Diversity-enhanced Probabilistic Ensemble For Uncertainty Estimation

Abstract

Ensemble methods combine multiple individual models for prediction, which have demonstrated their effectiveness in accurate uncertainty quantification (UQ) and strong robustness. Obtaining a diverse ensemble set of model parameters results in better model averaging performance and better approximation of the true posterior distribution of model parameters. In this paper, we propose the diversity-enhanced probabilistic ensemble method with the adaptive uncertainty-guided ensemble learning strategy for better quantifying uncertainty and further improving the model robustness. Specifically, we construct the probabilistic ensemble model by building a Gaussian distribution of the model parameters for each ensemble component using Laplacian approximation in a post-processing manner. Then a mixture of Gaussian model is established with learnable and refinable parameters in an EM-like algorithm. During ensemble training, we leverage the uncertainty estimated from previous models as guidance when training the next one such that the new model will focus more on the less explored regions by previous models. Various experiments including out-of-distribution detection and image classification under distributional shifts have demonstrated better uncertainty estimation and improved model generalization ability for our proposed method.

1 INTRODUCTION

The real world is full of uncertainty. However, deterministic deep learning models might be overconfident in some predictions where they actually do not know due to the lack of knowledge of those data regions [Lakshminarayanan et al., 2017a]. Hence, establishing deep learning models in a probabilistic manner is very important for a trusted system, which will enable us to tell when the models will fail in their predictions and guide human behaviors with confidence. There are mainly two types of uncertainty, namely, epistemic uncertainty and aleatoric uncertainty [Kendall and Gal, 2017]. Epistemic uncertainty represents the prediction uncertainty due to the lack of knowledge when building the models. Aleatoric uncertainty measures the inherent data noise in the distribution, which is irreducible. For quantifying those uncertainties, we can rely on Bayesian neural networks (BNNs) which aim at constructing the posterior distribution of the neural network parameters. However, the Bayesian inference performs marginalization over the posterior distribution, which is often intractable in practice.

Alternatively, the deep ensemble method [Lakshminarayanan et al., 2017a] trains an ensemble of deep neural networks from random initializations, which demonstrates great success in predictive uncertainty calibration and outperforms various approximate BNNs. Generating sufficient and diverse ensemble components can better approximate the complex posterior distribution. Ensemble diversity is also a good indicator of uncertainty quantification performance and model robustness Dusenberry et al. [2020]. Higher diversity also enables different models to make independent errors such that their individual mistakes will be canceled out during majority voting and model averaging, leading to better prediction accuracy and improved generalization ability [Bian and Chen, 2021, Zhang et al., 2020]. However, traditional ensemble methods have limited diversity since each component is trained independently with only different initializations. Generating sufficient and diverse ensemble models requires many initializations and is hence computationally expensive. With limited computational resources, ensemble-based methods can only provide several modes to approximate the posterior distribution, which is hard to describe the complex posterior landscape. Moreover, previous methods often train each component independently and ignore the important knowledge from previous models when getting a new model. Finally, there are also multi-

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ple resources that we can gain additional diversity during ensemble training besides random initializations.

To overcome the above limitations, we propose the diversity-enhanced probabilistic ensemble (PE) method, which has the following contributions.

- We propose the PE, a Bayesian framework to model aleatoric and epistemic uncertainty by combining the ensemble method and Laplacian approximation (LA) [MacKay, 1992] for Bayesian inference. The diversity of ensemble components is enhanced through exploring the neighborhood of each ensemble member by LA, where performance guarantees are provided.
- Given the LA for ensemble members, a mixture of Gaussian (MoG) is constructed with learnable and refinable parameters in an EM-like algorithm, enabling a better posterior approximation of model parameters.
- We propose an adaptive uncertainty-guided ensemble training strategy (AUEL), where the new ensemble model is trained based on the knowledge of previous models with the guidance of uncertainty, leading to improved ensemble diversity and better joint model averaging performance.
- Various applications have been conducted including out-of-distribution detection and image classification under distributional shifts, which demonstrate competitive performance in uncertainty estimation and domain generalization.

2 RELATED WORK

Laplacian Approximation Laplace approximation assumes a Gaussian posterior distribution by performing Taylor expansion around the mode. However, constructing the Gaussian posterior for large models by LA is not applicable mainly because of the computational difficulty of the large covariance matrix for high-dimensional model parameters. Several methods are proposed to improve the efficiency of LA. For example, subnetwork LA [Daxberger et al., 2021b] and last-layer LA [Kristiadi et al., 2020] reduce the number of Bayesian parameters by constructing the posterior distribution only for partial neural network weights. Different Hessian matrix factorization methods are also proposed such as Kronecker-factored approximation curvature (KFAC) [Ritter et al., 2018] and low-rank KFAC [Lee et al., 2020]. Please refer to the review paper [Daxberger et al., 2021a] for more information.

