Sparse Convolved Multiple Output Gaussian Processes

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Abstract

Recently there has been an increasing interest in methods that deal with multiple outputs. This has been motivated partly by frameworks like multitask learning, multisensor networks or structured output data. From a Gaussian processes perspective, the problem reduces to specifying an appropriate covariance function that, whilst being positive semi-definite, captures the dependencies between all the data points and across all the outputs. One approach to account for non-trivial correlations between outputs employs convolution processes. Under a latent function interpretation of the convolution transform we establish dependencies between output variables. The main drawbacks of this approach are the associated computational and storage demands. In this paper we address these issues. We present different sparse approximations for dependent output Gaussian processes constructed through the convolution formalism. We exploit the conditional independencies present naturally in the model. This leads to a form of the covariance similar in spirit to the so called PITC and FITC approximations for a single output. We show experimental results with synthetic and real data, in particular, we show results in pollution prediction, school exams score prediction and gene expression data.

Keywords: Gaussian processes, convolution processes, sparse approximations, multitask learning, structured outputs, multivariate processes.

1. Introduction

Accounting for dependencies between model outputs has important applications in several areas. In sensor networks, for example, missing signals from temporal failing sensors may be predicted due to correlations with signals acquired from other sensors (Osborne et al. 2008). In geostatistics, prediction of the concentration of heavy pollutant metals (for example, Copper), that are expensive to measure, can be done using inexpensive and over-sampled variables (for example, pH) as a proxy. Within the machine learning community this approach is sometimes known as multitask learning. The idea in multitask learning is that information shared between the tasks leads to improved performance in comparison to learning the same tasks individually (Caruana 1997).

In this paper, we consider the problem of modeling related outputs in a Gaussian process (GP). A Gaussian process specifies a prior distribution over functions. When using a GP for multiple related outputs, our purpose is to develop a prior that expresses correlation between the outputs. This information is encoded in the covariance function. The class of valid
covariance functions is the same as the class of reproducing kernels. Such kernel functions for single outputs are widely studied in machine learning (see, for example, Rasmussen and Williams 2006). More recently the community has begun to turn its attention to covariance functions for multiple outputs. One of the paradigms that has been considered (Teh et al. 2005; Osborne et al. 2008; Bonilla et al. 2008) is known in the geostatistics literature as the linear model of coregionalization (LMC) (Journel and Huijbregts 1978; Goovaerts 1997). In the LMC, the covariance function is expressed as the sum of Kronecker products between coregionalization matrices and a set of underlying covariance functions. The correlations across the outputs are expressed in the coregionalization matrices, while the underlying covariance functions express the correlation between different data points.

Multitask learning has also been approached from the perspective of regularization theory (Evgeniou and Pontil 2004; Evgeniou et al. 2005). These multitask kernels are obtained as generalizations of the regularization theory to vector-valued functions. They can also be seen as examples of LMCs applied to linear transformations of the input space.

The linear model of coregionalization is a rather restrictive approach to constructing multiple output covariance functions. Each output can be thought of as an instantaneous mixing of the underlying signals/processes. An alternative approach to constructing covariance functions for multiple outputs employs convolution processes (CP). To obtain a CP in the single output case, the output of a given process is convolved with a smoothing kernel function. For example, a white noise process may be convolved with a smoothing kernel to obtain a covariance function (Barry and Hoef 1996; Hoef and Barry 1998). Higdon (2002) noted that if a single input process was convolved with different smoothing kernels to produce different outputs, then correlation between the outputs could be expressed. This idea was introduced to the machine learning audience by Boyle and Frean (2005). We can think of this approach to generating multiple output covariance functions as a non-instantaneous mixing of the base processes.

The convolution process framework is an elegant way for constructing dependent output processes. However, it comes at the price of having to consider the full covariance function of the joint GP. For \( D \) output dimensions and \( N \) data points the covariance matrix scales as \( DN \) leading to \( O(N^3D^3) \) computational complexity and \( O(N^2D^2) \) storage. We are interested in exploiting the richer class of covariance structures allowed by the CP framework, but reducing the additional computational overhead they imply.

In this paper, we propose different sparse approximations for the full covariance matrix involved in the multiple output convolution process. We exploit the fact that, in the convolution framework, each of the outputs is conditional independent of all others if the input process is fully observed. This leads to an approximation that turns out to be strongly related to the partially independent training conditional (PITC) (Quiñonero Candela and Rasmussen 2005) approximation for a single output GP. This analogy inspires us to consider a further conditional independence assumption across data points. This leads to an approximation which shares the form of the fully independent training conditional (FITC) approximation (Snelson and Ghahramani 2006; Quiñonero Candela and Rasmussen 2005).

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1. In this paper we will use kernel to refer to both reproducing kernels and smoothing kernels. Reproducing kernels are those used in machine learning that conform to Mercer’s theorem. Smoothing kernels are kernel functions which are convolved with a signal to create a smoothed version of that signal.
This reduces computational complexity to $O(NDK^2)$ and storage to $O(NDK)$ with $K$ representing a user specified value for the number of inducing points in the approximation.

The rest of the paper is organized as follows. First we give a more detailed review of related work, with a particular focus on relating multiple output work in machine learning to other fields. Despite the fact that there are several other approaches to multitask learning (see for example Caruana (1997); Heskes (2000); Bakker and Heskes (2003); Xue et al. (2007) and references therein), in this paper, we focus our attention to those that address the problem of constructing the covariance or kernel function for multiple outputs, so that it can be employed, for example, together with Gaussian process prediction. Then we review the convolution process approach in Section 3 and Section 4. We demonstrate how our conditional independence assumptions can be used to reduce the computational load of inference in Section 5. Experimental results are shown in Section 6 and finally some discussion and conclusions are presented in Section 7.

2. Related Work

In geostatistics, multiple output models are used to model the co-occurrence of minerals or pollutants in a spatial field. Many of the ideas for constructing covariance functions for multiple outputs have first appeared within the geostatistical literature, where they are known as linear models of coregionalization (LMC). We present the LMC and then review how several models proposed in the machine learning literature can be seen as special cases of the LMC.

2.1 The Linear Model of Coregionalization

The term linear model of coregionalization refers to models in which the outputs are expressed as linear combinations of independent random functions. If the independent random functions are Gaussian processes then the resulting model will also be a Gaussian process with a positive semi-definite covariance function. Consider a set of $D$ output functions \( \{f_d(x)\}_{d=1}^D \) where $x \in \mathbb{R}^p$ is the input domain. In a LMC each output function, $f_d(x)$, is expressed as (Journel and Huijbregts, 1978)\[ f_d(x) = \sum_{q=1}^Q a_{d,q} u_q(x) + \mu_d, \] (1)

Under the GP interpretation of the LMC the functions $\{u_q(x)\}_{q=1}^Q$ are taken (without loss of generality) to be drawn from a zero-mean GP with $\text{cov}[u_q(x), u_{q'}(x')] = k_q(x, x')$ if $q = q'$ and zero otherwise. Some of these base processes might have the same covariance, i.e. $k_q(x, x') = k_{q'}(x, x')$, but they would still be independently sampled. We can group together (Journel and Huijbregts, 1978; Goovaerts, 1997) the base processes that share latent functions, allowing us to express a given output as \[ f_d(x) = \sum_{q=1}^Q \sum_{i=1}^{R_q} a_{d,q,i}^p u_q^i(x) + \mu_d, \]
where the functions \( \{ u_q^i(x) \}_{i=1}^{R_q} \), \( i = 1, \ldots, R_q \), represent the latent functions that share the same covariance matrix \( k_q(x, x') \). There are now \( Q \) groups of functions, each member of a group shares the same covariance, but is sampled independently.

In geostatistics it is common to simplify the analysis of these models by assuming that the processes \( f_d(x) \) are stationary (Cressie 1993). The stationarity and ergodicity conditions are introduced so that the prediction stage can be realized through an optimal linear predictor using a single realization of the process (Cressie 1993). Such linear predictors receive the general name of cokriging. The cross covariance between any two functions \( f_d(x) \) and \( f_{d'}(x) \) is given in terms of the covariance functions for \( u_q^i(x) \)

\[
\text{cov}[f_d(x), f_{d'}(x')] = \sum_{q=1}^{Q} \sum_{q'=1}^{Q} \sum_{i=1}^{R_q} \sum_{i'=1}^{R_{q'}} a_{d,q}^i a_{d',q'}^{i'} \text{cov}[u_q^i(x), u_{q'}^{i'}(x')].
\]

Because of the independence of the latent functions \( u_q^i(x) \), the above expression can be reduced to

\[
\text{cov}[f_d(x), f_{d'}(x')] = \sum_{q=1}^{Q} \sum_{i=1}^{R_q} a_{d,q}^i a_{d',q}^{i'} k_q(x, x') = \sum_{q=1}^{Q} b_{d,d'}^q k_q(x, x'),
\]

with \( b_{d,d'}^q = \sum_{i=1}^{R_q} a_{d,q}^i a_{d',q}^{i'} \).

For a number \( N \) of input vectors, let \( f_d \) be the vector of values from the output \( d \) evaluated at \( X = \{ x_n \}_{n=1}^{N} \). If each output has the same set of inputs the system is known as isotopic. In general, we can allow each output to be associated with a different set of inputs, \( X^{(d)} = \{ x_n^{(d)} \}_{n=1}^{N_d} \), this is known as heterotopic. For notational simplicity, we restrict ourselves to the isotopic case, but our analysis can also be completed for heterotopic set ups. The covariance matrix for \( f_d \) is obtained expressing equation (2) as

\[
\text{cov}[f_d, f_{d'}] = \sum_{q=1}^{Q} \sum_{i=1}^{R_q} a_{d,q}^i a_{d',q}^{i'} K_q = \sum_{q=1}^{Q} b_{d,d'}^q K_q,
\]

where \( K_q \in \mathbb{R}^{N \times N} \) has entries given by computing \( k_q(x, x') \) for all combinations from \( X \).

