Improving Regression Uncertainty Estimation Under Statistical Change

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Abstract

While deep neural networks are highly performant and successful in a wide range of real-world problems, estimating their predictive uncertainty remains a challenging task. To address this challenge, we propose and implement a loss function for regression uncertainty estimation based on the Bayesian Validation Metric (BVM) framework while using ensemble learning. A series of experiments on in-distribution data show that the proposed method is competitive with existing state-of-the-art methods. In addition, experiments on out-of-distribution data show that the proposed method is robust to statistical change and exhibits superior predictive capability.

1 Introduction

The proven utility of accurate data analysis has caused machine learning (ML) and deep neural networks (NNs) to emerge as crucially important tools in academia, industry, and society (LeCun, Bengio, and Hinton 2015). NNs have many documented successes in a wide variety of critical domains such as natural language processing (Collobert and Weston 2008; Mikolov et al. 2013; Sutskever, Vinyals, and Le 2014), computer vision (Krizhevsky, Sutskever, and Hinton 2012), and speech recognition (Hinton et al. 2012; Hannun et al. 2014). The main aspect that differentiates ML methods from traditional statistical modeling techniques is their ability to provide tractable analysis on large and informationally dense datasets. As the amount of data being produced each year continues to accelerate, ML-based techniques are expected to dominate the future of data analysis.

Unless NN models are trained in a way to make predictions that indicate uncertainty when they are not confident, these models can make overly confident, yet incorrect, predictions. While these models can guarantee a level of accuracy for data that is statistically similar to the data they trained on, they have no guarantee to make accurate predictions on statistically different (known as out-of-distribution (Hendrycks and Gimpel 2016)) data. For instance, after training a vanilla NN to classify the hand written digits in the MNIST dataset, one observes (far more often than not) that feeding the NN a uniformly randomly generated image results in a prediction probability one for the predicted digit. This overly certain and wrong prediction is in stark contrast with what the modeler would desire, e.g. a uniform distribution that indicates uncertainty (Sensoy, Kaplan, and Kandemir 2018).

The field of probabilistic machine learning seeks to avoid overly confident, yet incorrect, predictions by quantifying and estimating the predictive uncertainty of NN models (Krzywinski and Altman 2013; Ghahramani 2015). Given that these models are being integrated into real decision systems (e.g. self-driving vehicles, infrastructure control, medical diagnosis, etc.), a decision system should incorporate the uncertainty of a prediction to avoid ill-informed choices or reactions that could potentially lead to heavy or undesired losses (Amodei et al. 2016).

A comparative review of the progress made regarding predictive uncertainty estimation for NN models may be found in (Snoek et al. 2019). Most of the early proposed approaches are Bayesian in nature (Bernardo and Smith 2009). These methods assign prior distributions to the NN’s parameters (weights) and the training process updates these distributions to the “learned” posterior distributions. The residual uncertainty in the posterior distribution of the parameters allow the network to estimate predictive uncertainty. Several methods were suggested for learning Bayesian NNs including Laplace approximation (MacKay 1992), Hamiltonian methods (Springenberg et al. 2016), Markov Chain Monte Carlo (MCMC) methods (Neal 1996), expectation propagation (Jylänki, Nummenmaa, and Vehtari 2014; Li, Hernández-Lobato, and Turner 2015; Hasenclever et al. 2017), and variational inference (Graves 2011; Louizos and Welling 2016). Implementing Bayesian NNs is generally difficult and training them is computationally expensive. Recent state-of-the-art methods for predictive uncertainty estimation include probabilistic backpropagation (PBP) (Hernández-Lobato and Adams 2015), Monte Carlo dropout (MC-dropout) (Gal and Ghahramani 2016), and Deep Ensembles (Lakshminarayanan, Pritzel, and Blundell 2017). These state-of-the-art methods achieve top performance when estimating predictive uncertainty.

Average generalization error captures the expected ability of a model to generalize to new in-distribution data due to the i.i.d. nature of train-test data split. Among several of the error functions that can be used, log of the predictive probi...
abilities takes the predictive uncertainty into account while assessing the error. Thus, the log of the predictive probabilities is typically used for assessing the quality of predictive methods that quantify uncertainty in regression problems (Nix and Weigend 1994; Lakshminarayanan, Pritzel, and Blundell 2017).

Contributions: We present a new approach to quantify predictive uncertainty in NNs for regression tasks based on the Bayesian Validation Metric (BVM) framework proposed in (Vanslette, Tohme, and Youcef-Toumi 2020). Using this framework, we propose a new loss function (log-likelihood cumulative distribution function difference) and use it to train an ensemble of NNs (inspired by the work of (Lakshminarayanan, Pritzel, and Blundell 2017)). The proposed loss function reproduces maximum likelihood estimation in the limiting case. Our method is very simple to implement and only requires minor changes to the standard NN training procedure. We assess our method both qualitatively and quantitatively through a series of experiments on toy and real-world datasets, and show that our approach provides well-calibrated uncertainty estimates and is competitive with the existing state-of-the-art methods (when tested on in-distribution data). We introduce and utilize the concept of “outlier train-test splitting” to evaluate a method’s predictive ability on out-of-distribution examples whenever their presence in a dataset is not guaranteed. We show that our method has superior predictive power compared to Deep Ensembles (Lakshminarayanan, Pritzel, and Blundell 2017) when tested on out-of-distribution (outlier) samples. As the statistics of training datasets often differ from the statistics of the environment of deployed systems, our method can be used to improve safety and decision-making in the deployed environment by better estimating out-of-distribution uncertainty.

2 The Bayesian Validation Metric for predictive uncertainty estimation

2.1 Notation and problem setup

Consider the following supervised regression task. We are given a dataset \( D = \{x_n, t_n\}_{n=1}^N \), consisting of \( N \) i.i.d. paired examples, where \( x_n \in \mathbb{R}^d \) denotes the input vector, \( t_n \in \mathbb{R} \) denotes the corresponding continuous target variable (or label). We aim to learn the probabilistic distribution \( \rho(t|x) \) over the targets \( t \) for given inputs \( x \) using NNs.