Ensemble Methods for Uncertainty Estimation Besides the deep ensemble method, different ensemble-based variants have been proposed to improve the efficiency or uncertainty quantification accuracy. For improving efficiency, deep sub-ensemble [Valdenegro-Toro, 2019] ensembles only the layers close to the output. The snapshot ensemble [Huang et al., 2017] method collects different ensemble components in different epochs in one training attempt. Considering weight sharing, the batch-ensemble [Wen et al., 2020] method proposes a parameter-efficient representation of ensemble weights. For improving the accuracy, some ensemble methods further explore each ensemble subspace with approximate posterior estimation such as Multi-SWAG [Wilson and Izmailov, 2020] and ensemble with subspace sampling [Fort et al., 2019]. Multi-SWAG combines deep ensemble with SWAG to form a mixture of Gaussian distribution with uniform coefficients while Fort et al. [2019] built an ensemble model by training multiple variational BNNs with empirical analysis. Recently, Eschenhagen et al. [2021] connected ensemble methods with LA for better uncertainty quantification. Some ensemble techniques such as MIMO [Havasi et al., 2020] and Rank-1 BNN [Dusenberry et al., 2020] also use a mixture approximate posterior to capture ensemble components. However, they are mainly designed for training multiple subnetworks in one model's capacity, which is less accurate. Compared to the above methods, we focus on diversity-enhanced ensemble learning for improving UQ accuracy and proposed three sub-modules, including probabilistic ensemble, adaptive uncertainty-guided ensemble learning, and the MoG refinement.

Diversity-enhanced Ensemble Learning Diversity matters for improving ensemble performance. One line of work trains ensemble models with special diversity regularization [Zhang et al., 2020, Zaid et al., 2021, Jain et al., 2020, Liu and Yao, 1999, Pearce et al., 2018, Wabartha et al., 2021]. For example, Zhang et al. [2020] utilized the pair-wise difference between classifiers as regularization. Zaid et al. [2021] created a diversity-promoted ensemble loss based on mutual information. Jain et al. [2020] leveraged out-of-distribution samples as regularization to increase ensemble diversity. Another line of work focuses on training each ensemble component with a subset of data so that each ensemble model has its own learning specialty to increase diversity [Lee et al., 2015, Zhou et al., 2018]. Moreover, EDST [Liu et al., 2021] and SeBayS [Jantre et al., 2022] make adjustments to the learning process to obtain ensembles sequentially from diverse models. Finally, Wenzel et al. [2020] tried to increase ensemble diversity by training with different hyperparameters. Zaidi et al. [2020] further constructed the ensemble models with different architectures and proposed a special selection procedure for choosing diverse ensemble members from a pretrained ensemble model pool. Recently, several particle-based function-space variational inference methods [Tiulpin and Blaschko, 2021, D'Angelo and Fortuin, 2021, Yashima et al., 2022] try to utilize a finite number of models to approximate the Bayesian posterior distribution through optimization, where they often consider the interaction between models with an explicit diversity measurement as regularization. We exclude them from comparisons since our proposed method is in weight space and is a randomization-based method, which is often more efficient than function-space methods. In the development of

diversity-enhanced learning, different diversity metrics are studied [Wu et al., 2020, 2021]. There are also many related applications such as active learning [Tan et al., 2021] and computer vision tasks [Dvornik et al., 2019].

3 PROPOSED METHOD

3.1 BACKGROUND

General Notations and Assumptions. Denote the input as x, the target variable as y, the training data as $\mathcal{D} = \{x_m, y_m\}_{m=1}^M$. In this paper, we will focus on classification tasks. We denote $f(x, \theta) \in \mathcal{R}^C$ as the output of the neural network with input x parameterized by θ, which is the probability logit before the softmax layer. C represents the number of classes. When constructing the ensemble models, $f(x, \theta_i)$ represents the output of the ith ensemble component. β represents the hyperparameter of LA for the prior distribution of θ. $\mathbb{E}(\cdot)$ represents the expectation. $\mathcal{H}(\cdot)$ represents the entropy.

Laplacian Approximation. The LA constructs the posterior distribution $p(\theta|\mathcal{D}, \beta)$ by a Gaussian distribution around the MAP estimate θ_{map} where

$$\theta_{map} = \arg\max_{\theta} \log p(\theta|\mathcal{D}, \beta)$$

By taking the second-order Taylor expansion of $\log p(\theta|\mathcal{D}, \beta)$ around θ_{map}, we can observe that

$$p(\theta|\mathcal{D}, \beta) \approx \mathcal{N}(\theta_{map}, \Sigma) \tag{1}$$

where $\Sigma = -(H)^{-1}$ and $H = \nabla_\theta^2 \log p(\theta|\mathcal{D}, \beta)|_{\theta=\theta_{map}}$.

Please refer to Appendix Sec. A.1 for more details. This paper utilizes the last-layer LA [Kristiadi et al., 2020] to achieve competitive accuracy with high efficiency.

Uncertainty Quantification. For classification problems, we estimate the epistemic uncertainty and the aleatoric uncertainty by the mutual information and the expected entropy [Depeweg et al., 2018]. Details can be found in Appendix Sec. A.2.

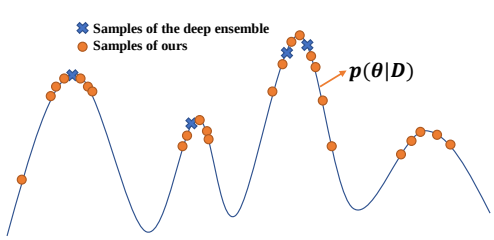


Figure 1: Posterior Approximation by Samples.

