Multi-Output Convolution Spectral Mixture for Gaussian Processes

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Abstract

Multi-output Gaussian processes (MOGPs) are recently extended by using spectral mixture kernel, which enables expressively pattern extrapolation with a strong interpretation. In particular, Multi-Output Spectral Mixture kernel (MOSM) is a recent, powerful state of the art method. However, MOSM cannot reduce to the ordinary spectral mixture kernel (SM) when using a single channel. Moreover, when the spectral density of different channels is either very close or very far from each other in the frequency domain, MOSM generates unreasonable scale effects on cross weights which produces an incorrect description of the channel correlation structure. In this paper, we tackle these drawbacks and introduce a principled multi-output convolution spectral mixture kernel (MOCSM) framework. In our framework, we model channel dependencies through cross convolution of time and phase delayed components between different channels. Results of extensive experiments on synthetic and real datasets demonstrate the advantages of MOCSM and its state of the art performance.

1 Introduction

Gaussian processes (GPs) [1][2] are an elegant Bayesian approach to model an unknown function. They provide regression models where a posterior distribution over the unknown function is maintained as evidence is accumulated. This allows GPs to learn complex functions if a large amount of evidence is available and makes them robust against overfitting in the presence of little evidence. A GP can model a large class of phenomena through the choice of its kernel which characterizes one’s assumption on how the unknown function autocovaries [1]. The choice of the kernel is a core aspect of GP design, since the posterior distribution can significantly vary for different kernels.
As a consequence, various kernels, e.g., Squared Exponential, Periodic, Matérn, and kernel design methods have been proposed [2].

The extension of GPs to predict multiple output variables (or channels, tasks) simultaneously is known as multi-output Gaussian processes (MOGPs). Usually MOGPs are also called multi-task Gaussian processes (MTGPs). For convenience, in some cases, MOGPs and MTGPs are used alternately. MOGPs model temporal or spatial relationships among infinitely many random variables, as scalar GPs, but also account for the statistical dependence across different sources of data (or channels) [3]. How to choose an appropriate kernel to jointly model the cross covariance between channels and auto-covariance within each channel is the core aspect of MOGPs design.

Early approaches to MOGPs, like Linear Model of Coregionalization (LMC [4] [5] [6], focused on linear combinations of shared kernels. More expressive methods like the multi-kernel method [7] and the convolved latent function framework [8] consider convolution to construct cross covariance functions, and assume that each channel has its own kernel. Recently spectral mixture (SM) kernels have been used and extended for MOGPs resulting in a principled method for constructing cross-covariance functions which are easier to interpret. Initially, the SM-LMC kernel [9] [10] was proposed, which uses shared components. A more flexible kernel is the Cross-Spectral Mixture (CSM) kernel [11], which considers the power and phase correlations between multiple outputs. The CSM kernel, however, cannot capture time delayed cross correlations between channels. The Multi-Output Spectral Mixture kernel (MOSM) [3] addresses this limitation, but has some other drawbacks. First, MOSM cannot reduce to the ordinary spectral mixture kernel (SM) when using a single channel. Second, when the spectral density of different channels is either very close or very far from each other in the frequency domain, MOSM generates unreasonable scale effects on cross weights which produces an incorrect description of the channel correlation structure.

In this paper, in order to address these drawbacks in MOSM, we propose a multi-output convolution spectral mixture kernel (MOCSM) framework based on convolution of components which is a direct generalization of single task GP that better captures cross covariance than MOSM. MOCSM shows a stronger ability of discovering channel correlation in each component. Particularly the cross weights reflecting channel correlations in MOCSM are more accurate than MOSM. Although MOCSM and MOSM have the same parameter space, MOCSM gives a more accurate closed form of multi-output spectral mixture kernel. The aforementioned approaches can be seen as specific instances of MOCSM.

The paper is mainly structured as follows. In Section 3 we show how to construct cross component with time and phase delay through convolution, extend the cross component to multi-output scenario, and compare MOCSM and MOSM. In Section 4 we describe further the difference between MOCSM and aforementioned cross SM approaches for MOGPs. Section 5 discusses the experiments of our approach on synthetic and real dataset. Some summary, concluding remarks and future work on this topic are given in the final Section 6.

2 Background

We start with some background information on GPs, multi-output GPs, and spectral mixture kernels.

2.1 Gaussian processes

A Gaussian process defines a distribution over functions, specified by its mean function \( m(x) \) and covariance function \( k(x, x') \) [2] for given input vector \( x \in \mathbb{R}^P \). Thus we can define a GP as

\[
f(x) \sim \mathcal{GP}(m(x), k(x, x'))
\]

Without loss of generality we assume the mean of a GP to be zero. The covariance function is applied to construct a positive definite covariance matrix on input points \( X \), here denoted by \( K = K(X, X) \). By placing a GP prior over functions through the choice of a kernel and parameter initialization, from the training data \( X \) we can predict the unknown function value \( \mathring{y}_s \) and its variance \( \mathbb{V}[y_s] \) (that is, its uncertainty) for a test point \( x_s \) using the following key predictive equations for GP regression [2]:

\[
\mathring{y}_s = \mathbf{k}_s^\top (K + \sigma_n^2 I)^{-1} \mathbf{y}
\]

\[
\mathbb{V}[y_s] = k(x_s, x_s) - \mathbf{k}_s^\top (K + \sigma_n^2 I)^{-1} \mathbf{k}_s
\]
where $k_{ij}^T$ is the covariances vector between $x_i$ and $X$, and $y$ are the observed values corresponding to $X$. Typically, GPs contain free parameters $\Theta$, called hyper-parameters, which can be optimized by minimizing the Negative Log Marginal Likelihood (NLML) as follows:

$$\text{NLML} = -\log p(y|x, \Theta) = \frac{1}{2} y^T (K + \sigma_n^2 I)^{-1} y + \frac{1}{2} \log |K + \sigma_n^2 I|$$

where $\sigma_n^2$ is the noise level. This formulation follows directly from the fact that $y \sim \mathcal{N}(0, K + \sigma_n^2 I)$.

