A sparse expansion for deep Gaussian processes

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ABSTRACT
In this work, we use Deep Gaussian Processes (DGPs) as statistical surrogates for stochastic processes with complex distributions. Conventional inferential methods for DGP models can suffer from high computational complexity, as they require large-scale operations with kernel matrices for training and inference. In this work, we propose an efficient scheme for accurate inference and efficient training based on a range of Gaussian Processes, called the Tensor Markov Gaussian Processes (TMGP). We construct an induced approximation of TMGP referred to as the hierarchical expansion. Next, we develop a deep TMGP (DTMGP) model as the composition of multiple hierarchical expansion of TMGPs. The proposed DTMGP model has the following properties: (i) the outputs of each activation function are deterministic while the weights are chosen independently from standard Gaussian distribution; (ii) in training or prediction, only $O(\text{polylog}(M))$ (out of $M$) activation functions have non-zero outputs, which significantly boosts the computational efficiency. Our numerical experiments on synthetic models and real datasets show the superior computational efficiency of DTMGP over existing DGP models.

1. Introduction
This work is partially motivated by surrogate modeling of stochastic computer simulations (Ankenman et al., 2010; Plumlee and Tuo, 2014). The ultimate goal in this field is to approximate an underlying stochastic process, defined by a complex stochastic computer simulation code, using a surrogate stochastic process that is computationally efficient. Among existing statistical surrogates, the Deep Gaussian Process (DGP) proposed by Damianou and Lawrence (2013) has recently become a popular choice, due to its exceptional performance and flexibility in fitting the complex distributions from the stochastic processes in real applications (Radaideh and Kozlowski, 2020; Sauer, Gramacy and Higdon, 2022).

DGPs are multi-layer compositions of multi-variate Gaussian Processes (GPs). The deep probabilistic structures of DGPs allows a Bayesian formulation to model complex stochastic systems, such as computer vision, natural language processing, etc. However, the cost of expressiveness and flexibility of DGPs is the extreme difficulties in training and inference, due to the propagation of randomness throughout the layers of DGPs being nonlinear and correlated among layers. Existing approaches for overcoming these difficulties can be separated into two classes – one class focuses on approximating the Bayesian formulations of DGPs, such as Variational Inference (VI) (Blei et al., 2017), Expectation Propagation (EP) (Bui et al., 2016), or Vecchia approximation (Sauer, Cooper and Gramacy, 2022), whereas the other class considers simplified representations of the structures of DGPs such as inducing-variable approximation (Hensman and Lawrence, 2014) and random Fourier feature expansion (Cutajar et al., 2017).

Simplifications based on inducing variables and random Fourier features (Rahimi and Recht, 2008) partially address the computational issue of DGPs. However, they are still hard to implement. This is because these simplifications of DGPs are Deep Neural Networks (DNN) with kernel-based activations, correlated random weights and bias parameters, which is equivalent to Bayesian Neural Networks (BNN) (MacKay, 1992; Neal, 1996) with dense and highly correlated structures. Training and inference of these simplifications are at least as hard as existing BNN models.

In this work, we focus on introducing an accurate and efficient simplification of DGPs. We propose a sparse reduced-rank approximation, referred as Hierarchical Expansion, for DGPs. Our expansion is specialized for DPGs that are the compositions of multi-variate tensor Markov GPs (TMGP) (Ding and Zhang, 2020), so we call this expanded DGP deep TMGP (DTMGP). One of our main contributions lies in constructing a sparse representation of DGPs. There are only a poly-logarithmic number of activations in our model with non-zero outputs each time we run the model. Because of this sparse property, training of DTMGPs are much faster and easier compared with existing DGP models, avoiding commonly seen numerical issues in training deep models. Another contribution is to show that hierarchical expansion is also highly accurate. Unlike many
other sparse approximations for GPs/DGPs, the difference between sample paths generated by any DGP and those generated by its hierarchical expansion is small. This property allows DTMGPs to model complex stochastic systems with satisfactory performance, as shown in our numerical experiments.

We use VI to train a DTMGP on data generated from simulations and real data and compare it with other existing DGP models. We conduct simulation studies by running experiments on an artificial random field and simulator of a stochastic activity network (Pasupathy and Henderson, 2011). We also use the RC-49 data set, which is publicly available on the web https://paperswithcode.com/dataset/rc-49, to demonstrate the performance of the proposed approach. In these numerical studies, we find that the training process of a DTMGP is more stable, and the training loss converges faster compared with its competitors. In addition, we compare the similarities between instances from the underlying systems and instances generated from competing statistical surrogate models. The results show that DTMGP outperforms the alternative DGPs in all experiments.

The remainder of this article is organized as follows. We will review the related literature in Section 2. We introduce general DGP models and an approximation of DGPs called an induced approximation in Section 3. The methodology and detailed implementation of a DTMGP are introduced in Section 4. Simulation studies are given in Section 5 and experiments on real data are given in 6. Concluding remarks are made in Section 7. The Appendix includes the required mathematical tools and technical proofs.

2. Literature review

The state-of-the-art deep learning techniques have brought probabilistic modeling with DNN structures to popularity. Based on the concept of Deep Belief Network (DBN) Hinton et al. (2006), and Damianou and Lawrence (2013) generalized the Restricted Boltzmann Machine (Hinton, 2010), which is a DBN with binary output, to a deep based on Gaussian process mapping. DGPs have been a popular probabilistic modeling with DNN structures to popularity. Based on the concept of Deep Belief Network (DBN) Hinton et al. (2006), and Damianou and Lawrence (2013) generalized the Restricted Boltzmann Machine (Hinton, 2010), which is a DBN with binary output, to a deep based on Gaussian process mapping. DGPs have been a popular tool in several applications. Their prowess has been demonstrated on many classification tasks (Damianou and Lawrence, 2013; Fei et al., 2018; Yang and Klabjan, 2021). Compared with traditional DNNs, the flexibility in uncertainty quantification of DGPs makes them ideal candidates for surrogate modeling (Radaideh and Kozlowski, 2020; Sauer, Gramacy and Higdon, 2022). DGPs are commonly used statistical surrogate models. The results show that DTMGP outperforms the alternative DGPs in all experiments.

3. General DGP models

3.1. DGPs

A GP $\mathcal{G}$ is a random function characterized by its mean function $\mu$ and covariance function $k$. To be more specific, given any input $x$, the output $\mathcal{G}(x)$ has a Gaussian distribution with mean $\mu(x)$ and variance $k(x,x)$, and given any pair of inputs $x$ and $x'$, the covariance between $\mathcal{G}(x)$ and $\mathcal{G}(x')$ is $k(x,x')$:

$$
\mathcal{G}(x) \sim \mathcal{N}(\mu(x), k(x,x)).
$$

A W-variate GP is simply a $W$-vector of GPs $[\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_W]$. Without loss of generality, we assume that any multivariate GP in the following content has mean function $\mu=0$ and independently distributed entries. A $H$-layer DGP $f^{(H)}$ is then the composition of $H$ multi-variate GPs:

$$
f^{(H)}(x') = G^{(H)} \circ \cdots \circ G^{(2)} \circ G^{(1)}(x'),
$$

where $f \circ g$ denotes the composition function $f(g(\cdot))$, $G^{(h)}$ denotes a $W^{(h)}$-variate GP $[G^{(h)}_1, G^{(h)}_2, \ldots, G^{(h)}_W]$, and $W^{(h)}$ is called the width of layer $h$. The formulation (2) of DGP can be viewed as a DNN with random activations $\{G^{(h)}_i\}$.