3.2 PROBABILISTIC ENSEMBLE

Given N pretrained ensemble models, we denote θ_i as the MAP estimation of the ith ensemble component parameters. We perform the Laplacian approximation for each ensemble component as an approximation of the true posterior, denoted as $\mathcal{N}(\theta; \theta_i, \Sigma_i)$. A mixture of Gaussian model is constructed for better approximating the posterior distribution shown in Eq. (2).

$$p(\theta|D, \beta) \approx \sum_{i=1}^{N} \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i) \tag{2}$$

where $\lambda_i \in [0, 1], i = 1, 2, ..., N$ are the coefficients such that $\sum_{i=1}^N \lambda_i = 1$. As shown in Figure 1, PE can better approximate the posterior distribution than the deep ensemble method by exploring each ensemble subspace. Given the probabilistic ensemble model, the Bayesian inference is performed shown in Eq. (3).

$$\begin{aligned} p(y|x, D) &\approx \int p(y|x, \theta) \sum_{i=1}^{N} \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i) d\theta \\ &\approx \frac{1}{S} \sum_{s=1}^{S} p(y|x, \theta^s) \end{aligned} \tag{3}$$

where $\theta^s \sim \sum_{i=1}^N \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i)$ represents the sth sample from the Gaussian mixture model. Several propositions are shown to demonstrate the effectiveness of the probabilistic ensemble model with theoretical guarantees. All the proofs can be found in Appendix Sec. B. Specifically, approximation guarantees are shown in Proposition 3.1 and 3.2. When the sample size is large, Proposition 3.1 guarantees that the PE model converges to the true posterior distribution. Otherwise, Proposition 3.2 shows theoretical evidence that the PE model bridges the connection of the deep ensemble method to approximate Bayesian inference and has better posterior approximation than single LA.

Proposition 3.1 (Convergence of PE)**.** *Denote the data samples as $\mathcal{D} = \{x_m, y_m\}_{m=1}^M$. Under mild regularity conditions [Gelman, 2011], as the sample size $M \to \infty$, the probabilistic ensemble representation of θ approaches its posterior distribution. For example,*

$$\sup_{\theta} |p(\theta|\mathcal{D}) - \sum_{i=1}^{N} \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i)| \to 0 \tag{4}$$

Proposition 3.2 (Better posterior approximation)**.** *PE models extend the deep ensembles for approximate Bayesian inference. Denote $p_{PE}(\theta) = \sum_{i=1}^N \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i), p_{LA}^{(i)}(\theta) = \mathcal{N}(\theta; \theta_i, \Sigma_i)$ as the PE approximation and the ith-network LA, respectively. The PE model has better posterior approximation compared to the single LA with a measure of KL divergence.*

$$KL(p(\theta|\mathcal{D})||p_{PE}(\theta)) \leq \sum_{i=1}^{N} \lambda_i KL(p(\theta|\mathcal{D})||p_{LA}^{(i)}(\theta)) \tag{5}$$

Proposition 3.3 (Error reduction of the PE and the role of diversity)**.** *Denote $\theta \sim \sum_{i=1}^N \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i)$ as PE parameters, x as the input, and y^* as the corresponding label. The*

PE model fulfills

$$-\log \mathbb{E}_\theta[p(y^*|x,\theta)] \leq \mathbb{E}_\theta[-\log p(y^*|x,\theta)] - \inf_\theta \frac{1}{2p(y^*|x,\theta)^2}\mathbb{V}_\theta[p(y^*|x,\theta)] \tag{6}$$

where $\inf_\theta \frac{1}{p(y^*|x,\theta)^2}$ *is bounded given* $p(y^*|x,\theta) \in [0,1]$ *and* $\mathbb{V}_\theta[p(y^*|x,\theta)]$ *is the variance of probabilistic ensemble model prediction.*

$$\mathbb{V}_\theta[p(y^*|x,\theta)] = \mathbb{E}_\theta[(p(y^*|x,\theta) - \mathbb{E}_\theta[p(y^*|x,\theta)])^2] \tag{7}$$

Proposition 3.3 shows that the errors of the PE model are reduced compared to single models, which are also bounded by variance $\mathbb{V}_\theta[p(y^*|x,\theta)]$. The diversity measurement $\mathbb{V}_\theta[p(y^*|x,\theta)]$ can be applied for both regression and classification tasks since $p(y^*|x,\theta)$ is a scalar variable parameterized by θ given label y^*. With a larger variance, the upper bound of the NLL is reduced. As a result, we can theoretically show that enhancing diversity improves the prediction performance when $\mathbb{E}_\theta[-\log p(y^*|x,\theta)]$ remains similar. Moreover, Proposition 3.4 shows that PE has better diversity compared to deep ensemble method as the theoretical basis of the improved performance.

Proposition 3.4 (Enhanced diversity of PE)**.** *Let* μ_D, Σ_D *be the mean and covariance matrix of the deep ensemble representation* $p_{DE}(\theta) = \sum_{i=1}^N \lambda_i \delta(\theta, \theta_i)$ *where* δ *represents the delta function. Let* μ_P, Σ_P *be the mean and covariance matrix of* $p_{PE}(\theta)$*. We show that*

$$\mu_D = \mu_P \qquad \Sigma_P \geq \Sigma_D \tag{8}$$

where $\Sigma_P \geq \Sigma_D$ *means* $\Sigma_P - \Sigma_D$ *is positive semi-definite. Compared to deep ensemble method, the PE model gains improved diversity.*

