Being Bayesian, Even Just a Bit, 
 Fixes Overconfidence in ReLU Networks

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Abstract
The point estimates of ReLU classification networks—arguably the most widely used neural network architecture—have been shown to yield arbitrarily high confidence far away from the training data. This architecture, in conjunction with a maximum a posteriori estimation scheme, is thus not calibrated nor robust. Approximate Bayesian inference has been empirically demonstrated to improve predictive uncertainty in neural networks, although the theoretical analysis of such Bayesian approximations is limited. We theoretically analyze approximate Gaussian posterior distributions on the weights of ReLU networks and show that they fix the overconfidence problem. Furthermore, we show that even a simplistic, thus cheap, Bayesian approximation, also fixes these issues. This indicates that a sufficient condition for a calibrated uncertainty on a ReLU network is “to be a bit Bayesian”. These theoretical results validate the usage of last-layer Bayesian approximation and motivate a range of a fidelity-cost trade-off. We further validate these findings empirically via various standard experiments using common deep ReLU networks and Laplace approximations.

1. Introduction
As neural networks have been successfully applied in ever more domains, including safety-critical ones, the robustness of their predictions and the calibration of their predictive uncertainty have moved into focus, subsumed under the notion of AI safety (Amodei et al., 2016). A principal goal of uncertainty calibration is that learning machines and neural networks in particular, should assign low confidence to test cases not explained well by the training data or prior information (Gal, 2016). The most obvious cases are test points that lie “far away” from the training data. Many methods to achieve this goal have been proposed, both Bayesian (e.g. Blundell et al., 2015; Louizos & Welling, 2017; Zhang et al., 2018) and non-Bayesian (e.g. Lakshminarayanan et al., 2017; Liang et al., 2018; Hein et al., 2019).

ReLU networks are currently among the most widely used neural architectures. This class comprises any network that can be written as a composition of linear layers (including fully-connected, convolutional, and residual layers) and a ReLU activation function. But, while ReLU networks often achieve high accuracy, the uncertainty of their predictions has been shown to be miscalibrated (Guo et al., 2017). Indeed, Hein et al. (2019) demonstrated that ReLU networks are always overconfident “far away from the data”: scaling a training point \( x \) (a vector in a Euclidean input space) with a scalar \( \delta \) yields predictions of arbitrarily high confidence in the limit \( \delta \to \infty \). This means ReLU networks are susceptible to out-of-distribution (OOD) examples. Meanwhile, Bayesian methods have long been known empirically to improve the predictive uncertainty calibration. MacKay (1992a) demonstrated experimentally that the predictive uncertainty of Bayesian neural networks will naturally be high in regions not covered by training data. Although the theoretical analysis is still lacking, results like this raise the hope that the overconfidence problem of ReLU networks, too, might be mitigated by the use of Bayesian methods.

This paper offers a theoretical analysis of the binary classification case of ReLU networks with a logistic output layer. We show that equipping such networks with a Gaussian-approximated posterior—obtained via e.g. a Laplace approximation or variational Bayes—malignates the aforementioned theoretical problem, in the sense that the predictive confidence far away from the training data approaches a known limit, bounded away from one, whose value is controlled by the covariance. At the same time, in the case of Laplace approximations (MacKay, 1992b; Ritter et al., 2018), this treatment does not change the decision boundary of the trained network, so it has no negative effect on the predictive performance (cf. Figure 1). Furthermore, we show that a sufficient condition for this desirable property to hold is to apply a Bayesian method only to the last layer of a ReLU network. This motivates the commonly used
approximation scheme where an $L$-layer network is decomposed into a fixed feature map composed by the first $L-1$ layers and a Bayesian linear classifier (Snoek et al., 2015; Wilson et al., 2016; Brosse et al., 2020, etc.). This particular result implies that just being “a bit” Bayesian—at low cost overhead—already gives desirable benefits.

We empirically validate our results through Laplace approximations on common deep ReLU networks. Furthermore, while our theoretical analysis is focused on the binary classification case, we also experimentally show that these Bayesian approaches yield good performance in the multi-class classification setting, suggesting that our analysis may carry over to this case.

To summarize, our contributions are three-fold:

(i) we provide theoretical analysis on why Bayesian ReLU networks mitigate the overconfidence problem in the binary classification setting,

(ii) we show that a sufficient condition for having this property is to be “a bit” Bayesian: employing a last-layer Bayesian approximation, and

(iii) we validate our theoretical findings via a series of comprehensive experiments involving commonly-used deep ReLU networks and Laplace approximations in both binary and multi-class cases.

Section 2 begins with definitions, assumptions, and the problem statement, then develops the main theoretical results. Proofs are available in Appendix A. We discuss related work in Section 3, while empirical results are shown in Section 4.

2. Analysis

2.1. Preliminaries

Definitions

We call a function $f: \mathbb{R}^n \rightarrow \mathbb{R}^k$ piecewise affine if there exists a finite set of polytopes $\{Q_r\}_{r=1}^R$, referred to as the linear regions of $f$, such that $\bigcup_{r=1}^R Q_r = \mathbb{R}^n$ and $f|_{Q_r}$ is an affine function for every $Q_r$. ReLU networks are networks that result in piecewise affine classifier functions (Arora et al., 2018), which includes networks with fully-connected, convolutional, and residual layers where just ReLU or leaky-ReLU are used as activation functions and max or average pooling are used in convolution layers. Let $D := \{x_i \in \mathbb{R}^n, t_i\}_{i=1}^m$ be a dataset, where the targets are $t_i \in \{0, 1\}$ or $t_i \in \{1, \ldots, k\}$ for the binary and multi-class case, respectively. Let $\phi: \mathbb{R}^n \rightarrow \mathbb{R}^d$ be an arbitrary fixed feature map and write $\phi := \phi(x)$ for a given $x$. We define the logistic (sigmoid) function as $\sigma(z) := 1/(1 + \exp(-z))$ for $z \in \mathbb{R}$ and the softmax function as $\text{softmax}(\mathbf{z}, i) := \exp(z_i) / \sum_j \exp(z_j)$ for $\mathbf{z} \in \mathbb{R}^k$ and $i \in \{1, \ldots, k\}$. Given a neural network $f_\theta$, we consider the posterior distribution $p(\theta|D)$ over its parameters. The predictive distribution for the binary case is

$$p(y = 1|x, D) = \int \sigma(f_\theta(x)) p(\theta|D) d\theta,$$

and for the multi-class case

$$p(y = i|x, D) = \int \text{softmax}(f_\theta(x), i) p(\theta|D) d\theta.$$
exist) of their matrix argument, respectively.\footnote{We assume they are sorted in a descending order.} Similarly for the function $s_i(\cdot)$, $s_{\text{max}}(\cdot)$, and $s_{\text{min}}(\cdot)$ which return singular values instead. Finally, we always assume that the bias trick is used and $\| \cdot \|$ is the $\ell^2$ norm.

**Problem statement**

The following theorem from Hein et al. (2019) shows that ReLU networks exhibit arbitrarily high confidence far away from the training data: If a point $x \in \mathbb{R}^n$ is scaled by a sufficiently large scalar $\delta > 0$, the input $\delta x$ attains arbitrarily high confidence.

**Theorem 2.1** (Hein et al., 2019). Let $\mathbb{R}^d = \bigcup_{r=1}^{R} Q_r$ and $f_{Q_r}(x) = U_r x + c_r$ be the piecewise affine representation of the output of a ReLU network on $Q_r$. Suppose that $U_r$ does not contain identical rows for all $r = 1, \ldots, R$, then for almost any $x \in \mathbb{R}^n$ and any $\epsilon > 0$, there exists a $\delta > 0$ and a class $i \in \{1, \ldots, k\}$ such that it holds $\text{softmax}(f(\delta x), i) \geq 1 - \epsilon$. Moreover, $\lim_{\delta \to \infty} \text{softmax}(f(\delta x), i) = 1$.\hfill \qed

It is standard to treat neural networks as probabilistic models of the conditional distribution $p(y|x, \theta)$ over the prediction $y$. In this case, we define the confidence of any input point $x$ as the maximum predictive probability, which in the case of a binary problem, can be written as $\max_{x \in \{0,1\}} p(y = i|x, \theta) = \sigma(|f_\theta(x)|)$. Standard training involves assigning a maximum a posteriori (MAP) estimate $\theta_{\text{MAP}}$ to the weights, ignoring potential uncertainty on $\theta$. We will show that this lack of uncertainty is the primary cause of the overconfidence discussed by Hein et al. (2019) and argue that it can be fixed by considering the Bayesian predictive distribution (1) instead.

Even for a linear classifier parametrized by a single weight matrix $\theta = w$, there is generally no analytic solution for (1). But, good approximations exist when the distribution over the weights is a Gaussian $p(w|D) \approx \mathcal{N}(w|\mu, \Sigma)$ with mean $\mu$ and covariance $\Sigma$. One such approximation (Spiegelhalter & Lauritzen, 1990; MacKay, 1992a) is constructed by scaling the input of the probit function $\Phi$ by a constant $\lambda = \sqrt{\pi/8}$. Using this approximation and the Gaussian assumption, if we let $a := \frac{w^\top \phi}{\sqrt{8/\pi}}$, we get

$$p(y = 1|x, D) \approx \int \Phi(\sqrt{\pi/8} a) \mathcal{N}(a|\mu^\top \phi, \phi^\top \Sigma \phi) da$$

$$= \Phi\left(\frac{\mu^\top \phi}{\sqrt{8/\pi + \phi^\top \Sigma \phi}}\right) \approx \sigma(z(x)),$$

(3)

where the last step uses the approximation $\Phi(\sqrt{\pi/8} x) \approx \sigma(x)$ a second time, with

$$z(x) := \frac{\mu^\top \phi}{\sqrt{1 + \pi/8 \phi^\top \Sigma \phi}}.$$

In the case of $\mu = w_{\text{MAP}}$, Equation (3) can be seen as the “softened” version of the MAP prediction of the classifier, using the covariance of the Gaussian. The confidence in this case is $\max_{i \in \{0,1\}} p(y = i|x, D) = \sigma(|z(x)|)$.