While DGP yields a non-parametric and Bayesian formulation of DNNs, computations for inference/prediction of DGPs are cumbersome. For example, given a set of input-output...
pairs \((X, Y) \in \mathbb{R}^{n \times d} \times \mathbb{R}^n\), the conditional probability distribution \(P(Y|X)\) induced by (2) is
\[
\mathbb{P}(Y|X) = \prod_{h=1}^{H} \mathbb{P}\left(Y|\mathbf{f}(H)\right) \mathbb{P}\left(\mathbf{f}(H-1)|\mathbf{f}(H-2)\right) \ldots \mathbb{P}(\mathbf{f}(1)|X) d\mathbf{f}(1) \ldots d\mathbf{f}(H),
\]
where \(\mathbf{f}(h)\) denotes the output vector from layer \(h\):
\[
\mathbf{f}(h) = \mathcal{G}(h) \circ \mathcal{G}(h-1) \circ \ldots \circ \mathcal{G}(1),
\]
with \(h = 1, \ldots, H\). Evidently, the integral (3) is intractable, leading to the intractability of inference and predictions of DGP \(\mathbf{f}(H)\) conditioned on any observed data \((X, Y)\).

### 3.2. Induced approximation of DGPs

The inference of a GP, which acts as a single activation in a DGP, is also time and space consuming. A challenge for GPs lies in their computational complexity and storage for the inverse of the covariance matrix \(k(X, X)\) which are \(O(n^3)\) and \(O(n^2)\), respectively, when the covariance matrix is of size \(n\). To alleviate this computational problem, current methods, such as the inducing-variable approximation in Hensman and Lawrence (2014) and Dai et al. (2016) and random Fourier feature approximation in Cutajar et al. (2017), focus on approximating the covariance matrix \(k(X, X)\) by some low-rank matrices.

Instead of approximating the covariance matrix, we directly approximate the GP activations in a DGP. In the following content, we will construct a reduced-rank approximation called the induced approximation. Induced approximation can bring a more flexible and clear DNN representation of DGPs.

Without loss of generality, let \(\mathcal{G}\) defined in (1) be a GP with constant mean \(\mu\) and covariance function \(k\). Inspired by the kriging method (Matheron, 1963; Sacks et al., 1989), we can approximate GP \(\mathcal{G}\) defined in (1) by the following finite-rank approximation:
\[
\tilde{\mathcal{G}}(x^*) := \mu + k(x^*, U)[k(U, U)]^{-1}G(U)
\]
where we call \(U = \{u_i \in \mathbb{R}^{d \times m}\}_{i=1}^m\) the inducing points and \(\tilde{\mathcal{G}}(U)\) are the values of \(\mathcal{G}\) on \(U\). According to theory (Ding and Zhang, 2020; Ritter, 2000; Wang et al., 2020), the required number of inducing points to achieve the optimal statistical error is much lower than the size \(n\) provided that the inducing points \(U\) are well-chosen. Hence, (4) can be computed in a highly efficient way.

Finite-rank approximation (4) can be represented as a one-layer neural network with correlated Gaussian distributed weights \(w = [k(U, U)]^{-1}G(U)\) and bias \(\mu\) as shown in Figure 1. However, the correlated Gaussian distributed weights still make training and inference difficult. In order to write the finite-rank approximation (4) in the form of a neural network with independently distributed weights, we can simply apply Cholesky decomposition to the kernel matrix \(k(U, U)\), which leads to the following equation:
\[
\tilde{\mathcal{G}}(x^*) = \mu + k(x^*, U)R_U^{-1}Z := \mu + \phi^T(x^*)Z,
\]
where \(R_U\) is the Cholesky decomposition of matrix \(k(U, U)\) and \(Z = [R_U^{-1}]^T\mathcal{G}(U)\) are independent and identically distributed (i.i.d.) distributed standard Gaussian random variables. We call approximation (5) the induced approximation and Figure 2 shows that the induced approximation can be represented as a two-layer network where the functions \(\phi\) act as an extra hidden layer. As the approximation (5) consists of only \(m\) Gaussians, the time and space complexity for its inference are then reduced to \(O(m^2 n)\) and \(O(mn)\), respectively.

The induced approximation of a DGP is to approximate each random activation by corresponding induced approximation. For example, suppose that in a DGP \(\mathbf{f}(H)\), all activations in the same layer are characterized by the same covariance function \(k^{(h)}\). Then, the induced approximation \(\tilde{\mathbf{f}}^{(H)}(x^*)\) of \(\mathbf{f}^{(H)}\) is
\[
\tilde{\mathbf{f}}^{(H)}(x^*) = [Z^{(H)}\phi^{(H)}(\cdot) + \mu^{(H)}] \circ \ldots \circ [Z^{(1)}\phi^{(1)}(x^*) + \mu^{(1)}],
\]
where, for \(h = 1, \ldots, H\), \(Z^{(h)} \in \mathbb{R}^{W^{(h)} \times m^{(h)}}\) is a matrix with i.i.d. standard Gaussian entries, \(U^{(h)}\) are the total \(m^{(h)}\) inducing variables for kernel \(k^{(h)}\), \(R_h \in \mathbb{R}^{m^{(h)} \times m^{(h)}}\) is the Cholesky decomposition of the covariance matrix \(k^{(h)}(U^{(h)}, U^{(h)})\), and \(\mu^{(h)} \in \mathbb{R}^{W^{(h)}}\) is the mean vector and can be treated as the bias of layer \(h\).
In the next section, we will show that if kernel $k$ is in a class of kernel function called a tensor Markov kernel and inducing points $U$ are a specific design called a sparse grid, then induced approximations (5) and (6) can be further written as a sparse approximation.

4. Methodology of DTMGP

In this section, we first introduce the concept of TMGs. We then introduce hierarchical expansion of TMGs and how it leads to mutually orthogonal feature functions with hierarchical supports. Based on hierarchical expansion, we can introduce the implementation and training of DTMGPs.

