partial z$, i.e. derivatives are taken elementwise. The two identities below are useful:

$$\frac{\partial}{\partial z}\operatorname{tr}\Sigma = \operatorname{tr}\frac{\partial\Sigma}{\partial z} \tag{A.1}$$

$$\frac{\partial}{\partial z}\log|\Sigma| = \operatorname{tr}\left(\Sigma^{-1}\frac{\partial\Sigma}{\partial z}\right) \tag{A.2}$$

$$\frac{\partial\Sigma^{-1}}{\partial z} = -\Sigma^{-1}\frac{\partial\Sigma}{\partial z}\Sigma^{-1} \tag{A.3}$$

A useful reference for these identities is Petersen, Pedersen, et al. (2008).

Taking derivative of the log-likelihood for θ with respect to the i'th component yields

$$\begin{aligned}\frac{\partial}{\partial\theta_i}L(\theta|X) &= -\frac{1}{2}\frac{\partial}{\partial\theta_i}\log|\Sigma_\theta| - \frac{1}{2}\frac{\partial}{\partial\theta_i}\operatorname{tr}(\Sigma_\theta^{-1}XX^\top) \\ &= -\frac{1}{2}\operatorname{tr}\left(\Sigma_\theta^{-1}\frac{\partial\Sigma_\theta}{\partial\theta_i}\right) - \frac{1}{2}\operatorname{tr}\left(\frac{\partial\Sigma_\theta^{-1}}{\partial\theta_i}XX^\top\right) \\ &= -\frac{1}{2}\operatorname{tr}\left(\Sigma_\theta^{-1}\frac{\partial\Sigma_\theta}{\partial\theta_i} - \Sigma_\theta^{-1}\frac{\partial\Sigma_\theta}{\partial\theta_i}\Sigma_\theta^{-1}XX^\top\right).\end{aligned}$$

Taking derivatives again, this time with respect to θ_j, we get

$$\begin{aligned}\frac{\partial^2}{\partial\theta_i\theta_j}L(\theta|X) &= -\frac{1}{2}\frac{\partial}{\partial\theta_j}\operatorname{tr}\left(\Sigma_\theta^{-1}\frac{\partial\Sigma_\theta}{\partial\theta_i} - \Sigma_\theta^{-1}\frac{\partial\Sigma_\theta}{\partial\theta_i}\Sigma_\theta^{-1}XX^\top\right) \\ &= -\frac{1}{2}\operatorname{tr}\bigg(\frac{\partial\Sigma_\theta^{-1}}{\partial\theta_j}\frac{\partial\Sigma_\theta}{\partial\theta_i} + \Sigma_\theta^{-1}\frac{\partial^2\Sigma_\theta}{\partial\theta_i\theta_j} - \frac{\partial\Sigma_\theta^{-1}}{\partial\theta_j}\frac{\partial\Sigma_\theta}{\partial\theta_i}\Sigma_\theta^{-1}XX^\top \\ &\qquad\qquad - \Sigma_\theta^{-1}\frac{\partial^2\Sigma_\theta}{\partial\theta_i\theta_j}\Sigma_\theta^{-1}XX^\top - \Sigma_\theta^{-1}\frac{\partial\Sigma_\theta}{\partial\theta_i}\frac{\partial\Sigma_\theta^{-1}}{\partial\theta_j}XX^\top\bigg).\end{aligned}$$

The Fisher information matrix U contains (i,j) entries equal to the expectation of $-\frac{\partial^2}{\partial\theta_i\theta_j}L(\theta|X)$. Using the fact that 1) $\mathrm{E}[\operatorname{tr}\Sigma] = \operatorname{tr}(\mathrm{E}\,\Sigma)$, 2) $\mathrm{E}[XX^\top] = \Sigma_\theta$; and 3) the trace is invariant under cyclic permutations, we get

$$\begin{aligned}
U_{ij} &= \frac{1}{2}\operatorname{tr}\left(\cancel{\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j}\frac{\partial \Sigma_\theta}{\partial \theta_i}} + \cancel{\Sigma_\theta^{-1}\frac{\partial^2 \Sigma_\theta}{\partial \theta_i \theta_j}} - \cancel{\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j}\frac{\partial \Sigma_\theta}{\partial \theta_i}} - \cancel{\Sigma_\theta^{-1}\frac{\partial^2 \Sigma_\theta}{\partial \theta_i \theta_j}} - \frac{\partial \Sigma_\theta}{\partial \theta_i}\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j} \right) \\
&= \frac{1}{2}\operatorname{tr}\left(\Sigma_\theta^{-1}\frac{\partial \Sigma_\theta}{\partial \theta_i}\Sigma_\theta^{-1}\frac{\partial \Sigma_\theta}{\partial \theta_j} \right)
\end{aligned}$$

as required.

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