Gaussian Process Regression in the Flat Limit

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January 11, 2022

Abstract

Gaussian process (GP) regression is a fundamental tool in Bayesian statistics. It is also known as kriging and is the Bayesian counterpart to the frequentist kernel ridge regression. Most of the theoretical work on GP regression has focused on a large-\(n\) asymptotics, characterising the behaviour of GP regression as the amount of data increases. Fixed-sample analysis is much more difficult outside of simple cases, such as locations on a regular grid.

In this work we perform a fixed-sample analysis that was first studied in the context of approximation theory by Driscoll & Fornberg (2002), called the “flat limit”. In flat-limit asymptotics, the goal is to characterise kernel methods as the length-scale of the kernel function tends to infinity, so that kernels appear flat over the range of the data. Surprisingly, this limit is well-defined, and displays interesting behaviour: Driscoll & Fornberg showed that radial basis interpolation converges in the flat limit to polynomial interpolation, if the kernel is Gaussian. Subsequent work showed that this holds true in the multivariate setting as well, but that kernels other than the Gaussian may have (polyharmonic) splines as the limit interpolant.

Leveraging recent results on the spectral behaviour of kernel matrices in the flat limit, we study the flat limit of Gaussian process regression. Results show that Gaussian process regression tends in the flat limit to (multivariate) polynomial regression, or (polyharmonic) spline regression, depending on the kernel. Importantly, this holds for both the predictive mean and the predictive variance, so that the posterior predictive distributions become equivalent.

For the proof, we introduce the notion of prediction-equivalence of semi-parametric models, which lets us state flat-limit results in a compact and unified manner. Our results have practical consequences: for instance, they show that optimal GP predictions in the sense of leave-one-out loss may occur at very large length-scales, which would be invisible to current implementations because of numerical difficulties.

Gaussian processes are a cornerstone of modern Bayesian methods, used almost wherever one may require nonparametric priors. Quite naturally, the theory of Gaussian Process methods is well-developed. Aside from limited special cases in which Fourier analysis is applicable, GP-based methods have mostly been studied under large-\(n\) asymptotics (see, e.g. [30, 25, 34]), which involve treating measurement locations as random and letting their number go to infinity. In this paper we report intriguing theoretical results obtained under a different asymptotic, one that treats the data as fixed, rather than random, with fixed sample size. The limit we look at is the so-called “flat limit”, pioneered by [8] in 2002. The flat limit consists in letting the spatial width of the kernel function go to infinity, which results in the covariance function becoming flat over the range of the data.

Studying Gaussian processes under the flat limit may seem at first sight to be entirely pointless - does that not correspond to a prior that contains only flat functions? The answer is no, because covariance functions have a second hyperparameter that sets the vertical scale (pointwise variance). When one lets pointwise variance grow as the covariance becomes wider, the actual function space spanned by Gaussian processes remains interesting and useful. In the cases studied here, they are (multivariate) polynomials and (polyharmonic) splines.

A first hint that such would be the case was obtained in [8], where Driscoll & Fornberg examined Radial Basis Function interpolation in the flat limit, a popular method in approximation theory that corresponds to noiseless GP regression. Driscoll & Fornberg found that under certain conditions, the RBF interpolant tends to the Lagrange polynomial interpolant in the flat limit. The result is very
surprising, since the RBF interpolation problem may seem at first sight to become ill-defined in the flat limit. Subsequent papers generalised this result to multivariate interpolation \[17\], and finitely-smooth kernels \[31\]. Our contribution can be seen as an extension of these results, since RBF interpolation features as a special case.

Further evidence that GPs may be interesting in the flat limit comes from the study of the spectrum and eigenvectors of kernel matrices performed in \[3\]. The full story is complicated, but the key phenomenon is that the eigenvectors of kernel matrices tend in the flat limit to orthogonal multivariate polynomials or polyharmonic spline bases. Based on these results, we have been able to study the flat limit of determinantal point processes (DPPs), a type of point process that is in some sense dual to Gaussian processes \[4\].

To give some highlights, we show the following:

1. GP regression tends in the flat limit to either polynomial regression or (polyharmonic) spline regression
2. Which it is depends on the smoothness of the kernel, and on the amount of regularisation enforced by the prior
3. The specific kernel has only a minor influence on the limit, influencing only the part of the function space that is most heavily regularised.
4. There is nothing in theory that prevents the optimal GP model (according to hyperparameter selection criteria) from being arbitrarily close to the flat limit. Such solutions are invisible in practice because of numerical issues, or because they are obscured by a nugget term.
5. In some cases, we show empirically that the flat limit is a good approximation for GP regression even when the actual kernel is far from flat

We shall now introduce our results informally, by way of a few pictures. Fig. 1 shows a synthetic dataset, fitted using various methods. A very classical way of fitting such data is to use polynomials, which results in the curves on panel (a). Another classical way is to use smoothing splines, which results in panel (c), where the different curves correspond to different values of the regression parameter. A more modern way of producing a fit is to use a Gaussian process. Gaussian process regression requires a covariance function, which determines the behaviour of the fit. The ever-popular Gaussian or “squared-exponential” covariance function is

\[
\kappa_\varepsilon(x, y) = \gamma \exp \left(-\varepsilon^2 \|x - y\|^2\right)
\]  

where \(x\) and \(y\) are two points in \(\mathbb{R}^d\). In this definition \(\gamma\) and \(\varepsilon\) are hyperparameters. \(\varepsilon\) sets the horizontal scale (the width of the Gaussian), and \(\gamma\) sets the vertical scale (its height). For a fixed value of \(\varepsilon\), changing the value of \(\gamma\) produces different fits. Increasing \(\gamma\) increases the degrees of freedom, resulting in a tighter fit to the data. Decreasing \(\gamma\) decreases the degrees of freedom, as \(\gamma \to 0\) the fit goes to a horizontal line at 0. Panel (b) shows the fits for a few different values of \(\gamma\), for a fixed value of \(\varepsilon = 0.5\). Panel (d) is the same, but for a different covariance function, specifically one in the Matérn family, which has the property of being only once differentiable at 0. For reasons that cannot be succinctly explained, differentiability of the kernel function plays a large role – see \[3\].

Our analysis consists in letting \(\varepsilon \to 0\), making the covariance functions “flat” over the range of the data. One outcome is that in the flat limit, to put things very roughly, panel (a) \(\approx\) panel (b) and panel(c) \(\approx\) panel (d). The next set of figures should explain this a bit better. For a given value of \(\varepsilon\) and \(\gamma\), the fit produced by a Gaussian process is a function from (in this case) \([0, 1]\) to \(\mathbb{R}\). Call it \(f_{\varepsilon, \gamma}(x)\). If we leave \(\varepsilon\) fixed and vary \(\gamma\), we obtain a family of functions \(F_\varepsilon = \{f_{\varepsilon, \gamma} | \gamma \in \mathbb{R}^+\}\). Panel (b) shows a few elements from \(F_\varepsilon\) for the Gaussian kernel. A polynomial fit is another function from \([0, 1]\) to \(\mathbb{R}\), this time parameterised by the degree of the polynomial. Call \(p_r(x)\) the polynomial fit of degree \(r\). An implication of our results (theorem \[4.2\]) is that as \(\varepsilon \to 0\) the set \(F_\varepsilon\) intersects (goes through) the polynomial fits.
Figure 1: Various fits of the same data. a. Polynomials of degree 0 to 3. b. Gaussian process regression, with a Gaussian kernel, $\varepsilon = 0.5$ and different values of $\gamma$ (see text). c. Quadratic smoothing splines. d. GP regression, with a Matérn kernel (see text).
Figure 2: Predictions at $x = 0.2$ and $x = 0.8$ from different models. The numbered dots correspond to the polynomial fits with degree 0 to 6. The continuous curves are the predictions from GP regression with Gaussian kernel, fixing $\varepsilon$ but letting $\gamma$ vary. We show the two limits $\gamma \to 0$ and $\gamma \to \infty$, which correspond respectively to a maximally penalised fit and to a minimally constrained one (an interpolation). The two individual curves are for two different values of $\varepsilon$. Theorem 4.2 states that as $\varepsilon \to 0$ the continuous curve goes through the blue dots in a piecewise linear manner.

This is best understood graphically. We cannot plot $F_\varepsilon$, but we can plot the following: we choose two locations on the x-axis (at $x_a = 0.2$ and $x_b = 0.8$), and plot the value of the fit at these locations. For fixed $\varepsilon$, we can think of the pair $(\hat{f}_{\varepsilon,\gamma}(x_a), \hat{f}_{\varepsilon,\gamma}(x_b))$ as a parametric curve in $\mathbb{R}^2$, parameterised by $\gamma$. The curves on fig. 2 are two such parametric curves, for the Gaussian kernel and two different values of $\varepsilon$. The predictions of the polynomial fits at $x_a$ and $x_b$ are just a set of points in $\mathbb{R}^2$. What theorem 4.2 implies is that as $\varepsilon \to 0$, the parametric curves will go through each polynomial fit (and more than that, interpolate linearly between these points).

For the Matérn kernel, following again theorem 4.2, the comparison should be to another parametric curve, corresponding to the smoothing splines for all possible values of the regularisation parameter. Barring very high values of $\gamma$ (for which the behaviour of the GP becomes polynomial), the GP fit should behave like a spline and therefore tend to the parametric curve produced by the smoothing splines. That is exactly the behaviour observed on fig. 3.

Theorem 4.2 is actually a bit more informative than what we have just shown, since it deals for instance with the predictive variance as $\varepsilon \to 0$. Theorem 6.2 generalises the result to fits in $\mathbb{R}^d$ with $d > 1$. It is stated abstractly in terms of asymptotically equivalent models, but figs. 2 and 3 are useful to keep in mind to visualise what happens to GP fits as $\varepsilon \to 0$.

**Organisation of the paper**

Section 1 introduces GP regression, the main formulas and notation. Taking GPs to the flat limit produces improper, semi-parametric GP models which have a penalised and an unpenalised part. Section 2 introduces some notation and useful facts on semi-parametric models for GP regression. Section 3 sets the main theoretical framework, where we develop an equivalence relation on semi-parametric models from the point of view of prediction-equivalence. Roughly, two models are prediction-equivalent...
Figure 3: Predictions at $x = 0.2$ and $x = 0.8$ from different models. The dashed line corresponds to smoothing spline fits for all possible values of the regularisation parameter. The continuous curves are the predictions from GP regression with a once-differentiable Matérn kernel, fixing $\varepsilon$ but letting $\gamma$ vary. The two individual curves are for two different values of $\varepsilon$. Theorem 4.2 states that as $\varepsilon$ the continuous curve tends to the dashed curve.
if they lead to the same predictive distributions. Subsequent results are stated in terms of prediction equivalence.

Section 3 contains results on limits of GP regressions in the univariate case, which are generalised in section 6 to the multivariate case. Section 5 contains additional results on hyperparameter selection and degrees of freedom. Section 4.3 shows how to construct matched flat-limit approximations to GP regressions, and includes numerical results. The discussion in section 7 highlights some limitations and directions for future work.

1 Background on GP regression and related methods

Gaussian processes are used in a variety of statistical models, but the simplest and most elegant is GP regression, also known as kriging. GP regression is a Bayesian procedure for non-parametric regression, in which we assume that a function \( f(x) \) has been measured (with noise) at \( n \) locations \( x_1, \ldots, x_n \) and the goal is to infer \( f \) given these measurements and some vague prior knowledge, for instance that \( f \) is smooth. The procedure is called non-parametric because we do not assume that \( f \) has some parametric form. Instead, a Gaussian process prior is used to capture some basic prior knowledge about \( f \), for instance its smoothness or its periodicity.

A Gaussian process is a random function \( f(x) : \Omega \to \mathbb{R} \) that has multivariate Gaussian marginals. For simplicity we take \( \Omega \subset \mathbb{R} \) in this introduction, but higher dimensions are dealt with further down. We note \( f \sim GP(\mu, \kappa) \), where \( \mu(x) : \Omega \to \mathbb{R} \) is a mean function and \( \kappa(x, y) : \Omega^2 \to \mathbb{R} \) is a covariance function, if for all finite subsets \( X = \{x_1, \ldots, x_n\} \) of \( \Omega \), the random vector \( f_X = [f(x_1), \ldots, f(x_n)]^\top \) has a multivariate Gaussian distribution, specifically \( f_X \sim N(\mu_X, K_X) \), where \( \mu_X = [\mu(x_1), \ldots, \mu(x_n)]^\top \) and \( K_X = [\kappa(x_i, x_j)]_{i,j=1}^n \). In most cases, the covariance \( \kappa(x, y) \) is a decreasing function of the distance between \( x \) and \( y \), which ensures that \( f(x_i) \) and \( f(x_j) \) have similar values if \( x_i \) is close to \( x_j \) and so that the random function is smooth (smoothness order of \( f \) is in fact a function of smoothness order of \( \kappa \)). In GP regression the GP plays the role of a prior. We assume \( f \sim GP(0, \kappa) \) and in addition that the measurements are i.i.d. and Gaussian, namely

\[
y_i \sim N(f(x_i), \sigma^2)
\]  

for \( i = 1, \ldots, n \). Then the posterior distribution \( f|y \) is also a Gaussian process. This can be verified by writing the joint distribution of \( y \) and \( f_X \) for any finite set \( X' \subset \Omega \). By hypothesis, that joint distribution is a multivariate Gaussian, and so the (posterior) conditional \( f_{X'}|y \) is Gaussian as well. The posterior mean and covariance functions can be easily derived by applying the usual Gaussian conditioning formulas, and read:

\[
E(f(x)|y) = k_{x,X} (K_X + \sigma^2 I)^{-1} y
\]

with \( k_{x,X} = [\kappa(x_1, x_1) \ldots \kappa(x, x_n)] \), and

\[
\text{Cov}(f(x), f(x'))|y) = \kappa(x, x') - k_{x,X} (K_X + \sigma^2 I)^{-1} k_{X,x'}. \tag{4}
\]

The posterior expectation, \( \tilde{f}(x) = E(f(x)|y) \) is naturally used as an estimator for \( f(x) \). Two remarks are in order:

1. \( \tilde{f} \) is a linear function of \( y \), which makes GP regression a member of the family of linear smoothers studied by, e.g., [9]

2. \( \tilde{f} \) can be written as \( \tilde{f}(x) = \sum \kappa(x, x_i) \alpha_i \), so that \( \tilde{f} \) belongs to the reproducing kernel Hilbert space generated by \( \kappa \), which relates GP regression to classical kernel methods [29]

In fact, most of the results given below apply (with appropriate modifications) to related methods like kernel ridge regression or support vector regression.
1.1 Covariance functions, and the problem of hyperparameters

So far, we have not defined our covariance function. We shall focus on stationary covariance functions, meaning that \( \kappa(x, y) = \psi(||x - y||) \) for some function \( \psi \), i.e. the covariance only depends on the (Euclidean) distance between \( x \) and \( y \). For \( \kappa \) to be a valid covariance function, it needs to be positive definite, and for stationary covariance functions this is equivalent (by Bochner’s theorem) to requiring that \( \psi \) be the Fourier transform of a non-negative measure.

The prototypical choice in ML is to use the squared-exponential (also known as Gaussian) covariance function, eq. (1). In this formulation \( \varepsilon \) acts like an inverse horizontal scale (an inverse bandwidth) while \( \gamma \) acts like an inverse vertical scale (a gain parameter). These parameters are usually unknown and must be estimated from the data, using one of the methods outlined below in section 1.4. In addition, the noise variance \( \sigma^2 \) (see eq. (2)) may not be known either, in which case it needs to be estimated too, bringing the number of hyperparameters to three: \( \varepsilon, \gamma, \sigma^2 \).

The goal here is to characterise the flat limit of GP regression, which is the regime where \( \varepsilon \to 0 \). This essentially fixes \( \varepsilon \) and leaves only two hyperparameters to be estimated. We describe below (section 5) how to understand this limit in the context of hyperparameter selection.

While in ML the squared-exponential kernel is the most popular, in spatial statistics the Matérn class of kernels [32] is very often preferred. These kernels feature an additional hyperparameter \( \nu \in \mathbb{R}^+ \) which determines regularity, and have a somewhat unwieldy expression ([37], p. 83):

\[
\kappa_\varepsilon(x, y) = \gamma \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \sqrt{2\nu} \varepsilon \|x - y\| \right)^\nu K_\nu \left( \sqrt{2\nu} \varepsilon \|x - y\| \right)
\]

where \( K_\nu \) is a modified Bessel function. The expression simplifies when \( 2\nu \) is an integer. For instance, with \( \nu = 1/2 \) we obtain the exponential kernel:

\[
\kappa_\varepsilon(x, y) = \gamma \exp(-\varepsilon \|x - y\|)
\]

The value of \( \nu \) determines the regularity of \( f \) in the sense that if \( f \) is drawn from a Matérn kernel with parameter \( \nu, \) \( f \) is \( \lceil \nu \rceil \) times mean-square differentiable. This implies for instance that if \( f \) is drawn from an exponential kernel it is continuous but nowhere differentiable.

More generally, and beyond Matérn kernels, the regularity of \( f \) is determined by the differentiability of the covariance \( \kappa(x, y) \) in both variables. Heuristically, it is easy to see that \( f \) is m.s. differentiable if and only if \( \kappa(x, y) \) is differentiable in both \( x \) and \( y \). m.s. differentiability is equivalent to requiring that \( \frac{f(x+\delta)-f(x)}{\delta} \) has finite variance in the limit \( \delta \to 0 \). By writing the covariance of \( f(x+\delta) \) and \( f(x) \) one can check that \( \text{Var}(\frac{f(x+\delta)-f(x)}{\delta}) = \delta^{-2}(\kappa(x+\delta, x+\delta) + \kappa(x, x) - 2\kappa(x+\delta, x)) \) which has a finite limit if and only if \( \kappa(x, y) \) is differentiable in both variables at \( y = x \). Repeating the argument we see that m.s. differentiability of order \( s \) requires that the kernel be \( s \) times differentiable in both variables at \( y = x \).