2.2 Maximum likelihood estimation

In regression tasks, it is common practice to train a NN with a single output node (corresponding to the predicted mean), say \( \mu(x) \), such that the network parameters (or weights) are optimized by minimizing the mean squared error (MSE) cost (or loss) function, expressed as

\[
C_{\text{MSE}} = \frac{1}{N} \sum_{n=1}^{N} (t_n - \mu(x_n))^2.
\]  

Note that the network output \( \mu(x) \) can be thought of as an estimate of the true mean of the noisy target distribution for a given input feature (Nix and Weigend 1994). However, this does not take into account the uncertainty or noise in the data.

To capture predictive uncertainty, an alternative approach based on maximum likelihood was proposed in (Nix and Weigend 1994), and it consists of adding another node to the output layer of the neural network, \( \sigma^2(x) \), that estimates the true variance of the target distribution. In other words, we train a network with two nodes in its output layer: \( (\mu(x), \sigma^2(x)) \). By assuming the target values \( t_n \) to be drawn from a Gaussian distribution with the predicted mean \( \mu(x_n) \equiv \mu_n \) and variance \( \sigma^2(x_n) \equiv \sigma_n^2 \), we can express the likelihood \( \rho(t_n|x_n) \) of observing the target value \( t_n \) given the input vector \( x_n \) as follows:

\[
\rho(t_n|x_n) \equiv \rho(t_n|\mu_n, \sigma_n^2) = \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp\left\{ -\frac{(t_n - \mu_n)^2}{2\sigma_n^2} \right\}.
\]  

The aim is to train a network that infers \( (\mu(x), \sigma^2(x)) \) by maximizing the likelihood function in (2). This is equivalent to minimizing its negative log-likelihood, expressed as

\[
-\log \rho(t_n|\mu_n, \sigma_n^2) = \frac{1}{2} \log 2\pi \sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2}.
\]  

Hence the overall negative log-likelihood (NLL) cost function is given by

\[
C_{\text{NLL}} = \frac{1}{N} \sum_{n=1}^{N} \left( \frac{1}{2} \log 2\pi \sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} \right).
\]  

Note that \( \sigma^2(x) > 0 \); we impose this positivity constraint on the variance by using the sigmoid function (instead of softplus as in (Lakshminarayanan, Pritzel, and Blundell 2017)) as our data will be standardized.

2.3 The Bayesian Validation Metric

The Bayesian Validation Metric (BVM) is a general model validation and testing tool that was shown to generalize Bayesian model testing and regression (Vanslette, Tohme, and Youcef-Toumi 2020; Tohme, Vanslette, and Youcef-Toumi 2020). The BVM measures the probability of agreement \( A \) between the model \( M \) and the data \( D \) given the Boolean agreement function \( B \), denoted as \( 0 \leq p(A|M, D, B) \leq 1 \). The probability of agreement is

\[
p(A|M, D, B) = \int_{\hat{y}, y} \rho(\hat{y}|M) \cdot \Theta(B(\hat{y}, y)) \cdot \rho(y|D) \, d\hat{y} \, dy,
\]  

where \( \hat{y} \) and \( y \) correspond to the model output and observed data respectively, \( \rho(\hat{y}|M) \) is the probability density function (pdf) representing the model predictive uncertainty, \( \rho(y|D) \) is the data uncertainty pdf, and \( \Theta(B(\hat{y}, y)) \) is the indicator function of the Boolean \( B \) that defines the meaning of model-data agreement. The indicator function behaves as a probabilistic kernel between the data and model prediction pdfs.
2.4 The BVM reproduces the NLL loss as a special case

We show that the BVM is capable of replicating the maximum likelihood NN framework by representing the NLL cost function $C_{\text{NLL}}$ described in (4) as a special case. In terms of the BVM framework, the maximum likelihood formulation is achieved by modeling the predictions using a Gaussian likelihood given by

$$
\rho(\hat{y}_n | M(x_n)) = \rho(\hat{y}_n | \mu_n, \sigma^2_n) = \frac{1}{\sqrt{2\pi\sigma^2_n}} \exp\left\{-\frac{(\hat{y}_n - \mu_n)^2}{2\sigma^2_n}\right\},
$$

(6)

and by assuming the target variables to be deterministic, i.e. $\rho(y_n | D) = \delta(y_n - t_n)$, where $\delta(\cdot)$ is the Dirac delta function. In addition, the Boolean agreement function is defined such that the model and the data are required to “agree exactly” (as is the case with Bayesian model testing (Vanslette, Tohme, and Youcef-Toumi 2020; Tohme 2020)), and is given by $\Theta(B(\hat{y}_n, y_n)) = \delta(\hat{y}_n - y_n)$, when $p(A | M, D, B) \rightarrow \rho(A | M, D, B)$ is a probability density.

For a particular input feature vector $x_n$, the probability density of agreement between the model and data is equal to

$$
p(A | M, D, B, x_n) = \int \rho(\hat{y}_n | M(x_n)) \cdot \Theta(B(\hat{y}_n, y_n)) \cdot \rho(y_n | D) d\hat{y}_n dy_n
$$

$$
= \int \rho(\hat{y}_n | \mu_n, \sigma^2_n) \cdot \delta(\hat{y}_n - y_n) \cdot \delta(y_n - t_n) d\hat{y}_n dy_n
$$

$$
= \int \rho(\hat{y}_n | \mu_n, \sigma^2_n) \cdot \delta(\hat{y}_n - t_n) d\hat{y}_n
$$

$$
= \rho(t_n | \mu_n, \sigma^2_n)
$$

$$
= \frac{1}{\sqrt{2\pi\sigma^2_n}} \exp\left\{-\frac{(t_n - \mu_n)^2}{2\sigma^2_n}\right\}.
$$

(7)

Maximizing the BVM probability density of agreement is equivalent to minimizing its negative log-likelihood,

$$
-\log \rho(A | M, D, B, x_n) = -\log \rho(t_n | \mu_n, \sigma^2_n)
$$

(8)

which is Equation (3). Therefore, the negative log-likelihood BVM cost function over the set of all input feature vectors $x = \{x_1, \ldots, x_N\}$ is given by

$$
C_{\text{BVM}} = -\frac{1}{N} \log \rho(A | M, D, B, x)
$$

$$
= -\frac{1}{N} \log \prod_{n=1}^{N} \rho(t_n | \mu_n, \sigma^2_n)
$$

$$
= \frac{1}{N} \sum_{n=1}^{N} -\log \rho(t_n | \mu_n, \sigma^2_n)
$$

(9)

which is Equation (4). Thus, with the assumptions put on the data, model, and agreement definition, the BVM method can reproduce the maximum likelihood method as a special case. That is, minimizing the BVM negative log-probability density of agreement is mathematically equivalent to minimizing the NLL loss, which was essentially used in Deep Ensembles (Lakshminarayanan, Pritzel, and Blundell 2017).