In multi-output GPs (MOGPs), we have multiple sources of data which specify related outputs. The construction of the MOGP covariance function $k_{\text{MOGP}}(x^i, x^j)$ models covariances of each output and dependencies between pairs of different outputs [12] where $x^i$ and $x^j$ are respectively from $i$-th and $j$-th outputs.

### 2.2 Spectral mixture kernels

Usually, the smoothness and generalization properties of GPs depend on the kernel function and its hyper-parameters $\Theta$. Choosing an appropriate kernel function and its initial hyper-parameters based on prior knowledge from the data are the core steps of a GP. Various kernel functions have been proposed [2], such as Squared Exponential (SE), Periodic (PER), and general Matérn (MA). Recently new covariance kernels have been proposed in [9, 13], called Spectral Mixture (SM) kernels. An SM kernel, here denoted by $k_{\text{SM}}$, is derived through modeling a spectral density (Fourier transform of a kernel) with a mixture of Gaussians. A desirable property of SM kernels is that they can be used to reconstruct other popular standard covariance kernels. According to Bochner’s Theorem [14], the properties of a stationary kernel entirely depend on its spectral density. With enough mixture components, $k_{\text{SM}}$ can approximate any stationary covariance kernel [13].

$$k_{\text{SM}}(\tau) = \sum_{i=1}^{Q} w_i k_{\text{SM}_i}(\tau)$$  \hspace{1cm} (5)

$$k_{\text{SM}_i}(\tau) = \cos (2\pi \tau^T \mu_i) \prod_{p=1}^{P} \exp \left(-2\pi^2 \tau^2 \Sigma_i^{(p)}\right)$$  \hspace{1cm} (6)

where $\tau = x - x'$, $Q$ is the number of components, $k_{\text{SM}_i}$ is the $i$-th component, $P$ is the dimension of input, $w_i$, $\mu_i = [\mu_i^{(1)}, \ldots, \mu_i^{(P)}]$, and $\Sigma_i = \text{diag} \left([\sigma_i^2(1), \ldots, \sigma_i^2(P)]\right)$ are weight, mean, and variance of the $i$-th component in frequency domain, respectively. The variance $\sigma_i^2$ can be thought of as an inverse length-scale, $\mu_i$ as a frequency, and $w_i$ as a contribution.

Bochner’s Theorem [14, 15] indicates a direction on how to construct a valid kernel from the frequency domain. We will use $\hat{k}(s)$ to denote the spectral density of a covariance function $k(\tau)$ in the frequency domain. Using the following definition, the spectral density of kernel function $k(\tau)$ can be given by its Fourier transform:

$$\hat{k}(s) = \int k(\tau) e^{-2\pi i \tau s} \, d\tau$$  \hspace{1cm} (7)

where $i$ is the imaginary number. Furthermore, the inverse Fourier transform of a spectral density $\hat{k}(s)$ is the original kernel function $k(\tau)$.

$$k(\tau) = \int \hat{k}(s) e^{2\pi i \tau s} \, ds$$  \hspace{1cm} (8)

For SM kernel [9], using inverse Fourier transform of the spectral density $\hat{k}_{\text{SM}_i}(s) = [\varphi_{\text{SM}_i}(s) + \varphi_{\text{SM}_i}(-s)]/2$ where $\varphi_{\text{SM}_i}(s) = \mathcal{N}(s; \mu_i, \Sigma_i)$ is a symmetrized scale-location Gaussian in the frequency domain, we have

$$k_{\text{SM}}(\tau) = \mathcal{F}^{-1}_{s \rightarrow \tau} \left[ \sum_{i=1}^{Q} w_i \hat{k}_{\text{SM}_i}(s) \right](\tau)$$

$$= \sum_{i=1}^{Q} w_i \mathcal{F}^{-1}_{s \rightarrow \tau} \left[ (\varphi_{\text{SM}_i}(s) + \varphi_{\text{SM}_i}(-s))/2 \right](\tau)$$  \hspace{1cm} (9)
where $\mathcal{F}_{s \to \tau}^{-1}$ denotes inverse Fourier transform.

3 Multi-output convolution spectral mixture kernel

We can now address the following questions. (1) How to construct cross component with time and phase delay through convolution? (2) How to extend the cross component to multi-output scenario? (3) What is the relationship between MOCSM and MOSM?

3.1 Time and phase dependent component through convolution

Recently the Generalized Convolution Spectral Mixture (GCSM) kernel was introduced [16], which uses convolution to model dependencies between components $i$ and $j$ in a single task setting, through the cross component $k_{GCSM}^{i \times j}$ defined as:

$$k_{GCSM}^{i \times j}(\tau) = \mathcal{F}_{s \to \tau}^{-1} \left[ \frac{1}{2} \left( \hat{k}_{GCSM}^{i \times j}(s) + \hat{k}_{GCSM}^{i \times j}(-s) \right) \right](\tau)$$

$$= w_{ij} a_{ij} \exp \left( -\frac{1}{4} \pi^2 (2\tau - \theta_{ij})^T \Sigma_{ij} (2\tau - \theta_{ij}) \right) \times \cos \left( \pi \left( (2\tau - \theta_{ij})^T \mu_{ij} - \phi_{ij} \right) \right)$$

(10)

Here

- $w_{ij} = \sqrt{w_i w_j}$ is the cross weight;
- $a_{ij} = \left| \frac{\sqrt{2} \Sigma_i \Sigma_j}{\Sigma_i + \Sigma_j} \right|^\frac{1}{2} \exp \left( -\frac{1}{4} (\mu_i - \mu_j)^T (\Sigma_i + \Sigma_j)^{-1} (\mu_i - \mu_j) \right)$ is the cross amplitude;
- $\mu_{ij} = \frac{\Sigma_i \mu_j + \Sigma_j \mu_i}{\Sigma_i + \Sigma_j}$ is the cross mean;
- $\Sigma_{ij} = \frac{2 \Sigma_i \Sigma_j}{\Sigma_i + \Sigma_j}$ is the cross covariance;
- $\theta_{ij} = \theta_i - \theta_j$ is the cross time delay; and
- $\phi_{ij} = \phi_i - \phi_j$ is the cross phase delay.