Proposition 3.5 (Overconfidence reduction of PE)**.** *Given a probabilistic ensemble model with* N *components, let* $f_{\theta_i} : R^{|x|} \to R^C$ *be a ReLU network parameterized by* θ_i*. Let* $|x|$ *represent the dimension of* x *and* $\theta \sim \sum_{i=1}^N \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i)$*. Then for any input* x*, the estimated probability based on multi-class probit approximation (see Appendix Sec. A.1) of the PE fulfills*

$$\lim_{\eta\to\infty} p_{PE}(y=c|\eta x) \leq \sum_{i=1}^N \frac{\lambda_i}{1 + \sum_{j\neq c} \exp\{-t_i^{(j)} - t_i^{(c)}\}} \tag{9}$$

where

$$t_i^{(k)} = \frac{||w_i^{(k)}||}{s_{min}(J_i^{(k)})\sqrt{\frac{\pi}{8}\lambda_{min}(\Sigma_i)}} \qquad k = 1, 2, \cdots, C$$

and $w_i = [w_i^{(1)}, w_i^{(2)}, \cdots, w_i^{(C)}] \in R^{|x|\times C}$ *is a matrix that only depends on* θ_i*.* $J_i^{(j)} = \frac{\partial w_i^{(j)}}{\partial \theta}|_{\theta=\theta_i}$ *is the Jacobian matrix of* $w_i^{(j)}$ *at* $\theta = \theta_i$*.* λ_{min} *represents the minimum eigenvalue.* s_{min} *represents the minimum singular value.*

Deterministic models suffer from the overconfidence issue such that the estimated probability is very high even if the input is far away from the data distribution. The Proposition 3.5 builds an upper bound for the predictive probability of samples $\{\eta x\}$ when $\eta \to \infty$, which prevents $p_{PE}(y = c|\eta x)$ to be extremely large. The Proposition 3.5 also shows that the confidence for far-away samples is upper bounded by the uncertainty estimated from LA. Especially, when the uncertainty is large, i.e., $\lambda_{min}(\Sigma_i) \to \infty, i = 1, 2, \cdots, N$, we have $\lim_{\eta\to\infty} p_{PE}(y = c|\eta x) \leq \frac{1}{C}$.

3.3 ADAPTIVE UNCERTAINTY-GUIDED ENSEMBLE LEARNING

The deep ensemble method trains ensemble models independently, which ignores the information obtained from previous models when getting a new one. This may cause knowledge redundancy that limits the diversity among ensemble models. The key idea of the proposed adaptive uncertainty-guided ensemble learning is to always make the new model focus on the regions which previous models have less explored, measured by uncertainty. Thus the new model will have the ability to provide complementary information to the previous models, which will improve the model averaging performance as well as implicitly enhance the diversity.

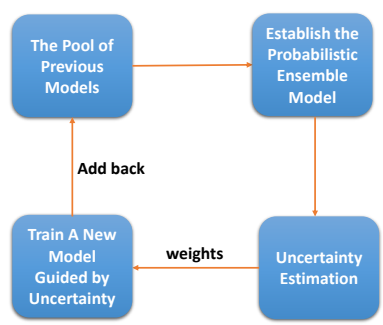


Figure 2: The Adaptive Uncertainty-guided Ensemble Learning Framework

Given k trained deterministic models with parameters $\{\theta_i\}_{i=1}^k$, we perform the adaptive uncertainty-guided ensemble learning to get the $(k+1)$th model in the following steps. First, we construct the probabilistic ensemble illustrated in Sec. 3.2 such that $\theta \sim \sum_{i=1}^k \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i)$. Then, the epistemic uncertainty $u(x)$ of each training data x is computed. Finally, we use the estimated epistemic uncertainty $u(x)$ from previous models as weights to guide the training of the $(k+1)$th model. Given a batch of data $\mathcal{D}_B = \{x_m, y_m\}_{m=1}^B$ of size B, the uncertainty-guided training loss can be expressed as

$$\mathcal{L}_{nll}(\theta) = -\frac{1}{B}\sum_{m=1}^B w(x_m) \log p(y_m|x_m,\theta) \tag{10}$$

where $w(x_m)$ is the weight for sample x_m as a function of $u(x_m)$, which is shown in Eq. (11).

$$w(x_m) = \frac{\exp(a * \log(u(x_m)) + b)}{\sum_{j=1}^{B} \exp(a * \log(u(x_j)) + b)} \tag{11}$$

Eq. (11) guarantees that samples with larger uncertainty will receive larger weights and the weights for a batch of data sum to 1. A $\log$ function is applied on $u(x_m)$ since the epistemic uncertainty is usually small. $a, b > 0$ are hyper-parameters that can be tuned. The following propositions provide some theoretical evidence of the proposed method with proofs shown in Appendix Sec. C.

Proposition 3.6 (Prediction error bound)**.** *The prediction error is bounded by the total uncertainty. The epistemic uncertainty is positively correlated with the prediction error.*

Proposition 3.7 (Striking the right balance with uncertainty [Khan et al., 2019])**.** *For the imbalanced classification problems, minimizing the empirical loss results in a hypothesis that the classification boundary is towards the minority classes, leading to a larger classification region for the majority ones.*

Proposition 3.6 provides theoretical support for uncertainty-guided learning. By putting higher weights on problematic samples, the proposed method can reduce their uncertainty through adaptive ensemble learning to improve overall accuracy. Proposition 3.7 shows that a single model tends to sacrifice minority samples to obtain a good overall performance. It motivates us to adaptively learn complementary models focusing on minority samples, in order to achieve better ensemble performance.

Although our method is similar to boosting methods [Freund and Schapire, 1997, Hastie et al., 2009] in terms of reweighing the samples, they, however, are fundamentally different. As a discriminative model, boosting methods build an ensemble classifier by combining a set of weak classifiers to better classify the data. In contrast, we construct a generative ensemble that better models the posterior distribution of model parameters, through which we perform uncertainty quantification. Moreover, instead of using classification errors to weigh the samples, we use epistemic uncertainty to weigh the training samples. As epistemic uncertainty inversely measures training sample density, training of the next model will focus more on the samples that are not well represented by previous models.