We now define \( f \) to be a stacked version of the outputs so that \( f = [f_1^\top, \ldots, f_D^\top]^\top \). We can now write the covariance matrix for the joint process over \( f \) as

\[
K_{f,f} = \sum_{q=1}^{Q} A_q A_q^\top \otimes K_q = \sum_{q=1}^{Q} B_q \otimes K_q,
\]

where the symbol \( \otimes \) denotes the Kronecker product, \( A_q \in \mathbb{R}^{D \times R_q} \) has entries \( a_{d,q}^i \) and \( B_q = A_q A_q^\top \in \mathbb{R}^{D \times D} \) has entries \( b_{d,d'}^q \) and is known as the coregionalization matrix. The covariance matrix \( K_{f,f} \) is positive semi-definite as long as the coregionalization matrices \( B_q \) are positive semi-definite and \( k_q(x, x') \) is a valid covariance function. By definition, coregionalization matrices \( B_q \) fulfill the positive semi-definiteness requirement. The covariance

2. These names come from geostatistics.
functions for the latent processes, $k_q(x, x')$, can simply be chosen from the wide variety of covariance functions (reproducing kernels) that are used for the single output case. Examples include the squared exponential (sometimes called the Gaussian kernel or RBF kernel) and the Matérn class of covariance functions (see Rasmussen and Williams, 2006, chap. 4).

The linear model of coregionalization represents the covariance function as a product of the contributions of two covariance functions. One of the covariance functions models the dependence between the functions independently of the input vector $x$, this is given by the coregionalization matrix $B_q$, whilst the other covariance function models the input dependence independently of the particular set of functions $f_d(x)$, this is the covariance function $k_q(x, x')$.

We can understand the LMC by thinking of the functions having been generated as a two step process. Firstly we sample a set of independent processes from the covariance functions given by $k_q(x, x')$, taking $R_q$ independent samples for each $k_q(x, x')$. We now have $R = \sum_{q=1}^{Q} R_q$ independently sampled functions. These functions are instantaneously mixed in a linear fashion. In other words the output functions are derived by application of a scaling and a rotation to an output space of dimension $D$.

2.1.1 INTRINSIC CORREGIONALIZATION MODEL

A simplified version of the LMC, known as the intrinsic coregionalization model (ICM) (see Goovaerts, 1997), assumes that the elements $b_{d,d'}^q$ of the coregionalization matrix $B_q$ can be written as $b_{d,d'}^q = v_{d,d'} b_q$. In other words, as a scaled version of the elements $b_q$ which do not depend on the particular output functions $f_d(x)$. Using this form for $b_{d,d'}^q$, equation (2) can be expressed as

$$\text{cov}[f_d(x), f_d'(x')] = \sum_{q=1}^{Q} v_{d,d'} b_q k_q(x, x') = v_{d,d'} \sum_{q=1}^{Q} b_q k_q(x, x').$$

The covariance matrix for $f$ takes the form

$$K_{f,f} = \Upsilon \otimes K,$$

where $\Upsilon \in \mathbb{R}^{D \times D}$ with entries $v_{d,d'}$ and $K = \sum_{q=1}^{Q} b_q K_q$ is an equivalent valid covariance function. This is also equivalent to a LMC model where we have $Q = 1$. As pointed out by Goovaerts (1997), the ICM is much more restrictive than the LMC since it assumes that each basic covariance $k_q(x, x')$ contributes equally to the construction of the autocovariances and cross covariances for the outputs.

2.1.2 LINEAR MODEL OF CORREGIONALIZATION IN MACHINE LEARNING

Several of the approaches to multiple output learning in machine learning based on kernels can be seen as examples of the linear model of coregionalization.

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3. The term instantaneous mixing is taken from blind source separation. Of course if the underlying processes are not temporal but spatial, instantaneous is not being used in its original sense. However, it allows us to distinguish this mixing from convolutional mixing.
Semiparametric latent factor model. In Teh et al. (2005), the model proposed to construct the covariance function for multiple outputs turns out to be a simplified version of equation (3). In particular, if $R_q = 1$ (see equation (1)), we can rewrite equation (3) as

$$K_{f,f} = \sum_{q=1}^{Q} a_q a_q^\top \otimes K_q,$$

where $a_q \in \mathbb{R}^{D \times 1}$ with elements $a_{d,q}$. With some algebraic manipulations that exploit the properties of the Kronecker product we can write

$$K_{f,f} = \sum_{q=1}^{Q} (a_q \otimes I_N)K_q(a_q^\top \otimes I_N) = (\tilde{A} \otimes I_N)\tilde{K}(\tilde{A}^\top \otimes I_N),$$

where $I_N$ is the $N$-dimensional identity matrix, $\tilde{A} \in \mathbb{R}^{D \times Q}$ is a matrix with columns $a_q$ and $\tilde{K} \in \mathbb{R}^{QN \times QN}$ is a block diagonal matrix with blocks given by $K_q$.

The functions $u_q(x)$ are considered to be latent factors and the model for the outputs was named semiparametric latent factor model (SLFM). The semiparametric name comes from the fact that it is combining a nonparametric model, i.e. a Gaussian process with a parametric linear mixing of the functions $u_q(x)$. The kernel for each basic process $q$, $k_q(x,x')$, is assumed to be of Gaussian type with a different length scale per input dimension. For computational speed up the informative vector machine (IVM) is employed (Lawrence et al., 2003).

Multi-task Gaussian processes. The intrinsic coregionalization model has been employed in Bonilla et al. (2008) for multitask learning. The covariance matrix is expressed as $K_{\vec{f}(x),\vec{f}(x')} = K^f \otimes k(x,x')$, with $\vec{f}(x) = [f_1(x), \ldots, f_D(x)]^\top$, $K^f$ being constrained positive semi-definite and $k(x,x')$ a covariance function over inputs. It can be noticed that this expression has is equal to the one in (4), when it is evaluated for $x,x' \in X$. In Bonilla et al. (2008), $K^f$ (equal to $\Upsilon$ in equation (4)) expresses the correlation between tasks or inter-task dependencies and it is represented through a PPCA model, with the spectral factorization in the PPCA model replaced by an incomplete Cholesky decomposition to keep numerical stability. For $k(x,x')$ (the function used in equation (4) to compute $K$), the squared-exponential kernel is employed. To reduce computational complexity, the Nyström approximation is applied.

It can be shown that if the outputs are considered to be noise-free, prediction using the intrinsic coregionalization model under an isotopic data case is equivalent to independent prediction over each output (Helterbrand and Cressie, 1994). This circumstance is also known as autokrigeability (Wackernagel, 2003) and it can also be seen as the cancellation of inter-task transfer (Bonilla et al., 2008).

Multi-output Gaussian processes. The intrinsic coregionalization model has been also used in Osborne et al. (2008). Matrix $\Upsilon$ in expression (4) is assumed to be of the spherical parametrisation kind, $\Upsilon = \text{diag}(e^\top S^\top S \text{diag}(e))$, where $e$ gives a description for the length scale of each output variable and $S$ is an upper triangular matrix whose $i$-th column is

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4. See Brookes (2005) for a nice overview.
associated with particular spherical coordinates of points in \( \mathbb{R}^i \) (for details see Osborne and Roberts, 2007, sec. 3.4). Function \( k(x, x') \) is represented through a M\'atern kernel, where different parametrisations of the covariance allow the expression of periodic and non-periodic terms. Sparsification for this model is obtained using an IVM style approach.

**Multi-task kernels.** Kernels for multiple outputs have also been studied in the context of regularization theory. The approach is based mainly on the definition of kernels for multitask learning provided in Evgeniou and Pontil (2004) and Evgeniou et al. (2005), derived based on the theory of kernels for vector-valued functions. Let \( D = \{1, \ldots, D\} \). According to Evgeniou et al. (2005), the following lemma can be used to construct multitask kernels,

**Lemma 1** If \( G \) is a kernel on \( T \times T \) and, for every \( d \in D \) there are prescribed mappings \( \Phi_d : \mathcal{X} \rightarrow T \) such that

\[
k_{d,d'}(x, x') = k((x, d), (x', d')) = G(\Phi_d(x), \Phi_{d'}(x')) , \quad x, x' \in \mathbb{R}^p , \quad d, d' \in D,
\]

then \( k(\cdot) \) is a multitask or multioutput kernel.

A linear multitask kernel can be obtained if we set \( T = \mathbb{R}^m \), \( \Phi_d(x) = C_d x \) with \( \Phi_d \in \mathbb{R}^{m \times p} \) and \( G : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R} \) as the polynomial kernel \( G(z, z') = (z^\top z')^n \) with \( n = 1 \), leading to \( k_{d,d'}(x, x') = x^\top C_d^\top C_d x' \). Lemma 1 can be seen as the result of applying kernel properties to the mapping \( \Phi_d(x) \) (see Genton, 2001, pag. 2). Notice that this corresponds to the linear model of coregionalization where each output is expressed through its own basic process acting over the linear transformation \( C_d x \), this is, \( u_d(\Phi_d(x)) = u_d(C_d x) \).

### 3. Convolution processes for multiple outputs

The approaches introduced above all involve some form of instantaneous mixing of a series of independent processes to construct correlated processes. Instantaneous mixing has some limitations. If we wanted to model two output processes in such a way that one process was a blurred version of the other, we cannot achieve this through instantaneous mixing. We can achieve blurring through convolving a base process with a smoothing kernel. If the base process is a Gaussian process, it turns out that the convolved process is also a Gaussian process. We can therefore exploit convolutions to construct covariance functions (Barry and Hoef, 1996; Hoef and Barry, 1998; Higdon, 1998; 2002). A recent review of several extensions of this approach for the single output case is presented in Calder and Cressie (2007). Applications include the construction of nonstationary covariances (Higdon, 1998; Higdon et al., 1998; Fuentes, 2002a, b; Paciorek and Schervish, 2004) and spatiotemporal covariances (Wikle et al., 1998; Wikle, 2002, 2003).

