Accelerating Monte Carlo Bayesian Inference via Approximating Predictive Uncertainty over Simplex

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Abstract

Estimating the uncertainty of a Bayesian model has been investigated for decades. The model posterior is almost always intractable, such that approximation is necessary. In many real-world cases, even though a decent estimation of the model posterior is obtained, another approximation is required to compute the predictive distribution over the desired output. However, it needs to maintain a large number of samples, evaluate the model repeatedly and average multiple model outputs. In this paper, we propose a method to approximate the probability distribution over the simplex induced by model posterior, enabling tractable computation of the predictive distribution for classification. The aim is to approximate the induced uncertainty of a specific Bayesian model, meanwhile alleviating the heavy workload of MC integration in testing time. Methodologically, we adapt Wasserstein distance to learn the induced conditional distributions, which is novel for Bayesian learning. The proposed method is universally applicable to Bayesian classification models that allow for posterior sampling. Empirical results validate the strong practical performance of our approach.

1 Introduction

Bayesian inference is a principled method to estimate the uncertainty of probabilistic models. In most applications, especially in deep learning, the likelihood model and model prior are not conjugate hence marginalizing over model prior or posterior cannot be performed analytically, which hinders the practical applicability. For tractability, a simple point estimate such as maximum a posteriori (MAP) estimate could be used to approximate the full model posterior. However, the disadvantage is the loss of model uncertainty due to the incomplete characterization of the model posterior. Approximate inference methods, such as Markov chain Monte Carlo and variational inference, enhance the approximate posterior by a better probability distribution while keeping tractability. A set of posterior samples can be drawn by running the chain for a sufficiently long time and the particle distribution is used as an approximate posterior \cite{16, 6, 20}. However, even though a decent estimate of posterior is obtained, the computation load of predictive distribution is heavy.

To introduce the problem, we consider a Bayesian classification problem with a size-$N$ dataset $D = \{(y_n, x_n)\}_{n=1}^N$, where $x_n \in \mathcal{X}$ is the $n$th input and $y_n \in \mathcal{Y}$ is the $n$th output. Let the posterior $p(\theta|D)$ be approximated by particles $q(\theta) = \frac{1}{S} \sum_{s=1}^{S} \delta(\theta - \theta_s)$, and the predictive distribution (a categorical distribution parametrized by the predicted class probabilities) is thus approximated by

$$p(y|x, D) \approx \int p(y|x, \theta)q(\theta) d\theta = \frac{1}{S} \sum_{s=1}^{S} p(y|x, \theta_s).$$

The predictive distribution can be accurately estimated as $S \to \infty$. However, to perform the computation, we need to maintain a large number of samples, repeatedly evaluate the model for $S$ times and finally average the model outputs. Note that even if a full approximation $q(\theta)$ is utilized,
usually it does not maintain conjugacy with the likelihood, and we need to resort to MC integration to calculate the predictive distribution. In many real-world cases, this is not applicable due to limited computational resources and storage [1][12][1][4].

To alleviate the computation of MC integration, previous works, such as CompactApprox [16] and Bayesian Dark Knowledge (BDK) [3], have considered approximating the class probabilities (i.e., the predictive distribution) as a point estimate rather than with an MC ensemble. However, the disadvantage is that the class uncertainty (due to overlapping classes), the model uncertainty (due to data sampling), and the distribution uncertainty (due to out-of-sample data) are all entangled in the class probabilities, due to the limited expressiveness of the categorical distribution. Thus, the confidence about the predictions is not directly available in those methods.

In this work, aiming at a richer characterization of the prediction, we propose to approximate the distribution of class probabilities over the simplex induced by the posterior \( p(\theta|D) \). We call this distribution the “Bayes teacher” due to the analogy with teacher-student learning. Suppose we have an estimate of the Bayes teacher in the form of an MC ensemble. Based on the observation in Fig. 1 on real-world datasets, the MC ensemble is able to capture both class probability and confidence of the prediction by its location and concentration on the simplex. For example, tightly concentrated samples on the simplex indicate a confident prediction (either a particular class as in \( x_1 \) or an unknown class as in \( x_2 \)), while dispersed samples indicate an input outside of the training domain (as in \( x_3 \)). We use a Dirichlet distribution as the approximation model (the “student”) due to its expressiveness, conjugacy to categorical distribution and its efficient reparameterization for training. We term our approximation method as One-Pass Uncertainty (OPU) as it simplifies real-world evaluation of Bayesian models by computing the predictive distribution with only one model evaluation.

