
Non-linear process convolutions for multi-output Gaussian processes

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Abstract

The paper introduces a non-linear version of the process convolution formalism for building covariance functions for multi-output Gaussian processes. The non-linearity is introduced via Volterra series, one series per each output. We provide closed-form expressions for the mean function and the covariance function of the approximated Gaussian process at the output of the Volterra series. The mean function and covariance function for the joint Gaussian process are derived using formulae for the product moments of Gaussian variables. We compare the performance of the non-linear model against the classical process convolution approach in one synthetic dataset and two real datasets.

1 INTRODUCTION

A multi-output Gaussian process (MOGP) is a Gaussian process (GP) with a covariance function that accounts for dependencies between multiple and related outputs [Bonilla et al., 2008]. Having models that exploit such dependencies is particularly important when some of the outputs are expensive to measure and the other more inexpensive outputs can be used as surrogates of the expensive output to improve its prediction. A typical example comes from geostatistics, where the accuracy of predicting the concentration of toxic heavy metals like lead or copper, which can be expensive to measure, can be improved by including measurements of pH as secondary variables, something that is significantly less expensive to measure [Goovaerts, 1997].

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One of the challenges in multi-output GPs is defining a cross-covariance function between outputs that leads to a valid covariance function for the joint GP. There is extensive literature looking at ways to build such types of cross-covariance functions [Álvarez et al., 2012]. One such approach is known as process convolution, for which each output is the convolution integral between a smoothing kernel and a latent random process. The approach was introduced by Barry and Ver Hoef [1996] to build covariance functions for single-output GPs, and later for multi-outputs in Ver Hoef and Barry [1998] and Higdon [2002]. The convolution integral linearly transforms the underlying latent process, which is usually assumed to be a Gaussian process. The output process is then a GP with a covariance equal to the convolution operators acting to modify the covariance function of the latent GP.

The main contribution in this paper is the introduction of a non-linear version of the process convolution construction suitable both for single-output and multi-output GPs. The non-linear model is constructed using a Volterra series where the input function is a latent random process. The Volterra series has been widely studied in the literature of non-linear dynamical systems [Haber and Keviczky, 1999]. They generalise the Taylor expansion for the case of non-instantaneous input functions. We treat the latent process as a Gaussian process and, using formulae for the product moments of Gaussian variables, we provide closed-form expressions for the mean function and covariance function of the output process. We approximate the output as a Gaussian process using these mean and covariance functions.

Most attempts to generate non-linear models that involve Gaussian processes come from an alternative representation of the convolution integral based on state space approaches [Hartikainen and Särkkä, 2011, Särkkä et al., 2013]. Exceptions include the works by Lawrence et al. [2007] and Titsias et al. [2009] where the non-linearity is a *static transformation* of the underlying latent GP. We review these and other approaches

in the Section 4.

We compare the performance of the non-linear model against the classical process convolution approach in one synthetic dataset and two real datasets and show that the non-linear version provides better performance than the traditional approach.

2 BACKGROUND

In this section, we briefly review the MOGP with process convolutions. We will refer to this particular construction as the convolved MOGP (CMOGP). We also briefly review the Volterra series and the formulae for the product moments of Gaussian variables that we use to construct our non-linear model.

2.1 Process convolutions for multi-output Gaussian processes

We want to jointly model the set of processes $[f_d(t)]_{d=1}^D$ using a joint Gaussian process. In the process convolution approach to building such a Gaussian process, dependencies between different outputs are introduced by assuming that each output $f_d(t)$ is the convolution integral between a smoothing kernel $G_d(t)$ and some latent function $u(t)$,

$$f_d(t) = \int_{\tau} G_d(t - \tau)u(\tau)d\tau, \quad (1)$$

where the smoothing kernel $G_d(t - \tau)$ should have finite energy. Assuming that the latent process $u(t)$ is a GP with zero mean function and covariance function $k(t, t')$, the set of processes $f_1(t), f_2(t), \dots, f_D(t)$ are jointly Gaussian with zero mean function and cross-covariance function between $f_d(t)$ and $f_{d'}(t')$ given by

$$k_{d,d'}(t, t') = \text{cov}[f_d(t), f_{d'}(t')] = \int \int G_d(t - \tau_i)G_{d'}(t' - \tau_j)k(\tau_i, \tau_j)d\tau_i d\tau_j. \quad (2)$$

In Álvarez et al. [2012], the authors have shown that the covariance function above generalises the well-known linear model of coregionalization, a form of covariance function for multiple outputs commonly used in machine learning and geostatistics.

The expression for $f_d(t)$ in the form of the convolution integral in (1) is also the representation of a linear dynamical system with impulse response $G_d(t)$. In the context of latent force models, such convolution expressions have been used to compute covariance functions informed by physical systems where the smoothing kernel is related to the so-called Green's function representation of an ordinary differential operator [Álvarez et al., 2013].

2.2 Representing non-linear dynamics with Volterra series

We borrow ideas from the representation of non-linear systems to extend the CMOGP to the non-linear case. One such representation is the Taylor series, which is the expansion of a time-invariant non-linear system as a polynomial about a fixed working point:

$$f(t) = \sum_{c=0}^{\infty} g_c u^c(t) = g_0 + g_1 u(t) + g_2 u^2(t) + \dots$$

While the Taylor series is widely used in the approximation of non-linear systems, it can only approximate systems for which the input has an instantaneous effect over the output [Haber and Keviczky, 1999].

By the Stone-Weierstraß theorem, a given continuous non-linear system with finite-dimensional vector input can be uniformly approximated by a finite polynomial series [Gallman and Narendra, 1976]. The Volterra series is such a polynomial expansion, describing a series of nested convolution operators:

$$\begin{aligned} f(t) &= \sum_{c=0}^{\infty} \int \dots \int G^{(c)}(t - \tau_1, \dots, t - \tau_c) \prod_{j=1}^c u(\tau_j) d\tau_j \\ &= G^{(0)} + \int G^{(1)}(t - \tau_1)u(\tau_1)d\tau_1 \\ &\quad + \iint G^{(2)}(t - \tau_1, t - \tau_2)u(\tau_1)u(\tau_2)d\tau_1 d\tau_2 \\ &\quad + \dots \end{aligned}$$

The leading term $G^{(0)}$ is a constant term, which in practise is assumed to be zero-valued and the series is incremented from $c = 1$. Because of the convolutions involved, the series is no longer modelling an instantaneous input at t , giving the series a so-called *memory effect* [Haber and Keviczky, 1999]. As with the Taylor series, the approximant needs a cut-off for the infinite sum, denoted C ; a Volterra series with C sum terms is called C -order.

