Multilevel Bayesian Deep Neural Networks

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Abstract

In this article we consider Bayesian inference associated to deep neural networks (DNNs) and in particular, trace-class neural network (TNN) priors [52] which can be preferable to traditional DNNs as (a) they are identifiable and (b) they possess desirable convergence properties. TNN priors are defined on functions with infinitely many hidden units, and have strongly convergent Karhunen-Loeve-type approximations with finitely many hidden units. A practical hurdle is that the Bayesian solution is computationally demanding, requiring simulation methods, so approaches to drive down the complexity are needed. In this paper, we leverage the strong convergence of TNN in order to apply Multilevel Monte Carlo (MLMC) to these models. In particular, an MLMC method that was introduced in [5] is used to approximate posterior expectations of Bayesian TNN models with optimal computational complexity, and this is mathematically proved. The results are verified with several numerical experiments on model problems arising in machine learning, including regression, classification, and reinforcement learning.

Keywords: Deep Neural Networks, Multilevel Monte Carlo, Sequential Monte Carlo, Trace-Class, Reinforcement Learning

AMS subject classifications: 62M20, 62M45, 62F15, 93E35

1 Introduction

Deep neural networks (DNNs) [27] are a popular and powerful parametric model class which can be used for solving a variety of machine learning problems. These architectures are very much applicable to a wide array of disciplines and applications, where a major advantage of DNNs is that one attains the universal approximation theorem, which in brief states that the NN can approximate a wide class of target functions [33]. For this work our interest in DNNs are w.r.t. generating random processes. There has been extensive work on connecting DNN with Gaussian and non-Gaussian processes [2, 39, 44, 46]. Deep Gaussian and α-stable process priors for fully Bayesian edge-preserving inversion have been employed in the context of inverse problems in [14, 15], but these studies have typically been limited to low input dimensionality due to the debilitating computational complexity. Sell et al. introduce trace-class DNN (TNN) priors [52], which are non-stationary, non-Gaussian, and well-defined in the infinite-width limit, yet scale well with input dimension. For example, they have been successfully applied to problems with up to \( n = 17 \) dimensions. Fitting such model often require Monte Carlo (MC) methods. Monte Carlo methods are well-known class of methods aimed to solve stochastic computation problems. Such developments have been primarily in the fields of computational physics, statistics and numerical analysis. In particular one methodology which improves on vanilla MC is multilevel Monte Carlo (MLMC). MLMC aims to reduce the computational cost, and complexity, to attain a particular order of mean square error (MSE), i.e. \( O(\varepsilon^2) \) for \( \varepsilon > 0 \). First introduced in [22, 23, 30] and primarily applied to diffusion processes in mathematical finance, it has seen since since various extensions to other fields. Related to this work, it has been applied to MC methods within computational statistics which includes sequential Monte Carlo (SMC), Markov Chain Monte Carlo (MCMC) [4, 5, 31, 36, 37] and other related methods, based on sampling from a distribution of interest. However in terms of the application of MLMC to machine learning, there has been limited work on this. Notable works along this direction include the improvement of complexity in gradient estimators within variational inference [20, 53], and improved complexity for
data-driven surrogate modelling of high-dimensional PDE and SDE models \cite{16, 24, 41}. However as of yet this has not been exploited for the use of statistical inference problems in machine learning. In this paper our focus is on fully Bayesian inference with DNNs for machine learning problems, through the aid and use of Monte Carlo simulation methods. We will provide a new methodology, multilevel Bayesian deep neural networks, which combines TNN prior models with an advanced multilevel sequential Monte Carlo (MLSMC) algorithm \cite{5}. This methodology combines the advantages of the TNN model in terms of scalability and flexibility, with the efficiency of MLSMC to achieve the canonical computational complexity of $1/\text{MSE}$. For problems of this form, where MC is used to simulate from an approximate distribution, such complexity can only be attained in a MLMC framework, and it is impossible to do better.

1.1 Contributions
Our contributions of this work are summarized through the following points.

- We show how to use MLMC in the context of Bayesian inference for deep neural networks. The specific method we use is MLSMC samplers. Our motivation is to reduce the computational complexity, where we show it is possible to attain the canonical rate of convergence \( \text{Cost} = \frac{1}{\text{MSE}} \).

- We prove two key results within our work. First, we are able to derive strong rates of convergence for TNN priors in a multilevel setting. Secondly, we establish a bound on the MSE, which can be decomposed into a variance and bias term. By leveraging these two results, we establish that our method converges to the true underlying posterior with the canonical rate.

- Various numerical experiments are presented to verify the theoretical findings discussed above. This is related to both demonstrating that the strong convergence rate is attained, and also that the MLSMC sampler with TNN priors can reduce the cost to attain a particular order of MSE. The experiments are conducted on machine learning examples including regression, classification and reinforcement learning.

1.2 Outline
The outline of this article is structured as follows. In Section 2 we present preliminary material related to both the model problem and multilevel Monte Carlo. This leads onto Section 3 where we present our numerical algorithm coupled with our main mathematical result, which is a bound on the MSE establishing convergence of our method. We then discuss and introduce our multilevel trace-class priors in Section 4 where we demonstrate they attain the canonical rate of convergence, with numerical verification. In Section 5 our numerical results are presented on a range of machine learning tasks, verifying the improved gains on computational cost using the MLSMC sampler, combined with TNN priors. Finally we conclude, and remark on future directions, in Section 6. The proof of our main theorem is deferred to the Appendix.

2 Model Formulation
In this section we provide a preliminary background on the setting, and formulation of the model problem. This will include an initial discussion on our setup, which will discuss neural networks and how they related to Bayesian modeling, as well as introducing the key concepts of multilevel Monte Carlo.

Suppose we have data \( D = \{(x_1, y_1), \ldots, (x_N, y_N)\} \), \( N \in \mathbb{N}, \) where, for \( i \in \{1, \ldots, N\} \), \( x_i \in \mathcal{X} \) and \( y_i \in \mathcal{Y}. \) The objective is to infer a predictive model \( f : \mathcal{X} \rightarrow \mathcal{Y} \) based on the data. One way to do this is with a parametric model of the form \( f : \mathcal{X} \times \Theta \rightarrow \mathcal{Y} \), with \( \Theta \subseteq \mathbb{R}^{d_{\theta}}. \) It is assumed that \( x_{1:N} \) are deterministic.

Suppose further that \( \mathcal{Y} = \mathbb{R}^m, \) then we will assume that for \( i \in \{1, \ldots, N\} \)

\begin{equation}
    y_i = f(x_i, \theta) + \epsilon_i, \quad \epsilon_i \overset{\text{ind}}{\sim} \mathcal{N}(0, \Sigma_i),
\end{equation}

(2.1)
where ind denotes independence across the indices \( i \in \{1, \ldots, N\} \) and \( \mathcal{N}_m(\mu, \Sigma) \) denotes the \( m \)-dimensional Gaussian distribution with mean \( \mu \) and covariance matrix \( \Sigma \). From this we have \( y_i|\theta \sim (f(x_i, \theta), \Sigma_i) \).

Now consider the case that \( \mathcal{Y} = \{1, \ldots, m\} \), for some \( m \in \mathbb{N} \). Let \( f : X \times \Theta \to \mathbb{R}^m \), with \( f(x, \theta) = (f_1(x, \theta), \ldots, f_m(x, \theta)) \), and we define the so-called softmax function as

\[
  h_k(x, \theta) := \frac{\exp(f_k(x, \theta))}{\sum_{j=1}^K \exp(f_j(x, \theta))}, \quad k \in \mathcal{Y},
\]

(2.2)

We will assume that \( y_i \sim h(x_i, \theta) \), independently for \( i \in \{1, \ldots, N\} \), where \( h(x, \theta) = (h_1(x, \theta), \ldots, h_m(x, \theta)) \) denotes a categorical distribution on \( m \) outcomes, given input \( x \).

A popular parametric model is deep neural networks (DNN) [27]. In this scenario, affine functions are composed with simple element-wise activation functions \( \sigma : \mathbb{R} \to \mathbb{R} \). For \( z \in \mathbb{R}^n \), including the limit \( n \to \infty \), we define \( \sigma(z) := (\sigma(z_1), \ldots, \sigma(z_k))^\top \). An example is \( \nu(z) = \max\{0, z\} \) for \( z \in \mathbb{R}_+ \), the so-called ReLU activation. Let \( X = \mathbb{R}^n \) and \( \mathcal{Y} = \mathbb{R}^m \). The DNN itself can be defined in the following way. Let \( D \in \mathbb{N}, (n_0, \ldots, n_D) \in \mathbb{N}^{D+1} \) be given, with the constraint that \( n_0 = n \) for the input layer and \( n_D = m \) for the output layer. Now for weights \( A_d \in \mathbb{R}^{n_d \times n_{d-1}} \) and biases \( b_d \in \mathbb{R}^{n_d} \), \( d \in \{1, \ldots, D\} \) also given, we use the notation \( \theta := ((A_1, b_1), \ldots, (A_D, b_D)) \) and so \( \theta \in \Theta = \bigotimes_{d=1}^D \{ \mathbb{R}^{n_d \times n_{d-1}} \times \mathbb{R}^{n_d} \} \). Now set

\[
  g_0(x, \theta) := A_1x + b_1, \\
  g_d(x, \theta) := A_d\sigma_{n_{d-1}}(g_{d-1}(x)) + b_d, \quad d \in \{1, \ldots, D-1\}, \\
  f(x, \theta) := A_D\sigma_{n_{D-1}}(g_{D-1}(x)) + b_D,
\]

(2.3)

where \( f(x, \theta) \) is the output of the final layer of the DNN. For any given \( f(x, \theta) \) and parameter space \( \Theta \) one can place a prior \( \pi \) on \( \Theta \). Given the structure in (2.1) one then has a posterior

\[
  \pi(\theta|y_{1:N}) \propto p(y_{1:N}|\theta)\pi(\theta),
\]