We can generalize the previous insight to the case where the feature map $\phi$ is also assumed to be a Bayesian NN. Let $\theta \in \mathbb{R}^p$ be the parameter vector of a NN $f_\theta : \mathbb{R}^n \to \mathbb{R}$ with a given Gaussian approximate posterior $p(\theta|D) \approx \mathcal{N}(\theta|\mu, \Sigma)$. Let $x \in \mathbb{R}^n$ be an arbitrary input point. Letting $d := \nabla f_\theta(x)\mu$, we do a first-order Taylor expansion of $f_\theta$ at $\mu$ (MacKay, 1995): $f_\theta(x) \approx f_\mu(x) + d^\top(\theta - \mu)$. This implies that the distribution over $f_\theta(x)$ is given by $p(f_\theta(x)|x, D) \approx \mathcal{N}(f_\theta(x)|f_\mu(x), d^\top \Sigma \Sigma d)$. Therefore, we have

$$z(x) := \frac{f_\mu(x)}{\sqrt{1 + \pi/8 d^\top \Sigma d}}.$$  (5)

It is easy to see that (4) is indeed a special case of (5).

As the first notable property of this approximation, we show that, in contrast to some other methods for uncertainty quantification (e.g. Monte Carlo dropout, Gal & Ghahramani, 2016) it preserves the decision boundary induced by the MAP estimate.

**Proposition 2.2** (Invariant property). Let $f_\theta : \mathbb{R}^n \to \mathbb{R}$ be a binary classifier network parametrized by $\theta$ and let $\mathcal{N}(\theta|\mu, \Sigma)$ be the posterior over $\theta$ where $\mu = \theta_{\text{MAP}}$. Then for any $x \in \mathbb{R}^n$, we have $\sigma(f_{\theta_{\text{MAP}}}(x)) = 0.5$ if and only if $\sigma(z(x)) = 0.5$.

This property is useful in practice since it guarantees that employing the Bayesian technique on top of a MAP-trained network will not reduce the original classification accuracy. Virtually all state-of-the-art models in deep learning are trained via MAP estimation and sacrificing the classification performance that makes them attractive in the first place would be a waste.

### 2.2 Main results

As our central theoretical contribution, we show that for any $x \in \mathbb{R}^n$, asymptotically, the value of $|z(x)|$ in (5) goes to a quantity that only depends on the mean and covariance of the Gaussian over the weights. Moreover, this property also holds in the non-asymptotic regime far enough from the training data. This result implies that one can drive the confidence closer to the uniform (one-half) far away from the training points by shifting $|z(x)|$ closer to zero by controlling the Gaussian. We formalize this result in the following theorem. The situation is illustrated in Figure 2.
Theorem 2.3 (All-layer Bayesian). Let \( f_\theta : \mathbb{R}^n \to \mathbb{R} \) be a binary ReLU classification network parametrized by \( \theta \in \mathbb{R}^p \) with \( p \geq n \), and let \( \mathcal{N}(\theta|\mu, \Sigma) \) be the posterior. Then for any input \( x \in \mathbb{R}^n \), there exists an \( \alpha > 0 \) such that for any \( \delta \geq \alpha \), the confidence \( \sigma(|z(\delta x)|) \) is bounded from above by the limit \( \lim_{\delta \to \infty} \sigma(|z(\delta x)|) \). Furthermore,

\[
\lim_{\delta \to \infty} \sigma(|z(\delta x)|) \leq \sigma \left( \frac{\|u\|}{s_{\min}(J) \sqrt{\pi/8 \lambda_{\min}(\Sigma)}} \right),
\]

where \( u \in \mathbb{R}^n \) is a vector depending only on \( \theta \) and the \( n \times p \) matrix \( J := \frac{\partial u}{\partial \theta} \| \mu \) is the Jacobian of \( u \) w.r.t. \( \theta \) at \( \mu \).

The following question is practically interesting: Do we have to give a Bayesian treatment to the whole ReLU network for the previous property (Theorem 2.3) to hold? Surprisingly, the answer is no. The following theorem establishes that a guarantee similar to Theorem 2.3, is feasible even if only the last layer is given a Bayesian treatment.

Theorem 2.4 (Last-layer Bayesian). Let \( g : \mathbb{R}^d \to \mathbb{R} \) be a binary linear classifier defined by \( g(w(x)) := w^T \phi(x) \) where \( \phi : \mathbb{R}^n \to \mathbb{R}^d \) is a fixed ReLU network and let \( \mathcal{N}(w|\mu, \Sigma) \) be the posterior. Then for any input \( x \in \mathbb{R}^n \), there exists an \( \alpha > 0 \) such that for any \( \delta \geq \alpha \), the confidence \( \sigma(|z(\delta x)|) \) is bounded from above by the limit \( \lim_{\delta \to \infty} \sigma(|z(\delta x)|) \). Furthermore,

\[
\lim_{\delta \to \infty} \sigma(|z(\delta x)|) \leq \sigma \left( \frac{\|\mu\|}{\sqrt{\pi/8 \lambda_{\min}(\Sigma)}} \right).
\]

We show, using the same toy dataset as in Figure 1, an illustration of the previous results in Figure 3. Confirming the findings, for each input \( x \), the Bayesian treatment drives \( |z(\delta x)| \) to a constant for sufficiently large \( \delta \). Note that on true data points (\( \delta = 1 \)), the confidences remain high and the convergence occurs at some small \( \delta \).

Taken together, the results above formally validate the usage of Bayesian treatments on ReLU networks for mitigating overconfidence problems. Furthermore, Theorem 2.4 shows that a full-blown Bayesian treatment (i.e. on all layers of a NN) is not required to achieve control over the confidence far away from the training data. Indeed, it formally validates the usefulness of “being a bit Bayesian”.

We will show in extensive experiments (Section 4.3) that Bayesian treatments also mitigate asymptotic confidence in the multi-class case. However, extending the theoretical guarantees to this case is currently hampered by the lack of an analytic approximation of the integral in (2).

2.3. Laplace approximations

The results in the previous section imply that the asymptotic confidence of a Bayesian binary ReLU classifier—either via a full or last-layer Bayesian treatment—can be driven closer to uniform by controlling the posterior covariance. In this section, we analyze the case when a Laplace approximation is employed for obtaining the posterior. Although Laplace approximations are currently less popular than variational Bayes (VB), they have useful practical benefits: (i) they can be applied to any pre-trained network, (ii) whenever the approximation (5) can be employed, Proposition 2.2 holds, and (iii) no re-training is needed. Indeed, Laplace approximations can be attractive to practitioners who already have a working MAP-trained network, but want to enhance its uncertainty calibration further without decreasing performance.

The principle of Laplace approximations is as follows. Let \( p(\theta|D) \propto p(\theta) \prod_{t \in D} p(y = t|x, \theta) \) be the posterior of a network \( f_\theta \). Then we can obtain a Gaussian approximation \( p(\theta|D) \approx \mathcal{N}(\theta|\mu, \Sigma) \) of the posterior by setting \( \mu = \theta_{\text{MAP}} \)
and \( \Sigma = H^{-1} := (-\nabla^2 \log p(\theta | D)|_{\theta_{\text{MAP}}})^{-1} \), the inverse Hessian of the negative log-posterior at the mode. In the binary classification case, the likelihood \( p(y|x, w) \) is assumed to be a Bernoulli distribution \( B(\sigma(f_0(x))) \). The prior \( p(\theta) \) is assumed to be an isotropic Gaussian \( \mathcal{N}(\theta | 0, \sigma_0^2 I) \).

One needs to pick a value for the hyperparameter \( \sigma_0^2 \), the prior variance. In the following proposition, we analyze the effect of \( \sigma_0^2 \) on the asymptotic confidence presented by Theorem 2.3 in the previous section, for the all-layer Bayesian case. The statement for the case of last-layer Laplace is analogous and presented in Appendix A.

**Proposition 2.5** (All-layer Laplace). Let \( f_0 \) be a binary ReLU classification network modeling a Bernoulli distribution \( p(y|x, \theta) = B(\sigma(f_0(x))) \) with parameter \( \theta \in \mathbb{R}^p \). Let \( \mathcal{N}(\theta | \mu, \Sigma) \) be the posterior obtained via a Laplace approximation with prior \( \mathcal{N}(\theta | 0, \sigma_0^2 I) \) and \( J \) be the Jacobian as in Theorem 2.3. Then for any input \( x \in \mathbb{R}^n \), the confidence \( \sigma(|z(x)|) \) is a decreasing function of \( \sigma_0^2 \) with limits

\[
\lim_{\sigma_0^2 \to 0} \sigma(|z(x)|) = \sigma(|f_\mu(x)|), \\
\lim_{\sigma_0^2 \to \infty} \sigma(|z(x)|) \leq \sigma \left( \frac{|f_\mu(x)|}{1 + \sqrt{\frac{\pi}{8}} \lambda_{\text{max}}(H)||Jx||^2} \right).
\]

The result above shows that the confidence decreases (up to some limit) as the prior variance increases. Meanwhile, we recover the confidence induced by the MAP estimate as the prior variance goes to zero. One could therefore pick a value of \( \sigma_0^2 \) as high as possible for mitigating overconfidence. However, this is undesirable since it also lowers the confidence of the training data and test data around them (i.e. the so-called in-distribution data), thus, causing underconfident predictions. Another common way to set this hyperparameter is by maximizing the validation log-likelihood (Guo et al., 2017; Ritter et al., 2018). This is also inadequate for our purpose since it only considers points close to the training data.

Inspired by Hendrycks et al. (2019) and Hein et al. (2019), we simultaneously prefer high confidence on the in-distribution validation set and low confidence (high entropy) on the out-of-distribution validation set. Let \( \mathcal{D} := \{ (x_i, t_i) \}_{i=1}^m \) be a validation set and \( \tilde{\mathcal{D}} := \{ (\tilde{x}_i) \}_{i=1}^m \) be an out-of-distribution dataset. We then pick the optimal \( \sigma_0^2 \) by solving the following one-parameter optimization problem:

\[
\arg\min_{\sigma_0^2} -\frac{1}{m} \sum_{i=1}^m \log p(y = t_i | \tilde{x}_i, \mathcal{D}) + \lambda H[p(y|\tilde{x}_i, \mathcal{D})],
\]

where \( \lambda \in [0, 1] \) is controlling the trade-off between both terms. The first term in (8) is the standard cross-entropy loss over \( \mathcal{D} \) while the second term is the negative predictive entropy over \( \tilde{\mathcal{D}} \). Alternatively, the second term can be replaced by the cross-entropy loss where the target is the uniform probability vector. In all our experiments, we assume that \( \mathcal{D} \) is a collection of uniform noise in the input space.