The representation of a c^{th} degree kernel, i.e. $G^{(c)}(t - \tau_1, \dots, t - \tau_c)$, can be expressed in different forms, such as in symmetric or triangular form [Haber and Keviczky, 1999]. A common assumption is that the kernels are homogeneous and separable, such that $G^{(c)}$ is the product of c first degree kernels. The assumption of separability is stronger but reduces the number of unique parameters, which can be very large for a full Volterra series [Schetzen, 1980]. It should also be noted that a truncated Volterra series with separable homogeneous kernels is equivalent to a Wiener model [Cheng et al., 2017].

2.3 Product moments for multivariate Gaussian random variables

Several of the results that we will present in the following section involve the computation of the expected value of the product of several multivariate Gaussian random variables. For this, we will use results derived in Song and Lee [2015]. We are interested in those results for which the Gaussian random variables have zero mean. In particular, let $[X_i]_{i=1}^c$ be multivariate Gaussian random variables with zero mean values and covariance between X_i and X_j given as ϕ_{ij} . According to Corollary 1 in Song and Lee [2015], the expression for $\mathbb{E}[\prod_{i=1}^c X_i^{a_i}]$, follows as

$$\mathbb{E}\left[\prod_{i=1}^c X_i^{a_i}\right] = \sum_{\mathbf{L} \in T_{\mathbf{a}}} \frac{\prod_{k=1}^c a_k!}{2^{\text{tr}[\mathbf{L}]} \prod_{i=1}^c \prod_{j=1}^c l_{ij}!} \prod_{i=1}^c \prod_{j=i}^c (\phi_{ij})^{l_{ij}}, \quad (3)$$

where $\mathbf{a} = [a_i]_{i=1}^c$ is a vector consisting of the random variable exponents and $T_{\mathbf{a}}$ is the set of $c \times c$ symmetric matrices¹ that meet the condition $L_{\mathbf{a},k} = 0$ for $k = 1, \dots, c$, as defined by

$$T_{\mathbf{a}} = \left\{ [l_{pq}]_{c \times c} \mid \underbrace{a_k - l_{kk} - \sum_{j=1}^c l_{jk}}_{L_{\mathbf{a},k}} = 0, \forall k \in \{1, \dots, c\} \right\}. \quad (4)$$

If the sum of exponents, $\sum_{k=1}^c a_k$, is an odd number, then $\mathbb{E}[\prod_{i=1}^c X_i^{a_i}] = 0$ for the zero mean value case, as described in Corollary 2 in Song and Lee [2015].

An additional result used later is that if $a_k = 1, \forall a_k$ then (3), by Remark 5 in Song and Lee [2015], reduces to

$$\mathbb{E}\left[\prod_{i=1}^c X_i\right] = \sum_{\mathbf{L} \in T_{\mathbf{a}}} \prod_{i=1}^c \prod_{j=i}^c \phi_{ij}^{l_{ij}}. \quad (5)$$

3 A NON-LINEAR CMOGP BASED ON VOLTERRA SERIES

We represent a vector-valued non-linear dynamic system with a system of Volterra series of order C . For a given output dimension, d , we approximate the function with a truncated Volterra series as follows

$$f_d^{(C)}(t) = \sum_{c=1}^C \int \dots \int G_d^{(c)}(t - \tau_1, \dots, t - \tau_c) \prod_{j=1}^c u(\tau_j) d\tau_j, \quad (6)$$

where $G_d^{(c)}$ are c^{th} degree Volterra kernels.

Our approach is to assume that $u(t)$, the latent driving function, follows a GP prior. For $C = 1$, we recover the

¹In Song and Lee [2015], the authors denote $T_{\mathbf{a}}$ as a collection of sets-of-sets, but we interpret the elements as symmetric matrices for notational clarity.

the expression for the process convolution construction of a multi-output GP as defined in (1). In contrast to the linear case, the output $f_d^{(C)}$ is no longer a GP. However, we approximate $f_d^{(C)}$ with a GP $\tilde{f}_d^{(C)}(t)$ with a mean and covariance function computed from the moments of the output process $f_d^{(C)}$:

$$\tilde{f}_d^{(C)}(t) \sim \mathcal{GP}(\mu_d^{(C)}(t), k_{d,d'}^{(C)}(t, t')), \quad (7)$$

where $\mu_d^{(C)}(t) = \mathbb{E}[f_d^{(C)}(t)]$ and $k_{d,d'}^{(C)}(t, t') = \text{cov}[f_d^{(C)}(t), f_{d'}^{(C)}(t')]$. Approximating a non-Gaussian distribution with a Gaussian, particularly for non-linear systems, is common in state space modelling, for example in the unscented Kalman filter [Särkkä, 2013]; or as a choice of variational distribution in variational inference [Blei et al., 2017]. We refer to the joint process $[\tilde{f}_d^{(C)}(t)]_{d=1}^D$ as the *non-linear convolved multi-output GP* (NCMOGP).

Furthermore, we will assume that the c^{th} degree Volterra kernels are separable, such that

$$G_d^{(c)}(t - \tau_1, \dots, t - \tau_c) = \prod_{i=1}^c G_d^{(c,i)}(t - \tau_i), \quad (8)$$

where $G_d^{(c,i)}$ are first degree Volterra kernels.