2.5 The $\epsilon$-BVM loss: a relaxed version of the NLL loss

We now consider the $\epsilon$-Boolean agreement function $B(\hat{y}_n, y_n, \epsilon)$ being true iff $|\hat{y}_n - y_n| \leq \epsilon$. In the limit $\epsilon \to 0$, this Boolean function requires the model output and data to “agree exactly”, which leads to the maximum likelihood NN limit of the BVM discussed above. Again, assuming the model predictive uncertainty to be Gaussian, the target variables to be deterministic and the agreement function to be $B(\hat{y}_n, y_n, \epsilon)$, the $\epsilon$-BVM probability of agreement for a given input feature vector $x_n$ can be expressed as

$$
p(A | M, D, B(\epsilon), x_n)
$$

$$
= \int_{\hat{y}_n, y_n} \rho(\hat{y}_n | \mu_n, \sigma^2_n) \cdot \Theta(|\hat{y}_n - y_n| \leq \epsilon) \cdot \delta(y_n - t_n) d\hat{y}_n dy_n
$$

$$
= \int_{\hat{y}_n, y_n} \rho(\hat{y}_n | \mu_n, \sigma^2_n) \cdot \Theta(|\hat{y}_n - t_n| \leq \epsilon) d\hat{y}_n
$$

$$
= \int_{t_n - \epsilon}^{t_n + \epsilon} \rho(\hat{y}_n | \mu_n, \sigma^2_n) d\hat{y}_n
$$

$$
= \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right),
$$

(10)

where $\Phi(\cdot)$ is the cumulative distribution function (cdf) of the standard normal distribution. Thus, this $\epsilon$-BVM probability of agreement becomes the difference in likelihood cdfs around the mean. Taking its (overall) negative log gives

$$
C_{\text{BVM}}(B(\epsilon)) = \frac{1}{N} \sum_{n=1}^{N} -\log p(A | M, D, B(\epsilon), x_n)
$$

$$
= \frac{1}{N} \sum_{n=1}^{N} -\log \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right].
$$

(11)

Having this looser definition of model-data agreement effectively coarse-grains the in-distribution data and prevents overfitting. While Section 3.3 shows that this coarse-graining increases the bias of the in-distribution test results, Section 3.4 shows that our method better generalizes to out-of-distribution sample predictions.

2.6 Implementation and ensemble learning

Implementing our proposed method is straightforward and requires little modifications to typical NNs. We simply train a NN using the BVM loss function. Since our aim is to estimate and quantify the predictive uncertainty, our NN will have two nodes in its output layer, corresponding to the predicted mean $\mu(x)$ and variance $\sigma(x)^2$, as we mentioned earlier. More details about our NN architecture will be discussed in the next section.
Training an ensemble of NNs independently and statistically integrating their results was shown to improve predictive performance (Lakshminarayanan, Pritzel, and Blundell 2017). This class of ensemble methods is known as a randomization-based approach (such as random forests (Breiman 2001)) in contrast to a boosting-based approach where NNs are trained sequentially. Due to the randomized and independent training procedure, the local minima the NNs settle into vary across the ensemble. This causes the ensemble to “agree” where there is training data and “disagree” elsewhere, which increases the variance of the statistically integrated predictive distribution.

We follow (Lakshminarayanan, Pritzel, and Blundell 2017) and adopt their ensemble learning procedure by training an ensemble of NNs (the effect of ensemble learning becomes more apparent as we move further away from the training data). Note that the results we get using the BVM loss function results in better predictive uncertainty estimation.

The results are shown in Figure 1. From Figure 1, it is clear that predictive uncertainty estimation can be improved by learning the variance through training using the BVM loss, and it can be further improved by training an ensemble of NNs (the effect of ensemble learning becomes more apparent as we move further away from the training data).

3 Experimental results

We evaluate our proposed method both qualitatively and quantitatively through a series of experiments on regression benchmark datasets. In particular, we first conduct a regression experiment on a one-dimensional toy dataset, and then experiment with well-known, real world datasets.

3.1 Toy dataset

We first qualitatively assess the performance of our proposed method on a toy dataset that was used in (Hernández-Lobato and Adams 2015; Lakshminarayanan, Pritzel, and Blundell 2017). The dataset is produced by uniformly sampling (at random) 20 inputs $x$ in the interval $[-4, 4]$. The label $t$ corresponding to each input $x$ is obtained by computing $t = x^3 + \xi$ where $\xi \sim \mathcal{N}(0, 3^2)$. The NN architecture consists of one layer with 100 hidden units and the value of $\epsilon$ in the BVM loss is set to 1 as the data is not normalized.

In order to measure and estimate uncertainty, a commonly used approach is to train multiple NNs independently (i.e. an ensemble of NNs) to minimize MSE, and compute the variance of the networks’ generated point predictions. We show that learning the variance by training using the BVM loss function results in better predictive uncertainty estimation.

The results are shown in Figure 1.

The datasets can be found at the University of California, Irvine (UCI) machine learning data repository.
3.2 Training using MSE vs NLL vs BVM

This section shows that the predicted variance (using our method) is as well-calibrated as the one from Deep Ensembles (using NLL) and is better calibrated than the empirical variance (using MSE). In (Lakshminarayanan, Pritzel, and Blundell 2017), it was shown that training an ensemble of NNs with a single output (representing the mean) using MSE and computing the empirical variance of the networks’ predictions to estimate uncertainty does not lead to well-calibrated predictive probabilities. This was due to the fact that MSE does not capture predictive uncertainty. It was then shown that learning the predictive variance by training an ensemble of NNs with two outputs (corresponding to the mean and variance) using NLL (i.e. Deep Ensembles) results in well-calibrated predictions. We show that this is also the case for the proposed BVM loss.