Furthermore we have $\hat{k}_{GCSM}^{i \times j}(s) = \hat{g}_{GCSM_i}(s) \overline{\hat{g}_{GCSM_j}(s)}$, and

$$\hat{g}_{GCSM_i}(s) = \sqrt{w_i \phi_{SM_i}(s)} \exp \left( -\pi i (\theta_i s + \phi_i) \right)$$

(11)

is a base function of a complex-valued Gaussian with time delay $\theta_i$ and phase delay $\phi_i$. Here the overline denotes the complex conjugate operator.

3.2 Multi-output convolution spectral mixture kernel

$k_{GCSM}^{i \times j}(\tau)$ can be easily extended to the MOGP scenario. We can treat $k_{GCSM}^{i \times j}(\tau)$ with $\tau = x^i - x^j$ as a MOGP covariance function $k_{MOGP}(x^i, x^j)$, called MOCSM kernel, which models the covariances of the $i$-th and $j$-th channels corresponding to different outputs. First define the cross spectral density in MOCSM as $\hat{k}_{MOCSM}^{i \times j}(s) = \hat{k}_{GCSM}^{i \times j}(s)$, where $\{i, j\} \in \{1, ..., M\}$ are channel identifiers in MOCSM rather than indices of components in GCSM. Kernel $k_{MOCSM}^{i \times j}(\tau)$ is positive semi-definite if and only if its spectral density $\hat{k}_{MOCSM}^{i \times j}(s)$ is positive semi-definite [14][15]. For one spectral density $\hat{k}_{MOCSM}^{i \times j}(s)$ in MOCSM, given any finite set of non-zero vectors $[z_1, ..., z_M]^T \in \mathbb{C}^M \times P$ with complex values
entries for $M$ outputs, $s \in \mathbb{R}^P$, we have

\[
\sum_{i,j=1}^{M} \left( z_i k^{i \times j}_{\text{MOCSM}}(s) z_j \right) = \sum_{i,j=1}^{M} \left( z_i \left( \hat{y}_{\text{GCSM}_i}(s) \cdot \hat{y}_{\text{GCSM}_j}(s) \right) z_j \right) \\
= \sum_{i,j=1}^{M} (z_i \hat{y}_{\text{GCSM}_i}(s)) \cdot (z_j \hat{y}_{\text{GCSM}_j}(s)) \\
= \left| \sum_{i=1}^{M} z_i \hat{y}_{\text{GCSM}_i}(s) \right|^2 \geq 0
\]

where $z_i^\dagger$ denotes the conjugate transpose of $z_i$. Therefore $\tilde{k}^{i \times j}_{\text{MOCSM}}(s)$ satisfies the positive definite condition. However, up till now we only considered one component. For $Q$ symmetric components on multidimensional inputs the MOCSM kernel must also be positive definite with the following form:

\[
k_{\text{MOCSM}}(\tau) = \sum_{q=1}^{Q} c_{ij}^{(q)} \exp \left( -\frac{1}{2} \pi^2 \left( 2\tau - \theta_{ij}^{(q)} \right) \Sigma_{ij}^{(q)} \left( 2\tau - \theta_{ij}^{(q)} \right)^{\top} \right) \\
\times \cos \left( \pi \left( 2\tau - \theta_{ij}^{(q)} \right)^{\top} \mu_{ij}^{(q)} - \phi_{ij}^{(q)} \right)
\]

where the $q$-th cross contribution $c_{ij}^{(q)} = w_{ij}^{(q)} a_{ij}^{(q)}$ incorporates the $q$-th cross weight and the $q$-th cross amplitude between $i$-th and $j$-th channels. Here

- $w_{ij}^{(q)} = \sqrt{w_i^{(q)} w_j^{(q)}}$ is $q$-th cross weight;
- $a_{ij}^{(q)} = \sqrt{\frac{a_{ij}^{(q)} a_{ji}^{(q)}}{\Sigma_{ij}^{(q)} + \Sigma_{ji}^{(q)}}}$ is the $q$-th cross amplitude; 
- $\mu_{ij}^{(q)} = \frac{\Sigma_{ij}^{(q)} \mu_{ij} + \Sigma_{ji}^{(q)} \mu_{ji}}{\Sigma_{ij}^{(q)} + \Sigma_{ji}^{(q)}}$ is the $q$-th cross mean;
- $\Sigma_{ij}^{(q)} = \frac{2\Sigma_{ij}^{(q)} \Sigma_{ji}^{(q)}}{\Sigma_{ij}^{(q)} + \Sigma_{ji}^{(q)}}$ is the $q$-th cross covariance;
- $\theta_{ij}^{(q)} = \theta_{ij}^{(q)} - \theta_{ji}^{(q)}$ is the $q$-th cross time delay; and
- $\phi_{ij}^{(q)} = \phi_{ij}^{(q)} - \phi_{ji}^{(q)}$ is the $q$-th cross phase delay.

In the above Equations, $\Sigma_i$, $\mu_i$, $\theta_i$, $\phi_i$ have the same dimension $P$ as in Equation (5). In our MOCSM kernel, one can also employ angular frequencies instead of ordinary frequencies in the convolution and the inverse Fourier transform (see Equations (15), (17), (19), and (20)).