(2.4)

assuming it is well-defined. The likelihood function, in the case (2.1) is exactly

\[
  p(y_{1:N}|\theta) = \prod_{i=1}^N \phi_m(y_i; f(x_i, \theta), \Sigma_i),
\]

(2.5)

where \( \phi_m(y; \mu, \Sigma) \) is the \( m \)-dimensional Gaussian density of mean \( \mu \), covariance \( \Sigma \) evaluated at \( y \) given. In the case of classification, the likelihood function associated to (2.2) is exactly

\[
  p(y_{1:N}|\theta) = \prod_{i=1}^N \prod_{k=1}^m h_k(x_i, \theta)^{[y_i=k]}.
\]

(2.6)

### 2.1 Multilevel Bayesian Neural Networks

We shall begin with a short review of MLMC. Let us assume that we are given a probability density \( \Psi \), on a state-space \( U \) and it is of interest to compute expectations of \( \Psi - \)integrable functions, \( \varphi : U \to \mathbb{R} \):

\[
  \Psi(\varphi) := \int_U \varphi(u)\Psi(u)\,du \text{ with } du \text{ a dominating } \sigma - \text{finite measure (often Lebesgue).}
\]

Now, we assume that working with \( \Psi \) is not computationally feasible (e.g. has an infinite computational cost) but there exist a scalar parameter \( l \in \mathbb{N} \) which parameterises an approximation \( \Psi_l \) of \( \Psi \), where \( \Psi_l \) a density on a state-space \( U_l \subseteq U \) such that:

1. For any \( \varphi : U \to \mathbb{R} \) that is both \( \Psi_l \) and \( \Psi - \)integrable we have \( \lim_{l \to \infty} \Psi_l(\varphi) = \Psi(\varphi) \), where
   \[
   \Psi_l(\varphi) = \int_{U_l} \varphi(u)\Psi_l(u)\,du.
   \]
2. The cost of computing with \( \Psi_l \) is increasing in \( l \).
Let \( L \in \{2, 3, \ldots \} \) be given, we have the telescoping sum identity

\[
\Psi_L(\varphi) = \Psi_1(\varphi) + \sum_{i=2}^{L} [\Psi_i \Psi_{i-1}](\varphi),
\]

(2.7)

with \( [\Psi_i \Psi_{i-1}](\varphi) = \Psi_i(\varphi) - \Psi_{i-1}(\varphi) \). The idea behind MLMC is to try and approximate the R.H.S. of (2.7) in such a way as to reduce the cost of a particular order of mean square error (MSE) versus approximating the L.H.S. of (2.7). The way in which this is achieved is to construct couplings of \( (\Psi_1, \Psi_{i-1}) \), \( l \in \{2, \ldots, L \} \), that is, joint densities \( \Psi_l \), on \( U_1 \times U_{l-1} \) such that \( \int_{U_1} \Psi_l(u_l, u_{l-1})du_l = \Psi_{l-1}(u_{l-1}) \) and \( \int_{U_{l-1}} \Psi_l(u_l, u_{l-1})du_{l-1} = \Psi_l(u_l) \).

Then, we have the approximation

\[
\Psi^M_L(\varphi) := \frac{1}{P_1} \sum_{i=1}^{P_1} \varphi(U_1^i) + \sum_{l=2}^{L} \frac{1}{P_l} \sum_{i=1}^{P_l} (\varphi(U_1^i) - \varphi(U_{l-1}^i)),
\]

(2.8)

Now, alternatively, one can use i.i.d. samples \( U_1^1, \ldots, U_1^P \) from \( \Psi_1 \) to approximate \( \Psi_L(\varphi) \):

\[
\Psi^{ID}_L(\varphi) := \frac{1}{P} \sum_{i=1}^{P} \varphi(U_1^i),
\]

(2.9)

In either scenario one would have a standard, variance (assuming it exists) plus square bias decomposition of the MSE; e.g. for the MLMC estimator:

\[
\mathbb{E}[(\Psi^M_L(\varphi) - \Psi(\varphi))^2] = \mathbb{Var}[\Psi^M_L(\varphi)] + [\Psi_L - \Psi](\varphi)^2,
\]

(2.10)

with \( \mathbb{Var} \) representing the variance operator. The bias is of course the same for both estimators (2.8) and (2.9) and so, if there is to be an advantage for using (2.8) under an MSE criterion, it would be via the variance. The variance of (2.8) is

\[
\mathbb{Var}[\Psi^M_L(\varphi)] = \frac{\mathbb{Var}[\varphi(U_1^1)]}{P_1} + \sum_{l=2}^{L} \frac{\mathbb{Var}[\varphi(U_1^i) - \varphi(U_{l-1}^i)]}{P_l},
\]

whereas for (2.9)

\[
\mathbb{Var}[\Psi^{ID}_L(\varphi)] = \frac{\mathbb{Var}[\varphi(U_1^1)]}{P}.
\]

Now, if the couplings \( \Psi_l \) are constructed so that \( \mathbb{Var}[\varphi(U_1^i) - \varphi(U_{l-1}^i)] \) falls sufficiently quickly with \( l \) then it can be possible to achieve an MSE (as in (2.10)) for the estimator (2.8) which is of the same order as (2.9) except for a cost that is lower. This is characterized in the following result. Below \( \text{Cost}(\Psi_l) \) is the cost of one sample from \( \Psi_l \).

**Theorem 2.1** (Giles [22]). Suppose that there exists constants \( (\alpha, \beta, \gamma) \in \mathbb{R}^3_+ \) with \( \alpha \geq \frac{\min(\beta, \gamma)}{2} \) such that

(i) \( |\Psi_l(\varphi) - \Psi(\varphi)| = O(2^{-\alpha l}) \).

(ii) \( \mathbb{Var}[\varphi(U_1^i) - \varphi(U_{l-1}^i)] = O(2^{-\beta l}) \).
(iii) $\text{Cost}(\Psi_l) = \mathcal{O}(2^{nl})$.

Then for any $\varepsilon < 1$ and $L := \lceil \log(1/\varepsilon) \rceil$, there exists $(P_1, \ldots, P_L) \in \mathbb{N}^L$ such that

$$\text{MSE} = \mathbb{E}[(\Psi_{ML}^L(\varphi) - \Psi(\varphi))^2] = \mathcal{O}(\varepsilon^2),$$

and

$$\text{Cost}(\text{MLMC}) := \sum_{l=0}^{L} P_l C_l = \begin{cases} \mathcal{O}(\varepsilon^{-2}), & \text{if } \beta > \gamma, \\ \mathcal{O}(\varepsilon^{-2}(\log \varepsilon)^2), & \text{if } \beta = \gamma, \\ \mathcal{O}(\varepsilon^{-2} - \frac{(\gamma - \beta)}{\alpha}), & \text{if } \beta < \gamma, \end{cases}$$

(2.11)

where $C_l$ is the cost for one sample of $\varphi(U_l^i) - \varphi(U_{l-1}^i)$.

We remark that the cost in (2.11) can be lower than that of using the estimator (2.9), depending upon the parameters $(\alpha, \beta, \gamma)$, and simultaneously, the estimator (2.11) having an MSE of $\mathcal{O}(\varepsilon^2)$. The case of $\beta > \gamma$ is referred to as the optimal, or canonical, rate of convergence, i.e. $\mathcal{O}(\varepsilon^{-2})$, in other words this is the best rate that one can obtain. In the original work of Giles [22] the methodology of MLMC was motivated and applied to diffusion processes with applications in financial mathematics. In [22], $\beta \in \mathbb{R}$ relates to the strong rate of convergence, and $\alpha \in \mathbb{R}$ the weak rate of convergence. In our context, as we do not work with diffusion processes, not only is strong and weak convergence not required, i.i.d. sampling of couplings is not achievable in our context (to be defined below) and thus an alternative methodology to reducing the variance of the higher level $l$ differences are required.

### 2.1.1 Multilevel Neural Networks

We now consider the question of choosing the dimension of $\theta$, in particular $n_d$ for $d \in \{1, \ldots, D - 1\}$ (since $n_0$ and $n_D$ are fixed to the input and output dimensions). For simplicity, here we assume $D$ is fixed and the NN width is the same for all layers other than the input or the output, i.e. $n_d = n_d'$ for $d, d' \in \{1, \ldots, D - 1\}$, but dependent upon some resolution parameter $l \in \mathbb{N}$. We can now re-define $n_l = 2^l$, noting that $n_0 = n$ and $n_D = m$, so those variables are no longer needed. We will denote the corresponding vector of parameters by $\theta_l := ((A_{1,l}, b_{1,l}), \ldots, (A_{D,l}, b_{D,l}))$, with prior $\pi_l(\theta_l)$, and the parameter space is $\Theta_l = \{R^{n_l \times n} \times R^{m_l}\} \otimes \{R^{n_l \times n} \times R^{m_l}\} \otimes \{R^{m \times n_l} \times R^m\}$, thus $\theta_l \in \Theta_l$. The NN’s output function $f(x, \theta_l)$ (see (2.3)) for resolution $l$ is denoted by $f_l(x, \theta_l)$, the likelihood by $p_l(y_{1:N} | \theta_l)$, and the posterior distribution by

$$\pi_l(\theta_l | y_{1:N}) \propto p_l(y_{1:N} | \theta_l)\pi_l(\theta_l),$$

(2.12)

where $p_l(y_{1:N} | \theta_l)$ is the likelihood function using $\theta_l$ parameters as in (2.5), and (2.6) for the second example discussed. We view this posterior (and the corresponding $f_l(x, \theta_l)$) as a finite approximation of the posterior associated to the non-parametric limiting DNN as $l \to \infty$, assuming it exists.

### 3 Algorithm and Main Result

In this section we introduce our methodology related to the Bayesian machine learning tasks, which we numerically test in Section 5. Namely we consider the ML sequential Monte Carlo method, and present it in our given framework. This will lead to the our main mathematical result, which is the convergence of our ML estimator, provided in terms of a bound on the MSE.