Higdon (2002) suggested using convolutions to construct multiple output covariance functions. The approach was introduced to the machine learning community by Boyle and Frean (2005). Consider again a set of \( D \) functions \( \{f_d(x)\}_{d=1}^D \). Now each function could be expressed through a convolution integral between a smoothing kernel, \( \{G_d(x)\}_{d=1}^D \), and a latent function \( u(x) \),

\[
f_d(x) = \int_{\mathcal{X}} G_d(x - \mathbf{z}) u(\mathbf{z}) d\mathbf{z}.
\]
More generally, we can consider the influence of more than one latent function, \( \{u_q(z)\}_{q=1}^Q \), and corrupt each of the outputs of the convolutions with an independent process (which could also include a noise term), \( w_d(x) \), to obtain

\[
y_d(x) = f_d(x) + w_d(x) = \sum_{q=1}^Q \int_\mathcal{X} G_{d,q}(x - z) u_q(z) \, dz + w_d(x)
\]

(6)

The covariance between two different outputs \( y_d(x) \) and \( y_{d'}(x') \) is then recovered as

\[
\text{cov} \left[ y_d(x), y_{d'}(x') \right] = \text{cov} \left[ f_d(x), f_{d'}(x') \right] + \text{cov} \left[ w_d(x), w_{d'}(x') \right] \delta_{d,d'},
\]

where \( \delta_{d,d'} \) is the Kronecker delta function and

\[
\text{cov} \left[ f_d(x), f_{d'}(x') \right] = \sum_{q=1}^Q \sum_{q'=1}^Q \int_\mathcal{X} G_{d,q}(x - z) \int_\mathcal{X} G_{d',q'}(x' - z') \text{cov} \left[ u_q(z), u_{q'}(z') \right] \, dz \, dz'.
\]

(7)

Specifying \( G_{d,q}(x - z) \) and \( \text{cov} \left[ u_q(z), u_{q'}(z') \right] \) in (7), the covariance for the outputs \( f_d(x) \) can be constructed indirectly. Note that if the smoothing kernels are taken to be the Dirac delta function such that,

\[
G_{d,q}(x - z) = \delta_{d,d} \delta(x - z'),
\]

where \( \delta(\cdot) \) is the Dirac delta function the double integral is easily solved and the linear model of coregionalization is recovered. This matches to the concept of instantaneous mixing we introduced to describe the LMC. In a convolutional process the mixing is more general, for example the latent process could be smoothed for one output, but not smoothed for another allowing correlated output functions of different length scales.

The traditional approach to convolution processes in statistics and signal processing is to assume that the latent functions \( u_q(z) \) are independent white Gaussian noise processes, \( \text{cov} \left[ u_q(z), u_{q'}(z') \right] = \sigma^2_{u_q} \delta_{q,q'} \delta(z - z') \). This allows us to simplify (7) as

\[
\text{cov} \left[ f_d(x), f_{d'}(x') \right] = \sum_{q=1}^Q \sigma^2_{u_q} \int_\mathcal{X} G_{d,q}(x - z) G_{d',q}(x' - z) \, dz.
\]

In general though, we can consider any type of latent process, for example, we could assume independent GPs for the latent functions so that we have \( \text{cov} \left[ u_q(z), u_{q'}(z') \right] = k_{u_q,u_{q'}}(z,z') \delta_{q,q'} \). With this form of the latent functions, (7) can be written as

\[
\text{cov} \left[ f_d(x), f_{d'}(x') \right] = \sum_{q=1}^Q \int_\mathcal{X} G_{d,q}(x - z) \int_\mathcal{X} G_{d',q}(x' - z') k_{u_q,u_{q'}}(z,z') \, dz \, dz'.
\]

(8)

As well as this correlation across outputs, the correlation between the latent function, \( u_q(z) \), and any given output, \( f_d(x) \), can be computed,

\[
\text{cov} \left[ f_d(x), u_q(z) \right] = \int_\mathcal{X} G_{d,q}(x - z') k_{u_q,u_{q'}}(z,z') \, dz'.
\]

(9)

5. We have slightly abused of the delta notation to indicate the Kronecker delta for discrete arguments and the Dirac function for continuous arguments. The particular meaning should be understood from the context.
Higdon (2002) proposed the direct use of convolution processes for constructing multiple output Gaussian processes. Lawrence et al. (2007) arrive at a similar construction from solving a physical model: a first order differential equation (see also Gao et al., 2008). This idea of using physical models to inspire multiple output systems has been further extended in Alvarez et al. (2009) who give examples using the heat equation and a second order system. A different approach using Kalman Filtering ideas has been proposed in Calder (2003, 2007). Calder proposed a model that incorporates dynamical systems ideas to the process convolution formalism. Essentially, the latent processes are of two types: random walks and independent cyclic second-order autoregressions. With this formulation, it is possible to construct a multivariate output process using convolutions over these latent processes. Particular relationships between outputs and latent processes are specified using a special transformation matrix ensuring that the outputs are invariant under invertible linear transformations of the underlying factor processes (this matrix is similar in spirit to the sensitivity matrix of Lawrence et al. (2007) and it is given a particular form so that not all latent processes affect the whole set of outputs (Calder 2007)).

Bayesian kernel methods. The convolution process is closely related to the Bayesian kernel method (Pillai et al., 2007; Liang et al., 2009) for constructing reproducible kernel Hilbert spaces (RKHS), assigning priors to signed measures and mapping these measures through integral operators. In particular, define the following space of functions,

\[ \mathcal{F} = \left\{ f \mid f(x) = \int_{\mathcal{X}} G(x, z) \gamma(dz), \gamma \in \Gamma \right\}, \]

for some space \( \Gamma \subseteq \mathcal{B}(\mathcal{X}) \) of signed Borel measures. In Pillai et al. (2007, proposition 1), the authors show that for \( \Gamma = \mathcal{B}(\mathcal{X}) \), the space of all signed Borel measures, \( \mathcal{F} \) corresponds to a RKHS. Examples of these measures that appear in the form of stochastic processes include Gaussian processes, Dirichlet processes and Lévy processes. This framework can be extended for the multiple output case, expressing the outputs as

\[ f_d(x) = \int_{\mathcal{X}} G_d(x, z) \gamma(dz). \]

The analysis of the mathematical properties of such spaces of functions are beyond the scope of this paper and are postponed for future work.

4. Constructing Multiple Output Convolution Processes

We now consider practical examples of how these multiple output convolution processes can be constructed. We start with a more generic example (although it has an underlying physical interpretation (Alvarez et al., 2009)), which can be seen as the equivalent of the squared exponential covariance function for multiple outputs. We will then consider a particular physical model: a simple first order differential equation for modeling transcription.

Example 1. A general purpose convolution kernel for multiple outputs. A simple general purpose kernel for multiple outputs based on the convolution integral can be constructed assuming that the kernel smoothing function, \( G_{d,r}(x) \), and the covariance...
for the latent function, \( k_{u_q,u_q}(x,x') \), follow both a Gaussian form. The kernel smoothing function is given as

\[
G_{d,q}(x) = S_{d,q}N(x|0,P_d^{-1}),
\]

where \( S_{d,q} \) is a variance coefficient that depends both of the output \( d \) and the latent function \( q \) and \( P_d \) is the precision matrix associated to the particular output \( d \). The covariance function for the latent process is expressed as

\[
k_{u_q,u_q}(x,x') = N(x - x'|0,\Lambda_q^{-1}),
\]

with \( \Lambda_q \) the precision matrix of the latent function \( q \).

Expressions for the kernels are obtained applying systematically the identity for the product of two Gaussian distributions. Let \( N(x|\mu,P^{-1}) \) denotes a Gaussian for \( x \), then

\[
N(x|\mu_1,P_1^{-1})N(x|\mu_2,P_2^{-1}) = N(\mu_1|\mu_2,P_1^{-1} + P_2^{-1})N(x|\mu_c,P_c^{-1}),
\]

where \( \mu_c = (P_1 + P_2)^{-1}(P_1\mu_1 + P_2\mu_2) \) and \( P_c^{-1} = (P_1 + P_2)^{-1} \). For all integrals we assume that \( \mathcal{X} = \mathbb{R}^p \). Using these forms for \( G_{d,q}(x) \) and \( k_{u_q,u_q}(x,x') \), expression (8) can be written as

\[
k_{f_d,f_d'}(x,x') = \sum_{q=1}^Q S_{d,q}S_{d',q} \int_\mathcal{X} N(x - z|0,P_d^{-1}) \int_\mathcal{X} N(x' - z'|0,P_d'^{-1})N(z - z'|0,\Lambda_q^{-1})dz' dz.
\]

Since the Gaussian covariance is stationary and isotropic, we can write it as \( N(x - x'|0,P^{-1}) = N(x'|x, P^{-1}) = N(x'|x, P^{-1}) = N(x'|x, P^{-1}) \). Using the identity in equation (10) twice, we get

\[
k_{f_d,f_d'}(x,x') = \sum_{q=1}^Q S_{d,q}S_{d',q}N(x - x'|0,P_d^{-1} + P_d'^{-1} + \Lambda_q^{-1}).
\]

For a high value of the input dimension, \( p \), the term \( 1/[(2\pi)^{p/2}|P_d^{-1} + P_d'^{-1} + \Lambda_q^{-1}|^{1/2}] \) in each of the Gaussian’s normalization terms will dominate, making values go quickly to zero. We can fix this problem, by scaling the outputs using the factors \( 1/[(2\pi)^{p/4}|2P_d^{-1} + \Lambda_q^{-1}|^{1/4}] \) and \( 1/[(2\pi)^{p/4}|2P_d'^{-1} + \Lambda_q^{-1}|^{1/4}] \). Each of these scaling factors correspond to the standard deviation associated to \( k_{f_d,f_d}(x,x) \) and \( k_{f_d',f_d'}(x,x) \).

Equally for the covariance \( \text{cov} [f_d(x), u_q(x')] \) in equation (9), we obtain

\[
k_{f_d,u_q}(x,x') = S_{d,q}N(x - x'|0,P_d^{-1} + \Lambda_q^{-1}).
\]

Again, this covariance must be standardized when working in higher dimensions.