4.1. TMGPs

Hierarchical expansion is applied to a class of GPs called a TMGP. In one dimension, a Markov GP is characterized by the following Lemma in Marcus and Rosen (2006):

**Lemma 1** (Marcus and Rosen (2006) Lemma 5.1.8). Let $I \subseteq \mathbb{R}$. Let $G$ be a zero mean GP defined on $I$ with continuous positive definite kernel $k$. Then, $G$ is a Markov GP and $k$ is Markov kernel if and only if there exist positive functions $p$ and $q$ on $I$ with $p/q$ strictly increasing such that

$$ k(x,x') = p'(\min(x,x'))q'(\max(x,x'))], \quad x,x' \in I. \quad (7) $$

For any Markov GP $G$ we have that, conditioned on its distribution at a point $x$, its distributions at any point $x_{0} < x$ are independent: $\mathcal{G}(x_{0}) \perp \mathcal{G}(x) \mid \mathcal{G}(x_{0})$, whence Markov GP. Markov GPs have two advantages in computations. First, given any ordered inducing points $\{u_{1} \prec \cdots \prec u_{i}\}$, the distribution of $\mathcal{G}(x)$ at any $x$, where $u_{i} < x < u_{i+1}$, depends only on its left and right inducing points $\mathcal{G}(u_{i})$ and $\mathcal{G}(u_{i+1})$. Second, for any induced approximation, accuracy of the approximation at $x$ only depends on the distances between $x$ and its left and right neighbors, respectively. Therefore, evenly distributed inducing variables can achieve an accurate approximation that is also cheap to compute.

The following purely additive and purely tensor structure of a one-dimensional Markov kernel can both extend Markov GPs to multi-dimensions:

$$ k(x,x') = \prod_{j=1}^{d} k_{j}(x_{j},x'_{j}), \quad k(x,x') = \prod_{j=1}^{d} k_{j}(x_{j},x'_{j}). \quad (8) $$

We generalize the additive and tensor form in (8) to the following GP, which has additive and tensor structure simultaneously:

**Definition 1.** A GP is called TMGP if and only if it is a zero mean GP with covariance function of the form

$$ k(x,x') = \sum_{i=1}^{s} \prod_{j \in U_{i}} k_{i,j}(x_{j},x'_{j}), \quad (9) $$

where $U_{i} \subseteq \{1,2,\cdots,d\}$ and $k_{i,j}$ is a 1-D Markov kernel for any $l,j$. A kernel of the form (10) is called a tensor Markov kernel (TMK).

A TMGP $G$ with kernel (9) can be factorized to a sum of $s$ mutually independent GPs: $G = \sum_{i=1}^{s} G_{i}$ where each $G_{i}$ is with kernel function $\prod_{j \in U_{i}} k_{i,j}(x_{j},x'_{j})$. To achieve an accurate approximation of TMGP using the smallest number of inducing variables, we can only focus on TMGP with a purely tensor structure. By combining mutually independent approximations, we can arrive at a solution. Therefore, in the following content, we only study approximation for TMGP with a purely tensor structure:

$$ k(x,x') = \prod_{j=1}^{d} k_{j}(x_{j},x'_{j}), \quad (10) $$

and the general TMGP with kernel (9) is a straightforward extension that involves combining approximations of GPs with purely tensor kernels.

Commonly used TMKs with purely tensor structure include the Laplace kernel $k(x,x') = \exp(\sum_{j=1}^{d} \theta_{j}|x_{j} - x'_{j}|)$ and Brownian sheet kernel $k(x,x') = \prod_{j=1}^{d}(1 + \theta_{j}|x_{j} - x'_{j}|)$. The challenge in extending the inducing approximation of a 1-D Markov GP to multiple dimensions lies in properly defining the “left” and “right” neighbors in a multidimensional space, similar to how it is done on the real line. To address this, we introduce the hierarchical expansion method, which is explained in the following section.

4.2. Hierarchical expansion

To construct the hierarchical expansion, we let inducing variables $U$ be an experimental design $X_{l}^{SG}$ called level-$l$ Sparse Grid (SG) (Bungartz and Griebel, 2004; Plumlee, 2014), where level $l$ determines the number of inducing variables. Furthermore, the SG inducing variables must be sorted in a specific order. A detailed introduction to SGs and the required order are provided in Appendix A, and MATLAB codes for generating SGs satisfying the requirement can be found in the Sparse Grid Designs package (Plumlee, 2021). Examples of two-dimensional SGs are shown in Figure 3. From the examples, we can see that the incremental points from the next level of a SG exhibit a hierarchical structure—higher level SG consists of local SGs of smaller levels.

Hierarchical expansion of a TMGP $G$ with inducing points $X_{l}^{SG}$ is then simply:

$$ G(x') \approx k(x',X_{l}^{SG})R_{l}^{-1}Z := \phi^{T}(x')Z, \quad (11) $$

where $k(x',X_{l}^{SG}) = [k(x',x_{1}),\cdots,k(x',x_{m})]$ is the covariance vector, $k(X_{l}^{SG},X_{l}^{SG}) = [k(x_{i},x_{j})]_{i,j=1}^{m}$ is the covariance matrix, $R_{l}$ is the Cholesky decomposition of $k(X_{l}^{SG},X_{l}^{SG})$, $Z = [Z_{1},\cdots,Z_{m}]$ are i.i.d. standard Gaussian random variables and $\phi = [\phi_{i}]_{i=1}^{m}$ are called hierarchical features. Hierarchical expansion (11) yields a sparse approximation of TMGP that is easy to compute as shown in the following theorems.

**Theorem 1.** The number of non-zero entries on $R_{l}^{-1}$ is $O(m_{l})$ and $R_{l}^{-1}$ can be computed in $O(m_{l})$ operations.
Theorem 2. Given any input point \( \mathbf{x}^* \), the number of non-zero entries on the vector of hierarchical features \( \phi(\mathbf{x}^*) \) is \( O(\log m_1^{2d-1}) \).

The algorithm for computing \( R_i^{-1} \) in \( O(m_i) \) operations is given in Appendix B, and proofs for Theorems 1 and 2 are provided in supplementary material. Since we can compute \( R_i^{-1} \) in \( O(m_i) \) operations and the numbers of non-zero entries on \( R_i^{-1} \) is \( O(m_i) \), hierarchical expansion can be computed in \( O(m_i) \) operations. Moreover, if matrix \( R_i^{-1} \) is given, because the numbers of non-zero entries on \( \phi(\mathbf{x}^*) \) is only \( O(\log m_i^{2d-1}) \), the computational time of the hierarchical expansion can be further reduced to \( O(\log m_i^{2d-1}) \). The sparsity of hierarchical feature vector \( \phi \) relies on the fact that the supports of \( \{\phi_i\} \) are either nested or disjoint and, hence, form a hierarchical structure as shown in Figure 4.

\( X_i^{S} \) is also regarded as the index set of \( \phi \), because instead of labeling each hierarchical feature by number \( i \), we can also label it by the corresponding inducing variable \( \mathbf{x}_i \in X_i^{S} \). As shown in Figure 5, for any \( i \), \( \mathbf{x}_i \) is the only point at which \( \phi_i \) is not differentiable along all dimensions. Hence, we call \( \mathbf{x}_i \) the center of \( \phi_i \). From this perspective, we can claim that, given any \( \mathbf{x}^* \), the distribution of the approximation at \( \mathbf{x}^* \) only depends on \( O(\log m_i^{2d-1}) \) inducing variables. As a result, the hierarchical expansion generalizes the one-dimensional Markov property while still remaining a high accuracy approximate. We discuss the approximation error of hierarchical expansion in the supplementary material.