We begin this section by firstly presenting our algorithm for approximating functional expectations, with respect to the posterior $\pi$, such as

$$\mathbb{E}_\pi[f(x, \theta)],$$

as well as some mathematical results which justify their implementation. The choice of posterior predictive expectation as a quantity of interest is motivated by the goal of our inference procedure, i.e. to make predictions related to the output of the neural network $f$. The form of our results are such that they extend trivially to objective functions $\varphi \circ f$, for Lipschitz $\varphi$, for example. We note that our results
extend to a whole class of possible test functions beyond the neural network itself. The results will be presented first for the posterior predictive, and then extended as a corollary. Noting that \( \mathbb{E}_\pi[f(x, \theta)] = \mathbb{E}_{\pi L}[f_L(x, \theta_L)] + (\mathbb{E}_\pi[f(x, \theta)] - \mathbb{E}_{\pi L}[f_L(x, \theta_L)]) \), our main objective is to construct a multilevel Monte Carlo estimator:

\[
\mathbb{E}_{\pi L}[f_L(x, \theta_L)] = \sum_{l=2}^L \left\{ \mathbb{E}_{\pi L}[f_L(x, \theta_l)] - \mathbb{E}_{\pi_{l-1}}[f_{l-1}(x, \theta_{l-1})] \right\} + \mathbb{E}_{\pi L}[f_1(x, \theta_1)],
\]

(3.1)

whose variance matches the discretization bias \( \mathbb{E}_\pi[f(x, \theta)] - \mathbb{E}_{\pi L}[f_L(x, \theta_L)] \), by approximating each summand on the R.H.S., as well as \( \mathbb{E}_{\pi L}[f_1(x, \theta_1)] \), using a suitable simulation method. Then we will show that the computational cost for doing so, versus, simply approximating \( \mathbb{E}_{\pi L}[f_L(x, \theta_L)] \) can be lower, when seeking to achieve a pre-specified mean square error.

### 3.1 Algorithm

The approach we construct follows that in [4, 5] and in order to directly apply some of its results, we introduce additional notation. Throughout this exposition \((x, L) \in \mathbb{X} \times \mathbb{N}\) are fixed and given. Define the state-spaces for \( l \in \{2, \ldots, L\} \)

\[
\hat{\Theta}_l := \{\mathbb{R}^{(n_1^{l_1-1}) \times n} \times \mathbb{R}^{n_1^{l_1-1}}\} \otimes \{\mathbb{R}^{(n_1^{l_1-1}) \times n_1^{l_2-1}} \times \mathbb{R}^{n_1^{l_2-1}}\} \times \cdots \times \{\mathbb{R}^{n_1^{L_1-1}}\}
\]

and we set \( \hat{\Theta}_1 = \Theta_1 \); the significance of these spaces will be made clear below. Set \( \theta_i \equiv \hat{\theta}_i \in \Theta_i \) and for \( l \in \{2, \ldots, L\} \)

\[
\theta_l = (\hat{\theta}_1, \ldots, \hat{\theta}_l) \in \Theta_l.
\]

The quantities \((\hat{\theta}_2, \ldots, \hat{\theta}_l)\) will be used to denote the increase in dimension between \( \theta_{l-1} \) and \( \theta_l \) say, which is pivotal to the algorithm that we will present. We will suppress the data \((x_{1:N}, y_{1:N})\) from the notation and set for \( l \in \{1, \ldots, L\} \)

\[
\pi_l(\theta_l) \propto p_l(y_{1:N} | \theta_l) \pi_l(\theta_l) =: \kappa_l(\theta_l).
\]

For any \( l \in \{2, \ldots, L\} \) and \( \theta_{l-1} \in \Theta_{l-1} \), let \( q_l(\cdot | \theta_{l-1}) \) be a positive probability density on \( \hat{\Theta}_l \) and \( q_1(\theta_1) \) a positive probability density on \( \Theta_1 \). Set \( G_1(\theta_1) = \kappa_1(\theta_1) / q_1(\theta_1) \) and for \( l \in \{2, \ldots, L\} \)

\[
G_l(\theta_l) = \frac{\kappa_l(\theta_l)}{\kappa_{l-1}(\theta_{l-1}) q_l(\theta_l | \theta_{l-1})},
\]

define our weights. Let \((K_l)_{l \in \{1, \ldots, L-1\}}\) be a sequence of \((\pi_l)_{l \in \{1, \ldots, L-1\}}\)–invariant Markov kernels and define for \( l \in \{1, \ldots, L-1\} \)

\[
M_l(\theta_l, d\theta_{l+1}) = K_l(\theta_l, d\theta_{l+1}) q_{l+1}(\theta_{l+1} | \theta_l) d\theta_{l+1},
\]

(3.2)

where \( \theta_{l+1} = (\theta_l', \hat{\theta}_{l+1}) \) and \( d\theta_{l} \) is the appropriate dimensional Lebesgue measure. This kernel is invoked in Step 4 of Algorithm 1.

Set \( \eta_l(\theta_l) = q_l(\theta_l) \) and for \( l \in \{2, \ldots, L\} \)

\[
\eta_l(\theta_l) = \pi_{l-1}(\theta_{l-1}) q_l(\theta_l | \theta_{l-1}).
\]

The algorithm to be presented will provide a sample-based approximation of these probability densities and in particular, associated expectations. In other words we will have access to \( P \in \mathbb{N} \) samples \((\theta_1^P, \ldots, \theta_L^P) \in \Theta_L^P\) so that

\[
\eta_l^P(\varphi_l) := \frac{1}{P} \sum_{i=1}^P \varphi_l(\theta_l^P).
\]

(3.3)

will be an almost surely convergent estimator of \( \int_{\Theta_l} \varphi_l(\theta_l) \eta_l(\theta_l) d\theta_l \), where \( \varphi_l : \Theta_l \to \mathbb{R} \) is \( \eta_l \)–integrable. In the subsequent exposition given \((\theta_1^P, \ldots, \theta_L^P) \in \Theta_L^P \) \( \eta_l^P \) will denote the so-called \( P \)–empirical measure.
We stress that the superscript of $\theta_i^j$ is used to denote a simulated sample (the simulation is given in the algorithm to be described) and the subscript relates to the subscript associated to the posterior $\pi_i$.

We are now in a position to define our algorithm which can approximate expectations w.r.t. the sequence of posteriors $(\pi_{1:\ell})_{\ell \in \{1,\ldots,L\}}$ and this is given in Algorithm 1.

**Algorithm 1 Multilevel Sequential Monte Carlo Sampler for Deep Neural Networks.**

1. **Input:** $L \in \mathbb{N}$ the highest resolution and the number of samples at each level $(P_0, \ldots, P_{L-1}) \in \mathbb{N}^L$, with $+\infty > P_1 \geq P_2 \geq \cdots \geq P_L \geq 1$.
2. **Initialize:** For $i \in \{1,\ldots,P_1\}$ independently sample $\theta_i^1$ using $q_1(\theta_1) d\theta_1$. Set $l = 1$. Go to step 3.
3. **Iterate:** If $l = L$ go to step 4. Otherwise for $i \in \{1,\ldots,P_{l+1}\}$ sample $\theta_{l+1} | \theta_l^1, \ldots, \theta_l^{P_l}$ independently using:
   
   $\sum_{j=1}^{P_l} \frac{G_l(\theta_l^j)}{\sum_{s=1}^{P_l} G_l(\theta_l^s)} M_l(\theta_l^j, d\theta_{l+1})$.
   
   Set $l = l + 1$ and go to the start of step 4.
4. **Output:** $(\theta_1^1, \ldots, \theta_1^{P_1}, \ldots, \theta_L^1, \ldots, \theta_L^{P_L})$, from which (3.5) is constructed.

Now, recalling (3.1), our objective is to approximate the difference, for $(x,l) \in X \times \{2,\ldots,L\}$:

$E_{\pi_l}[f_l(x, \theta_l)] - E_{\pi_{l-1}}[f_{l-1}(x, \theta_{l-1})] =: \pi_l(f_l) - \pi_{l-1}(f_{l-1}),$

where $E_{\pi_l}$ denotes expectation w.r.t. $\pi_l$. Now, we have the simple identity

$$E_{\pi_l}[f_l(x, \theta_l)] - E_{\pi_{l-1}}[f_{l-1}(x, \theta_{l-1})] = E_{\pi_{l-1} \otimes q_l} \left[ \frac{\kappa_{l}(\theta_l) Z_{l-1}}{\kappa_{l-1}(\theta_{l-1}) q_l(\theta_l | \theta_{l-1}) Z_l} f_l(x, \theta_l) - f_{l-1}(x, \theta_{l-1}) \right]$$

$$= E_{\pi_{l-1} \otimes q_l} \left[ \frac{Z_{l-1}}{Z_l} G_l(\theta_l) f_l(x, \theta_l) - f_{l-1}(x, \theta_{l-1}) \right],$$

where $E_{\pi_{l-1} \otimes q_l}$ denotes expectation w.r.t. $\pi_{l-1}(\theta_{l-1}) q_l(\theta_l | \theta_{l-1}) = \eta_l$ and for any $l \in \{1,\ldots,L\}$ and $Z_l = \int_{\Theta_l} \kappa_l(\theta_l) d\theta_l$. One can approximate the R.H.S. of (3.4) as

$$\frac{\eta_l^P(G_l f_l)}{\eta_l^P(G_l)} - \eta_l^P(f_{l-1}).$$

The justification of this estimator is informally as follows. $\eta_l^P(f_{l-1})$ will converge in probability (as $P_l \to \infty$) to $\pi_{l-1}(f_{l-1}) = \int_{\Theta_{l-1}} f_{l-1}(x, \theta_{l-1}) \pi_{l-1}(\theta_{l-1}) d\theta_{l-1}$ (see [10]), which justifies the term $\eta_l^P(f_{l-1})$. Then $\eta_l^P(G_l)$ will converge to

$$\int_{\Theta_l} \pi_{l-1}(\theta_{l-1}) q_l(\theta_l | \theta_{l-1}) \frac{\kappa_{l}(\theta_l)}{\kappa_{l-1}(\theta_{l-1}) q_l(\theta_l | \theta_{l-1})} d\theta_l = \frac{1}{Z_{l-1}} \int_{\Theta_l} \kappa_l(\theta_l) d\theta_l = \frac{Z_l}{Z_{l-1}}.$$