**Example 2. Convolution kernels constructed through a first order differential equation.** The convolution integral appears naturally when solving ordinary differential equations. In this case, the smoothing kernel function corresponds to the impulse response
of the system described by the differential equation. As an example consider the following set of first order differential equations where the input variable is time, \( t \),

\[
\frac{df_d(t)}{dt} = \sum_{q=1}^{Q} S_{d,q} u_q(t) - \gamma_d f_d(t), \quad d = 1, \ldots, D,
\]

where \( \gamma_d \) is a parameter of the particular system (electrical circuit, mechanical system, among others) and \( S_{d,q} \) quantifies the influence of latent function \( q \) over output \( d \). Assuming initial conditions equal to zero, the solution to the above equation is given as

\[
f_d(t) = \sum_{q=1}^{Q} S_{d,q} \int_0^t \exp(-\gamma_d(t-\tau)) u_q(\tau) d\tau. \tag{11}
\]

If the functions \( \{u_q(t)\}_{q=1}^Q \) are Gaussian processes with squared exponential kernel

\[
k_{u_q,u_q}(t,t') = \exp\left(-\frac{(t-t')^2}{\ell_q^2}\right),
\]

where \( \ell_q \) represents the length-scale parameter, the covariance for the outputs can be found (Lawrence et al., 2007; Gao et al., 2008) as

\[
k_{f_d,f_d'}(t,t') = \sum_{q=1}^{Q} S_{d,q} S_{d',q} \sqrt{\pi \ell_q} \exp\left(-\gamma_d^2 \ell_q^2/2\right) \exp\left(-\gamma_d (t-t')/2\right) \mathcal{H}_q(\gamma_d, t, t') - \mathcal{H}_q(\gamma_d, 0, t'),
\]

Solving the above equation, the covariance \( k_{f_d,f_d'}(t,t') \) is given as

\[
k_{f_d,f_d'}(t,t') = \sum_{q=1}^{Q} S_{d,q} S_{d',q} \sqrt{\pi \ell_q} \exp\left(-\gamma_d^2 \ell_q^2/2\right) \exp\left(-\gamma_d (t-t')/2\right) \mathcal{H}_q(\gamma_d, t, t') - \mathcal{H}_q(\gamma_d, 0, t'),
\]

where

\[
h_q(\gamma_d, \gamma_d', t, t') = \frac{\exp\left[\left(\gamma_d \ell_q/2\right)^2\right]}{\gamma_d + \gamma_d'} \left[ \exp[(\gamma_d + \gamma_d')t] \mathcal{H}_q(\gamma_d, t, t') - \mathcal{H}_q(\gamma_d, 0, t') \right],
\]

and

\[
\mathcal{H}_q(\gamma_d, t, t') = \text{erf}\left(\frac{t}{\ell_q} + \frac{\gamma_d \ell_q}{2}\right) - \text{erf}\left(\frac{t-t'}{\ell_q} + \frac{\gamma_d \ell_q}{2}\right).
\]

In the above expression, the function \( \text{erf}(x) \) is the so called error function and it is defined as \( \text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\xi^2) d\xi \). The covariance between \( f_d(t) \) and \( u_q(t') \) is given as

\[
k_{f_d,u_q}(t,t') = \frac{S_{d,q} \sqrt{\pi \ell_q}}{2} \exp\left[-\gamma_d^2 \ell_q^2/2\right] \exp[-\gamma_d (t-t')] \mathcal{H}_q(\gamma_d, t', t).
\]
5. Sparse Approximations for Convolutional Processes

Assuming that the double integral is tractable, the principle challenge for the convolutional framework is computing the inverse of the covariance matrix associated with the outputs. For $D$ outputs, each having $N$ data points, the inverse has computational complexity $O(D^3N^3)$ and associated storage of $O(D^2N^2)$. We show how through making specific conditional independence assumptions, inspired by the model structure (Alvarez and Lawrence, 2009), we arrive at a sparse approximation similar in form to the partially independent training conditional model (PITC, see Quiñonero Candela and Rasmussen, 2005). The relationship with PITC inspires us to make further conditional independence assumptions.

5.1 Full Dependence

Given the convolution formalism, we can construct a full GP over the set of outputs. The likelihood of the model is given by

$$p(y|X, \theta) = \mathcal{N}(0, K_{f,f} + \Sigma),$$

(12)

where $y = [y_1^\top, \ldots, y_D^\top]^\top$ is the set of output functions with $y_d = [y_d(x_1), \ldots, y_d(x_N)]^\top$; $K_{f,f} \in \mathbb{R}^{DN \times DN}$ is the covariance matrix arising from the convolution. It expresses the covariance of each data point at every other output and data point and its elements are given by $\text{cov}[f_d(x), f_{d'}(x')]$ in (8). The term $\Sigma$ represents the covariance associated with the independent processes in (6), $w_d(x)$. It could contain structure, or alternatively could simply represent noise that is independent across the data points. The vector $\theta$ refers to the hyperparameters of the model. For exposition we will focus on the isotopic case (although our implementations allow heterotopic modeling), so we have a matrix $X = \{x_1, \ldots, x_N\}$ which is the common set of training input vectors at which the covariance is evaluated.

The predictive distribution for a new set of input vectors $X_*$ is (Rasmussen and Williams, 2006)

$$p(y_*|y, X, X_*, \theta) = \mathcal{N}(K_{f,f}^{-1}y, K_{f,f} - K_{f,f}^{-1}K_{f,f})$$

where we have used $K_{f,f}$ as a compact notation to indicate when the covariance matrix is evaluated at the inputs $X_*$, with a similar notation for $K_{f,f}$. Learning from the log-likelihood involves the computation of the inverse of $K_{f,f} + \Sigma$ giving the problematic complexity of $O(N^3D^3)$. Once the parameters have been learned, prediction is $O(ND)$ for the predictive mean and $O(N^2D^2)$ for the predictive variance.

5.2 Latent functions as conditional means

We restrict the analysis of the approximations to one latent function $u(x)$. The key to all approximations is based on the form we assume for the latent functions. From the perspective of a generative model, equation (5) can be interpreted as follows: first we draw a sample from the Gaussian process prior $p(u(z))$ and then solve the integral for each of the outputs $f_d(x)$ involved. Uncertainty about $u(z)$ is also propagated through the convolution transform.

For the set of approximations, instead of drawing a sample from $u(z)$, we first draw a sample from a finite representation of $u(z)$, $u(Z) = [u(z_1), \ldots, u(z_K)]^\top$, where $Z = \{z_k\}_{k=1}^K$. 

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is the set of input vectors at which \( u(z) \) is evaluated. Due to the properties of a Gaussian process, \( p(u(Z)) \) follows a multivariate Gaussian distribution. Conditioning on \( u(Z) \), we next sample from the conditional prior \( p(u(z)|u(Z)) \) and use this function to solve the convolution integral for each \( f_d(x) \). Under this generative approach, we can approximate each function \( f_d(x) \) using

\[
f_d(x) \approx \int_X G_d(x - z) E[u(z)|u] \, dz. \tag{13}
\]

Replacing \( u(z) \) for \( E[u(z)|u] \) is a reasonable approximation as long as \( u(z) \) be a smooth function so that the infinite dimensional object \( u(z) \) can be summarized by \( u \). Figure 1 shows a cartoon example of the quality of the approximations for two outputs as the size of the set \( Z \) increases. The first column represents the conditional prior \( p(u(z)|u) \) for a particular choice of \( u(z) \). The second and third columns represent the outputs \( f_1(x) \) and \( f_2(x) \) obtained when using equation 13.

Using expression 13, the likelihood function for \( f \) follows

\[
p(f|u, Z, X, \theta) = \mathcal{N} \left( K_{f,u} K_{u,u}^{-1} u, K_{f,f} - K_{f,u} K_{u,u}^{-1} K_{f,u}^\top \right),
\]

where \( K_{u,u} \) is the covariance matrix between the samples from the latent function \( u(Z) \), with elements given by \( k_{u,u}(z, z') \) and \( K_{f,u} = K_{u,f}^\top \) is the cross-covariance matrix between the latent function \( u(z) \) and the outputs \( f_d(x) \), with elements \( \text{cov} [f_d(x), u(z)] \) in 9. Given the set of points \( u \), we can have different assumptions about the uncertainty of the outputs in the likelihood term. For example, we could assume that the outputs are independent or uncorrelated, keeping only the uncertainty involved for each output in the likelihood term. Other approximation would assume that the outputs are deterministic, this is \( K_{f,f} = K_{f,u} K_{u,u}^{-1} K_{f,u}^\top \). The only uncertainty left would be due to the prior \( p(u) \). Next, we present different approximations of the covariance of the likelihood that lead to a reduction in computational complexity.

### 5.2.1 Partial Independence

We assume that the set of outputs \( f \) are independent given the latent function \( u \), leading to the following expression for the likelihood

\[
p(f|u, Z, X, \theta) = \prod_{d=1}^D p(f_d|u, Z, X, \theta) = \prod_{d=1}^D \mathcal{N} \left( K_{f_d,u} K_{u,u}^{-1} u, K_{f_d,f_d} - K_{f_d,u} K_{u,u}^{-1} K_{f_d,u}^\top \right).
\]

We rewrite this product of multivariate Gaussians as a single Gaussian with a block diagonal covariance matrix, including the uncertainty about the independent processes

\[
p(y|u, Z, X, \theta) = \mathcal{N} \left( K_{f,u} K_{u,u}^{-1} u, D + \Sigma \right) \tag{14}
\]

where \( D = \text{blockdiag} \left[ K_{f,f} - K_{f,u} K_{u,u}^{-1} K_{u,f} \right] \), and we have used the notation \( \text{blockdiag} [G] \) to indicate that the block associated with each output of the matrix \( G \) should be retained, but all other elements should be set to zero. We can also write this as \( D = \)

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6. For simplicity in the notation, we just write \( u \) to refer to \( u(Z) \).
[\mathbf{K}_{u,f}^{-1} \otimes \mathbf{M}] \mathbf{M} = \mathbf{I}_D \otimes \mathbf{1}_N, \mathbf{1}_N \text{ being the } N \times N \text{ matrix of ones. We now marginalize the values of the samples from the latent function by using its process prior, this means } p(\mathbf{u}|\mathbf{Z}) = \mathcal{N}(0, \mathbf{K}_{u,u}). \text{ This leads to the following marginal likelihood,}

\begin{equation}
    p(\mathbf{y}|\mathbf{Z}, \mathbf{X}, \theta) = \int p(\mathbf{y}|\mathbf{u}, \mathbf{Z}, \mathbf{X}, \theta)p(\mathbf{u}|\mathbf{Z})d\mathbf{u} = \mathcal{N}(0, \mathbf{D} + \mathbf{K}_{u,u}^{-1} \mathbf{K}_{u,f} + \Sigma).
\end{equation}

Figure 1: Conditional prior and two outputs for different values of $K$. The first column, figures (a), (d) and (g), shows the mean and confidence intervals of the conditional prior distribution using one input function and two output functions. The dashed line represents one sample from the prior. Conditioning over a few points of this sample, shown as black dots, the conditional mean and conditional covariance are computed. The solid line represents the conditional mean and the shaded region corresponds to 2 standard deviations away from the mean. The second column, (b), (e) and (h), shows the solution to equation (5) for output one using the sample from the prior (dashed line) and the conditional mean (solid line), for different values of $K$. The third column, (c), (f) and (i), shows the solution to equation (5) for output two, again for different values of $K$. 

\[ \begin{bmatrix}
    \mathbf{K}_{f,f} - \mathbf{K}_{f,u} \mathbf{K}_{u,u}^{-1} \mathbf{K}_{u,f} \nabla \mathbf{M}
\end{bmatrix} \]
Notice that, compared to (12), the full covariance matrix $K_{f,f}$ has been replaced by the low rank covariance $K_{f,u}K_{u,u}^{-1}K_{u,f}$ in all entries except in the diagonal blocks corresponding to $K_{f,f}$. Depending on our choice of $K$ the inverse of the low rank approximation to the covariance is either dominated by a $O(DN^3)$ term or a $O(K^2DN)$ term. Storage of the matrix is $O(N^2D + O(NDK))$. Note that if we set $K = N$ these reduce to $O(N^3D)$ and $O(N^2D)$ respectively. Rather neatly this matches the computational complexity of modeling the data with $D$ independent Gaussian processes across the outputs.