3.4 MIXTURE OF GAUSSIAN REFINEMENT

In this section, we will establish an EM-like algorithm for refining the mixture of Gaussian parameters. To our knowledge, most of the ensemble methods assume that each ensemble component has the same importance, which may not be the case for real-world applications. Denote $\phi = \{\{\lambda_i\}_{i=1}^N, \{\theta_i\}_{i=1}^N, \{\Sigma_i\}_{i=1}^N\}$ as the mixture of Gaussian parameters, $\phi^0 = \{\{\lambda_i^0\}_{i=1}^N, \{\theta_i^0\}_{i=1}^N, \{\Sigma_i^0\}_{i=1}^N\}$ as the previous learned parameters before the refinement, and the training data as $\mathcal{D} = \{\mathcal{D}_m\}_{m=1}^M = \{x_m, y_m\}_{m=1}^M$. Let $Z \sim Cat(\lambda_1, \lambda_2, \ldots, \lambda_N)$ be the latent variable indicating membership of (x, y) belonging to which ensemble component. We learn non-uniform $\{\lambda_i\}_{i=1}^N$ and refine $\{\{\theta_i\}_{i=1}^N, \{\Sigma_i\}_{i=1}^N\}$ in the following EM steps.

E-step: construct the loss function $Q(\phi|\phi^0, \mathcal{D})$ as the expected value of the log likelihood function of ϕ with respect to the current conditional distribution of Z given ϕ^0 and $\mathcal{D}$

$$\begin{aligned}
\log p(\mathcal{D}|\phi) &= \sum_{m=1}^{M} \log p(\mathcal{D}_m|\phi) \\
&= \sum_{m=1}^{M} \log \sum_{i=1}^{N} \frac{p(Z=i|\mathcal{D}_m, \phi^0)}{p(Z=i|\mathcal{D}_m, \phi^0)} p(\mathcal{D}_m, Z=i|\phi) \\
&\geq \sum_{m=1}^{M} \sum_{i=1}^{N} p(Z=i|\mathcal{D}_m, \phi^0) \log \frac{p(\mathcal{D}_m, Z=i|\phi)}{p(Z=i|\mathcal{D}_m, \phi^0)} \\
&:= Q(\phi|\phi^0, \mathcal{D})
\end{aligned} \tag{12}$$

M-step: maximize $Q(\phi|\phi^0, \mathcal{D})$ with respect to ϕ.

$$\phi^* = \arg\max_{\phi} Q(\phi|\phi^0, \mathcal{D}) \tag{13}$$

Optimizing Eq. (13) returns a close-form expression of $\{\lambda_i^*\}_{i=1}^N$.

$$\lambda_i^* = \frac{\sum_{m=1}^{M} p(Z=i|\mathcal{D}_m, \phi^0)}{\sum_{m=1}^{M} \sum_{j=1}^{N} p(Z=j|\mathcal{D}_m, \phi^0)} \tag{14}$$

Letting $p_m(\theta) = p(y_m|x_m, \theta)$,

$$p(Z=i|\mathcal{D}_m, \phi^0) = \frac{\lambda_i^0 \int p_m(\theta) \mathcal{N}(\theta; \theta_i^0, \Sigma_i^0) d\theta}{\sum_{j=1}^{N} \lambda_j^0 \int p_m(\theta) \mathcal{N}(\theta; \theta_j^0, \Sigma_j^0) d\theta} \tag{15}$$

Then given the distribution $Z \sim Cat(\{\lambda_i^*\}_{i=1}^N)$, we assign each data samples to its top l nearest components based on their weighted log-likelihood (i.e., $l = N/2$). The refinement is conducted by fine-tuning the existing ensemble components on the data samples they receive to further strengthen the specialty and diversity of each ensemble model. Details can be found in Appendix Sec. D.

3.5 PROBABILISTIC ENSEMBLE TRAINING STRATEGY

In this paper, three sub-modules are proposed: the probabilistic ensemble built by LA, the uncertainty-guided ensemble learning, and the mixture of Gaussian refinement. The pseudocode of the overall proposed method is shown in Algorithm 1, consisting of four steps. Although the final refinement step can further improve performance, it is not required.

During training, we admit that AUEL requires sequential training, which takes more time than parallel training. However, our methods can achieve similar UQ results with fewer ensemble components, compared to other ensemble baselines in Sec. 4.4. It could be more useful when there are limited capacities for parallel training or when there exist parallelly trained ensemble models with low diversity and we want to add a new one for providing complementary information. PE can be applied to any trained ensemble models with high efficiency. The last-layer LA is efficient whose complexity is $O(m + c^3 + p^3)$, where m, c, p represents the total number of parameters, the number of classes, and the number of last-layer parameters. For the inference complexity of PE, we can generate an arbitrary number of samples from the mixture of Gaussian. Compared to the deep ensemble method, the additional cost to obtain one more sample is $O(p)$, which is minimal since we only sample the last-layer parameters and reuse the intermediate outputs. More importantly, each sub-module can be applied to other ensemble methods separately to make further improvements. Although incorporating all sub-modules leads to the best performance, only applying PE could be an alternative way for efficient training.