Similarly $\eta_l^P(G_l f_l)$ converges to

$$\int_{\Theta_l} \pi_{l-1}(\theta_{l-1}) q_l(\theta_l | \theta_{l-1}) \frac{\kappa_{l}(\theta_l)}{\kappa_{l-1}(\theta_{l-1}) q_l(\theta_l | \theta_{l-1})} f_l(x, \theta_l) d\theta_l.$$
which yields the appropriate identity on the R.H.S. of (3.4). As a result of this exposition, one can use the following approximation of \( \pi_L(f_L) \):

\[
\hat{\pi}_L(f_L) = \sum_{l=2}^{L} \left\{ \frac{\eta_l G_l f_l}{\eta_l G_l} - \frac{\eta_l f_{l-1}}{\eta_l f_{l-1}} \right\} + \frac{\eta_1 G_1 f_1}{\eta_1 G_1}. \tag{3.5}
\]

### 3.2 Mathematical Result

We consider the convergence of (3.5) in the case \( m = 1 \); this latter constraint can easily be removed with only minor changes to the subsequent notations and arguments. The analysis of Algorithm 1 has been considered in [4, 5]. However, there are some nuances that need to be adapted for the context under study. Throughout, we will suppose that for each \( l \in \{2, 3, \ldots\} \) we have chosen \( q_l \) so that for each \( \theta_l \in \Theta_l \)

\[
\pi_l(\theta_l) = \pi_{l-1}(\theta_{l-1}) g_l(\theta_l|\theta_{l-1}). \tag{3.6}
\]

This means that

\[
G_l(\theta_l) = \frac{p_l(y_l|\theta_l)}{p_{l-1}(y_l|\theta_{l-1})}.
\]

This convention is not entirely necessary, but it will facilitate a simplification of the resulting calculations. We discuss this point after stating our assumptions. We will use the following assumptions, which are often used in the analysis of approaches of the type described in Algorithm 1. Below \( \mathcal{B}(\Theta_l) \) is the Borel \( \sigma \)-field associated to \( \Theta_l \). We also consider, as is the case for the DNN model and priors, that the indices associated to \( p_l, \pi_l, f_l, q_l, K_l \) can be indefinitely extended (i.e. beyond \( L \)).

**A1**

1. There exists a \( 0 < C < \overline{C} < +\infty \) such that for any \( x \in X \):

\[
\inf_{l \in \mathbb{N}} \inf_{\theta_l \in \Theta_l} \min\{p_l(y_1|\theta_l), \pi_l(\theta_l)\} \geq C \tag{3.7}
\]

\[
\sup_{l \in \mathbb{N}} \sup_{\theta_l \in \Theta_l} \max\{p_l(y_1|\theta_l), \pi_l(\theta_l), f_l(x, \theta_l)\} \leq \overline{C}. \tag{3.8}
\]

2. There exists a \( \rho \in (0, 1) \) such that for any \( (l, \theta_l, \theta_{l+1}, B) \in \mathbb{N} \times \Theta_l^2 \times \mathcal{B}(\Theta_{l+1}) \):

\[
\int_B M_l(\theta_l, d\theta_{l+1}) \geq \rho \int_{\Theta_{l+1}} M_l(\theta_{l+1}, d\theta_{l+1}).
\]

3. There exists a \( C < \infty \) and \( \beta > 0 \) such that for any \( (l, x) \in \{2, 3, \ldots\} \times X \):

\[
\int_{\Theta_l} (f_l(x, \theta_l) - f_{l-1}(x, \theta_{l-1}))^2 \pi_l(\theta_l)d\theta_l \leq C n_l^{-\beta}.
\]

4. There exists a \( C < \infty \) such that for any \( (l, \theta_l, x) \in \{2, 3, \ldots\} \times \Theta_l \times X \),

\[
|p_l(y_1|\theta_l) - p_{l-1}(y_1|\theta_{l-1})| \leq C |f_l(x, \theta_l) - f_{l-1}(x, \theta_{l-1})|.
\]

5. There exists a \( r \geq 3, C < \infty \), possibly depending on \( r \), such that for \( \beta > 0 \) as in 3. and any \( (l, \theta, x) \in \{2, 3, \ldots\} \times \Theta_{l-1} \times X \):

\[
\left( \int_{\Theta_l} |f_l(x, \theta_l) - f_{l-1}(x, \theta_{l-1})|^r M_{l-1}(\theta, d\theta_l) \right)^{1/r} \leq C n_l^{-\beta/2}.
\]
Admittedly, the minimum bound in (3.7) is not satisfied for most applications but does significantly simplify the proof. An approach similar to [4] can be used to relaxed this assumption. To deal with the general case of $G_l$ (i.e. without the condition (3.6)) one could specify $q_l$ so that (A1) 4. can be modified to: There exists a $C < \infty$ such that for any $(l, \theta_l, x) \in \{2, 3, \ldots \} \times \Theta_l \times X$,

$$|p_l(y_{l1:N}|\theta_l)\pi_l(\theta_l) - p_{l-1}(y_{l1:N}|\theta_{l-1})\pi_{l-1}(\theta_{l-1})q_{l}(\theta_l|\theta_{l-1})| \leq C|f_l(x, \theta_l) - f_{l-1}(x, \theta_{l-1})|.$$  

Such a specification may require considerable work, but essentially the point is that one must be able to sufficiently control $|G_l(\theta_l) - 1|$. This is what the combination of (3.6) and (A1) 4. allow us to do with the current proof. We then have the following result, whose proof is in Supplementary material A.

**Proposition 3.1.** Assume (A1). Then there exists a $C < \infty$ and $\zeta \in (0, 1)$ such that for any $L \in \{2, 3, \ldots \}$

$$\mathbb{E}[(\tilde{\pi}_L(f_L) - \pi_L(f_L))^2] \leq C \left( \frac{1}{P_1} + \sum_{i=2}^{L} \frac{1}{P_i n_i^\beta} + \sum_{i=2}^{L-1} \sum_{q=i+1}^{L} \frac{1}{(n_i n_q)^{\beta/2}} \left( \frac{\zeta^{q-1}}{P_i} + \frac{1}{P_l^{1/2} P_q} \right) \right).$$

Connecting to the discussion of Section 2.1 if $\beta$ is large enough (we have $\beta = 3$ later, which is large enough) then as $\zeta = 1$ one can choose $P_1, \ldots, P_L$ to achieve a MSE of $O(\varepsilon^2)$ for the optimal cost of $O(\varepsilon^{-2})$.

### 4 Trace class priors

In this section we briefly discuss our trace class priors, which we aim to analyze and motivate for numerical experiments later within the manuscript. We will begin with a formal definition, before providing a result related to convergence of the predictive model $f$. Given the rate obtained, we will then verify this rate through the demonstration of a simple numerical experiment.

The neural network priors we consider are the trace class neural networks, first proposed by Sell et al. [52]. These priors were introduced to mimic Gaussian priors $\pi_0 \sim \mathcal{N}(0, C)$, for function-space inverse problems, where a common way to simulate Gaussian random fields is to use the Karhunen-Loève expansion

$$f = \sum_{j \in \mathbb{Z}^+} \sqrt{\lambda_j} \psi_j, \quad \psi_j \sim \mathcal{N}(0, 1),$$

(4.1)

where $(\lambda_j, \psi_j)_{j \in \mathbb{Z}^+}$ are the associated eigenbasis of the covariance operator $C$, and $\{\psi_j\}_{j \in \mathbb{Z}^+}$ is Gaussian white noise. For a detail description of the derivation of (4.1) and its application to stochastic numerical problems, we refer the reader to [48]. An issue that can arise with using (4.1) is that using such priors do not scale well with high-dimensional problems. This acts as the initial motivation for trace-class neural network (TNN) priors, where the work of Sell et al. [52] provided a justification for such priors. Specifically if one considers an infinite width network $n_l = \infty$, then the variances can be summarized in a diagonal covariance operator $C$. Such a result is presented as [Theorem 1., [52]]. If we consider the TNN prior for $\theta_l := ((A_{l1}^1, b_{l1}^1), \ldots, (A_{lD}^l, b_{lD}^l))$, then for $d = 1, \ldots, D$, the associated weights and bias are defined as

$$A_{lj,d}^i \sim \mathcal{N}(0, (ij)^{-\alpha}), \quad b_{ld}^i \sim \mathcal{N}(0, i^{-\alpha}),$$

(4.2)

where at level $l$ a coupling can be constructed by letting $A_{lj,d}^i = A_{lj,d}^{l-1}$ and $b_{ld}^i = b_{ld}^{l-1}$ for $i, j \in \{1, \ldots, n_l-1\}$ and $d \in \{2, D-1\}$; a similar assignment between layers $l$ and $l-1$ is to be adopted for $(A_{lj,d}^i, b_{ld}^i)$ and $(A_{lj,d}^{l-1}, b_{ld}^{l-1})$. The notation $A_i, b_i$, for $i = 1, \ldots, D$, and $\theta$, will be used to denote the limits $\lim_{n_l \to \infty} A_{lj,d}^i, b_{ld}^i, \theta^i$.

The limiting TNN prior uses (2.3) in place of (4.1), with parameters defined in (4.2). The approximation at level $l$, $f_l$, simply replaces all limiting objects with the level $l$ approximations (with width $n_l = 2^l$ for all hidden layers). The tuning parameter $\alpha$ controls how much information one believes concentrates on the first nodes. In the case of $\alpha > 1$, we refer to the prior as trace-class, which results in the term trace-class neural network prior.
As we are concerned with combining such priors to the MLMC sampler, it would be of interest to analyze the convergence of such neural networks which use (4.2). Therefore we provide a result establishing Assumption 3, in terms of the parameters \( l \) and \( \alpha \), which is given through the following proposition.