The functional form of (15) is almost identical to that of the PITC approximation (Quinonero Candela and Rasmussen, 2005), with the samples we retain from the latent function providing the same role as the inducing values in the partially independent training conditional (PITC) approximation. This is perhaps not surprising given that the PITC approximation is also derived by making conditional independence assumptions. A key difference is that in PITC it is not obvious which variables should be grouped together when making these conditional independence assumptions, here it is clear from the structure of the model that each of the outputs should be grouped separately. However, the similarities are such that we find it convenient to follow the terminology of Quinonero Candela and Rasmussen (2005) and also refer to our approximation as a PITC approximation.

5.2.2 FULL INDEPENDENCE

We can be inspired by the analogy of our approach to the PITC approximation and consider a more radical factorization of the likelihood term. In the fully independent training conditional (FITC) (Snelson and Ghahramani, 2006; 2007) a factorization across the data points is assumed. For us that would lead to the following expression for conditional distribution of the output functions given the inducing variables,

$$p(f|u, Z, X, \theta) = \prod_{d=1}^{D} \prod_{n=1}^{N} p(f_{n,d}|u, Z, X, \theta),$$

which can be briefly expressed through (14) with $D = \text{diag} [K_{f,f} - K_{f,u}K_{u,u}^{-1}K_{u,f}] = [K_{f,f} - K_{f,u}K_{u,u}^{-1}K_{u,f}] \odot \mathbf{M}$, with $\mathbf{M} = I_D \otimes I_N$. The marginal likelihood, including the uncertainty about the independent processes is given by equation (15) with the diagonal form for $D$, leading to the fully independent training conditional (FITC) approximation (Snelson and Ghahramani, 2006; Quinonero Candela and Rasmussen, 2005).

5.2.3 DETERMINISTIC LIKELIHOOD

In Quinonero Candela and Rasmussen (2005) the relationship between the projected process approximation and the FITC and PITC approximations is elucidated. They show that if, given the set of values $u$, the outputs are deterministic, the likelihood term of equation (13) can be simplified as

$$p(f|u, Z, X, \theta) = \mathcal{N} \left( K_{f,u}K_{u,u}^{-1}u, 0 \right).$$

Marginalizing with respect to the latent function using $p(u|Z) = \mathcal{N}(0, K_{u,u})$ and including the uncertainty about the independent processes, we obtain the marginal likelihood as

$$p(y|Z, X, \theta) = \int p(y|u, Z, X, \theta)p(u|Z)du = \mathcal{N} \left( 0, K_{f,u}K_{u,u}^{-1}K_{f,u}^{\top} + \Sigma \right).$$
In other words, we approximate the full covariance \( K_{f,f} \) using the low rank approximation \( K_{f,u}K_{u,u}^{-1}K_{f,u}^\top \). Using this new marginal likelihood to estimate the parameters \( \theta \) reduces computational complexity to \( O(K^2DN) \). The approximation obtained has similarities with the projected latent variables (PLV) method also known as the projected process approximation (PPA) or the deterministic training conditional (DTC) approximation (Csató and Opper, 2001; Seeger et al., 2003; Quinonero Candela and Rasmussen, 2005; Rasmussen and Williams, 2006). For this reason we refer to this approximation as the deterministic training conditional approximation (DTC) for multiple output Gaussian processes.

5.2.4 Additional independence assumptions.

As mentioned before, we can consider different conditional independence assumptions for the likelihood term. One further assumption that is worth mentioning considers conditional independencies across data points and dependence across outputs. This would lead to the following likelihood term

\[
p(f|u, Z, X, \theta) = \prod_{n=1}^{N} p(\tilde{f}_n|u, Z, X, \theta),
\]

where \( \tilde{f}_n = [f_1(x_n), f_2(x_n), \ldots, f_D(x_n)]^\top \). We can use again equation (14) to express the likelihood. In this case, if the matrix \( D \) is a partitioned matrix with blocks \( D_{d,d'} \in \mathbb{R}^{N \times N} \), each block \( D_{d,d'} \) would be given as \( D_{d,d'} = \text{diag} \left[ K_{f_d,f_d'} - K_{f_d,u}K_{u,u}^{-1}K_{u,f_d'} \right] \). For cases in which \( D > N \), that is, the number of outputs is greater than the number of data points, this approximation may be more accurate than PITC. For cases where \( D < N \) it may be less accurate than PITC, but faster to compute\(^7\).

5.3 Posterior and predictive distributions

Combining the likelihood term for each approximation with \( p(u|Z) \) using Bayes’ theorem, the posterior distribution over \( u \) is obtained as

\[
p(u|y, X, Z, \theta) = \mathcal{N} \left( K_{u,u}A^{-1}K_{u,f}(D + \Sigma)^{-1}y, K_{u,u}A^{-1}K_{u,u} \right) \tag{16}
\]

where \( A = K_{u,u} + K_{u,f}(D + \Sigma)^{-1}K_{f,u} \) and \( D \) follows a particular form according to the different approximations: for PITC it equals \( D = \text{blockdiag} \left[ K_{f,f} - K_{f,u}K_{u,u}^{-1}K_{u,f} \right] \), for FITC \( D = \text{diag} \left[ K_{f,f} - K_{f,u}K_{u,u}^{-1}K_{u,f} \right] \) and for DTC \( D = 0 \). The predictive distribution is expressed through the integration of the likelihood term, evaluated at \( X_s \), with (16), giving

\[
p(y_s|y, X, X_s, Z, \theta) = \int p(y_s|u, Z, X_s, \theta)p(u|y, X, Z, \theta)du = \mathcal{N} \left( K_{f_s,f_s}^{-1}K_{u,f_s}(D + \Sigma)^{-1}y, D_s + K_{f_s,u}A^{-1}K_{u,f_s} + \Sigma \right),
\]

with \( D_s = \text{blockdiag} \left[ K_{f_s,f_s} - K_{f_s,u}K_{u,u}^{-1}K_{u,f_s} \right] \) for PITC, \( D_s = \text{diag} \left[ K_{f_s,f_s} - K_{f_s,u}K_{u,u}^{-1}K_{u,f_s} \right] \) for FITC and \( D_s = 0 \) for DTC.

\(^7\) Notice that if we work with the block diagonal matrices \( D_{d,d'} \), we would need to invert the full matrix \( D \). However, since the blocks \( D_{d,d'} \) are diagonal matrices themselves, the inversion can be done efficiently using, for example, a block Cholesky decomposition. Furthermore, we would be restricted to work with isotopic input spaces. Alternatively, we could rearrange the elements of the matrix \( D \) so that the blocks of the main diagonal are the covariances associated with the vectors \( \tilde{f}_n \).
5.4 Fitting the Model

The marginal likelihood approximation for the PITC, FITC and DTC variants for sparse multioutput Gaussian processes is a function of both the parameters of the covariance function and the location of the inputs for the inducing variables. One of the key ideas presented in Snelson and Ghahramani (2006) was that we should optimize with respect to the location of these inducing variables. Previously, the inducing variables were taken to be a subset of the data variables (Csató and Opper [2001], Williams and Seeger [2001]). However, a method of choosing which subset of the data is required (Smola and Bartlett [2001], Seeger et al. [2003]). Such criteria can be expensive to compute and also lead to fluctuations in the approximation to the log-likelihood when the subset changes. This causes problems as while the parameters of the Gaussian process are optimized, the optimal subset of the inducing inputs will also change. Convergence is therefore difficult to monitor. The key advantage of optimizing the inducing input locations, $\mathbf{Z}$, across the entire input domain is that convergence of the likelihood will be smooth. In appendix A.1 we include the derivatives of the marginal likelihood with respect to the matrices $K_{f_f}, K_{u_f}$ and $K_{u_u}$.

6. Experimental evaluation

In this section we present results of applying the sparse methods in pollutant metal prediction, exam score prediction and the prediction of transcription factor behavior in a gene-network. First, though, we illustrate the performance of the sparse method in a toy example.

6.1 A toy example

For the toy experiment, we employ the kernels constructed in Example 1 of section 4. The toy problem consists of $D = 4$ outputs, one latent function, $Q = 1$ and one input dimension. The training data was sampled from the full GP with the following parameters, $S_{1,1} = S_{2,1} = 1$, $S_{3,1} = S_{4,1} = 5$, $P_{1,1} = P_{2,1} = 50$, $P_{3,1} = 300$, $P_{4,1} = 200$ for the outputs and $\Lambda_1 = 100$ for the latent function. For the independent processes, $w_d(\mathbf{x})$, we simply added white noise separately to each output so we have variances $\sigma_1^2 = \sigma_2^2 = 0.0125$, $\sigma_3^2 = 1.2$ and $\sigma_4^2 = 1$. We generate $N = 500$ observation points for each output and use 200 observation points (per output) for training the full and the sparse multiple output GP and the remaining 300 observation points for testing. We repeated the same experiment setup 10 times and compute the standardized mean square error (SMSE) and the mean standardized log loss (MSLL) as defined in Rasmussen and Williams (2006). For the sparse methods we use $K = 30$ inducing inputs. We sought the kernel parameters and the positions of the inducing inputs through maximizing the marginal likelihood using a scaled conjugate gradient algorithm. Initially the inducing inputs are equally spaced between the interval $[-1, 1]$.

Figure 2 shows the training result of one of the ten repetitions. The predictions shown correspond to the full GP (Figure 2(a)), the DTC approximation (Figure 2(b)), the FITC approximation (Figure 2(c)) and the PITC approximation (Figure 2(d)).