The regularity of the kernel essentially determines its flat limit behaviour. We use the following definition:

**Definition 1.1** (Regularity parameter). We say a kernel \( k(x, y) \) has regularity parameter \( r \) if it is \( (r - 1) \)-times differentiable in both \( x \) and \( y \) at \( x = 0, y = 0 \), but not \( r \)-times differentiable.

**Example 1.1.** The exponential kernel (eq. (6)) is not differentiable at \( y = x \), because the distance function is not. It therefore has regularity parameter \( r = 1 \). In dimension \( d = 1 \), one can check directly that the Matérn kernel

\[
k(x, y) = (1 + |x - y|) \exp(|x - y|)
\]

is once-differentiable and therefore has \( r = 2 \). The Gaussian kernel is infinitely differentiable in both variables, and therefore has \( r = \infty \).

For stationary kernels, the regularity parameter is easy to determine based on the power spectral density, see [32] or appendix 10.1.
1.2 Other linear smoothers

In this section we introduce other linear smoothers which are related to GP regression in the flat limit. The first is polynomial regression, which is very simple when \( d = 1 \) (the multivariate case introduces some complexity, dealt with in section 6). Here we assume \( f \) is a polynomial of degree \( s \), noted \( f \in \mathcal{P}_s \), i.e. \( f(x) = \sum_{i=0}^s \alpha_i x^i \), with \( \alpha \in \mathbb{R}^{s+1} \). \( f \) is estimated by maximum likelihood, i.e. via least-squares:

\[
\hat{f}(\cdot) = \arg \min_{f \in \mathcal{P}_s} \sum (y_i - f(x_i))^2 = \mathbf{v}_{\leq s}(\cdot)^\top (V_{\leq s}^\top V_{\leq s})^{-1} V_{\leq s}^\top \mathbf{y} \tag{7}
\]

where \( \mathbf{v}_{\leq s}(x) = [x^0 \ x^1 \ \ldots \ x^s]^\top \) is the column vector in \( \mathbb{R}^{s+1} \) that contains the first \( s \) order monomials at \( x \), and where the Vandermonde matrix \( V_{\leq s} = [\mathbf{v}_{\leq s}(x_1), \ldots, \mathbf{v}_{\leq s}(x_n)]^\top \) of \( \mathbb{R}^{n \times (s+1)} \) collects these vectors at the locations \( x_1, \ldots, x_n \). This matrix and the space it spans are fundamental objects in the paper. Eq. (4) shows that \( \hat{f}_s \) depends linearly on \( \mathbf{y} \), so that polynomial regression is a linear smoother.

The only hyperparameter in this case is the degree \( s \). The polynomial regression fit can also be thought of as a Bayesian \textit{a posteriori} estimate, specifically \( \text{E}(f|\mathbf{y}) \) under a (improper), flat prior over the coefficients \( \alpha \). In this case the posterior variance equals:

\[
\text{Var}(f|\mathbf{y}) = \sigma^2 \mathbf{v}_{\leq s}(x)^\top (V_{\leq s}^\top V_{\leq s})^{-1} \mathbf{v}_{\leq s}(x). \tag{8}
\]

A different and very popular family of smoothers are the smoothing splines, which generalise to the polyharmonic splines when \( d > 1 \). Here \( f \) is only assumed to be \( p \)-times differentiable, and estimated using penalised maximum likelihood. The penalty equals the energy of the \( p \)-th derivative of \( f \):

\[
\hat{f} = \arg \min_{f \in \mathcal{C}_p(\Omega)} \sum (y_i - f(x_i))^2 + \eta \int_\Omega f^{(p)}(x)^2 dx. \tag{9}
\]

An important feature of the \( \int_\Omega f^{(p)}(x)^2 dx \) regulariser is that it has a null space, since any polynomial of degree \( (p - 1) \) has zero penalty.

A famous result known as the “representer theorem” ([35, 29]) states that this variational optimisation problem collapses to a finite-dimensional optimisation problem: the solution \( \hat{f} \) belongs to a finite dimensional space of functions, the splines of order \( p \) with knots at \( x_1 \ldots x_n \). The argument is quite simple [29]. Without using the RKHS formalism, it can be sketched as follows: the error \( \sum (y_i - f(x_i))^2 \) is indifferent to the values of \( f \) outside of the measurements \( \mathcal{X} \), so we need to look for the function that minimises the penalty given certain values \( \mathbf{f}_\mathcal{X} \). The solution turns out to be a spline of order \( p \) with knots at \( \mathcal{X} \), and so the solution of the overall optimisation problem is just to find the optimal such spline.

Classical results on splines show that a basis for this space is given by functions of the form:

\[
g(x) = \sum_{i=1}^n (x - x_i)^{2p-1} \alpha_i + \sum_{j=0}^{p-1} x^j \beta_j. \tag{10}
\]

Here \( g \) is a sum of a piecewise polynomial term and a polynomial term. Note that the latter spans the null space of the regulariser. This form has \( n + p \) degrees of freedom, but the regularisation term imposes \( V_{\leq p}^\top \alpha = 0 \), which removes \( p \) degrees of freedom.

We can inject eq. (10) into the smoothing splines optimisation problem (eq. (9)) to turn into a finite dimensional problem over \( \alpha \) and \( \beta \). Some calculus shows that the problem is equivalent to inverting the following “saddle-point” system:

\[
\begin{pmatrix}
(-1)^p D^{(2p-1)} & \eta I \\
V_{\leq p}^\top & 0
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\beta
\end{pmatrix}
= 
\begin{pmatrix}
\mathbf{y} \\
0
\end{pmatrix}
\tag{11}
\]

where \( D^{(2p-1)} \) is a symmetric matrix with entries \( D_{ij}^{(2p-1)} = |x_i - x_j|^{2p-1} \).

Recall that \( \eta \) is a regularisation parameter: the smaller \( \eta \), the closer \( f \) must fit the data. In the \( \eta \to 0 \), regularisation turns into interpolation, and the system above turns into:

\[
\begin{pmatrix}
(-1)^p D^{(2p-1)} & \eta I \\
V_{\leq p}^\top & 0
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\beta
\end{pmatrix}
= 
\begin{pmatrix}
\mathbf{y} \\
0
\end{pmatrix}
\tag{12}
\]
which is the classical system for polyharmonic spline interpolation \cite{5, 36}. On the other hand, letting \( \eta \) go to \( \infty \) in the optimisation problem (eq. \cite{5}) effectively imposes that the solution belongs to the null space of the regulariser, i.e. the space of polynomials of degree up to \( p-1 \). In this limit we therefore recover polynomial regression. The same sort of relationships are present in the flat limit of GP regression. The limit is sometimes a spline, sometimes a polynomial, sometimes a regression and sometimes an interpolant. Exactly what happens depends on \( n \), on the regularity of the kernel, and on how much regularisation is applied.

1.3 Degrees of freedom of a linear smoother

The notion of degrees of freedom is important in the analysis of linear smoothers (see \cite{6}). If \( \hat{f}_X = MY \), where \( M \) is the smoother matrix, the degrees of freedom is simply defined as \( \text{Tr} M \). For instance, if \( M \) is a projection (as in the case of polynomial regression), then \( \text{Tr} M \) is just the dimension of the space \( y \) is projected to (the image space). For regularised regressions, the matrix \( M \) is not a projection but the eigenvalues are in \([0, 1]\), and summing these eigenvalues, which is what the trace does, is a natural way of defining a “dimension” for the image space.

In the case of polynomial regression of degree \( p \), the number of degrees of freedom of the smoother simply equals \( p+1 \), the dimension of the space of polynomials of degree \( p \). In the case of GP smoothers, the number of degrees of freedom equals (from eq. \cite{4}):

\[
\text{Tr} \left( K(K + \sigma^2 I)^{-1} \right) = \sum_{i=1}^{n} \frac{\lambda_i}{\lambda_i + \sigma^2}
\]

where the \( \lambda_i \)'s are the eigenvalues of \( K \). On the right-hand side, each term in the sum is between 0 and 1. If \( \lambda_i \) is much larger than \( \sigma^2 \), then the term is close to 1. If \( \lambda_i \) is much smaller than \( \sigma^2 \), then the term is close to 0. If there is an index \( j \) such that \( \lambda_j \gg \lambda_{j+1} \), and \( \lambda_j > \sigma^2 > \lambda_{j+1} \), then the smoother matrix is close to a projection matrix. Such a scenario arises in the flat limit.

The number of degrees of freedom of (polyharmonic) spline interpolants are a bit more intricate to work out, because the smoothing matrix does not take a very convenient form. The result can be obtained either by a brute-force calculation or by noticing that the problem is the same as computing the expected size of an extended L-ensemble \cite{33, Eq. (17)}, yielding the following figure:

\[
\text{Tr}(M) = p + \sum_{i=1}^{n-p} \frac{\lambda_i}{\lambda_i + \eta}
\]

where here the \( \lambda_i \)'s are the eigenvalues of the matrix \((-1)^p Q_\perp D^{2(p-1)} Q_\perp \), \( Q_\perp \) being an orthonormal basis of the orthogonal of span \( V_{ \leq p} \). Recall that when \( \eta \) goes to 0 regression turns into interpolation, so that \( MY = y \). One can verify from eq. \cite{14} that the number of degrees of freedom indeed goes to \( n \). In the other limit, when \( \eta \to \infty \) we perform a polynomial regression of degree \( p-1 \), and accordingly the number of degrees of freedom goes to \( p \).

1.4 Hyperparameter selection

There are several methods available for hyperparameter selection in GP regression. The most satisfactory is certainly to avoid hyperparameter selection entirely by computing the marginal posterior expectation (integrating over the hyperparameters). This is not tractable analytically and somewhat expensive in practice, so alternative methods are often preferred. Let us set up more appropriate notation. The vector of hyperparameters is \( \theta = (\gamma, \epsilon, \sigma^2) \) if \( \sigma^2 \) is unknown, and \( \theta = (\gamma, \epsilon) \) if \( \sigma^2 \) it considered known.

A method for hyperparameter selection popularised by \cite{20}, but equivalent to a form of Empirical Bayes \cite{24}, is to set \( \theta \) to its maximum-likelihood value. The probability of the observations \( y \) given the hyperparameters (marginalising over \( f \)) is:

\[
p(y|\theta) = \det (2\pi(K_{\theta} + \sigma^2 I))^{-1/2} \exp(-\frac{1}{2} y^T(K_{\theta} + \sigma^2 I)^{-1/2} y)
\]
The maximum likelihood estimate of $\theta$ is obtained by maximising eq. (15). For our purposes here it is not very fruitful to compute the asymptotics of eq. (15) in the flat limit because it is divergent, as the prior becomes improper. We therefore focus our efforts on other selection criteria which are not divergent, as we show in section 5.

The non-divergent criteria we study are also very popular, and consist of (a) Stein’s Unbiased Risk Estimator and (b) two different forms of cross-validation. We believe AIC and Generalised Cross-Validation should show qualitatively the same behaviour, but we do not study them here.

For all these criteria, the smoother matrix plays a central role. Recall that the smoother matrix $M_\theta$ is defined via the posterior expectation at the sampled locations which equals:

$$E(f_X | y, \theta) = \gamma K_\varepsilon \left( \gamma K_\varepsilon + \sigma^2 I \right)^{-1} y = K_\varepsilon \left( K_\varepsilon + \frac{\sigma^2}{\gamma} I \right)^{-1} y = M_\theta y$$  (16)

Cross-validation is a natural way of picking hyperparameters, but one needs to pick a cost function and a way of splitting the datasets. Leave-one-out (LOO) is popular with GPs because there are closed-form formulas for two loss functions. One is the squared-loss. LOO cross-validation with the squared-loss reads:

$$C_{\text{loo}}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \left( y_i - E(f(x_i) | y_{-i}, \theta)) \right)^2$$  (17)

Here $E(f(x_i) | y_{-i}, \theta)$ is the posterior expectation of $f(x_i)$ conditional on all the data except $y_i$. Standard calculations using the Woodbury lemma show that an alternative formula for the LOO loss is [13] :

$$C_{\text{loo}}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \left( y_i - (M_\theta y)_{i} \right)^2 \left( 1 - M_\theta(i,i) \right)$$  (18)

Evident from this formula is that LOO squared-error loss only depends on the smoother matrix. A different choice, one that takes uncertainty into account, is to use the negative log-likelihood as a cost:

$$C_{\ell}(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \log p(y_i | y_{-i}, \theta) = \frac{1}{n} \left\{ \sum_{i=1}^{n} \frac{1}{2} \log (2\pi \text{Var}(y_i | y_{-i}, \theta)) + \frac{1}{2} \left( y_i - E(y_i | y_{-i}, \theta)) \right)^2 \frac{\text{Var}(y_i | y_{-i}, \theta)}{\text{Var}(y_i | y_{-i}, \theta)} \right\}$$  (19)

Eq. (19) also has an equivalent form that is faster to compute and involves the smoother matrix, see [37] (p. 117).

Finally, another way of selecting a hyperparameter, popular in the signal processing community, is Stein’s Unbiased Risk Estimate (SURE, [18]), which assumes that $\sigma^2$ is known.

$$C_{\text{SURE}}(\theta) = -\sigma^2 + \frac{1}{n} \sum_{i=1}^{n} \left( y_i - (M_\theta y)_{i} \right)^2 + \frac{2\sigma^2}{n} \text{Tr} M_\theta$$  (20)

SURE is quite similar to AIC in that it features a loss term corrected by a measure of model complexity, quantified here by the degrees of freedom of the smoother matrix $\text{Tr} M_\theta$.

2 Semi-Parametric models

The goal of this section is to introduce some notation to unify linear smoothers like GP regression, polynomial regression and polyharmonic spline regression; we shall describe them all as “semi-parametric” GP models. Semi-parametric regression [27] is not a new concept at all, and the results in this section are not novel. However, we introduce some notation that allows us to describe what happens in the flat limit in a compact and unified way.

Semi-parametric Gaussian process models assume the unknown function $f(x)$ to be of the form:

$$f(x) = g(x) + \sum_{i} \alpha_i v_i(x)$$  (21)
where \( g(x) \) is non-parametric and \( \mathcal{V} = \{ v_1(x), \ldots, v_m(x) \} \) is a set of basis functions forming the parametric part. \( g(x) \) is given a Gaussian process prior, and the prior on the weights \( \alpha_i \) is the improper uniform prior \( p(\alpha_i) \propto 1 \). Despite the improper prior, the posterior is well-defined under mild conditions (see below), and the resulting fit has useful properties. Of course, if no basis functions are included, then the model is a (non-parametric) GP regression, and if no non-parametric term is included, then we have a parametric model.

We use the following notation for describing semi-parametric models:

**Definition 2.1** (Semi-parametric model). A semi-parametric model (SPM) over \( \Omega \subseteq \mathbb{R}^d \) is a tuple \( (l; \mathcal{V}) \), where \( l(x, y) \) is a (conditionally)-positive definite kernel on \( \Omega \), and \( \mathcal{V} = \{ v_1(x), \ldots, v_m(x) \} \) is a set of linearly-independent basis functions.

**Example 2.1.** The following describes a SPM over \( \mathbb{R} \): \( \mathcal{M} = (\exp(-(x-y)^2); \{1, x, x^2\}) \). The non-parametric part is a Gaussian kernel, and the parametric part are the basis functions \( 1, x, x^2 \). It corresponds to a standard GP regression with a Gaussian kernel, except that polynomial trends of degree \( \leq 2 \) are unpenalised.

A parametric model over \( \mathbb{R} \) is the special case where the kernel is uniformly 0 or (equivalently) missing, e.g. \( \mathcal{M} = (0; \{\sin(x), \cos(x)\}) \) is a parametric model with two sinusoidal basis functions. A purely non-parametric model has \( \mathcal{V} = \emptyset \), e.g. \( \mathcal{M} = (\exp(-(x-y)^2); \emptyset) \) is a standard GP model with Gaussian covariance.

The possibility for the non-parametric kernel to be conditionally positive definite rather than positive definite is probably non-obvious to the reader (especially since we have not yet defined the term). Our first example is smoothing spline regression with linear splines, which may be cast as \( \mathcal{M} = (-|x-y|; \{1\}) \), i.e. with a single basis function, namely the constant function. The function \( l(x, y) = -|x-y| \) is not positive definite, as can be easily verified. If we evaluate the kernel matrix for \( l \) at the locations \( x_1 = 0, x_2 = 1 \), we find \( \mathbf{L} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \), which has eigenvalues equal to \(-1\) and \(1\), whereas a positive definite kernel would give non-negative eigenvalues. Nonetheless, the smoothing splines SPM is well-defined, because, as we shall explain soon, kernels only need to be positive definite along the directions orthogonal to the span of the basis functions.

**Definition 2.2** (unisolvent sets, conditional positive-definiteness). A set of locations \( \mathcal{X} = \{ \mathbf{x}_1, \ldots, \mathbf{x}_n \} \subset \Omega \) is said to be unisolvent for the SPM \( \mathcal{M} = (l; \{v_1, \ldots, v_m\}) \) if the matrix

\[
\mathbf{V} = [v_j(\mathbf{x}_i)]_{i=1}^n_{j=1}^{m}
\]

has rank \( m \). \( \mathbf{V} \) corresponds to the evaluation of the \( m \) basis functions (along columns) at the points in \( \mathcal{X} \) (along rows). We call it the basis matrix. It has a QR decomposition \( \mathbf{V} = \mathbf{QR} \), where \( \mathbf{Q} \) is an orthonormal basis for \( \text{span} \mathbf{V} \).