In summary, we make the following contributions:

- We propose the One-Pass Uncertainty (OPU) framework to accelerate Monte Carlo Bayesian inference. With only one evaluation, OPU obtains both class probabilities and prediction confidence. In contrast, MC integration requires large number of evaluations and other approximation methods ignore confidence of prediction. Furthermore, we derive OPU when the Bayes teacher is a non-parametric Gaussian Process, which shows that OPU is a universal approximation method for Bayesian classification.

- We propose to explicitly disentangle the parameters of the student into a prediction model (PM) and concentration model (CM), which capture class probability and sharpness of Dirichlet respectively. The CM output can directly be used as a measure for detecting out-of-domain (OOD) data. We empirically show that this disentangling improves OOD detection performance.

- We use Wasserstein distance for Bayesian teacher-student learning, and adapt it to our training objective using implicit reparameterization and adversarial training. Since adversarial training has poor scalability as each input data requires its own local witness function, we propose a global meta-network for generating the witness functions for each data point.

- Empirical evaluations show that OPU performs better in misclassification detection and OOD detection than CompactApprox and BDK. OPU does not require OOD data for training, and obtains similar comparable performance to Deep Prior Network [13] (DPN) which is explicitly trained using OOD data.

2 Related Work

CompactApprox was proposed in [16] to approximate the Bayesian predictive distribution by selecting samples from the MC ensemble. A parametric model composed of a small subset of “best samples” selected from the original MC samples is used to approximate the MC estimate of the predictive distribution. The forward KL divergence between the predictive distribution and the approximating distribution is minimized. Extending the approximation to Bayesian neural networks, Balan et al. [3] proposes BDK, which uses a parametric neural network to approximate the predictive distribution (a Categorical) of a Bayesian neural network trained by stochastic gradient Langevin dynamics (SGLD). Specifically, the teacher network generates samples via SGLD and the KL divergence between the two distributions is minimized in an online fashion.

Different from these previous works that only approximate the class probabilities, we approximate the distribution of class probabilities using a Dirichlet, from which the Categorical predictive distribution can be derived. In contrast, Snelson and Ghahramani [16], Balan et al. [3] directly approximate the Categorical distribution. Simply changing BDK’s approximation model to a Dirichlet fails because
the KL training objective is unstable due to sample degeneracy on the simplex (see Section 3.2), causing the concentration parameter to degenerate during training (see Section 4). To address these issues, we explicitly model the location and concentration of Dirichlet and design a novel learning method based on Wasserstein distance, which leads to substantial performance improvements.

Using a Dirichlet to estimate uncertainty has also been explored by Deep Prior Network (DPN) [13], where a parameterized Dirichlet is used in a Bayesian model to characterize the "distributional uncertainty"; i.e., to tell if the data is in the training domain or not. However, DPN adds a stochastic layer in the Bayes model, rather than approximating a well-trained Bayes teacher. Due to the high computational cost of MC estimation, DPN uses an MAP estimate of the model posterior. To compensate for the lost characterization of uncertainty, DPN uses a hand-crafted training goal that explicitly requires OOD samples (which are typically unavailable in real-world applications). In contrast, our OPU achieves comparable performance to DPN without requiring OOD training data.

3 One-Pass Uncertainty Framework

In this section we derive our OPU framework with a general Bayesian parametric classifier, including Bayesian logistic regression, Bayesian neural networks (NN), etc. The extension to nonparametric GP classifiers is deferred to the appendix. Specifically, let there be a Bayesian classifier with categorical likelihood in parametric form, i.e.,

\[ p(y|x, \theta) = \text{Cat}(y|T(x; \theta)) \]  

and a prior distribution \( p(\theta) \) be specified over the parameter space \( \Theta \), where \( T(\cdot; \theta) : \mathcal{X} \rightarrow \mathcal{Y}^{K-1} \) is any parametric function from input space to a \( (K-1) \)-simplex, e.g., a neural network (NN) with softmax output layer, where \( K \) is the number of classes.