### 3. Related work

The overconfidence problem of deep neural networks, and thus ReLU networks, has long been known in the deep learning community (Nguyen et al., 2015), although a formal description was only delivered recently. Many methods have been proposed to combat or at least detect this issue. Post-hoc heuristics based on temperature or Platt scaling (Platt et al., 1999; Guo et al., 2017; Liang et al., 2018) are unable to detect inputs with arbitrarily high confidence far away from the training data (Hein et al., 2019).

Many works on uncertainty quantification in deep learning have recently been proposed. Malinin & Gales (2018; 2019); Sensoy et al. (2018) used a Dirichlet distribution to model the distribution of a network’s output. Lakshminarayanan et al. (2017) quantify predictive uncertainty based on the idea of model ensembling and frequentist calibration. Hein et al. (2019) proposed enhanced training objectives based on robust optimization to mitigate this issue. However, the theoretical justification of these methods is still lacking. We argue that Bayesian methods provide the best of both worlds: they are principled methods and have empirically been shown to perform well for quantifying NNs’ predictive uncertainty.

Bayesian methods have long been thought to mitigate the overconfidence problem on any neural network (MacKay, 1992a). Empirical evidence supporting this intuition has also been presented (Liu et al., 2019; Wu et al., 2019, etc.). Our results complement these with a theoretical justification for the ReLU-logistic case. Furthermore, our theoretical results show that, in some cases, an expensive Bayesian treatment over all layers of a network is not necessary (Theorem 2.4), thus validating the usage of last-layer Bayesian methods such as Snoek et al. (2015) and Wilson et al. (2016).

### 4. Experiments

We corroborate our theoretical results via three experiments. In Section 4.1 we visualize the confidence of 2D binary and multi-class toy datasets. In Section 4.2 we empirically validate our main result that the confidence of binary classification datasets approaches finite constants as \( \delta \) increases. Furthermore, we show empirically that this property also holds in the multi-class case, along with the usefulness of Bayesian methods in standard OOD detection tasks in Section 4.3.

Unless stated otherwise, we use LeNet (for MNIST) or ResNet-18 (for CIFAR-10, SVHN, CIFAR-100) architec-
Being Bayesian, Even Just a Bit, Fixes Overconfidence in ReLU Networks

Figure 4. Binary (top) and multi-class (bottom) toy classification problem. Background color represents confidence.

Figure 5. Confidence of MAP (top row), temperature scaling (middle row), and LLLA (bottom row) as functions of $\delta$ over the test sets of binary classification datasets. Thick blue lines and shades correspond to means and ±3 standard deviations, respectively. Dashed lines signify the desirable confidence for $\delta$ sufficiently high.

We train these networks by following the procedure described by Meinke & Hein (2020) (Appendix C). To obtain the optimal hyperparameter $\sigma_0^2$, we follow (8) with $\lambda$ set to 0.25. We mainly use a last-layer Laplace approximation (LLLA) where a Laplace approximation with an exact Hessian or its Kronecker factors is applied only to the last layer of a network (Appendix B). Whenever the approximations of predictive distribution in (4) and (5) cannot be used, we compute them via Monte Carlo integrations with 100 posterior samples. Other Laplace approximations that we use will be introduced in the subsection where they are first employed. Besides the vanilla MAP method, we use the temperature scaling method (Guo et al., 2017) as a baseline since it claims to give calibrated predictions. In particular, the optimal temperature is found via a validation log-likelihood maximization using PyCalib Wenger et al. (2019). For each dataset that we use, we obtain a validation set via a random split from the respective test set.$^3$ Lastly, all numbers reported in this section are averages along with their standard deviations over 10 trials.

$^3$We use 50, 1000, and 2000 points for the toy, binary, and multi-class classification cases, respectively.
Table 1. OOD detection for far-away points in binary classification settings. The in-distribution datasets are Binary-MNIST, Binary-CIFAR10, Binary-SVHN, and Binary-CIFAR100. Each OOD dataset is obtained by scaling uniform noise images in the corresponding input space of the in-distribution dataset with $\delta = 100$. All values are means and standard deviations over 10 trials.

| MAP +Temp. | +LLL A |
|------------|---------|
|            | MMC ↓ | AUR ↑ | MMC ↓ | AUR ↑ | MMC ↓ | AUR ↑ |
| Binary-MNIST Noise ($\delta = 100$) | 99.9±0.0 | - | 100.0±0.0 | 45.1±5.8 | 79.4±0.9 | - |
| Binary-CIFAR10 Noise ($\delta = 100$) | 96.3±0.3 | - | 90.5±0.6 | - | 76.4±0.3 | - |
| Binary-SVHN Noise ($\delta = 100$) | 99.4±0.0 | - | 98.2±0.1 | - | 80.7±0.1 | - |
| Binary-CIFAR100 Noise ($\delta = 100$) | 94.5±0.5 | - | 74.5±2.9 | - | 66.7±0.5 | - |

Table 2. Multi-class OOD detection results for MAP, last-layer Laplace (LLL A), (all-layers) diagonal Laplace (DLA), and (all-layers) Kronecker-Factored Laplace (KFLA). Each “far-away” Noise dataset is constructed as in Table 1 with $\delta = 2000$. All values are averages and standard deviations over 10 trials.

| MAP +Temp. | +LLL A |
|------------|---------|
|            | MMC ↓ | AUR ↑ | MMC ↓ | AUR ↑ | MMC ↓ | AUR ↑ |
| MNIST - MNIST | 99.2±0.0 | - | 95.4±0.2 | - | 92.8±1.1 | - |
| MNIST - EMNIST | 82.3±0.0 | 82.9±0.1 | 87.6±1.4 | 88.9±0.2 | 70.2±1.9 | 92.0±0.4 |
| MNIST - FMNIST | 66.3±0.0 | 97.4±0.0 | 75.2±2.5 | 97.1±0.1 | 56.0±1.8 | 98.2±0.2 |
| MNIST - Noise ($\delta = 2000$) | 100.0±0.0 | 0.1±0.0 | 100.0±0.0 | 6.8±1.1 | 99.9±0.0 | 9.6±0.7 |
| CIFAR10 - CIFAR10 | 971.1±0.1 | - | 95.4±0.2 | - | 92.8±1.1 | - |
| CIFAR10 - SVHN | 62.5±0.0 | 95.8±0.1 | 54.6±0.6 | 96.1±0.0 | 45.9±1.6 | 96.4±0.1 |
| CIFAR10 - LSUN | 74.5±0.0 | 91.9±0.1 | 66.9±0.6 | 92.2±0.1 | 57.4±1.9 | 92.7±0.4 |
| CIFAR10 - Noise ($\delta = 2000$) | 98.7±0.2 | 10.9±0.4 | 98.4±0.2 | 10.0±0.5 | 17.4±0.0 | 100.0±0.0 |
| SVHN - SVHN | 98.5±0.0 | - | 974.2±0.0 | - | 93.2±1.0 | - |
| SVHN - CIFAR10 | 70.4±0.0 | 95.4±0.0 | 64.1±0.9 | 95.4±0.0 | 43.4±2.1 | 97.2±0.1 |
| SVHN - LSUN | 71.7±0.0 | 95.5±0.0 | 65.4±1.0 | 95.6±0.0 | 44.3±2.3 | 97.3±0.1 |
| SVHN - Noise ($\delta = 2000$) | 98.7±0.1 | 11.9±0.6 | 98.4±0.1 | 11.0±0.6 | 27.5±0.1 | 99.6±0.0 |
| CIFAR100 - CIFAR100 | 81.2±0.1 | - | 78.9±0.8 | - | 74.6±0.2 | - |
| CIFAR100 - SVHN | 53.5±0.0 | 78.8±0.1 | 49.2±1.2 | 79.2±0.1 | 42.7±0.3 | 80.4±0.2 |
| CIFAR100 - LSUN | 50.7±0.0 | 81.0±0.1 | 46.8±1.1 | 81.1±0.1 | 39.8±0.2 | 82.6±0.2 |
| CIFAR100 - Noise ($\delta = 2000$) | 99.5±0.1 | 2.8±0.2 | 99.4±0.1 | 2.6±0.2 | 5.9±0.0 | 99.9±0.0 |

4.1. Toy dataset

Here, the dataset is constructed by sampling the input points from $k$ independent Gaussians. The corresponding targets indicate from which Gaussian the point was sampled. We use a 3-layer ReLU network with 20 hidden units at each layer. We use the exact Hessian and the full generalized-Gauss-Newton (GGN) approximation of the Hessian for the case of LLLA and all-layer Laplace approximations, respectively.

We show the results for the binary and multi-class cases in Figure 4. The MAP predictions have high confidence everywhere except at the region close to the decision boundary. Temperature scaling assigns low confidence to the training data, while assigning high confidence far away from them. LLLA, albeit simple, yields calibrated predictions—high confidence close to the training points and high uncertainty otherwise—while maintaining the MAP’s decision boundary. Furthermore, we found that the all-layer Laplace approximation makes the aforementioned finding stronger: the boundaries of the high-confidence regions are now closer to the training data.

4.2. Binary classification

We validate our theoretical finding by plotting the test confidence of various binary classification datasets as functions of $\delta$. Each dataset is constructed by picking two classes which are most difficult to distinguish, based on the confusion matrix of the corresponding multi-class problem.

As shown in Figure 5, both MAP (top row) and temperature scaling (middle row) methods are overconfident for sufficiently large $\delta$. Meanwhile, LLLA which represents Bayesian methods, fixes this issue: As $\delta$ increases, the confidence converges to some constant close to the uniform confidence (one-half). Moreover, when $\delta = 1$ (the case of in-distribution data), LLLA retain higher confidence.

Table 1 further quantifies the results where we treat collections of 2000 uniform noise images scaled by $\delta = 100$
as the OOD datasets. Note that, while the resulting data points are not in the image space anymore, this construction is useful to assess the effectiveness of the Bayesian methods in unbounded problems. We report the standard metrics proposed by Hendrycks & Gimpel (2017): maximum-confidence (MMC) and area-under-ROC-curve (AUR). Confirming our finding in Figure 5, LLLA is able to detect OOD data with high accuracy: for the chosen values of $\delta$, the MMC and AUR values are close to the ideal values of 50 and 100, respectively. Both MAP and temperature scaling fail to do so since their confidence saturate to one. These results (i) confirm our theoretical analysis in Section 2, (ii) show that even a simple Bayesian method yields calibrated uncertainty, and (iii) temperature scaling is not calibrated for outliers far-away from the training data.\footnote{This confirms the theoretical arguments of Hein et al. (2019).}

4.3. Multi-class classification

We also show empirically that Bayesian methods yield a similar behavior in multi-class settings. On top of LLLA, representing Bayesian methods, we employ various other scalable Laplace approximation techniques: diagonal Laplace approximation (DLA) where a diagonal Gaussian is used to approximate the posterior over all layers of a network, and Kronecker-factored Laplace approximation (KFLA) (Ritter et al., 2018) where a matrix-variate normal is used to approximate the posterior over all layers. We use 20 posterior samples for both DLA and KFLA. We refer the reader to Appendix B for details.