The kernel matrix equals

\[
\mathbf{L} = [l(\mathbf{x}_i, \mathbf{x}_j)]_{i=1}^n_{j=1}^{n}
\]

and we use “kernel matrix” rather than covariance matrix because \( \mathbf{L} \) may not be positive definite.

The condition that the kernel \( l \) be conditionally positive-definite with respect to \( \mathbf{V} \) corresponds to the requirement that for all unisolvent \( \mathcal{X} \), the matrix

\[
\tilde{\mathbf{L}} = (\mathbf{I} - \mathbf{Q} \mathbf{Q}^\top) \mathbf{L} (\mathbf{I} - \mathbf{Q} \mathbf{Q}^\top)
\]

be positive definite. Note that \( \mathbf{I} - \mathbf{Q} \mathbf{Q}^\top \) is a projector on the space orthogonal to \( \text{span} \mathbf{V} \); the requirement is therefore that \( \mathbf{L} \) be positive semi-definite on the space orthogonal to \( \text{span} \mathbf{V} \).

**Example 2.2.** We return to \( \mathcal{M} = (-|x-y|; \{1\}) \), linear smoothing splines, on the set \( \mathcal{X} = \{0, 1\} \).

Here \( \mathbf{V} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \), which has (trivially) full column rank, so that \( \mathcal{X} \) is unisolvent. The orthonormal form of the basis matrix is \( \mathbf{Q} = \begin{pmatrix} 1 / \sqrt{2} \\ 1 / \sqrt{2} \end{pmatrix} \). As before \( \mathbf{L} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \), and \( \tilde{\mathbf{L}} = \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix} \).
\[
\begin{pmatrix}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}
\end{pmatrix},
\] so that \( \tilde{L} \) is indeed positive semi-definite. More generally, since in this case the basis function is unique, all sets \( \mathcal{X} \in \mathbb{R} \) of size at least 1 are unisolvent. The fact that \( l(x, y) = -|x - y| \) is conditionally positive-definite w.r.t. the constant function is shown in [27].

The requirement that the measurement locations \( \mathcal{X} \) be unisolvent is necessary when using a SPM, because it essentially states that the basis functions need to be identifiable from \( \mathcal{X} \), or equivalently that the posterior distribution be proper, despite the improper prior on the parametric part. We do not wish to linger too much on unisolvent sets, except to note that there are non-trivial sets in \( \mathbb{R} \) because it essentially states that the basis functions need to be identifiable from \( \mathcal{X} \).

is conditionally positive-definite w.r.t. the constant function is shown in [21].

The conditional expectation in a SPM has the following form:

\[
E(f(x)|y) = (l_{x,X} \ v_x) \begin{pmatrix} L + \sigma^2 I & V \\ V^\top & 0 \end{pmatrix}^{-1} \begin{pmatrix} y \\ 0 \end{pmatrix}
\] (24)

where \( l_{x,X} = [l(x, x_1) \ldots l(x, x_n)] \) and \( v_x = [v_1(x) \ldots v_m(x)] \). One may check that this generalises the non-parametric case by removing the basis functions, and the parametric case by setting \( l = 0 \) (which implies \( L = 0 \) and \( l_{x,X} = 0 \)). In addition, we can see in eq. [24] that a SPM results in a linear smoother (in the sense that the fit is a linear function of \( y \)), and that the fit takes the form

\[
\hat{f}(x) = \sum_{i=1}^{n} \alpha_i l(x, x_i) + \sum_{j=1}^{m} \beta_j v_j(x)
\]

where the coefficients \( \alpha \) and \( \beta \) depend on \( y \) and \( \sigma^2 \). Although the fit seems to take its value in a \( n + m \)-dimensional space of functions, eq. [24] actually implies the condition \( V^\top \alpha = 0 \) which removes \( m \) degrees of freedom. This generalises the case of smoothing splines introduced earlier ((eq. see [10]).

\(^{1}\)These directions correspond to the space spanned by the eigenvectors associated with negative eigenvalues of \( L \).
An expression for the smoother matrix can be derived either by taking $x = x_i$ in eq. (24), or by using the correspondence between SPMs and extended-L-ensembles [33, 10] to get

$$M = QQ^\top + L (L + \sigma^2 I)^{-1}$$

(25)

where $Q$ is an orthonormal basis for $V$ and $\tilde{L} = (I - QQ^\top)L(I - QQ^\top)$. Eq. (25) is the sum of a projection matrix (as arises in a least-squares fit of a parametric model), and a regularised fit (as arises in a non-parametric GP model), limited to the subspace orthogonal to $V$.

The conditional variance takes a similar form to eq. (24), namely:

$$\text{Var}(f(x)|y) = l_{x,x} - (l_{x,x} v_x) \begin{bmatrix} L + \sigma^2 I & V \\ V^\top & 0 \end{bmatrix}^{-1} (l_{x,x} v_x^\top)$$

(26)

where again the parametric and non-parametric special cases can be recovered by setting $l = 0$ or removing the basis functions.

3 Prediction-equivalence of semi-parametric models

In the flat limit, standard GP models become equivalent to certain semi-parametric models (SPMs), in the sense that they give the same predictions (conditional expectation and conditional variance) regardless of what the value of $\sigma^2$ is, where the measurements $X$ occur and where the prediction is sought. The aim of this section is to formalise the notion of predictive-equivalence of SPMs, and to exhibit a simple criterion for proving equivalence based on the smoother matrix.

Definition 3.1 (Prediction-equivalence for semiparametric models). Two semi-parametric models $M = (l; V)$ and $M' = (l'; V')$ are said to be prediction-equivalent over a domain $\Omega \subset \mathbb{R}^d$, noted $M \sim M'$, if $|V| = |V'|$, and for any finite $X \subset \Omega$ unisolvent for $V$ and $V'$, for all $x \in \Omega$, $y \in V[|X|]$, $\sigma^2 \in \mathbb{R}^+$:

1. The predictive expectations (eq. (24)) are equal: $E_{M}(f(x)|y) = E_{M'}(f(x)|y)$
2. The predictive variances (eq. (26)) are equal: $\text{Var}_{M}(f(x)|y) = \text{Var}_{M'}(f(x)|y)$

i.e., the predictive distributions are equal.

In some cases the predictive-equivalence of two models is easy enough to establish. For instance, if $V$ and $V'$ are two sets of basis functions for the same function space, then whatever $l$, $(l; V) \sim (l; V')$. To take a concrete example, $V = \{x_1, x_2\}$ spans the same space as $V' = \{x_1 - x_2, x_1 + x_2\}$ and so using one rather than the other changes nothing to the model (theoretically, if not numerically). If the intuitive argument does not convince, one can also check equivalence directly via eq. (24) and (26).

A more subtle source of prediction-equivalence is the following: if $v_i \in V$, then

$$(l(x, y) + \alpha v_i(x)v_i(y); V) \sim (l(x, y); V)$$

This form of prediction-equivalence follows directly from the argument outlined in section 9.1, or again can be checked via eqs. (24) and (26). By extension,

$$(l(x, y) + \sum_{i=1}^{m} \alpha_i v_i(x)v_i(y); V) \sim (l(x, y); V)$$

In our flat limit computations however, we cannot show equivalence so directly. What we have access to are smoother matrices, but it turns out that this is enough. The next lemma is essential for our proofs, and concerns prediction-equivalence of two non-parametric models.

Lemma 3.2. These two statements are equivalent:
The following formula: predictive variances are equal. For the predictive means, one can repeat a similar computation with which is obtained from the conditional posterior over \( f \) l.h.s in equation (27), since we have equivalent to proving formula (5.26) in [13].

By equality of the smoother matrices \( M_X = K_X(K_X + \sigma^2 I)^{-1} \) and \( M'_X = K'_X(K'_X + \sigma^2 I)^{-1} \) are equal.

Proof. We prove each implication separately. (a) \( \implies \) (b) is straightforward. Since \((k; \emptyset) \sim (k'; \emptyset)\), then \( E_k(x|y) = E_k(x|y) \) for all \( x \), including \( x \in X \), implying that:

\[
\delta_r M_X y = \delta_r M'_X y
\]

for all \( i \in \{1, \ldots, |X|\} \) and \( y \in \mathbb{R}^{|X|} \). This implies equality of \( M_X \) and \( M'_X \) (i.e., take \( y \) to be any \( \delta_j \)).

(b) \( \implies \) (a) is less direct, but essentially the same as the derivation for the fast formula for leave-one-out cross-validation.

The main trick is that the prediction mean and variance at \( x \) given observations at \( X \) can be computed from the smoother matrix for \( Y = X \cup x \). Let \( |Y| = n \). We begin with the variance. The predictive variance at \( x \) for kernel \( k \) equals

\[
v_x = k_{x,x} - k_{x,X}(K_X + \sigma^2 I)^{-1} k_{Y,x}
\]

which is a Schur complement in the block matrix

\[
\begin{pmatrix}
K_x + \sigma^2 I & k_{X,x} \\
k_{x,X} & k_{x,x}
\end{pmatrix} = K_Y + \sigma^2 I - \sigma^2 \delta_n \delta_n^T
\]

i.e., we have

\[
\frac{1}{v_x} = \delta_n^T (K_Y + \sigma^2 I - \sigma^2 \delta_n \delta_n^T)^{-1} \delta_n
\]

Applying the Woodbury lemma, we have

\[
\frac{1}{v_x} = \delta_n^T (P + \frac{\sigma^2 P \delta_n \delta_n^T P}{1 - \sigma^2 \delta_n \delta_n^T}) \delta_n
\]

where \( P = (K_Y + \sigma^2 I)^{-1} = \sigma^{-2}(I - M_Y) \). Noting \( c = \delta_n^T M_Y \delta_n \) and simplifying, we obtain:

\[
v_x = \sigma^2 \frac{c}{1 - c}
\]

By equality of the smoother matrices \( M_Y = M'_Y \) for any \( Y \), we have \( c' = c \) and \( v'_x = v_x \), thus the predictive variances are equal. For the predictive means, one can repeat a similar computation with the following formula:

\[
E(f(x)|y) = \sigma^{-2} \delta_n^T (K_Y^{-1} + \sigma^{-2} I - \sigma^{-2} \delta_n \delta_n^T)^{-1} \begin{pmatrix} y \\ 0 \end{pmatrix}
\]

which is obtained from the conditional posterior over \( f_X, f(x) \) given \( y \). Applying the Woodbury lemma again, we see that the expectation depends only on the smoother matrix for \( Y \). The calculation is equivalent to proving formula (5.26) in [13].

An alternative way of proving the same result uses the block inverse formula for the matrix of the l.h.s in equation (27), since we have

\[
\frac{-E(f(x)|y)}{v_x} = \delta_n^T (K_Y + \sigma^2 I - \sigma^2 \delta_n \delta_n^T)^{-1} \begin{pmatrix} y \\ 0 \end{pmatrix}
\]

which leads using the previous calculations to

\[
E(f(x)|y) = \frac{\delta_n^T M_Y \begin{pmatrix} y \\ 0 \end{pmatrix}}{1 - c}
\]

which shows again that the a posteriori mean at \( x \) only depends on the full smoother matrix \( M_Y \). \( \square \)
With the above lemma in hand, extension to semi-parametric models is straightforward: As with standard kernels, predictive equivalence can be assessed from equality of smoother matrices:

**Proposition 3.3.** These two statements are equivalent: letting $M = (l; V), M' = (l'; V')$

a) $M \sim M'$.

b) For all finite $X \subset \Omega$ unisolvent for $V$ and $V'$, $\sigma^2 \in \mathbb{R}^+$, the smoother matrices for $M$ and $M'$ at $X$ are equal.

**Proof.** The proof is a variant of lemma 3.2. (a) $\Rightarrow$ (b) follows from the same argument.

For (b) $\Rightarrow$ (a), we use the characterisation of semi-parametric models as limits. $k_\varepsilon(x, y) = l(x, y) + \varepsilon^{-1} \sum_{v \in V} v(x)v(y)$ converges in $\varepsilon \to 0$ to the semi-parametric model $S$, and similarly $k'_\varepsilon(x, y) = l'(x, y) + \varepsilon^{-1} \sum_{v' \in V'} v'(x)v'(y)$ goes to $S'$, in the sense that the predictive means and variances converge to that of $S$ and $S'$. By corollary 3.4, we know that the smoother matrix if $k_\varepsilon$ equals $M_\varepsilon = M_0 + O(\varepsilon)$, its counterpart $M'_\varepsilon = M'_0 + O(\varepsilon)$ and, by assumption, since the smoother matrices for $S$ and $S'$ are equal then $M_0 = M'_0$. From the proof of lemma 3.2 we know that the predictive means and variances for $k_\varepsilon$ and $k'_\varepsilon$ are continuous functions of $M(\varepsilon)$ and $M'(\varepsilon)$, and therefore have the same limit as $\varepsilon \to 0$. 

In practice, as mentioned in section 1.4, a “vertical scale” hyperparameter is present in GP models. For semiparametric models, this means that we consider the family $M(\gamma) = (\gamma l; V)$ indexed by $\gamma \in \mathbb{R}^+$, and $\gamma$ is set by minimising a hyperparameter selection criterion like those in section 1.4. The marginal likelihood cannot be used here (unmodified, at least), because the prior is improper. This leaves us with cross-validation and SURE. An important property of predictive-equivalent models is that two equivalent models remain equivalent post-selection: the value of these selection criteria are equal for all values of $\sigma^2$ and $\gamma$.

**Proposition 3.4 (Post-selection equivalence).** Let $M = (l; V) \sim M' = (l'; V)$ on $\Omega$, and consider the families of models $M(\gamma) = (\gamma l; V)$ and $M'(\gamma) = (\gamma l'; V)$. Then for any data $y$ and noise variance $\sigma^2$, the value of the selection criteria given by eq. (17), eq. (19) and eq. (20) are the same for $M(\gamma)$ and $M'(\gamma)$. Consequently, if $\gamma^*$ is the optimal value of the criterion for $M$, it equals the optimal value for $M'$, and the selected models $M(\gamma^*)$ and $M'(\gamma^*)$ are prediction-equivalent.

**Proof.** First, it is is easy to check that if $(l; V) \sim (l'; V)$ then $(\gamma l; V) \sim (\gamma l'; V)$. The leave-one-out criteria rely on predictive means and variances so the result follows directly from the definition of predictive equivalence. For the SURE criterion, the result follows because eq. (20) only depends on the smoother matrix.

**Remark 3.5.** The result can be extended to selection of $\sigma^2$ as well, if $\sigma^2$ is unknown and selected via eq. (19).

Because the vertical scale hyperparameter $\gamma$ is always present in practice in a SPM, it is useful to introduce a notion of equivalence “up to a constant”:

**Definition 3.6.** We say that $M = (l; V)$ and $M' = (l'; V')$ are equivalent up to a constant, noted $M \propto M'$, if there exists $\alpha \in \mathbb{R}'$ such that $(l; V) \sim (\alpha l'; V')$.

This relaxed form of equivalence also holds post-selection. By prop. 3.4, if $\gamma^*$ is the optimal value of $\gamma$ for the family $M(\varepsilon)$, then $\frac{\alpha}{\gamma^*}$ is the optimal value for the family $M'(\varepsilon)$, and $M(\varepsilon) \sim M'(\frac{\alpha}{\gamma^*} \varepsilon)$. Therefore, because two models $M \propto M'$ define effectively the same family of models up to a change of scale, we shall use the $\propto$ notation in our results to hide irrelevant multiplicative factors.

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\(^2\)AIC and Generalised Cross Validation would work as well.
4 Main result in the univariate case

We use the notation \( a_\varepsilon \xrightarrow{\varepsilon \to 0} \mathcal{M} \) to denote models that become prediction-equivalent in the flat limit, in the sense that the predictive distributions of \( a_\varepsilon \) converge to that of \( \mathcal{M} \). The precise definition we use is an asymptotic variant of definition \[ \ref{def:prediction_equivalence} \].

**Definition 4.1** (Asymptotic prediction-equivalence). A model \( k_\varepsilon \) is said to be asymptotically prediction-equivalent to a fixed (semi)-parametric model \( \mathcal{M} = (l; \mathcal{V}) \) over a domain \( \Omega \subset \mathbb{R}^d \), noted \( k_\varepsilon \xrightarrow{\varepsilon \to 0} \mathcal{M} \), if \( |\mathcal{V}| = |\mathcal{V}'| \), and for any finite \( \mathcal{X} \subset \Omega \) such that \( \mathcal{V}_\mathcal{X} \) and \( \mathcal{V}'_\mathcal{X} \) have full column rank, for all \( x \in \Omega \), \( y \in \mathcal{R}^{|\mathcal{X}|} \), \( \sigma^2 \in \mathbb{R}^+ \):

1. The predictive expectations are such that: \( \mathbb{E}_{k_\varepsilon}(f(x)|y) = \mathbb{E}_{\mathcal{M}}(f(x)|y) + \mathcal{O}(\varepsilon) \)
2. The predictive variances are such that: \( \text{Var}_{k_\varepsilon}(f(x)|y) = \text{Var}_{\mathcal{M}}(f(x)|y) + \mathcal{O}(\varepsilon) \)

We use the short-hand \( k_\varepsilon \xrightarrow{\varepsilon \to 0} \mathcal{M} \) if there exists \( \mathcal{M}' \propto \mathcal{M} \) such that \( k_\varepsilon \xrightarrow{\varepsilon \to 0} \mathcal{M}' \).

We are now ready to state our main result in the one-dimensional case. We look at models of the form \( k_\varepsilon(x,y)\varepsilon^{-r} \), where the vertical scale hyperparameter \( (\gamma) \) grows as \( \varepsilon \to 0 \). This lets us control the degrees of freedom of the fit in the flat limit; the higher the value of \( p \), the more degrees of freedom we allow. A more thorough discussion of degrees of freedom can be found below (section 5). What the equivalent model turns out to be in the flat limit depends on \( p \) and \( r \), the regularity of the kernel, and nothing else.