Further, let the model be trained in a fully Bayesian way on \( \mathcal{D} = \{(y_n, x_n)\}_{n=1}^N \) and the posterior distribution is either available in closed-form or approximated by \( q(\theta) \approx p(\theta|\mathcal{D}) \). For example, \( q(\theta) \) can be chosen within some simple family if variational inference is employed, or taken as set of particles if sampling method is used. With a full posterior or posterior samples on hand, we are interested in computing the predictive distribution.

From a dual perspective, with some input \( x \) fixed, the mapping \( T(x; \cdot) \) is also understood as \( T(x; \cdot) : \Theta \rightarrow \mathcal{Y}^{K-1} \), which transforms the posterior \( p(\theta|\mathcal{D}) \) to an unknown conditional distribution defined over the simplex. We can define a random variable \( \pi = T(x; \theta) \) with randomness induced by \( \theta \sim p(\theta|\mathcal{D}) \). Given a testing point \( x \), the predictive distribution can be alternatively written as

\[ p(y|x, \mathcal{D}) = \int_{\Theta} \text{Cat}(y|T(x; \theta)) p(\theta|\mathcal{D}) \, d\theta = \int_{\mathcal{Y}^{K-1}} \text{Cat}(y|\pi) p(\pi|x, \mathcal{D}) \, d\pi, \]  

where \( p(\pi|x, \mathcal{D}) \) is the distribution of \( \pi = T(x; \theta) \) with \( x \) fixed. Our key insight is that \( p(\pi|x, \mathcal{D}) \) contains all information we need to compute the predictive distribution. Hence \( \pi \) is sufficient in the sense that \( y \) will be independent of both \( \theta \) and \( x \), given \( \pi \). This isolation combines the complexities in both the likelihood and posterior into a single object, namely \( p(\pi|x, \mathcal{D}) \), and keeps a simple dependence structure between \( y \) and \( \pi \).

In light of this, we propose to directly learn a parameterized conditional distribution \( q(\pi|x; \phi) \) that approximates the complex \( p(\pi|x, \mathcal{D}) \), where \( \phi \) is a set of global adaptive parameters. \( p(\pi|x, \mathcal{D}) \) can be considered as an induced penultimate layer of a generic Bayesian classifier, whereas the raw predictive \( p(y|x, \mathcal{D}) \) acts as the last layer. We denote \( p(\pi|x, \mathcal{D}) \) as the “Bayes teacher” and \( q(\pi|x; \phi) \) as the “student”. In our method, as seen in graphical representation in Fig. 2 by proper approximation, the stochasticity in node \( \theta \) of the teacher is transferred into node \( \pi \) of the student model, such that the predictive uncertainty is maintained. This can also be regarded as a type of “amortization” of local “Bayes teachers” by a global predictive network.

The intuition of our choice on approximating uncertainty of the penultimate layer is two-fold. First, compared with the last layer \( p(y|x, \mathcal{D}) \) that only gives the confidence on class labels, our approximation provides more options on estimating uncertainty and more flexible designs on the approximation model, as illustrated in Fig. 1 which gives an example of a teacher’s MC ensembles and student’s approximation on a 2-simplex. \( x_1 \) is similar to the training data (images of digits 0, 1, and 2). The Bayes teacher generates samples gathering around the corner of the simplex, indicating a confident prediction. \( x_2 \) is a digit image but was not seen by the Bayes teacher. Therefore, the MC ensemble gather around the center, indicating the teacher is certain that the input is on decision
boundary. $x_3$ is an image of a shoe (out-of-domain), the MC ensemble spread over the simplex, which means the teacher has a high uncertainty about $x_3$.

Second, the above benefit does not introduce any concession on generalizability. Our approximation can be applied to any Bayesian classifier, since it is based on approximating the distribution of the output class probabilities, which is common for all classifiers. In contrast, an approximation for a specific layer (e.g., a hidden layer of NN) may not be applicable to other models (a non-NN model or an NN with a different structure). With a parameterized $q$, the uncertainty is approximated with only one forward pass of an NN. As a result, we denote $q$ as the One-Pass Uncertainty (OPU) model.