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8. Code to run all simulations in this section is available at [http://www.cs.manchester.ac.uk/~neill/multigp/](http://www.cs.manchester.ac.uk/~neill/multigp/)
Tables 1 and 2 show the average prediction results over the test set. Table 1 shows that the SMSE of the sparse approximations is similar to the one obtained with the full GP. However, there are important differences in the values of the MSLL shown in Table 2. DTC offers the worst performance. It gets better for FITC and PITC since they offer a more precise approximation to the full covariance.

Also, the training times for iteration of each model are 1.97 ± 0.02 secs for the full GP, 0.20 ± 0.01 secs for DTC, 0.41 ± 0.03 for FITC and 0.59 ± 0.05 for the PITC.

As we have mentioned before, one important feature of multiple output prediction is that we can exploit correlations between outputs to predict missing observations. We used a simple example to illustrate this point. We removed a portion of one output between \([-0.8, 0]\) from the training data in the experiment before (as shown in Figure 3) and train the different models to predict the behavior of \(y_4(x)\) for the missing information. The predictions shown correspond to the full GP (Figure 3(a)), an independent GP (Figure 3(b)), the DTC approximation (Figure 3(c)), the FITC approximation (Figure 3(d)) and the PITC approximation (Figure 3(e)).

Figure 2: Predictive mean and variance using the full multi-output GP and the sparse approximations for output 4. The solid line corresponds to the predictive mean, the shaded region corresponds to 2 standard deviations of the prediction. The dashed line corresponds to the ground truth signal, that is, the sample from the full GP model without noise. In these plots the predictive mean overlaps almost exactly with the ground truth. The dots are the noisy training points. The crosses in figures 2(b), 2(c) and 2(d) correspond to the locations of the inducing inputs after convergence.
Cokriging is the generalization of kriging to multiple outputs. Within cokriging there are several alternative predictors, including simple and ordinary cokriging. Interested readers are referred to (Goovaerts, 1997, ch. 6) for details. In the geostatistics literature, the usual procedure is to use the linear model of coregionalization to construct a valid covariance function and then use the cokriging estimator for making predictions.

| Method | SMSE $y_1(x)$ | SMSE $y_2(x)$ | SMSE $y_3(x)$ | SMSE $y_4(x)$ |
|--------|---------------|---------------|---------------|---------------|
| Full GP | $1.06 \pm 0.08$ | $0.99 \pm 0.06$ | $1.10 \pm 0.09$ | $1.05 \pm 0.09$ |
| DTC    | $1.06 \pm 0.08$ | $0.99 \pm 0.06$ | $1.12 \pm 0.09$ | $1.05 \pm 0.09$ |
| FITC   | $1.06 \pm 0.08$ | $0.99 \pm 0.06$ | $1.10 \pm 0.08$ | $1.05 \pm 0.08$ |
| PITT    | $1.06 \pm 0.08$ | $0.99 \pm 0.06$ | $1.10 \pm 0.09$ | $1.05 \pm 0.09$ |

Table 1: Standardized mean square error (SMSE) for the toy problem over the test set. All numbers are to be multiplied by $10^{-2}$. The experiment was repeated ten times. Table includes the value of one standard deviation over the ten repetitions.

| Method | MSLL $y_1(x)$ | MSLL $y_2(x)$ | MSLL $y_3(x)$ | MSLL $y_4(x)$ |
|--------|---------------|---------------|---------------|---------------|
| Full GP | $-2.27 \pm 0.04$ | $-2.30 \pm 0.03$ | $-2.25 \pm 0.04$ | $-2.27 \pm 0.05$ |
| DTC    | $-0.98 \pm 0.18$ | $-0.98 \pm 0.18$ | $-1.25 \pm 0.16$ | $-1.25 \pm 0.16$ |
| FITC   | $-2.26 \pm 0.04$ | $-2.29 \pm 0.03$ | $-2.16 \pm 0.04$ | $-2.23 \pm 0.05$ |
| PITT    | $-2.27 \pm 0.04$ | $-2.30 \pm 0.03$ | $-2.23 \pm 0.04$ | $-2.26 \pm 0.05$ |

Table 2: Mean standardized log loss (MSLL) for the toy problem over the test set. More negative values of MSLL indicate better models. The experiment was repeated ten times. Table includes the value of one standard deviation over the ten repetitions.

Due to the strong dependencies between the signals, our model is able to capture the correlations and predicts accurately the missing information.

6.2 Heavy Metals in the Swiss Jura

The first example with real data that we consider is the prediction of the concentration of several metal pollutants in a region of the Swiss Jura. The data consist of measurements of concentrations of several heavy metals collected in the topsoil of a 14.5 km$^2$ region of the Swiss Jura. The data is divided into a prediction set (259 locations) and a validation set (100 locations). In a typical situation, referred to as undersampled or heterotopic case, a few expensive measurements of the attribute of interest are supplemented by more abundant data on correlated attributes that are cheaper to sample. We follow the experiment described in Goovaerts (1997, p. 248, 249) in which a primary variable (cadmium) at prediction locations in conjunction with some secondary variables (nickel and zinc) at prediction and validation locations, are employed to predict the concentration of the primary variable at validation locations. We compare results of independent GP, the different approximations described before, the full GP and ordinary cokriging.

9. This data is available at [http://www.ai-geostats.org/](http://www.ai-geostats.org/).
10. Cokriging is the generalization of kriging to multiple outputs. Within cokriging there are several alternatives, including simple and ordinary cokriging. Interested readers are referred to (Goovaerts, 1997, ch. 6) for details. In the geostatistics literature, the usual procedure is to use the linear model of coregionalization to construct a valid covariance function and then use the cokriging estimator for making predictions.
Figure 3: Predictive mean and variance using the full multi-output GP, the sparse approximations and an independent GP for output 4 with a range of missing observations in the interval [−0.8, 0.0]. The solid line corresponds to the mean predictive, the shaded region corresponds to 2 standard deviations away from the mean and the dash line is the actual value of the signal without noise. The dots are the noisy training points. The crosses in figures 3(c), 3(d) and 3(e) correspond to the locations of the inducing inputs after convergence.

GPs, we use one ($Q = 1$) latent function. For the sparse approximations results, a $k$-means procedure is employed first to find the initial locations of the inducing values and then these locations are optimized in the same optimization procedure used for the parameters.
Each experiment is repeated ten times. The result for ordinary cokriging was obtained from Goovaerts (p. 248, 249 1997). In this case, no values for standard deviation are reported. Figure 4 shows the results of prediction for cadmium (Cd). It can be noticed that as more inducing values are included, the approximations follow the performance of the full GP, as would be expected. For this particular dataset, FITC and PITC exhibit lower variances compared to DTC. In terms of the performance, it can be seen that PITC outperforms FITC and DTC when compared in terms of the number of inducing points. FITC and PITC also outperform the independent GP method, and for 200 and 500 inducing points, they outperform the cokriging method.

Figure 4: Mean absolute error and standard deviation for prediction of the pollutant metal Cadmium. The experiment was repeated ten times. In the bottom of the figure D\text{K}, F\text{K}, P\text{K} stands for DTC, FITC and PITC with K inducing values, respectively, FGP stands for full GP, CK stands for ordinary cokriging using the linear model of coregionalization (see Goovaerts (1997) for detailed description of the ordinary cokriging estimator) and IND stands for independent GP.

6.3 Exam score prediction

In the second experiment with real data the goal is to predict the exam score obtained by a particular student belonging to a particular school. The data comes from the Inner London Education Authority (ILEA). It consists of examination records from 139 secondary schools in years 1985, 1986 and 1987. It is a random 50% sample with 15362 students. The input space consists of four features related to each student (year in which each student took the exam, gender, VR band and ethnic group) and four features related to each school.

11. This data is available at http://www.cmm.bristol.ac.uk/learning-training/multilevel-m-support/datasets.shtml
(percentage of students eligible for free school meals, percentage of students in VR band one, school gender and school denomination). From the multiple output point of view, each school represents one output and the exam score of each student a particular instantiation of that output or \( D = 139 \).

We follow the same preprocessing steps employed in Bonilla et al. (2008). The only features used are the student-dependent ones, which are categorial variables. Each of them is transformed to a binary representation. For example, the possible values that the variable year of the exam can take are 1985, 1986 or 1987 and are represented as 100, 010 or 001. The transformation is also applied to the variables gender (two binary variables), VR band (four binary variables) and ethnic group (eleven binary variables), ending up with an input space with 20 dimensions. The categorial nature of the data restricts the input space to \( N = 202 \) unique input feature vectors. However, two students represented by the same input vector \( x \), and belonging both to the same school, \( d \), can obtain different exam scores. To reduce this noise in the data, we take the mean of the observations that, within a school, share the same input vector and use a simple heteroskedastic noise model in which the variance for each of these means is divided by the number of observations used to compute it.\(^{12}\) For the convolved GPs, we use one (\( Q = 1 \)) latent function. The performance measure employed is the percentage of explained variance defined as the total variance of the data minus the sum-squared error on the test set as a percentage of the total data variance. It can be seen as the percentage version of the coefficient of determination between the test targets and the predictions. The performance measure is computed for ten repetitions with 75% of the data in the training set and 25% of the data in the testing set.

As in the Jura dataset experiment, the initial positions of the inducing points are selected using the \( k \)-means algorithm with the data points as inputs to the algorithm. The positions of these points are optimized in a scaled conjugate gradient procedure together with the parameters of the model. Figure 5 shows results of the sparse methods, the ICM model and independent GPs. The results for the ICM model are the best results presented in Bonilla et al. (2008). The independent GPs result was also obtained from Bonilla et al. (2008). It can be seen that the sparse convolved multiple output GP framework outperforms the ICM model and the independent GPs, even with as few as 5 inducing points. FITC and PITC slightly outperform the DTC method, which also has greater variances. This dataset was also employed to evaluate the performance of the multitask kernels in Evgeniou and Pontil (2004). The best result presented in this work was 34.37 \( \pm \) 0.3. However, due to the averaging of the observations that we employed here, it is not fair to compare directly against those results.