**Theorem 4.2.** Let \( k_\varepsilon(x,y) \) be a stationary positive-definite kernel for \( x, y \) in \( \mathbb{R} \), with regularity parameter \( r \). Let \( p \) be an integer. Then the following asymptotic equivalence holds:

\[
k_\varepsilon \varepsilon^{-p} \xrightarrow{\varepsilon \to 0} (l_p; \mathcal{V}_p)
\]

where \( l_p(x,y) \) and \( \mathcal{V}_p \) depend on the interplay between \( p \) and \( r \). There are four different cases:

- \( p < 2r - 1 \) and \( p \) is even, i.e., \( \exists m < r \text{ s.t. } p = 2m \). Then \( l(x,y) = x^{m+1}y^{m+1} \) and \( \mathcal{V} = \{x^0, x^1, \ldots, x^m\} \). This case amounts to penalised polynomial regression.
- \( p < 2r - 1 \) and \( p \) is odd, i.e., \( \exists m < r - 1 \text{ s.t. } p = 2m + 1 \). Then \( l(x,y) = 0 \) and \( \mathcal{V} = \{x^0, x^1, \ldots, x^{m+1}\} \). This case amounts to unpenalised polynomial regression.
- \( p = 2r - 1 \). In this case, \( l(x,y) = (-1)^r|x-y|^{2r-1} \) and \( \mathcal{V} = \{x^0, x^1, \ldots, x^{r-1}\} \), which amounts to smoothing spline regression.
- \( p > 2r - 1 \). This case leads to an interpolant independently of the value of \( \sigma^2 \).

**Proof.** A full proof is given in appendix \[ \ref{app:proofs} \]. The bulk of the proof consists in obtaining the limit of the smoother matrix corresponding to model \( k_\varepsilon \varepsilon^{-p} \) as \( \varepsilon \to 0 \). We can work this out from the results in \[ \ref{sec:asymptotic_eigenvalues} \], which provide the asymptotic eigenvalues and eigenvectors of \( K_\varepsilon \). From this we obtain an expression for the smoother matrix as \( M_\varepsilon = M_0 + \mathcal{O}(\varepsilon) \) where \( M_0 \) depends on \( p \) and \( r \). The proof is completed by appealing to lemma \[ \ref{lem:asymptotic_eigenvalues} \] and proposition \[ \ref{prop:asymptotic_eigenvectors} \] which allows us to deduce equivalence of models from equality of smoother matrices.

Examining the proof of lemma \[ \ref{lem:asymptotic_eigenvalues} \] and proposition \[ \ref{prop:asymptotic_eigenvectors} \] we see that the predictive mean and variance depend smoothly on \( M_\varepsilon \) and so we have asymptotic predictive equivalence in the sense of definition \[ \ref{def:prediction_equivalence} \]. The different cases are the different cases for smoother matrices.

**Example 4.1.** If \( k_\varepsilon(x,y) \) is the exponential kernel, which has \( r = 1 \), then \( \varepsilon^{-1}k_\varepsilon(x,y) \) is asymptotically equivalent to the model \( (|x-y|; 1) \), i.e. the parametric part is the constant function and the non-parametric part is the kernel \( l(x,y) = |x-y| \). By eq. \[ \ref{eq:exponential_kernel} \], it implies that \( \hat{f} = E(f|y) \) goes to:

\[
\hat{f}(x) = -\sum_{i=1}^{n} \beta_i |x - x_i| + \alpha + \mathcal{O}(\varepsilon)
\]
The kernel functions $|x-x_i|$ are piecewise linear and so the fit goes in the limit to a linear spline. Recall that $\beta$ is constrained: $V^T\beta = 0$, which here simplifies to $\sum \beta_i = 0$. This sets the boundary conditions, as one may easily check by looking at derivatives outside the range of the data: $\frac{d}{dx}\hat{f}(x) = 0$ if $x$ is to the left or right of the observations $X$, so that the fit has a built-in, implicit Neumann boundary condition. Generalising further, if $k_\varepsilon(x,y)$ is a kernel with finite $r$, and setting $p = 2r - 1$, $\varepsilon^p k_\varepsilon(x,y)$ is asymptotically equivalent to the model $S = \{((-1)^r|x-y|^{2r-1};\{1,x,\ldots,x^{2r-1}\}\}$, which leads to the asymptotic fit:

$$\hat{f}(x) = (-1)^r \sum_{i=1}^{n} \beta_i |x-x_i|^{2r-1} + \sum_{j=0}^{r-1} \alpha_j v^j + O(\varepsilon)$$

with the constraint $V^T\beta = 0$.

The multivariate counterpart of theorem 4.2 can be found in section 6. The multivariate theorem resembles the univariate one, but requires quite a bit of notation. Instead of going directly to multivariate equivalent models, we take a look instead at degrees of freedom and hyperparameter selection in the flat limit.

5 Degrees of freedom, hyperparameter selection, and practical consequences

In this section we study the behaviour of the degrees of freedom, and the various hyperparameter selection methods as $\varepsilon \to 0$. All results are applicable to the multivariate case even though the numerical examples concern the univariate case.

Since degrees of freedom play such an important role in hyperparameter selection, we also look at their asymptotics and show that scaling $\gamma$ as $\gamma_0 \varepsilon^p$ for some well-chosen $\gamma_0$ and $p$ keeps the degrees of freedom constant as $\varepsilon \to 0$. We stress two practical implications of these results.

First, for certain datasets, very low values of $\varepsilon$ may be appropriate or even optimal (in terms of prediction performance). In practice low values of $\varepsilon$ are never used because either (a) kernel matrices become numerically non-invertible or (b) a nugget term is used which “hides” useful eigenvectors. There are specially constructed bases for some kernels with better numerical properties (e.g., [12]), and our analysis supports their use.

Second, we use the theoretical results on degrees of freedom to formulate a “matched approximation” for a given GP model. The matched approximation to a kernel $k_\varepsilon$ is the flat limit model with the same regularity and degrees of freedom for the measurement locations $X$. An interpretation of theorem 4.2 is that the matched approximation becomes exact as $\varepsilon \to 0$.

5.1 Degrees of freedom and isofreedom curves

As explained in section 1.3, the degrees of freedom of a linear smoother measure in some sense the “dimension” of the range of the smoother matrix. Given a GP model defined by a kernel $k$ and measurements at $X$, the degrees of freedom typically increase with larger $\varepsilon$ and larger $\gamma$. We show an example in figure 4 where the degrees of freedom are displayed as a function of $\gamma$ and $\varepsilon$ for a randomly drawn point set $X$ in $\mathbb{R}$. Because degrees of freedom decrease as $\varepsilon \to 0$, in section 4 we let $\gamma$ increase as $\varepsilon \to 0$ so that a nontrivial smoother matrix could arise in the limit. The particular form chosen is $\gamma = \gamma_0 \varepsilon^{-p}$, which looks like a choice of convenience but actually has a deeper motivation. What one might notice on figure 4, which has log-log axes, is that the contours become lines in small $\varepsilon$. We dub these contours “iso-freedom curves”, because they correspond to sets of the form

$$F_m = \{(\varepsilon, \gamma) | \text{Tr}(\gamma K_\varepsilon(\gamma K_\varepsilon + \sigma^2 I)^{-1}) = m\}$$
for fixed values of \(m\). Given \(m\), \(\sigma^2\) and \(\varepsilon\), we can solve for the value of \(\gamma\) such that the degrees of freedom equal \(m\). \(\gamma\) should verify:

\[
\text{Tr}(\gamma K_\varepsilon (\gamma K_\varepsilon + \sigma^2 I)^{-1}) = m \\
\Leftrightarrow \sum \gamma \lambda_i(\varepsilon) (\gamma \lambda_i(\varepsilon) + \sigma^2) - m = 0
\] (28)

Eq. (28) is a rational equation in \(\gamma\), and the eigenvalues of \(\lambda_i(\varepsilon)\) are analytic in \(\varepsilon\). Call \(\gamma_m(\varepsilon)\) the solution of eq. (28) as a function of \(\varepsilon\), and note that it is a parametrisation of the iso-freedom curve, giving \(\gamma\) as a function of \(\varepsilon\). The Newton-Puiseux theorem implies that \(\gamma_m(\varepsilon)\) can be expanded as a Puiseux series in small \(\varepsilon\) (see [4]), i.e. that there exist \(\gamma_0, l, s \in \mathbb{Z}\), \(s \in \mathbb{Z}^+\) such that:

\[
\gamma_m(\varepsilon) = \varepsilon^{\frac{1}{s}} (\gamma_0 + O(\varepsilon^{\frac{1}{s}}))
\] (29)

A Puiseux series is just a power series in \(\varepsilon^{\frac{1}{s}}\), and if \(s = 1\) it is actually a power series. Notice that \(\log \gamma_m(\varepsilon) \approx \frac{1}{s} \log \varepsilon + \log \gamma_0\), which explains why the iso-freedom curves look linear in log-log coordinates. In equation (29), \(l, s\) and \(\gamma_0\) depend on \(m\) (the desired number of degrees of freedom), and the kernel function. They can actually be determined in closed-form using the Newton polygon [22], but that would carry us outside the scope of this manuscript. Among other things, it is not too hard to show that \(s = 1\) here, so that the iso-freedom curves have integer slopes in small \(\varepsilon\).

## 5.2 Hyperparameter selection in the flat limit

In section 1.4, we introduced three hyperparameter selection methods: the SURE criterion, and two criteria based on leave-one-out cross-validation. Given the results above, one can verify that all three criteria are constant in \(\varepsilon \to 0\) along iso-freedom lines. Figure 5 gives a visual illustration of this fact.

To see why the three criteria are asymptotically constant along iso-freedom lines, consider theorem 4.2 and equation (29) jointly. We shall state the result informally. Following a contour with constant degrees of freedom to the limit \(\varepsilon \to 0\), we need to set \(\gamma(\varepsilon) = \varepsilon^{-p}(\gamma_0 + O(\varepsilon))\) (by eq. 29). This is identical in \(\varepsilon \to 0\) to setting \(\gamma(\varepsilon) = \varepsilon^{-p}\gamma_0\) (up to negligible terms), and we may apply theorem 4.1.
Figure 5: Asymptotics of hyperparameter selection. A synthetic dataset is shown in the upper-left panel. The three other panels are contour plots for three different hyperparameter selection criteria. We set $\sigma^2 = (0.1)^2$ and used a Gaussian kernel. Note that these three criteria are mostly constant along lines, which have asymptotically constant degrees of freedom (see fig. 4).
which tells us that the predictive mean and variance converge to finite quantities. It is clear from the
formulas of the two leave-one-out criteria (eq. (17) and (19)) that they must then converge to finite
quantities as well. The SURE criterion (eq. (20)) must converge as well since the degrees of freedom
are asymptotically constant and the smoother matrix converges.

5.3 Why low ε solutions are invisible in practice

One implication of the fact that selection criteria do not diverge is that, for some datasets, the optimal
solutions may be in small ε. However, these solutions may be invisible or unattainable when using
naïve numerical methods. The main source of numerical difficulty arises when computing the smoother
matrix:

\[
M_\varepsilon = K_\varepsilon (K_\varepsilon + \sigma^2 \gamma I)^{-1}
\]

Since γ becomes very large as ε → 0, σ^2 is small, and one must invert a poorly conditioned matrix. A
Cholesky decomposition in standard floating point precision may fail, so that the small-ε part of the
space is inaccessible. In practice sometimes a “nugget term” is used to alleviate numerical difficulties:
one replaces \(K_\varepsilon\) with \(K_\varepsilon + \nu I\), where \(\nu\) is small. However, once the nugget term is added, increasing
γ beyond \(\nu\) has no effect. Some useful eigenvectors are made invisible by the nugget term and this has
the effect of “clipping” the surface of hyperparameter selection criteria, as shown in fig. 6 Since this
is clearly undesirable, a better option in the future may be to adapt existing methods for stable RBF
interpolation (e.g., [11, 12]) to GP regression problems.

5.4 Towards practical approximations

Our limit results are not directly applicable when faced with the question: “what is a useful approxima-
tion of a particular GP model at a particular value of ε”? We do not claim to have a universal recipe,
but we shall present in this section a particular approximation that gives surprisingly good results in
certain cases.

This approximation is best understood graphically. We take as input a certain kernel function,
and a certain value for \(\sigma^2, \gamma\) and \(\epsilon\). We can think of it as occupying a certain position in the space
of hyperparameters as shown on figure 4 or 5 for example. The approximation we suggest, which we
call the matched approximation, consists in following the iso-freedom line from that point to \(\epsilon \to 0\).
Following theorem 4.2, the matched approximation will be either or polynomial or a spline regression,
with the same number of degrees of freedom as the original GP regression. The process is illustrated
graphically in figure 7 and 8 for two different kernels.

Let us sketch a concrete algorithm for kernels with \(r = \infty\) and degrees of freedom set to \(m \in \mathbb{R}^+\).
By theorem 4.2, the equivalent semiparametric models are of the form \(S = (\gamma x^p y^p; \{x^0, \ldots, x^{p-1}\})\) for
some degree \(p\). The corresponding fit will have between \(p\) and \(p + 1\) degrees of freedom, where the
former is attained with \(\gamma = 0\) and the latter with \(\gamma \to \infty\). We therefore need to set \(p = \lceil m \rceil\) and adjust
\(\gamma\) such that the \(m\)-th eigenvalue of the smoother matrix equals \(m - p\). A similar algorithm applies for
finite \(r\).

The matched approximation is illustrated on figs. 7 to 10 for kernels with different regularities,
and for different values of ε. For the Matérn kernel the quality of the approximation is excellent even
though ε = 2; it is hard to account for this fact in our current perturbative framework.

6 Results in the multivariate case

To deal with the multivariate case, we require a bit of background on multivariate polynomials and
polyharmonic splines.
Figure 6: Effect of a nugget term on hyperparameter selection as $\varepsilon \to 0$. A “nugget term” is a small multiple of the identity that is added to the kernel matrix to get around numerical issues. We show the degrees of freedom (top row) and the LOO-NLL criteria (bottom row) with and without the nugget term (left and right columns). The nugget term equals $10^{-6}I$, we use the Gaussian kernel and the same data as in figure 5.
Figure 7: The matched approximation. The fit in green on the left-hand panel is a GP regression with $\varepsilon = 4$ and 5 degrees of freedom. The kernel is Gaussian. The other coloured curves are other models along the isofreedom curve, with lower values of $\varepsilon$. The isofreedom curve is shown on the right-hand panel. The matched approximation is the limit obtained by following the isofreedom curve all the way to $\varepsilon \to 0$. The corresponding fit is the dashed black curve on the left. See fig. 8 for the same thing with a Matern kernel.

Figure 8: Same as fig. 7 but the kernel used is a Matern kernel with regularity order $r = 2$. The other parameters are identical. Note that the matched approximation fit is now very close to the original fit (even though the original fit has $\varepsilon = 4$).
Figure 9: GP regression compared to its matched approximation (dashed curve). Here we use the Gaussian kernel and $\varepsilon = 2$. The bands around the fit show $\pm$ the standard deviation of the predictive distribution. We denote by $\delta$ the degrees of freedom for the different fits.

Figure 10: Same as fig. 9 but with a Matérn kernel with regularity $r = 3$. 
6.1 Preliminaries and notation

Much of the material here is drawn from \[4, 3\], please refer to these papers for a more extensive background. Much information can also be found in e.g. \[36\].

Let \(x = (x_1, x_2, \ldots, x_d)^\top \in \mathbb{R}^d\). A monomial in \(x\) is a function of the form:

\[
x^\alpha = \prod_{i=1}^{d} x_i^{\alpha_i}
\]

for \(\alpha \in \mathbb{N}^d\) (a multi-index). The degree of a monomial is defined \(|\alpha| = \sum_{i=1}^{d} \alpha_i\). For instance: \(x^{(1,3,1)} = x_1^1x_2^3x_3^1\) has degree 5.

A multivariate polynomial in \(x\) is a weighted sum of monomials in \(x\), and its degree is equal to the maximum of the degrees of its component monomials. As an example, 

\[
-x^{(1,2,1)} + x^{(0,1,1)} + 2x^{(1,0,0)} - 1
\]

is a multivariate polynomial of degree 4 in \(\mathbb{R}^3\).

An important difference between the univariate and the multivariate case is that when \(d > 1\), there are several monomials of any given degree, instead of just one. For instance, with \(d = 2\), the first few monomials are \(x^{(0,0)}\) of degree 0; \(x^{(1,0)}\), \(x^{(0,1)}\) of degree 1; \(x^{(2,0)}\), \(x^{(1,1)}\), \(x^{(0,2)}\) of degree 3. The number of monomials of degree \(k\) in dimension \(d\) is:

\[
\mathcal{H}_{k,d} = \binom{k+d-1}{d-1}\quad \text{(30)}
\]

The notation \(\mathcal{H}_{k,d}\) comes from the notion of homogeneous polynomials.

A homogeneous polynomial is a polynomial made up of monomials with equal degree. Therefore, the set of homogeneous polynomials of degree \(k\) has dimension \(\mathcal{H}_{k,d}\). The set of polynomials of degree \(k\) is spanned by the sets of homogeneous polynomials up to \(k\), and has dimension:

\[
\mathcal{P}_{k,d} = \mathcal{H}_{0,d} + \mathcal{H}_{1,d} + \cdots + \mathcal{H}_{k,d} = \binom{k+d}{d}\quad \text{(31)}
\]

Note that \(\mathcal{P}_{0,d} = 1\) and \(\mathcal{P}_{1,d} = d + 1\). By convention, we will also set \(\mathcal{P}_{-1,d}\) to be equal to 0.