Algorithm 1 Probabilistic Ensemble with Adaptive Uncertainty-guided Ensemble Learning

Input: Training data $\mathcal{D} = \{x_m, y_m\}_{m=1}^{M}$. Initialize the model pool $P = \{\}$
Ouput: The probabilistic ensemble model parameters $\theta \sim \sum_{i=1}^{N} \lambda_i \mathcal{N}(\theta; \theta_i, \Sigma_i)$
Step 1 (single model): Train the first model using NLL loss to obtain θ_1; $P = P + \{\theta_1\}$
Step 2 (AUEL): Perform the adaptive uncertainty-guided ensemble learning to obtain $\{\theta_i\}_{i=2}^{N}$
for $k = 2 : N$ **do**
(1) Given P, construct the probabilistic ensemble model with uniform weights.
$$\theta \sim p_{k-1}(\theta) = \frac{1}{k-1} \sum_{i=1}^{k-1} \mathcal{N}(\theta; \theta_i, \Sigma_i)$$
(2) Estimate the epistemic uncertainty $\{u(x_m)\}_{m=1}^{M}$ using $\theta \sim p_{k-1}(\theta)$
(3) Use the weighted loss in Eq. (10) to train θ_k
(4) Update the model pool: $P = P + \{\theta_k\}$
end for
Step 3 (AUEL+PE): Based on current $P = \{\theta_i\}_{i=1}^{N}$, construct the probabilistic ensemble model
Step 4 (AUEL+RPE): We refine the Gaussian mixture model parameters based on Sec. 3.4

4 EXPERIMENT

4.1 OUT-OF-DISTRIBUTION DETECTION

Out-of-distribution (OOD) detection tries to detect anomalous data that is inconsistent with the training data distribution. Utilizing epistemic uncertainty as a measure for out-of-distribution detection is one of the major applications for demonstrating the quality of UQ performance. We evaluate our methods on benchmark image classification datasets MNIST [Deng, 2012] and CIFAR-10 (C10) [Krizhevsky et al., 2014], respectively. We choose Omniglot [Lake et al., 2015], EMNIST [Cohen et al., 2017], and KMNIST [Clanuwat et al., 2018] as OOD datasets for MNIST. For C10 dataset, the SVHN [Netzer et al., 2011], LSUN [Yu et al., 2015] and CIFAR-100 (C100) [Krizhevsky et al., 2009] are the OOD datasets. We compare our proposed method (AUEL+PE) with ensemble-based method (i.e., Ensemble (as the deep ensemble method)[Lakshminarayanan et al., 2017b], Batch Ensemble [Wen et al., 2020], Hyper Ensemble [Wenzel et al., 2020], Bayesian Ensemble [Pearce et al., 2018], Multi-SWAG [Wilson and Izmailov, 2020]) and approximate BNNs (i.e., LPBNN [Franchi et al., 2020], LA). We exclude sequential ensemble methods (EDST [Liu et al., 2021], SeBayS [Jantre et al., 2022]) and other mixture posterior approximation methods (MIMO [Havasi et al., 2020], Rank-1 BNN [Dusenberry et al., 2020]) for comparison since they are shown to perform worse than Ensemble method. The evaluation metrics include the area under the receiver operating characteristic curve (AUROC ↑) and the area under the precision-recall curve (AUPR ↑). All ensemble-based methods have size 5. The experiment settings and implementation details can be found in Appendix Sec. E.

The out-of-distribution detection performance is shown in Table 1. It is obvious that the proposed method (AUEL+PE) can achieve significant improvement over recent ensemble-based methods on various OOD detection tasks. Additional OOD detection experiments are shown in Sec. 4.2 for MNIST and C10 under different levels of distributional shifts. Since the post-processing refinement of the MoG is not required, we will show the effectiveness of the refinement (AUEL+RPE) in Sec. 4.4. Compared to diversity-enhanced ensemble learning such as Hyper Ensemble and Multi-SWAG, our better OOD detection performance also indicates enhanced diversity.

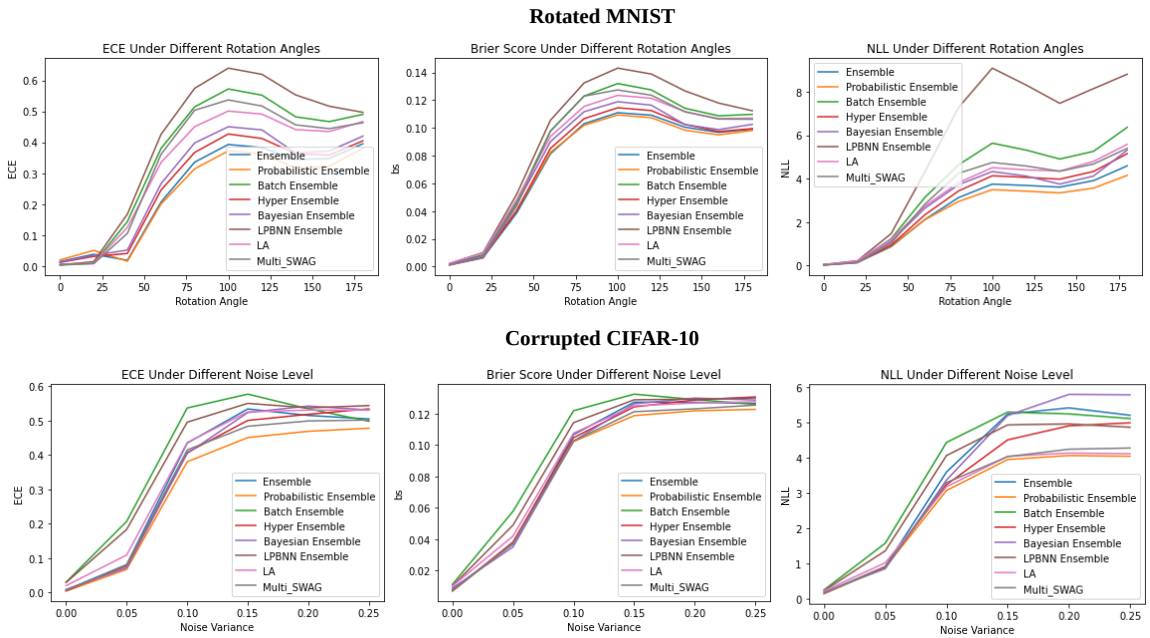
4.2 IMAGE CLASSIFICATION UNDER DISTRIBUTIONAL SHIFT