6.4 Transcription factor regulation in the cell cycle of Yeast

We now consider an application of the multiple output convolutional model in transcriptional regulation. Microarray studies have made the simultaneous measurement of mRNA from thousands of genes practical. Transcription is governed by the presence of absence of transcription factor proteins that act as switches to turn on and off the expression of the genes. The active concentration of these transcription factors is typically much more diffi-
Figure 5: Mean and standard deviation of the percentage of explained variance for exam score prediction results on the ILEA dataset. The experiment was repeated ten times. In the bottom of the figure D\_K, F\_K, P\_K stands for DTC, FITC and PITC with K inducing values, respectively, ICM stands for intrinsic coregionalization model and IND stands for independent GPs. The ICM and the independent GPs results were obtained from Bonilla et al. (2008).

cult to measure. Several alternative methods have been proposed to infer these activities using gene expression data and information about the network architecture. However, most of these methods are based on assuming that there is an instantaneous linear relationship between the gene expression and the protein concentration. This simplifying assumption allows these methods to be applied on a genome wide scale. However, it is possible to obtain a more detailed description of the dynamics of this interaction using more realistic models that employ differential equations. One example of this type of modeling was presented in Barenco et al. (2006). Barenco et al. (2006) used an ordinary first order differential equation to model the interaction between a single transcription factor and a number of genes in a biological network motif known as a single input module. A typical dataset of this type consists of \( N \) measurements of the mRNA abundance level of \( D \) genes. The expression level \( f_d(t) \) of gene \( d \) at time \( t \) is related with the transcription factor protein \( u(t) \) through

\[
\frac{df_d}{dt} = B_d + S_d u(t) - \gamma_d f_d(t),
\]

where \( B_d \) is the basal transcription rate of gene \( d \), \( S_d \) is the sensitivity of gene \( d \) to the transcription factor and \( \gamma_d \) is the decay rate of mRNA. Solution for \( f_d(t) \) was given in
equation (11) with \( Q = 1 \) and taking into account the additional parameter \( B_d \), it follows

\[
f_d(t) = \frac{B_d}{\gamma_d} + S_d \int_0^t \exp(-\gamma_d(t-\tau)) u(\tau) d\tau.
\]

Given some training data for \( f_d(t) \), the usual way to estimate the dynamics of \( u(t) \) is to establish an error function and minimize it with respect to each value of \( u(t) \) and the parameters of the differential equation.

An alternative way to deal with these differential equations was proposed by Lawrence et al. (2007); Gao et al. (2008). Instead of finding a point estimate for \( u(t) \), these authors proposed to put a Gaussian process prior over \( u(t) \) and use Bayesian analysis to infer the posterior distribution for \( u(t) \) using the data for \( f_d(t) \). This corresponds exactly to the multiple output convolved Gaussian process framework that we have described in Section 3. In this case, the latent functions \( u_q(t) \) correspond to the transcription factor proteins and the outputs \( f_d(t) \) represent the gene expression data. Due to the computational complexity issue that we have already discussed, Lawrence et al. (2007); Gao et al. (2008) only dealt with a reduced number of genes. The first order differential equation model is obviously an oversimplification of transcriptional regulation. However, it considers more aspects of the system than clustering, or factor analysis. The sparse approach allows us to apply this richer model on a genome wide scale. Also, because this is done within the framework of Gaussian processes, it is always possible to add other, perhaps independent, terms to the covariance function to deal with any model mismatch.

As an example, we tested the PITC approximation for the multiple output Gaussian process using the benchmark yeast cell cycle dataset of Spellman et al. (1998). Data is preprocessed as described in Sanguinetti et al. (2006) with a final dataset of \( D = 1975 \) genes and \( Q = 104 \) transcription factors. The data also contains information about the structure of the network, basically a matrix of connectivities between transcription factors and genes. This is a matrix of size 1975\( \times \)104, where each entry is either a 0 or a 1, indicating the absence or presence of a link between the gene and the transcription factor protein. There are \( N = 24 \) time points for each gene. For the PITC approximation, we used \( K = 15 \) fixed inducing points, equally spaced in the input range. We optimize the approximated marginal likelihood through scaled conjugate gradient using 1000 iterations, where each iteration takes about 0.72 minutes. Figure 6(a) shows the expression level \( f_d(t) \) for ACE2 and in figure 6(b) the inferred transcription factor \( u_q(t) \). Equally, figure 6(c) shows the expression level \( f_d(t) \) for SWI5 and in figure 6(d) the inferred transcription factor \( u_q(t) \). The resulting shape of the transcription factors can be seen as offset versions of the shape of the gene expression data, which is a feature in this kind of networks. We can also use the sensitivity parameters \( S_{d,q} \) for ranking the relative influence of a particular transcription factor \( q \), over a particular gene \( d \). In more detail, we use the signal-to-noise ratio (SNR) \( \hat{S}_{d,q}/\sigma_{S_{d,q}} \), defined as the point estimate \( \hat{S}_{d,q} \) of the sensitivity parameter \( S_{d,q} \), obtained after the optimization procedure, over the standard deviation for that sensitivity \( \sigma_{S_{d,q}} \). An ad-hoc method to estimate this standard deviation consists of approximating the mode of the posterior density for the parameters \( S_{d,q} \) with a second order Taylor expansion: this is known as Laplace’s approximation. For details, the reader is referred to appendix A.2. Figure 7(a) shows a histogram of the values of the signal-to-noise ratio of the sensitivities of all genes in the dataset with respect to ACE2, this is,
all the genes that, according to the connectivity matrix, are regulated by ACE2. Some of
the highest SNR values are obtained for genes CTS1, SCW11, DSE1 and DSE2, while, for
example, NCE4 appears to be repressed with a low SNR value. Similar results have been
reported in other studies [Spellman et al. 1998; Sanguinetti et al. 2006].

Figure 6: Gene expression profile and inferred protein concentration for ACE2 and SWI5. The first
column shows the gene expression level. The second column shows the mean posterior over the
transcription factor \( u_q(t) \) and two standard deviations for the uncertainty.

Figure 7(b) shows the signal-to-noise ratio for the sensitivities of all the genes associated
to the transcription factor SWI5. Among others, genes AMN1 and PLC2 appear to be
activated by SWI5, as it has been confirmed experimentally by Colman-Lerner et al. (2001).

7. Conclusions

We have presented several sparse approximations for multiple output GPs, in the context
of convolution processes. Using these approximations we can capture the correlated in-
formation among outputs while reducing the amount of computational load for prediction
and optimization purposes. The computational complexity for the DTC and the FITC
approximations is \( O(NDK^2) \). The reduction in computational complexity for the PITC
approximation is from \( O(N^3D^3) \) to \( O(N^3D) \). This matches the computational complexity
for modeling with independent GPs. However, as we have seen, the predictive power of in-
dependent GPs is lower. Also, since PITC makes a better approximation of the likelihood,
the variance of the results is usually lower and approaches closely to the performance of the full GP, when compared to DTC and FITC.

With an appropriate selection of the kernel smoothing function we have an indirect way to generate different forms for the covariance function in the multiple output setup. We showed examples with Gaussian kernels, for which a suitable standardization of the kernels can be made, leading to competitive results in high-dimensional input regression problems, as seen in the school exam score prediction problem. The authors are not aware of other work in which this convolution process framework has been applied in problems with high input dimensions. Likewise, convolution appears naturally when solving differential equations in dynamical systems and we showed how the sparse methods can be applied to a large scale network inference problem. In general, we do not have access to the connectivity matrix, so to use this model in those situations we need to put sparse priors over the sensitivity parameters. However, our motivation was to show an example where sparse methods like the ones we proposed are needed. We obtained sensible results that agree with previous literature.

Recently, Titsias (2009) highlighted how approximations like FITC or PITC can exhibit a tendency to overfit when inducing inputs are optimized. Titsias (2009) proposed a variational method with an associated lower bound to overcome to some extent the overfitting problem. Following the ideas presented here, we can combine easily the method of Titsias (2009) and propose a lower bound for the multiple output case. This is part of the future work.

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Appendix A. Derivatives for the sparse methods

In this appendix, we present the derivatives needed to apply the gradient methods in the optimization routines. We present the first order derivatives of the log-likelihood with respect to $K_f$, $f$, $K_u$, $f$ and $K_u$, $u$. These derivatives can be combined with the derivatives of $K_f$, $f$, $K_u$, $f$ and $K_u$, $u$ with respect to $\theta$ and employ these expressions in a gradient-like optimization procedure.

We also present the expressions for the Hessian matrix in Laplace’s approximation employed to compute the uncertainty of the sensitivity parameters in the yeast cell cycle example.

We follow the notation of Brookes (2005) obtaining similar results to Lawrence (2007). This notation allows us to apply the chain rule for matrix derivation in a straightforward manner. Let’s define $G = \text{vec} G$, where vec is the vectorization operator over the matrix $G$. For a function $L$ the equivalence between $\partial L / \partial G$ and $\partial L / \partial G: = \left( \partial L / \partial G \right):^\top$ is given through $\partial L / \partial G: = \left( \partial L / \partial G \right) \delta_{GK}$.