The fact that there are several monomials for each degree in dimension \(d\) is reflected in the structure of the eigenvalues in the flat limit. Previously, in the \(r = \infty\) case, each eigenvalue had a different order in \(\varepsilon\). In the multivariate case, there are blocks of eigenvalues with the same order in \(\varepsilon\), corresponding to a block of homogeneous polynomials of a given degree \(m\). For instance, in \(d = 2\), there is one monomial of degree 0, two monomials of degree 1 (\(x_1, x_2\)), three monomials of degree 2 (\(x_1^2, x_1x_2, x_2^2\)), and in general \(m + 1\) monomials of order \(m\). As first shown in \[28\], these give rise to a single eigenvalue of order \(\varepsilon^0\), two eigenvalues of order \(\varepsilon^2\), three eigenvalues of order \(\varepsilon^4\), etc.

6.1.1 Polynomial bases and orderings

The multivariate flat limit is more complicated than the univariate case, even though the results are substantially the same. The reason why the results are more complicated is fairly deep and boils down to the lack of a natural order on the set of multivariate monomials.

We use in section \[4\] the fact that eigenvectors of smooth kernel matrices tend to discrete polynomials. In dimension \(d = 1\), there is an obvious way to construct a basis of orthogonal polynomials, which is just to apply the Gram-Schmidt process to the monomials \((1, x, x^2, x^3, \ldots)\). The monomials in dimension 1 are naturally ordered by increasing degree. In dimension two, the degree only gives a partial order. For instance, at degree one, even though the constant polynomial is a consensus starting point, we have to decide at degree 1 which of \(x_1\) or \(x_2\) should come first in the Gram-Schmidt process. Depending on which we pick, we get a different orthogonal basis spanning polynomials of degree \(\leq 1\). We could also decide to orthogonalise \(x_1 + x_2\) followed by \(x_1 - x_2\), and get yet another basis. Multivariate orthogonal polynomials are non-unique, and therefore both richer and more complicated than univariate orthogonal polynomials.
To state our results, we need to pick an ordering on the monomials, even though the ordering is immaterial to the actual limits (kernel matrices do not care how we order monomials). The need for an ordering is an annoyance that can probably be lifted by finding a representation that is intrinsically invariant, but we have not found one as yet.

In any event, given an ordering, for an ordered set of points \( \Omega = \{x_1, \ldots, x_n\} \), all in \( \mathbb{R}^d \), we define the multivariate Vandermonde matrix as:

\[
V_{\leq k} = [V_0 \quad V_1 \quad \cdots \quad V_k] \in \mathbb{R}^{n \times \mathcal{P}_{k,d}},
\]

where each block \( V_i \in \mathbb{R}^{n \times \mathcal{P}_{i,d}} \) contains the monomials of degree \( i \) evaluated on the points in \( \Omega \). As an example, consider \( n = 3, d = 2 \) and the ground set

\[
\Omega = \{[y_{01}^1], [y_{02}^2], [y_{03}^3]\}.
\]

One has, for instance for \( k = 2 \):

\[
V_{\leq 2} = \begin{bmatrix}
1 & y_1 & z_1 & y_1^2 & y_1 z_1 & z_1^2
\end{bmatrix},
\]

where the ordering within each block is arbitrary.

We will use \( V_{\leq k}(\mathcal{X}) \) to denote the matrix \( V_{\leq k} \) reduced to its lines indexed by the elements in \( \mathcal{X} \). As such, \( V_{\leq k}(\mathcal{X}) \) has \( |\mathcal{X}| \) rows and \( \mathcal{P}_{k,d} \) columns. The QR decomposition of \( V_{\leq k} \) inherits a natural block structure from \( V_{\leq k} \) corresponding to the degrees of the monomials, i.e., we may split \( Q_{\leq k} \) into blocks \( Q_0, Q_1, \ldots \) where \( Q_i \) comes from the Gram-Schmidt process applied to monomials of degree \( i \) on monomials of lower degree.

What this means for kernel matrices is that the particular limiting eigenbasis that appears as \( \varepsilon \to 0 \) depends more strongly on the kernel than in the univariate case. In a sense, the kernel implicitly selects a particular family of orthogonal polynomials. The specific basis is determined by the so-called Wronskian matrix of the kernel, defined as:

\[
W_{\leq k} = \begin{bmatrix}
k^{(\alpha, \beta)}(0,0)
\end{bmatrix} \in \mathbb{R}^{\mathcal{P}_{k,d} \times \mathcal{P}_{k,d}},
\]

where \( k^{(\alpha, \beta)} \) is the partial derivatives of \( k(x, y) \) with respect to \( x^\alpha \) and \( y^\beta \). Here we index the matrix using multi-indices (equivalently, monomials), so that an element of \( W_{\leq k} \) is e.g., \( W_{(0,2), (2,1)} \) which is a scaled derivative of \( k(x, y) \) of order \((0, 2)\) in \( x \) and \((2, 1)\) in \( y \). For example, for \( d = 2 \) and \( k = 2 \) we may write

\[
W_{\leq 2} = \begin{bmatrix}
k^{((0,0),(0,0))} & k^{((0,0),(1,0))} & k^{((0,0),(1,1))} & k^{((0,0),(2,0))} & k^{((0,0),(2,1))} & k^{((0,0),(2,2))}
\end{bmatrix} \in \mathbb{R}^{\mathcal{P}_{2,2} \times \mathcal{P}_{2,2}}
\]

for a given ordering of the monomials, and where all the derivatives are taken at \( x = 0, y = 0 \). Eq. (33) makes Wronskian matrices look more daunting to compute than they really are. We explain in the appendix how the Wronskian may easily be computed in the stationary case from the Fourier transform of the kernel.

### 6.1.2 Polyharmonic splines

Polyharmonic splines [9] generalise smoothing splines in \( d > 1 \), and play the same role in the flat limit. For our purposes here, the space of polyharmonic splines of order \( r \) in dimension \( d \) for a point set \( \mathcal{X} \) is
given by functions of the form:

\[ f(x) = \sum_{i=1}^{n} \beta_i \|x - x_i\|^{2r-1} + \sum_{|\gamma| < k} \alpha_{\gamma} x^\gamma \]  

(34)

where \( V_{ij}^T \beta = 0 \).

We recognise the general form of semi-parametric models (eq. (49)), where here the parametric part is played by monomials of degree less than \( r \), and the non-parametric part by the radial basis function \( \|x - x_i\|^{2r-1} \). In our notation, polyharmonic spline models are therefore semiparametric models given by

\[ M_r = \left((-1)^r \|y - y\|^{2r-1}; \{x^\alpha | \alpha < r\}\right) \]

Note that polyharmonic splines generalise splines to \( d > 1 \), but they are not piecewise polynomials.

6.2 Smoother matrices in \( d > 1 \)

The smoother matrices in \( d > 1 \) have the same kind of limit as in the univariate case. Depending on the growth rate of \( \gamma, n \) and the regularity of the kernel, sometimes one has polynomials, sometimes splines. The next lemma gives a complete picture, and reexpresses theorem 6.4 from [4] in a form adapted to the GP context. To lighten the notation in the lemma, we define the following matrices, which appear in the flat limit of the eigenvectors:

\[ P_l = Q_l V_l W_l V_l^T Q_l^T \]

(35)

where \( \bar{W}_l \in \mathbb{R}^{H_l,d \times H_l,d} \) is the Schur complement:

\[ \bar{W}_l = W_l - W_l (W_{\leq l-1})^{-1} W_l \]

(36)

in the block description of \( W_{\leq l} \) or

\[ \begin{pmatrix} W_{\leq l-1} & W_l \\ W_l & W_{\leq l} \end{pmatrix} \]

We recall that \( \widetilde{D}^{(2r-1)} \) is the matrix \( D^{(2r-1)} = \left[ \|x_i - x_j\|^{2r-1} \right]_{i,j} \) with monomials of degree \( < r \) projected out, i.e.

\[ \widetilde{D}^{(2r-1)} = (I - Q_{<r} Q_{<r}^T)D^{(2r-1)}(I - Q_{<r} Q_{<r}^T) \]

(37)

The following lemma is not particularly easy to read and the reader may skip ahead to the theorem at no great loss. It generalizes to the multivariate setting the first steps in the proof of theorem 4.2 in the univariate case (see Th. 9.9 and subsections 9.2.2 and 9.2.3).

Lemma 6.1. Let \( \mathcal{X} \subset \Omega \subset \mathbb{R}^d \) with a set of \( |\mathcal{X}| = n \) measurement locations, \( k_\varepsilon \) a kernel with regularity \( r \), \( p \) an integer and \( \gamma(\varepsilon) = \gamma_0 \varepsilon^{-p} \). Then the smoother matrix

\[ M_\varepsilon = K_\varepsilon \left( K_\varepsilon + \frac{\sigma^2}{\gamma(\varepsilon)} I \right)^{-1} \]

has the following expansion in \( \varepsilon \rightarrow 0 \):

\[ M_\varepsilon = A + B \Gamma B^T + \mathcal{O}(\varepsilon) \]

(38)

where \( A \) is a projection matrix, \( B^T A = 0 \), and \( \Gamma \) is diagonal (and in some cases null). \( A, B \) and \( \Gamma \) depend on \( r, n \) and \( p \). First, \( p \) is either even or odd, meaning that only one out of the two following values \( \frac{p}{2}, \frac{p+1}{2} \) is an integer. We call that integer \( l \). The possible limits are:

\[ \text{More precisely, it is a minor variant of the functions actually studied.} \]

\[ \text{26} \]
• If $\mathcal{P}_{l-1,d} \geq n$ or $r < \frac{p + 1}{2}$ then $M_\varepsilon = I + O(\varepsilon)$

• If $r > \frac{p + 1}{2}$ and $p$ is odd, then $\Gamma = 0$ and $A = Q_{<l} Q_{<l}^T$

• If $r > \frac{p + 1}{2}$ and $p$ is even, then $A = Q_{<l} Q_{<l}^T$, $B$ are the (non-null) eigenvectors of $P_l$ (defined above) and $\gamma_{ii} = \frac{\gamma_{0}}{1 + \gamma_0 \lambda_i}$, where $\lambda_i$ is the $i$-th eigenvalue of $P_l$.

• If $r = \frac{p + 1}{2}$, then $A = Q_{\leq r-1} Q_{\leq r-1}^T$ and $B$ are the non-null eigenvectors of $f_{2r-1} D^{(2r-1)}$, $\lambda_i$ its eigenvalues, and $\gamma_{ii} = \frac{\gamma_{0}}{1 + \gamma_0 \lambda_i}$.

In a nutshell, the smoother matrices are in the limit either projection matrices, or the sum of a projection matrix and a smoother matrix. This indicates that the limiting models are generally semi-parametric and occasionally parametric.

### 6.3 Main result in $d > 1$

The generalisation of theorem 4.2 to the multivariate case is:

**Theorem 6.2.** Let $k_r(x, y)$ be a stationary positive-definite kernel for $x, y$ in $\mathbb{R}^d$, with regularity parameter $r$. Let $p$ be an integer. Then the following asymptotic equivalence holds:

$$k_\varepsilon \propto \frac{(l_p; V_p)}{\varepsilon_{\to 0}}$$

where $l_p(x, y)$ and $V_p$ depend on the interplay between $p$ and $r$. There are four different cases:

1. $p < 2r - 1$ and $p$ is even, i.e., $\exists m < r$ s.t. $p = 2m$. Then $l(x, y) = \sum_{|\alpha| = m, |\beta| = m} W_m(\alpha, \beta) x^\alpha y^\beta$, $V = \{x^\gamma | |\gamma| < m\}$. This case amounts to penalised polynomial regression.

2. $p < 2r - 1$ and $p$ is odd, i.e., $\exists m < r - 1$ s.t. $p = 2m + 1$. Then $l(x, y) = 0$, $V = \{x^\gamma | |\gamma| < m\}$.

   This case amounts to unpenalised polynomial regression.

3. $p = 2r - 1$. In this case, $l(x, y) = (-1)^r \|x - y\|^{2r-1}$, $V = \{x^\gamma | |\gamma| < r\}$, which amounts to polyharmonic spline regression.

4. $p > 2r - 1$. This case leads to an interpolant independently of the value of $\sigma^2$ and is not meaningful.

**Proof.** Identical to the final step in the proof of 4.2 after applying lemma 6.1.

We show in appendix 10.1.4 that for separable kernels the Schur complements of the Wronskian (eq. 36) are actually diagonal. For the Gaussian kernel a further simplification is possible, and gives a very compact limit result. The “polynomial kernel” of order $m$ is

$$\rho_m(x, y) = (x^T y)^m$$

and its associated reproducing kernel Hilbert space is the set of monomials in $\mathbb{R}^d$ of degree $m$.

**Corollary 6.3 (Flat limit of Gaussian kernels).** For the Gaussian kernel in $\mathbb{R}^d$, the following equivalence holds as $\varepsilon \to 0$:

1. For even $p = 2m$,

$$k_\varepsilon \propto \frac{(\rho_m; \{x^\gamma | |\gamma| < m\})}{\varepsilon_{\to 0}}$$

2. For odd $p = 2m + 1$

$$k_\varepsilon \propto \frac{\{x^\gamma | |\gamma| < m\}}{\varepsilon_{\to 0}}$$

The proof is given in section 10.1.4. The corollary states that in the flat limit, depending on the level of regularisation, the GP model is either plain (multivariate) polynomial regression, or a SPM with a parametric part of polynomials of degree $< m$, and a “non-parametric” part which is given by the polynomial kernel of degree $m$. 27
6.4 Numerical results

We illustrate our results with a few simulations in dimension 2. We generated a set of 30 random locations in $[0,1]^2$ (sampled uniformly and independently), and noiseless observations $y_i$ from the function $f(x_1, x_2) = \exp \left(-3((x_1 - 0.5)^2 + (x_2 - 0.5)^2) \sin(3(x_1 + x_2))\right)$. Fig. 11 shows (on the left) the contour lines of two GP regressions with $\varepsilon = 1$, one with a Gaussian kernel, the other with a Matérn kernel with $r = 3$. $\gamma$ has been adjusted so that the degrees of freedom equal approximately 12 in both cases. On the right, the corresponding matched approximations (as in section 5.4), respectively multivariate polynomials and polyharmonic splines. Over this range and for this value of $\varepsilon$ the agreement is excellent (but see later for caveats).

While the matched approximation may be surprisingly accurate close to the measurement locations, polynomials and polyharmonic splines generally diverge as $\|x\| \to \infty$, unlike GP models, which return to a baseline of 0. Consequently, the matched approximations are very inaccurate far from the data, as shown in fig. 12, which is just a zoomed-out version of fig. 11. There are ways of tapering the matched approximation to prevent divergence, but we leave the details for future work.

Finally, in the introduction we described the flat limit in terms of the family of fits, seen as a parametric curve (parameterised by $\gamma$). The predictions for the GP with a Gaussian kernel “go through” the polynomial predictions in the limit. The same holds true in the multidimensional case, as per theorem 6.2. For some appropriate value of $\gamma$, the prediction of the GP will come to match that of the model $\left(0; \sum_{|\alpha| \leq k} x^{\alpha}\right)$, a multivariate polynomial model of degree $k$. We show this on fig. 13, which is similar to fig. 2, the prediction of the model at locations $x_a = (0.2, 0.1)$ and $x_b = (0.8, 0.8)$ are plotted for different values of $\gamma$ and fixed $\varepsilon$. 

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Figure 12: Same contents as in fig. 11 but over a broader domain, to show the divergence in the matched approximations.
Figure 13: Prediction of GP model (with Gaussian kernel) vs. polynomial models. We show the predictions of the model for the data shown on fig. 11 for a range of values of $\gamma$ (continuous curves), and two different values of $\varepsilon$. The labelled points are the prediction of the polynomial models of degree 0 to 5. As per theorem 6.2 as $\varepsilon \to 0$, the continuous curve must go through the labelled points.

For kernels with finite regularity index, theorem 6.2 shows that the behaviour in the flat limit depends on $\gamma$. For low values of $\gamma$, they behave like polynomial models. For high values, like polyharmonic splines. This is the behaviour that appears on fig. 14.

7 Conclusion

The flat limit of Gaussian process regression highlights the very strong connections GP methods share with classical methods like polynomial regression and smoothing splines. The fact that, at least in certain cases, the flat limit gives a very good approximation for large values of $\varepsilon$ shows that it may be useful in practice once the limits of the approximation are better understood.

We conclude with some open questions and directions. First, while smoothing splines in $d = 1$ can be implemented at cost $O(n)$ [23], polyharmonic splines in $d > 1$ have cost $O(n^3)$. On the other hand, for Matèrn models with low regularity coefficient, there exist efficient (approximate) methods based on a stochastic PDE formulation [19]. Since such GP models have polyharmonic splines as their flat limit, this suggests that stochastic PDE methods should be applicable.

Second, regression is only one special case of GP methods. GP classification and other latent Gaussian models are even more interesting, although harder to study because the posterior mean and variance do not have a closed form. We believe our results can be extended to general latent Gaussian models via lemma 1 in [7], but this needs to be checked.

Finally, if a tractable “sharp limit” ($\varepsilon \to \infty$) expansion were available, there might be a way of finding good approximations that work over a broad range of values of $\varepsilon$, for instance via matched asymptotic approximations. Such an approximation would be both interesting theoretically and practically useful.

8 Acknowledgments

The authors would like to thank Julyan Arbel for his helpful comments on a preliminary version of this manuscript.