For each training dataset we evaluate all methods both in the non-asymptotic (the corresponding OOD test datasets, e.g. SVHN and LSUN for CIFAR-10) and asymptotic (Noise datasets) regime. Each “far-away” Noise dataset is constructed by scaling 200 uniform noise images in the corresponding input space with $\delta = 2000$. As in the previous section, we report the MMC and AUR metrics.

As presented in Table 2, all the Bayesian methods improve the OOD detection performance of the base models both in the non-asymptotic and asymptotic regime. Especially in the asymptotic regime, all the Bayesian methods perform well, empirically confirming our hypothesis that our theoretical analysis carries over to the multi-class setting. Meanwhile, both MAP’s and temperature scaling’s MMC and AUR are close to 100 and 0, respectively.\footnote{I.e. the worst values for those metrics.} Moreover, while LLLA is the most simple Bayesian method in this experiment, it often outperforms DLA and KFLA. Our finding agrees with the prior observation that last-layer Bayesian approximations are often sufficient (Brosse et al., 2020). Furthermore, in Appendix D we also show that we can apply Laplace approximations on top of prior OOD detection methods such as ACET (Hein et al., 2019) and Outlier-Exposure (Hendrycks et al., 2019) to achieve state-of-the-art performance in the non-asymptotic regime, while also enjoying calibrated uncertainty in the asymptotic regime.

In Table 3, we present the computational cost analysis in terms of wall-clock time. We measure the time required for each method to do posterior inference (or finding the optimal temperature) and to make predictions. While MAP and temperature scaling are fast, as we have shown in the previous results, they fail to address the overconfidence problem. Among the Bayesian methods, since the cost of LLLA is constant w.r.t. the network depth, we found that it is up to two orders of magnitude faster than DLA and KFLA when making predictions. All in all, this finding, combined with the previous results, makes this simple Bayesian method attractive in applications.

5. Conclusion

We have shown analytically that Bayesian methods, especially when applied on ReLU classification networks, can mitigate the overconfidence problem that plagues deep learning. While this behavior does not seem surprising—indeed, Bayesian methods have empirically been known to give calibrated uncertainties—formal statements regarding this property had been missing. Our results provide some of these statements. Furthermore, we have shown, both theoretically and empirically, that a sufficient condition for a calibrated uncertainty in ReLU networks is to be “a bit Bayesian”: apply a Bayesian method to the last layer of the network. This result further validates the common usage of last-layer approximate Bayesian methods. Moreover, while this paper focuses only in the case of Laplace approximations, our results also hold for any Gaussian approximate Bayesian inference methods.
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A. Proofs

In the followings, the norm $\| \cdot \|$ is the standard $\ell^2$-norm.

**Proposition A.1.** Let $f_\theta : \mathbb{R}^n \to \mathbb{R}$ be a binary classifier network parametrized by $\theta$ and let $N(\theta | \mu, \Sigma)$ be the posterior over $\theta$ where $\mu = \theta_{MAP}$. Then for any $x \in \mathbb{R}^n$, we have $\sigma(f_{\theta_{MAP}}(x)) = 0.5$ if and only if $\sigma(z(x)) = 0.5$.

**Proof.** Let $x \in \mathbb{R}^n$ be arbitrary and denote $\mu_f := f_{\theta_{MAP}}(x)$ and $v_f := d(x)^T \Sigma d(x)$. For the forward direction, suppose that $\sigma(\mu_f) = 0.5$. This implies that $\mu_f = 0$, and we have $\sigma(0) = 0.5$. For the reverse direction, suppose that $\sigma(\mu_f) = 0.5$. This implies $\mu_f = 0$, and since the denominator of the l.h.s. is positive, it follows that $\mu_f$ must be 0, implying that $\sigma(\mu_f) = 0.5$.

**Lemma A.2 (Hein et al., 2019).** Let $\{Q_t\}_{t=1}^T$ be the set of linear regions associated to the ReLU network $f : \mathbb{R}^n \to \mathbb{R}^k$. For any $x \in \mathbb{R}^n$ there exists an $\alpha > 0$ and $t \in \{1, \ldots, T\}$ such that $\delta x \in Q_t$ for all $\delta \geq \alpha$. Furthermore, the restriction of $f$ to $Q_t$ can be written as an affine function $U^T x + c$ for some suitable $U \in \mathbb{R}^{n \times k}$ and $c \in \mathbb{R}$.

**Theorem A.3 (All-layer Bayesian).** Let $f_\theta : \mathbb{R}^n \to \mathbb{R}$ be a binary ReLU classification network parametrized by $\theta \in \mathbb{R}^p$ with $p \geq n$, and let $N(\theta | \mu, \Sigma)$ be the posterior. Then for any input $x \in \mathbb{R}^n$, there exists an $\alpha > 0$ such that for any $\delta \geq \alpha$, the confidence $\sigma(|\delta(\delta x)|)$ is bounded from above by the limit $\lim_{\delta \to 0} \sigma(|\delta(\delta x)|)$.

**Proof.** We prove the second statement—the upper-bound of the limit—first. By Lemma 3.1 of Hein et al. (2019) (also presented in Theorem A.2) there exists an $\alpha > 0$ and a linear region $R$, along with $u \in \mathbb{R}^n$ and $c \in \mathbb{R}$, such that for any $\delta \geq \alpha$, we have that $\delta x \in R$ and the restriction $f_{\theta_{R}}$ can be written as $U^T x + c$. Note that, for any such $\delta$, the vector $u^T$ and scalar $c$ are constant w.r.t. $\delta$. Therefore for any such $\delta$, we can write the gradient $d(\delta x)$ as follows:

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$$
\frac{\partial d(\delta x)}{\partial \theta} = \begin{bmatrix} \partial \Sigma d(\delta x) \end{bmatrix} + \begin{bmatrix} \partial c \end{bmatrix} \mu = \begin{bmatrix} \delta \Sigma d(\delta x) \end{bmatrix} + \begin{bmatrix} \delta c \end{bmatrix} \mu = \delta \left( J^T x + \frac{1}{\delta} \nabla_\theta c \right).
$$

**Using the Cauchy-Schwarz inequality and Lemma A.5, we can upper-bound this limit with**

$$
\lim_{\delta \to 0} |\delta(\delta x)| \leq \frac{\|u\| \|x\|}{\sqrt{\pi/8 \lambda_{\min}(\Sigma)} \|J^T x\|^2}.
$$

The following lemma is needed to get the desired result.

**Lemma A.4.** Let $A = U S V^T$ and $z \in \mathbb{R}^n$ with $m \geq n$, then $\|A z\|^2 \geq s_{\min}(A) \|z\|^2$.

**Proof.** By SVD, $A = U S V^T$. Notice that $U, V$ are orthonormal and thus are isometries, and that $S$ is a rectangular diagonal matrix with $n$ non-zero elements. Therefore,

$$
\|U(SV^T z)\|^2 = \|SV^T z\|^2 = \sum_{i=1}^n s_i^2(A)(V^T z)_i^2 \\
\geq s_{\min}(A) \sum_{i=1}^n (V^T z)_i^2 \\
= s_{\min}(A) \|V^T z\|^2 = s_{\min}(A) \|z\|^2,
$$

thus the proof is complete.

Notice that $J^T \in \mathbb{R}^{p \times n}$ with $p \geq n$ by our hypothesis. Therefore, using the previous lemma on $\|J^T x\|^2$ in conjunction with $s_{\min}(J) = s_{\min}(J^T)$, we conclude that

$$
\lim_{\delta \to 0} |z(\delta x)| \leq \frac{\|u\| \|x\|}{\sqrt{\pi/8 \lambda_{\min}(\Sigma)} s_{\min}(J) \|x\|^2} \\
= \frac{\|u\|}{s_{\min}(J) \sqrt{\pi/8 \lambda_{\min}(\Sigma)}},
$$

thus the upper-bound of the limit is proved.

To prove the first statement, let $L := \lim_{\delta \to 0} |z(\delta x)|$. Since $L$ is the limit of $|z|_{Q}(\delta x)$ in the linear region $Q$
given by Lemma A.2, it is sufficient to show that the function $(0, \infty) \to \mathbb{R}$ defined by $\delta \mapsto |z|_Q(\delta x)$ is increasing.

For some suitable choices of $u \in \mathbb{R}^n$ and $c \in \mathbb{R}$ that depends on the parameter $\theta$, we write the restriction of the ReLU network $f_{\theta}|_Q(x) = u^\top x + c$ as $\check{u}^\top x$ via the application of the bias trick, where $\check{u} := (u_1, \ldots, u_n, c)^\top$ and $x := (x_1, \ldots, x_n, 1)^\top$. Furthermore, we let the matrix $J := \frac{\partial}{\partial \theta} \check{u}$ to be the Jacobian of $\check{u}$ w.r.t. $\theta$ at $\mu$. Therefore for any $\delta \geq \alpha$, we can write as a function of $\delta$:

$$|z|_Q(\delta x) = \frac{|\delta \check{u}^\top|}{\sqrt{1 + \pi/8 \delta^2 (J^\top x)^\top \Sigma(J^\top x)}}$$

where for simplicity we have let $a := \check{u}^\top x$ and $b := (J^\top x)^\top \Sigma(J^\top x)$. The derivative is therefore given by

$$\frac{d}{d\delta}|z|_Q(\delta x) = \frac{\delta|a|}{(1 + \delta^2 b)\frac{1}{2}\delta}$$

and since $\Sigma$ is positive-definite, it is non-negative for $\delta \in (0, \infty]$. Thus we conclude that $|z|_Q(\delta x)$ is an increasing function. \hfill \Box

**Lemma A.5.** Let $x \in \mathbb{R}^n$ be a vector and $A \in \mathbb{R}^{n \times n}$ be an SPD matrix. If $\lambda_{\text{min}}(A)$ is the minimum eigenvalue of $A$, then $x^\top A x \geq \lambda_{\text{min}}||x||^2$.