**Proposition 4.1.** Assume that for all \( z \in \mathbb{R} \), \( \sigma(z) \leq |z| \). Then for \( \alpha > 1/2 \), the priors defined as in (4.2) are trace-class. Furthermore, let \( x \in \mathbf{X} \), and consider the TNN \( f_l(x, \theta_l) \) truncated at \( n_l = 2^l \) terms, for \( l \in \mathbb{N} \), with the limit denoted \( f(x, \theta) = \lim_{l \to \infty} f_l(x, \theta_l) \), as described above. Then there is a \( C(x) < +\infty \) such that

\[
\mathbb{E} \left[ |f_l(x, \theta_l) - f(x, \theta)|^2 \right] \leq C 2^{-(2\alpha - 1)l}.
\]

**Proof.** First assume that \( D = 2 \), i.e. there is a single hidden layer, and \( m = 1 \). Let \( x \in \mathbf{X} \) be fixed, but allow the possibility that \( n \to \infty \), provided that \( \sum_j |x_j|^2 < \infty \) almost surely.

Let \( A_{k,1}^l \) denote the \( k \)-th row of \( A_1^l \), allowing the possibility that \( l \to \infty \) (denoted simply \( A_1 \), as described above), and observe that

\[
\mathbb{E} \left[ A_{k,1}^l x + b_{k,1}^l \right] = 0, \quad \mathbb{E} \left[ (A_{k,1}^l x + b_{k,1}^l)^2 \right] = k^{-\alpha} \left( \sum_{j=1}^n j^{-\alpha} x_j^2 + 1 \right) \leq k^{-\alpha} (|x|^2 + 1),
\]

where \( |x|^2 := \sum_{j=1}^n x_j^2 \).

Let \( A_{k,2}^l \) denote the \( k \)-th entry of the vector \( A_2^l \in \mathbb{R}^n \), again allowing \( l \to \infty \) (and denote the limit by \( A_2 \)). Using the shorthand notation \( \xi_{k,1}^l = A_{k,1}^l x + b_{k,1}^l \) (and \( \xi_{k,1} = A_{k,1} x + b_{k,1} \)), we are concerned with

\[
\mathbb{E} \left[ f^2(x, \theta) \right] = \sum_{k=1}^\infty \mathbb{E} \left[ A_{k,2}^l \right]^2 \mathbb{E} \left[ \sigma(\xi_{k,1}^l)^2 \right] + \mathbb{E} \left[ b_2 \right]^2 \leq \sum_{k=1}^\infty \mathbb{E} \left[ A_{k,2}^l \right]^2 \mathbb{E} \left[ \xi_{k,1}^l \right]^2 + 1 \leq C \sum_{k=1}^\infty k^{-2\alpha} + 1.
\]

This shows that the output has finite second moment for \( \alpha > 1/2 \). Furthermore, a simple extension of the above calculation shows that the rate of convergence is given by

\[
\mathbb{E} \left[ |f_l(x, \theta_l) - f(x, \theta)|^2 \right] \leq C \sum_{k \geq 2^l} k^{-2\alpha} \leq C 2^{-(2\alpha - 1)l}.
\]

Now, regarding multiple levels, we can proceed by induction. Assume we have (4.5) at level \( d \), with \( \xi_{d,i}^l \in \mathbb{R}^{n_i} \) denoting the output at level \( d \) (e.g. \( \xi_{i,2}^l \) replaces \( f \) in (4.5), for \( i = 1, \ldots \)). As above, let \( A_{k,d+1}^l \) denote the \( k \)-th row of the matrix \( A_{d+1}^l \). Then, by iterating expectations, we have a \( C < +\infty \) such that

\[
\mathbb{E} \left[ (A_{k,d+1}^l \xi_{d+1}^l + b_{k,d+1}^l)^2 \right] \leq C k^{-\alpha},
\]

as in (4.4). This brings us back to (4.5) at level \( d + 1 \), and we are done for \( D > 2 \).

The extension to finite \( m > 1 \) is trivial by repeating the arguments above. For example, the result (4.6) holds for each of the \( m \) outputs.

The result above establishes Assumption (A1.3) for \( \beta = 2\alpha - 1 \). It also provides (A1.5) for \( r = 2 \) when combined with (A1.1), (A1.2) and the definition (3.2).

**Remark 4.1.** Strong convergence is required to use the MLMC method, and is one attractive property of TNN. Standard NNGP derived as the infinite-width limit of i.i.d. weights with variance proportional to the inverse width do not have this property.
**Corollary 4.1.** Let $\tilde{A}^l, \tilde{b}^l, \tilde{\theta}^l$ denote the embedding of $\theta^l$ into $\Theta$, by setting $\tilde{A}^l, \tilde{b}^l$ to be 0 for rows higher than $n_l$. Then there is a $C > 0$ s.t.

$$
\mathbb{E} \left[ \| (\tilde{A}^l, \tilde{b}^l)_d - (A, b)_d \|^2 \right] \leq C 2^{-(\alpha - 1)l},
$$

for all layers $d \in \{1, \ldots, D\}$, where $\| \cdot \|$ denotes the induced operator norm.

**Remark 4.2.** The corollary above provides an important extension from the posterior predictive, covered in the basic propositions 4.1 and 3.1 to the important and challenging problem of inference over the parameter posterior.

### 4.1 Numerical Result

To verify the rate which was obtained in Proposition 4.1, we provide a simple numerical example which analyzes (4.3), in the context of our trace class priors. For our experiment we consider a setup of $\gamma = 2$ and $\alpha = 2$, implying that our decay rate is $\beta = 2\alpha - 1 = 3$. We test this on both a 2 layer and 3 layer NN, and with a ReLU activation function $\sigma(z) = \max\{z, 0\}$, and $\sigma(z) = \tanh(z)$ activation function. Our experiment is presented in Figures 1 - 2.

We observe that in both figures, as a result of using TNN priors, our decay rate matches that of (4.3), where we obtain the canonical rate of convergence. As a side example, to show that this is not attained with other choices, we compare this other choices of priors. This can be seen from Figure 2, where we notice that the rates are not as expected, implying that they are sub-canonical. Therefore this provides a motivation in using trace class NN priors, coupled with MLMC, which we exploit in the succeeding subsection.

![Figure 1: Increment 2nd moment vs. levels. The decay is $O(2^{-3l})$. Therefore the variance decays faster than $1/$cost, which is the canonical regime. Left: activation function of ReLU($z$) = $\max\{0, z\}$. Right: activation function of $\sigma(z) = \tanh(z)$.

### 5 Numerical Experiments

For this section we provide our main numerical experiments, which is to use our TNN priors on various Bayesian tasks related to machine learning. Specifically we will aim to use these priors with the proposed methodology of Algorithm 1, comparing it to single-level Monte Carlo SMC sampler which use the same priors. We will test this on a range of machine learning tasks, which include regression, classification (spiral and MNIST data set) and reinforcement learning, where we hope to show the benefit of using MLMC, by attaining the canonical rate of convergence.
Figure 2: Increment 2nd moment vs. levels. The decay is $O(2^{-l})$ Therefore the variance decays slower than 1/cost, which is a sub-canonical regime. Left: activation function of ReLU$(z) = \max\{0, z\}$. Right: activation function of $\sigma(z) = \tanh(z)$.

5.1 Regression Problem

Our first numerical experiment will be based on a Bayesian regression problem given in (2.1). Our objective is to identify the posterior distribution on $\theta$ specified in (2.4) with the likelihood specified in (2.5)

$$\pi(\theta|y_{1:N}) \propto p(y_{1:N}|\theta)\pi(\theta), \quad p(y_{1:N}|\theta) = \prod_{i=1}^{N} \phi_{m}(y_i; f(x_i, \theta), \Sigma_i),$$

where $\pi(\theta)$ is the TNN prior (4.2), discussed in Section 4. This can subsequently be used for prediction at a new test data point $x^*$

$$\mathbb{E}[f(x^*, \theta)|y_{1:N}] = \int_{\Theta} f(x^*, \theta)\pi(\theta|y_{1:N})d\theta,$$

as well as for the computation of other posterior predictive quantities such as the variance

$$\text{Var}[f(x^*, \theta)|y_{1:N}] = \int_{\Theta} (f(x^*, \theta) - \mathbb{E}[f(x^*)|y_{1:N}])^2 \pi(\theta|y_{1:N})d\theta.$$ 

For our observational noise we take $\Sigma_i^2 = 0.01^2 I$. We use a TNN prior with a tanh activation function, i.e. $\sigma(z) = \tanh(z)$. As we have no explicit form for our “ground-truth", we run a high-level simulation to attain a posterior, which we take as our reference solution. For this we take $n_1 = 2^l$ where $l = 7$. For this model we specify $N = 200$, and consider $X = \mathbb{R}^{10}$ so the input NN width is $n_0 = 10$, and the data points are generated as normal distributed random variables, i.e. $x_i \in \mathbb{R}^{10} \sim N(2, 0.5)$. Then for each $x_i$, the following model produces $y_i$. To compute the MSE we consider 100 replications, and then take the MSE.

We will compare and apply an SMC sampler and multilevel counterpart, i.e. a MLSMC sampler. The setup of the MLSMC sampler is presented in Algorithm 1. In this first experiment we will apply both these methodologies and observe the error-to-cost rate $\xi$ such that $\text{cost} \propto \text{MSE}^{-\xi}$. Recall the cost can be computed using equation (2.11). We will compare this for different values of $\beta = 2\alpha - 1$. Also recall that the cost (per one sample) is of the order $O(2^{-l})$, with $\gamma = 2$, so as a rule of thumb one should expect the attain a canonical rate of convergence when $\alpha > 1.5$ and $\beta > \gamma$.

