Simple and Principled Uncertainty Estimation with Deterministic Deep Learning via Distance Awareness

Jeremiah Zhe Liu
Google Research & Harvard University
jereliu@google.com

Zi Lin
Google Research
lzi@google.com

Shreyas Padhy
Google Research
shreyaspadhy@google.com

Dustin Tran
Google Research
trandustin@google.com

Tania Bedrax-Weiss
Google Research
tbedrax@google.com

Balaji Lakshminarayanan
Google Research
balajiiln@google.com

Abstract
Bayesian neural networks and deep ensembles are principled approaches to estimate the predictive uncertainty of a deep learning model. However their practicality in real-time, industrial-scale applications are limited due to their heavy memory and inference cost. This motivates us to study principled approaches to high-quality uncertainty estimation that require only a single deep neural network (DNN). By formalizing the uncertainty quantification as a minimax learning problem, we first identify distance awareness, i.e., the model’s ability to properly quantify the distance of a testing example from the training data manifold, as a necessary condition for a DNN to achieve high-quality (i.e., minimax optimal) uncertainty estimation. We then propose Spectral-normalized Neural Gaussian Process (SNGP), a simple method that improves the distance-awareness ability of modern DNNs, by adding a weight normalization step during training and replacing the output layer with a Gaussian Process. On a suite of vision and language understanding tasks and on modern architectures (Wide-ResNet and BERT), SNGP is competitive with deep ensembles in prediction, calibration and out-of-domain detection, and outperforms the other single-model approaches.

1 Introduction
Efficient methods that reliably quantify a deep neural network (DNN)’s predictive uncertainty are important for industrial-scale, real-world applications, which include examples such as object recognition in autonomous driving [22], ad click prediction in online advertising [76], and intent understanding in a conversational system [84]. For example, for a natural language understanding (NLU) model built for a domain-specific chatbot service (e.g., weather inquiry), the user’s input utterance to the model can be of any topic, and the model needs to understand reliably and in real-time whether to abstain or to trigger one of its known APIs.

When deep classifiers make predictions on input examples that are far from the support of the training set, their performance can be arbitrarily bad [4, 14]. This motivates the need for methods that are aware of the distance between an input test example and previously seen training examples, so they can return a uniform (i.e., maximum entropy) distribution over output labels if the input is too far from the training set (i.e., the input is out-of-domain) [30]. Gaussian processes (GPs) with suitable kernels enjoy such a property. However, to apply Gaussian processes to a high-dimensional machine

*Work done at Google Research.
†Work done as a Google AI Resident.
3Code available at https://github.com/google/uncertainty-baselines/tree/master/baselines.

34th Conference on Neural Information Processing Systems (NeurIPS 2020), Vancouver, Canada.
learning problem, it is usually necessary to perform some form of feature extraction or dimensionality reduction using a DNN. Ideally, the hidden representation of a DNN should reflect a meaningful distance in the data manifold (e.g., the semantic textual similarity between two sentences), such that this “distance aware” property is preserved. However, as we will show in the experiments, this is often not guaranteed for common deep learning models (cf. Figure 1).

We propose a simple solution to this problem, namely adding spectral normalization to the weights in each (residual) layer [54]. We refer to our method as “Spectral-normalized Neural Gaussian Processes” (SNGP). We show that this provides bounds on $\|h(x) - h(x')\|_H$ relative to $\|x - x'\|_X$, where $x$ and $x'$ are two inputs, $h(x)$ is a deep feature extractor, and $\|\cdot\|_X$ a semantically meaningful distance for the data manifold. We can then safely pass $h(x)$ into a distance-aware GP output layer. To ensure computational scalability, we approximate the GP posterior using a Laplace approximation to the random feature expansion of the GP, which gives rise to a model posterior that can be learned scalably and in closed-form with minimal modification to the training pipeline of a deterministic DNN, and allows us to efficiently compute the predictive uncertainty on a per-input basis without Monte Carlo sampling.

In the rest of this paper, we first theoretically motivate the importance of distance awareness for a model’s ability uncertainty estimation by studying it as a minimax learning problem (Section 2). We then introduce our SNGP method in detail in Section 3, and experimentally evaluate its performance against other single-model approaches as well as deep ensembles in Section 5 [42]. On two challenging real world problems, namely image classification (using a Wide Resnet model on CIFAR-10 and CIFAR-100) and conversational intent understanding (using a BERT model on CLINC out-of-scope (OOS) intent dataset), we show that the SNGP method attains an uncertainty performance (e.g., calibration and out-of-domain (OOD) detection) that is competitive with that of a deep ensemble, while maintaining the accuracy and latency of a single deterministic DNN.

2 Distance Awareness: An Important Condition for High-Quality Uncertainty Estimation

Notation and Problem Setup Consider a data-generating distribution $p^*(y|x)$, where $y \in \{1, \ldots, K\}$ is the space of $K$-class labels, and $x \in \mathcal{X} \subset \mathbb{R}^d$ is the input data manifold equipped with a suitable metric $\|\cdot\|_X$. In practice, the training data $\mathcal{D} = \{(y_i, x_i)\}_{i=1}^N$ is often collected from a subset of the full input space $\mathcal{X}_{100} \subset \mathcal{X}$. As a result, the full data-generating distribution $p^*(y|x)$ is in fact a mixture of an in-domain (IND) distribution $p_{100}(y|x) = p^*(y|x, x \in \mathcal{X}_{100})$ and also an OOD distribution $p_{OOD}(y|x) = p^*(y|x, x \notin \mathcal{X}_{100})$ [52, 66]:

$$
p^*(y|x) = p^*(y|x, x \in \mathcal{X}_{100}) + p^*(y|x, x \notin \mathcal{X}_{100}) = p^*(y|x, x \in \mathcal{X}_{100}) \ast p^*(x, x \notin \mathcal{X}_{100}) + p^*(y|x, x \notin \mathcal{X}_{100}) \ast p^*(x, x \notin \mathcal{X}_{100}). \tag{1}
$$

Figure 1: The uncertainty surface of a GP and different DNN approaches on the two ovals (Top Row) and two moons (Bottom Row) 2D classification benchmarks. SNGP is the only DNN-based approach achieving a distance-aware uncertainty similar to the gold-standard GP. Training data for positive (Orange) and negative classes (Blue). OOD data (Red) not observed during training. Background color represents the estimated model uncertainty (See 1e and 1j for color map). See Section 5.1 for details.
During training, the model learns the in-domain distribution $p^*(y|x, x \in \mathcal{X}_{\text{IND}})$ from the data $\mathcal{D}$, but does not have knowledge about $p^*(y|x, x \notin \mathcal{X}_{\text{IND}})$. In the weather-service chatbot example, the out-of-domain space $\mathcal{X}_{\text{OOD}} = \mathcal{X} / \mathcal{X}_{\text{IND}}$ is the space of all natural utterances not related to weather queries, whose elements usually do not have a meaningful correspondence with the in-domain intent labels $y_k \in \{1, \ldots, K\}$. Therefore, the out-of-domain distribution $p^*(y|x, x \notin \mathcal{X}_{\text{IND}})$ can be very different from the in-domain distribution $p^*(y|x, x \in \mathcal{X}_{\text{IND}})$, and we only expect the model to generalize well within $\mathcal{X}_{\text{IND}}$. However, during testing, the model needs to construct a predictive distribution $p(y|x)$ for the entire input space $\mathcal{X} = \mathcal{X}_{\text{IND}} \cup \mathcal{X}_{\text{OOD}}$, since the users’ utterances can be of any topic.