We reproduce an experiment from (Lakshminarayanan, Pritzel, and Blundell 2017) using the BVM loss function (with $\epsilon = 0.01$), where we construct reliability diagrams (also known as calibration curves) on the benchmark datasets. The procedure is as follows: (i) we calculate the $z\%$ prediction interval for each test point (using the predicted mean and variance), (ii) we then measure the actual fraction of test observations that fall within this prediction interval, and (iii) we repeat the calculations for $z = 10\%, \ldots, 90\%$ in steps of 10. If the actual fraction is close to the expected fraction (i.e. $\approx z\%$), this indicates that the predictive probabilities are well-calibrated. The ideal output would be a diagonal line. In other words, a regressor is considered to be well-calibrated if its calibration curve is close to the diagonal.

![Reliability diagram for the Energy dataset](image)

Figure 2: Reliability diagram for the Energy dataset. The predicted variance using our approach is as well-calibrated as the one from Deep Ensembles (using NLL) and is better calibrated than the empirical variance using MSE, which is overconfident.

We report the reliability diagram for the Energy dataset in Figure 2; diagrams for the other benchmark datasets are reported in Appendix A (the trend is the same for all datasets). We find that our method provides well-calibrated uncertainty estimates with a calibration curve very close to the diagonal (and almost overlapping with the curve of Deep Ensembles (Lakshminarayanan, Pritzel, and Blundell 2017)). We also find that the predicted variance (learned using BVM or NLL) is better calibrated than the empirical variance (computed by training five NNs using MSE) which is overconfident. For instance, for the 40% prediction interval (i.e. the expected fraction is equal to 0.4), the actual fraction of test observations that fall within the interval is only 10% (i.e. the observed fraction is around 0.1). In other words, the empirical variance (using MSE) underestimates the true uncertainty.

3.3 Real world datasets

We further evaluate our proposed method by comparing it to existing state-of-the-art methods. We adopt the same experimental setup as in (Hernández-Lobato and Adams 2015) for evaluating PBP, (Gal and Ghahramani 2016) for evaluating MC-dropout, and (Lakshminarayanan, Pritzel, and Blundell 2017) for evaluating Deep Ensembles. We use one-hidden-layer NNs with Rectified Linear Unit (ReLU) activation function (Nair and Hinton 2010), consisting of 50 hidden units for all datasets except for the largest one (i.e. Protein) where we use NNs with 100 hidden units. We train NNs using the BVM loss function with $\epsilon = 0.01$. Each dataset is randomly split into training and test sets with 90% and 10% of the available data, respectively. For each train-test split, we train an ensemble of 5 networks. We repeat the splitting process 20 times and report the average test performance of our proposed method. For the larger Protein dataset, we perform the train-test splitting 5 times (instead of 20).

In our experiments, we run the training for 40 epochs, using mini-batches of size 32 and AdamW optimizer with fixed learning rate of $3 \times 10^{-4}$. For all the datasets, we apply feature scaling by standardizing the input features to have zero mean and unit variance, and normalize the targets to have a range of $[0, 1]$ (in the training set). Before evaluating the predictions, we invert the normalization factor on the predictions so they are back to the original scale of the targets for the purpose of error evaluation. Note that a sigmoid activation function is applied to the outputs of the NNs corresponding to the mean and variance. We summarize our results in Table 1, along with the results of PBP, MC-dropout, and Deep Ensembles as were outlined in their respective papers. For each dataset, the best method(s) is (are) highlighted in bold.

The results in Table 1 clearly demonstrate that our proposed method is competitive with existing state-of-the-art methods. As might be expected, our method performs suboptimally compared to other methods in terms of RMSE (e.g. on the Energy dataset). Since our method optimizes for the BVM loss, which learns both the mean and the variance (to better capture uncertainties) rather than learning only the mean, it gives less optimal RMSE values. Also note that, although our method outperforms PBP and MC-dropout in terms of NLL on many datasets, it did not outperform Deep Ensembles (e.g. on the Energy dataset, our method produces the second lowest NLL average of 1.67 behind Deep Ensembles whose NLL average is 1.38). Since the Deep Ensembles method optimizes for NLL, it is expected to perform better than the BVM approach for $\epsilon > 0$ – at least when the splitting of the data into training and test sets is done randomly (i.e. when tested on in-distribution datasets).
The methods are comparable and identical in the limit $\epsilon \to 0$, because the BVM loss becomes equivalent to NLL. We intentionally used a nonzero $\epsilon$ to highlight its effect on the predictions (compared to Deep Ensembles) when tested on in-distribution samples. We later introduce and apply the concept of “outlier train-test splitting”, and show that our method outperforms Deep Ensembles when evaluated on out-of-distribution samples (see Section 3.4).

### 3.4 Robustness and out-of-distribution generalization

We aim to show that our proposed method is robust and able to generalize better to out-of-distribution (OOD) data than Deep Ensembles. That is, if we evaluate our method on data that is statistically different from the training data, we observe more robustness and higher predictive uncertainties.

**Experiment 1** We consider a training set consisting of Google stock prices for a period of 5 years (from the beginning of 2012 till the end of 2016) and a test set containing the stock prices of January 2017 (see Figure 3). In particular, we consider the Google opening stock price, i.e. the stock price at the beginning of the financial/trading day. It is worth noting that the input feature vector is 60-dimensional corresponding to a 60-day window, i.e. for a given day, the NN will consider the stock prices for the past 60 days, and based on the trends captured during this time window, it will predict the corresponding stock price (with its uncertainty).

We train an ensemble of 5 NNs consisting of 4 hidden layers with 50 hidden units per layer. We run the training for 40 epochs, using batch size of 32 and Adam optimizer with fixed learning rate of $1 \times 10^{-3}$. We repeat this process for three different loss functions: (i) The NLL loss in (4) used in Deep Ensembles (Lakshminarayanan, Pritzel, and Blundell 2017), (ii) the BVM loss in (17) with $\epsilon = 0.01$, and (iii) the BVM loss with $\epsilon = 0.1$. We plot the predicted mean stock price along with the 95% prediction interval corresponding to January 2017. The results are shown in Figure 3.