### 3.3 Comparison between MOCSM and MOSM

Here for simplicity of exposition we compare MOCSM and MOSM employing angular frequencies with only one component and one-dimensional input. We consider the parameters described in the last section. For both MOSM and MOCSM we have

\[
k^{i \times j}_{\text{MOSM}}(\tau) = \sqrt{2\pi} w_{ij}^{2}(\sigma_i^{2} \sigma_j^{2})^{\frac{1}{4}} a_{ij} \exp \left( -\frac{1}{2} (\tau - \theta_{ij}) \Sigma_{ij}^{2}(\tau - \theta_{ij}) \right) \\
\times \cos \left( ((\tau - \theta_{ij}) \Sigma_{ij}^{2}) \Sigma_{ij}^{2}(\tau - \theta_{ij}) \right) \\
\times \cos \left( ((\tau - \theta_{ij}) \Sigma_{ij}^{2}) \Sigma_{ij}^{2}(\tau - \theta_{ij}) \right)
\]

\[
k^{i \times j}_{\text{MOCSM}}(\tau) = w_{ij} a_{ij} \exp \left( -\frac{1}{2} (\tau - \theta_{ij}) \Sigma_{ij}^{2}(\tau - \theta_{ij}) \right) \\
\times \cos \left( ((\tau - \theta_{ij}) \Sigma_{ij}^{2}) \Sigma_{ij}^{2}(\tau - \theta_{ij}) \right)
\]
With no time and phase delay between channels MOSM and MOCSM become

\[ k_{\text{MOSM}}^{ij}(\tau) = \sqrt{2\pi w_i^2} w_{ij} \exp \left( -\frac{1}{2} \tau^2 \sigma_i^2 \right) \cos (\tau \mu_{ij}) \] (16)

\[ k_{\text{MOCSM}}^{ij}(\tau) = w_{ij} a_{ij} \exp \left( -\frac{1}{2} \tau^2 \sigma_i^2 \right) \cos (\tau \mu_{ij}) \] (17)

Furthermore, when the \( i \)-th and \( j \)-th channel are equal we have

\[ k_{\text{MOSM}}^{ii}(\tau) = w_i^2 \sqrt{2\pi \sigma_i^2} \exp \left( -\frac{1}{2} \tau^2 \sigma_i^2 \right) \cos (\tau \mu_i) \] (18)

\[ k_{\text{MOCSM}}^{ii}(\tau) = w_i \exp \left( -\frac{1}{2} \tau^2 \sigma_i^2 \right) \cos (\tau \mu_i) \] (19)

The ordinary SM kernel with angular frequencies, is defined as

\[ k_{\text{SM}}^{i}(\tau) = w_i \exp \left( -\frac{1}{2} \tau^2 \sigma_i^2 \right) \cos (\tau \mu_i) \] (20)

which shows that MOCSM (Equation (19)) reduces to the standard SM kernel when there is only one channel, while MOSM [3], does not. Notably in Equation (18) the term \( w_i^2 \sqrt{2\pi \sigma_i^2} \) involves \( w_i \) and \( \sigma_i \), which may produce inaccurate channel correlations. Comparing the one dimensional Equations (15) and (14) we can observe that one dimensional MOCSM and MOSM have the same \( exp \) and \( cos \) terms, but have different cross weight terms (see also Table 1).

Table 1: Cross weight and its difference in MOS and MOCSM.

| Kernel     | Single channel weight | Cross channel weight | Design method          |
|------------|-----------------------|----------------------|------------------------|
| SM         | \( w_i \)             | Not available        | Bochner’s Theorem      |
| MOSM       | \( w_i^2 \sqrt{2\pi \sigma_i^2} \) | \( \sqrt{2\pi w_i^2} (\sigma_i^2 \sigma_j^2)^{1/2} \) | Matrices decomposition |
| MOCSM      | \( w_i \)             | \( w_{ij} \)        | Spectral convolution   |

Here one dimensional MOCSM and MOSM have the same parameter space, but the cross weights of MOCSM are more accurate in the following sense. When weights \( (w_i, w_j) \) and variances \( (\sigma_i^2, \sigma_j^2) \) of channels 1 and 2 are close to each other, in MOSM the cross weight term will amplify the cross correlation if \( |w_i| > 1 \), \( |w_j| > 1 \), \( |\sigma_i| > 1 \), and \( |\sigma_j| > 1 \), otherwise the cross weight term will shrink the cross correlation, since MOSM contains squared weights and variances (see also Table 1). In Figure 1 we illustrate this problematic behaviour of MOSM by setting the channel weights to \( w = \{0.5, 0.6, 2.0, 2.1\} \) and channel variances to \( \sigma^2 = \{0.4, 0.5, 2.0, 2.1\} \) corresponding to channel 1, channel 2, channel 3, and channel 4, respectively. The figure clearly shows that the cross weights in MOSM may be amplified or may shrink because of the square used in the cross channel weights. Therefore, in MOSM (second row), cov(channel\(^{(1)}\), channel\(^{(2)}\)) (in red solid line) is smaller than that of MOCSM (in first row), while cov(channel\(^{(2)}\), channel\(^{(3)}\)) (in blue solid line) is larger than that of MOCSM, and particular cov(channel\(^{(3)}\), channel\(^{(3)}\)) (in green solid line) is much larger in MOSM than in MOCSM.