### 2.1 Uncertainty Estimation as a Minimax Learning Problem

To formulate the uncertainty estimation as a learning problem under (1), we need to define a loss function to measure a model $p(y|x)$’s quality of predictive uncertainty. A popular uncertainty metric is Expected Calibration Error (ECE), defined as

$$ECE(p, \hat{p}^*; \mathcal{D}) = \frac{1}{|\mathcal{D}|} \sum_{y \in \mathcal{Y}} \frac{1}{N_y} \sum_{x \in \mathcal{X}_y} \left| \hat{p}^*(y|x) - \frac{1}{N_y} \sum_{x \in \mathcal{X}_y} p(y|x) \right|,$$

where $N_y$ is the number of samples in class $y$.

Unfortunately, directly minimizing (2) over the entire input space $\mathcal{X}$ is not possible even with infinite amounts of data. This is because since the data is collected only from $\mathcal{X}_{\text{IND}}$, the true OOD distribution $p^*(y|x, x \notin \mathcal{X}_{\text{IND}})$ is never learned by the model, and generalization is not guaranteed since $p^*(y|x, x \in \mathcal{X}_{\text{IND}})$ and $p^*(y|x, x \notin \mathcal{X}_{\text{IND}})$ are not assumed to be similar. As a result, the naïve practice of using a model trained only with in-domain data to generate OOD predictions can lead to arbitrarily bad results, since nature can happen to produce an OOD distribution $p^*(y|x, x \notin \mathcal{X}_{\text{IND}})$ that is at odds with the model prediction. This is clearly undesirable for safety-critical applications.

To this end, a more prudent strategy is to instead minimize the worst-case risk with respect to all possible $p^* \in \mathcal{P}$, i.e., construct $p(y|x)$ to minimize the Minimax Uncertainty Risk:

$$\inf_{p \in \mathcal{P}} \sup_{p^* \in \mathcal{P}} S(p, p^*).$$

In game-theoretic nomenclature, the uncertainty estimation problem acts as a two-player game of model vs. nature, where the goal of the model is to produce a minimax strategy $p$ that minimizes the risk $S(p, p^*)$ against all possible (even adversarial) moves $p^*$ of nature. Under the classification task and for Brier score, the solution to the minimax problem (3) adopts a simple and elegant form:

$$p(y|x) = p(y|x, x \in \mathcal{X}_{\text{IND}}) \ast p^*(x \in \mathcal{X}_{\text{IND}}) + p_{\text{uniform}}(y|x, x \notin \mathcal{X}_{\text{IND}}) \ast p^*(x \notin \mathcal{X}_{\text{IND}}).$$

This is very intuitive: if an input point is in the training data domain, trust the model, otherwise use a uniform (maximum entropy) prediction. For the practice of uncertainty estimation, (4) is conceptually important in that it verifies that there exists a unique optimal solution to the uncertainty estimation problem (3). Furthermore, this optimal solution can be constructed conveniently. Specifically, it can be constructed as a mixture of a discrete uniform distribution $p_{\text{uniform}}$ and the in-domain predictive distribution $p(y|x, x \in \mathcal{X}_{\text{IND}})$ that the model has already learned from data, assuming one can quantify $p^*(x \in \mathcal{X}_{\text{IND}})$ well. In fact, the expression (4) can be shown to be optimal for a broad family of scoring rules known as the Bregman score, which includes the Brier score and the widely used log score as the special cases. We derive (4) in Appendix B.

### 2.2 Input Distance Awareness as a Necessary Condition

In light of Equation (4), a key capacity for a deep learning model to reliably estimate predictive uncertainty is its ability to quantify, either explicitly or implicitly, the domain probability $p(x \in \mathcal{X}_{\text{IND}})$. 


This requires the model to have a good notion of the distance (or dissimilarity) between a testing example \( x \) and the training data \( \mathcal{X}_{1\text{RD}} \) with respect to a meaningful distance \( \| \cdot \|_X \) for the data manifold (e.g., semantic textual similarity [12] for language data). Definition 1 makes this notion more precise:

**Definition 1 (Input Distance Awareness).** Consider a predictive distribution \( p(y|x) \) trained on a domain \( \mathcal{X}_{1\text{RD}} \subset \mathcal{X} \), where \( (\mathcal{X}, \| \cdot \|_X) \) is the input data manifold equipped with a suitable metric \( \| \cdot \|_X \). We say \( p(y|x) \) is input distance aware if there exists \( u(x) \) a summary statistic of \( p(y|x) \) that quantifies model uncertainty (e.g., entropy, predictive variance, etc) that reflects the distance between \( x \) and the training data with respect to \( \| \cdot \|_X \), i.e.,

\[
u(x) = v(d(x, \mathcal{X}_{1\text{RD}}))\]

where \( v \) is a monotonic function and \( d(x, \mathcal{X}_{1\text{RD}}) = E_{x' \sim \mathcal{X}_{1\text{RD}}} \| x - x' \|_X^2 \) is the distance between \( x \) and the training data domain.

A classic model that satisfies the distance-awareness property is a Gaussian process (GP) with a radial basis function (RBF) kernel. Its predictive distribution \( p(y|x) = \text{softmax}(g(x)) \) is a softmax transformation of the GP posterior \( g \sim \text{GP} \) under the cross-entropy likelihood, and its predictive uncertainty can be expressed by the posterior variance \( u(x') = \text{var}(g(x')) = 1 - k'\top Vk' \) for \( k' = \exp(-\frac{1}{2} ||x' - x||_X^2) \) and \( V_{N \times N} \) a fixed matrix determined by data. Then \( u(x') \) increases monotonically toward 1 as \( x' \) moves further away from \( \mathcal{X}_{1\text{RD}} \) [61]. In view of the expression (4), the input distance awareness property is important for both calibration and OOD detection. However, this property is not guaranteed for a typical deep learning model [33]. Consider a discriminative deep classifier with dense output layer \( \logit(x) = h(x)' \beta_k \), whose model confidence (i.e., maximum predictive probability) is characterized by the magnitude of the class logits, which is defined by the inner product distances between the hidden representation \( h(x) \) and the decision boundaries \( \{ \beta_k \}_{k=1}^K \) (see, e.g., Figure 1b-1c and 1g-1h). As a result, the model computes confidence for a \( x' \) based not on its distance from the training data \( \mathcal{X}_{1\text{RD}} \), but based on its distance from the decision boundaries, i.e., the model uncertainty is not input distance aware.

**Two Conditions for Input Distance Awareness in Deep Learning** Notice that a deep learning model \( \logit(x) = g \circ h(x) \) is commonly composed of a hidden mapping \( h: \mathcal{X} \rightarrow \mathcal{H} \) that maps the input \( x \) into a hidden representation space \( h(x) \in \mathcal{H} \), and an output layer \( g \) that maps \( h(x) \) to the label space. To this end, a DNN \( \logit(x) = g \circ h(x) \) can be made input distance aware via a combination of two conditions: (1) make the output layer \( g \) distance aware, so it outputs an uncertainty metric reflecting distance in the hidden space \( ||h(x) - h(x')||_H \) (in practice, this can be achieved by using a GP with a shift-invariant kernel as the output layer), and (2) make the hidden mapping distance preserving (defined below), so that the distance in the hidden space \( ||h(x) - h(x')||_H \) has a meaningful correspondence to the distance \( ||x - x'||_X \) in the data manifold. From the mathematical point of view, this is equivalent to requiring \( h \) to satisfy the bi-Lipschitz condition [67]:

\[
L_1 * ||x_1 - x_2||_X \leq ||h(x_1) - h(x_2)||_H \leq L_2 * ||x_1 - x_2||_X,
\]