Finally, we note that DPN [13] has a similar structure with (2), using a Dirichlet to model $p(\pi|x, D)$. The main difference from OPU is that DPN directly trains the Dirichlet to perform out-of-domain detection, by specifying a uniform Dirichlet distribution for OOD samples and peaky Dirichlet distributions for in-domain samples. This special training procedure is required because DPN uses an MAP model estimate where the predictive uncertainty is lost. In contrast, the goal of our OPU is to learn a parametrized Dirichlet that best represents the uncertainty induced by the Bayesian posterior; thus OPU is a higher fidelity representation of the original Bayesian predictive model.

### 3.1 Student Model

We choose the student model $q$ to be a Dirichlet distribution, $q(\pi|x, \phi) = \text{Dir}(\pi|\alpha(x; \phi))$, where $\alpha$ is the Dirichlet parameter which is a function of input $x$ and model parameter $\phi$. The reasons for choosing the Dirichlet distribution are three-fold: 1) expressiveness: for the predictive distribution in (2), any class probability vector can be obtained by appropriate choice of $\alpha$; 2) tractability: the Dirichlet is the conjugate prior to the Categorical, and thus enables tractable integration of (2) given the parameters. 3) implementation: the Dirichlet allows for an efficient reparameterization as a product Gamma distribution, and hence the gradient can be computed for back-propagation.

To better disentangle the uncertainty measures, we use the design $\alpha(x; \phi) = h(\langle x; \phi_1 \rangle) \cdot e^{\phi(\langle x; \phi_2 \rangle)}$, where $h(\cdot; \phi_1)$ and $g(\cdot; \phi_2)$ are two neural networks, and the vector output $h$ sums to 1. Vector output $h$ determines the mean of the Dirichlet (i.e., the predicted class probabilities), and $g$ determines the concentration of the Dirichlet (i.e., the prediction confidence). To see this, the posterior of the class labels is the Dirichlet mean,

$$p(y_\ell|1|x, \phi) = \int \text{Cat}(y_\ell = 1|\pi)\text{Dir}(\pi|\alpha(x; \phi)) \, d\pi = \frac{\alpha_\ell(x; \phi)}{\sum_c \alpha_c(x; \phi)} = h_\ell(x; \phi_1),$$

where $y_\ell$ and $\alpha_\ell$ are the $\ell$-th coordinate of $y$ and $\alpha$ respectively. Therefore, we call $h(\cdot; \phi_1)$ as the “prediction model” (PM). Similarly, the precision parameter (determines sharpness) of the Dirichlet solely depends on $g(\cdot; \phi_2)$,

$$\alpha_0 = \sum_c \alpha_c(x; \phi) = \sum_c h_c(x; \phi_1) e^{\phi(\langle x; \phi_2 \rangle)} = e^{\phi(\langle x; \phi_2 \rangle)}.$$
Therefore, we term \( g(\cdot; \phi_2) \) as the “concentration model” (CM). Based on this property, whether the Dirichlet is flat or not, can be fully characterized by CM. According to the analysis by [13], the designed CM fully captures “distributional” uncertainty. For example, in Fig. [1] CM outputs high values for \( x_1 \) and \( x_2 \) such that the corresponding distributions are sharp, which means high confidence. CM outputs a low value for \( x_3 \), yielding a flat distribution and low confidence.

### 3.2 Learning with Wasserstein-1 Metric

The KL divergence (forward KL) has been applied as a metric in approximating the Bayes teacher with the student in CompactApprox [16] and BDK [5]. However, there are some cases that KL might fail. For example, the unknown Bayes teacher \( p(\pi|x, D) \) might be supported on a low-dimensional manifold in the simplex \( \mathcal{S}_{K-1} \), in which case KL might provide no useful gradients [2] [17]. To observe this, \( K \) does not have to be very large. As illustrated in Figure [3], the input image is digit 2 that could be confused as a digit 0. In this case, the Bayes teacher generates samples spreading along the line between two corners, which is a low dimensional manifold on a higher dimensional simplex. The situation would be more serious if \( K \) gets larger [4]. As seen in WGAN [2] and WAE [17], the Wasserstein metric is able to provide more stable behaviour under such case. Hence, we choose Wasserstein metric as a loss measure to train the proposed OPU model. Using Wasserstein distance is appropriate for the situations where number of class is very large, making OPU applicable for more interesting applications.