4 Related work

There is an abundant literature on GPs related to MOGPs [3,5,7,8,10,11,17]. Here we mainly focus on MOGPs methods based on spectral mixture kernels, because of their expressiveness and recent use in MOGPs. Since the introduction of SM kernels [9,13], various MOGP methods have been introduced [9,17,18,19,20]. The first such MOGP kernel, based on the LMC framework introduced in [10] was defined as

\[ K_{\text{SM-LMC}} = \sum_{i=1}^{Q} B_i \otimes K_{\text{SM}_i} \]
Here $B_i$ encodes cross weights to represent channel correlations and involves a linear combination of components. The CSM kernel [11] improved the expressiveness of SM-LMC by introducing a cross phase spectrum and was also defined within the LMC framework as

$$K_{CSM} = \sum_{i=1}^{Q} B_i k_{SG_i}(\tau; \Theta_i)$$

where $k_{SG_i}(\tau; \Theta_i)$ is phasor notation of the spectral Gaussian kernel. However the kernels $k_{SG_i}(\tau; \Theta_i)$ used in the CSM are only phase dependent, but not time dependent. The more recent MOSM kernel [3] provided a principled framework to construct multivariate covariance functions with a better interpretation of cross correlations between channels. SM-LMC and CSM are instances of MOSM. However, MOSM cannot reduce to the SM kernel when using only one channel and in certain situations produces inaccurate channel correlations, for example, when patterns between channels are close to each other (see Table 1). Note that $\phi_i$ is a $P$-dimensional phase delay vector in MOCSM rather than a scalar in MOSM. More detailed comparisons between SM-LMC, CSM, MOSM, and MOCSM in terms of hyper-parameters and degrees of freedom are given in Table 2. In Table 2 all LMC-based kernels use free form parameterization, $\theta_f$ and $\theta_c$ are length-scale and x-scale in SE and Matérn kernel, respectively. Here we use $q$ instead of $i$ as a sub-index of a component. For SM-LMC, CSM, MOSM and MOCSM, $Q$ denotes the number of components, and $M$ the number of channels (outputs).

5 Experiments

We consider the empirical spectral density $s$ as derived from the data, and then applied a Bayesian Gaussian mixture model $p(\Theta|s) = \sum_{i=1}^{Q} \tilde{w}_i N(\tilde{\mu}_i, \tilde{\Sigma}_i)$ in order to get the $Q$ cluster centers of Gaussian spectral densities [21]. We use the Expectation Maximization algorithm [22] to estimate the parameters $\tilde{w}_i$, $\tilde{\mu}_i$, and $\tilde{\Sigma}_i$. The results are used as initial values of $w_i$, $\mu_i$, and $\Sigma_i$, respectively, for each channel in MOCSM.

We compare MOCSM with existing MOGP methods, namely SM-LMC, CSM, MOSM, on an artificial dataset and three real world datasets. First, we show the ability of MOCSM in modeling nonlinear correlated outputs simultaneously by considering a mixed signal sampled from a Gaussian
We designed an artificial experiment inspired by [3] but more complex, to model multiple non-linear factors in affecting local air pollution levels because it determines chemical reaction and change of air pollutant. There are multiple global trends and local patterns which can shape temperature evolution. Global trends are natural evolution mechanisms within the global climate system itself.

5.1 Artificial data: learning nonlinear correlated mixed signals simultaneously

We designed an artificial experiment inspired by [3] but more complex, to model multiple non-linear correlated channels simultaneously. The three channels consist of a mixed signal, its integral, and its derivative. Specifically, the signal of the first channel is sampled from $\mathcal{GP}(0, K_{SM}(Q = 4))$ with length 300 in the interval [-10, 10], and then its first integral and derivative are numerically computed to be the signals of the second and third channel. This experiment is intended to validate the interpolation, extrapolation, and signal recovery ability of MOCSM as well as to compare its pattern recognition performance with that of other MOGP approaches. For the first channel, we randomly choose half of the data as training data, and the rest as test data. The integral signal in the interval [-10, 0] is used for training (in gray), the rest of the signal is used for testing (in green). The derivative of the signal in the interval [0, 10] is used for training and the rest of the signal is used for testing.

The performance of MOCSM (in dashed red line) on the first channel is shown in Figure 2 (a). Although MOCSM performed a bit better, the difference in performance among these methods is not so evident: all mentioned GP methods learned the covariance and interpolated the missing values well. Next, the extrapolation performance of MOCSM and other methods on the integral and the derivative of the signal are shown in Figure 2 (b) and Figure 2 (c), respectively. For instance, the integral of the signal contains more complex patterns, which is difficult to recognize and extrapolate. Here MOCSM performs better than other methods with lowest MAE (see Table 3) and smallest confidences interval.

Predictions obtained using SE-LMC and Matérn-LMC kernels are of low quality, especially for the extrapolation tasks (integral and derivative signals): it is very hard for them to find valid patterns in the data, like the evolution of trend over time. Overall, results on the artificial dataset indicate the capability of MOCSM to model integration and differentiation patterns of the generated signal simultaneously.

5.2 Temperature extrapolation

Sensor networks monitoring climate change and global warming in Stockholm provide real time surveillance, historical analysis, and future forecasting of the regional environment. Particularly extrapolating future temperature values help to guide policy making and social development. We know that, as a result of global warming, the fluctuation of temperature becomes a sensitive topic with regard to balance of survival and development. On the other hand, temperature is one of main factors in affecting local air pollution levels because it determines chemical reaction and change of air pollutant. There are multiple global trends and local patterns which can shape temperature evolution. Global trends are natural evolution mechanisms within the global climate system itself.