(5)

for positive and bounded constants \( 0 < L_1 < 1 < L_2 \). It is worth noting that for a deep learning model, the bi-Lipschitz condition (5) usually leads the model’s hidden space to preserve a semantically meaningful distance in the input data manifold \( \mathcal{X} \), rather than a naive metric such as the square distance in the pixel space. This is because that the upper Lipschitz bound \( ||h(x_1) - h(x_2)||_H \leq L_2 * ||x_1 - x_2||_X \) is an important condition for the adversarial robustness of a deep network, which prevents the hidden representations \( h(x) \) from being overly sensitive to the semantically meaningless perturbations in the pixel space [65, 80, 75, 37, 71]. On the other hand, the lower Lipschitz bound \( ||h(x_1) - h(x_2)||_H \geq L_1 * ||x_1 - x_2||_X \) prevents the hidden representation from being unnecessarily invariant to the semantically meaningful changes in the input manifold [38, 77]. Combined together, the bi-Lipschitz condition essentially encourages \( h \) to be an approximately isometric mapping, thereby ensuring that the learned representation \( h(x) \) has a robust and meaningful correspondence with the semantic properties of the input data \( x \). Although not stated explicitly, learning an approximately isometric and geometry-preserving mapping is a common goal in machine learning. For example, image classifiers strive to learn a mapping from image manifold to a hidden space that can be well-separated by a set of linear decision boundaries, and sentences encoders aim to project sentences into a vector space where the cosine distance reflects the semantic similarity in natural language. Finally, it is worth noting that preserving such approximate isometry in a neural network is possible even after significant dimensionality reduction [8, 32, 59, 64].
3 SNGP: A Simple Approach to Distance-aware Deep Learning

In this section we propose Spectral-normalized Neural Gaussian Process (SNGP), a simple method to improve the input distance awareness ability of a modern residual-based DNN (e.g., ResNet, Transformer) by (1) making the output layer distance aware and (2) making the hidden layers distance preserving, as discussed in Section 2.2. Full method is summarized in Algorithms 1-2.

3.1 Distance-aware Output Layer via Laplace-approximated Neural Gaussian Process

To make the output layer $g : \mathcal{H} \to \mathcal{Y}$ distance aware, SNGP replaces the typical dense output layer with a Gaussian process (GP) with an RBF kernel, whose posterior variance at $x^*$ is characterized by its $L_2$ distance from the training data in the hidden space. Specifically, given $N$ training samples $\mathcal{D} = \{y_i, x_i\}_{i=1}^N$ and denoting $h_i = h(x_i)$, the Gaussian-process output layer $g_{N \times 1} = [g(h_1), \ldots, g(h_N)]^\top$ follows a multivariate normal distribution a priori:

$$g_{N \times 1} \sim MN(0_{N \times 1}, K_{N \times N}), \quad \text{where} \quad K_{i,j} = \exp(-||h_i - h_j||_2^2/2), \quad (6)$$

and the posterior distribution is computed as $p(g|\mathcal{D}) \propto p(\mathcal{D}|g)p(g)$ where $p(g)$ is the GP prior in (6) and $p(\mathcal{D}|g)$ is the data likelihood for classification (i.e., the exponentiated cross-entropy loss).

However, computing the exact Gaussian process posterior for a large-scale classification task is both analytically intractable and computationally expensive. In this work, we propose a simple approximation strategy for GP that is based on a Laplace approximation to the random Fourier feature (RFF) expansion of the GP posterior [61]. Our approach gives rise to a closed-form posterior that is end-to-end trainable with the rest of the neural network, and empirically leads to an improved quality in estimating the posterior uncertainty. Specifically, we first approximate the GP prior in (6) by deploying a low-rank approximation to the kernel matrix $K = \Phi \Phi^\top$ using random features [60]:

$$g_{N \times 1} \sim MN(0_{N \times 1}, \Phi \Phi^\top), \quad \text{where} \quad \Phi_{i,D_L \times 1} = \sqrt{2/D_L} \cos(-W_i h_i + b_i), \quad (7)$$

where $h_i = h(x_i)$ is the hidden representation in the penultimate layer with dimension $D_{L-1}$. $\Phi$ is the final layer with dimension $D_{L}$, it contains $W_i,D_L \times D_{L-1}$ a fixed weight matrix whose entries are sampled i.i.d. from $\mathcal{N}(0,1)$, and $b_i,D_L \times 1$ a fixed bias term whose entries are sampled i.i.d. from $\mathcal{U}niform(0,2\pi)$. As a result, for the $k^{th}$ logit, the RFF approximation to the GP prior in (6) can be written as a neural network layer with fixed hidden weights $W$ and learnable output weights $\beta_k^*:

$$g_k(h_i) = \sqrt{2/D_L} \cos(-W_i h_i + b_k^\top) \beta_k^*, \quad \text{with prior} \quad \beta_k^* \sim \mathcal{N}(0, I_{D_L \times 1}) \quad (8)$$

Notice that conditional on $h$, $\beta = \{\beta_k\}_{k=1}^K$ is the only learnable parameter in the model. As a result, the RFF approximation in (8) reduces an infinite-dimensional GP to a standard Bayesian linear model, for which many posterior approximation methods (e.g., expectation propagation (EP) can be applied [53]. In this work, we choose the Laplace method due to its simplicity and the fact that its posterior variance has a convenient closed form [61]. Briefly, the Laplace method approximates the RFF posterior $p(\beta|\mathcal{D})$ using a Gaussian likelihood centered around the maximum a posterior (MAP) estimate $\hat{\beta} = \arg\max_\beta p(\beta|\mathcal{D})$, such that $p(\hat{\beta} | \mathcal{D}) \approx MN(\hat{\beta}, \Sigma_k = \hat{\Sigma}_{k}^{-1})$, where $\hat{H}_{k(i,j)} = \frac{\partial^2}{\partial \beta_i \partial \beta_j} \log p(\beta_k | \mathcal{D}) |_{\beta = \hat{\beta}_k}$ is the $D_L \times D_L$ Hessian matrix of the log posterior likelihood evaluated at the MAP estimates. Under the linear-model formulation of the RFF posterior, the posterior precision matrix (i.e., the inverse covariance matrix) adopts a simple expression $\hat{\Sigma}_k^{-1} = I + \sum_{i=1}^N \hat{p}_{i,k}(1 - \hat{p}_{i,k}) \Phi_i \Phi_i^\top$, where $\hat{p}_{i,k}$ is the model prediction softmax($\hat{g}_i$) under the MAP estimates $\hat{\beta} = \{\beta_k\}_{k=1}^K$ [61]. To summarize, the Laplace posterior for GP under the RFF approximation is:

$$\beta_k | \mathcal{D} \sim MN(\hat{\beta}_k, \hat{\Sigma}_k), \quad \text{where} \quad \hat{\Sigma}_k^{-1} = I + \sum_{i=1}^N \hat{p}_{i,k}(1 - \hat{p}_{i,k}) \Phi_i \Phi_i^\top. \quad (9)$$

During minibatch training, the posterior mean $\hat{\beta}$ is updated via regular stochastic gradient descent (SGD) with respect to the (unnormalized) log posterior $-\log p(\beta | \mathcal{D}) = -\log p(\mathcal{D} | \beta) + \frac{1}{2} ||\beta||^2$ where $-\log p(\mathcal{D} | \beta)$ is the cross-entropy loss. The posterior precision matrix is updated cheaply as $\hat{\Sigma}_k^{-1} = (1 - m) \cdot \hat{\Sigma}_{k-1}^{-1} + m \cdot \sum_{i=1}^M \hat{p}_{i,k}(1 - \hat{p}_{i,k}) \Phi_i \Phi_i^\top$ for a minibatch of size $M$ and $m$ a small scaling coefficient. This computation only needs to be performed by passing through training data once at the final epoch. As a result, the GP posterior (9) can be learned scalably and in closed-form with minimal modification to the training pipeline of a deterministic DNN. It is worth noting that the Laplace approximation to the RFF posterior is asymptotically exact by the virtue of the Bernstein-von Mises (BvM) theorem and the fact that (8) is a finite-rank model [16, 23, 46, 57].
3.2 Distance-preserving Hidden Mapping via Spectral Normalization