Using this separable form, we express the output $f_d^{(C)}(t)$ as

$$\sum_{c=1}^C \prod_{i=1}^c \int_{\tau_i} G_d^{(c,i)}(t - \tau_i) u(\tau_i) d\tau_i = \sum_{c=1}^C \prod_{i=1}^c f_d^{(c,i)}(t),$$

where we define

$$f_d^{(c,i)}(t) = \int_{\tau_i} G_d^{(c,i)}(t - \tau_i) u(\tau_i) d\tau_i.$$

Assuming $u(t)$ has a GP prior with zero mean and covariance $k(t, t')$, and due to the linearity of the expression above, we can compute the corresponding mean and covariance functions for the joint Gaussian process $[f_d^{(c,i)}(t)]_{d=1}^D$. We compute the cross-covariance function between $f_d^{(c,i)}(t)$ and $f_{d'}^{(c',j)}(t')$ using

$$k_{d,d'}^{(c,i),(c',j)}(t, t') = \text{cov}[f_d^{(c,i)}(t), f_{d'}^{(c',j)}(t')] = \iint G_d^{(c,i)}(t - \tau_i) G_{d'}^{(c',j)}(t' - \tau_j) k(\tau_i, \tau_j) d\tau_i d\tau_j. \quad (9)$$

This is a similar expression to the one in (2) for the CMOGP. For some particular forms of the Volterra kernels $G_d^{(c,i)}$ and covariance $k(t, t')$ of the latent process $u(t)$, the covariance $k_{d,d'}^{(c,i),(c',j)}(t, t')$ can be computed analytically.

3.1 NCMOGP with separable Volterra kernels

In this section, we derive expressions for $\mu_d^{(C)}(t)$ and $k_{d,d'}^{(C)}(t, t')$ with the assumption of separability of the Volterra kernels in (8).

3.1.1 Mean function

Let us first compute the mean function, $\mu_d^{(C)}(t) = \mathbb{E}[f_d^{(C)}(t)]$. Using the definition for the expected value, we get

$$\mathbb{E}[f_d^{(C)}(t)] = \sum_{c=1}^C \mathbb{E} \left[\prod_{i=1}^c f_d^{(c,i)}(t) \right]. \quad (10)$$

The expected value of the product of the Gaussian processes, $\mathbb{E}[\prod_{i=1}^c f_d^{(c,i)}(t)]$, can be computed using results obtained for the expected value of the product of multivariate Gaussian random variables as introduced in Section 2.3.

Applying the result in (5) to the expression of the expected value in (10), we get

$$\mathbb{E} \left[\prod_{i=1}^c f_d^{(c,i)}(t) \right] = \sum_{\mathbf{L} \in T_{\mathbf{a}}} \prod_{i=1}^c \prod_{j=i}^c \left(k_{d,d}^{(c,i),(c,j)}(t,t) \right)^{l_{ij}}, \quad (11)$$

where

$$k_{d,d}^{(c,i),(c,j)}(t,t) = \text{cov}[f_d^{(c,i)}(t), f_d^{(c,j)}(t)].$$

Note that only the terms for which c is even are non-zero.

Example 1 To see an example of the kind of expressions that the expected value takes, let us assume that $c = 4$. We then have

$$\mathbb{E} \left[\prod_{i=1}^4 f_d^{(4,i)}(t) \right] = \sum_{\mathbf{L} \in T_{\mathbf{a}}} \prod_{i=1}^4 \prod_{j=i}^4 \left(k_{d,d}^{(4,i),(4,j)}(t,t) \right)^{l_{ij}},$$

where

$$k_{d,d}^{(4,i),(4,j)}(t,t) = \text{cov}[f_d^{(4,i)}(t), f_d^{(4,j)}(t)].$$

We now need to find the set $T_{\mathbf{a}}$ containing all $c \times c$ symmetric matrices \mathbf{L} , the elements of which meet the condition described in (4), where $\mathbf{a} = [1 \ 1 \ 1 \ 1]$. This leads to the following system of equations

$$\begin{aligned} 2l_{11} + l_{12} + l_{13} + l_{14} &= 1 \\ l_{12} + 2l_{22} + l_{23} + l_{24} &= 1 \\ l_{13} + l_{23} + 2l_{33} + l_{34} &= 1 \\ l_{14} + l_{24} + l_{34} + 2l_{44} &= 1, \end{aligned}$$

where we have used the symmetry of \mathbf{L} , so $l_{ij} = l_{ji}$. It can be seen from the above system that the set $T_{\mathbf{a}}$ contains three unique symmetric matrices:

$$T_{\mathbf{a}} = \left\{ \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \right\}.$$

We now have an expression for the expected value, by (11):

$$\begin{aligned} \mathbb{E} \left[\prod_{i=1}^4 f_d^{(4,i)}(t) \right] &= k_{d,d}^{(4,1),(4,2)}(t,t) k_{d,d}^{(4,3),(4,4)}(t,t) \\ &+ k_{d,d}^{(4,1),(4,3)}(t,t) k_{d,d}^{(4,2),(4,4)}(t,t) \\ &+ k_{d,d}^{(4,1),(4,4)}(t,t) k_{d,d}^{(4,2),(4,3)}(t,t). \end{aligned}$$

3.1.2 Cross-covariance function

For computing the covariance function, $k_{d,d'}^{(C)}(t,t') = \mathbb{E}[f_d^{(C)}(t)f_{d'}^{(C)}(t')] - \mathbb{E}[f_d^{(C)}(t)]\mathbb{E}[f_{d'}^{(C)}(t')]$, we first need to compute the second moment between $f_d^{(C)}(t)$ and $f_{d'}^{(C)}(t')$. The second moment is given as

$$\begin{aligned} &\mathbb{E} \left[f_d^{(C)}(t) f_{d'}^{(C)}(t') \right] \\ &= \mathbb{E} \left[\sum_{c=1}^C \prod_{i=1}^c f_d^{(c,i)}(t) \sum_{c'=1}^C \prod_{j=1}^{c'} f_{d'}^{(c',j)}(t') \right] \\ &= \sum_{c=1}^C \sum_{c'=1}^C \mathbb{E} \left[\prod_{i=1}^c \prod_{j=1}^{c'} f_d^{(c,i)}(t) f_{d'}^{(c',j)}(t') \right] \\ &= \sum_{c=1}^C \sum_{c'=1}^C \mathbb{E} \left[\prod_{i=1}^{c+c'} \bar{f}_{d,d'}^{(i)}(t) \right], \end{aligned} \quad (12)$$

where $\bar{f}_{d,d'}^{(i)}$ is the i^{th} output of a vector-valued function consisting of all functions in the product

$$\bar{\mathbf{f}}_{d,d'}(t) = \left[f_d^{(c,1)}(t) \dots f_d^{(c,c)}(t) f_{d'}^{(c',1)}(t') \dots f_{d'}^{(c',c')}(t') \right]^{\top}.$$