The results clearly demonstrate that the value of $\epsilon$ in the BVM loss affects the predictive uncertainty (i.e. the prediction interval). A small value of $\epsilon$ corresponds to a stricter agreement condition between the NN predictive means and the observed targets, which results in a narrower prediction interval (i.e. lower variance values). Note that using $\epsilon = 0.01$ results in a predictive envelope that almost overlaps with the prediction interval of Deep Ensembles. When we increase the value of $\epsilon$ to 0.1 in the BVM loss, the agreement conditions become less stringent, and this leads to a wider prediction interval, which better captures the uncertainty of the stock price in the test set. This results in a lower NLL for this highly volatile test set.

The NLL results are summarized in Table 2. Due to the out-of-distribution nature of the test data, the BVM loss with a relatively large $\epsilon = 0.1$ results in the lowest NLL. Since this loss leads to the largest variances (or uncertainties), its corresponding likelihood (2) will be the largest, which is equivalent to the lowest NLL. Using a very large $\epsilon$ will overly coarse grain the data and one will lose predictive power.

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**Table 1**: Average test performance in RMSE and NLL on regression benchmark datasets.

| Dataset       | N  | d   | Avg. Test RMSE and Std. Errors | BVM | Avg. Test NLL and Std. Errors |
|---------------|----|-----|-------------------------------|-----|-------------------------------|
|               |    |     | PBP | MC-dropout | Deep Ensembles |       | PBP | MC-dropout | Deep Ensembles |
| Boston housing| 506| 13  | 3.01 ± 0.18 | 2.97 ± 0.19 | 3.28 ± 1.00 | 3.06 ± 0.22 | 2.57 ± 0.09 | 2.46 ± 0.06 | 2.41 ± 0.25 | 2.52 ± 0.08 |
| Concrete      | 1,030| 8   | 1.80 ± 0.05 | 1.66 ± 0.04 | 2.09 ± 0.29 | 2.16 ± 0.07 | 2.04 ± 0.02 | 1.99 ± 0.02 | 1.38 ± 0.22 | 1.67 ± 0.13 |
| Energy        | 768| 8   | 8.192 | 8.064 | 8.192 | 8.192 | 8.192 | 8.192 | 8.192 | 8.192 |
| Kin8nm        | 15,934| 16  | 0.01 ± 0.00 | 0.01 ± 0.00 | 0.00 ± 0.00 | 0.01 ± 0.00 | -0.90 ± 0.01 | -0.95 ± 0.01 | -1.20 ± 0.02 | -0.85 ± 0.10 |
| Naval propulsion plant | 4,020 | 10  | 0.01 ± 0.00 | 0.01 ± 0.00 | 0.00 ± 0.00 | 0.01 ± 0.00 | -3.73 ± 0.01 | -3.80 ± 0.01 | -5.63 ± 0.05 | -3.92 ± 0.01 |
| Protein       | 45,730| 9   | 0.01 ± 0.00 | 0.01 ± 0.00 | 0.00 ± 0.00 | 0.01 ± 0.00 | 2.84 ± 0.01 | 2.80 ± 0.01 | 2.79 ± 0.04 | 3.07 ± 0.08 |
| Wine          | 1,599| 11  | 0.01 ± 0.00 | 0.01 ± 0.00 | 0.00 ± 0.00 | 0.01 ± 0.00 | 2.97 ± 0.00 | 2.89 ± 0.00 | 2.83 ± 0.02 | 3.02 ± 0.03 |
| Yacht         | 506| 8   | 0.01 ± 0.00 | 0.01 ± 0.00 | 0.00 ± 0.00 | 0.01 ± 0.00 | 0.97 ± 0.01 | 0.93 ± 0.01 | 0.94 ± 0.12 | 1.01 ± 0.09 |

**Table 2**: Test performance in NLL on Google stocks dataset.

| Dataset       | N  | d   | Deep Ensembles | BVM $(\epsilon = 0.01)$ | BVM $(\epsilon = 0.1)$ |
|---------------|----|-----|----------------|-------------------------|-------------------------|
| Google stocks | 1,198| 60  | 5.23 | 5.19 | 5.13 |
Table 3: Test performance in NLL on top 10% outliers in regression benchmark datasets, along with the statistical differences between the normalized train-test targets. The datasets with large statistical differences are highlighted in gray.

| Dataset            | N  | d  | Statistical Difference | Test NLL | Deep Ensembles | BVM |
|--------------------|----|----|------------------------|---------|----------------|-----|
| Boston housing     | 506| 13 | 0.05                   | 0.06    | 4.51           | 3.92|
| Concrete           | 1,030| 8  | 0.14                   | -0.01   | 4.12           | 3.84|
| Energy             | 768 | 8  | 0.06                   | 0.01    | 2.98           | 2.57|
| Kin8nm             | 8,192| 8 | -0.04                  | 0.01    | -0.85          | -0.87|
| Naval propulsion plant | 11,934| 16 | 0.01                   | 0.02    | -4.42          | -3.84|
| Power plant        | 9,568| 4  | -0.01                  | 0.02    | 2.82           | 3.18|
| Protein            | 45,730| 9 | 0.00                   | 0.01    | 2.86           | 3.09|
| Wine               | 1,599| 11 | 0.04                   | 0.02    | 3.15           | 1.47|
| Yacht              | 308 | 6  | 0.26                   | 0.10    | 3.95           | 1.83|

Taylor expanding around $\epsilon = 0$ leads to

\[
- \log \left( \frac{1}{2e} \left[ \Phi \left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) - \Phi \left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] \right)
\]

\[\approx \frac{1}{2} \log 2\pi \sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} - \frac{\epsilon^2}{6} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - \frac{1}{\sigma_n^2} \right] + O(\epsilon^3) \] (13)

The proof can be found in Appendix B. Thus, the minimizer of the BVM loss over the set of all input feature vectors can be approximated as

\[
\arg\min_{\mu_n, \sigma_n} \frac{1}{N} \sum_{n=1}^{N} \left( \frac{1}{2} \log 2\pi \sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} - \frac{\epsilon^2}{6} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - \frac{1}{\sigma_n^2} \right] \right) \] (14)

We can clearly see that for $\epsilon = 0$, the minimizer of the BVM loss is indeed the minimizer of the NLL loss in Equation (4). For a nonzero $\epsilon$, $\sigma_n$ will increase linearly with $\epsilon$ (see proof in Appendix B) leading to a larger variance, and hence a wider distribution (or prediction interval). Thus, the OOD samples near the tails (i.e. the outliers) will be more probable resulting in lower NLL values compared to Deep Ensembles (keeping in mind that the in-distribution samples near the mean will be less probable resulting in higher NLL values compared to Deep Ensembles, which was the case in Table 1).