Replacing the output layer $g$ with a Gaussian process only allows the model $\logit(x) = g \circ h(x)$ to be aware of the distance in the hidden space $||h(x_1) - h(x_2)||_H$. It is also important to ensure the hidden mapping $h$ is distance preserving so that the distance in the hidden space $||h(x) - h(x')||_H$ has a meaningful correspondence to the distance in the input space $|x - x'|_X$. To this end, we notice that modern deep learning models (e.g., ResNets, Transformers) are commonly composed of residual blocks, i.e., $h(x) = h_{L-1} \circ \cdots \circ h_2 \circ h_1(x)$ where $h_l(x) = x + g_l(x)$. For such models, there exists a simple method to ensure $h$ is distance preserving: by bounding the Lipschitz constants of all nonlinear residual mappings $\{g_l\}_{l=1}^{L-1}$ to be less than 1. We state this result formally below:

**Proposition 1** (Lipschitz-bounded residual block is distance preserving [3]). Consider a hidden mapping $h : \mathcal{X} \rightarrow \mathcal{H}$ with residual architecture $h = h_{L-1} \circ \cdots \circ h_2 \circ h_1$ where $h_l(x) = x + g_l(x)$. If for $0 < \alpha \leq 1$, all $g_l$’s are $\alpha$-Lipschitz, i.e., $||g_l(x) - g_l(x')||_H \leq \alpha ||x - x'||_X \forall (x, x') \in \mathcal{X}$. Then:

$$L_1 * ||x - x'||_X \leq ||h(x) - h(x')||_H \leq L_2 * ||x - x'||_X,$$

where $L_1 = (1 - \alpha)^{L-1}$ and $L_2 = (1 + \alpha)^{L-1}$, i.e., $h$ is distance preserving.

Proof is in Appendix E.1. The ability of a residual network to construct a geometry-preserving metric transform between the input space $\mathcal{X}$ and the hidden space $\mathcal{H}$ is well-established in learning theory and generative modeling literature, but the application of these results in the context of uncertainty estimation for DNN appears to be new [3, 5, 32, 64].

Consequently, to ensure the hidden mapping $h$ is distance preserving, it is sufficient to ensure that the weight matrices for the nonlinear residual block $g_l(x) = \sigma(W_l x + b_l)$ to have spectral norm (i.e., the largest singular value) less than 1, since $||g_l||_{Lip} \leq ||W_l x + b_l||_{Lip} \leq ||W_l||_2 \leq 1$. In this work, we enforce the aforementioned Lipschitz constraint on $g_l$’s by applying the spectral normalization (SN) on the weight matrices $\{W_l\}_{l=1}^{L-1}$ as recommended in [5]. Briefly, at every training step, the SN method first estimate the spectral norm $\hat{\lambda} \approx ||W_l||_2$ using the power iteration method [26, 54], and then normalizes the weights as:

$$W_l = \begin{cases} c * W_l / \hat{\lambda} & \text{if } c < \hat{\lambda} \\ W_l & \text{otherwise} \end{cases}$$

(10)

where $c > 0$ is a hyperparameter used to adjust the exact spectral norm upper bound on $||W_l||_2$ (so that $||W_l||_2 \leq c$). This hyperparameter is useful in practice since the other regularization mechanisms (e.g., Dropout, Batch Normalization) in the hidden layers can rescale the Lipschitz constant of the original residual mapping [26]. Therefore, (10) allows us more flexibility in controlling the spectral norm of the neural network weights so it is the most compatible with the architecture at hand.

**Method Summary** We summarize the method in Algorithms 1-2. As shown, for every minibatch step, the model first updates the hidden-layer weights $\{W_l, b_l\}_{l=1}^{L-1}$ and the trainable output weights $\beta = \{\beta_k\}_{k=1}^K$ via SGD, then performs spectral normalization, and finally (if in the final epoch) performs precision matrix update (Equation (9)). We discuss further details (e.g. computational complexity) in Appendix A.

**Algorithm 1 SNGP Training**

1: **Input:**
Minibatches $\{D_l\}_{l=1}^L$ for $D_l = \{y_{ml}, x_{ml}\}_{m=1}^M$.
2: **Initialize:**
$\hat{\Sigma} = 1, W_L \sim N(0, 1), b_L \sim U(0, 2\pi)$
3: **for** $\text{train/step} = 1$ to max/step **do**
4: SGD update $\{\beta, \{W_l\}_{l=1}^{L-1}, \{b_l\}_{l=1}^{L-1}\}$
5: **Spectral Normalization** $\{W_l\}_{l=1}^{L-1}$ (10).
6: **if** final/epoch **then**
7: Update precision matrix $\{\Sigma_k^{-1}\}_{k=1}^K$ (9).
8: **end if**
9: **end for**
10: Compute posterior covariance $\hat{\Sigma}_k = \text{inv}(\Sigma_k^{-1})$.

**Algorithm 2 SNGP Prediction**

1: **Input:** Testing example $x$.
2: **Compute Feature:**
$\Phi_{D_{k \times 1}} = \sqrt{2/D_k} \cos(W_L h(x) + b_L)$.
3: **Compute Posterior Mean:**
$logit(x) = \Phi^T \beta_k$
4: **Compute Posterior Variance:**
$\text{var}(x) = \Phi^T \hat{\Sigma}_k \Phi$
5: **Compute Predictive Distribution:**
$p(y|x) = \int_{m \sim N(\logit(x), \text{VAR}(x))} \text{softmax}(m)$
We first study the behavior of the uncertainty surface of a SNGP model under a suite of 2D classification benchmarks. Specifically, we consider the two ovals benchmark (Figure 1, row 1) and the two moons benchmark (Figure 1, row 2). The two ovals benchmark consists of two near-flat Gaussian distributions, which represent the two in-domain classes (orange and blue) that are separable by a linear decision boundary. There also exists an OOD distribution (red) that the model doesn’t observe during training. Similarly, the two moons dataset consists of two banana-shaped distributions separable by a nonlinear decision boundary. We consider a 12-layer, 128-unit deep architecture ResFFN-12-128. The full experimental details are in Appendix C.

Figure 1 shows the results, where the background color visualizes the uncertainty surface output by each model. We first notice that the shallow Gaussian process models (Figures 1a and 1f) exhibit an expected behavior for high-quality predictive uncertainty: it generates low uncertainty in $\mathcal{X}_{\text{IND}}$ that is supported by the training data (purple color), and generates high uncertainty when $x$ is far from $\mathcal{X}_{\text{IND}}$ (yellow color), i.e., input distance awareness. As a result, the shallow GP model is able to assign low confidence to the OOD data (colored in red), indicating reliable uncertainty quantification. On the other hand, deep ensembles (Figures 1b, 1g) and MC Dropout (Figures 1c, 1h) are based on dense output layers that are not distance aware. As a result, both methods quantify their predictive uncertainty based on the distance from the decision boundaries, assigning low uncertainty to OOD examples even if they are far from the data. Finally, the DNN-GP (Figures 1d and 1i) and SNGP (Figures 1e and 1j) both use GP as their output layers, but with SNGP additionally imposing the spectral normalization on its hidden mapping $h(\cdot)$. As a result, the DNN-GP’s uncertainty surfaces are still strongly impacted by the distance from decision boundary, likely caused by the fact that the un-regularized hidden mapping $h(x)$ is free to discard information that is not relevant for prediction. On the other hand, the SNGP is able to maintain the input distance awareness property via its...
bi-Lipschitz constraint, and exhibits a uncertainty surface that is analogous to the gold-standard model (shallow GP) despite the fact that SNGP is based on a 12-layer network.