We have assumed that both $f_d^{(C)}(t)$ and $f_{d'}^{(C)}(t')$ share the same value of C , although a more general expression can be obtained where each output can have its own C value. We can apply the expressions in Song and Lee [2015] to the above moment of the product of Gaussian random variables as we did for computing the mean function in Section 3.1.1. Using the expression for the expected value of the product of Gaussian variables, we get

$$\mathbb{E} \left[\prod_{i=1}^{c+c'} \bar{f}_{d,d'}^{(i)}(t) \right] = \sum_{\mathbf{L} \in T_{\mathbf{a}}} \prod_{i=1}^{c+c'} \prod_{j=i}^{c+c'} \left(\text{cov} \left[\bar{f}_{d,d'}^{(i)}(t), \bar{f}_{d,d'}^{(j)}(t) \right] \right)^{l_{ij}},$$

where the covariance element is defined in (9) as the cross-covariance of two latent functions.

Example 2 For illustration purposes, let us assume that $c = 3$ and $c' = 1$. In this case, we would have

$$\begin{aligned} &\mathbb{E} \left[\prod_{i=1}^3 f_d^{(3,i)}(t) f_{d'}^{(1,1)}(t') \right] \\ &= \sum_{\mathbf{L} \in T_{\mathbf{a}}} \prod_{i=1}^3 \prod_{j=i}^3 \left(\text{cov} \left[\bar{f}_{d,d'}^{(i)}(t), \bar{f}_{d,d'}^{(j)}(t) \right] \right)^{l_{ij}}, \end{aligned}$$

where we have defined $\bar{\mathbf{f}}_{d,d'}$ as

$$\bar{\mathbf{f}}_{d,d'} = \left[f_d^{(3,1)}(t) \ f_d^{(3,2)}(t) \ f_d^{(3,3)}(t) \ f_{d'}^{(1,1)}(t') \right]^{\top}.$$

The set $T_{\mathbf{a}}$ contains the same matrices as we found in Example 1 in Section 3.1.1 leading to

$$\begin{aligned} &\mathbb{E} \left[\prod_{i=1}^3 f_d^{(3,i)}(t) f_{d'}^{(1,1)}(t') \right] \\ &= k_{d,d}^{(3,1),(3,2)}(t,t) k_{d,d'}^{(3,3),(1,1)}(t,t') \\ &+ k_{d,d}^{(3,1),(3,3)}(t,t) k_{d,d'}^{(3,2),(1,1)}(t,t') \\ &+ k_{d,d}^{(3,1),(1,1)}(t,t') k_{d,d}^{(3,2),(3,3)}(t,t). \end{aligned}$$

The cross-covariance function between $f_d^{(C)}(t)$ and $f_{d'}^{(C)}(t')$ is then computed using

$$\begin{aligned} \text{cov}[f_d^{(C)}(t), f_{d'}^{(C)}(t')] \\ = \mathbb{E}[f_d^{(C)}(t)f_{d'}^{(C)}(t')] - \mathbb{E}[f_d^{(C)}(t)]\mathbb{E}[f_{d'}^{(C)}(t')]. \end{aligned}$$

We have expressions for both $\mathbb{E}[f_d^{(C)}(t)f_{d'}^{(C)}(t')]$ and $\mathbb{E}[f_d^{(C)}(t)]$ by (10) and (12) respectively.

3.2 NCMOGP with separable and homogeneous Volterra kernels

In the section above, we introduced a model that allows for different first-order Volterra kernels $G_d^{(c,i)}(x)$, when building the general Volterra kernel of order c . A further assumption we can make is that all first-order Volterra kernels are the same, i.e., $G_d^{(c,i)}(t - \tau_i) = G_d(t - \tau)$, $\forall c, \forall i$, meaning that $f_d^{(c,i)}(t) = f_d(t)$, for all c and for all i . We will refer to this as the separable and homogeneous version of the NCMOGP.

We then get

$$f_d^{(C)}(t) = \sum_{c=1}^C \prod_{i=1}^c f_d^{(c,i)}(t) = \sum_{c=1}^C \prod_{i=1}^c f_d(t) = \sum_{c=1}^C f_d^c(t),$$

where $f_d(t) = \int G_d(t - \tau)u(\tau)d\tau$, and $u(t) \sim \mathcal{GP}(0, k(t, t'))$. The cross-covariance function between $f_d(t)$ and $f_{d'}(t')$ is again $k_{d,d'}(t, t')$ as in (2).

As we did in Section 3.1, we can compute the mean function for $f_d^{(C)}(t)$ and cross-covariance functions between $f_d^{(C)}(t)$ and $f_{d'}^{(C)}(t')$.

3.2.1 Mean function

Using Eq. (3), the mean function $\mathbb{E}[f_d^{(C)}(t)]$ follows as

$$\begin{aligned} \mathbb{E}[f_d^{(C)}(t)] &= \mathbb{E}\left[\sum_{c=1}^C f_d^c(t)\right] = \sum_{c=1}^C \mathbb{E}[f_d^c(t)] \\ &= \sum_{c=1}^C \frac{c!}{2^{l_{11}}l_{11}!} (k_{d,d}(t, t))^{l_{11}}, \end{aligned}$$

where l_{11} is such that satisfies $2l_{11} = c$. This means that the above expression only has solutions for even-valued c , and $l_{11} = c/2$. Then,

$$\mathbb{E}[f_d^{(C)}(t)] = \sum_{c=1}^C \frac{c!}{2^{c/2}(\frac{c}{2})!} (k_{d,d}(t, t))^{c/2},$$

for even c and $C \geq 2$.