4 Conclusion

In this work, we proposed a new loss function for regression uncertainty estimation (based on the BVM framework) which reproduces maximum likelihood estimation in the limiting case. This loss, boosted by ensemble learning, improves predictive performance when the training and test sets are statistically different. Experiments on in-distribution data show that our method generates well-calibrated uncertainty estimates and is competitive with existing state-of-the-art methods. When tested on out-of-distribution samples (outliers), our method exhibits superior predictive power by consistently displaying improved predictive log-likelihoods. Because the data source statistics in the learning and deployed environments are often known to be different, our method can be used to improve safety and decision-making in the deployed environment. Our future work involves expanding the BVM framework to address predictive uncertainty estimation in classification problems.
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Vanslette, K.; Tohme, T.; and Youcef-Toumi, K. 2020. A general model validation and testing tool. Reliability Engineering & System Safety, 195: 106684.
A Training using MSE vs NLL vs BVM

This section shows that the predicted variance (using our method) is as well-calibrated as the one from Deep Ensembles (using NLL) and is better calibrated than the empirical variance (using MSE). In (Lakshminarayanan, Pritzel, and Blundell 2017), it was shown that training an ensemble of NNs with a single output (representing the mean) using MSE and computing the empirical variance of the networks’ predictions to estimate uncertainty does not lead to well-calibrated predictive probabilities. This was due to the fact that MSE does not capture predictive uncertainty. It was then shown that learning the predictive variance by training NNs with two outputs (corresponding to the mean and variance) using NLL (i.e. Deep Ensembles) results in well-calibrated predictions. We show that this is also the case for the proposed BVM loss.

We reproduce an experiment from (Lakshminarayanan, Pritzel, and Blundell 2017) using the BVM loss function, where we construct reliability diagrams (also known as calibration curves) on the benchmark datasets. The procedure is as follows: (i) we calculate the $z\%$ prediction interval for each test point (using the predicted mean and variance), (ii) we then measure the actual fraction of test observations that fall within this prediction interval, and (iii) we repeat the calculations for $z = 10\%, \ldots, 90\%$ in steps of 10. If the actual fraction is close to the expected fraction (i.e. $\approx z\%$), this indicates that the predictive probabilities are well-calibrated. The ideal output would be the diagonal line. In other words, a regressor is considered to be well-calibrated if its calibration curve is close to the diagonal.

We report the reliability diagrams for the benchmark datasets in Figure 4. We find that our method provides well-calibrated uncertainty estimates with a calibration curve very close to the diagonal (and almost overlapping with the curve of Deep Ensembles (Lakshminarayanan, Pritzel, and Blundell 2017)). We also find that the predicted variance (learned using BVM or NLL) is better calibrated than the empirical variance (computed by training five NNs using MSE) which is overconfident. For instance, if we consider the reliability diagram for the Boston Housing dataset, for the 60% prediction interval (i.e. the expected fraction is equal to 0.6), the actual fraction of test observations that fall within the interval is only 20% (i.e. the observed fraction is around 0.2). In other words, the empirical variance (using MSE) underestimates the true uncertainty. The trend is the same for all datasets.

![Figure 4: Reliability diagrams for the benchmark datasets. The predicted variance using our approach is as well-calibrated as the one from Deep Ensembles (using NLL) and is better calibrated than the empirical variance using MSE.](image-url)
B Why does BVM outperform Deep Ensembles on OOD samples? (detailed proof)

Recall from Section 2.5 that the $\epsilon$-BVM probability of agreement for a given input feature vector $x_n$ can be expressed as

$$p(A|M, D, B(\epsilon), x_n) = \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right),$$  

(15)

where $\Phi(\cdot)$ is the cumulative distribution function (cdf) of the standard normal distribution:

$$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx.$$  

(16)

Also recall that the (overall) negative log $\epsilon$-BVM probability of agreement (i.e. the BVM loss function) over the set of all input feature vectors $x = \{x_1, \ldots, x_N\}$ is

$$C_{BVM}(B(\epsilon)) = \frac{1}{N} \sum_{n=1}^{N} - \log p(A|M, D, B(\epsilon), x_n) = \frac{1}{N} \sum_{n=1}^{N} - \log \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right].$$  

(17)

Note that for a given input feature vector $x_n$, the minimizer of the BVM loss function satisfies

$$\arg\min_{\mu_n, \sigma_n} \log \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] = \arg\min_{\mu_n, \sigma_n} \log \left( \frac{1}{2\epsilon} \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] \right).$$  

(18)

Taylor expanding around $\epsilon = 0$ leads to

$$- \log \left( \frac{1}{2\epsilon} \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] \right) \approx \frac{1}{2} \log 2\pi\sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} - \frac{\epsilon^2}{6} \frac{(t_n - \mu_n)^2}{\sigma_n^4} - \frac{1}{\sigma_n^2} + O(\epsilon^3)$$  

(19)

Proof. Let for a given input feature vector $x_n$ the function $g(\epsilon, x_n)$ be defined by

$$g(\epsilon, x_n) = \frac{1}{2\epsilon} p(A|M, D, B(\epsilon), x_n) = \frac{1}{2\epsilon} \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right]$$  

(20)

Then, we have

$$g'(\epsilon, x_n) = \frac{1}{4\epsilon^2} \left[ 2\epsilon \left( \frac{1}{\sigma_n} \varphi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) + \frac{1}{\sigma_n} \varphi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right) - 2 \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] \right]$$

$$= \frac{1}{2\epsilon^2} \left( \frac{\epsilon}{\sigma_n} \left[ \varphi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) + \varphi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] - \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] \right]$$  