### Table 2: Comparisons between MOCSM and other kernels [5].

| Kernel       | Parameters                                                                 | Degrees of freedom |
|--------------|-----------------------------------------------------------------------------|--------------------|
| SE-LMC       | $\{B, \theta_f, \theta_r\}$                                                | $(M^2 + M)/2 + P + 1$ |
| Matérn-LMC   | $\{B, \theta_f, \theta_r\}$                                                | $(M^2 + M)/2 + P + 1$ |
| SM-LMC       | $\{B_q, w_q, \mu_q, \Sigma_q\}_{q=1}^Q$                                    | $Q((M^2 + M)/2 + 2P + 1)$ |
| CSM          | $\{\sigma^q, \mu^q, \{w^q, \phi^q\}_{r=1}^M\}_{q=1}^Q$                   | $2Q + M(2Q - 1)$   |
| MOSM         | $\{\{w^q, \mu^q, \Sigma^q\}_{m=1}^M, \phi^q\}_{m=1}^M\}_{q=1}^Q$         | $QM(3P + 2)$       |
| MOCSM        | $\{\{w^q, \mu^q, \Sigma^q, \phi^q\}_{m=1}^M, \phi^q\}_{m=1}^M\}_{q=1}^Q$ | $QM(4P + 1)$       |

1http://slb.nu/slbanalys/historiska-data-luft/
Local patterns are external forces caused by local surroundings and industry activities. Usually global trends affect long term evolution of temperature at a large scale. Local patterns always shape the short term and medium-term change of temperature at a small scale. Both global trends and local patterns are time and phase dependent and tightly coupled together. Here we use temperature recordings as a real world example to show extrapolating ability of MOCSM in sensor networks. Based on the extrapolation results, suggestions may be given on measures to mitigate global warming.

The temperature monitoring recordings are recorded from a number of stations (Torkel Knutsson-sgatan, Marsta, Norr Malma) in Stockholm and outside. For instance: Torkel Knutsson-sgatan’s measurement at the urban background, Marsta’s measurement at a high-altitude tower, North Malma’s measurement at the regional background. We consider each station to be a channel: Torkel Knutsson-sgatan as channel 1, Marsta as channel 2, and Norr Malma as channel 3. We observe from Figure 3 that the change of temperature has an apparent oscillatory behavior. In this case, we use temperature time series from 22 June 2017 to 12 July 2017, in 1 hour intervals. Here we just focus on the task in channel 2. Specifically, a randomly chosen half of the temperature data in Torkel Knutsson-sgatan, the first half of the temperature data in Marsta, and the last half of the temperature data in Norr Malma are used for training. The last half of temperature data in Marsta is used for testing. The change of temperature in each channel is affected by their nonlinear interaction of time and phase related local patterns and global trends.

From Figure 3 as a result of time and phase dependent local patterns within channels (local patterns depend on surroundings) and time and phase dependent global trends between channels (global trends depend on seasonal or yearly factors), changes in temperature are fluctuating. MOCSM, however, consistently outperform others with lowest MAE and smallest predicted confidence interval (see Figure 3 and Table 3).
Secondly, we use an 8-hour average Ozone concentrations dataset. The Ozone dataset comes from an air pollution monitoring sensor network in Stockholm. The Ozone concentration is recorded from 5 April, 2017 to 25 April, 2017, in one-hour intervals at Torkel Knutssonsgatan, Norr Malma, and Hornsgatan stations. As a result of moving average, noise was smoothed and therefore the evolution of ozone concentration is more smooth and less fluctuant. In other words, patterns from the frequency domain should become more clear. However, Ozone concentration depends more on local environment and human activities. Thus its extrapolations is more difficult than temperature. Although the Ozone concentration data was smoothed by a sliding window of 8-hour values, local patterns in each channel depending on surroundings and global trends related to large-scale climate change still exist. Both local patterns and global trends are time and phase dependent over the period of recording. Modeling from multiple channels can benefit the long range extrapolating rather than learning one channel alone, because the evolution of Ozone concentration in each station is a result of nonlinear interaction of these local patterns and global trends. Here randomly chosen half of data in Torkel Knutssonsgatan (channel 1), first half of data in Norr Malma (channel 2), and the last half of data in Hornsgatan (channel 3) are used for training and the remaining data in Norr Malma as a testing. In this case we still aim to extrapolate the long range trends of sliding mean Ozone concentration in Norr Malma. With the same setting in the first experiments, the performance of SM-LMC, CSM, MOSM, MOCSM are shown in Figure 4 and Table 3.

As seen in Figure 4 patterns in sliding mean Ozone concentration are more difficult and less clear to capture than temperature. It is even hard for human to find any quasi periodical or periodical trends. Although all MOGPs methods can extrapolate trends of sliding mean Ozone concentration, but MOCSM is the best, which be able to correctly predict the appearance of all low peaks and high peaks. No doubt MOCSM achieves better performance (see Figure 3 and Table 3) in terms of MAE and confidence interval. This experiment shows again that MOCSM has stronger pattern learning abilities.

5.4 Global radiation backward extrapolation

After two extrapolating experiments, we conduct a backward extrapolation on global radiation recordings of the sensor networks in order to validate the long range back extrapolating capability and historical signal recovery ability of MOCSM and other methods. The global radiation is an important parameter reflecting global climate evolution and change of atmosphere. Global radiation is the total amount of direct, diffuse, and reflected solar energy received by the Earth’s surface, which is mainly affected by sun altitude and cloud cover.
Figure 4: Sliding mean Ozone concentration extrapolation. Performance comparison between MOCSM and recently proposed spectral mixture kernels: (a) MOCSM (in red dashed line), (b) MOSM (in blue dashed line), (c) CSM (in purple dashed line), (d) SM-LMC (in cyan dashed line).

The changes of sun altitude has a global influence on earth with a one-year period, while the cloud cover has a local influence with an a-periodic behavior. These global and local patterns show time and phase related variability over the period of recording. Usually for small scale variation (1 hour interval), the global radiation depends more on its surroundings and location because local weather condition determines the cloud cover. Empirical analysis shows various time and phase dependent characteristics of this global radiation: short term variations, medium term monthly patterns and non-strict periodic long term trends related to position of moon and sun, and some white noises. The time of appearance of high peak in global radiation is not periodical and its amplitude is always irregular.