Specifically, we consider the commonly used Kantorovich-Rubinstein dual representation [18] of Wasserstein-1 metric based on \( \ell_1 \) norm defined as

\[
W_1(p, q) = \sup_{\|\psi\|_{\text{Lip}} \leq 1} E_{p(z)}[\psi(z)] - E_{q(z)}[\psi(z)],
\]

(5)

where \( \| \cdot \|_{\text{Lip}} \) denotes the Lipschitz norm and \( \psi \) is known as the witness function. Based on this, we then define the loss incurred by replacing \( p(z) \) and \( q(z) \) by \( p(\pi|x, D) \) and \( q(\pi|x, \phi) \) as

\[
\mathcal{L}(\phi|x) = \sup_{\|\psi_x\|_{\text{Lip}} \leq 1} E_{p(\theta|D)}[\psi_x(T(x; \theta))] - E_{q(\pi|x; \phi)}[\psi_x(\pi)],
\]

(6)

where \( \psi_x \) is a local witness for each \( x \). The parameters \( \phi \) of the approximation are trained by minimizing the aggregated loss with respect to a training distribution \( p(x) \),

\[
\phi^* = \arg \min_{\phi} \mathbb{E}_{p(x)}[\mathcal{L}(\phi|x)] = \arg \min_{\phi} \int p(x) \mathcal{L}(\phi|x) \, dx,
\]

(7)

where we use an empirical estimate \( p(x) = |D'|^{-1} \sum_{x_m \in D'} \delta(x - x_m) \), and \( x_m \in D' \) are samples from a held-out dataset \( D' \) for OPU training (different from the dataset \( D \) used to train the Bayes teacher [3]). In addition, the first expectation in (6) is approximated by its MC estimate based on global posterior samples.

We make two other major adaptations. First, to obtain efficient gradient estimator and reduce variance, we reparameterize the Dirichlet by an equivalent product of \( K \) independent Gamma distributions. If \( \tilde{\pi} \sim \text{PG}(\pi|\alpha) \), then \( \pi = (\sum_{k=1}^{K} \tilde{\pi}_k)^{-1} \tilde{\pi} \sim \text{Dir}(\pi|\alpha) \). By Thm. 3 in [2], in each \( \mathcal{L}(\phi|x) \), the supremum is attained at \( \psi_x^* \in \text{Lip}_1 \) and the gradient is \( \nabla_{\phi} \mathcal{L}(\phi|x) = -\nabla_{\phi} E_{q(\pi|x; \phi)}(\psi_x^*(\pi)) \). Then as noted by [5], the gradient \( \nabla_{\phi} \mathcal{L}(\phi|x) \) can be implicitly computed without knowing the inverse of standardization function (e.g., CDF). Specifically, by Eq. 5 in [5], \( \nabla_{\phi} E_{q(\pi|x; \phi)}(\psi_x^*(\pi)) = \mathbb{E}_{\tilde{\pi}\sim\text{PG}(\tilde{\pi}|\tilde{\phi})}[\nabla_{\tilde{\pi}} \psi_x^*(\pi)] \nabla_{\tilde{\phi}} \tilde{\pi} \), where the first term \( \nabla_{\tilde{\pi}} \psi_x^*(\pi) \) is computed via the chain rule and the second term \( \nabla_{\tilde{\phi}} \tilde{\pi} \) is obtained by solving a local diagonal linear system. Refer to [5] and references therein for details.