This work was supported by MIAI at Univ. Grenoble Alpes (ANR-19-P3IA-0003), ANR project GenGP (ANR-16-CE23-0008), ANR project LeaFleT (ANR-19-CE23-0021-01), LabEx PERSYVAL-
Figure 14: Prediction of GP model (with Matérn covariance, \( r = 3 \)) vs. polynomial models and polyharmonic spline kernels. The figure uses the same data and principle as in fig. 13 but according to theorem 6.2 this GP model matches polynomials of degree up to 2 at low \( \gamma \), and polyharmonic splines at higher values of \( \gamma \). Accordingly, we show the polynomial predictions for degree up to two (labelled points). The three curves are for decreasing values of \( \varepsilon \), \( \varepsilon = 0.5 \) is in red, \( \varepsilon = 0.15 \) in green and \( \varepsilon = 0.05 \) in purple. The panel to the right shows a zoomed-in version of the rectangle highlighted in the first panel. The dotted curve corresponds to the polyharmonic splines.

Lab (ANR-11-LABX-0025-01), Grenoble Data Institute (ANR-15-IDEX-02), LIA CNRS/Melbourne Univ Geodesic, and partial funding from the IRS (Initiatives de Recherche Stratégiqques) of the IDEX Université Grenoble Alpes.

9 Appendix

9.1 Semi-parametric models as limits

In this section we introduce SPMs as a limit (we do not claim that this is particularly original). This section parallels section 4 in [33]. Readers familiar with DPPs may be interested to note that extended L-ensembles are to semi-parametric GPs what L-ensembles are to GPs, see [10].

Our definition of regression with semi-parametric Gaussian fields is as follows: let \( l(x, y) \) be a kernel (not necessarily positive definite, as we will see), and \( v_1(x), \ldots, v_r(y) \) a set of basis functions. Then semi-parametric GP regression is just GP regression with the kernel

\[
\kappa_\varepsilon(x, y) = l(x, y) + \varepsilon^{-1} \sum_i v_i(x)v_i(y)
\]

in the limit \( \varepsilon \to 0 \). Even though the prior variance goes to infinity along some directions, the posterior distribution is generally well-defined, and quantities like the smoother matrix tend to finite limits. Although the construction naturally works for \( l(x, y) \) positive definite, recall that this is not a requirement, and \( l(x, y) \) may have negative eigenvalues, so long as they align with the subspace spanned by the \( v_i \)'s.

We introduce some notation, borrowed from [33], that will be used throughout this section. A non-negative pair is the discrete counterpart to a SPM \((l; V)\).

**Definition 9.1.** A Nonnegative Pair, noted \((L; V)\) is a pair \( L \in \mathbb{R}^{n \times n}, V \in \mathbb{R}^{n \times p}, 0 \leq p \leq n \), such that \( L \) is symmetric and conditionally positive semi-definite with respect to \( V \), and \( V \) has full column rank. Wherever a NNP \((L; V)\) appears below, we consistently use the following notation:

- \( Q \in \mathbb{R}^{n \times p} \) is an orthonormal basis of span \( V \), such that \( I - QQ^\top \) is a projector on orth \( V \)

---

4Sampling measurement locations from the appropriate extended L-ensemble guarantees for instance that the posterior distribution is proper (integrable).
• \( \tilde{L} = (I - QQ^\top)L(I - QQ^\top) \in \mathbb{R}^{n \times n} \) is also symmetric and thus diagonalisable. From [33, Prop. 2.3] we know that all its eigenvalues are non-negative. We will denote by \( q \) the rank of \( \tilde{L} \). Note that \( q \leq n - p \) as the \( p \) columns of \( Q \) are trivially eigenvectors of \( \tilde{L} \) associated to 0. We write

\[
\tilde{L} = \tilde{U}\tilde{\Lambda}\tilde{U}^\top
\]

its truncated spectral decomposition; where \( \tilde{\Lambda} = \text{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_q) \in \mathbb{R}^{q \times q} \) and \( \tilde{U} \in \mathbb{R}^{n \times q} \) are the diagonal matrix of nonzero eigenvalues and the matrix of the corresponding eigenvectors of \( \tilde{L} \), respectively.

Saddle-point systems feature prominently in our formulas:

**Definition 9.2.** The saddle-point system associated with a NNP \((L, V)\) is the \((2n) \times (n + p)\) matrix:

\[
S(L, V) = \begin{pmatrix} L & V \\ V^\top & 0 \end{pmatrix}
\]

It has the same form as the system that appears in polyharmonic spline interpolation, and this is no accident. Our first step will be to find the limit of the smoother matrix, which here reads:

\[
M_\varepsilon = (L + \varepsilon^{-1}VV^\top)(L + \sigma^2I + \varepsilon^{-1}VV^\top)^{-1} = (\varepsilon L + VV^\top) (\varepsilon(L + \sigma^2I) + VV^\top)^{-1}
\]

(39)

To do so we use matrix perturbation theory (treating \( \varepsilon L \) as a perturbation), and specifically the approach of [2]. The difficulty lies in dealing with \((\varepsilon(L + \sigma^2I) + VV^\top)^{-1}\), which is divergent as \( \varepsilon \to 0 \) since \( VV^\top \) is not invertible. Because of that, it does not admit a power series. However, it does admit a Laurent series, which is an expansion involving negative orders of \( \varepsilon \). We do not need the theory developed in [2] in its full generality for our purposes here. We introduce a simplified version tailored to our needs.

**Theorem 9.3.** Let \( A(\varepsilon) = VV^\top + \varepsilon C \), invertible for \( \varepsilon > 0 \), with \( C \in \mathbb{R}^{n \times n} \) symmetric and \( V \in \mathbb{R}^{n \times p} \), \( p < n \), so that \( VV^\top \) is non-invertible. Then:

\[
A(\varepsilon)^{-1} = \varepsilon^{-1}(B_0 + \varepsilon B_1 + \varepsilon^2 B_2 + \ldots)
\]

(40)

This is a Laurent expansion around \( \varepsilon = 0 \), and its terms \( B_0, B_1, \ldots \) are the solutions of the following equation, called the “master equation”:

\[
VV^\top B_0 = 0 \\
VV^\top B_1 + CB_0 = I \\
VV^\top B_2 + CB_1 = 0 \\
VV^\top B_3 + CB_2 = 0 \\
\vdots
\]

or equivalently:

\[
VV^\top B_i + CB_{i-1} = \delta_{i,1}I
\]

(41)

for \( i \) going from 1 to \( \infty \). In addition, all the terms \( B_0, B_1, \ldots \) are symmetric.

The proof can be found in [2] but straightforward to sketch. The existence of the Laurent expansion (eq. 40) is a consequence of Cramer’s rule. The master equation is obtained by plugging eq. 40 into \( AA^{-1} = I \) and matching terms by order.

Using the Laurent expansion we find:
The conditional expectation way. This fits in with the “semi-parametric regression” interpretation.

\[ M_\varepsilon = QQ^\top + \tilde{U} \tilde{\Lambda} (\tilde{\Lambda} + \sigma^2 I)^{-1} \tilde{U}^\top + O(\varepsilon) \]  

(42)

\[ M_\varepsilon = QQ^\top + \tilde{L} (\tilde{L} + \sigma^2 I)^{-1} + O(\varepsilon) \]  

(43)

**Proof.** We use theorem 9.3 with \( C = L + \sigma^2 I \) in eq. (39), which gives

\[ M_\varepsilon = (\varepsilon (L + VV^\top) (\varepsilon (L + \sigma^2 I) + VV^\top)^{-1} = \varepsilon^{-1}(\varepsilon L + VV^\top)(B_0 + \varepsilon B_1 + \ldots) \]  

(44)

where \( B_0 \) and \( B_1 \) verify the master equation:

\[ VV^\top B_0 = 0 \]

\[ VV^\top B_1 + (L + \sigma^2 I)B_0 = I \]

Expanding in eq. (45), we find:

\[ M_\varepsilon = \varepsilon^{-1}(VV^\top B_0) + (LB_0 + VV^\top B_1) + O(\varepsilon) \]  

(45)

The diverging term \( VV^\top B_0 \) is null by the master equation. Again by the master equation, the constant-order term equals \( I - \sigma^2 B_0 \). We now solve for \( B_0 \). Note that \( VV^\top B_0 = 0 \) implies \( V^\top B_0 = 0 \) (\( V \) is \( n \) times \( p \) and has full rank). Therefore, \( B_0 \) is orthogonal to span \( V \) and we may express \( B_0 \) in a basis that spans the complement of span \( V \). Recall that the notation we introduced, \( Q \) is an orthogonal basis for \( V, \tilde{L} = (I - QQ^\top)L(I - QQ^\top) \in \mathbb{R}^{n \times n} \), and so \( \tilde{L} \) lies in the complement of span \( V \). The (non-null) eigenvectors of \( \tilde{U} \) of \( \tilde{L} \) may therefore be taken as a basis for the complement of span \( V \), and we have that \( B_0 = \tilde{U}Z_0 \) for some matrix \( Z_0 \). Inserting this form into the master equation (in the second term), we have:

\[ VV^\top B_1 + (L + \sigma^2 I)\tilde{U}Z_0 = I \]

Multiplying to the left by \( \tilde{U}^\top \), we have:

\[ \tilde{U}^\top (L + \sigma^2 I)\tilde{U}Z_0 = \tilde{U}^\top \]

\[ \Leftrightarrow Z_0 = \left( \tilde{U}^\top (L + \sigma^2 I)\tilde{U} \right)^{-1} \tilde{U}^\top \]

\[ \Leftrightarrow B_0 = \tilde{U} \left( \tilde{U}^\top (L + \sigma^2 I)\tilde{U} \right)^{-1} \tilde{U}^\top = \left( \tilde{U} \tilde{L} (\tilde{L} + \sigma^2 I)^{-1} \tilde{U}^\top \right)^\dagger \]

by analogy with \( \tilde{L} = (\tilde{U} \tilde{L} \tilde{U} \tilde{L})^\dagger \), we have \( B_0 = (L + \sigma^2 I)^\dagger = (\tilde{L} + \sigma^2 \tilde{U} \tilde{U}^\top)^\dagger = \tilde{U} (\tilde{\Lambda} + \sigma^2 I)^{-1} \tilde{U}^\top \). Inserting this result in eq. (45), we obtain \( M_\varepsilon = I - \sigma^2 \tilde{U} (\tilde{\Lambda} + \sigma^2 I)^{-1} \tilde{U}^\top + O(\varepsilon) \).

Then observe that \( M_\varepsilon \) diagonalises in \((Q, U)\) to finally obtain:

\[ M_\varepsilon = QQ^\top + \sigma^2 \tilde{U} \tilde{\Lambda} (\tilde{\Lambda} + \sigma^2 I)^{-1} \tilde{U}^\top + O(\varepsilon) \]

hence completing the proof.

The expression for the smoother matrix has a simple interpretation: anything in the span of \( V \) goes through unpenalised (for instance, constant and linear trends), and the rest is penalised in the usual way. This fits in with the “semi-parametric regression” interpretation.

Next, we examine the conditional expectation at an unobserved location:

**Corollary 9.5.** The conditional expectation \( \text{E}(f(x)|y) \) has the following expansion in the semi-parametric limit:

\[ \text{E}(f(x)|y) = (I_{x,X} \ v_x) \begin{pmatrix} L + \sigma^2 I & V \\ V^\top & 0 \end{pmatrix}^{-1} \begin{pmatrix} y \\ 0 \end{pmatrix} + O(\varepsilon) \]  

(46)
Proof. We start with:

\[ E(f(x)|y) = (l_{x,X} + \varepsilon^{-1}v_xV^\top)(L + \sigma^2 I + \varepsilon^{-1}VV^\top)^{-1}y \]

and insert the Laurent expansion as previously, to obtain:

\[ E(f(x)|y) = \varepsilon^{-1}(v_xV^\top B_0 y) + (l_{x,X}B_0 + v_xV^\top B_1) y + O(\varepsilon) \]  \hspace{1cm} (47)

As previously, the diverging term disappears since \( V^\top B_0 = 0 \). The master equation for \( B_0 \) can be rewritten as:

\[ \begin{pmatrix} V + \sigma^2 I & V \\ V^\top & 0 \end{pmatrix} \begin{pmatrix} B_0 \\ V^\top B_1 \end{pmatrix} = \begin{pmatrix} I \\ 0 \end{pmatrix} \]  \hspace{1cm} (48)

We may rewrite eq. \( 47 \) as:

\[ E(f(x)|y) = (l_{x,X} v_x) \begin{pmatrix} B_0 \\ V^\top B_1 \end{pmatrix} y + O(\varepsilon) \]

and eq. \( 24 \) is obtained by solving eq. \( 48 \) and injecting the result. \( \square \)

Remark 9.6. By setting \( \sigma^2 = 0 \) in the equation, we recover the interpolation case. One may also verify that setting \( x \in X \) recovers a column of the smoother matrix. In addition, eq. \( 24 \) implies that the function \( f = E(f|y) \) belongs in \( \varepsilon \rightarrow 0 \) to a specific function space:

\[ \hat{f}(x) = \sum_{i=1}^{n} \beta_i l(x, x_i) + \sum_{j=1}^{p} \alpha_j v_j(x) + O(\varepsilon) \]  \hspace{1cm} (49)

This looks at first sight like a function space of dimension \( n + p \) but by eq. \( 24 \) \( V^\top \beta = 0 \), which removes \( p \) degrees of freedom. The first term corresponds to the non-parametric part, the second to the parametric part. The spline basis of eq. \( 10 \) is a special case of this general form.

Finally, we may also obtain the asymptotic predictive variance using the same technique (although it requires going a step further in the master equation):

Corollary 9.7. The conditional expectation \( \text{Var}(f(x)|y) \) has the following expansion in the semi-parametric limit:

\[ \text{Var}(f(x)|y) = l_{x,X} - (l_{x,X} v_x) \begin{pmatrix} L + \sigma^2 I & V \\ V^\top & 0 \end{pmatrix}^{-1} \begin{pmatrix} l_{x,X} \\ v_x \end{pmatrix} + O(\varepsilon) \]  \hspace{1cm} (50)

Proof. We follow the same steps as above, starting with:

\[ \text{Var}(f(x)|y) = l_{x,X} + \varepsilon^{-1}v_xv_x^\top + (l_{x,X} + \varepsilon^{-1}v_xV^\top)(L + \sigma^2 I + \varepsilon^{-1}VV^\top)^{-1}(l_{x,X} + \varepsilon^{-1}Vv_x^\top) \]

\[ = l_{x,X} + \varepsilon^{-1}v_xv_x^\top + \varepsilon^{-2}(l_{x,X} + v_xV^\top)(B_0 + \varepsilon B_1 + \varepsilon B_2 + \ldots)(\varepsilon l_{x,X} + Vv_x^\top) \]

We now extract the terms in the expansion, starting with the lowest valuation:

\[ [\varepsilon^{-2}]\text{Var}(f(x)|y) = -v_xV^\top B_0 Vv_x^\top \]

This term is zero by the master equation. The next order is:

\[ [\varepsilon^{-1}]\text{Var}(f(x)|y) = v_xv_x^\top - v_xV^\top B_1 Vv_x^\top - 2l_{x,X} B_0 Vv_x^\top \]  \hspace{1cm} (51)

The master equation implies \( B_0 V = 0 \), so the last term drops out. We also have \( B_0(L + \sigma^2 I) + B_1 VV^\top = I \), and multiplying to the left by \( VV^\top \) yields \( VV^\top B_1 VV^\top = VV^\top \). Let \( \alpha \) any vector such that \( \alpha V = v_x \). Then

\[ \alpha VV^\top B_1 VV^\top \alpha^\top = v_x V^\top B_1 Vv_x = v_x v_x^\top \]
This shows that \( \varepsilon^{-1} \text{Var}(f(x)|y) = 0 \), and therefore that the conditional variance is not divergent as \( \varepsilon \to 0 \). We now compute the constant-order term:

\[
\varepsilon^0 \text{Var}(f(x)|y) = l_{x,x} - v_x V^T B_2 V v_x^T - 2l_{x,x} B_1 V v_x^T - l_{x,x} B_0 l_{x,x}
\]

(52)

The next order in the master equation is:

\[
VV^T B_2 + (L + \sigma^2 I)B_1 = 0
\]

Multiplying to the right by \( VV^T \), we have:

\[
VV^T B_2 VV^T = -(L + \sigma^2 I)B_1 VV^T
\]

Again using \( \alpha \) such that \( \alpha V = v_x \), we obtain

\[
v_x V^T B_2 V v_x^T = -\alpha (L + \sigma^2 I)B_1 v_x^T
\]

We now inject this result in eq. (52), and re-express it in the following form:

\[
\varepsilon^0 \text{Var}(f(x)|y) = l_{x,x} + \alpha (L + \sigma^2 I)B_1 V v_x^T - 2l_{x,x} B_1 V v_x^T - l_{x,x} B_0 l_{x,x}
\]

(53)

We already note that the master equation for \( B_0 \) is equivalent to (45). Solving for \( B_0 \) and \( V^T B_1 \) is easy and gives in particular \( V^T B_1 = (V^T (V^T (L + \sigma^2 I)^{-1} V)^{-1} V^T (L + \sigma^2 I)^{-1} V)^{-1} v_x^T \). Thus the term containing \( \alpha \) equals \( \alpha (L + \sigma^2 I)B_1 V v_x^T = v_x (V^T (L + \sigma^2 I)^{-1} V)^{-1} v_x^T \).