3.2.2 Cross-covariance function

We can compute the second moment $\mathbb{E}[f_d^{(C)}(t)f_{d'}^{(C)}(t')]$ using

$$\begin{aligned} \mathbb{E}[f_d^{(C)}(t)f_{d'}^{(C)}(t')] &= \mathbb{E}\left[\sum_{c=1}^C f_d^c(t) \sum_{c'=1}^C f_{d'}^{c'}(t')\right] \\ &= \sum_{c=1}^C \sum_{c'=1}^C \mathbb{E}[f_d^c(t)f_{d'}^{c'}(t')]. \end{aligned}$$

Once again we use expression (3) to compute $\mathbb{E}[f_d^c(t)f_{d'}^{c'}(t')]$, leading to

$$\begin{aligned} \mathbb{E}[f_d^c(t)f_{d'}^{c'}(t')] &= \\ \sum_{\mathbf{L} \in T_{\mathbf{a}}} A_{c,c',\mathbf{L}} (k_{d,d}(t, t))^{l_{11}} (k_{d,d'}(t, t'))^{l_{12}} (k_{d',d'}(t', t'))^{l_{22}}, \end{aligned}$$

where $A_{c,c',\mathbf{L}}$ is defined as

$$A_{c,c',\mathbf{L}} = \frac{c!c'}{2^{l_{11}+l_{22}}l_{11}!l_{12}!l_{22}!},$$

and $k_{d,d'}(t, t')$ is defined in (2). To avoid computer overflow due to the factorial operators when computing $A_{c,c',\mathbf{L}}$, we compute $\exp(\log(A_{c,c',\mathbf{L}}))$ instead. As stated previously, the expected value will be 0 if $c + c'$ is not even.

Example 3 Let us assume that $c = 3$ and $c' = 3$. The expected value $\mathbb{E}[f_d^3(t)f_{d'}^3(t')]$ follows as

$$\sum_{\mathbf{L} \in T_{\mathbf{a}}} A_{3,3,\mathbf{L}} (k_{d,d}(t, t))^{l_{11}} (k_{d,d'}(t, t'))^{l_{12}} (k_{d',d'}(t', t'))^{l_{22}},$$

where $A_{3,3,\mathbf{L}} = (3!3!)/2^{l_{11}+l_{22}}l_{11}!l_{12}!l_{22}!$. To find the elements in $\mathbf{L} \in T_{\mathbf{a}}$, we need to solve similar equations to the ones in Example 1. We would have

$$\begin{aligned} 2l_{11} + l_{12} &= c = 3 \\ l_{12} + 2l_{22} &= c' = 3. \end{aligned}$$

We can see that there are two valid solutions for \mathbf{L} :

$$T_{\mathbf{a}} = \left\{ \begin{bmatrix} 0 & 3 \\ 3 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \right\}.$$

The expression for $\mathbb{E}[f_d^3(t)f_{d'}^3(t')]$ is thus

$$6k_{d,d'}^3(t, t') + 9k_{d,d}(t, t)k_{d,d'}(t, t')k_{d',d'}(t', t').$$

We compute the covariance $\text{cov}[f_d^{(C)}(t), f_{d'}^{(C)}(t')]$ now that we have expressions to compute the mean for $f_d^{(C)}(t)$ and the expected value for the product between $f_d^{(C)}(t)$ and $f_{d'}^{(C)}(t')$.

4 RELATED WORK

In the work by Lawrence et al. [2007], non-linear dynamics are introduced with a GP prior within a non-linear function, which are inferred using the Laplace approximation, with the convolution operator itself approximated as a discrete sum. Similarly, Titsias et al. [2009] approximate the posterior to the non-linear system over a GP using an MCMC sampling approach. Approaches to non-linear likelihoods with GP priors, not limited to MOGPs, include the warped GP model [Lázaro-Gredilla, 2012] and chained GPs [Saul et al., 2016] which make use of variational approximations. Techniques from state space modelling, including Taylor series linearisation and sigma points used to approximate Gaussians in the extended and unscented Kalman filters respectively have been applied to non-linear Gaussian processes, both for single output and multitask learning [Steinberg and Bonilla, 2014, Bonilla et al., 2016].

An alternative perspective to the linear convolution process, in particular latent force models, is to construct it as a continuous-discrete state space model (SSM) driven by white noise [Hartikainen and Särkkä, 2011, Särkkä et al., 2013]. Hartikainen et al. [2012] use this approach for the general case of non-linear Wiener systems, approximating the posterior with an unscented versions of the Kalman filter and Rauch-Tung-Streifel smoother. The SSM approach benefits from inference being performed in linear time, but relies on certain constraints on the nature of the underlying covariance functions. In particular, a kernel must have a rational power spectrum to be used in exact form, which precludes the use of, for example, the exponentiated quadratic kernel for exact Gaussian process regression without introducing an additional approximation error [Särkkä et al., 2013]. Wills et al. [2013] also use a state space representation to approximate Hammerstein-Wiener models, albeit with sequential Monte Carlo and a maximum-likelihood approach.

5 IMPLEMENTATION

Multi-output regression with NCMOGP In this paper, we are interested in the multi-output regression case. Therefore, we restrict the likelihood models for each output to be Gaussian. In particular, we assume that each observed output $y_d(t)$ follows $y_d(t) = \tilde{f}_d^{(C)}(t) + w_d(t)$, where $w_d(t)$ is a white Gaussian noise process with covariance function $\sigma_d^2 \delta_{t,t'}$. Other types of likelihoods are possible as for example in Moreno-Muñoz et al. [2018].

Kernel functions In all the experiments, we use an exponentiated quadratic (EQ) form for the smoothing kernels $G_d(t - \tau)$ and an EQ form for the kernel of the latent functions $u(t)$. With these forms, the kernel $k_{d,d'}(t, t')$ also follows an EQ form. We use the expressions for $k_{d,d'}(t, t')$ obtained by Álvarez and Lawrence [2011].

