Frequentist Uncertainty Estimates for Deep Learning

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Abstract

We provide frequentist estimates of aleatoric and epistemic uncertainty for deep neural networks. To estimate aleatoric uncertainty we propose simultaneous quantile regression, a loss function to learn all the conditional quantiles of a given target variable. These quantiles can be used to compute well-calibrated prediction intervals. To estimate epistemic uncertainty we propose orthonormal certificates, a collection of diverse non-constant functions that map all training samples to zero. These certificates map out-of-distribution examples to non-zero values, signaling high epistemic uncertainty. Our uncertainty estimators are computationally attractive, since they do not require training an ensemble of deep models. Throughout a variety of real-world datasets and tasks, we show the state-of-the-art performance of our uncertainty estimators.

1. Introduction

Deep learning permeates our lives, with prospects to drive our cars and decide on our medical treatments. These ambitions will not materialize if deep learning models remain unable to assess their confidence when performing under diverse situations. Being aware of uncertainty in prediction is crucial in multiple scenarios. First, uncertainty plays a central role on deciding when to abstain from prediction. Abstention is a reasonable strategy to deal with anomalies (Chandola et al., 2009), outliers (Hodge & Austin, 2004), out-of-distribution examples (Shafaei et al., 2018), defend against adversarial examples (Szegedy et al., 2014), or delegate high-risk predictions to humans (Cortes et al., 2016). Deep classifiers that “do not know what they know” may confidently assign one of the training categories to objects that they have never seen. Second, uncertainty is the backbone of active learning (Settles, 2014), the problem of deciding what examples should humans annotate to maximally improve the performance of a model. Third, uncertainty estimation is important when analyzing the structure of noise in predictions, such as in causal discovery (Lopez-Paz, 2016) and in the estimation of predictive intervals. Fourth, uncertainty quantification is one of the first steps towards model interpretability (Alvarez-Melis & Jaakkola, 2017).

Being a wide-reaching concept, most taxonomies consider three sources of uncertainty: approximation, aleatoric, and epistemic uncertainties (Der Kiureghian & Ditlevsen, 2009). First, approximation uncertainty describes the errors made by simplistic models unable to fit complex data (e.g., the error made by a linear model fitting a sinusoidal curve). Since the sequel focuses on deep neural networks, which are known to be universal approximators (Cybenko, 1989), we assume that the approximation uncertainty is negligible and omit its analysis. Second, aleatoric uncertainty (from the Greek word *alea*, meaning “rolling a dice”) accounts for the stochasticity of the data. Aleatoric uncertainty describes the variance of the conditional distribution of our target variable given our features. This type of uncertainty arises due to hidden variables or measurement errors, and cannot be reduced by collecting more data under the same experimental conditions. Third, epistemic uncertainty (from the Greek word *episteme*, meaning “knowledge”) describes
the errors associated to the lack of experience of our model at certain regions of the feature space. Therefore, epistemic uncertainty is inversely proportional to the density of features as given by the training distribution, and could be reduced by collecting data in those low density regions. Figure 1 depicts the aleatoric uncertainty (gray shade) and epistemic uncertainty (pink shade) for a simple one-dimensional regression example.

In general terms, accurate estimation of aleatoric and epistemic uncertainty would allow machine learning models to know better about their limits, acknowledge doubtful predictions, and signal test instances that do not resemble anything seen during their training regime. As argued by Begoli et al. (2019), uncertainty quantification is a problem of paramount importance when deploying machine learning models in sensitive domains such as information security (Smith et al., 2011), engineering (Wen et al., 2003), transportation (Zhu & Laptev, 2017), or medicine (Begoli et al., 2019), to name a few.

Despite its importance, uncertainty quantification is a largely unsolved problem. Prior literature on uncertainty estimation for deep neural networks is dominated by Bayesian methods (Hernández-Lobato & Adams, 2015; Blundell et al., 2015; Gal & Ghahramani, 2016; Kendall & Gal, 2017; Khan et al., 2019), frequentist approaches relying on expensive ensembling of models (Begoli et al., 2019), uncertainty quantification is a problem for deep neural networks is dominated by Bayesian methods. In general terms, accurate estimation of aleatoric and epistemic uncertainty is inversely proportional to the density of our features as given by the training distribution, and could be reduced by collecting data in those low density regions. Figure 1 depicts the aleatoric uncertainty (gray shade) and epistemic uncertainty (pink shade) for a simple one-dimensional regression example.

We propose the following contributions:

1. We propose simultaneous quantile regression and apply it to aleatoric uncertainty estimation (Section 2).
2. We propose orthonormal certificates and apply them to epistemic uncertainty estimation (Section 3).
3. Throughout experiments concerning a variety of tasks on real-world data, we show the state-of-the-art performance of our uncertainty estimators (Section 4).
4. We close by providing an unified literature review on uncertainty estimation (Section 5) and perspectives for future work (Section 6).