Collecting the different terms, we can write

\[
\varepsilon^0 \text{Var}(f(x)|y) = l_{x,x} + (l_{x,x} v_x) \begin{pmatrix} B_0 & B_1 V \\ V^T B_1 & - (V^T (L + \sigma^2 I)^{-1} V)^{-1} \end{pmatrix} \begin{pmatrix} l_{x,x} v_x^T \\ 1 \end{pmatrix}
\]

Now, using the block inverse formula allows to show that if \( A \in \mathbb{R}^{n \times n} \) is an invertible matrix \( B \in \mathbb{R}^{n \times p}, p \leq n \) is full rank, then

\[
\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}^{-1} = \begin{pmatrix} A^{-1} - A^{-1} B (B^T A^{-1} B)^{-1} B^T A^{-1} & A^{-1} B (B^T A^{-1} B)^{-1} \\ B^T A^{-1} & - (B^T A^{-1} B)^{-1} \end{pmatrix}
\]

Using this result, we observe that the matrix involved in Eq. (53) is the inverse of

\[
\begin{pmatrix} L + \sigma^2 I & V \\ V^T & 0 \end{pmatrix}
\]

hence finishing the proof. \( \square \)

**Remark 9.8.** It is interesting to develop the inverse of the saddle point matrix. The a posteriori mean then reads

\[
E(f(x)|y) = v_x \beta + l_{x,x} (L + \sigma^2 I)^{-1} (y - V \beta)
\]

(54)

where \( \beta = (V^T (L + \sigma^2 I)^{-1} V)^{-1} V^T (L + \sigma^2 I)^{-1} y \). The estimation is performed after the polynomial trend has been removed. Note that the preceding results corresponds to the Bayesian approach in which \( g \) admits a Gaussian prior and \( \beta \) is chosen Gaussian with an infinite variance, an uninformative prior which however leads to a proper posterior (see e.g. [14]).

### 9.2 Proof of theorem 4.2

As stated in the proof sketch, most of the proof consists in working out what the limiting smoother matrices are. These results can be found implicitly in [4]. The approach we use here is much more direct, however, and hopefully easier to follow.

We start by recalling results from [3] on eigenvalues and eigenvectors in the flat limit. There are two essential facts to keep in mind. One is that most eigenvalues of kernel matrices go to 0 in the flat limit, but they do so at different speeds. The other is that the eigenvectors go to orthogonal polynomials or splines, depending on the regularity of the kernel and the magnitude of the associated eigenvalues.
9.2.1 Asymptotics of the eigenvalues

In the cases we examine, the smoother matrix reads:

\[ M_{\varepsilon} = K_{\varepsilon}(K_{\varepsilon} + \frac{\sigma^2}{\gamma} I)^{-1} = U_{\varepsilon} \text{diag}(\frac{\lambda_i(\varepsilon)}{\lambda_i(\varepsilon) + \frac{\sigma^2}{\gamma}}) U_{\varepsilon}^T \]

We will review the behaviour of the eigenvectors \( U_{\varepsilon} \) later. An interpretation that is helpful to keep in mind is that the smoother matrix acts like a filter: the measurement \( y \) is transformed to the eigenbasis, then (by analogy with the Fourier transform) each discrete “frequency” is scaled by \( \frac{\lambda_i(\varepsilon)}{\lambda_i(\varepsilon) + \frac{\sigma^2}{\gamma}} \), after which the data is transformed back to its original space. The function \( s(\lambda) = \frac{\lambda_i(\varepsilon)}{\lambda_i(\varepsilon) + \frac{\sigma^2}{\gamma}} \) is analogous to a filter response function. It is an increasing function of \( \lambda \) and maps \( \mathbb{R}^+ \) to \([0, 1]\). Notably, if \( \lambda \) is small compared to \( \frac{\sigma^2}{\gamma} \), then \( s(\lambda) \approx 0 \), and if it is large \( s(\lambda) \approx 1 \). In a nutshell, what happens in the flat limit is that eigenvalues grow apart (by orders of magnitude), so that the eigenvalues separate into three groups. A first group is much larger than \( \sigma \), and these have \( s(\lambda) \approx 0 \); a second has approximately the same magnitude as \( \sigma \), and finally a third group is much smaller, and have \( s(\lambda) \approx 0 \). That explains why GPs behave in the flat limit like semiparametric regression (like intrinsic GPs): some directions in \( y \) go through the smoother matrix unchanged, some are penalised, and some are clamped down to 0.

The asymptotics of the eigenvalues of kernel matrices in the flat limit are as follows. If the kernel matrix is analytic in \( \varepsilon \), then the eigenvalues can also be written as analytic functions of \( \varepsilon \), i.e.

\[ \lambda_i(\varepsilon) = \varepsilon^\nu_i \left( \tilde{\lambda}_i + O(\varepsilon) \right) \]

The coefficient \( \nu_i \) is the valuation of the \( i \)-th eigenvalue, and gives the rate at which it vanishes as \( \varepsilon \to 0 \). In a log-log plot of eigenvalues versus \( \varepsilon \), it defines the limiting slope. When \( d = 1 \), the valuation of the eigenvalues is given by the following result (from [3])

\[ \nu_i = \begin{cases} 2(i - 1) & \text{if } i \leq r \\ 2r - 1 & \text{otherwise} \end{cases} \]

Note the dependency on \( r \), the smoothness order of the kernel. Two extreme cases are the Gaussian kernel (\( r = +\infty \)), for which the eigenvalues are \( O(1), O(\varepsilon^2), O(\varepsilon^4), O(\varepsilon^6), \ldots \) and the exponential kernel, which has \( r = 1 \) and eigenvalues that are \( O(1), O(\varepsilon), O(\varepsilon), O(\varepsilon), \ldots \). Kernels with \( r > 1 \) behave like the Gaussian kernel for the first \( r \) eigenvalues, then the next \( n - r \) eigenvalues are all of the same order.

Now consider the asymptotics of terms of the form \( \frac{\lambda_i}{\lambda_i + \frac{\sigma^2}{\gamma}} \), as they appear in the spectral form of the smoother matrix. If \( \gamma \) is constant as a function of \( \varepsilon \), then, for all kernels with \( r \leq 1 \),

\[ \frac{\lambda_1}{\lambda_1 + \frac{\sigma^2}{\gamma}} = \frac{\tilde{\lambda}_1}{\tilde{\lambda}_1 + \frac{\sigma^2}{\gamma}} + O(\varepsilon) \]

and for all \( i > 1 \)

\[ \frac{\lambda_i}{\lambda_i + \frac{\sigma^2}{\gamma}} = O(\varepsilon) \]

All but the first term go to 0 in \( \varepsilon \to 0 \). In the filtering interpretation, that means the smoothing matrix will only let through the part of \( y \) that is proportional to the first eigenvector and everything else will be clamped down to zero. The associated eigenvector is the constant vector, so that the output of the smoother is a constant function. In addition, there will be some regularisation, given by

\[ 0 < \frac{\tilde{\lambda}_1}{\tilde{\lambda}_1 + \frac{\sigma^2}{\gamma}} < 1 \]

The smoother matrix for constant \( \gamma \) then becomes effectively the smoother matrix for a (penalised) polynomial regression of degree 0.

---

\(^{5}\)The requirement that \( K_{\varepsilon} \) be analytic is probably artificial, see [1]
Thus, taking the limit $\varepsilon \to 0$ while keeping $\gamma$ fixed does not lead to very interesting results, since the GP fit tends in that case to a constant function. Precise examination of the asymptotics (more on which below) leads to the conclusion that $\gamma$ must scale as $\varepsilon^{-p}$ for the number of degrees of freedom to stay constant as $\varepsilon$.

As an example, we may take $\gamma = \bar{\gamma} \varepsilon^{-1}$. There are two cases we need to distinguish: $r = 1$ and $r > 1$. If $r > 1$, one may check that $\frac{\lambda_i(\varepsilon)}{\lambda_i(\varepsilon) + \frac{\sigma^2}{\gamma \varepsilon}}$ goes to 1 for $i = 1$, and goes to 0 for $i > 1$. Thus, the fit will now correspond to an unpenalised polynomial regression of degree 0. If $r = 1$, then $\frac{\lambda_i(\varepsilon)}{\lambda_i(\varepsilon) + \frac{\sigma^2}{\gamma \varepsilon}}$ goes to 1 for $i = 1$, then all subsequent terms (from 2 to $n$) equal $\frac{\lambda_i}{\lambda_i + \frac{\sigma^2}{\gamma \varepsilon}} + O(\varepsilon)$. From the filtering point of view, the first eigenvector goes through unpenalised, then everything goes through with a penalty. This is the signature of a semiparametric model, and indeed it is. As we will see later, in this case the parametric part is the constant function, and the non-parametric part is made up of linear splines.

The general pattern of the results has much in common with what we have seen so far. $\gamma$ needs to rise as $\varepsilon \to 0$, and by controlling the ratio $\gamma/\varepsilon$, we control how many eigenvectors go through unpenalised, penalised, or not at all. Asymptotically we need $\gamma = \bar{\gamma} \varepsilon^{-p}$, and the asymptotics will depend on the parity of $p$.

In the theorems stated here we take $\gamma = \varepsilon^{-p} \bar{\gamma}$. The first result concerns the smoother matrix and follows directly from the spectral asymptotics in [3]. We introduce $D^{(2r-1)}$ the matrix $D^{(2r-1)} = \left[\left\|x_i - x_j\right\|^{2(r-1)}\right]_{i,j}$ with monomials of degree $< r$ projected out, i.e. obtained using a QR decomposition.

$$D^{(2r-1)} = (I - Q_<,Q_>^\top)D^{(2r-1)}(I - Q_<,Q_>)$$ (55)

$Q_<$ being and orthogonal basis for $V_{<r}$, e. g. obtained using a QR decomposition. We can state:

**Theorem 9.9.** Let $k$ a stationary kernel with regularity order $r \in \mathbb{N}^+$, given $n$ observations on the real line $\{x_1, \ldots, x_n\}$ the smoother matrix $M_\varepsilon = \gamma K(\gamma K + \sigma^2 I)^{-1}$ has the following expansion as $\varepsilon \to 0$: $M_\varepsilon = \tilde{U} F_\varepsilon \tilde{U}^\top + O(\varepsilon)$ where $\tilde{U}$ is the matrix of limiting eigenvectors and $F_\varepsilon$ is a diagonal (“filter”) matrix with entries

$$F_{\varepsilon,i,i} = \begin{cases} \frac{\tilde{\lambda}_i}{\lambda_i + \frac{\gamma^2}{\sigma^2} \varepsilon^{p-2(i-1)}} & \text{if } i \leq r \\ \frac{\tilde{\lambda}_i}{\lambda_i + \frac{\gamma^2}{\sigma^2} \varepsilon^{p-2(r-1)}} & \text{otherwise} \end{cases}$$ (56)

The limiting eigenvectors are similarly partitioned as:

$$U = \left[Q_{\leq \min(n,r)} \tilde{U}\right]$$

where $V = QR$ is the QR decomposition of $V$ and $\tilde{U}$ are the eigenvectors of $D^{(2r-1)}$, as defined above. If $r > n$ then $U = Q$.

**Proof.** This follows directly from noting that (by Rellich’s theorem) $\gamma K(\gamma K + \sigma^2 I)^{-1} = U(\varepsilon) \tilde{F}_\varepsilon U(\varepsilon)^\top$ with $U(\varepsilon)$ analytic, and $F_{\varepsilon,i,i} = \frac{\tilde{\lambda}_i(\varepsilon)}{\lambda_i(\varepsilon) + \frac{\gamma^2}{\sigma^2} \varepsilon^{p-2(i-1)}}$ and filling in the results of [3].

Note that the theorem includes the case $r \geq n$. In this case, the result is independent of the regularity parameter $r$ and is equivalent to the infinite smooth case.

We can now study the flat limit when $\varepsilon$ goes to 0.

**9.2.2 Smooth case, or $r > n$**

In this case all the eigenvalues are $O(\varepsilon^{2(i-1)})$. Thus we get:

- $p \geq 2n - 1$, then $F_{\varepsilon,i,i} \to i = 1, \ldots, n, M_\varepsilon \to I$ and $\text{Tr}(M_\varepsilon) \to n$.

This corresponds to the polynomial interpolation of $n$ points by a polynomial of order $n - 1$. 37
In the non-smooth case, all eigenvalues have order at most 2.

2.3 Non-smooth case or $r < n$

1. For every odd $r$ and restricting to the case equivalence in the sense of definition 4.1. Then we obtain, using the results of the two preceding sections, that the predictive mean and variance depend smoothly on $M$ always of the form $M = \frac{\lambda_{n+1} - 1}{\lambda_i + \frac{2}{r}}$, 0 otherwise.

Thus $M \rightarrow Q \leq l, Q^T \leq l$ and $\text{Tr}(M) \rightarrow l$.

This corresponds to a (unpenalised) regression by a polynomial of order $l - 1$.

• for $p > 2r - 1$, we obtain an interpolation, since all eigenvalues of the smoother matrix go to 1.

• for $p = 2r - 1$, $F_{r,i} \rightarrow r, \forall i = 1, \ldots, l = [p/2 + 1]$, 0 otherwise. Thus $M \rightarrow Q \leq l + \frac{\lambda_{p/2+1}^{r+1}}{\lambda_{p/2+1}^{r+1} + \sigma^2} q_{p/2+1} q^T_{p/2+1}$ and $\text{Tr}(M) \rightarrow p/2 + \frac{\lambda_{p/2+1}^{r+1}}{\lambda_{p/2+1}^{r+1} + \sigma^2}$.

This corresponds to a penalised polynomial regression (the order is controlled by a balance between the observation noise and the importance (as measured by the eigenvalue) of a higher order monomial).

9.2.3 Non-smooth case or $r < n$

In the non-smooth case, all eigenvalues have order at most $2r - 1$ in $\varepsilon$.

• for $p > 2r - 1$, we obtain an interpolation, since all eigenvalues of the smoother matrix go to 1.

• for $p = 2r - 1$, $F_{r,i} \rightarrow r, \forall i = 1, \ldots, r$ and $\frac{\lambda_i - 1}{\lambda_i + \frac{2}{r}}$, $\forall i = r + 1, \ldots, n$.

Thus $M \rightarrow Q \leq l + \frac{\lambda_{p/2+1}^{r+1}}{\lambda_{p/2+1}^{r+1} + \sigma^2} q_{p/2+1} q^T_{p/2+1}$ and $\text{Tr}(M) \rightarrow p/2 + \frac{\lambda_{p/2+1}^{r+1}}{\lambda_{p/2+1}^{r+1} + \sigma^2}$.

This corresponds to a penalised polynomial regression (the order is controlled by a balance between the observation noise and the importance (as measured by the eigenvalue) of a higher order monomial).

Remark 9.10. Some examples will clarify the meaning of this result. For the Gaussian kernel, $r = \infty$ and so for every odd $r$ the smoother matrix goes to $Q \leq l, Q^T \leq l$ ($l = (r - 1)/2$), the smoother matrix of a polynomial regression of degree $l$. For the exponential kernel, $r = 1$, and so for $p = 1$ the smoother matrix goes to the smoother matrix of a polyharmonic spline regression of degree 1. For $p$ larger than 1 all eigenvalues go to 1 and so the limit is an interpolation.

9.2.4 Final step of the proof, equivalent asymptotic models

The final step of the proof uses the results of section 3. The limit of smoother matrices, which is always of the form $M = M_0 + O(\varepsilon)$. Examining the proof of lemma 3.2 and proposition 3.3, we see that the predictive mean and variance depend smoothly on $M$ and so we have asymptotic predictive equivalence in the sense of definition 4.1. Then we obtain, using the results of the two preceding sections, and restricting to the case $r < n$:

• $p$ even: The model converges to $(l_p, V_p)$ where the kernel associated is $l_p(x, y) = x^{p/2+1} y^{p/2+1}$ and the basis functions given by the monomials up to order $p/2$, or $V_p = (1, x, x^2, \ldots, x^{p/2})$.

• $p$ odd: The model converges in this case to $(l_p, V_p)$ where the kernel associated is $l_p(x, y) = 0$ and the basis functions given by the monomials up to order $[p/2 + 1]$, or $V_p = (1, x, x^2, \ldots, x^{p/2+1})$.

• $p = 2r - 1$: The model converges to $(l_p, V_p)$ where the kernel associated is $l_p(x, y) = (-1)^r |x - y|^{2r-1}$ and the basis functions given by the monomials up to order $r - 1$, or $V_p = (1, x, x^2, \ldots, x^{r-1})$.

This concludes the proof.
10 Wronskians

10.1 Wronskian matrices from spectral representation

In this section we derive some properties of the Wronskian matrices of stationary kernel functions from their spectral representation. For stationary kernels, we may write \( k(\mathbf{x}, \mathbf{y}) = \kappa(\mathbf{x} - \mathbf{y}) \).

Bochner’s theorem \[32\] tells us that \( \kappa \) may be written as:

\[
\kappa(\mathbf{x} - \mathbf{y}) = \int_{\mathbb{R}^d} \exp(\mathbf{i} \omega^\top (\mathbf{x} - \mathbf{y})) \, d\mu(\omega)
\]

(57)

where \( \mu \) is a positive measure (the spectral measure). In fact, there is a one-to-one correspondence between measures and kernel functions. Assume further that \( \mu \) has a density \( i.e. is absolutely continuous relative to the Lebesgue measure on \( \mathbb{R}^d \)). Then eq. (57) can be rewritten as:

\[
\kappa(\mathbf{x} - \mathbf{y}) = \int_{\mathbb{R}^d} \exp(\mathbf{i} \omega^\top (\mathbf{x} - \mathbf{y})) \, g(\omega) \, d\omega
\]

(58)

where \( g = \mu' \) is the density corresponding to the spectral measure \( \mu \), called the spectral density. Eq. (58) implies that in this case \( \kappa \) and \( g \) are Fourier transform pairs. Since integrable functions have continuous Fourier transforms, if \( \kappa \) is integrable it has a spectral density.