High-dimensional inputs The resulting mean function $\mathbb{E}[f_d^{(C)}(t)]$ and covariance function $\text{cov}[f_d^{(C)}(t), f_{d'}^{(C)}(t')]$ assume that the input space is one-dimensional. We can extend the approach to high-dimensional inputs, $\mathbf{x} \in \mathbb{R}^p$ by assuming that both the mean function and covariance function factorise across the input dimension, and using the same expressions for the kernels for each factorised dimension.

Hyperparameter learning We optimise the log-marginal likelihood for finding point estimates of the hyperparameters θ of the NCMOGP. Hyperparameters include the parameters for the smoothing kernels $G_d(\cdot)$, the kernel function $k(t, t')$ and the variances for the white noise processes $w_d(t)$, σ_d^2 . For simplicity in the notation, we assume that all the outputs are evaluated at the same set of inputs $\mathbf{t} = \{t_n\}_{n=1}^N$. Let $\mathbf{y} = [\mathbf{y}_1^\top, \dots, \mathbf{y}_D^\top]^\top$, with $\mathbf{y}_d = [y_d(t_1), \dots, y_d(t_N)]^\top$. The log-marginal likelihood $\log p(\mathbf{y}|\mathbf{t})$ is then given as

$$-\frac{ND}{2} \log(2\pi) - \frac{1}{2} (\mathbf{y} - \boldsymbol{\mu}^{(C)})^\top (\mathbf{K}_{\mathbf{f},\mathbf{f}}^{(C)} + \boldsymbol{\Sigma})^{-1} \times (\mathbf{y} - \boldsymbol{\mu}^{(C)}) - \frac{1}{2} \log |\mathbf{K}_{\mathbf{f},\mathbf{f}}^{(C)} + \boldsymbol{\Sigma}|,$$

where $\boldsymbol{\mu}^{(C)} \in \mathbb{R}^{ND \times 1}$ has entries given by $\mu_d^{(C)}(t)$, $\mathbf{K}_{\mathbf{f},\mathbf{f}}^{(C)} \in \mathbb{R}^{ND \times ND}$ has entries computed using $k_{d,d'}^{(C)}(t, t')$ and $\boldsymbol{\Sigma}$ is

a diagonal matrix containing the variances of the noise processes per output. We use a gradient-based optimization procedure to estimate the hyperparameters that maximize the log-marginal likelihood. Computational complexity for this model grows as $\mathcal{O}(D^3 N^3)$, related to the inversion of the matrix $\mathbf{K}_{\mathbf{f},\mathbf{f}}^{(C)} + \boldsymbol{\Sigma}$. This is the typical complexity in a full multi-output Gaussian process model [Álvarez and Lawrence, 2011].

Predictive distribution The predictive distribution is the same one used for the single-output case. Let $\mathbf{t}_* = [t_{n,*}]_{n=1}^{N_*}$ be the input test set. The predictive distribution follows as $p(\mathbf{y}_*|\mathbf{y}) = \mathcal{N}(\mathbf{y}_*|\boldsymbol{\mu}_{\mathbf{y}_*|\mathbf{y}}, \mathbf{K}_{\mathbf{y}_*|\mathbf{y}})$, with $\boldsymbol{\mu}_{\mathbf{y}_*|\mathbf{y}} = \boldsymbol{\mu}_*^{(C)} + \mathbf{K}_{\mathbf{f}_*,\mathbf{f}}^{(C)} (\tilde{\mathbf{K}}_{\mathbf{f},\mathbf{f}}^{(C)})^{-1} \boldsymbol{\mu}^{(C)}$ and $\mathbf{K}_{\mathbf{y}_*|\mathbf{y}} = \mathbf{K}_{\mathbf{f}_*,\mathbf{f}_*}^{(C)} - \mathbf{K}_{\mathbf{f}_*,\mathbf{f}}^{(C)} (\tilde{\mathbf{K}}_{\mathbf{f},\mathbf{f}}^{(C)})^{-1} \mathbf{K}_{\mathbf{f},\mathbf{f}}^{(C)} + \boldsymbol{\Sigma}_*$, where $\tilde{\mathbf{K}}_{\mathbf{f},\mathbf{f}}^{(C)} = \mathbf{K}_{\mathbf{f},\mathbf{f}}^{(C)} + \boldsymbol{\Sigma}$. In these expressions, $\boldsymbol{\mu}_*^{(C)}$ has entries given by $\mu^{(C)}(t_{n,*})$; $\mathbf{K}_{\mathbf{f}_*,\mathbf{f}_*}^{(C)}$ has entries given by $k_{d,d'}^{(C)}(t_{n,*}, t_{m,*})$; and $\mathbf{K}_{\mathbf{f},\mathbf{f}}^{(C)}$ has entries given by $k_{d,d'}^{(C)}(t_{n,*}, t_m)$.

6 EXPERIMENTAL RESULTS

Experimental results are provided for the NCMOGP with homogeneous and separable kernels. In all the experiments that follow, hyperparameter estimation is performed through maximization of the log-marginal likelihood as explained in section 5. We use the normalised mean squared-error (NMSE) and the negative log-predictive density (NLPD) to assess the performance.

6.1 Toy example

We set a problem of $D = 3$ outputs where the smoothing kernels are given as $G_d(t - \tau) = S_d \exp(-P_d(t - \tau)^2)$, with parameters $S_1 = 5, S_2 = 1, S_3 = 2$, and $P_1 = 200, P_2 = 0.1$ and $P_3 = 100$. The latent function follows as $u(t) = \sum_{k=1}^4 \left(\frac{1}{k^2}\right) \cos(2k\pi t)$. We then numerically solve the convolution integral $f_d(t) = \int_0^t G_d(t - \tau) u(\tau) d\tau$ for 200 datapoints in the input range $[0, 1]$. We compute $f_d^{(C=3)}(t) = \sum_{c=1}^3 f_d^c(t)$ and the observed data is obtained by adding Gaussian noise with a variance of $\sigma_d^2 = 0.005 \times \text{var}[f_d^{(C=3)}(t)]$. We randomly split the dataset into a train set of $N = 50$ per output and the rest of the datapoints are used for assessing the performance.