5.2 Vision and Language Understanding

Baseline Methods All methods included in the vision and language understanding experiments are summarized in Table 1. Specifically, we evaluate SNGP on a Wide ResNet 28-10 [83] for image classification, and BERTbase [18] for language understanding. We compare against a deterministic baseline and two ensemble approaches: MC Dropout (with 10 dropout samples) and deep ensembles (with 10 models), all trained with a dense output layer and no spectral regularization. We consider three single-model approaches: MCD-GP (with 10 samples), Deterministic Uncertainty Quantification (DUQ) (see Section 4). For all models that use GP layer, we keep $D_L = 1024$ and compute predictive distribution by performing Monte Carlo averaging with 10 samples. We also include two ablated version of SNGP: DNN-SN which uses spectral normalization on its hidden weights and a dense output layer (i.e. distance preserving hidden mapping without distance-aware output layer), and DNN-GP which uses the GP as output layer but without spectral normalization on its hidden layers (i.e., distance-aware output layer without distance-preserving hidden mapping). Further experiment details and recommendations for practical implementation are in Appendix C. All baselines are built on the uncertainty baselines framework.

| Methods                          | Additional Regularization | Output Layer | Ensemble Training | Multi-pass Inference |
|----------------------------------|---------------------------|--------------|-------------------|----------------------|
| Deterministic                    | -                         | Dense        | -                 | -                    |
| MC Dropout                       | Dropout                   | Dense        | -                 | Yes                  |
| Deep Ensemble                    | -                         | Dense        | Yes               | Yes                  |
| MCD-GP                           | Dropout                   | GP           | -                 | Yes                  |
| DUQ                              | Gradient Penalty          | RBF          | -                 | -                    |
| DNN-SN                           | Spec Norm                 | Dense        | -                 | -                    |
| DNN-GP                           | Spec Norm                 | GP           | -                 | -                    |
| SNGP                             | Spec Norm                 | GP           | -                 | -                    |

Table 1: Summary of methods used in experiments. Multi-pass Inference refers to whether the method needs to perform multiple forward passes to generate the predictive distribution.

CIFAR-10 and CIFAR-100 We evaluate the model’s predictive accuracy and calibration error under both clean CIFAR testing data and its corrupted versions termed CIFAR-*-C [34]. To evaluate the model’s OOD detection performance, we consider two tasks: a standard OOD task using SVHN as the OOD dataset for a model trained on CIFAR-10/-100, and a difficult OOD task using CIFAR-100 as the OOD dataset for a model trained on CIFAR-10, and vice versa. We compute the uncertainty score for OOD using the Dempster-Shafer metric as introduced in [68], which empirically leads to better performance for distance-aware models (see Appendix C). Table 2-3 reports the results. As shown, for predictive accuracy, SNGP is competitive with that of a deterministic network, and outperforms the other single-model approaches. For calibration error, SNGP clearly outperforms the other single-model approaches and is competitive with the deep ensemble. Finally, for OOD detection, SNGP outperforms not only the deep ensembles and MC Dropout approaches that are based on a dense output layer, but also the MCD-GP and DUQ that are based on the GP layer, illustrating the importance of the input distance awareness property for high-quality performance in uncertainty quantification.

| Method  | Accuracy (%) | ECE (%) | NLL (%) | OOD AUPR (%) | Latency (ms / example) |
|---------|--------------|---------|---------|--------------|------------------------|
| Clean   | Corrupted    | Clean   | Corrupted | Clean        | Corrupted   | SVHN | CIFAR-100 | Clean   | Corrupted | Clean        | Corrupted   | Clean | Corrupted | Clean        | Corrupted   | Clean | Corrupted | Clean        | Corrupted   | Clean | Corrupted | Clean        | Corrupted   | Clean | Corrupted | Clean        | Corrupted   | Clean | Corrupted | Clean        | Corrupted   |
| Deterministic | 96.0 ± 0.01 | 72.9 ± 0.01 | 0.023 ± 0.002 | 0.135 ± 0.011 | 0.158 ± 0.004 | 0.159 ± 0.02 | 0.781 ± 0.00 | 0.835 ± 0.01 | 3.91       |
| Deep Ensembles | 96.6 ± 0.01 | 77.9 ± 0.01 | 0.010 ± 0.001 | 0.087 ± 0.004 | 0.114 ± 0.001 | 0.815 ± 0.01 | 0.691 ± 0.01 | 0.832 ± 0.01 | 27.10      |
| MCD-GP | 95.5 ± 0.02 | 70.0 ± 0.01 | 0.054 ± 0.004 | 0.100 ± 0.007 | 0.172 ± 0.001 | 1.157 ± 0.01 | 0.960 ± 0.01 | 0.863 ± 0.01 | 29.53      |
| DUQ    | 94.7 ± 0.02 | 71.6 ± 0.02 | 0.034 ± 0.002 | 0.183 ± 0.011 | 0.239 ± 0.002 | 1.348 ± 0.01 | 0.973 ± 0.01 | 0.854 ± 0.01 | 8.68       |
| DNN-GP | 95.9 ± 0.01 | 71.7 ± 0.01 | 0.029 ± 0.002 | 0.175 ± 0.008 | 0.221 ± 0.002 | 1.380 ± 0.01 | 0.976 ± 0.01 | 0.887 ± 0.01 | 5.58       |
| SNGP(Ours) | 95.9 ± 0.01 | 74.6 ± 0.01 | 0.018 ± 0.001 | 0.090 ± 0.012 | 0.138 ± 0.001 | 0.935 ± 0.01 | 0.990 ± 0.01 | 0.905 ± 0.01 | 6.25       |

Table 2: Results for Wide ResNet-28-10 on CIFAR-10, averaged over 10 seeds.

Detecting Out-of-Scope Intent in Conversational Language Understanding To validate the method beyond image modalities, we also evaluate SNGP on a practical language understanding task where uncertainty quantification is of natural importance: dialog intent detection [44, 78, 82, 84]. In a goal-oriented dialog system (e.g. chatbot) built for a collection of in-domain services, it is important for the model to understand if an input natural utterance from an user is in-scope (so it can activate
one of the in-domain services) or out-of-scope (where the model should abstain). To this end, we consider training an intent understanding model using the CLINC OOS intent detection benchmark dataset [44]. Briefly, the OOS dataset contains data for 150 in-domain services with 150 training sentences in each domain, and also 1500 natural out-of-domain utterances. We train the models only on in-domain data, and evaluate their predictive accuracy on the in-domain test data, their calibration and OOD detection performance on the combined in-domain and out-of-domain data. The results are in Table 4. As shown, consistent with the previous vision experiments, SNGP is competitive in predictive accuracy when compared to a deterministic baseline, and outperforms other approaches in calibration and OOD detection.

| Method        | Accuracy (↑) | ECE (↓) | NLL (↓) | OOD AUROC (↑) | Latency (ms / example) |
|---------------|-------------|--------|--------|---------------|------------------------|
| Deterministic | 96.5 ± 0.11 | 0.024 ± 0.002 | 3.559 ± 0.11 | 0.897 ± 0.01 | 0.757 ± 0.02 | 10.42 |
| MC Dropout    | 96.1 ± 0.10 | 0.021 ± 0.001 | 1.658 ± 0.05 | 0.938 ± 0.01 | 0.799 ± 0.01 | 85.62 |
| Deep Ensemble | 97.5 ± 0.03 | 0.013 ± 0.002 | 1.062 ± 0.02 | 0.964 ± 0.01 | 0.862 ± 0.01 | 84.46 |
| MCD-GP        | 95.9 ± 0.05 | 0.015 ± 0.003 | 1.664 ± 0.04 | 0.906 ± 0.02 | 0.803 ± 0.01 | 88.38 |
| DUQ           | 96.0 ± 0.04 | 0.009 ± 0.002 | 4.015 ± 0.08 | 0.917 ± 0.01 | 0.806 ± 0.01 | 15.60 |
| DNN-SN        | 95.6 ± 0.10 | 0.037 ± 0.004 | 3.563 ± 0.03 | 0.922 ± 0.02 | 0.733 ± 0.01 | 17.36 |
| DNN-GP        | 95.9 ± 0.07 | 0.075 ± 0.003 | 3.594 ± 0.02 | 0.941 ± 0.01 | 0.831 ± 0.01 | 18.93 |
| SNGP          | 96.6 ± 0.05 | 0.014 ± 0.005 | 1.218 ± 0.03 | 0.969 ± 0.01 | 0.880 ± 0.01 | 17.36 |

Table 4: Results for BERT on CLINC OOS, averaged over 10 seeds.