Below in Figure 3 we present results of applying both SMC sampler and a MLSMC sampler. As mentioned, further details on the MLSMC sampler can be found in [5]. We conduct our numerical experiment with levels $L \in \{3, 4, \ldots, 7\}$. The first numerical results are presented in Figure 3 which compares values of $\alpha = \{1.7, 1.9, 2, 3\}$. We plot both the SMC sampler and MLSMC sampler where the prior for each method is our TNN prior. Furthermore we also plot the credible sets around the MSE values, given by the thin blue and red curves.
As we can observe from the results, The MLMC methodology shows computational benefits, where for a fixed MSE the cost associated with attaining that order of MSE is smaller than the SMC sampler. We can see that the difference in cost for the lowest MSE is approximately a factor of 10. This indicates that the error-to-cost rates are different, and to verify our theoretical findings we plot the canonical rate in black, which matches that of our proposed methodology.

Figure 3: Regression problem: error vs cost plots for SMC and MLSMC using TNN priors. Top left: \( \alpha = 3 \). Top right: \( \alpha = 2.0 \). Bottom left: \( \alpha = 1.9 \). Bottom right: \( \alpha = 1.7 \). Credible sets are provided in the thin blue and red curves.

5.1.1 Sub-canonical rates

The results thus far are for values of \( \alpha \) which attain the canonical rate. Now let us consider alternative choices of \( \alpha \), which should result in a sub-canonical rate. We now modify the parameter values of \( \alpha \leq 1.5 \). In this case, \( \beta \leq \gamma = 2 \), where the cost of a single simulation of \( f \) is \( O(2^\gamma) \), so sub-canonical convergence is expected. We will consider two choices of \( \alpha \in \{1.1, 1.4\} \), where we keep the experiment and the parameter choices the same. Our results are presented in Figure 4. As expected, the complexity rate is closer to the single level case, but an improvement factor of around 3 is still observed at the resolutions considered.

The results from Figure 4 indicate that if we consider TNN priors of lower regularity, then we can expect to achieve sub-canonical rates, in the complexity related to the MSE-to-cost ratio. This promotes the question, of whether canonical rates, in our setup and framework are possible for non-smooth random fields. This, and related questions, will be considered for future work.
5.2 Spiral Classification Problem

Following the definition of the classification model (2.2), just as we considered the likelihood (2.5) for the regression problem, we consider the likelihood (2.6) for the classification problem. The posterior is again given by (2.4). Again predictions at an input \( x^* \) not part of the data are delivered by the posterior predictive distribution. For example, the marginal posterior class probability \( P(k|x^*, y_{1:N}) \) is given by

\[
P(k|y_{1:N}) = \int_\Theta h_k(x^*, \theta)\pi(\theta|y_{1:N})d\theta,
\]

and the variance associated to a prediction of class \( k \) for input \( x^* \) is given by

\[
\text{Var}[k|y_{1:N}] = \int_\Theta h_k(x^*, \theta)^2\pi(\theta|y_{1:N})d\theta - P(k|y_{1:N})^2.
\]

For our classification problem we are interested in classifying two data sets, where the data is based on a 2D spiral. In other words, the data for class \( k = 1 \) is generated through the following equations, for \( i = 1, \ldots, N = 500 \)

\[
x_{i1} = a \upsilon_i^p \cos(2\upsilon_i^p \pi) + \epsilon_{i1},
\]

\[
x_{i2} = a \upsilon_i^p \sin(2\upsilon_i^p \pi) + \epsilon_{i2},
\]

where \( \upsilon_i, t_i \sim \mathcal{U}[0, 1] \) uniform, \( \epsilon_i \sim \mathcal{N}(0, 0.1^2) \) and the parameter choices are \( a = 16 \) and \( p = 0.05 \). The data associated to class \( k = 2 \) is generated similarly, except with a shift of \( \pi \) in the arguments of the trigonometric functions. This data can be seen in Figure 5, where our two classes correspond to the colors, i.e. data labelled as Class \( k = 1 \) is blue and data labelled as Class \( k = 2 \) is yellow. The setup for the classification problem is similar to the regression problem. Again we conduct experiments for different choices of \( \alpha \), i.e. \( \alpha \in \{1.7, 1.9, 2, 3\} \) and levels \( L \in \{3, 4, \ldots, 7\} \). Our parameter choices are the same as the regression problem. For our reference solution we again use \( n_7 = 2^7 \) with a tanh activation function, for the prior and take a high-resolution solution. We present firstly in Figure 6 the results related to the canonical rates obtained for the MSE-to-cost rates. As we observe, we see a clear distinction in the difference in costs as the MSE is decreased, with again roughly a magnitude of \( \sim O(10^1) \). This again highlights the computationally efficiency of our proposed methodology, with the combination of our TNN prior. For our final experiments for the classification problem, we consider alternative values of \( \alpha \), i.e., \( \alpha \in \{1.1, 1.4\} \), which are presented in Figure 7. Again, similar to the regression problem, we observe that sub-canonical rates are obtained for \( \alpha < 1.5 \), where the difference in cost for the lower value of MSEs is not as significant.
Figure 5: Classification problem: Our data is generated as a 2D spiral with two classes, Class $k = 1$ being in blue and Class $k = 2$ in yellow.

Figure 6: Classification problem: error vs cost plots for SMC and MLSMC, using TNN priors. Top left: $\alpha = 3$. Top right: $\alpha = 2.0$. Bottom left: $\alpha = 1.9$. Bottom right: $\alpha = 1.7$. Credible sets are provided in the thin blue and red curves.

5.3 Binary MNIST Classification

We now turn our attention to a more realistic classification example, which is based on the well-known MNIST dataset. This dataset is relatively high-dimensional dataset which contains handwritten digits
from 0 to 9. Our problem that we consider now is a binary MNIST classification problem, where we are interested in two classes. One class corresponds to a collection of zeros and the other is related to the class of ones. This can be seen in Figure 8. Our methodology and experimental setup remains the same, where we refer the reader to the previous subsection on specific choices on our MLSMC algorithm. The main difference we have now is related to dimensionality and number of samples, where this is chosen now as $d = 784$ and $m = 400$. To overcome this challenging dimensionality issues, we apply principle component analysis (PCA) which reduces the dimension to $d = 100$.

Our numerical experiments are provided in Figure 9 - 10. From analyzing Figure 9 we notice again that there is a clear difference in the MSE-to-cost plots for both methods. Specifically, by exploiting a TNN prior within our MLSMC methodology we attain the canonical rate of convergence. This is consistent amongst all subplots for values of $\alpha = \{1.7, 1.9, 2, 3\}$. Again, if we do not consider the TNN prior, what we observe is an improvement compared to the SMC sampler methodology, however we do not attain the canonical rate. This is observed in Figure 10, where we have $\alpha = \{1.1, 1.4\}$.

Figure 8: Random selection of 0’s and 1’s from the MNIST dataset.

5.4 Reinforcement Learning

5.4.1 Setup

Our final numerical example will consist of an inverse reinforcement learning problem. Unlike the previous two examples, reinforcement learning is not concerned with pattern formations, but instead decision making. Specifically it is used to solve stochastic optimal control problems. Before we continue with the specific example, we first recall some common notation and provide our setup for Bayesian reinforcement learning, which is largely motivated and taken from [52].
Figure 9: MNIST Classification problem: error vs cost plots for SMC and MLSMC, using TNN priors. Top left: $\alpha = 3$. Top right: $\alpha = 2.0$. Bottom left: $\alpha = 1.9$. Bottom right: $\alpha = 1.7$. Credible sets are provided in the thin blue and red curves.

Figure 10: MNIST Classification problem: error vs cost plots for SMC and MLSMC, using TNN priors. Left: $\alpha = 1.4$. Right: $\alpha = 1.1$. Credible sets are provided in the thin blue and red curves.

A Markov decision process is defined by a controlled Markov chain $\{X_t\}_{t\in\mathbb{N}}$, referred to as the state process, the control process $\{A_t\}_{t\in\mathbb{N}}$ and the an optimality criterion. The state process takes values in a bounded set $\mathcal{X} \subset \mathbb{R}^d$. The control process is $\mathcal{A}$-valued with $\mathcal{A} = \{1, \ldots, M\}$. Therefore the state process
propagates by

\[ X_{t+1}|(X_{1:t} = x_{1:t}, A_{1:t} = a_{1:t}) \sim p(\cdot|x_{t}, a_{t}), \]

where for any state-action pair \((x_{t}, a_{t})\), \(p(\cdot|x_{t}, a_{t})\) is a probability density. Now let \(r : \mathcal{X} \to \mathbb{R}\) be the reward function, then the accumulated reward given in a policy and initial state \(X_{1} = x_{1}\) is

\[ C_{\mu}(x_{1}) = \mathbb{E}_{\mu}\left[ \sum_{t=1}^{\infty} \beta^{t} r(X_{t}) | X_{1} = x_{1} \right], \]

where \(\beta \in (0, 1)\) is a discount factor and \(\mu : \mathcal{X} \to \mathbb{R}\) is the policy mapping. A policy \(\mu^{*}\) is optimal if

\[ C_{\mu^{*}}(x_{1}) > C_{\mu}(x_{1}), \]

for all \((\mu, x_{1}) \in \mathcal{X} \times \mathbb{R}\), and can be found by solving Bellman’s fixed point equation [3]. Using this fixed point solution \(v : \mathcal{X} \to \mathbb{R}\), we can derive the optimal policy by

\[ \mu^{*}(x) = \arg \max_{a \in A} \left[ \int_{X} p(x'|x, a)v(x')dx' \right], \quad (5.1) \]

that is, the optimal action at any state is the one that maximizes the expected value function at the next state. It is assumed that the state evolution is deterministic, i.e., there is a map \(T : \mathcal{X} \times A \to \mathcal{X}\) such that

\[ p(x'|x, a) = \delta_{T(x,a)}(x'). \]