**Proof.** Since $A$ is SPD, it admits an eigendecomposition $A = Q\Lambda Q^\top$ and $\Lambda = \Lambda^\frac{1}{2}\Lambda^\frac{1}{2}$ makes sense. Therefore, by keeping in mind that $Q^\top x$ is a vector in $\mathbb{R}^n$, we have

$$x^\top A x = x^\top Q\Lambda Q^\top x = ||\Lambda^\frac{1}{2} Q^\top x||^2$$

$$= \sum_{i=1}^{n} \lambda_i(A)(Q^\top x)_i^2 \geq \lambda_{\text{min}}(A) \sum_{i=1}^{n} (Q^\top x)_i^2$$

$$= \lambda_{\text{min}}(A)||Q^\top x||^2 = \lambda_{\text{min}}(A)||x||^2,$$

where the last equality is obtained since $||Q^\top x||^2 = x^\top Q^\top Q x$ and by noting that $Q$ is an orthogonal matrix. \hfill \Box

**Theorem A.6 (Last-layer Bayesian).** Let $g : \mathbb{R}^d \to \mathbb{R}$ be a binary linear classifier defined by $g(\phi(x)) := w^\top \phi(x)$ where $\phi : \mathbb{R}^n \to \mathbb{R}^d$ is a fixed ReLU network and let $N(w|\mu, \Sigma)$ be the posterior. Then for any input $x \in \mathbb{R}^n$, there exists an $\alpha > 0$ such that for any $\delta \geq \alpha$, the confidence $\sigma(|z|_Q(\delta x))$ is bounded from above by the limit $\lim_{\delta \to \infty} \sigma(|z|_Q(\delta x)))$. Furthermore,

$$\lim_{\delta \to \infty} \sigma(|z|_Q(\delta x))) \leq \sigma\left(\frac{||\mu||}{\sqrt{\pi/8 \lambda_{\text{min}}(\Sigma)}}\right). \quad (13)$$

**Proof.** We prove the second statement—i.e. the upper-bound of the limit—first. By Lemma 3.1 of Hein et al. (2019) there exists $\alpha > 0$ and a linear region $R$, along with $U \in \mathbb{R}^{d \times n}$ and $c \in \mathbb{R}^d$, such that for any $\delta \geq \alpha$, we have that $\delta x \in R$ and the restriction $\phi_R$ can be written as $Ux + c$. Therefore, for any such $\delta$,

$$|z \circ \phi_R(\delta x)| = \frac{|\mu^\top (\delta Ux + c)|}{\sqrt{1 + \pi/8 (\delta Ux + b)^\top \Sigma(\delta Ux + c)}}$$

$$= \frac{|\mu^\top (Ux + \frac{1}{2}c)|}{\sqrt{1 + \pi/8 (Ux + \frac{1}{2}c)^\top \Sigma(Ux + \frac{1}{2}c)}}$$

Now, notice that as $\delta \to \infty$, $1/\delta^2$ and $1/\delta$ goes to zero. So, in the limit, we have that

$$\lim_{\delta \to \infty} |z \circ \phi_R(\delta x)| = \frac{|\mu^\top (Ux)|}{\sqrt{\pi/8 (Ux)^\top \Sigma(Ux)}}.$$

Using Cauchy-Schwarz and Lemma A.5, we can upper-bound this limit with

$$\lim_{\delta \to \infty} |z \circ \phi_R(\delta x)| \leq \frac{||\mu|| ||Ux||}{\sqrt{\pi/8 \lambda_{\text{min}}(\Sigma)||Ux||^2}}$$

$$= \frac{||\mu||}{\sqrt{\pi/8 \lambda_{\text{min}}(\Sigma)}},$$

which concludes the proof for the second result.

For the first result, since $L$ is the limit of $|z|_{\theta}(\delta x)$ in the linear region $R$, it is sufficient to show that the function $(0, \infty) \to \mathbb{R}$ defined by $\delta \mapsto |z|_R(\delta x)$ is increasing.

We write the restriction of the ReLU network $\phi_R(x) = Ux + c$ as $\check{U}x$ via the application of the bias trick. Therefore for any $\delta \geq \alpha$, we can write as a function of $\delta$:

$$|z|_R(\delta x) = \frac{\delta|a|}{\sqrt{1 + \pi/8 \delta^2 (Ux)^\top \Sigma(Ux)}}$$

$$= \frac{|\delta a|}{\sqrt{1 + \pi/8 \delta^2 b}},$$

where for simplicity we have let $a := \mu^\top \check{U}x$ and $b := (Ux)^\top \Sigma(Ux)$. The derivative is therefore given by

$$\frac{d}{d\delta}|z|_R(\delta x) = \frac{\delta|a|}{(1 + \delta^2 b)\frac{1}{2}\delta},$$

and since $\Sigma$ is positive-definite, it is non-negative for $\delta \in (0, \infty]$. Thus we conclude that $|z|_R(\delta x)$ is an increasing function. \hfill \Box

**Proposition A.7 (All-layer Laplace).** Let $f_{\theta}$ be a binary ReLU classification network modeling a Bernoulli distribution $p(y|x, \theta) = B(\sigma(f_{\theta}(x)))$ with parameter $\theta \in \mathbb{R}^p$. Let
\( \mathcal{N}(\theta | \mu, \Sigma) \) be the posterior obtained via a Laplace approximation with prior \( \mathcal{N}(\theta | 0, \sigma_0^2 \mathbf{I}) \) and \( \mathbf{J} \) be the Jacobian as in Theorem 2.3. Then for any input \( x \in \mathbb{R}^n \), the confidence \( \sigma(|z(x)|) \) is a decreasing function of \( \sigma_0^2 \) with limits

\[
\lim_{\sigma_0^2 \to \infty} \sigma(|z(x)|) \leq \sigma \left( \frac{|f_\mu(x)|}{1 + \sqrt{\pi/8} \lambda_{\max}(\mathbf{H}) \| \mathbf{J} x \|^2} \right),
\]
\[
\lim_{\sigma_0^2 \to 0} \sigma(|z(x)|) = \sigma(|f_\mu(x)|).
\]

Proof. The assumption on the prior implies that

\(- \log p(\theta) = 1/2 \theta \top \left( 1/\sigma_0^2 \mathbf{I} \right) \theta + \text{const}, \)

which has Hessian \( 1/\sigma_0^2 \mathbf{I} \). Thus, the Hessian of the negative log posterior

\(- \log p(\theta | D) = - \log p(\theta) - \log \prod_{x, t \in D} p(y|x, \theta) \)

is \( 1/\sigma_0^2 \mathbf{I} + \mathbf{H} \). This implies that the posterior covariance \( \Sigma \) of the Laplace approximation is given by

\[
\Sigma = \left( \frac{1}{\sigma_0^2} \mathbf{I} + \mathbf{H} \right)^{-1}.
\]

Therefore, the \( i \)th eigenvalue of \( \Sigma \) for any \( i = 1, \ldots, n \) is

\[
\lambda_i(\Sigma) = \frac{1}{1/\sigma_0^2 + \lambda_i(\mathbf{H})} = \frac{\sigma_0^2}{1 + \sigma_0^2 \lambda_i(\mathbf{H})}.
\]

For all \( i = 1, \ldots, n \), the derivative of \( \lambda_i(\Sigma) \) w.r.t. \( \sigma_0^2 \) is \( 1/(1 + \sigma_0^2 \lambda_i(\mathbf{H}))^2 \) which is non-negative. This tells us that \( \lambda_i(\Sigma) \) is a non-decreasing function of \( \sigma_0^2 \). Furthermore, it is also clear that \( \sigma_0^2/(1 + \sigma_0^2 \lambda_i(\mathbf{H})) \) goes to \( 1/\lambda_i(\mathbf{H}) \) as \( \sigma_0^2 \) goes to infinity, while it goes to \( 0 \) as \( \sigma_0^2 \) goes to zero.

Now, we can write

\[
|z(x)| = \frac{|f_\mu(x)|}{\sqrt{1 + \pi/8 \sum_{i=1}^d \lambda_i(\Sigma)(\mathbf{Q}^\top \mathbf{d})^2}},
\]

where \( \Sigma = \mathbf{Q} \text{diag}(\lambda_1(\Sigma), \ldots, \lambda_d(\Sigma)) \mathbf{Q}^\top \) is the eigendecomposition of \( \Sigma \). It is therefore clear that the denominator of the r.h.s. is a non-decreasing function of \( \sigma_0^2 \). This implies \( |z(x)| \) is a non-increasing function of \( \sigma_0^2 \).

For the limits, it is clear that \( \lambda_{\min}(\Sigma) \) has limits \( 1/\lambda_{\max}(\mathbf{H}) \) and \( 0 \) whenever \( \sigma_0^2 \to \infty \) and \( \sigma_0^2 \to 0 \), respectively. From these facts, the right limit is immediate from Lemma A.5 while the left limit is directly obtained by noticing that the denominator goes to \( 1 \) as \( \sigma_0^2 \to 0 \).

**Proposition A.8** (Last-layer Laplace). Let \( g : \mathbb{R}^d \to \mathbb{R} \) be a binary linear classifier defined by \( g \circ \phi(x) := \mathbf{w}^\top \phi(x) \) where \( \phi : \mathbb{R}^n \to \mathbb{R}^d \) is a ReLU network, modeling a Bernoulli distribution \( p(y|x, \mathbf{w}) = \mathcal{B}(\sigma(g \circ \phi(x))) \) with parameter \( \mathbf{w} \in \mathbb{R}^d \). Let \( \mathcal{N}(\mathbf{w} | \mu, \Sigma) \) be the posterior obtained via a Laplace approximation with prior \( \mathcal{N}(\theta | 0, \sigma_0^2 \mathbf{I}) \).