6 Conclusion

We propose SNGP, a simple approach to improve a single deterministic DNN’s ability in predictive uncertainty estimation. It makes minimal changes to the architecture and training/prediction pipeline of a deterministic DNN, only adding spectral normalization to the hidden mapping, and replacing the dense output layer with a random feature layer that approximates a GP. We theoretically motivate input distance awareness, the key design principle behind SNGP, via a learning-theoretic analysis of the uncertainty estimation problem. We also propose a closed-form approximation method to make the GP posterior end-to-end trainable in linear time with the rest of the neural network. On a suite of vision and language understanding tasks and on modern architectures (ResNet and BERT), SNGP is competitive with a deep ensemble in prediction, calibration and out-of-domain detection, and outperforms other single-model approaches.

A central observation we made in this work is that good representational learning is important for good uncertainty quantification. In particular, we highlighted bi-Lipschitz (Equation (5)) as an important condition for the learned representation of a DNN to attain high-quality uncertainty performance, and proposed spectral normalization as a simple approach to ensure such property in practice. It is worth noting that there exists other representation learning techniques, e.g., data augmentation or unsupervised pretraining, that are known to also improve a network’s uncertainty performance [35, 36]. Analyzing whether and how these approaches contribute to improve a DNN bi-Lipschitz condition, and whether the bi-Lipschitz condition is sufficient in explaining these methods’ success, are interesting avenues of future work. Furthermore, we note that the spectral norm bound \( \alpha < 1 \) in Proposition 1 forms only a sufficient condition for ensuring bi-Lipschitz [5]. In practice, we observed that for convolutional layers, a looser norm bound is needed for state-of-the-art performance (see Section C), raising questions of whether the current regularization approach is precise enough in controlling the spectral norm of a convolutional kernel, or if there is an alternative mechanism at play in ensuring the bi-Lipschitz criterion. Finally, from a probabilistic learning perspective, SNGP focuses on learning a single high-quality model \( p_\theta(y|x) \) for a deterministic representation. Therefore we expect it to provide complementary benefits to approaches such as (efficient) ensembles and Bayesian neural networks [21, 42, 79] which marginalize over the representation parameters as well.
Acknowledgements We would like to thank Kevin Murphy, Deepak Ramachandran, Jasper Snoek, and Timothy Nguyen at Google Research for the insightful comments and fruitful discussion.

Broader Impact

This work proposed a simple and practical methodology to improve the uncertainty estimation performance of a deterministic deep learning model. Experiment results showcased the method’s ability in improving model performance in calibration and OOD detection while maintaining similar level of accuracy and latency, therefore illustrating its feasibility for industrial-scale applications. We hope the proposed approach can be used to bring concrete improvements to AI-driven, socially-relevant services where uncertainty is of natural importance. Examples include medical and policy decision making, online toxic comment management, fairness-aware recommendation systems, etc.

Nonetheless, we do not claim that the improvement illustrated in this paper solve the problem of model uncertainty entirely. This is because the analysis and experiments in this study may not capture the full complexity of the real-world use cases, and there will always be room for improvement. Designers of machine learning systems are encouraged to proactively confront the shortcomings of model uncertainty and the underlying models that generate these confidences. Even with a proper user interface, there is always room to misinterpret model outputs and probabilities, such as with nuanced applications such as election predictions, and users of these models should to be properly trained to take these factors into account.

References

[1] S. An, F. Boussaid, and M. Bennamoun. How Can Deep Rectifier Networks Achieve Linear Separability and Preserve Distances? In International Conference on Machine Learning, pages 514–523, June 2015. ISSN: 1938-7228 Section: Machine Learning.

[2] C. Anil, J. Lucas, and R. Grosse. Sorting Out Lipschitz Function Approximation. In International Conference on Machine Learning, pages 291–301, May 2019. ISSN: 1938-7228 Section: Machine Learning.

[3] P. Bartlett, S. Evans, and P. Long. Representing smooth functions as compositions of near-identity functions with implications for deep network optimization. arXiv, 2018.

[4] P. L. Bartlett and M. H. Wegkamp. Classification with a Reject Option using a Hinge Loss. Journal of Machine Learning Research, 9(Aug):1823–1840, 2008.

[5] J. Behrmann, W. Grathwohl, R. T. Q. Chen, D. Duvenaud, and J.-H. Jacobsen. Invertible Residual Networks. In International Conference on Machine Learning, pages 573–582, May 2019. ISSN: 1938-7228 Section: Machine Learning.

[6] A. Bendale and T. E. Boult. Towards Open Set Deep Networks. 2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR), 2016.

[7] J. O. Berger. Statistical Decision Theory and Bayesian Analysis. Springer Series in Statistics. Springer-Verlag, New York, 2 edition, 1985.

[8] A. Blum. Random Projection, Margins, Kernels, and Feature-Selection. In C. Saunders, M. Grobelnik, S. Gunn, and J. Shawe-Taylor, editors, Subspace, Latent Structure and Feature Selection, Lecture Notes in Computer Science, pages 52–68, Berlin, Heidelberg, 2006. Springer.

[9] J. Bradshaw, A. G. d. G. Matthews, and Z. Ghahramani. Adversarial Examples, Uncertainty, and Transfer Testing Robustness in Gaussian Process Hybrid Deep Networks. arXiv:1707.02476 [stat], July 2017. arXiv: 1707.02476.

[10] J. Bröcker. Reliability, sufficiency, and the decomposition of proper scores. Quarterly Journal of the Royal Meteorological Society: A journal of the atmospheric sciences, applied meteorology and physical oceanography, 135(643):1512–1519, 2009.

[11] R. Calandra, J. Peters, C. E. Rasmussen, and M. P. Deisenroth. Manifold Gaussian Processes for regression. 2016 International Joint Conference on Neural Networks (IJCNN), 2016.
[12] D. Cer, M. Diab, E. Agirre, I. Lopez-Gazpio, and L. Specia. SemEval-2017 Task 1: Semantic Textual Similarity Multilingual and Crosslingual Focused Evaluation. In Proceedings of the 11th International Workshop on Semantic Evaluation (SemEval-2017), pages 1–14, Vancouver, Canada, Aug. 2017. Association for Computational Linguistics.

[13] A. Chernodub and D. Nowicki. Norm-preserving Orthogonal Permutation Linear Unit Activation Functions (OPLU). arXiv:1604.02313 [cs], Jan. 2017. arXiv: 1604.02313.

[14] C. Cortes, M. Mohri, and A. Rostamizadeh. Learning Non-Linear Combinations of Kernels. In Y. Bengio, D. Schuurmans, J. D. Lafferty, C. K. I. Williams, and A. Culotta, editors, Advances in Neural Information Processing Systems 22, pages 396–404. Curran Associates, Inc., 2009.