Bayesian models marginalize all possible solutions for the final prediction, leading to improved robustness. In this section, we will demonstrate the effectiveness of the proposed method for image classification tasks on MNIST and C10 with synthetic distributional shifts. For MNIST, we create the synthetic rotated MNIST dataset, where we increasingly rotate the MNIST testing data from 0° to 180° with a step of 20°. For the C10 dataset, we add the Gaussian noise with 0 mean and variance ranging from 0 to 0.25 with a step of 0.05 to the testing data as the corrupted C10 dataset. Additional adversarial shifts can be found in Sec. 4.4. Note that we keep the original training strategy on MNIST/C10 training

Table 1: OOD Detection Results for AUROC (%) and AUPR (%) on MNIST-related and C10-related Datasets with Epistemic Uncertainty. Each experiment result is aggregated over 3 independent runs.

Method	MNIST → Omniglot		MNIST → EMNIST		MNIST→ KMNIST	
	AUROC	AUPR	AUROC	AUPR	AUROC	AUPR
Ours	**97.25** ± 0.14	**96.72** ± 0.25	**96.49** ± 0.04	**95.36** ± 0.07	**97.02** ± 0.12	**96.06** ± 0.19
Ensemble	96.73 ± 0.14	95.80 ± 0.27	96.15 ± 0.17	94.81 ± 0.19	96.59 ± 0.17	95.31 ± 0.20
Batch Ensemble	95.95 ± 0.17	94.74 ± 0.22	95.79 ± 0.70	93.76 ± 0.75	96.59 ± 0.45	94.72 ± 0.43
Hyper Ensemble	96.98 ± 0.20	96.44 ± 0.16	96.21 ± 0.26	95.26 ± 0.35	96.87 ± 0.26	**96.06** ± 0.27
Bayesian Ensemble	96.22 ± 0.20	95.63 ± 0.23	95.55 ± 0.21	94.22 ± 0.19	96.49 ± 0.07	95.18 ± 0.09
LPBNN	95.09 ± 0.78	93.01 ± 1.27	91.72 ± 0.74	91.75 ± 0.85	95.15 ± 2.25	92.05 ± 3.87
LA	94.45 ± 0.34	93.26 ± 0.45	94.44 ± 0.35	92.91 ± 0.46	94.92 ± 0.26	92.99 ± 0.31
Multi-SWAG	96.42 ± 0.37	94.56 ± 0.84	95.81 ± 0.60	90.64 ± 1.70	96.70 ± 0.42	94.34 ± 0.98

Method	C10 → SVHN		C10 → LSUN		C10→ C100	
	AUROC	AUPR	AUROC	AUPR	AUROC	AUPR
Ours	93.88 ± 0.57	90.58 ± 1.58	**89.57** ± 0.08	**86.81** ± 0.14	**93.80** ± 0.11	**91.67** ± 0.36
Ensemble	91.23 ± 1.35	86.16 ± 1.73	88.42 ± 0.85	84.99 ± 0.65	91.87 ± 0.58	88.69 ± 0.55
Batch Ensemble	90.40 ± 1.62	85.12 ± 2.64	86.10 ± 0.24	81.42 ± 0.40	90.15 ± 0.18	85.48 ± 0.49
Hyper Ensemble	91.11 ± 0.32	85.86 ± 0.46	88.82 ± 0.15	85.29 ± 0.25	92.59 ± 0.24	89.65 ± 0.71
Bayesian Ensemble	90.96 ± 3.35	86.57 ± 5.27	87.85 ± 1.22	84.56 ± 1.01	91.80 ± 0.45	88.83 ± 0.02
LPBNN	89.99 ± 2.44	85.18 ± 4.00	86.87 ± 0.01	82.14 ± 0.49	90.80 ± 0.22	85.62 ± 1.59
LA	93.39 ± 0.46	91.17 ± 0.98	87.27 ± 0.19	85.77 ± 0.21	93.45 ± 1.17	92.59 ± 1.47
Multi-SWAG	**94.06** ± 0.54	**93.92** ± 0.59	87.23 ± 0.29	85.44 ± 0.61	90.24 ± 0.86	88.05 ± 1.02



(a) ECE **(b) Brier Score** **(c) NLL**

Figure 3: Predictive Calibration Analysis of Rotated MINST and Corrupted C10 Datasets. The first row shows the results for MNIST while the second row represents C10. There are three different metrics (ECE, Brier Score, NLL) that are analyzed in each column, respectively. Each experiment result is aggregated over 3 independent runs.

data but test on the shifted testing data. During the evaluation, the uncertainty calibration metrics include negative log-likelihood (NLL ↓), accuracy (ACC ↑), expected calibration error (ECE ↓), maximum calibration error (MCE ↓), and brier score (BS ↓). We also provide the OOD detection results of MNIST → Rotated MNIST and C10 → Corrupted C10 in terms of AUROC and AUPR. The comparisons are conducted under the same experiment settings as Sec. 4.1. In Figure 3, partial results for ECE, BS, and NLL are shown. Additional analysis can be found in Appendix Sec. F.