Then for any input \( x \in \mathbb{R}^n \), the confidence \( \sigma(|z(x)|) \) is a non-increasing function of \( \sigma_0^2 \) with limits

\[
\lim_{\sigma_0^2 \to \infty} \sigma(|z(x)|) \leq \sigma \left( \frac{|\mu^\top \phi|}{1 + \sqrt{\pi/8} \lambda_{\max}(\mathbf{H}) \| \phi \|^2} \right),
\]
\[
\lim_{\sigma_0^2 \to 0} \sigma(|z(x)|) = \sigma(|\mu^\top \phi|).
\]

Proof. The assumption on the prior implies that

\(- \log p(\mathbf{w}) = 1/2 \mathbf{w} \top \left( 1/\sigma_0^2 \mathbf{I} \right) \mathbf{w} + \text{const}, \)

which has Hessian \( 1/\sigma_0^2 \mathbf{I} \). Thus, the Hessian of the negative log posterior

\(- \log p(\mathbf{w} | D) = - \log p(\mathbf{w}) - \log \prod_{x, t \in D} p(y|x, \mathbf{w}) \)

is \( 1/\sigma_0^2 \mathbf{I} + \mathbf{H} \). This implies that the posterior covariance \( \Sigma \) of the Laplace approximation is given by

\[
\Sigma = \left( \frac{1}{\sigma_0^2} \mathbf{I} + \mathbf{H} \right)^{-1}.
\]

Therefore, the \( i \)th eigenvalue of \( \Sigma \) for any \( i = 1, \ldots, n \) is

\[
\lambda_i(\Sigma) = \frac{1}{1/\sigma_0^2 + \lambda_i(\mathbf{H})} = \frac{\sigma_0^2}{1 + \sigma_0^2 \lambda_i(\mathbf{H})}.
\]

For all \( i = 1, \ldots, n \), the derivative of \( \lambda_i(\Sigma) \) w.r.t. \( \sigma_0^2 \) is \( 1/(1 + \sigma_0^2 \lambda_i(\mathbf{H}))^2 \) which is non-negative. This tells us that \( \lambda_i(\Sigma) \) is a non-decreasing function of \( \sigma_0^2 \). Furthermore, it is also clear that \( \sigma_0^2/(1 + \sigma_0^2 \lambda_i(\mathbf{H})) \) goes to \( 1/\lambda_i(\mathbf{H}) \) as \( \sigma_0^2 \) goes to infinity, while it goes to \( 0 \) as \( \sigma_0^2 \) goes to zero.

Now, we can write

\[
|z(x)| = \frac{|\mu^\top \phi|}{\sqrt{1 + \pi/8 \sum_{i=1}^d \lambda_i(\Sigma)(\mathbf{Q}^\top \mathbf{d})^2}},
\]

where \( \Sigma = \mathbf{Q} \text{diag}(\lambda_1(\Sigma), \ldots, \lambda_d(\Sigma)) \mathbf{Q}^\top \) is the eigendecomposition of \( \Sigma \). It is therefore clear that the denominator of the r.h.s. is a non-decreasing function of \( \sigma_0^2 \). This implies \( |z(x)| \) is a non-increasing function of \( \sigma_0^2 \).

For the limits, it is clear that \( \lambda_{\min}(\Sigma) \) has limits \( 1/\lambda_{\max}(\mathbf{H}) \) and \( 0 \) whenever \( \sigma_0^2 \to \infty \) and \( \sigma_0^2 \to 0 \), respectively. From these facts, the right limit is immediate from Lemma A.5 while the left limit is directly obtained by noticing that the denominator goes to \( 1 \) as \( \sigma_0^2 \to 0 \).

**B. Laplace Approximations**

The theoretical results in the main text essentially tell us that if we have a Gaussian approximate posterior that comes from a Laplace approximation, then using eq. (1) (and eq. (2)) to make predictions can remedy the overconfidence problem on any ReLU network. In this section, we describe LLLA, DLA, and KFLA: the Laplace methods being used in the main text. For the sake of clarity, we omit biases in the following and revisit the case where biases are included at the end of this section.
B.1. LLLA

In the case of LLLA, we simply perform a Laplace approximation to get the posterior of the weight of the last layer \(w\) while assuming the previous layer to be fixed. I.e. we infer 
\[
p(w|D) = \mathcal{N}(w|w_{\text{MAP}}, H^{-1})
\]
where \(H\) is the Hessian of the negative log-posterior w.r.t. \(w\) at \(w_{\text{MAP}}\). This Hessian could be easily obtained via automatic differentiation. We emphasize that we only deal with the weight at the last layer and not the weight of the whole network, thus the inversion of \(H\) is rarely a problem. For instance, even for large models like DenseNet-201 (Huang et al., 2017) and ResNet-152 (He et al., 2016) have \(d = 1920\) and \(d = 2048\) respectively,\(^6\) implying that we only need to do the inversion of a single \(1920 \times 1920\) or \(2048 \times 2048\) matrix once.

In the case of multi-class classification, we now have 
\[
f : \mathbb{R}^d \to \mathbb{R}^k
\]
defined by \(\phi \mapsto W_{\text{MAP}} \phi\). We obtain the posterior over a random matrix \(W \in \mathbb{R}^{k \times d}\) in the form
\[
\mathcal{N}(\text{vec}(W)|\text{vec}(W_{\text{MAP}}), \Sigma)
\]
for some \(\Sigma \in \mathbb{R}^{dk \times dk}\) SPD. The procedure is still similar to the one described above, since the exact Hessian of the linear multi-class classifier can still be easily and efficiently obtained via automatic differentiation. Note that in this case we need to invert a \(dk \times dk\) matrix, which, depending on the size of \(k\), can be quite large.\(^7\)

For a more efficient procedure, we can make a further approximation to the posterior in the multi-class case by assuming the posterior is a matrix Gaussian distribution. We can use the Kronecker-factored Laplace approximation (KFLA) (Ritter et al., 2018), but only for the last layer of the network. That is, we find the Kronecker factorization of the Hessian \(H^{-1} \approx V^{-1} \otimes U^{-1}\) via automatic differentiation (Dangel et al., 2020).\(^8\) Then by definition of a matrix Gaussian (Gupta & Nagar, 1999), we immediately obtain the posterior \(\mathcal{MV}(W|W_{\text{MAP}}, U, V)\). The distribution of the latent functions is Gaussian, since fixed \(w := W \phi\) and 
\[
p(W|D) = \mathcal{MV}(W|W_{\text{MAP}}, U, V) \implies
\]
\[
p(f|D) = \mathcal{MV}(f|W_{\text{MAP}} \phi, \mu, \Sigma)
\]
implies
\[
\begin{align}
N(f|W_{\text{MAP}} \phi, (\phi^T V \phi) \otimes U) \\
= N(f|W_{\text{MAP}} \phi, (\phi^T V \phi) U)
\end{align}
\]
where the last equality follows since \((\phi^T V \phi)\) is a scalar. We then have the following integral
\[
p(y = i|x, \mathcal{D}) = \int \text{softmax}(f, i) N(f|W_{\text{MAP}} \phi, (\phi^T V \phi) U) df,
\]
which can be approximated via a MC-integral.

While one can always assume that the bias trick is already used, i.e. it is absorbed in the weight matrix/vector, in practice when dealing with pre-trained networks, one does not have such liberty. In this case, one can simply assume that the bias \(b\) is independent of the weight \(w\) or \(W\), respectively in the two- and multi-class cases. By using the same Laplace approximation procedure, one can easily get
\[
p(b|D) := \mathcal{N}(b|\mu_b, \sigma_b^2)
\]
and
\[
p(b|D) := \mathcal{N}(b|\mu_b, \Sigma_b).
\]
This implies \(w^T \phi + b =: f\) and \(W \phi + b =: f\) are also Gaussians given by
\[
\begin{align}
\mathcal{N}(f|\mu^T \phi + \mu_b, \phi^T H^{-1} \phi + \sigma_b^2) & \quad (19) \\
\mathcal{N}(f|W_{\text{MAP}} \phi + \mu_b, (\phi^T V \phi) U + \Sigma_b) & \quad (20)
\end{align}
\]
respectively, with \(I \in \mathbb{R}^{k \times k}\) if \(W \in \mathbb{R}^{k \times d}\) and \(\phi \in \mathbb{R}^d\).

Similarly, in the case when the Kronecker-factored approximation is used, we have
\[
p(f|D) = \mathcal{N}(f|W_{\text{MAP}} \phi + \mu_b, (\phi^T V \phi) U + \Sigma_b).
\]
(21)

We present the pseudocodes of LLLA in Algorithms 1 and 2.

Algorithm 1 LLLA with exact Hessian for binary classification.

**Input:**
- A pre-trained network \(f \circ \phi\) with \(w_{\text{MAP}}\) as the weight of \(f\), (averaged) cross-entropy loss \(\mathcal{L}\), training set \(\mathcal{D}_{\text{train}}\), test set \(\mathcal{D}_{\text{test}}\), mini-batch size \(m\), running average weighting \(\rho\), and prior precision \(\tau_0 = 1/\sigma_b^2\).

**Output:**
- Predictions \(P\) containing \(p(y = 1|x, \mathcal{D}_{\text{train}}) \forall x \in \mathcal{D}_{\text{train}}\).

1: \(\Lambda = 0 \in \mathbb{R}^{d \times d}\)
2: for \(i = 1, \ldots, |\mathcal{D}_{\text{train}}|/m\) do
3: \(X_i, y_i = \text{sampleMinibatch}(\mathcal{D}_{\text{train}}, m)\)
4: \(A_i, B_i = \text{getHessian}(\mathcal{L}(f \circ \phi(X_i), y_i), w_{\text{MAP}})\)
5: \(\Lambda = \rho \Lambda + (1 - \rho) A_i\)
6: end for
7: \(\Sigma = (|\mathcal{D}_{\text{train}}| \Lambda + \tau_0 I)^{-1}\)
8: \(p(w|D) = \mathcal{N}(w|w_{\text{MAP}}, \Sigma)\)
9: \(Y = \emptyset\)
10: for all \(x \in \mathcal{D}_{\text{test}}\) do
11: \(y = \sigma(w_{\text{MAP}} \phi/(1 + \pi/8 \phi^T \Sigma \phi)^{1/2})\)
12: \(Y = Y \cup \{y\}\)
13: end for

B.2. DLA

In this method, we aim at inferring the **diagonal** of the covariance of the Gaussian over the whole layer of a network. Instead of using the exact diagonal Hessian, we use the diagonal of the Fisher information matrix \(\mathbf{F}\) of the network.
**Algorithm 2** LLLA with Kronecker-factored Hessian for multi-class classification.