The global radiation dataset is collected from three stations in Stockholm city: Torkel Knutssonsgatan’s measurement at urban background, Marsta’s measurement at a high-altitude tower, Norr Malma’s measurement at regional background. All recordings cover 24 hours at 1 hour intervals and missing values are filtered. In this case, we consider a global radiation recording from 5 December, 2017 to 26 December, 2017. Interestingly, the changing of global radiation over time looks like a non-continuous impulse signal because the sun radiation at night is almost equal to zero. From Figure 5 we can observe that the appearance of high peak in global radiation is irregular and its time of duration is short and fluctuant. Thus, complicated patterns contained in this non-continuous impulse signal is very difficult to detect. Ordinary kernels cannot find any valid pattern in this dataset. In a multi-output scenario, the changing of global radiation in each channel is caused by their nonlinear interaction of time and phase related local and global patterns.

In our experiment, we randomly choose half of global radiation data in Torkel Knutssonsgatan, the first half of global radiation data in Marsta, and the last half of global radiation data in Norr Malma as training data in channel 1, channel 2, and channel 3, respectively. Different from the first and second real world experiment, the rest of the Norr Malma time series is used for testing. In this setting, MOCSM consistently outperforms the other baselines with a lower MAE (see Figure 5 and Table 3). Results indicate that all methods have difficulty to capture the trends of high peak appearance, and only MOCSM can forecast it without over estimation.

Table 3 summarizes the performance of the considered kernel methods. The MOCSM kernel consistently achieves the lowest MAE on the artificial and the real world datasets. Predictions obtained using the SE-LMC and Matérn-LMC kernels are very bad especially for extrapolation (Integral, Derivative signals, Temperature, and Sliding mean Ozone concentration) even if the methods achieve a good MAE. With these kernels it is very hard to find any valid pattern in the data. We use the temperature in Marsta, the sliding mean Ozone concentration in Norr Malma, and the radiation in Norr Malma as tasks to perform long range extrapolation.
Figure 5: Global radiation back extrapolation. Performance comparison between MOCSM and recently proposed spectral mixture kernels: (a) MOCSM (in red dashed line), (b) MOSM (in blue dashed line), (c) CSM (in purple dashed line), (d) SM-LMC (in cyan dashed line).

Table 3: Performance of MOCSM and other kernels on artificial and real world datasets.

| Kernel    | $GP(0, K_{SM})$ | Integral | Derivative | Temperature | Ozone | Radiation |
|-----------|-----------------|----------|------------|-------------|-------|-----------|
| SE-LMC    | 0.156           | 0.225    | 0.212      | 13.677      | 62.154| 5.499     |
| Matérn-LMC| 0.126           | 0.219    | 0.221      | 14.737      | 70.867| 5.230     |
| SM-LMC    | 0.124           | 0.195    | 0.195      | 2.081       | 6.591 | 5.671     |
| CSM       | 0.128           | 0.200    | 0.210      | 1.357       | 12.859| 6.072     |
| MOSM      | 0.133           | 0.175    | 0.231      | 1.611       | 14.440| 5.437     |
| MOCSM     | **0.084**       | **0.113**| **0.038**  | **1.109**   | **5.808**| **4.141**|

6 Conclusion

We proposed the generalized multi-output convolution spectral mixture (MOCSM) kernel with expressive closed form to describe cross covariance between multi-outputs in a principled way. In our method we incorporated time and phase delay in spectral density, then transform convolution into product through Fourier transform.

MOCSM shows stronger abilities in modeling complicated nonlinear correlation across multi-outputs than the considered baselines. Experiments on artificial datasets and real world datasets have shown that by using cross convolution of components within MOGPs, more irregular trends in the data can be recognized and learnt and long-term trends forecasting and long range back extrapolation can be performed in a more accurate way.

For example, they can be applied to fill in the gaps that cross correlations are not so precise in MOSM, and extend the extrapolating ability of MOSM without increasing complexity in training and inference steps. In this work we did not address efficient inference of the MOCSM. At present, efficient inference approximation methods like FITC and PITC \[8, 25, 26, 27, 28, 29, 30\], are not very effective for MOGPs. Interesting future research involves the development of sparse and efficient inference methods for MTGPs \[31, 32, 33\].

Global optimizing and initialization strategy of hyper-paramters are also very important for the MOGP performance. Here we considered the empirical spectral density as derived from the data, and then applied a Bayesian Gaussian mixture model. More advanced initialization strategies, like \[20, 34, 35, 36\] need to be investigated in future work.
References

[1] C. E. Rasmussen and H. Nickisch, “Gaussian processes for machine learning (gpml) toolbox,” *Journal of Machine Learning Research*, vol. 11, no. Nov, pp. 3011–3015, 2010.

[2] C. E. Rasmussen, *Gaussian processes for machine learning*, ser. Adaptive computation and machine learning, C. K. I. Williams, Ed. Cambridge, Massachussets: The MIT Press, 2006.

[3] G. Parra and F. Tobar, “Spectral mixture kernels for multi-output Gaussian processes,” in *Advances in Neural Information Processing Systems*, 2017, pp. 6684–6693.

[4] P. Goovaerts, “Geostatistics for natural resources evaluation. oxford univ. press, new york.” Geostatistics for natural resources evaluation. *Oxford Univ. Press, New York.*, 1997.

[5] E. V. Bonilla, K. M. Chai, and C. Williams, “Multi-task Gaussian process prediction,” in *Advances in neural information processing systems*, 2008, pp. 153–160.

[6] R. Dürichen, M. A. Pimentel, L. Clifton, A. Schweikard, and D. A. Clifton, “Multitask Gaussian processes for multivariate physiological time-series analysis,” *IEEE Transactions on Biomedical Engineering*, vol. 62, no. 1, pp. 314–322, 2015.

[7] A. Melkumyan and F. Ramos, “Multi-kernel Gaussian processes,” in *IJCAI Proceedings-International Joint Conference on Artificial Intelligence*, vol. 22, no. 1, 2011, p. 1408.

[8] M. Alvarez and N. D. Lawrence, “Sparse convolved Gaussian processes for multi-output regression,” in *Advances in neural information processing systems*, 2009, pp. 57–64.