The following numerical example illustrates the sparsity of the hierarchical expansion:

Example 1. Let two-dimensional TMK \( k(\mathbf{x}, \mathbf{x}') = \exp\{-\sum_{j=1}^{2} |x_j - x'_j|\} \). Let

\[
X_2^{S} = \left[ \begin{array}{cccc}
(1/2 & 1/2) & (1/2 & 1/4) & (1/2 & 3/4) & (1/2 & 1/2) & (3/4 & 1/2) \\
0 & 1.5942 & 0 & 0 & 0 & 0 & 1.5942 \\
0 & 0 & 1.5942 & 0 & 0 & 0 & 0.0000 \\
0 & 0 & 0 & 0 & 0 & 0 & 1.5942 \\
\end{array} \right].
\]

be the sorted level-2 SG. Then, we numerically compute the inverse Cholesky decomposition \( R_2^{-1} \) and we get

\[
R_2^{-1} = \left[ \begin{array}{cccccc}
1.0000 & -1.2416 & -1.2416 & -1.2416 & -1.2416 \\
0 & 1.5942 & 0.0000 & 0.0000 & 0.0000 \\
0 & 0 & 1.5942 & 0.0000 & 0.0000 \\
0 & 0 & 0 & 1.5942 & 0.0000 \\
0 & 0 & 0 & 0 & 1.5942 \\
\end{array} \right].
\]

Let \( \mathbf{x}_1 = (0.8147, 0.9058) \), and \( \mathbf{x}_2 = (0.2785, 0.5469) \) be two randomly chosen points. We numerically compute the hierarchical features at \( \mathbf{x}_1 \) and \( \mathbf{x}_2 \) and we get

\[
k(\mathbf{x}_1^{S}, \mathbf{x}_2^{S})R_2^{-1} = [0.4865, 0.3918, 0.0000, 0.3918],
\]

\[
k(\mathbf{x}_1^{S}, \mathbf{x}_2^{S})R_2^{-1} = [0.7646, 0.5291, 0.0, 0.0933].
\]

As we can see, matrix \( R_2^{-1} \) is sparse and each of \( k(\mathbf{x}_1^{S}, \mathbf{x}_2^{S})R_2^{-1} \) and \( k(\mathbf{x}_2^{S}, \mathbf{x}_2^{S})R_2^{-1} \) has two zero elements. The sparsity is even more visible as the number of inducing points increases.

4.3. DTMGPs

A H-layer DTMGP \( T^{(H)} \) is defined as the composition of \( H \) hierarchical expansions of multi-variate TMGP:

\[
T^{(H)}(\mathbf{x}^*) = \left[ Z^{(H)}(\phi(\mathbf{x}^*) + \mu^{(H)}) \right] \circ \cdots \circ \left[ Z^{(1)}(\phi^{(1)}(\mathbf{x}^*) + \mu^{(1)}) \right],
\]

where, for \( h = 1, \cdots, H \), \( Z^{(h)} \) is a \( W^{(h)} \)-by-\( m^{(h)} \) matrix with i.i.d. standard Gaussian entries, \( W^{(h)} \) is the dimension of the output (width of the neural network) of layer \( h \), \( m^{(h)} \) is the
number of hierarchical features for approximating a $W^{(h)}$-variate TMGP, $\phi^{(h)}$ consists of the $m^{(h)}$ hierarchical features for approximating the TMGP, acting as the activation functions in layer $h$, and $\mu^{(h)} \in \mathbb{R}^{W^{(h)}}$ is the parameterized mean for the TMGP in layer $h$.

Let us now focus on layer $h$ of $T^{(H)}$ to compare DTMGP with DNN. Let $T^{(h)} = (T^{(h)}_1, \ldots, T^{(h)}_{W^{(h)}})$ denote the $W^{(h)}$-dimensional output of layer $h$. We then have the following structure:

\[
T^{(h-1)} \rightarrow (\phi^{(h)}_1(T^{(h-1)}), \ldots, \phi^{(h)}_{m^{(h)}}(T^{(h-1)})) \quad \# \text{non-zero entries: } O(\log m^{(h)}2^{W^{(h)}-1})
\]

\[
\rightarrow \left[ T_j^{(h)} = \mu_j^{(h)} + \sum_{i=1}^{m^{(h)}} Z_{ij} \phi_j^{(h)}(T^{(h-1)}) \right]_{j=1}^{W^{(h)}},
\]

where $\phi_j^{(h)}(T^{(h-1)})$ is the $j$th entry of vector $k^{(h)}(T^{(h-1)}, X^{SG}^{(h)})[R^{(h)}]^{-1} k^{(h)}$ is the TMK for layer $h$, $X^{SG}^{(h)}$ is a level-$l^{(h)}$ SG of size $m^{(h)}$ for induced approximation, and $R^{(h)}$ is the Cholesky decomposition of covariance matrix $k^{(h)}(X^{SG}^{(h)}, X^{SG}^{(h)})$. This structure is also illustrated in Figure 6.

If we treat DTMGP as a DNN, then, for $h = 1, \ldots, H$, layer $h$ is equipped with $m^{(h)}$ activations $\{k^{(h)}(\cdot, x): x \in X^{SG}^{(h)}\}$, a sparse linear filter $[R^{(h)}]^{-1}$ which converts the dense input to sparse local hierarchical features, bias $\mu^{(h)}$, and i.i.d. standard Gaussian weights. Moreover, sparse linear filters $\{[R^{(h)}]^{-1}\}_{h=1}^{H}$ are fixed for a specific hierarchical expansion. Therefore, $\{[R^{(h)}]^{-1}\}_{h=1}^{H}$ can be computed and stored in advance. Due to Theorems 1 and 2, the space complexity for storing $\{[R^{(h)}]^{-1}\}_{h=1}^{H}$ is linear in the number of inducing points and the time complexity of any operation in layer $h$ of DTMGP is $O(\log m^{(h)}2^{W^{(h)}-1})$.

### 4.4. VI

The proposed DTMGP is mathematically equivalent to a DNN with biases $\{\mu_1^{(h)}\}_{h=1}^{H}$ and i.i.d. weights $\{Z^{(h)}\}_{h=1}^{H}$. So we can parameterize DTMGP as a BNN with i.i.d. weights. Specifically, we regard the variances and means of all Gaussian weights, and the biases as parameters of the BNN. A DTMGP can be represented as a stochastic process $f_{0}$ in the parameterized family $\mathcal{F}_{\Theta}$:

\[
\mathcal{F}_{\Theta} = \left\{ \left[ (\Sigma^{(h)} \odot Z^{(h)}) + m^{(h)} \right] \phi^{(h)} + \mu^{(h)} \right\}\]

\[
\cdots \left[ (\Sigma^{(1)} \odot Z^{(1)}) + m^{(1)} \right] \phi^{(1)} + \mu^{(1)} \right\}:
\]

\[
\{ (\Sigma^{(h)}, m^{(h)}, \mu^{(h)}) \}_{h=1}^{H} \in \Theta \}
\]

where $\Theta$ denotes the set of parameters.
and $A \odot B$ denotes the entry-wise multiplication of matrices $A$ and $B$, i.e., the Hadamard product. In other words, the family $F_{\Theta}$ consists of BNNs with activations $\{\phi^{(h)}\}_{h=1}^{H}$, parameterized biases, and normally distributed weights.