**Input:**
A pre-trained network \( f \circ \phi \) with \( W_{\text{MAP}} \) as the weight of \( f \), (averaged) cross-entropy loss \( L \), training set \( \mathcal{D}_{\text{train}} \), test set \( \mathcal{D}_{\text{test}} \), mini-batch size \( m \), number of samples \( s \), running average weighting \( \rho \), and prior precision \( \tau_0 = 1/\sigma_0^2 \).

**Output:**
- Predictions \( \mathcal{P} \) containing \( p(y = i|x, \mathcal{D}_{\text{train}}) \forall x \in \mathcal{D}_{\text{test}} \forall i \in \{1, \ldots, k\} \).
  - \( A = 0 \in \mathbb{R}^{k \times k} \), \( B = 0 \in \mathbb{R}^{d \times d} \)
  - for \( i = 1, \ldots, |\mathcal{D}_{\text{train}}|/m \) do
    - \( X_i, y_i = \text{sampleMinibatch}(\mathcal{D}_{\text{train}}, m) \)
    - \( A_{i}, B_{i} = \text{KronFactors}(L(f \circ \phi(X_i), y_i), W_{\text{MAP}}) \)
    - \( A = \rho A + (1 - \rho) A_i \)
    - \( B = \rho B + (1 - \rho) B_i \)
  - end for
  - for all \( x \in \mathcal{D}_{\text{test}} \) do
    - \( p(f(x)|D) = \mathcal{N}(W^{l}\text{MAP}, U^{l}, V^{l}) \)
    - \( U^{l} = (\sqrt{|\mathcal{D}_{\text{train}}|}A + \sqrt{\tau_0} 1) \)
    - \( V^{l} = (\sqrt{|\mathcal{D}_{\text{train}}|}B + \sqrt{\tau_0} 1) \)
    - \( p(W|D) = \mathcal{N}(W|W^{l}\text{MAP}, U^{l}, V^{l}) \)
  - end for

(Ritter et al., 2018) as follows

\[
\text{diag}(\Sigma) \approx (\sigma_0^2 + \text{diag}(F))^{-1} = (\sigma_0^2 + E_{y \sim p(y|x, \theta)} x \sim D(\nabla_\theta p(y|x, \theta))^2)^{-1}.
\]

Thus, one simply needs to do several backpropagation to compute the gradients of all weight matrices of the network. This gives rise to the Gaussian posterior \( \mathcal{N}(\theta|\theta_{\text{MAP}}, \text{diag}(\Sigma)) \). During prediction, an MC-integration scheme is employed: we repeatedly sample a whole network and average their predictions. That is, for each layer \( l \in \{1, \ldots, L\} \), we sample the \( l \)th layer’s weight matrix \( W^{l} \sim \mathcal{N}(W^{l}|W^{l}_{\text{MAP}}, \text{diag}(\Sigma)) \) by computing

\[
e \sim \mathcal{N}(0, I), \\
\text{vec}(W^{l}) = \text{vec}(W^{l}_{\text{MAP}}) + e \odot \text{diag}(\Sigma^{l})^{\frac{1}{2}},
\]

where we have denoted the covariance matrix of the \( l \)th layer as \( \Sigma^{l} \). Note that, the computational cost for doing prediction scales with the size of the network, thus this scheme is already orders of magnitude more expensive than LLLA, cf. Table 3.

**B.3. KFLA**

LLLA with a matrix normal distribution as described in the previous section is a special case of KFLA (Ritter et al., 2018). In KFLA, similar to DLA, we aim to infer the posterior of the whole network parameters and not just those of the last layer. Concretely, for each layer \( l \in \{1, \ldots, L\} \), we infer the posterior

\[
p(W^{l}|D) \approx \mathcal{N}(W^{l}|W^{l}_{\text{MAP}}, U^{l}, V^{l}) \]

where

\[
U^{l} = (\sqrt{|\mathcal{D}_{\text{train}}|}A + 1/\sigma_0^2 I)^{-1}, \\
V^{l} = (\sqrt{|\mathcal{D}_{\text{train}}|}B + 1/\sigma_0^2 I)^{-1},
\]

and \( A, B \) are the Kronecker-factors—e.g. obtained KFAC (Martens & Grosse, 2015)—of the Hessian of the loss w.r.t. \( W^{l} \).

During predictions, as in DLA, we also use MC-integration to compute the posterior predictive distribution. That is, at each layer \( l \in \{1, \ldots, L\} \), we sample the \( l \)th layer’s weight matrix \( W^{l} \) via

\[
E \sim \mathcal{N}(0, I), \\
W^{l} = W^{l}_{\text{MAP}} + (U^{l})^{\frac{1}{2}}E(V^{l})^{\frac{1}{2}},
\]

where \( S, T \) are the Cholesky factors such that \((U^{l})^{\frac{1}{2}}(U^{l})^{\frac{1}{2}}^{\top} = U \) and \((V^{l})^{\frac{1}{2}}(V^{l})^{\frac{1}{2}}^{\top} = V \). Again, the cost for doing prediction scales with the size of the network, and it is clear that KFLA is more expensive than DLA.

**C. Training detail**

We train all networks we use in Table 2 for 100 epochs with batch size of 128. We use ADAM and SGD with 0.9 momentum with the initial learning rates of 0.001 and 0.1 for MNIST and CIFAR-10/100 experiments, respectively, and we divide them by 10 at epoch 50, 75, and 95. Standard data augmentations, i.e. random crop and standardization are also used for training the network on CIFAR-10. We use a graphic card with 11GB memory for all computation.

**D. Further experimental results**

**D.1. Histograms**

To give a more fine-grained perspective of the results in Tables 1 and 2, we show the histograms in Figures 7 and 8.
The histograms of both the in-distribution data and far-away OOD data are close together in both MAP and temperature scaling methods, leading to low AUR scores. Meanwhile LLLA (representing Bayesian methods) yields clear separations.

D.2. Asymptotic regime of multi-class problems

In Figure 6, we present the multi-class counterpart of Figure 5. We found that, as in the binary case, the Bayesian method (LLLA) mitigates overconfidence in the asymptotic regime. We observed, however, that LLLA is less effective in MNIST, which might be due to the architecture choice and the training procedure used: The eigenvalues of the Gaussian posterior’s covariance might be too small such that (4) is still large.

D.3. Adversarial examples

The adversarial datasets (“Adversarial” and “FarAwayAdv”, cf. Table 2) are constructed as follows. For “Adversarial”: We use the standard PGD attack (Madry et al., 2018) on a uniform noise dataset of size 2000. The objective is to maximize the confidence of the MAP model (resp. ACET and OE below) inside of an $\ell^{\infty}$ ball with radius $\epsilon = 0.3$. The optimization is carried out for 40 iterations with a step size of 0.1. We ensure that the resulting adversarial examples are in the image space. For “FarAwayAdv”: We use the same construction, but start from the “far-away” Noise datasets as used in Table 2 and we do not project the resulting adversarial examples onto the image space.

D.4. Bayesian methods on top of state-of-the-art OOD detectors

We can also apply all methods we are considering here on top of the state-of-the-art models that are specifically trained to mitigate the overconfidence problem, namely ACET (Hein et al., 2019) and outlier exposure (OE) (Hendrycks et al., 2019). The results are presented in Tables 6 and 7. In general, applying the Bayesian methods improves the models further, especially in the asymptotic regime.

D.5. Frequentist calibration

Although calibration is a frequentist approach for predictive uncertainty quantification, it is nevertheless interesting to get an insight on whether the properties of the Bayesian predictive distribution lead to a better calibration. To answer this, we use a standard metric (Naeini et al., 2015; Guo et al., 2017): the expected calibration error (ECE). We use the same models along with the same hyperparameters as we have used in the previous OOD experiments. We present the results in Table 4. We found that all the Bayesian methods are competitive to the temperature scaling method, which is specifically constructed for improving the frequentist calibration.

| Table 4. Expected calibration errors (ECE). |
|------------------------------------------|
| MNIST | CIFAR10 | SVHN | CIFAR100 |
|-------|---------|------|---------|
| MAP  | 6.7 ± 0.3 | 13.1 ± 0.2 | 10.1 ± 0.2 | 8.1 ± 0.3 |
| +Temp. | 11.4 ± 2.2 | 3.6 ± 0.6 | 2.1 ± 0.5 | 6.4 ± 0.5 |
| +LLLA | 6.9 ± 0.3 | 3.6 ± 0.6 | 5.2 ± 0.8 | 4.8 ± 0.3 |
| +DLA  | 15.5 ± 0.2 | 6.9 ± 0.1 | 8.3 ± 0.0 | 4.7 ± 0.3 |
| +KFLA | 9.7 ± 0.3 | 7.9 ± 0.1 | 6.5 ± 0.1 | 5.6 ± 0.4 |
| ACET  | 5.9 ± 0.2 | 15.8 ± 0.4 | 11.9 ± 0.2 | 10.1 ± 0.4 |
| +Temp. | 11.0 ± 1.5 | 3.7 ± 0.8 | 2.3 ± 0.4 | 6.4 ± 0.4 |
| +LLLA | 6.1 ± 0.2 | 12.3 ± 0.7 | 9.3 ± 0.5 | 6.9 ± 0.3 |
| +DLA  | 6.2 ± 0.3 | 4.3 ± 0.3 | 2.0 ± 0.1 | 6.0 ± 0.3 |
| +KFLA | 6.1 ± 0.3 | 4.3 ± 0.2 | 2.1 ± 0.1 | 4.6 ± 0.2 |
| OE    | 14.7 ± 1.2 | 15.8 ± 0.3 | 11.0 ± 0.1 | 25.0 ± 0.2 |
| +Temp. | 9.0 ± 2.3 | 23.3 ± 0.7 | 3.7 ± 0.7 | 19.4 ± 0.2 |
| +LLLA | 6.5 ± 0.6 | 14.6 ± 0.2 | 4.1 ± 0.3 | 24.9 ± 0.4 |
| +DLA  | 9.1 ± 0.6 | 15.8 ± 0.3 | 7.2 ± 0.1 | 29.0 ± 0.2 |
| +KFLA | 10.1 ± 0.9 | 15.9 ± 0.3 | 6.4 ± 0.1 | 29.0 ± 0.2 |
Figure 6. The multi-class confidence of MAP (top row), temperature scaling (middle row), and LLLA (bottom row) as functions of $\delta$ over the test sets of the multi-class datasets. Thick blue lines and shades correspond to means and ±3 standard deviations. Dotted lines signify the desirable confidence for $\delta$ sufficiently high.