(21)

and

$$g''(\epsilon, x_n) = \frac{1}{4\epsilon^2} \left[ 2\epsilon^2 \left( \frac{1}{\sigma_n} \left[ \varphi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) + \varphi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] + \frac{\epsilon}{\sigma_n^2} \left[ \varphi'\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \varphi'\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] \right]$$

$$- \frac{1}{\sigma_n} \left[ \varphi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) + \varphi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right]$$

$$- 4\epsilon \left( \frac{\epsilon}{\sigma_n} \left[ \varphi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) + \varphi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] - \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] \right)$$

$$= \frac{1}{2\epsilon^3} \left[ \frac{\epsilon^2}{\sigma_n^2} \left[ \varphi'\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \varphi'\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] \right]$$

$$- 2 \left( \frac{\epsilon}{\sigma_n} \left[ \varphi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) + \varphi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] - \left[ \Phi\left(\frac{t_n + \epsilon - \mu_n}{\sigma_n}\right) - \Phi\left(\frac{t_n - \epsilon - \mu_n}{\sigma_n}\right) \right] \right)$$
where $\varphi(\cdot)$ is the probability density function (pdf) of the standard normal distribution:

$$
\varphi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}
$$

(22)

In what follows we will also use $\varphi'(\cdot)$ and $\varphi''(\cdot)$ which are expressed as

$$
\varphi'(x) = -\frac{x}{\sqrt{2\pi}} e^{-x^2/2} \quad \text{and} \quad \varphi''(x) = \frac{x^2 - 1}{\sqrt{2\pi}} e^{-x^2/2} = (x^2 - 1) \varphi(x)
$$

(23)

The Taylor series approximation of $g(\epsilon, x_n)$ near $\epsilon = 0$ is

$$
g(\epsilon, x_n) \simeq g(0, x_n) + \frac{g'(0, x_n)}{1!} (\epsilon - 0) + \frac{g''(0, x_n)}{2!} (\epsilon - 0)^2 + \mathcal{O}(\epsilon^3)
$$

$$
= g(0, x_n) + \epsilon g'(0, x_n) + \frac{\epsilon^2}{2} g''(0, x_n) + \mathcal{O}(\epsilon^3)
$$

(24)

where $g(0, x_n)$, $g'(0, x_n)$, and $g''(0, x_n)$ can be derived as follows:

**Term 1:**

$$
g(0, x_n) = \lim_{\epsilon \to 0} g(\epsilon, x_n)
$$

$$
= \lim_{\epsilon \to 0} \frac{1}{2\epsilon} \left[ \Phi \left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) - \Phi \left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right]
$$

$$
= \lim_{\epsilon \to 0} \frac{1}{2} \left[ \frac{1}{\sigma_n} \varphi \left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) + \frac{1}{\sigma_n} \varphi \left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] \quad \text{(using L'Hôpital's rule)}
$$

$$
= \frac{1}{2\sigma_n} \left[ \varphi \left( \frac{t_n - \mu_n}{\sigma_n} \right) + \varphi \left( \frac{t_n - \mu_n}{\sigma_n} \right) \right]
$$

$$
= \frac{1}{\sigma_n} \varphi \left( \frac{t_n - \mu_n}{\sigma_n} \right)
$$

(25)

It follows that $g(0, x_n)$ is the pdf of the general normal distribution:

$$
g(0, x_n) = \frac{1}{\sqrt{2\pi}\sigma_n^2} \exp \left\{ - \frac{(t_n - \mu_n)^2}{2\sigma_n^2} \right\}
$$

(26)

**Term 2:**

$$
g'(0, x_n) = \lim_{\epsilon \to 0} g'(\epsilon, x_n)
$$

$$
= \lim_{\epsilon \to 0} \frac{1}{2\epsilon} \left[ \frac{\epsilon}{\sigma_n} \left[ \varphi \left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) + \varphi \left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] - \left[ \Phi \left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) - \Phi \left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] \right]
$$

$$
= \lim_{\epsilon \to 0} \frac{1}{4\epsilon} \left[ \frac{\epsilon}{\sigma_n} \left[ \varphi \left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) + \varphi \left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] + \frac{\epsilon}{\sigma_n^3} \left[ \varphi' \left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) - \varphi' \left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] \right]
$$

(26)

(27)

(28)

It follows that

$$
g'(0, x_n) = 0
$$

(28)
Term 3:

\[ g''(0, x_n) = \lim_{\epsilon \to 0} g''(\epsilon, x_n) \]

\[ = \lim_{\epsilon \to 0} \frac{1}{2\epsilon^2} \left[ \frac{\epsilon^2}{\sigma_n^2} \left[ \varphi'\left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) - \varphi'\left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] \right. \]

\[ - 2 \left( \frac{\epsilon}{\sigma_n} \left[ \varphi\left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) + \varphi\left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] - \left[ \Phi\left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) - \Phi\left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] \right] \]

\[ = \lim_{\epsilon \to 0} \frac{1}{6\epsilon^2} \left[ \frac{2\epsilon}{\sigma_n^2} \left[ \varphi'\left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) - \varphi'\left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] + \frac{\epsilon^2}{\sigma_n^3} \left[ \varphi''\left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) + \varphi''\left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] \right. \]

\[ - 2 \left( \frac{1}{\sigma_n} \left[ \varphi\left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) + \varphi\left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] + \frac{\epsilon}{\sigma_n} \left[ \varphi'\left( \frac{t_n + \epsilon - \mu_n}{\sigma_n} \right) - \varphi'\left( \frac{t_n - \epsilon - \mu_n}{\sigma_n} \right) \right] \right] \]

\[ = \frac{\epsilon^2}{6\sigma_n^3} \left[ \varphi''\left( \frac{t_n - \mu_n}{\sigma_n} \right) + \varphi''\left( \frac{t_n - \mu_n}{\sigma_n} \right) \right] \]

\[ = \frac{1}{3\sigma_n^3} \varphi''\left( \frac{t_n - \mu_n}{\sigma_n} \right) \]

\[ = \frac{1}{3\sigma_n^3} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - 1 \right] \varphi\left( \frac{t_n - \mu_n}{\sigma_n} \right) \quad \text{(using } \varphi''(x) = (x^2 - 1) \varphi(x)) \]

(29)

It follows that

\[ g''(0, x_n) = \frac{1}{3\sigma_n^3} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - 1 \right] \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp \left\{ - \frac{(t_n - \mu_n)^2}{2\sigma_n^2} \right\} \]

(30)