Given observations $(X, Y)$, our goal is to search for the parameters $\theta'$ that maximize the marginal likelihood $\mathbb{P}(Y|X, \theta)$. The DTMGP $f_{\theta}$ can best interpret how $(X, Y)$ is generated. Computing $\mathbb{P}(Y|X, \theta)$ of any DGP involves intractable integral as shown in (3), but we can obtain a tractable lower bound using VI. VI first assigns a prior $f_{\theta}$ with some $\tilde{\theta} = \{\tilde{\Sigma}^{(h)}, \tilde{m}^{(h)}, \mu^{(h)}\}_{h=1}^{H}$ to the underlying stochastic process generating $(X, Y)$ and then maximizes the following evidence lower bound (ELBO):

$$\mathcal{E}(\theta) = \mathbb{E}_{\tilde{\theta}}[\log \mathbb{P}(Y|X, \theta)] - D_{\text{KL}}(f_{\theta}||\tilde{\theta}),$$

which is the lower bound of log-likelihood $\log \mathbb{P}(Y|X, \theta)$.

In our framework, the term $\mathbb{E}_{\tilde{\theta}}[\log \mathbb{P}(Y|X, \theta)]$ is called the negative energy and can be explicitly written as

$$\mathbb{E}_{\tilde{\theta}}[\log \mathbb{P}(Y|X, \theta)] = \mathbb{E}_{Z^{(1)}, \ldots, Z^{(H)}}[\log \mathbb{P}(Y|X, Z^{(1)}, \ldots, Z^{(H)}, \theta)].$$

This term now can be efficiently estimated by stochastic optimization based on Monte Carlo methods, such as doubly-stochastic approximation (Dai et al., 2014; Hensman and Lawrence, 2014; Salimbeni and Deisenroth, 2017). The term $D_{\text{KL}}(f_{\theta}||\tilde{\theta})$ is the KL-divergence between $f_{\theta}$ and the prior $f_{\tilde{\theta}}$ and it can be explicitly written

$$D_{\text{KL}}(f_{\theta}||\tilde{\theta}) = \frac{1}{2} \sum_{h=1}^{H} \sum_{i=1}^{W^{(h)}} \sum_{j=1}^{m^{(h)}} \left[ \frac{\Sigma^{(h)}_{i,j}}{\tilde{\Sigma}^{(h)}_{i,j}} \right]^2 + \frac{[\Sigma^{(h)}_{i,j}]^2}{[\tilde{\Sigma}^{(h)}_{i,j}]^2} - 1 - \log \frac{[\Sigma^{(h)}_{i,j}]^2}{[\tilde{\Sigma}^{(h)}_{i,j}]^2}.$$

The computation of $\mathcal{E}$ is efficient at any $\theta \in \Theta$, the training process of DTMGP is simply defined as

$$\theta^* = \arg \max_{\theta \in \Theta} \{ \mathbb{E}_{\tilde{\theta}}[\log \mathbb{P}(Y|X)] - D_{\text{KL}}(f_{\theta}||\tilde{\theta}) \}.$$ (14)

This optimization problem can also be treated as a penalized regression problem where the negative energy term is the model fitness level and the KL-divergence term is the penalty of being far from the DTMGP prior. Equation (14) can be solved efficiently by using the automatic differentiation technique (Neidinger, 2010; Baydin et al., 2018).

## 5. Simulation studies

In this section, we run simulations on systems with stochastic outputs to access DTMGP’s capacity in modeling stochastic processes. More specifically, in each experiment, output $Y$ of the underlying system at each input $x$ follows an unknown distribution $F(\cdot|x)$:

$$Y(x) \sim F(y|x).$$

A training set $(X_{\text{train}}, Y_{\text{train}})$ is independently collected where $Y_{\text{train}} = Y(X_{\text{train}})$ is the realization of the underlying system on inputs $X_{\text{train}}$. We then train competing models using training set $(X_{\text{train}}, Y_{\text{train}})$.

Let $\hat{Y}(\cdot)$ denote a trained model. We first choose a test set $X_{\text{test}}$ from the input space. For each input $x \in X_{\text{test}}$, we sample 100 independent realizations from the true underlying system and from the trained model to get data sets $\{Y_i(x)\}_{i=1}^{100}$ and $\{\hat{Y}_i(x)\}_{i=1}^{100}$, respectively. We then use the two-sample Kolmogorov–Smirnov (KS) statistic:

$$D_x = \sup_{y} \frac{1}{100} \sum_{i=1}^{100} 1[y_i(x) \leq y] - \frac{1}{100} \sum_{i=1}^{100} 1[\hat{Y}_i(x) \leq y]$$

to quantify the similarity between $Y$ and $\hat{Y}$ on input $x$. The smaller $D_x$ is, the closer are the two distributions. We access the overall performance of $\hat{Y}(\cdot)$ via the following averaged two-sample KS statistic over test set $X_{\text{test}}$:

$$\hat{D} = \frac{1}{R} \sum_{r=1}^{R} D_r,$$

$$\hat{\sigma} = \left[ \frac{1}{R} \sum_{r=1}^{R} (D_r - \hat{D})^2 \right]^{1/2}. $$

In all experiments, activations of DTMGP are hierarchical features generated from TMGPs with the Laplace covariance function $k(x, x') = \exp \left(-\frac{|x - x'|^2}{\ell^2}\right)$. We compare DTMGP with the following existing models:

1. **GP**: Standard Gaussian process with squared exponential covariance function.
2. **BNN-ReLU** (Schmidt et al., 1992; Graves, 2011; Blundell et al., 2015): ReLU deep neural networks (Glorot et al., 2011) with parameterized Gaussian distributed weights and biases. VI is used for training BNN-ReLU.
3. **DGP-RFF** (Cutajar et al., 2017): A Random Fourier feature expansion of DGP with each layer represented by Gaussian processes with the Gaussian kernel $\exp \left(-\sum_{j=1}^{p} w_j |x - x'_j|^2\right)$. DGP-RFF is trained with VI approximation provided in Cutajar et al. (2017).
4. **DGP-VEC** (Sauer, Cooper and Graacy, 2022) DGP where each activation is GP with Matérn-1/2 kernel. Posterior of the model is approximated through the incorporation of the Vecchia approximation (Katzfuss and Guinness, 2021).

Note that all deep models can be represented by the same architecture and the difference among them lies in their activations. For DTMGP, BNN-ReLU, and DGP-RFF,
they are BNN with different deterministic activations and random weights. For DGP-VEC, it is composition of GPs. Therefore, for each data set, we adopt the same architectures for fair comparisons. In other words, except for the specific activations, all deep models are with equal number of layers, widths, weights, and biases.

We conduct experiments with two simulation models: a two-dimensional non-Gaussian random field in Section 5.1, and the expected revenue of a 13-dimensional Stochastic Activity Network problem in Section 5.2. All the experiments are implemented on a computer with macOS, 3.3 GHz Intel Core i5 CPU, and 8 GB of RAM (2133Mhz).