Figure 1 shows qualitative results for predictions made by the CMOGP and a NCMOGP with $C = 3$. Although the outputs exhibit a smooth behavior, there are subtle non-linear characteristics that are not captured by the linear model. By zooming in on the interval $t \in [0.4, 0.6]$ for output $y_1(t)$ (first column in the Figure), we observe that the predictive mean of the linear model ($C = 1$) does not completely follow the data compared to the true non-linear model ($C = 3$). For output $y_3(t)$ (third column in the Figure), we observe a similar behavior in the predictive mean of the linear model in the intervals $t \in [0.4, 0.8]$ and $t > 0.9$ compared to the predictive mean of the non-linear model.

Table 1 shows the NMSE and the NLPD for different values of C for twenty different partitions of the original dataset into training and testing. We show the average of the metric plus-or-minus a standard deviation. The performance is

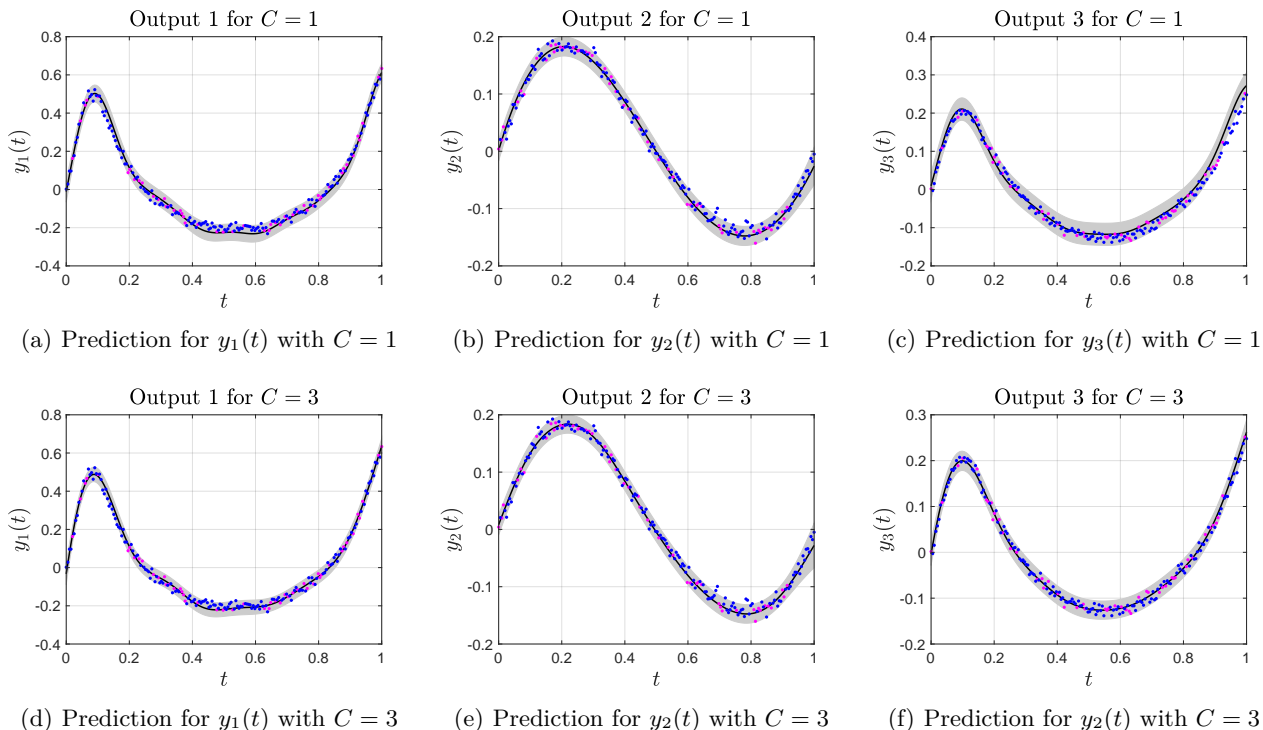


Figure 1: Comparison of the predictive performance of CMOGP (top row) and NCMOGP with $C = 3$ (bottom row) for the dataset synthetically generated. Each column is a different output. Training data is represented using red dots and Test data using blue dots. The black line in the mean over the predictive GP function, and the shaded region denotes two times the standard deviation.

similar for the non-linear models with $C \geq 3$, although the model for $C = 3$ shows the lowest standard deviation.

Table 1: Results for the Toy example.

C	NMSE	NLPD
1	0.0142 ± 0.0022	-2.6868 ± 0.0794
2	0.0075 ± 0.0012	-2.9641 ± 0.0665
3	0.0071 ± 0.0009	-2.9780 ± 0.0513
4	0.0072 ± 0.0010	-2.9546 ± 0.0960
5	0.0071 ± 0.0011	-2.9428 ± 0.0956

6.2 Weather data

We use the air temperature dataset considered previously by Nguyen and Bonilla [2014] and used in other multi-output GP papers. The dataset contains air temperature measurements at four spatial locations on the south coast of England: Bramble Bank, Southampton Dockhead, Chichester Harbour and Chichester Bar, usually refer to by the names Bramblemet, Sotonmet, Cambermet and Chimet, respectively. The measurements correspond to July 10 to July 15, 2013. The prediction problem as introduced in Nguyen and Bonilla [2014] corresponds to predicting consecutive missing data in the outputs Cambermet and Chimet, 173 and 201 observations, respectively, using observed data from all the stations: 1425 observations for Bramblemet, 1268 observations for Cambermet, 1235 for Chimet and

1097 for Sotonmet.