Second, a popular way (following WGAN [2]) to address the intractability of the supremum in (6) is to let each \( \psi_x(\cdot) \approx \psi(\cdot; w_x) \) be a family of parametric functions \( \Psi_W = \{\psi(\cdot; w) : w \in W\} \), where \( w \) is the parameter vector. Hence each \( \mathcal{L}(\phi|x) \) is approximated as

\[
\mathcal{L}(\phi|x) \approx \sup_{w_x \in W} \mathbb{E}_{p(\theta|D)}[\psi(T(x; \theta); w_x)] - \mathbb{E}_{q(\pi|x; \phi)}[\psi(\pi; w_x)].
\]

(8)

Besides the weight clipping heuristic considered in WGAN, more methods have been proposed to appropriately restrict \( W \) to enforce Lipschitz condition, including [7] [19].
3.3 Amortization of Local Witness Functions

Note that, in (5), for different $x$, the optimal $w^*_x$ are in general different. Hence in theory, the parameter $w$ should be understood in a local sense, which turns out to be impractical for large datasets. To address this, we propose to use a parametrized function to learn a map $\Omega : \mathcal{X} \to \mathcal{W}$ that generates the weight of a witness function $\psi(\pi; w)$ in an amortized way, i.e., $w^*_x = \Omega(x)$.

Particularly, we parameterize the function $\Omega(x)$ with a neural network with a new set of parameters $v$ to obtain a tractable implementation. This type of neural network has been widely adopted in the field of Auto-ML and meta-learning, where it is termed as meta-network as it generates the weight of another neural network. In summary, the local witness functions at each $x$ are modeled as $\psi_x(\cdot) = \psi(\cdot; \Omega(x; v))$, where $\psi$ is a neural network whose parameters are generated by the meta-network $\Omega$ with parameters $v$. The final optimization goal then becomes

$$\min_{\phi} \max_{\psi} \mathbb{E}_{p_D(x)} \left[ \mathbb{E}_{p(\theta|x)} [\psi(T(x; \theta); \Omega(x; v))] - \mathbb{E}_{q(\pi|x; \phi)} [\psi(\pi; \Omega(x; v))] \right] + \lambda \mathcal{R}(v), \quad (9)$$

where $\mathcal{R}(v)$ is the imposed gradient penalty [27] over the output of meta-network to achieve the Lipschitz constraint. An algorithm for optimizing (9) is given in Alg.1. The meta-network and OPU model are alternately trained while PM and CM are alternately trained within a student iteration. Details about meta-network architecture and training flowchart are in the appendix.

4 Experiments

4.1 Experimental Setup

We conduct experiments on three types of Bayesian model: Bayesian logistic regression (BLR), Bayesian neural network (BNN) and Gaussian process classification (GP). For each model, we choose a few Monte-Carlo methods as the Bayes teachers, and approximate them with our OPU. We also compare with state-of-the-art approximations that are proposed for the specific types of Bayes models. For BLR, we use Polya Gamma [15] as the teacher, and compare with CompactApprox [16]. For BNN, we use MCDP [5] and SGLD [20] as the teacher, and BDK [3] and DPN [13] for comparisons. For GP, we use SGPMC [9] as the teacher, and SVGP [10] for comparison. The methods for obtaining posterior samples from the Bayes teachers are in appendix B. For each type of model, in-domain misclassification (MisC) detection, out-of-domain (OOD) input detection, prediction performance and prediction time are presented. Specifically, the goal of misclassification detection is to detect whether a data point is correctly predicted with an uncertainty measure. OOD input detection involves detecting if an input is out-of-domain with an uncertainty measure.

For the Bayes teacher, discrete entropy (Ent) and maximum probability (MaxP) of the averaged MC ensemble are used as the uncertainty measures, while the students use discrete entropy (for CompactApprox, BDK, SVGP) or differential entropy (for DPN) and MaxP of the output distributions. For OPU, we consider the discrete entropy and MaxP of the prediction model, and the total concentration of the Dirichlet (CM) as the measures.

The in-domain dataset is split to training data and testing data, i.e., $D^{in} = \{D^{ir}, D^{iu}\}$, which is used for training models, evaluating prediction and MisC detection. The OOD dataset $D^{ood}$ is used for OOD detection. To assess the performance, we use accuracy, time, Area under the ROC (AUROC)
and Precision-Recall (AUPR), following the baseline proposed by [3]. Time is evaluated on the whole testing dataset. To save space, we only present the best performing uncertainty measure (Ent, MaxP, or CM) for each task and method. We use the MXNet implementation of BDK and GPflow implementation of GP, and the remaining models are implemented in Pytorch. All experiments run on a desktop with an i7-8700 CPU and an RTX-2080 Ti GPU.