5.1. A non-Gaussian random field

In this section, we use the following non-Gaussian and non-stationary random field in two dimensions to access the sample and computational efficiency of the proposed methodology:

\[ Y(x) = \frac{1}{1 + \exp \{B(x)\}}, \quad x \in [0,1]^2 \]

where \(B(x)\) is a Brownian sheet, which is defined as a zero-mean GP with covariance function \( \prod_{d=1}^{2} (1 + \min\{x_d, x_d'\}) \).

In this experiment, \(X_{\text{train}}\) is randomly collected from \([0,1]^2\) and \(Y_{\text{train}}\) is from independently sample paths of \(B(x)\) on \(X_{\text{train}}\). We investigate the performance of each method as the sizes of the training set \((X_{\text{train}}, Y_{\text{train}})\) increase. For each training set, we randomly select \(n_{\text{test}} = 100\) points from \([0,1]^2\) as the test set, denoted as \(X_{\text{test}}\). We run \(R = 20\) macro-replications and compute \(\hat{D}\) and the associated standard deviation \(\hat{\sigma}\) for each method.

All deep models are with two hidden layers where the first layers consists of 181 activations and one output, and the second layer consist of 127 activations and one output. Figure 7 shows the realization of the random field and architecture shared by all deep models. We let the i.i.d. prior of each coefficient in DTMGP be normal distributed with mean 0 and variance 1.

Our experiments reveal that DGP-VEC has a significantly longer training time compared to all other models. Specifically, Table 1 demonstrates that while DTMGP has the fastest convergence rate to stable training error, DGP-VEC exhibits the slowest. Consequently, to ensure a fair comparison, we report our results at different training times. First, we report the KS statistics of all models when DTMGP’s training error begins to converge, and then we report the KS statistics of all models when DGP-VEC’s training error begins to converge.

As shown in Figure 8, when given enough training time, DGP-VEC outperforms all other models. However, it’s worth noting that the performance of DTMGP is still comparable to that of DGP-VEC. If we limit the training time for all models to end once the training error of DTMGP begins to converge, we find that DTMGP - which has the fastest convergence rate - outperforms all other models, including DGP-VEC. This is despite the fact that DGP-VEC requires a training time that is three to four times longer than DTMGP, as it relies on MCMC for training. As it is widely acknowledged that VI is more efficient than MCMC, this serves as an important reminder of the tradeoffs we must consider when selecting a training method.

5.2. Stochastic activity network

In this subsection, we consider the Stochastic Activity Network (SAN) where the arcs are labeled from 1 through 13. The detailed explanation of SAN is available in Avramidis and Wilson (1996). As shown in the left of Figure 9, each arc \(i\) in the SAN is associated with a task with random duration \(D_i\) and task durations are mutually independent. Suppose that \(D_i\) is exponentially distributed with mean \(X_i\) for each \(i\). Suppose that we can control \(X_i > 0\) for each \(i\), but there is an associated cost. In particular, the overall cost is defined as

\[ C(X) = T(X) + f(X) \]

where \(X = (X_1, \cdots, X_{13})\), \(T(X)\) is the (random) duration of the longest path from a to \(i\), and \(f(X) = \sum_{i=1}^{13} X_i^{-1}\). The closed form of \(C(X)\) is unknown, but the MATLAB
The simulator of this problem is available in the SimOpt library (Pasupathy and Henderson, 2011).

In this experiment, data are collected from a maximin Latin Hypercube Design (LHD) that maximizes the minimum distance between points (van Dam et al., 2007). The LHD consists of 5000 sample points from the cube \([0.5, 5]^3\). At each sample point, \(m\) simulation replications are run with \(m = 2, 4, \ldots, 20\). In order to select a reasonable prior for the target stochastic process, we first normalize all the output so that all output data in the training set and testing set are distributed on \([0, 1]\). We then run \(m = 10\) replications at each design point during the training process to estimate the variance at each point. Based on the sample estimates, we let the i.i.d. prior of each coefficient in DTMGP be normal distributed with mean 0 and variance 0.04.

We examine the performance of each method as the number of replications \(m\) increase. Given \(m\), we construct the test set \(X_{\text{test}}\) of size \(n_{\text{test}} = 100\) by random samples from \([0.5, 5]^3\). We compute \(\hat{D}\) of each method, its associated standard deviation \(\hat{\sigma}\) based on \(R = 20\) macro-replications.

Similar to Section 5.1, all the competing models in this experiment share the same architecture. All deep models have two hidden layers. The first layer consists of 391 activations and its output is 10-dimensional. The second layer consists of 241 activations and its output is 1-dimensional. Such an architecture is flexible enough to capture the random process.

As before, the training time of DGP-VEC is much longer than other models. When \(m > 10\), the training time required for DGP-VEC is longer than 4 hours, which is unacceptable compared with DTMGP. Therefore, to ensure a fair comparison, we also report our results at different training times, see Table 2. First, we report the KS statistics of all models when DTMGP’s training error begins to converge, and then we report the KS statistics of all models when DGP-VEC’s training error begins to converge or the training time reaches 4 hours.

As demonstrated in Figure 10, DGP-VEC outperforms all other models when given sufficient training time. However, DGP-VEC’s training time exceeds 4 hours when \(m > 10\) or when the total training data size is greater than 50,000. Therefore, we only present the results of DGP-VEC for \(m \leq 10\). On the other hand, DTMGP demonstrates comparable performance, with a training time of roughly one-tenth that required by DGP-VEC. Similar to Section 5.1, when we restrict the training time for all models to stop once the training error of DTMGP starts to stabilize, we observe that DTMGP outperforms all other models, and DGP-VEC performs even worse than BNN-ReLU. This is because the training time is not sufficient for MCMC.

### 6. Experiment on real data

This section aims to evaluate the performance of the proposed methodology on a real dataset. To this end, we utilize
the RC-49 dataset (Ding et al., 2021), which is a synthetic collection of 49 3-D chair models rendered at yaw angles ranging from 0° to 90°. The RC-49 dataset consists of \( n = 176,400 \) data pairs \( \{(X_i, Y_i)\}_{i=1}^n \) where, for any \( i = 1, \ldots, n \), input \( X_i \in [0, 90] \) is a specific yaw angle and outputs \( Y_i \) is a 64 × 64 image of a chair rendered. The objective is to use the Bayesian formula to train a generative model, which is conditioned on the input variable \( x \). When provided with input yaw angle \( x \), the trained model should generate a random matrix output that is similar to the data \( Y \) at the same angle. In essence, the generative problem is a stochastic process \( Y(x) \in \mathbb{R}^{64 \times 64} \) where \( x \in [0, 90] \), and our aim is to employ a deep GP model to reconstruct \( Y(x) \) from observed data.