Figure 7. The histograms of MAP (top row), temperature scaling (middle row), and LLLA (bottom row) over the binary datasets. Each entry “Out - FarAway” refers to the OOD dataset obtained by scaling the corresponding in-distribution dataset with some $\delta > 0$. 
Figure 8. The histograms of MAP (top row), temperature scaling (middle row), and LLLA (bottom row) over the multi-class datasets. Each entry “Out - FarAway” refers to the OOD dataset obtained by scaling the corresponding in-distribution dataset with some $\delta > 0$.

Table 5. Adversarial OOD detection results.

|                   | MAP          | +Temp.        | +LLLA        | +DLA         | +KFLA        |
|-------------------|--------------|---------------|--------------|--------------|--------------|
|                   | MMC | AUR | MMC | AUR | MMC | AUR | MMC | AUR | MMC | AUR | MMC | AUR |
| MNIST - Adversarial | 100.0±0.0 | 0.3±0.0 | 100.0±0.0 | 6.8±4.1 | 100.0±0.0 | 5.3±0.1 | 99.6±0.2 | 2.0±0.9 | 91.3±1.2 | 69.2±3.5 |
| MNIST - FarAwayAdv | 100.0±0.0 | 0.1±0.0 | 100.0±0.0 | 6.8±4.1 | 99.9±0.0 | 9.3±0.6 | 85.3±1.4 | 53.0±3.8 | 55.6±2.0 | 97.4±0.3 |
| CIFAR10 - Adversarial | 100.0±0.0 | 0.0±0.0 | 100.0±0.0 | 0.0±0.0 | 99.7±0.0 | 9.1±0.1 | 99.3±0.1 | 9.0±1.0 | 99.2±0.0 | 5.8±0.4 |
| CIFAR10 - FarAwayAdv | 99.5±0.0 | 8.8±0.0 | 99.2±0.0 | 7.9±0.1 | 17.4±0.1 | 100.0±0.0 | 61.3±2.4 | 89.4±1.0 | 61.2±1.3 | 87.8±0.8 |
| SVHN - Adversarial | 100.0±0.0 | 0.0±0.0 | 100.0±0.0 | 0.0±0.0 | 97.6±0.0 | 32.5±0.3 | 98.6±0.0 | 6.8±0.3 | 98.6±0.1 | 9.6±0.4 |
| SVHN - FarAwayAdv | 99.7±0.0 | 7.7±0.0 | 99.5±0.0 | 6.9±0.1 | 27.5±0.1 | 99.6±0.0 | 61.7±1.4 | 92.4±0.9 | 61.0±1.2 | 94.4±0.3 |
| CIFAR100 - Adversarial | 100.0±0.0 | 0.0±0.0 | 100.0±0.0 | 0.0±0.0 | 100.0±0.0 | 0.2±0.0 | 100.0±0.0 | 0.1±0.0 | 100.0±0.0 | 0.0±0.0 |
| CIFAR100 - FarAwayAdv | 100.0±0.0 | 1.3±0.0 | 99.9±0.0 | 1.2±0.0 | 5.9±0.0 | 99.9±0.0 | 42.0±1.5 | 83.9±0.9 | 42.3±1.8 | 80.8±1.2 |
### Table 6. OOD detection results when applying post-hoc Bayesian methods on top of models trained with ACET (Hein et al., 2019).

| MAP      | +Temp. | +LLLA | +DLA | +KFLA |
|----------|--------|-------|------|-------|
| MMC      | AUR    | MMC   | AUR  | MMC   | AUR  |
| MNIST - MNIST | 98.9±0.0 | 99.5±0.0 | 99.8±0.0 | 99.8±0.0 |
| MNIST - EMNIST | 59.1±0.0 | 96.9±0.0 | 70.9±1.8 | 96.5±0.1 |
| MNIST - FMMIST | 10.2±0.0 | 100.0±0.0 | 10.3±0.0 | 100.0±0.0 |
| MNIST - Noise (δ = 2000) | 100.0±0.0 | 100.0±0.0 | 100.0±0.0 | 100.0±0.0 |
| MNIST - Adversarial | 10.0±0.0 | 100.0±0.0 | 10.0±0.0 | 100.0±0.0 |
| MNIST - FarAwayAdv | 100.0±0.0 | 100.0±0.0 | 100.0±0.0 | 100.0±0.0 |
| CIFAR10 - CIFAR10 | 97.3±0.0 | 95.2±0.2 | 96.7±0.1 | 94.7±0.0 |
| CIFAR10 - SVHN | 62.8±0.0 | 96.1±0.0 | 52.9±0.7 | 96.5±0.0 |
| CIFAR10 - LSUN | 72.1±0.0 | 92.8±0.0 | 62.6±0.7 | 93.2±0.0 |
| CIFAR10 - Noise (δ = 2000) | 100.0±0.0 | 0.0±0.0 | 100.0±0.0 | 0.0±0.0 |
| CIFAR10 - Adversarial | 78.1±0.0 | 83.1±0.1 | 71.1±0.5 | 84.1±0.1 |
| CIFAR10 - FarAwayAdv | 100.0±0.0 | 0.0±0.0 | 100.0±0.0 | 0.0±0.0 |
| SVHN - SVHN | 98.5±0.0 | 97.3±0.2 | 98.3±0.0 | 96.7±0.0 |
| SVHN - CIFAR10 | 65.9±0.0 | 95.6±0.0 | 58.5±0.8 | 95.7±0.0 |
| SVHN - LSUN | 28.0±0.0 | 99.3±0.0 | 24.6±0.3 | 99.4±0.0 |
| SVHN - Noise (δ = 2000) | 17.9±0.2 | 100.0±0.0 | 16.0±0.3 | 100.0±0.0 |
| SVHN - Adversarial | 104.2±0.0 | 100.0±0.0 | 103.2±0.0 | 100.0±0.0 |
| SVHN - FarAwayAdv | 17.6±0.0 | 100.0±0.0 | 15.7±0.2 | 100.0±0.0 |
| CIFAR10 - CIFAR100 | 82.0±0.1 | 78.1±0.5 | 79.6±0.1 | 78.7±0.1 |
| CIFAR100 - SVHN | 57.1±0.0 | 77.8±0.1 | 49.5±0.8 | 78.7±0.1 |
| CIFAR100 - LSUN | 55.1±0.0 | 78.8±0.1 | 48.3±0.7 | 79.0±0.1 |
| CIFAR100 - Noise (δ = 2000) | 99.3±0.1 | 4.2±0.2 | 99.2±0.1 | 3.8±0.2 |
| CIFAR100 - Adversarial | 15.1±0.0 | 100.0±0.0 | 1.4±0.0 | 100.0±0.0 |
| CIFAR100 - FarAwayAdv | 99.7±0.0 | 3.4±0.0 | 99.6±0.0 | 3.1±0.0 |

### Table 7. OOD detection results when applying post-hoc Bayesian methods on top of models trained with outlier exposure (OE) (Hendrycks et al., 2019).

| MAP      | +Temp. | +LLLA | +DLA | +KFLA |
|----------|--------|-------|------|-------|
| MMC      | AUR    | MMC   | AUR  | MMC   | AUR  |
| MNIST - MNIST | 99.6±0.0 | 99.4±0.1 | 97.8±0.8 | 99.4±0.0 |
| MNIST - EMNIST | 84.2±0.0 | 96.0±0.1 | 77.1±2.6 | 96.3±0.1 |
| MNIST - FMMIST | 27.9±0.0 | 99.9±0.0 | 22.8±1.5 | 99.9±0.0 |
| MNIST - Noise (δ = 2000) | 99.9±0.0 | 26.4±0.2 | 99.4±0.0 | 50.2±4.0 |
| MNIST - Adversarial | 40.5±0.0 | 98.8±0.0 | 35.2±1.1 | 99.1±0.0 |
| MNIST - FarAwayAdv | 100.0±0.0 | 25.5±0.2 | 100.0±0.0 | 3.6±2.4 |
| CIFAR10 - CIFAR10 | 89.4±0.1 | 92.5±0.4 | 89.2±0.1 | 89.3±0.1 |
| CIFAR10 - SVHN | 10.8±0.0 | 98.8±0.0 | 11.2±0.1 | 98.8±0.0 |
| CIFAR10 - LSUN | 10.4±0.0 | 98.6±0.0 | 10.7±0.1 | 98.6±0.0 |
| CIFAR10 - Noise (δ = 2000) | 99.1±0.1 | 6.5±0.6 | 99.4±0.1 | 7.0±6.7 |
| CIFAR10 - Adversarial | 98.5±0.0 | 2.4±0.0 | 98.8±0.0 | 2.6±0.2 |
| CIFAR10 - FarAwayAdv | 99.5±0.0 | 5.2±0.0 | 99.8±0.0 | 6.2±0.3 |
| SVHN - SVHN | 97.4±0.0 | 95.8±0.3 | 95.7±0.2 | 95.8±0.3 |
| SVHN - CIFAR10 | 10.2±0.0 | 100.0±0.0 | 10.1±0.0 | 100.0±0.0 |
| SVHN - LSUN | 10.1±0.0 | 100.0±0.0 | 10.1±0.0 | 100.0±0.0 |
| SVHN - Noise (δ = 2000) | 99.7±0.0 | 3.0±0.2 | 99.6±0.1 | 2.7±0.2 |
| SVHN - Adversarial | 44.9±0.0 | 98.2±0.0 | 34.4±0.7 | 98.5±0.0 |
| SVHN - FarAwayAdv | 99.9±0.0 | 2.4±0.0 | 99.8±0.0 | 2.2±0.0 |
| CIFAR100 - CIFAR100 | 59.6±0.2 | 71.8±0.5 | 54.9±0.2 | 51.5±0.2 |
| CIFAR100 - SVHN | 3.6±0.0 | 93.5±0.1 | 7.2±0.2 | 93.4±0.1 |
| CIFAR100 - LSUN | 2.6±0.0 | 95.4±0.1 | 5.0±0.1 | 95.3±0.1 |
| CIFAR100 - Noise (δ = 2000) | 100.0±0.0 | 1.3±0.0 | 100.0±0.0 | 7.3±0.7 |
| CIFAR100 - Adversarial | 95.6±0.0 | 21.7±0.1 | 96.7±0.0 | 24.6±0.4 |
| CIFAR100 - FarAwayAdv | 100.0±0.0 | 1.3±0.0 | 100.0±0.0 | 7.3±0.7 |