[15] J. Daunizeau. Semi-analytical approximations to statistical moments of sigmoid and softmax mappings of normal variables. Feb. 2017.

[16] G. P. Dehaene. A deterministic and computable Bernstein-von Mises theorem. ArXiv, 2019.

[17] J. S. Denker and Y. LeCun. Transforming Neural-Net Output Levels to Probability Distributions. In R. P. Lippmann, J. E. Moody, and D. S. Touretzky, editors, Advances in Neural Information Processing Systems 3, pages 853–859. Morgan-Kaufmann, 1991.

[18] J. Devlin, M.-W. Chang, K. Lee, and K. Toutanova. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. arXiv:1810.04805 [cs], Oct. 2018. arXiv: 1810.04805.

[19] L. Dinh, D. Krueger, and Y. Bengio. NICE: Non-linear Independent Components Estimation. arXiv:1410.8516 [cs], Oct. 2014. arXiv: 1410.8516.

[20] L. Dinh, J. Sohl-Dickstein, and S. Bengio. Density estimation using Real NVP. arXiv:1605.08803 [cs, stat], May 2016. arXiv: 1605.08803.

[21] M. Dusenberry, G. Jerfel, Y. Wen, Y. Ma, J. Snoek, K. Heller, B. Lakshminarayanan, and D. Tran. Efficient and Scalable Bayesian Neural Nets with Rank-1 Factors. Proceedings of the International Conference on Machine Learning, 1, 2020.

[22] D. Feng, L. Rosenbaum, and K. Dietmayer. Towards Safe Autonomous Driving: Capture Uncertainty in the Deep Neural Network For Lidar 3D Vehicle Detection. Apr. 2018.

[23] D. Freedman. Wald Lecture: On the Bernstein-von Mises theorem with infinite-dimensional parameters. The Annals of Statistics, 27(4):1119–1141, Aug. 1999.

[24] T. Gneiting, F. Baladadouai, and A. E. Raftery. Probabilistic forecasts, calibration and sharpness. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 69(2):243–268, Apr. 2007.

[25] T. Gneiting and A. E. Raftery. Strictly Proper Scoring Rules, Prediction, and Estimation. Journal of the American Statistical Association, 102(477):359–378, Mar. 2007.

[26] H. Gouk, E. Frank, B. Pfahringer, and M. Cree. Regularisation of Neural Networks by Enforcing Lipschitz Continuity. Apr. 2018.

[27] P. D. GräFenwald and A. P. Dawid. Game theory, maximum entropy, minimum discrepancy and robust Bayesian decision theory. Annals of Statistics, 32(4):1367–1433, Aug. 2004. Publisher: Institute of Mathematical Statistics.

[28] I. Gulrajani, F. Ahmed, M. Arjovsky, V. Dumoulin, and A. Courville. Improved training of wasserstein GANs. In Proceedings of the 31st International Conference on Neural Information Processing Systems, NIPS’17, pages 5769–5779, Long Beach, California, USA, Dec. 2017. Curran Associates Inc.

[29] C. Guo, G. Pleiss, Y. Sun, and K. Q. Weinberger. On Calibration of Modern Neural Networks. In International Conference on Machine Learning, pages 1321–1330, July 2017. ISSN: 1938-7228 Section: Machine Learning.
[30] D. Hafner, D. Tran, T. Lillicrap, A. Irpan, and J. Davidson. Reliable Uncertainty Estimates in Deep Neural Networks using Noise Contrastive Priors. July 2018.

[31] R. E. Harang and E. M. Rudd. Principled Uncertainty Estimation for Deep Neural Networks, 2018. Library Catalog: www.semanticscholar.org.

[32] M. Hauser and A. Ray. Principles of Riemannian Geometry in Neural Networks. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems 30, pages 2807–2816. Curran Associates, Inc., 2017.

[33] M. Hein, M. Andriushchenko, and J. Bitterwolf. Why ReLU Networks Yield High-Confidence Predictions Far Away From the Training Data and How to Mitigate the Problem. pages 41–50, 2019.

[34] D. Hendrycks and T. Dietterich. Benchmarking Neural Network Robustness to Common Corruptions and Perturbations. Sept. 2018.

[35] D. Hendrycks, K. Lee, and M. Mazeika. Using Pre-Training Can Improve Model Robustness and Uncertainty. In International Conference on Machine Learning, pages 2712–2721, May 2019. ISSN: 1938-7228 Section: Machine Learning.

[36] D. Hendrycks*, N. Mu*, E. D. Cubuk, B. Zoph, J. Gilmer, and B. Lakshminarayanan. AugMix: A Simple Method to Improve Robustness and Uncertainty under Data Shift. In International Conference on Learning Representations, 2020.

[37] J.-H. Jacobsen, J. Behrmann, R. Zemel, and M. Bethge. Excessive Invariance Causes Adversarial Vulnerability. Sept. 2018.

[38] J.-H. Jacobsen, J. Behrmann, N. Carlini, F. Tramãšr, and N. Papernot. Exploiting Excessive Invariance caused by Norm-Bounded Adversarial Robustness. Mar. 2019.

[39] r.-H. Jacobsen, A. W. M. Smeulders, and E. Oyallon. i-RevNet: Deep Invertible Networks. Feb. 2018.

[40] M. E. E. Khan, A. Immer, E. Abedi, and M. Korzepa. Approximate Inference Turns Deep Networks into Gaussian Processes. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d. AlchëBrown, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems 32, pages 3094–3104. Curran Associates, Inc., 2019.

[41] A. Kristiadi, M. Hein, and P. Hennig. Being Bayesian, Even Just a Bit, Fixes Overconfidence in ReLU Networks. arXiv:2002.10118 [cs, stat], Feb. 2020. arXiv: 2002.10118.

[42] B. Lakshminarayanan, A. Pritzel, and C. Blundell. Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems 30, pages 6402–6413. Curran Associates, Inc., 2017.

[43] J. Landes. Probabilism, entropies and strictly proper scoring rules. International Journal of Approximate Reasoning, 63:1–21, Aug. 2015.

[44] S. Larson, A. Mahendran, J. J. Peper, C. Clarke, A. Lee, P. Hill, J. K. Kummerfeld, K. Leach, M. A. Laurenzano, L. Tang, and J. Mars. An Evaluation Dataset for Intent Classification and Out-of-Scope Prediction. arXiv:1909.02027 [cs], Sept. 2019. arXiv: 1909.02027.

[45] N. D. Lawrence and J. Q. Candela. Local Distance Preservation in the GP-LVM Through Back Constraints. Jan. 2006.

[46] L. LeCam. Convergence of Estimates Under Dimensionality Restrictions. The Annals of Statistics, 1(1):38–53, Jan. 1973.

[47] K. Lee, H. Lee, K. Lee, and J. Shin. Training Confidence-calibrated Classifiers for Detecting Out-of-Distribution Samples. In International Conference on Learning Representations, 2018.
D. Macedo, T. I. Ren, C. Zanchettin, A. L. I. Oliveira, A. Tapp, and T. Ludermir. Isotropic Maximization Loss and Entropic Score: Fast, Accurate, Scalable, Unexposed, Turnkey, and Native Neural Networks Out-of-Distribution Detection. arXiv:1908.05569 [cs, stat], Feb. 2020.

D. J. C. MacKay. A practical Bayesian framework for backpropagation networks. Neural Computation, 4(3):448–472, May 1992. Number: 3 Publisher: MIT Press.

A. Malinin and M. Gales. Predictive Uncertainty Estimation via Prior Networks. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems 31, pages 7047–7058. Curran Associates, Inc., 2018.