Hence, the Taylor series approximation of \( g(\epsilon, x_n) \) around \( \epsilon = 0 \) is

\[ g(\epsilon, x_n) \approx g(0, x_n) + \epsilon g'(0, x_n) + \frac{\epsilon^2}{2} g''(0, x_n) + O(\epsilon^3) \]

\[ = \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp \left\{ - \frac{(t_n - \mu_n)^2}{2\sigma_n^2} \right\} + \frac{\epsilon^2}{2} \frac{1}{3\sigma_n^2} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - 1 \right] \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp \left\{ - \frac{(t_n - \mu_n)^2}{2\sigma_n^2} \right\} + O(\epsilon^3) \]

\[ = \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp \left\{ - \frac{(t_n - \mu_n)^2}{2\sigma_n^2} \right\} \left[ 1 + \frac{\epsilon^2}{2} \frac{1}{3\sigma_n^2} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - 1 \right] \right] + O(\epsilon^3) \]

(31)

Taking its negative log gives

\[ - \log g(\epsilon, x_n) \approx \frac{1}{2} \log 2\pi\sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} - \log \left( 1 + \frac{\epsilon^2}{2} \frac{1}{3\sigma_n^2} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - 1 \right] \right) + O(\epsilon^3) \]

\[ \approx \frac{1}{2} \log 2\pi\sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} - \frac{\epsilon^2}{2} \frac{1}{3\sigma_n^2} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - 1 \right] + O(\epsilon^3) \quad \text{(using } \log(1 + x) \approx x \text{ for } x \text{ near 0)} \]

\[ = \frac{1}{2} \log 2\pi\sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} - \frac{\epsilon^2}{6} \frac{1}{\sigma_n^4} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^2} - 1 \right] + O(\epsilon^3) \]

(32)
Thus, the minimizer of the BVM loss over the set of all input feature vectors can be approximated as

\[
\arg\min_{\mu_n, \sigma_n} \frac{1}{N} \sum_{n=1}^{N} \left( \frac{1}{2} \log 2\pi \sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} - \frac{e^2}{6} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^4} - \frac{1}{\sigma_n^2} \right] \right)
\]  
(33)

We can clearly see that for \( \epsilon = 0 \), the minimizer of the BVM loss is indeed the minimizer of the NLL loss in Equation (4). For a nonzero \( \epsilon \), \( \sigma_n \) will increase linearly with \( \epsilon \) (see proof below) leading to a larger variance, and hence a wider distribution (or prediction interval). Thus, the OOD samples near the tails (i.e., the outliers) will be more probable resulting in lower NLL values compared to Deep Ensembles (keeping in mind that the in-distribution samples near the mean will be less probable resulting in higher NLL values compared to Deep Ensembles).

**Proof.** Let for a given input feature vector \( x_n \) the function \( f(\epsilon, x_n) \) be defined by

\[
f(\epsilon, x_n) = \frac{1}{2} \log 2\pi \sigma_n^2 + \frac{(t_n - \mu_n)^2}{2\sigma_n^2} - \frac{e^2}{6} \left[ \frac{(t_n - \mu_n)^2}{\sigma_n^4} - \frac{1}{\sigma_n^2} \right]
\]  
(34)

For a fixed \( \epsilon \), the minimizers \( \mu_n \) and \( \sigma_n \) can be found by computing the gradients \( \nabla_{\mu_n} f \) and \( \nabla_{\sigma_n} f \) and setting them to zero:

\[
\nabla_{\mu_n} f = -\frac{t_n - \mu_n}{\sigma_n^2} + \frac{e^2}{3} \frac{t_n - \mu_n}{\sigma_n^3} = \frac{t_n - \mu_n}{\sigma_n^2} \left( -1 + \frac{e^2}{3\sigma_n^2} \right)
\]  
(35)

\[
\nabla_{\sigma_n} f = \frac{1}{\sigma_n} - \frac{(t_n - \mu_n)^2}{\sigma_n^3} - \frac{e^2}{6} \left[ -4 \frac{(t_n - \mu_n)^2}{\sigma_n^5} + \frac{2}{\sigma_n^3} \right]
\]  
(36)

Note that

\[
\nabla_{\mu_n} f = 0 \quad \text{for} \quad \mu_n = t_n \quad \text{or} \quad \sigma_n = \epsilon/\sqrt{3}
\]  
(37)

**Case 1:** \( \mu_n = t_n \)

In this case, we set \( \nabla_{\sigma_n} f \) to zero and we get

\[
\nabla_{\sigma_n} f = \frac{1}{\sigma_n} - \frac{(t_n - \mu_n)^2}{\sigma_n^3} - \frac{e^2}{6} \left[ -4 \frac{(t_n - \mu_n)^2}{\sigma_n^5} + \frac{2}{\sigma_n^3} \right] = \frac{1}{\sigma_n} - \frac{e^2}{3\sigma_n^3} = 0 \implies \sigma_n = \epsilon/\sqrt{3}
\]  
(38)

**Case 2:** \( \sigma_n = \epsilon/\sqrt{3} \)

In this case, we set \( \nabla_{\sigma_n} f \) to zero and we get

\[
\nabla_{\sigma_n} f = \frac{1}{\sigma_n} - \frac{(t_n - \mu_n)^2}{\sigma_n^3} - \frac{e^2}{6} \left[ -4 \frac{(t_n - \mu_n)^2}{\sigma_n^5} + \frac{2}{\sigma_n^3} \right]
\]

\[
= \frac{1}{\sigma_n} - \frac{(t_n - \mu_n)^2}{\sigma_n^3} \left[ 1 - 2 \frac{e^2}{3\sigma_n^2} \right] - \frac{1}{\sigma_n^3} \frac{e^2}{3\sigma_n^2}
\]

\[
= \frac{1}{\sigma_n^3} - \frac{(t_n - \mu_n)^2}{\sigma_n^3} (-1) - \frac{1}{\sigma_n^3}
\]

\[
= \frac{(t_n - \mu_n)^2}{\sigma_n^4} = 0 \implies \mu_n = t_n
\]  
(39)

Thus, in both cases, we have \( \mu_n = t_n \) and \( \sigma_n = \epsilon/\sqrt{3} \).

It follows that \( \sigma_n \) increases linearly with \( \epsilon \). The larger \( \epsilon \), the larger the variance and hence the more probable the OOD samples (and the less probable the in-distribution samples).