[9] A. G. Wilson, “Covariance kernels for fast automatic pattern discovery and extrapolation with Gaussian processes,” *University of Cambridge*, 2014.

[10] A. G. Wilson, D. A. Knowles, and Z. Ghahramani, “Gaussian process regression networks,” *arXiv preprint arXiv:1110.4411*, 2011.

[11] K. R. Ulrich, D. E. Carlson, K. Dzirasa, and L. Carin, “GP kernels for cross-spectrum analysis,” in *Advances in neural information processing systems*, 2015, pp. 1999–2007.

[12] M. G. Genton and W. Kleiber, “Cross-covariance functions for multivariate geostatistics,” vol. 30, pp. 147–163, 2015.

[13] A. Wilson and R. Adams, “Gaussian process kernels for pattern discovery and extrapolation,” in *Proceedings of the 30th International Conference on Machine Learning (ICML-13)*, 2013, pp. 1067–1075.

[14] S. Bochner, *Lectures on Fourier Integrals.(AM-42)*. Princeton University Press, 2016, vol. 42.

[15] M. Stein, “Interpolation of spatial data: some theory for kriging. 1999.”

[16] K. Chen, P. Groot, J. Chen, and E. Marchiori, “Spectral Mixture Kernels with Time and Phase Delay Dependencies,” *ArXiv e-prints*, Aug. 2018.

[17] D. Duvenaud, J. R. Lloyd, R. Grosse, J. B. Tenenbaum, and Z. Ghahramani, “Structure discovery in nonparametric regression through compositional kernel search,” *arXiv preprint arXiv:1302.4922*, 2013.

[18] S. Flaxman, A. Wilson, D. Neill, H. Nickisch, and A. Smola, “Fast kronecker inference in Gaussian processes with non-Gaussian likelihoods,” in *International Conference on Machine Learning*, 2015, pp. 607–616.

[19] J. B. Oliva, A. Dubey, A. G. Wilson, B. Póczos, J. Schneider, and E. P. Xing, “Bayesian nonparametric kernel-learning,” in *Artificial Intelligence and Statistics*, 2016, pp. 1078–1086.

[20] P. A. Jang, A. Loeb, M. Davidow, and A. G. Wilson, “Scalable Levy process priors for spectral kernel learning,” in *Advances in Neural Information Processing Systems*, 2017, pp. 3943–3952.

[21] W. Herlands, A. Wilson, H. Nickisch, S. Flaxman, D. Neill, W. Van Panhuis, and E. Xing, “Scalable gaussian processes for characterizing multidimensional change surfaces,” in *Artificial Intelligence and Statistics*, 2016, pp. 1013–1021.

[22] T. K. Moon, “The expectation-maximization algorithm,” *IEEE Signal Processing Magazine*, vol. 13, no. 6, pp. 47–60, 1997.

[23] M. Abadi, P. Barham, J. Chen, Z. Chen, A. Davis, J. Dean, M. Devin, S. Ghemawat, G. Irving, M. Isard et al., “Tensorflow: A system for large-scale machine learning. arxiv preprint,” *arXiv preprint arXiv:1605.08695*, 2016.
[24] A. G. d. G. Matthews, M. van der Wilk, T. Nickson, K. Fujii, A. Boukouvalas, P. León-Villagrá, Z. Ghahramani, and J. Hensman, “GPflow: A Gaussian process library using tensorflow,” Journal of Machine Learning Research, vol. 18, no. 40, pp. 1–6, 2017.

[25] M. Álvarez, D. Luengo, M. Titsias, and N. Lawrence, “Efficient multioutput Gaussian processes through variational inducing kernels,” in Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, 2010, pp. 25–32.

[26] M. A. Álvarez and N. D. Lawrence, “Computationally efficient convolved multiple output Gaussian processes,” Journal of Machine Learning Research, vol. 12, no. May, pp. 1459–1500, 2011.

[27] C. K. Williams and M. Seeger, “Using the nyström method to speed up kernel machines,” in Advances in neural information processing systems, 2001, pp. 682–688.

[28] J. Quiñonero-Candela and C. E. Rasmussen, “A unifying view of sparse approximate Gaussian process regression,” Journal of Machine Learning Research, vol. 6, no. Dec, pp. 1939–1959, 2005.

[29] E. Snelson and Z. Ghahramani, “Sparse Gaussian processes using pseudo-inputs,” in Advances in neural information processing systems, 2006, pp. 1257–1264.

[30] K. Chalupka, C. K. Williams, and I. Murray, “A framework for evaluating approximation methods for Gaussian process regression,” Journal of Machine Learning Research, vol. 14, no. Feb, pp. 333–350, 2013.

[31] B. Rakitsch, C. Lippert, K. Borgwardt, and O. Stegle, “It is all in the noise: Efficient multi-task Gaussian process inference with structured residuals,” in Advances in neural information processing systems, 2013, pp. 1466–1474.

[32] C. Guarnizo and M. A. Álvarez, “Fast kernel approximations for latent force models and convolved multiple-output Gaussian processes,” arXiv preprint arXiv:1805.07460, 2018.

[33] H. Liu, Y.-S. Ong, X. Shen, and J. Cai, “When Gaussian process meets big data: A review of scalable GPs,” arXiv preprint arXiv:1807.01065, 2018.

[34] K. Swersky, J. Snoek, and R. P. Adams, “Multi-task Bayesian optimization,” in Advances in neural information processing systems, 2013, pp. 2004–2012.

[35] R. Martinez-Cantin, “Bayesopt: A Bayesian optimization library for nonlinear optimization, experimental design and bandits,” The Journal of Machine Learning Research, vol. 15, no. 1, pp. 3735–3739, 2014.

[36] N. Knudde, J. van der Herten, T. Dhaene, and I. Couckuyt, “GPflowopt: A Bayesian optimization library using tensorflow,” arXiv preprint arXiv:1711.03845, 2017.