We compare DTMGP with BNN-ReLU and DGP-RFF introduced in Section 5. Other deep GP models are omitted due to their limited capacity for handling the large data size and complex model architecture. All competing deep GP models share the following architecture. We first apply the embedding technique on input \( x \), which uses a linear transformation \( A \) to map the single variable input \( x \in [0, 90] \) to a 100-dimensional vector \( x' \in \mathbb{R}^{100} \). We then adopt a four-layer BNN architecture where \( x' \) is the input layer, the first hidden layer consists of 201 activations and a 256-dimensional output, the second hidden layer consists of 513 activations and a 512-dimensional output, and the third hidden layer consists of 1025 activations and the final output is a 64 × 64 random matrix. Specifically, the architecture can be written as follows:

\[
\begin{align*}
    f_1^{(1)} &= \sum_{i=1}^{201} Z_{i,j}^{(1)} \phi_i^{(1)}(Ax), \quad j = 1, \ldots, 256, Z_{i,j}^{(1)} \sim \mathcal{N}(0,1), A \in \mathbb{R}^{100 \times 1}, \\
    f_2^{(2)} &= \sum_{i=1}^{513} Z_{i,j}^{(2)} \phi_i^{(2)}(f_1^{(1)}), \quad j = 1, \ldots, 512, Z_{i,j}^{(2)} \sim \mathcal{N}(0,1), \\
    \hat{Y}_{l,j} &= \sum_{i=1}^{1025} Z_{i,j}^{(3)} \phi_i^{(3)}(f_2^{(2)}), \quad l,j = 1, \ldots, 28, Z_{i,j}^{(3)} \sim \mathcal{N}(0,1).
\end{align*}
\]

Figure 11 provides an illustration of the above architecture.

We use 80,000 samples from the RC-49 dataset to train DTMGP and its competitors BNN-RELU and DGP-RFF. We train the models by mini-batch SGD and, in each epoch, we sample their random outputs at input \( x \), for \( x \in [0, 90] \). Because the output in this experiment is a 64 × 64 random matrix and we are unable to sample data from the true distribution of RC-49, the previous KS statistics cannot be used to access the accuracy. Instead, we directly examine the output images of each model to evaluate their performances.

Conditional samples generated by DTMGP, BNN-ReLU, and DGP-RFF at the third, sixth and ninth epochs are
shown in Figure 12. The results demonstrate that DTMGP generates samples that are closer to the actual data and performs the best, whereas other models fail to reconstruct the conditional samples. This is because, as observed in previous experiments, the hierarchical structure of DTMGP can effectively capture the local features whereas the ReLU or cosine activations of BNN-ReLU or DGP-RFF lack the ability to do so.

As depicted in Figure 13, DTMGP exhibits a faster convergence rate towards stability with more consistent generated results. The rapid convergence suggests that the model can be trained in few epochs, while the consistent performance implies that the model is reliable. This may be attributed to the sparsity introduced by our expansion approach, which facilitates feature detection and speeds up parameter determination.

Table 3 demonstrates that the training time per epoch of both BNN-ReLU and DGP-RFF is faster than that of DTMGP. This difference could be primarily attributed to the fact that BNN-ReLU and DGP-RFF are built using built-in functions and packages in the MATLAB, whereas our code for DTMGP does not take this advantage. Nonetheless, the training time per epoch of DTMGP is still comparable to that of BNN-ReLU and DGP-RFF.

7. Conclusions and discussion
We utilize hierarchical features to expand DGPs, which comprise TMGPs. Our expansion is known as DTMGP and is computationally efficient, resulting in a sparse representation of DGPs. The hierarchical nature of the features means
that their supports are either nested or disjoint, enabling a poly-logarithmic number of activations throughout a DTMGP to have non-zero output conditioned on any input or operation. Furthermore, hierarchical features can effectively capture local features from inputs, resulting in high performance in prediction and generative problems, as demonstrated in our experiments. In comparison with existing DGP models, DTMGP’s sparsity leads to efficient inference and training, while generated instances from DTMGP are also relatively accurate under the KS test.

The current article can potentially be extended in several ways. First, how to apply hierarchical expansion on DGP with more general structures, such as DGP with Måtern covariance functions, can be studied in future research. Second, it was pointed out by Stein (2014) that, approximating the likelihood function of GP by low-rank methods, such as inducing point and random features, may have an adverse effect on the performance. How large this effect is for the proposed DGP models should be studied in further investigation.

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**Appendix**

A. Sparse grid designs with required order

The class of SG adopted in this work is called Hyperbolic-cross SG, which is the union of Full Grids (FGs) with dyadic structures. Without loss of generality, we can assume that all design points are collected from the hypercube $(0,1)^d$, and we start constructing SGs satisfying the required order with the one-dimensional case, which is also called a dyadic point set.

A one-dimensional level-$l$ dyadic point set $X_l$ with increasing order is simply defined as $X_l = \{2^{-l} \cdot i : i \in \mathcal{P}(l)\}$.

Then given a level-$l$ dyadic point set $X_l$ and a level-$(l-1)$ dyadic point set $X_{l-1}$, we can define the sorted incremental set $D_l = X_l - X_{l-1} = \{2^{-l} \cdot i : i \in \mathcal{P}(l)\}$, with $D_0 = \emptyset$. It is straightforward to check that $X_l = \bigcup_{i=1}^l D_i$. $D_i \cap D_j = \emptyset$, if $i \neq j$. For any incremental set $D_i$, we can label any point in $D_i$ by $x_{l,i} \in \mathcal{P}(l)$ so that the label is unique for any point: $x_{l,i} \neq x_{l,j}$ if and only if $(l,i) \neq (l,j)$. Now we can define the following dyadic set with the required order:

$X_l^d = [D_1, D_2, \ldots, D_l] = [x_{l,i} : \ell \leq i, i \in \mathcal{P}(l)]$.

For example, $X_1 = [\frac{1}{8}, \frac{3}{8}, \frac{5}{8}, \frac{7}{8}]$ with $D_1 = [\frac{1}{8}, \frac{3}{8}, \frac{5}{8}, \frac{7}{8}]$ and $D_2 = [\frac{1}{4}, \frac{3}{4}, \frac{5}{4}, \frac{7}{4}]$, respectively.

We also define the Cartesian product of one-dimensional sorted $X_l^d$’s for later use in Algorithms and proofs. We call this sorted Cartesian product FG $X_l^d$ labeled by $I = (l_1, l_2, \ldots, l_d) \in \mathbb{N}^d$:

$X_l^d = \prod_{j=1}^d X_{l_j} = [x_{l_1,i_1}, x_{l_2,i_2}, \ldots, x_{l_d,i_d} : \ell_j \leq i_j, i_j \in \mathcal{P}(\ell_j), j = 1, \ldots, d]$.

For simplicity, we define the Cartesian product $\mathcal{P}(l) = \times_{j=1}^d \mathcal{P}(\ell_j)$ for any $l \in \mathbb{N}^d$ so that any points in $X_l^d$ can be represented as $x_{l,i} = (x_{l_1,i_1}, x_{l_2,i_2}, \ldots, x_{l_d,i_d})$ for any $l \in \mathbb{N}^d$ and $i \in \mathcal{P}(l)$. Then we have a more compact representation of $X_l^d$:

$X_l^d = [x_{l,i} : \ell \leq i, i \in \mathcal{P}(l)]$.