Noise is added to model imperfect action selections so that at each time step the chosen action is a random variable given by

\[ A_{t}(x_{t}) = \arg \max_{a \in A} \left[ v(T(x_{t}, a)) + \epsilon_{t}(a) \right], \quad \epsilon_{t} \sim \mathcal{N}(0, \sigma^{2}I). \quad (5.2) \]

Now what remains is to define our likelihood function associated to our example. Our data will consist of a collection of noise corrupted state-action pairs \(\{x_{t}, a_{t}\}_{t=1}^{T}\), and the aim is to infer the value function (5.1) that leads to the actions \(a_{t}\) for the current state \(x_{t}\). Using the noisy action selection process (5.2) we have the likelihood function defined as

\[ \mathcal{L}(a_{1:T}|x_{1:T}, v, \sigma) = \prod_{t=1}^{T} p(a_{t}|x_{t}, v, \sigma) = \prod_{t=1}^{T} p(a_{t}|v_{t}, \sigma), \quad (5.3) \]

where \(v_{t} \in \mathbb{R}^{M}\) is defined by \(v_{t,k} = v(T(x_{t}, a = k))\). Following from (5.2), the factors in (5.3) have a closed form expression

\[ p(a_{t}|v_{t}, \sigma) = \frac{1}{\sigma} \int_{\mathbb{R}} \phi \left( \frac{t - v_{t,a_{t}}}{\sigma} \right) \prod_{i \neq a_{t}}^{M} \Phi \left( \frac{t - v_{t,i}}{\sigma} \right) dt, \]

where \(\phi\) and \(\Phi\) denote the standard normal PDF and CDF, respectively. The derivation can be found in [52].

Figure 11: Plot of HalfCheetah, which has states \(x_{t} \in \mathbb{R}^{17}\). Its goal is to run as quickly as possible, while not moving its body parts more than necessary.
5.4.2 Experiment

For our Bayesian reinforcement learning example, we consider the HalfCheetah example [54], where the goal is for the HalfCheetah to run as fast as possible without moving its body more than necessary. The state space is \( X = \mathbb{R}^{17} \), and the action space is \( A = \{1, \ldots, 8\} \). We also take \( T = 100 \) for the observations, where the data generation is taken similarly to [52], and \( \sigma^2 = 0.01^2 \). As before we aim to show the benefit of MLMC for the SMC sampler, where we choose values \( \alpha = \{1.7, 1.9, 2.3\} \) with levels \( L \in \{3, 4, \ldots, 7\} \).

For our truth we again take a high-resolution solution to our problem, similarly to what was done for the 2D spiral experiment. These values are again chosen such that we can attain the canonical rate of convergence. Our results are presented in Figure 12 which compare both methodologies with TNN priors, for the different values of \( \alpha \). Similarly to our previous results we notice a a bigger difference is cost for lower values of the MSE, which indicate both error-to-cost rates are different. As done for the previous experiments, we plot the canonical rate in black to verify our methodology attains the rate.

Finally our last experiment is to verify that one cannot attain the canonical rate if we assume that \( \alpha < 1.5 \). In Figure 13 we present similar experiments to Figure 12, but with modified values of \( \alpha \in \{1.1, 1.4\} \). We can observe that the results are similar to the previously attained, in the sense that the complexity grows at a faster rate than it does in the canonical case, but still slower than for the single level approach. Again this verifies the theory.

![Figure 12: Reinforcement learning: error vs cost plots for SMC and MLSMC, using TNN priors. Top left: \( \alpha = 3.0 \). Top right: \( \alpha = 2.0 \). Bottom left: \( \alpha = 1.9 \). Bottom right: \( \alpha = 1.7 \). Credible sets are provided in the thin blue and red curves.](image-url)
6 Conclusion

The development of machine learning methodologies is of high relevance now, due to the availability of data and modern advanced algorithms. In this work we considered the application of multilevel Monte Carlo (MLMC) for various Bayesian machine learning problems, where we exploited the use of trace-class neural network priors. These priors had been previously used on a range of Bayesian inference tasks, where now we combined this with the methodology of multilevel sequential Monte Carlo (MLSMC) samplers, which is based on MLMC. In particular we motivated the use of such priors in a multilevel setting, where we were able to firstly prove that one does attain the canonical Monte Carlo rate, unlike others priors based on neural network methodologies, but also providing a bound on mean square error (MSE), using the methodology described above reducing the MSE-to-cost rate. Numerical experiments were conducted on a range of common machine learning problems, which includes regression, classification and reinforcement learning, where we were able to verify the reduction in computational cost to achieve a particular order of MSE.

For future considerations of work, one natural direction is to see if one can extend this work to multi-index Monte Carlo [28], which has shown to gain efficiency over MLMC methods. This requires more, especially related to choosing the optimal set, but can be viewed as a natural extension. Another direction is to consider other applications beyond this work, such as clustering. In a Bayesian context, such popular methods would be the likes of Bayesian hierarchical clustering [26, 35] which is related to mixture models. One could also exploit more advanced Monte Carlo proposal, based on gradient information, which could enhance the performance, such as related to the reinforcement learning example. Such examples could include, Metropolis-Hastings adjusted algorithm, or Hamiltonian Monte Carlo. This examples, and others, will be conducted for future work. As eluded to in the numerical experiments, one could consider alternative ways in which TNN priors, for a wider range of $\alpha \in \mathbb{R}$, could be analyzed where one attains a canonical rate of convergence. Finally it would be of interest to derive a full complexity analysis, for the application of MLMC to deep neural approximations of data-driven models [24, 41]. Deep learning is often applied to unstructured data with very high input dimension, which is extremely computationally intensive and goes well beyond the cases considered here. Indeed [34] leverage 1000s of TPU to apply MCMC to CIFAR-10. Our approach is more efficient, but still not nearly enough to look at such models on a laptop. Our approach is also amenable to parallelization [47], which can help to leverage supercomputers even more effectively. However, for the present work, we do not have access to such resources. It may also be useful to modify the depth of the network at the same time as the width, and find an optimal balance there. This requires further investigation, which requires a careful construction of a modified MLMC scheme.
A Proofs for Proposition 3.1

The proof of Proposition 3.1 essentially follows that of [4, Theorem 3.1], except there are some modifications required. We mainly provide details of these additional calculations, but we remark that to fully understand the proof, one must have read [4]. We recall that \( \eta_l = q_l \) and that for any \( l \in \{2, \ldots, L\} \) one can establish that
\[
\eta_l(d\theta_l) = \frac{\int_{\Theta_1 \times \ldots \times \Theta_{l-1}} \prod_{p=1}^{l-1} G_p(\theta_p) q_1(\theta_1) \prod_{p=1}^{l-1} M_p(u_{p-1}, du_p) d\theta_1}{\int_{\Theta_1 \times \ldots \times \Theta_{l-1}} \prod_{p=1}^{l-1} G_p(\theta_p) q_1(\theta_1) \prod_{p=1}^{l-1} M_p(u_{p-1}, du_p) d\theta_1}.
\]
One can show that for any \( l \in \{1, \ldots, L\} \) and any measurable \( \varphi_l : \Theta_l \to \mathbb{R} \) that is \( \pi_l \)-integrable that
\[
\pi_l(\varphi_l) = \int_{\Theta_l} \varphi_l(\theta_l) \pi_{l+1}(d\theta_{l+1})
\]
for \( l \in \{1, \ldots, L - 1\} \). Note that we need only approximate expectations associated to \( \pi_l, l \in \{1, \ldots, L - 1\} \) using our multilevel identity. From herein \( C \) is a finite constant whose value may change on each appearance, but, does not depend upon \( l \). We will also make use of the \( C_p \) inequality. For two real-valued random variables \( X \) and \( Y \) defined on the same probability space, with expectation operator \( \mathbb{E} \), suppose that for some fixed \( p \in (0, \infty) \), \( \mathbb{E}[|X|^p] \) and \( \mathbb{E}[|Y|^p] \) are finite, then the \( C_p \) inequality is
\[
\mathbb{E}[|X + Y|^p] \leq C_p \left( \mathbb{E}[|X|^p] + \mathbb{E}[|Y|^p] \right), \tag{A.1}
\]
where \( C_p = 1 \), if \( p \in (0, 1) \) and \( C_p = 2^{p-1} \) for \( p \in [1, \infty) \).

**Proof of Proposition 3.1.** For any \( l \in \{2, 3, \ldots, L\} \), we have the decomposition
\[
\eta_l^P(G_l f_l) \left( \frac{\eta_l}{\eta_l(G_l)} \right) - \eta_l^P(f_{l-1}) - \left\{ \eta_l(G_l f_l) \frac{\eta_l(G_l)}{\eta_l(G_l)} - \eta_l(f_{l-1}) \right\} = \sum_{j=1}^{3} T_j^P,
\]
where
\[
T_1^P = -\eta_l^P(G_l f_l) \left[ \eta_l^P - \eta_l \right] \left( \frac{Z_l}{Z_{l-1}} G_l - 1 \right),
\]
\[
T_2^P = \left[ \eta_l^P - \eta_l \right] \left( f_l \left\{ \frac{Z_l}{Z_{l-1}} G_l - 1 \right\} \right),
\]
\[
T_3^P = \left[ \eta_l^P - \eta_l \right] (f_l - f_{l-1}).
\]
As a result, by using the \( C_2 \)-inequality, from (A.1) we can consider
\[
\mathbb{E}[|\bar{\pi}_L(f_L) - \pi_L(f_L)|^2] \leq C \left( \mathbb{E} \left[ \left( \frac{\eta_l^P(G_l f_l)}{\eta_l^P(G_l)} - \eta_l(G_l f_l) \frac{\eta_l(G_l)}{\eta_l(G_l)} \right)^2 \right] + \sum_{j=1}^{3} \mathbb{E}[|\sum_{l=2}^{L} T_j^P|^2] \right). \tag{A.2}
\]
For the first-term on the R.H.S. of (A.2) by standard results (see e.g. [4, Lemma A.3]) we have
\[
\mathbb{E} \left[ \left( \frac{\eta_l^P(G_l f_l)}{\eta_l^P(G_l)} - \eta_l(G_l f_l) \frac{\eta_l(G_l)}{\eta_l(G_l)} \right)^2 \right] \leq \frac{C}{P_1}.
\]
For the summands on the R.H.S. of (A.2) we can apply Remark A.1 to conclude the proof. \( \square \)
To give our technical results, we require some notations. To connect with the appendix in [4], we use the same subscript conventions (i.e., $n, p$ instead of $l$). Let $p \in \mathbb{N}$ then $Q_p(\theta, d\theta') = G_p(\theta) M_p(\theta, d\theta')$ and for $1 \leq p \leq n \in \mathbb{N}$ we set for $\theta_p \in \Theta_p$ and $\varphi : \Theta_n \to \mathbb{R}$ bounded and measurable (write the collection of such functions as $B_b(\Theta_n)$)