We follow the normalisation convention of \[32\] and note:

\[
g(\omega) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(-\mathbf{i} \omega^\top \mathbf{x}) \, \kappa(\mathbf{x}) \, d\mathbf{x}
\]

(59)

the spectral density of the kernel. The spectral representation of \( k \) lets us link the Wronskian matrix to moments of \( g \). Partial derivatives \( k^{(\alpha, \beta)} \) of \( k \) may be computed as:

\[
\frac{\partial |\alpha|+|\beta|}{\partial x^\alpha \partial y^\beta} k(\mathbf{x}, \mathbf{y}) = \frac{\partial |\alpha|+|\beta|}{\partial x^\alpha \partial y^\beta} \int_{\mathbb{R}^d} \exp(\mathbf{i} \omega^\top (\mathbf{x} - \mathbf{y})) \, d\mu(\omega)
\]

\[
= \int_{\mathbb{R}^d} |\alpha|+|\beta| (\omega^{\alpha+\beta} \exp(\mathbf{i} \omega^\top (\mathbf{x} - \mathbf{y})) \, d\mu(\omega)
\]

Thus, the \((\alpha, \beta)\) element of the Wronskian matrix equals:

\[
W_{\alpha, \beta} = \frac{1}{\alpha! \beta!} k^{(\alpha, \beta)}(0, 0)
\]

\[
= \frac{1}{\alpha! \beta!} \int_{\mathbb{R}^d} |\alpha|+|\beta| (\omega^{\alpha+\beta} \exp(\mathbf{i} \omega^\top (\mathbf{x} - \mathbf{y})) \, d\mu(\omega)
\]

\[
= \frac{1}{\alpha! \beta!} |\alpha|+|\beta| (\omega^{\alpha+\beta} \exp(\mathbf{i} \omega^\top (\mathbf{x} - \mathbf{y})) \, d\mu(\omega)
\]

\[
= \frac{1}{\alpha! \beta!} |\alpha|+|\beta| (\omega^{\alpha+\beta} \exp(\mathbf{i} \omega^\top (\mathbf{x} - \mathbf{y})) \, d\mu(\omega)
\]

(60)

where \( E_\mu \) designates expectation under \( g \) (note that \( g \) is not normalised). In general, not all moments of \( g \) exist, which is an equivalent way of stating that not all derivatives exist \[32\]. The fact that \( g \) is symmetric around the origin immediately yields that \( E_\mu (\omega^{\alpha+\beta}) \neq 0 \) if and only if \( |\alpha + \beta| \) is even. We obtain the following compact expression:

\[
W_{\alpha, \beta} = \begin{cases}
\frac{1}{\alpha! \beta!} (-1)^{p+|\beta|} E_\mu (\omega^{\alpha+\beta}) & \text{if } |\alpha + \beta| = 2p, p \in \mathbb{Z} \\
0 & \text{otherwise}
\end{cases}
\]

Remark 10.1. In certain cases further simplification is possible. If the kernel function is separable (which is the case for instance for the squared-exponential kernel), then \( g \) is a product distribution: \( g(\omega) = \prod_{j=1}^d p(\omega_j) \), and \( E_\mu (\omega^{\alpha+\beta}) = \prod_{j=1}^d E_{\mu_j} (\omega_j^{\alpha_j+\beta_j}) \). In the special case of Matérn kernels, \( g \) is a multivariate Student’s \( t \) distribution, and a simple expression for the moments can be found in \[16\].
We now use eq. (60) to prove that Wronskians are positive-definite. The positive-definiteness is strict as long as the spectral density exists.

**Lemma 10.2.** Let \( W_m = [W_{\alpha,\beta}]_{\alpha,\beta \in \mathbb{P}_m} \) the Wronskian (of order \( m \)) of a stationary kernel of order \( r \geq m \). Then \( W_m \geq 0 \). Further, if the kernel has a spectral density then \( W_m > 0 \).

**Proof.** We will show that \( W_m \) is a Gram matrix, which implies positive-definiteness. Consider the following sequence of functions: \( \Psi_\gamma(\omega) = \frac{1}{\gamma!}(\omega)^\gamma \) where \( \gamma \) runs over \( \mathbb{P}_m \). We define a dot product from \( q \):

\[
<\phi, \eta> = \int_{\mathbb{R}^d} \phi(\omega)\overline{\eta(\omega)}d\mu(\omega)
\]

Then:

\[
<\psi_\alpha, \psi_\beta> = \int \frac{1}{\alpha!}(i\omega)^\alpha \overline{\frac{1}{\beta!}(i\omega)^\beta}d\mu(\omega) = \frac{1}{\alpha!\beta!}(-1)^{\beta - |\beta|} \int (\omega)^{\alpha+|\beta|}d\mu(\omega) = W_{\alpha,\beta}
\]

which verifies that \( W \) is indeed a Gram matrix, and implies \( W \geq 0 \). To go further and prove positive-definiteness, we now assume that the spectral density exists. Consider the quadratic form \( p^\top W p \), with \( p \neq 0 \):

\[
p^\top W p = \sum_{\alpha,\beta} p_\alpha W_{\alpha,\beta} p_\beta = \sum_{\alpha} p_\alpha <\psi_\alpha, \psi_\beta> p_\beta = <\sum_{\alpha} p_\alpha \psi_\alpha, \sum_{\beta} p_\beta \psi_\beta> = \left\| \sum_{\alpha} p_\alpha \psi_\alpha \right\|^2_\mu
\]

where \( \|f\|_\mu^2 \) is the norm induced by the dot product we have defined, i.e.:

\[
\|f\|_\mu^2 = \int_{\mathbb{R}^d} f(\omega)\overline{f(\omega)}q(\omega)d\omega
\]

Obviously, \( \|f\|_\mu^2 = 0 \) if and only if \( f \) vanishes almost everywhere on the support of \( \mu \).

Recall that the set of functions \( \psi_\alpha \) is a subset of the monomials (up to scaling). In eq. (61) \( \eta_\mu(\omega) = \sum p_\alpha \psi_\alpha(\omega) \) is a complex-valued polynomial of degree \( m \), so \( \|\eta_\mu(\omega)\|_\mu^2 \neq 0 \) unless \( \eta_\mu(\omega) = 0 \) almost everywhere on the support of \( \mu \). Since \( \mu \) is absolutely continuous w.r.t the Lebesgue measure on \( \mathbb{R}^d \), the support of \( \mu \) is a \( d \)-dimensional subset of \( \mathbb{R}^d \). Polynomials in \( \mathbb{R}^d \) can only vanish on a subspace of dimension less than \( d \), so \( \|\eta_\mu(\omega)\|_\mu^2 > 0 \) for all non-zero \( p \).

\[
\square
\]

### 10.1.1 Expressions for the Wronskian in some special cases

The Wronskian for the squared exponential kernel can be worked out directly from eq. (60) and known formulas for Gaussian moments. The spectral density of the squared exponential kernel equals:

\[
q(\omega) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(-i\omega^\top x)\exp(-\|x\|^2/2)dx = \frac{1}{(2\sqrt{\pi})^d} \exp(-\|\omega\|^2/4)
\]

which is the (normalised) density of a \( d \)-dimensional Gaussian vector with independent entries of variance \( \sigma^2 = 2 \). The \( p \)-th moment of a univariate, centered Gaussian variate \( z \) equals \( E(z^p) = \sigma^p(p-1)!! \).
In this section we consider Matérn kernels with regularity parameter $\nu$.

### 10.1.3 Wronskian matrix of Matérn kernels

In the exponential case the orthogonal polynomials of the measure are the Hermite polynomials.

If $p$ is even, and 0 otherwise. Here $n!!$ designates the so-called “double factorial”, which if $n$ is odd, equals the product $n(n-2)(n-4)\ldots 1$. Since $q$ is separable, we have:

$$E_\mu(\omega^\gamma) = \begin{cases} \prod_{i=1}^d 2^{\gamma_i/2}(\gamma_i - 1)!! & \text{if } \gamma_1, \ldots, \gamma_d \text{ even} \\ 0 & \text{otherwise} \end{cases}$$  \quad (64)

Injecting eq. (63) into eq. (60), we obtain:

$$W_{\alpha,\beta} = \begin{cases} \frac{(\alpha+\beta-1)!!}{\alpha!\beta!}(-2)^{\alpha+\beta}(-1)^\beta & \text{if } \alpha_1 + \beta_1, \ldots, \alpha_d + \beta_d \text{ even} \\ 0 & \text{otherwise} \end{cases}$$  \quad (65)

### 10.1.2 The Wronskian matrix and orthogonal polynomials

Let $h_0, \ldots, h_s$ denote the first $s$ orthogonal polynomials of the spectral measure. There is a close relationship between the orthogonal polynomials and the matrix of moments:

$$E(\omega^{\alpha+\beta}) = E(\omega^\alpha \omega^\beta)$$

$$= E\left( \sum_{|\gamma| \leq |\alpha|} A_{\gamma,\alpha} h_\gamma(\omega) \right) \left( \sum_{|\gamma| \leq |\beta|} A_{\gamma,\beta} h_\gamma(\omega) \right)$$

$$= \sum_{\beta,\gamma} A_{\gamma,\beta} A_{\gamma,\beta} E(h_\gamma h_{\gamma'})$$

$$= \sum_{\beta} A_{\gamma,\beta} A_{\gamma,\beta} E(h_\gamma^2)$$

$$= (AHA^\top)_{\alpha,\beta}$$  \quad (66)

which gives an LDLt decomposition of the matrix of moments (H is diagonal and its diagonal values are the energies of the orthogonal polynomials). Using the same trick as in the previous section, and defining $B_{\alpha,\gamma} = \frac{\alpha!}{\alpha!} A_{\alpha,\gamma}$, we find the LDL* decomposition of $W$, specifically:

$$W = BHB^*$$

\quad (67)

In certain cases the elements of $B$ are available in closed-form. For example in the squared-exponential case the orthogonal polynomials of the measure are the Hermite polynomials.

### 10.1.3 Wronskian matrix of Matérn kernels

In this section we consider Matérn kernels with regularity parameter $\nu$, with spectral density as in [37], p.84:

$$q(\omega) = \frac{(2\sqrt{\pi})^d \Gamma(\nu+d/2)(2\nu)^\nu}{\Gamma(n)} \left( 2\nu + 4\pi^2 \|\omega\|^2 \right)^{-\nu-d/2}$$

One may verify that this is also the density of a multivariate $t$-distribution, with degrees of freedom $2\nu$. The $t$-distribution has finite moments of order $2\nu - 1$, so that the order of regularity $r$ of the kernel equals $2\nu$. For instance, if $\nu = 1/2$, then $q(\omega)$ is integrable but has no other finite moments exist, meaning equivalently the kernel function is not differentiable. The Matérn kernel with $\nu = 1/2$ is actually the exponential kernel. The moments of $q$ are given in [16], p. 11. For all $\gamma$ such that $|\gamma| < 2\nu$:

$$E_\mu(\omega^\gamma) = \begin{cases} \prod_{i=1}^d \frac{2^{\gamma_i/2}(\gamma_i - 1)!!}{(2\nu-\gamma_i/2)!!} & \text{if } \gamma_1, \ldots, \gamma_d \text{ even} \\ 0 & \text{otherwise} \end{cases}$$  \quad (69)

Injecting (69) into (60), we obtain:

$$W_{\alpha,\beta} = \begin{cases} \frac{(\alpha+\beta-1)!!(2\nu-\alpha-\beta-2)!!}{\alpha!\beta!(2\nu-\alpha-\beta-2)!!}(-2\nu)^{\alpha+\beta}(-1)^\beta & \text{if } \alpha_1 + \beta_1, \ldots, \alpha_d + \beta_d \text{ even} \\ 0 & \text{otherwise} \end{cases}$$  \quad (70)
The multivariate t-distribution is a scale mixture of Gaussians, which makes the moments tractable. Other kernels that have a scale mixture as their spectral density should also have tractable Wronskians.

10.1.4 Inverse and Schur complements of Wronskian matrices for separable kernels

Theorem 6.2 involves Schur complements in the Wronskian matrix (eq. (36)). A result in [15] shows that these Schur complements are diagonal for separable kernels. Indeed, rephrased for our need, we have:

**Theorem 10.3** (Th. 3.1 in [15]). Consider a random vector $X$ with values in $\mathbb{R}^d$ and with product measure $p(X) = \prod_{i} p(X_i)$. Let $M_k \in \mathbb{R}^{P_k \times P_k}$ be the moment matrix with entries $M_{\alpha, \beta} = E_{p}[X^\alpha X^\beta]$. Note that the maximal degree of the multiindexes considered is $k$.

Then $M_{-1}^{-1}$ can be different from 0 if and only if $\sum_{i=1}^{d} \max(\alpha_i, \beta_i) \leq k$.

Alternately, $M_{-1}^{-1}$ is necessarily zero (called a congenital zero in [15]) iff $\sum_{i=1}^{d} \max(\alpha_i, \beta_i) > k$.

As an example, consider $d = 2$ and $k$ up to 3. The pattern provided by the theorem is depicted in the following matrices: all the entries $\star$ can take different values from zero, all the others are necessarily 0:

$$M_1^{-1} = \begin{pmatrix}
(0,0) & (1,0) & (0,1) \\
(1,0) & * & 0 \\
(0,1) & * & *
\end{pmatrix}$$

$$M_2^{-1} = \begin{pmatrix}
(0,0) & (1,0) & (0,1) & (2,0) & (1,1) & (0,2) \\
(0,1) & * & * & * & * & 0 \\
(2,0) & * & 0 & * & * & * \\
(1,1) & * & 0 & 0 & 0 & *
\end{pmatrix}$$

$$M_3^{-1} = \begin{pmatrix}
(0,0) & (1,0) & (0,1) & (2,0) & (1,1) & (0,2) & (3,0) & (2,1) & (1,2) & (0,3) \\
(1,0) & * & * & * & * & * & * & * & * & 0 \\
(0,1) & * & * & * & * & * & * & * & * & 0 \\
(2,0) & * & * & 0 & * & * & 0 & * & * & 0 \\
(1,1) & * & * & 0 & * & * & 0 & * & * & 0 \\
(0,2) & * & 0 & * & * & * & * & * & * & 0 \\
(3,0) & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(2,1) & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(1,2) & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(0,3) & * & * & * & * & * & * & * & * & *
\end{pmatrix}$$

Since the Schur complements we need are diagonal subblocks $M_{-1, \alpha}$ for $|\alpha| = k$, Th. 3.1 in [15] directly shows that these are diagonal! This result allows to prove corollary 6.3.

10.1.5 Proof of corollary 6.3

We just have to prove that the flat limit kernel for the Gaussian kernel rescaled by $\varepsilon^{-p}$ is $\rho_p(x, y) = (x^\top y)^{p/2}$ for even $p$.

From the main result 6.2 we know that the limiting kernel in this case is $l(x, y) = \sum_{|\alpha| = m, |\beta| = m} W_m(\alpha, \beta)x^\alpha y^\beta$. Since $W_m(\alpha, \beta)$ is diagonal this reduces to $l(x, y) = \sum_{|\alpha| = m} \mathcal{H}_{m,d} W_m(\alpha, \alpha)x^\alpha y^\alpha$, where we recall that $\mathcal{H}_{m,d}$ is the number of monomials of degree $m$ in dimension $d$. 

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\( W_m(\alpha, \alpha) \) are the diagonal terms of the Schur complement discussed above. From elementary block inverses lemma, we know that the Schur complement needed is the inverse of the corresponding block in the inverse of \( W_m \).

Let \( \Delta_\alpha \) be a diagonal matrix with elements \( i^{\alpha_1}/\alpha! \). Then \( W_m = \Delta_\alpha M_m \Delta_\alpha^{-1} \). Thus \( W_m^{-1} = \Delta_\alpha^{-1} M_m^{-1} \Delta_\alpha^{-1} \). Since the block we are interested in is diagonal, we end up with \( W_m(\alpha, \alpha) = 1/(\alpha!^2 M_m^{-1}(\alpha, \alpha)) \). We thus need to calculate the diagonal terms in the inverse of the moment matrix.

To do so, a trick is to use the orthonormal polynomials associated to the measure at end (here the isotropic Gaussian, see above). Writing the orthonormal polynomials as

\[ p_{\alpha} \]

implies that the orthonormal polynomials \( p_{\alpha} \) of degree \( \alpha \) is lower triangular (orthogonality) and invertible. Therefore, \( I = D M_m D^\top \) so that \( M_m^{-1} = D^\top D \). Thus, \( M_m^{-1}(\alpha, \alpha) = \sum_{\gamma \leq \alpha} d_{\alpha, \gamma} \), since in the block of order \( m \) all terms but the diagonal terms are equal to zero. Now, \( d_{\alpha, \alpha} \) may be found using the norm of the polynomial \( p_{\alpha} \) which writes \( E p_{\alpha} p_{\beta} = \delta_{\alpha, \beta} = \sum_{\gamma \leq \alpha, \rho \leq \beta} d_{\gamma, \rho} M_m(\gamma, \rho) d_{\beta, \rho} \). Note that the matrix \( D \) with entries \( d_{\alpha, \beta} \) is lower triangular (orthogonality) and invertible. Therefore, \( I = D M_m D^\top \) so that \( M_m^{-1} = D^\top D \).

The final twist here uses the fact that the measure is a product measure \( E \), thus simply the norm of the Hermite polynomial of degree \( \alpha \). For our case, \( d_{\alpha, \alpha} = 1/(2^\alpha \alpha! \alpha!) \) so that \( d_{\alpha, \alpha} = 1/(2^{\alpha(\alpha+1)} \alpha!) \) and \( W_m(\alpha, \alpha) = 2^{\alpha(\alpha+1)} \alpha! / \alpha! \). Thus \( l(x, y) \propto \sum_{|\alpha| = m!} \alpha!^2 x^\alpha y^\alpha = (x^T y)^m \). Since proportionality here leads do prediction-equivalence, this ends the proof of corollary 6.3.

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