For example, the sorted FG $X_{1,2}^d$ is

$X_{1,2}^d = \left[ \begin{array}{lll} 1 & 1 & 1 \\ 1 & 3 & 3 \\ 1 & 2 & 2 \\ \end{array} \right]$.

Finally, a level-$l$ SG satisfying our required order is the union of sorted FGs as follows:

$X_l^{SG} = \bigcup_{l_i=1}^{l_{\text{max}}} X_{l_i} = [x_{l,i} : \ell \leq i, i \in \mathcal{P}(l)]$.

where $\|l\|$ denotes the $l_1$-norm $\sum_{i=1}^d |l_i|$. To be more specific, a point $x_{l,i} \in X_l^{SG}$ must be ahead of any $x_l$ with $|l'| > |l|$. For example, the two-dimensional sorted SG $X_2^{SG}$ is
\[ \mathbf{x}^S_G = \begin{bmatrix} \begin{pmatrix} 1 & 1 \\ 2 & 2 \end{pmatrix} & \begin{pmatrix} 1 & 1 \\ 2 & 4 \end{pmatrix} & \begin{pmatrix} 1 & 3 \\ 4 & 2 \end{pmatrix} \end{pmatrix} \]

Unlike FG, whose size increases exponentially in dimension \( d \), the size of SGs increases relatively mildly in \( d \). Lemma 3.6 in Bungartz and Griebel (2004) stipulates that the sample size of a \( d \)-dimensional level-1 \( \mathbf{x}^S_G \) is given by

\[ |\mathbf{x}^S_G| = \sum_{l=0}^{l-1} 2^l \frac{(l + d - 1)!}{(d - 1)!} = 2^l \left( \frac{l^d - 1}{d - 1}! \right) + O(2^l l^{-2}). \]  

\[(15)\]

**B. Algorithms**

We first introduce how to compute \( R^{-1} \), with \( R \) the Cholesky decomposition of \( \mathbf{k}(\mathbf{x}_i^r, \mathbf{x}_i^r) \), \( \mathbf{k} \) is a one-dimensional Markov kernel and \( \mathbf{x}_i^r \) is a one-dimensional sorted level-1 dyadic point set. To present the algorithm for computing the inverse of Cholesky decomposition, we also label the entries on matrices by points in \( \mathbf{x}_i^r \). For example, \( [R^{-1}]_{x_i^r} \) represents the entry with row index corresponding to point \( x \in \mathbf{x}_i^r \) and column index corresponding to point \( x' \in \mathbf{x}_i^r \).

**Algorithm 1:** Computing \( R^{-1} \) for Markov kernel \( k \) and point set \( \mathbf{x}_i^r \).

**Input:** Markov kernel \( k \), level-1 dyadic points \( \mathbf{x}_i^r \)

**Output:** \( R^{-1} \)

1. Initialize \( R^{-1} \leftarrow \mathbf{0} \in \mathbb{R}^{(2^l-1) \times (2^l-1)} \), \( \mathbf{N} = (-\infty, \infty) \), define \( k(\pm \infty, \pm \infty) = 0 \), \( \forall x \)
2. for \( l \leftarrow 1 \) to \( l \) do
3. for \( i \in p(l) \) do
   4. search the closest left neighbor \( x_{\text{left}} \) and right neighbor \( x_{\text{right}} \) of \( x_{2i} \) in \( \mathbf{N} \)
5. Solve \( c_1, c_2, c_3 \) for the following system:
   \[
   \begin{align*}
   c_1 k(x_{\text{left}}, x_{\text{left}}) + c_2 k(x_{\text{left}}, x_{\text{right}}) + c_3 k(x_{\text{right}}, x_{\text{left}}) &= 0, \\
   c_1 k(x_{\text{left}}, x_{\text{right}}) + c_2 k(x_{\text{right}}, x_{\text{right}}) + c_3 k(x_{\text{right}}, x_{\text{left}}) &= 0, \\
   E \left[ c_1 \mathcal{G}(x_{\text{left}}) + c_2 \mathcal{G}(x_{\text{right}}) + c_3 \mathcal{G}(x_{\text{right}}) \right] &= 1 
   \end{align*}
   \]

\[(17)\]

6. if \( x_{\text{left}} \neq -\infty \), \( [R^{-1}]_{x_{\text{left}}, x_{\text{left}}} = c_1 \)
7. if \( x_{\text{right}} \neq \infty \), \( [R^{-1}]_{x_{\text{right}}, x_{\text{right}}} = c_3 \)
8. Let \( [R^{-1}]_{x_{\text{left}}, x_{\text{right}}} = c_2, x_{2i} \rightarrow \mathbf{N} \)
9. enddo
10. enddo
11. Return \( R^{-1} \)

Now let \( k = \prod_{i=1}^{d} k_i \) be a \( d \)-dimensional TMK and \( \mathbf{x}_i^r = \times_{i=1}^d \mathbf{x}_i^r \) be a sorted FG. Then, \( R_0^{-1} \), with \( R_0 \) the Cholesky decomposition of \( k(\mathbf{x}_i^r, \mathbf{x}_i^r) \) can be directly calculated as

\[ R_1^{-1} = \bigotimes_{i=1}^d R_i^{-1}, \]  

\[(16)\]

where \( \otimes \) denotes the Kronecker product between matrices and \( R_i^{-1} \) is the inverse Cholesky decomposition yielded by **Algorithm 1** with input \( k_i \) and \( \mathbf{x}_i^r \).

Let \( R_{\mathbf{x}_i^r \mathbf{x}_i^r} \) represent a sub-matrix of \( R \) consisting of entries \( R_{\mathbf{x}_i^r \mathbf{x}_i^r} \in \mathbf{x}_i^r \subset \mathbf{X}_i^G \). Now we can present the algorithm of constructing \( R_i^{-1} \).

**Algorithm 2:** Computing \( R_i^{-1} \) for TMK \( k \) and level-1 SG \( \mathbf{X}_i^G \)

**Input:** TMK \( k \), level-1 SG \( \mathbf{X}_i^G \)

**Output:** \( R_i^{-1} \)

1. Initialize \( R^{-1} \leftarrow \mathbf{0} \in \mathbb{R}^{m_i \times m_i} \)
2. for all \( i \in \mathbb{N} \) with \( 1 \leq |i| \leq l + d - 1 \) do
3. Compute \( R_i^{-1} \) associated to \( (k, \mathbf{x}_i^r) \) via **Algorithm 1** and (16)
4. Update \( R_i^{-1} \) via
   \[ [R_i^{-1}]_{\mathbf{x}_i^r \mathbf{x}_i^r} \leftarrow [R_i^{-1}]_{\mathbf{x}_i^r \mathbf{x}_i^r} + (-1)^{(l+d-1-|i|)} \left( \frac{d - 1}{l + d - 1 - |i|} \right) [R_{i+1}^{-1}]_{\mathbf{x}_i^r \mathbf{x}_i^r} \]

\[(18)\]

5. enddo
6. Return \( R_i^{-1} \)

We will prove the correctness of **Algorithm 1** and **Algorithm 2** in the supplementary material.