4.2 Bayesian Logistic Regression

This experiment uses Pima and Spambase datasets as $D_{\text{in}}$. Pima[2] is a medical dataset with 769 data points and 9 dimensions. Spambase[1] is a text dataset with 4601 data points and 57 dimensions for identifying spam email. We generate the same number of data points from a zero-mean multivariate Gaussian distribution for $D_{\text{ood}}$. For each dataset, $10\%$ of data points are uniformly selected into the testing set $D_{\text{te}}$. We normalize the data by features with L2 norm. For CM, we use a 2-layer MLP with size $d$-$2d$-$1$, where $d$ is the input dimension. For the meta-network $\Omega$, we use an MLP with size $d$-$2d$-$2d$ and ReLU activation. For the witness function, we use an MLP with size $K$-$10K$-$2K$-$1$ and ReLU activation, where $K$ is the number of classes.

We test two models in this experiment: Polya Gamma (PG), CompactApprox approximating PG (CA-PG) and OPU approximating PG (OPU-PG). We draw 500 posterior samples from PG and train OPU with the following hyperparameters: number of epochs 100, learning rate for student and meta-network $10^{-3}$, mini-batch size of 256, number of iterations to save space, we only present the best performing uncertainty measure (Ent, MaxP, or CM) for each task and method. We use the MXNet implementation of BDK and GPflow implementation of GP, and the remaining models are implemented in Pytorch. All experiments run on a desktop with an i7-8700 CPU and an RTX-2080 Ti GPU.

4.3 Bayesian Neural Network

The experiments for Bayesian neural network use MNIST dataset as $D_{\text{in}}$ and SEMEION dataset as $D_{\text{ood}}$, as in [13]. MNIST[3] is an image dataset of 28 × 28-dimensional handwritten digits from 0 to 9, which contains 60000 training data points and 10000 testing data points. SEMEION[4] is an image dataset that contains 1593 handwritten digits. We normalize the data with mean 0.5 and std 0.5.

There are 7 models in this experiment: MCDP, OPU approximating MCDP (OPU-MCDP), SGLD, OPU-SGLD, BDK-SGLD, BDK-Dir-SGLD and DPN. For BDK-Dir-SGLD, we replace the Categorical distribution in BDK by a Dirichlet without disentangling mean and concentration, then train it with the same MC ensemble as OPU-SGLD. The neural network architecture used by these models is an MLP with size $784$-$400$-$400$-$10$, ReLU activations, and softmax outputs, following Balan et al. [5]. For CM, we use an MLP with size $784$-$400$-$400$-$1$. We use an MLP with size $784$-$1024$-$1024$ for meta-network and use an MLP with size $10$-$400$-$128$-$1$. MCDP is trained by SGD with hyperparameters: dropout-rate of 0.5, learning rate $5 \times 10^{-4}$, mini-batch size of 256, number of iterations $10^3$. Then, 500 binary samples are generated by the dropout unit with the same rate which induces 500 samples of model parameters, as mentioned in appendix. OPU-MCDP is trained by SGD with

Table 1: Results on Bayesian logistic regression models.

| Data  | Model    | MisC detection | OOD detection | Accuracy | Time (sec.) |
|-------|----------|----------------|---------------|----------|-------------|
|       |          | AUROC AUPR    | AUROC AUPR    |          |             |
| Pima  | PG       | 60.0 (Ent) 24.2 (Ent) | 87.0 (Ent) 76.7 (Ent) | 64.4 | 1.01 ± 0.001 |
|       | CA-PG    | 58.2 (Ent) 24.2 (Ent) | 80.1 (Ent) 74.5 (Ent) | 62.3 | 0.18 ± 0.001 |
|       | OPU-PG   | 59.7 (Ent) 25.6 (Ent) | 100.0 (CM) 100.0 (CM) | 64.4 | 0.01 ± 0.002 |
| Spam  | PG       | 83.9 (Ent) 24.3 (Ent) | 54.6 (Ent) 53.5 (Ent) | 92.4 | 5.94 ± 0.001 |
|       | CA-PG    | 64.1 (Ent) 24.2 (Ent) | 71.5 (Ent) 67.5 (Ent) | 85.4 | 0.36 ± 0.001 |
|       | OPU-PG   | 83.9 (Ent) 23.8 (Ent) | 99.7 (CM) 99.3 (CM) | 92.4 | 0.01 ± 0.002 |