$$Q_{p,n}(\varphi)(\theta_p) := \int_{\Theta_{p+1} \times \ldots \times \Theta_n} \varphi(\theta_n) \prod_{q=p}^{n-1} Q_q(\theta_q, d\theta_{q+1}),$$

with $Q_{n,n}$ the identity operator. Then for $(\theta_p, \varphi_n) \in \Theta_p \times B_b(\Theta_n)$ set

$$D_{p,n}(\varphi_n)(\theta_p) = \frac{Q_{p,n}(\varphi_n - \eta_n(\varphi_n))(\theta_p)}{\eta_p(Q_{p,n}(1))},$$

with $D_{n,n}(\varphi_n)(\theta_n) = \varphi_n(\theta_n) - \eta_n(\varphi_n)$. Then we make the definitions, with $\mu$ a probability measure on $\Theta_{p-1}$, $(\varphi_{p}, \varphi_n) \in B_b(\Theta_p) \times B_b(\Theta_n)$, $\Phi_1(\eta_0^p)(\varphi_1) = \int_{\Theta_p} \varphi_1(\theta_1) q_1(\theta_1) d\theta_1$

$$\Phi_p(\mu)(\varphi) = \frac{\mu(G_{p-1} M_{p-1}(\varphi_p))}{\mu(G_{p-1})}, \quad p \geq 2$$

$$V_{p,r}^p(\varphi_p) = \sqrt{P_p(\eta_p^p - \Phi_p(\eta_{p-1}^p))(\varphi_p)},$$

$$R_{p+1}^p(D_{p,n}(\varphi_n)) = \frac{\eta_p^p(D_{p,n}(\varphi_n))}{\eta_p^p(G_p)}(\eta_p - \eta_p^p)(G_p).$$

The following decomposition is then well-known (see [4]) for $\varphi_n \in B_b(\Theta_n)$

$$[\eta_n^p - \eta_n(\varphi_n)](\varphi_n) = \sum_{p=1}^{n} \frac{V_{p,r}^p(D_{p,n}(\varphi_n))}{\sqrt{F_p}} + \sum_{p=1}^{n-1} R_{p+1}^p(D_{p,n}(\varphi_n)).$$

Given the terms in (A.2) it is then necessary to deal with the decomposition above. This has largely been done in the proof of Theorem 3.1. in [4]. However, in order to use the proof there, one must provide an appropriate adaptation of [4, Lemma A.1. (i)-(iii)] and this is the subject of the following result. Below, for a scalar random variable $Z$, we use the notation $\|Z\|_{r} = \mathbb{E}[|Z|^r]^{1/r}$.

**Lemma A.1.** Assume (A1). Then there exists a $C < \infty$, possibly depending upon $r$ in (A1) 5., and $\zeta \in (0, 1)$ such that for any $1 \leq p \leq n$,

$\varphi_n \in \{ f_n - f_{n-1}, \frac{Z_n}{Z_{n-1}} G_n - 1, f_n \left( \frac{Z_n}{Z_{n-1}} G_n - 1 \right) \}$ and $\beta$ as in (A1) 3.,

1. $\sup_{\theta_p \in \Theta_p} |D_{p,n}(\varphi_n)(\theta_p)| \leq C \zeta^{-p} n^{-\beta/2}, \ (1 \leq p < n).$
2. $\|V_{p}(D_{p,n}(\varphi_n))\|_{r} \leq C \zeta^{-p} n^{-\beta/2}, \ (r \text{ as in (A1) 5.}).$
3. $\|R_{p+1}^p(D_{p,n}(\varphi_n))\|_{r} \leq C \zeta^{-p} n^{-\beta/2}, \ (0 \leq p < n, \ r \text{ as in (A1) 5.}).$

**Proof.** Throughout the proof, we only consider the case $\varphi_n = \frac{Z_n}{Z_{n-1}} G_n - 1$. The other cases can be dealt with in a similar manner. We start with 1. and noting that

$$\frac{Z_n}{Z_{n-1}} G_n - 1 = \frac{Z_n}{Z_{n-1}} (G_n - 1) + \frac{Z_n}{Z_{n-1}} - 1.$$  \hspace{1cm} (A.3)

Therefore

$$D_{p,n}(\varphi_n)(\theta_p) = \frac{Z_n}{Z_{n-1}} D_{p,n}(G_n - 1)(\theta_p) \leq C |D_{p,n}(G_n - 1)(\theta_p)|,$$
so we need only work with $D_{p,n}(G_n - 1)(\theta_p)$. Now, we note that
\[
D_{p,n}(G_n - 1)(\theta_p) = \frac{\eta_p(Q_{p,n-1}(1))}{\eta_p(Q_{p,n}(1))} \left\{ D_{p,n-1}(Q_{n-1}(G_n - 1))(\theta_p) - \frac{\eta_{n-1}(G_{n-1}M_{n-1}(G_n - 1))}{\eta_{n-1}(G_{n-1})} D_{p,n-1}(G_{n-1})(\theta_p) \right\}.
\]

Now by using (A1) 1. & 2. we have
\[
\frac{\eta_p(Q_{p,n-1}(1))}{\eta_p(Q_{p,n}(1))} \leq C. \tag{A.4}
\]

In addition
\[
M_{n-1}(G_n - 1)(\theta_{n-1}) = \int_{\Theta_n} \left( \frac{p_n(y_{1:N}|\theta'_n)}{p_n(y_{1:N}|\theta_{n-1})} - 1 \right) M_{n-1}(\theta_{n-1}, d\theta'_n).
\]

Now by using (A1) 1. followed by (A1) 4. and then (A1) 5.
\[
|M_{n-1}(G_n - 1)(\theta_{n-1})| \leq C \int_{\Theta_n} |f_n(x, \theta'_n) - f_{n-1}(x, \theta'_{n-1})| M_{n-1}(\theta_{n-1}, d\theta'_n) \leq C n^{-\beta/2}. \tag{A.5}
\]

Therefore, we have
\[
D_{p,n}(G_n - 1)(\theta_p) = \frac{\eta_p(Q_{p,n-1}(1))}{\eta_p(Q_{p,n}(1))} \left\{ D_{p,n-1} \left( \frac{Q_{n-1}(G_n - 1)}{\|Q_{n-1}(G_n - 1)\|_\infty} \right) (\theta_p) \|Q_{n-1}(G_n - 1)\|_\infty - \frac{\eta_{n-1}(G_{n-1}M_{n-1}(G_n - 1))}{\eta_{n-1}(G_{n-1})} D_{p,n-1}(G_{n-1})(\theta_p) \right\}
\]

where for any $\varphi_p \in B_0(\Theta_p)$, $\|\varphi_p\|_\infty = \sup_{\theta_p \in \Theta_p} |\varphi_p(\theta_p)|$. Application of (A.4) and [4, Lemma A1. (i)] yields
\[
|D_{p,n}(G_n - 1)(\theta_p)| \leq C \zeta^{n-p} (\|Q_n\{G_n - 1\}\|_\infty + \|G_{n-1}\|_\infty).
\]

Then using (A1) 1. and (A.5) yields
\[
\sup_{\theta_p \in \Theta_p} |D_{p,n}(\varphi_n)(\theta_p)| \leq C \zeta^{n-p} n^{-\beta/2}.
\]

For the proof of 2. the case $1 \leq p < n$ follows immediately from 1. and the proof in [4, Lemma A1. (ii)]. So we need only consider $n = p$, which reads
\[
\sqrt{P_n} E[|\eta_n^p - \Phi_n(\eta_n^{p-1})|\varphi_n]|^1/r,
\]

and then using (A.3) we need only consider
\[
\sqrt{P_n} E[|\eta_n^p - \Phi_n(\eta_n^{p-1})|(G_n - 1)|^1/r.
\]

Using the conditional Marcinkiewicz-Zygmund inequality gives the upper-bound
\[
\|V_n(D_{n,n}(\varphi_n))\|_r \leq C E[|G_n(\theta_n^1) - 1|^1/r.
\]

Taking conditional expectations w.r.t. $M_{n-1}$ and using (A.5) yields
\[
\|V_n(D_{n,n}(\varphi_n))\|_r \leq C n_1^{-\beta/2},
\]

which is the desired result.

For the proof of 3. this follows immediately from 1. and the proof in [4, Lemma A1. (iii)].
Remark A.1. Given the results in Lemma A.1, one can follow the proofs of [4, Theorem 3.1.] to deduce that for any $j \in \{1, 2, 3\}$

$$
\mathbb{E}[\left(\sum_{l=2}^{L} T^P_{l,j}\right)^2] \leq C \left( \sum_{l=2}^{L} \frac{1}{P_l n_l^2} + \sum_{2 \leq l_1 < l_2 \leq L} \frac{1}{(n_{l_1} n_{l_2})^{3/2}} \left( \frac{\zeta^{l_1-1}}{P_{l_1}} + \frac{1}{P_{l_1}^{1/2} P_{l_2}} \right) \right),
$$

with the notations as in the statement of Proposition 3.1.

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