Based on Figure 3, we can observe that the probabilistic ensemble method can achieve better calibration performance for both rotated MNIST and corrupted C10 datasets. As the shift level increases, our proposed method consistently outperforms other ensemble-based methods, which demonstrates the great potential of our method in better generalization ability. Besides improved robustness of uncertainty

Table 2: Ablation Studies: OOD Detection Results and Robustness Analysis on MNIST/C10 Datasets. The first table shows the effectiveness of the sub-modules. The second table shows the improvement when PE serves as a plug-and-play module. Each experiment result is aggregated over 3 independent runs.

Method	MNIST → Omniglot		C10 → SVHN		Rotated MNIST 120°		Noisy C10 Level 0.1	
	AUROC	AUPR	AUROC	AUPR	NLL	ECE	NLL	ECE
Ensemble	96.59	95.31	91.23	86.16	3.69	0.383	3.58	0.435
AUEL	96.78	96.07	92.98	88.97	3.66	0.380	3.28	0.394
AUEL+PE	97.25	96.72	93.88	90.58	3.42	0.363	3.06	0.380
AUEL+RPE	**97.36**	**96.79**	**93.93**	**91.93**	**3.38**	**0.356**	**3.02**	**0.375**

Method	MNIST → Omniglot		C10 → SVHN		Rotated MNIST 60°		Noisy C10 Level 0.1	
	AUROC	AUPR	AUROC	AUPR	NLL	ECE	NLL	ECE
Hyper-E	96.98	96.44	91.11	85.86	4.36	0.432	3.23	0.407
Hyper-E + PE	**97.37**	**96.98**	**92.09**	**87.52**	**3.78**	**0.400**	**2.66**	**0.342**
Bayes-E	96.22	95.63	90.96	86.57	4.16	0.449	3.36	0.404
Bayes-E + PE	**96.75**	**96.31**	**93.27**	**90.41**	**3.65**	**0.422**	**2.40**	**0.298**

quantification, comparable within-dataset performance can be found in Appendix Sec. F.1.

4.3 DIVERSITY ANALYSIS

Besides theoretical evidence of enhanced diversity shown in Sec. 3.2 and 3.3, we also provide empirical analysis for the diversity gained from the proposed method. We utilize the diversity metrics introduced in Wu et al. [2020] including the pairwise diversity metrics such as Q Statistics (QS) and Binary Disagreement (BD) as well as non-pairwise diversity metrics such as Fleiss' Kappa (FK) and Kohavi-Wolpert Variance (KW). We perform normalization for all the scores so that smaller scores (↓) represent higher diversity. From Table 3, our method outperforms other ensemble-based methods in terms of diversity. Besides quantitative results, some visualizations for both the parameter space diversity and the prediction space diversity are provided in Appendix Sec. G using principal component analysis.

Table 3: Diversity Analysis of Ensemble-based Methods Trained on C10 dataset

Method	QS	BD	FK	KW
Ours	**0.174**	**0.538**	**0.383**	**0.857**
Ensemble	0.185	0.552	0.404	0.860
Batch Ensemble	0.284	0.576	0.422	0.868
Hyper Ensemble	0.199	0.554	0.406	0.861
Bayesian Ensemble	**0.174**	0.548	0.406	0.859
LPBNN	0.209	0.557	0.405	0.862
Multi-SWAG	0.246	0.566	0.418	0.865

4.4 ABLATION STUDIES

Effectiveness of Sub-modules. Table 2 shows the intermediate results for each step illustrated in Algorithm 1. Each proposed module helps further improve the OOD detection and uncertainty calibration performance. More results are shown in Appendix Sec. H.1.

Probabilistic Ensemble as a Plug-and-Play Module. Our probabilistic ensemble method can be a plug-and-play module for easily applying to other ensemble methods with further improvements. Given trained ensemble models from other ensemble methods, we apply the PE module to construct the mixture of Gaussian model in the post-processing way. For example, we combine the Hyper Ensemble (Hyper-E) with PE and the Bayesian Ensemble (Bayes-E) with PE to show further improvements in Table 2. Further analysis can be found in Appendix Sec. H.2.

Efficiency Analysis. In Appendix Sec. H.3, we empirically show the runtime of our method and further provide a comparison among the ensemble baselines with different numbers of ensemble components. It shows that our method requires fewer ensemble members to achieve similar results.

Application to Larger Datasets. In Appendix Sec. I, we show that our method is applicable for larger datasets such as CIFAR-100 and TinyImagenet [CS231N, 2017].

Other Distributional Shifts. In Appendix Sec. J, we perform adversarial perturbations with the fast gradient sign method Goodfellow et al. [2014] on C10 dataset to show the robustness of our method under various adversarial attacks.

Synthetic Experiments. In Appendix Sec. K, we provide some toy examples for one-dimensional regression problems and the two-moon classification problem to show that the estimated epistemic uncertainty of the PE model inversely matches well with the training data density.

5 CONCLUSION

In this paper, we propose the probabilistic ensemble method with adaptive uncertainty-guided ensemble training to construct the Gaussian mixture model with learnable and refinable parameters. Both theoretical and empirical evidence is provided to show that our proposed method can achieve a better approximation of the posterior distribution with enhanced diversity. Moreover, the proposed method has demonstrated better uncertainty quantification performance as well as improved uncertainty calibration ability for various applications including out-of-distribution detection and image classification under different settings.

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