A.1 First Derivatives of the log-likelihood for the gradient methods

The obtain the hyperparameters, we maximize the following log-likelihood function,

$$L(Z, \theta) \propto -\frac{1}{2} \log |D + K_{f,u} K_{u,u}^{-1} K_{u,f}| - \frac{1}{2} \text{trace} \left[ (D + K_{f,u} K_{u,u}^{-1} K_{u,f})^{-1} y y^\top \right]$$

where we have redefined $D$ as $D = \left[ K_{f,f} - K_{f,u} K_{u,u}^{-1} K_{u,f} \right] \odot M + \Sigma$, to keep a simpler notation. Using the matrix inversion lemma and its equivalent form for determinants, expression (17) can be written as

$$L(Z, \theta) \propto \frac{1}{2} \log |K_{u,u}| - \frac{1}{2} \log |A| - \frac{1}{2} \log |D| - \frac{1}{2} \text{trace} \left[ D^{-1} y y^\top \right] + \frac{1}{2} \text{trace} \left[ D^{-1} K_{f,u} A^{-1} K_{u,f} D^{-1} y y^\top \right].$$

We can find $\partial L / \partial \theta$ and $\partial L / \partial Z$ applying the chain rule to $L$ obtaining expressions for $\partial L / \partial K_{f,f} \delta_{GK}$ and $\partial L / \partial K_{u,u}$ and combining those with the relevant derivatives of the covariances wrt $\theta$ and $Z$,

$$\frac{\partial L}{\partial G:} = \frac{\partial L_A}{\partial A:} \frac{\partial A}{\partial D:} + \frac{\partial L_D}{\partial D:} \frac{\partial D}{\partial G:} + \left[ \frac{\partial L_A}{\partial A:} \frac{\partial A}{\partial G:} + \frac{\partial L_G}{\partial G:} \right] \delta_{GK},$$

where the subindex in $L_E$ stands for those terms of $L$ which depend on $E$, $G$ is either $K_{f,f}$, $K_{u,f}$ or $K_{u,u}$ and $\delta_{GK}$ is zero if $G$ is equal to $K_{f,f}$ and one in other case. Next we present
expressions for each partial derivative

\[
\frac{\partial \mathcal{L}_A}{\partial A} = -\frac{1}{2} \,(C:\,^T, \quad \frac{\partial A}{\partial D} = -(K_{u,f}D^{-1} \otimes K_{u,f}D^{-1}) \quad \frac{\partial \mathcal{L}_D}{\partial D} = -\frac{1}{2} \left((D^{-1}H^{-1}D^{-1})\right)\,^T
\]

\[
\frac{\partial D}{\partial K_{f,f}} = \text{diag}(M), \quad \frac{\partial D}{\partial K_{u,u}} = -\text{diag}(M) \left[ (I \otimes K_{f,u}K_{u,u}^{-1}) + (K_{f,u}K_{u,u}^{-1} \otimes I) \, T_D \right],
\]

\[
\frac{\partial D}{\partial K_{u,u}} = \text{diag}(M) \left( K_{f,u}K_{u,u}^{-1} \otimes K_{f,u}K_{u,u}^{-1} \right), \quad \frac{\partial A}{\partial K_{u,u}} = (K_{u,f}D^{-1} \otimes I) + (I \otimes K_{u,f}D^{-1}) \, T_A
\]

\[
\frac{\partial A}{\partial K_{f,f}} = I, \quad \frac{\partial \mathcal{L}_{K_{u,f}}}{\partial K_{u,u}} = \left((A^{-1}K_{u,f}D^{-1}yy^\top D^{-1})\right)\,^T, \quad \frac{\partial \mathcal{L}_{K_{u,u}}}{\partial K_{u,u}} = \frac{1}{2} \left((K_{u,u}^{-1})\right)\,^T
\]

where \( C = A^{-1} + A^{-1}K_{u,f}D^{-1}yy^\top D^{-1}K_{u,f}A^{-1} \), \( H = D - yy^\top + K_{f,u}A^{-1}K_{f,u}D^{-1}yy^\top + (K_{f,u}A^{-1}K_{u,u}D^{-1}yy^\top)^\top \) and \( T_D \) and \( T_A \) are vectorized transpose matrices (see, e.g., [Brookes, 2005]) and we have not included their dimensions to keep the notation clearer. We can replace the above expressions in (18) to find the corresponding derivatives, so

\[
\frac{\partial \mathcal{L}}{\partial K_{f,f}} = -\frac{1}{2} \, Q,
\]

where \( J = H - K_{f,u}CK_{u,f} \) and \( Q = (D^{-1}JD^{-1} \otimes M) \). We have used the property \((B:\,^T (F \otimes P) = ((P^\top BF)\,^T)\) in (19a) and the property \(\text{diag}(B:\,F) = (B \otimes F)\); to go from (19b) to (19c). We also have

\[
\frac{\partial \mathcal{L}}{\partial K_{u,u}} = \frac{1}{2} \left( (Q:\,^T \left[ (I \otimes K_{f,u}K_{u,u}^{-1}) + (K_{f,u}K_{u,u}^{-1} \otimes I) \, T_D \right] - \frac{1}{2} \,(C:\,^T \right.
\]

\[
\left. \left[ (K_{u,f}D^{-1} \otimes I) + (I \otimes K_{u,u}D^{-1}) \, T_A \right] + \left((A^{-1}K_{u,f}D^{-1}yy^\top D^{-1})\right)\,^T \right) \quad (20)
\]

or simply

\[
\frac{\partial \mathcal{L}}{\partial K_{u,f}} = K_{u,u}^{-1}K_{u,f}Q - CK_{u,f}D^{-1} + A^{-1}K_{u,f}D^{-1}yy^\top D^{-1},
\]

where in (20), \((Q:\,^T (F \otimes I) \, T_D = (Q:\,^T \, T_D (I \otimes F) = (T_D^\top Q:\,^T (I \otimes F) = (Q:\,)\,^T (I \otimes F). \)

A similar analysis is formulated for the term involving \( T_A \). Finally, results for \( \frac{\partial \mathcal{L}}{\partial K_{u,f}} \) and \( \frac{\partial \mathcal{L}}{\partial \Sigma} \) are obtained as

\[
\frac{\partial \mathcal{L}}{\partial K_{u,u}} = -\frac{1}{2} \,(K_{u,u}^{-1} - C - K_{u,u}^{-1}K_{u,f}QK_{f,u}K_{u,u}^{-1}), \quad \frac{\partial \mathcal{L}}{\partial \Sigma} = -\frac{1}{2} \, Q.
\]
A.2 Laplace approximation for the sensitivities

As an ad-hoc procedure to compute the uncertainty in the sensitivity parameters, we employ a Laplace approximation (see e.g. Chapter 4 of Bishop [2006]). In particular, consider \( Q = 1 \) and denote by \( s \in \mathbb{R}^D \) the vector of sensitivities with entries given by \( S_d \). The Laplace approximation \( q(s) \) for the random vector \( s \) follows

\[
q(s) = \mathcal{N}(s|s_0, \Gamma_{s_0}),
\]

where \( s_0 \) corresponds to a mode of the log-marginal likelihood for the sparse approximation and \( \Gamma_{s_0}^{-1} = -\nabla \nabla \mathcal{L}(Z, s, \eta) \big|_{s=s_0} \) with \( \eta \) representing the set of parameters belonging to the vector \( \theta \) without including \( s \). Assuming that after the optimization procedure we find a proper value for \( s_0 \), we need to compute \( \Gamma_{s_0}^{-1} \).

For simplicity, let us denote by \( Q_{f,f} \) the approximated covariance in the marginal likelihood, this is, \( Q_{f,f} = D + K_{f,u}K_{u,u}^{-1}K_{u,f} \). The log-marginal likelihood is given as

\[
\mathcal{L}(Z, \theta) \propto -\frac{1}{2} \log |Q_{f,f}| - \frac{1}{2} \left[ y^\top Q_{f,f}^{-1} y \right].
\]

The derivative \( \frac{\partial \mathcal{L}(Z, \theta)}{\partial S_d} \) is equal to

\[
\frac{\partial \mathcal{L}(Z, \theta)}{\partial S_d} = \frac{\partial \mathcal{L}}{\partial Q_{f,f}} \frac{\partial Q_{f,f}}{\partial S_d},
\]

where

\[
\frac{\partial \mathcal{L}}{\partial Q_{f,f}} = -\frac{1}{2} \left[ \left( Q_{f,f}^{-1} \right) : - \left( Q_{f,f}^{-1} y y^\top Q_{f,f}^{-1} \right) \right]^\top,
\]

where the inverse matrix \( Q_{f,f}^{-1} \) is computed using \( Q_{f,f}^{-1} = D^{-1} - D^{-1} K_{f,u} A^{-1} K_{u,f} D^{-1} \). We assume the sensitivities are independent random variables, so we only need to compute the elements in the diagonal of \( \Gamma_{s_0} \). Thus

\[
\frac{\partial^2 \mathcal{L}(Z, \theta)}{\partial S_d^2} = \frac{\partial}{\partial S_d} \left[ \frac{\partial \mathcal{L}}{\partial Q_{f,f}} \frac{\partial Q_{f,f}}{\partial S_d} \right] = \frac{\partial \mathcal{L}}{\partial Q_{f,f}} \frac{\partial^2 Q_{f,f}}{\partial S_d^2} + \frac{\partial}{\partial S_d} \left[ \frac{\partial \mathcal{L}}{\partial Q_{f,f}} \frac{\partial Q_{f,f}}{\partial S_d} \right].
\]

Finally, in the above expression, we need to compute

\[
\frac{\partial}{\partial S_d} \left[ \frac{\partial \mathcal{L}}{\partial Q_{f,f}} \right] = \frac{\partial}{\partial S_d} \left\{ -\frac{1}{2} \left[ \left( Q_{f,f}^{-1} \right) : - \left( Q_{f,f}^{-1} y y^\top Q_{f,f}^{-1} \right) \right]^\top \right\}
\]

\[
= -\frac{1}{2} \left[ \frac{\partial}{\partial S_d} \left( Q_{f,f}^{-1} \right) : - \frac{\partial}{\partial S_d} \left( Q_{f,f}^{-1} y y^\top Q_{f,f}^{-1} \right) \right]^\top
\]

\[
= -\frac{1}{2} \left\{ \left[ \frac{d}{d Q_{f,f}} \left( Q_{f,f}^{-1} \right) : - \frac{d}{d Q_{f,f}} \left( Q_{f,f}^{-1} y y^\top Q_{f,f}^{-1} \right) \right] \frac{\partial Q_{f,f}}{\partial S_d} \right\}^\top
\]

\[
= \frac{1}{2} \left\{ Q_{f,f}^{-1} \otimes Q_{f,f}^{-1} - Q_{f,f}^{-1} y y^\top Q_{f,f}^{-1} \otimes Q_{f,f}^{-1} - Q_{f,f}^{-1} \otimes Q_{f,f}^{-1} y y^\top Q_{f,f}^{-1} \right\} \frac{\partial Q_{f,f}}{\partial S_d} \right\}^\top.
\]

We do not need to compute the Kronecker products above. Instead, we use the property (PBF): = (F^\top \otimes P)B; leading to

\[
\frac{\partial}{\partial S_d} \left[ \frac{\partial \mathcal{L}}{\partial Q_{f,f}} \right] = \frac{1}{2} \left[ \left( Q_{f,f}^{-1} \frac{\partial Q_{f,f}}{\partial S_d} - Q_{f,f}^{-1} y y^\top Q_{f,f}^{-1} \frac{\partial Q_{f,f}}{\partial S_d} Q_{f,f}^{-1} - Q_{f,f}^{-1} \frac{\partial Q_{f,f}}{\partial S_d} Q_{f,f}^{-1} y y^\top Q_{f,f}^{-1} \right) \right]^\top.
\]
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