The missing data was artificially removed and we have access to the ground-truth measurements. We compare the non-linear convolution approach to the Intrinsic Coregionalization Model (ICM) [Goovaerts, 1997] and Dependent Gaussian processes (DGP) [Boyle and Frean, 2005]. Both models can be seen as particular cases of the non-linear model in Eq. (6). The ICM can be recovered from Eq. (6) by making $C = 1$ and $G_{d,1}(\cdot) = a_d \delta(\cdot)$, where a_d is a scalar that needs to be estimated and $\delta(\cdot)$ is the Dirac delta function.² DGP is also recovered from (6) assuming $C = 1$ and a white-Gaussian process noise model for $u(\cdot)$.

Table 2 reports the mean predictive performance for the missing observations for five random initialisations of the models. CMOGP refers to the NCMOGP with $C = 1$. The number at the end of NCMOGP indicates the order C of the non-linear model. Results are shown per output with missing data. Notice the reduction in the NMSE for Cambermet for all the non-linear models compared to the linear models (CMOGP and DGP). Here ICM performs better than any of the convolution approaches. For Chimet, there is also a reduction in the NMSE, but only for $C = 3$ (NCMOGP3) and $C = 5$ (NCMOGP5). In terms of the NLPD, the non-linear model with $C = 5$ (NCMOGP5) has a competitive performance when compared to the linear

²Notice that we use a rank one ICM since, similarly to the non-linear model, it only involves one latent function $u(\cdot)$ [Álvarez et al., 2012]

model (CMOGP). The averaged NSMEs for the two outputs are: 0.6989 ($C = 1$), 0.5717 ($C = 2$), 0.4309 ($C = 3$), 0.5456 ($C = 4$), 0.4753 ($C = 5$), 0.4425 (ICM) and 0.6431 (DGP). The averaged NLPDs for the two outputs are: 2.0613 ($C = 1$), 3.2479 ($C = 2$), 2.2550 ($C = 3$), 2.5460 ($C = 4$), 1.9600 ($C = 5$), 2.6848 (ICM) and 1.9925 (DGP). NCMOGP5 offers the best competitive performance both in terms of the NMSE and the NLPD compared to CMOGP, ICM and DGP.

Table 2: Results for the Weather dataset.

Model	Cambermet		Chimet	
	NMSE	NLPD	NMSE	NLPD
CMOGP	0.6004	1.9830	0.7974	2.1397
NCMOGP2	0.3080	2.1604	0.8354	4.3355
NCMOGP3	0.4366	2.3333	0.4252	2.1766
NCMOGP4	0.2676	2.1075	0.8235	2.9846
NCMOGP5	0.4499	2.0919	0.5007	1.8280
ICM	0.1048	3.2211	0.7801	2.1485
DGP	0.5513	1.9463	0.7349	2.0388

6.3 A high-dimensional input example

The NCMOGP can also be applied for datasets with an input dimension greater than one. We use a subset of the SARCOS dataset³ for illustration purposes. The prediction problem corresponds to map from positions, velocities and accelerations to the joint torques in seven degrees-of-freedom SARCOS anthropomorphic robot arm. The datasets contains $D = 7$ outputs and the dimension of the input space is $p = 21$, corresponding to seven positions, seven velocities, and seven accelerations. The kernels that we use follow the idea described in Section 5 for higher-dimensional inputs.

Our setup is as follows: from the file `sarcos_inv.mat` we randomly select $N = 500$ observations for each output for training and from the file `sarcos_inv_test.mat`, we randomly select another 500 observations for testing. We repeat the experiment ten times for different training and testing sets taken from the same two files.

Table 3: Results for a subset of the SARCOS dataset.

Model	NMSE	NLPD
CMOGP	0.0497 \pm 0.0252	1.4292 \pm 1.1080
NCMOGP2	0.0478 \pm 0.0238	1.4067 \pm 1.1032
NCMOGP3	0.0571 \pm 0.0377	1.4164 \pm 1.1401
NCMOGP4	0.0720 \pm 0.0855	1.4294 \pm 1.0787
NCMOGP5	0.0830 \pm 0.0809	1.4674 \pm 1.1449
ICM	0.0513 \pm 0.0246	1.4208 \pm 1.1286
DGP	0.0477 \pm 0.0237	1.4221 \pm 1.1088

Table 3 shows the averaged NMSE and averaged NLPD for the ten repetitions plus-or-minus a standard deviation.

³Available at <http://www.gaussianprocess.org/gpml/data/>

The non-linear model NCMOGP2 yields better averaged performance than CMOGP and ICM, in terms of NMSE and a very similar performance to DGP. In terms of NLPD, NCMOGP2 outperforms all the other models, indicating a better performance in terms of the predicted variance. Something to point out is that when looking at the predictive performance for the different NCMOGP, we noticed that each output is usually better predicted by different values of C . For example, in terms of NLPD, the best order to predict outputs $d = 1, 2, 3, 7$ would be a non-linear model with $C = 4$. The best model for predicting outputs $d = 4, 6$ would be $C = 3$, and the best model for predicting output $d = 5$ would be $C = 5$.

7 CONCLUSIONS AND FUTURE WORK

We have introduced a non-linear extension of the process convolution formalism to build multi-output Gaussian processes. We derived a novel mean function and covariance function from the non-linear operations introduced by the transformations in a Volterra series and showed experimental results that corroborate that these non-linear models have indeed an added benefit in real-world datasets.

We envision several paths for future work. The most pressing one is extending the framework to make it suitable for larger datasets. We can use similar ideas to the ones presented in Moreno-Muñoz et al. [2018] to establish a stochastic variational lower bound for the model introduced in this paper. Exploring the non-linear models for the case of latent force models is also an interesting venue. In this paper we use an smoothing kernel with an EQ form, but it is also possible to use smoothing kernels that correspond to Green’s function of dynamical systems. Automatically learning the smoothing kernel from data is also an alternative as for example in Guarnizo and Álvarez [2017].

An observation from both the Weather and SARCOS experiments, one that could have been expected, is that the predictive performances for the outputs are not all equally good for the same value of C . A potential extension of our model would be to allow the automatic learning of the order C per output dimension, say C_d . Additionally, the kernels we considered were derived assuming that the Volterra kernels were separable and homogeneous. Relaxing both assumptions is yet another path for future research.

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