A. Malinin and M. Gales. Prior Networks for Detection of Adversarial Attacks. arXiv:1812.02575 [cs, stat], Dec. 2018. arXiv: 1812.02575.

A. Meinke and M. Hein. Towards neural networks that provably know when they don’t know. In International Conference on Learning Representations, 2020.

T. P. Minka. A family of algorithms for approximate bayesian inference. phd, Massachusetts Institute of Technology, USA, 2001. AAI0803033.

T. Miyato, T. Kataoka, M. Koyama, and Y. Yoshida. Spectral Normalization for Generative Adversarial Networks. In International Conference on Learning Representations, 2018.

Y. Netzer, T. Wang, A. Coates, A. Bissacco, B. Wu, and A. Y. Ng. Reading Digits in Natural Images with Unsupervised Feature Learning. In NIPS Workshop on Deep Learning and Unsupervised Feature Learning 2011, 2011.

J. Nixon, M. W. Dusenberry, L. Zhang, G. Jerfel, and D. Tran. Measuring calibration in deep learning. In CVPR Workshop, 2019.

M. Panov and V. Spokoiny. Finite Sample Bernstein von Mises Theorem for Semiparametric Problems. Bayesian Analysis, 10(3):665–710, Sept. 2015.

M. Parry, A. P. Dawid, and S. Lauritzen. Proper local scoring rules. Annals of Statistics, 40(1):561–592, Feb. 2012. Publisher: Institute of Mathematical Statistics.

D. C. Perrault-Joncas. Metric Learning and Manifolds: Preserving the Intrinsic Geometry. 2017.

A. Rahimi and B. Recht. Random Features for Large-Scale Kernel Machines. In J. C. Platt, D. Koller, Y. Singer, and S. T. Roweis, editors, Advances in Neural Information Processing Systems 20, pages 1177–1184. Curran Associates, Inc., 2008.

C. E. Rasmussen and C. K. I. Williams. Gaussian Processes for Machine Learning. University Press Limited, Jan. 2006. Google-Books-ID: vWtwQgAACAAJ.

C. Riquelme, G. Tucker, and J. Snoek. Deep Bayesian Bandits Showdown: An Empirical Comparison of Bayesian Deep Networks for Thompson Sampling. In International Conference on Learning Representations, 2018.

H. Ritter, A. Botev, and D. Barber. A Scalable Laplace Approximation for Neural Networks. In International Conference on Learning Representations, 2018.

F. Rousseau, L. Drumetz, and R. Fablet. Residual Networks as Flows of Diffeomorphisms. Journal of Mathematical Imaging and Vision, 62(3):365–375, Apr. 2020.

W. Ruan, X. Huang, and M. Kwiatkowska. Reachability analysis of deep neural networks with provable guarantees. In Proceedings of the 27th International Joint Conference on Artificial Intelligence, IJCAI’18, pages 2651–2659, Stockholm, Sweden, July 2018. AAAI Press.

W. J. Scheirer, L. P. Jain, and T. E. Boult. Probability Models for Open Set Recognition. IEEE Transactions on Pattern Analysis and Machine Intelligence, 36(11):2317–2324, Nov. 2014. Conference Name: IEEE Transactions on Pattern Analysis and Machine Intelligence.
[67] M. O. Searcoid. *Metric Spaces*. Springer London, London, 2007 edition, Aug. 2006.

[68] M. Sensoy, L. Kaplan, and M. Kandemir. Evidential Deep Learning to Quantify Classification Uncertainty. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems 31*, pages 3179–3189. Curran Associates, Inc., 2018.

[69] L. Shu, H. Xu, and B. Liu. DOC: Deep Open Classification of Text Documents. *arXiv:1709.08716 [cs]*, Sept. 2017. arXiv: 1709.08716.

[70] J. Snoek, O. Rippel, K. Swersky, R. Kiros, N. Satish, N. Sundaram, M. M. A. Patwary, Prabhat, and R. P. Adams. Scalable Bayesian Optimization Using Deep Neural Networks. *arXiv:1502.05700 [stat]*, Feb. 2015. arXiv: 1502.05700.

[71] J. Sokolic, R. Giryes, G. Sapiro, and M. R. D. Rodrigues. Robust Large Margin Deep Neural Networks. *IEEE Transactions on Signal Processing*, 2017.

[72] N. Tagasovska and D. Lopez-Paz. Single-Model Uncertainties for Deep Learning. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d. AlchÉ-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems 32*, pages 6417–6428. Curran Associates, Inc., 2019.

[73] L. Tierney, R. E. Kass, and J. B. Kadane. Approximate Marginal Densities of Nonlinear Functions. *Biometrika*, 76(3):425–433, 1989. Publisher: [Oxford University Press, Biometrika Trust].

[74] G.-L. Tran, E. V. Bonilla, J. Cunningham, P. Michiardi, and M. Filippone. Calibrating Deep Convolutional Gaussian Processes. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 1554–1563, Apr. 2019. ISSN: 1938-7228 Section: Machine Learning.

[75] Y. Tsuzuku, I. Sato, and M. Sugiyama. Lipschitz-Margin Training: Scalable Certification of Perturbation Invariance for Deep Neural Networks. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems 31*, pages 6541–6550. Curran Associates, Inc., 2018.

[76] B. van Aken, J. Risch, R. Krestel, and A. Loser. Challenges for Toxic Comment Classification: An In-Depth Error Analysis. In *Proceedings of the 2nd Workshop on Abusive Language Online (ALW2)*, pages 33–42, Brussels, Belgium, Oct. 2018. Association for Computational Linguistics.

[77] J. van Amersfoort, L. Smith, Y. W. Teh, and Y. Gal. Simple and Scalable Epistemic Uncertainty Estimation Using a Single Deep Deterministic Neural Network. *arXiv:2003.02037 [cs, stat]*, Mar. 2020. arXiv: 2003.02037.

[78] N. Vedula, N. Lipka, P. Maneriker, and S. Parthasarathy. Towards Open Intent Discovery for Conversational Text. *arXiv:1904.08524 [cs]*, Apr. 2019. arXiv: 1904.08524.

[79] Y. Wen, D. Tran, and J. Ba. BatchEnsemble: an Alternative Approach to Efficient Ensemble and Lifelong Learning. In *International Conference on Learning Representations*, 2020.

[80] T.-W. Weng, H. Zhang, P.-Y. Chen, J. Yi, D. Su, Y. Gao, C.-J. Hsieh, and L. Daniel. Evaluating the Robustness of Neural Networks: An Extreme Value Theory Approach. In *International Conference on Learning Representations*, 2018.

[81] A. G. Wilson, Z. Hu, R. Salakhutdinov, and E. P. Xing. Stochastic Variational Deep Kernel Learning. In *Proceedings of the 30th International Conference on Neural Information Processing Systems*, NIPS’16, pages 2594–2602, USA, 2016. Curran Associates Inc.

[82] M.-A. Yaghoub-Zadeh-Fard, B. Benatallah, F. Casati, M. Chai Barukh, and S. Zamanirad. User Utterance Acquisition for Training Task-Oriented Bots: A Review of Challenges, Techniques and Opportunities. *IEEE Internet Computing*, pages 1–1, 2020. Conference Name: IEEE Internet Computing.

[83] S. Zagoruyko and N. Komodakis. Wide Residual Networks. *arXiv:1605.07146 [cs]*, June 2017. arXiv: 1605.07146.
[84] Y. Zheng, G. Chen, and M. Huang. Out-of-Domain Detection for Natural Language Understanding in Dialog Systems. *IEEE/ACM Transactions on Audio, Speech, and Language Processing*, 28:1198–1209, 2020. Conference Name: IEEE/ACM Transactions on Audio, Speech, and Language Processing.