1. https://www.kaggle.com/uclml/pima-indians-diabetes-database
2. https://archive.ics.uci.edu/ml/datasets/spambase
3. http://yann.lecun.com/exdb/mnist/
4. https://archive.ics.uci.edu/ml/datasets/semeion+handwritten+digit
hyper-parameters: number of iterations 100, learning rate for student and meta-network $10^{-5}$. The training of SGLD and BDK follows Balan et al. [3]. When SGLD training is finished, we obtain 500 samples of the model parameters by sampling at each step of SGLD. Then OPU-SGLD is trained with the same hyperparameter as OPU-MCDP. Results of DPN are from Malinin and Gales [13].

The results are shown in Table 2. OPU-MCDP has similar performance to MCDP on MisC detection and prediction accuracy, and better performance than MCDP on OOD detection. OPU-SGLD shows similar performance with SGLD on MisC detection and accuracy, and reports better performance on OOD detection. OPU-SGLD outperforms BDK-SGLD on all results except MisC detection AUPR. Furthermore, decoupling class probabilities and confidence (OPU-SGLD) consistently outperforms simple parameterization (BDK-Dir-SGLD). This demonstrates that explicitly disentangling the mean/scale of the Dirichlet parameter and our proposed training procedure yield a significant improvement. Finally, OPU offers a $\sim 500x$ speedup compared to the original MCDP/SGLD. Note that the time cost of MCDP/SGLD increases with more posterior samples involved. BDK is slightly faster than OPU because it runs one network while OPU runs both PM and CM.

The results of DPN on these tasks are also presented. Our OPU model (without OOD data in training) has comparable performance to DPN (which uses a hand-crafted goal and OOD data in training). Another reason that DPN performs slightly better is that DPN uses VGG-6 (4 Convolutional layer and 1 FC layer) which is a much stronger model than the 2-layer MLP model that other models use.

### 4.4 Gaussian Process

The experiments for Gaussian process use the same data setup as Bayesian logistic regression. There are 3 models tested: SGPMC, OPU approximating SGPMC (OPU-SGPMC) and SVGP. SGPMC and SVGP are trained with $\frac{1}{10} D^{in}$ data points randomly selected from $D^{in}$ as inducing points. Then 500 samples over functions of $D^{in}$ are generated from SGPMC.

The results are presented in Table 3. On MisC detection and prediction accuracy, OPU has similar performance to SGPMC, which indicates the effectiveness of approximating prediction results with ensemble of samples in the nonparametric family. With the same number of inducing points, SVGP performs slightly worse than SGPMC, because it incurs two-fold approximation. Measuring uncertainty with CM in OPU outperforms other measures and models, which indicates the sharpness of the logistic-normal distribution can be captured via the CM the designed Dirichlet.

SGPMC and SVGP are faster than OPU on Pima, but are slower than OPU on Spambase. This is due to the static latency for setting up the GP for OPU, which becomes the main time cost when the dataset is small (as in Pima). For the two GP methods, the computation time depends on the number of inducing points and the number of dimensions. Therefore, as the dataset becomes larger (Spambase), the computation time increases.

### 5 Discussion

In this article, we propose to approximate the induced Bayesian predictive distribution over simplex with a parameterized Dirichlet distribution, which significantly speeds up the predictive process and keeps Bayesian uncertainty. This method is particularly useful in the case where an accurate...
estimate of Bayesian uncertainty is required meanwhile the computational resources are limited, e.g., the assisted-driving systems and the embedded platforms for machine learning. In the future, the theoretical aspects of the proposed method and the potential use in other scenarios such as accelerating ensemble learning can be further investigated.

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