The code necessary to replicate all of our tables and figures is available at [github_repo_coming_soon](https://github.com/coming_soon). Without further ado, we start our exposition by exploring the estimation of aleatoric uncertainty, that is, the estimation of uncertainty related to the conditional distribution of the target variable given the feature variable.

## 2. Simultaneous Quantile Regression for Aleatoric Uncertainty

We start with some basic definitions. Let \( F(y) = P(Y \leq y) \) be the strictly monotone cumulative distribution function of a target variable \( Y \) taking real values \( y \). Consequently, let \( F^{-1}(\tau) = \inf \{ y : F(y) \geq \tau \} \) denote the quantile distribution function of the same variable \( Y \), for all quantile levels \( 0 \leq \tau \leq 1 \). The goal of quantile regression is to estimate a given quantile level \( \tau \) of the target variable \( Y \), when conditioned on the values \( x \) taken by a feature variable \( X \). That is, we are interested in building a model \( \hat{y} = f_\tau(x) \) approximating the conditional quantile distribution function \( y = F^{-1}(\tau|X = x) \). One strategy to estimate such models is to minimize the pinball loss (Fox & Rubin, 1964; Koenker & Bassett Jr, 1978; Koenker, 2005; Ferguson, 1967):

\[
\ell_\tau(y, \hat{y}) = \begin{cases} 
\tau(y - \hat{y}) & \text{if } y - \hat{y} \geq 0, \\
(1 - \tau)(\hat{y} - y) & \text{else}.
\end{cases}
\]

To see this, write

\[
\mathbb{E}[\ell_\tau(y, \hat{y})] = (\tau - 1) \int_{-\infty}^{\hat{y}} (y - \hat{y}) dF(y) + \tau \int_{\hat{y}}^{\infty} (y - \hat{y}) dF(y),
\]

where we omit the conditioning on \( X = x \) for clarity. Next,

\[
\mathbb{E}[\ell_\tau(y, \hat{y})] = (1 - \tau) \int_{-\infty}^{\hat{y}} dF(y) - \tau \int_{\hat{y}}^{\infty} dF(y) = (1 - \tau) F(\hat{y}) - \tau (1 - F(\hat{y})) = F(\hat{y}) - \tau = 0 \Rightarrow \hat{y} = F^{-1}(\tau),
\]

where the last line assumed a strictly monotone cumulative distribution function \( F \), which is to assume a target variable with a strictly positive density function. As expected, one recovers the absolute loss when building a quantile regressor for the level \( \tau = \frac{1}{2} \), associated to the estimation of the conditional median. The pinball loss \( \ell_\tau \) estimates the \( \tau \)-th quantile consistently (Steinwart et al., 2011).

Armed with the pinball loss, we collect a dataset of identically and independently distributed (iid) feature-target pairs \( (x_1, y_1), \ldots, (x_n, y_n) \) drawn from some unknown probability distribution \( P(X,Y) \). Then, we may estimate the conditional quantile distribution of \( Y \) given \( X \) at a single quantile level \( \tau \) as the empirical risk minimizer

\[
\hat{f}_\tau \in \arg \min_f \frac{1}{n} \sum_{i=1}^{n} \ell_\tau(f(x_i), y_i).
\]
Instead, we propose to estimate all the quantile levels simultaneously by solving:

\[
\hat{f} \in \arg\min_f \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\tau \sim U[0, 1]} \left[ \ell_r(f(x, \tau), y_i) \right].
\]

(1)

In practice, we minimize this expression using stochastic gradient descent, sampling fresh random quantile levels \(\tau \sim U[0, 1]\) for each training point and mini-batch during training. The resulting function \(\hat{f}(x, \tau)\) can be used to compute any quantile of the conditional variable \(Y|X = x\). This allows to compute the entire conditional distribution of one target variable in a flexible manner. After obtaining the function \(\hat{f}\), we are ready to propose our estimate of aleatoric uncertainty, the \(1 - \alpha\) prediction interval (\(\alpha\)-significance level) around the median:

\[
u_\alpha(x^*) := f(x^*, 1 - \alpha/2) - f(x^*, \alpha/2).
\]

(2)

In contrast to prior work (Gal & Ghahramani, 2016; Lakshminarayanan et al., 2017; Pearce et al., 2018), our solution provides a prediction model able to estimate the entire profile of non-Gaussian (e.g. skewed, asymmetric, multimodal) heteroskedastic noises in data. Moreover, we use a single model instead of training a model for each quantile level separately. This reduces training time, evaluation time, and storage requirements.

We conclude this section with two implementation details.

First, many quantile regression techniques meet an undesirable phenomenon known as crossing quantiles (Koenker, 2005): that is, obtaining predictions \(f(x, \tau) > f(x, \tau + \epsilon)\) for some \(\epsilon > 0\). This contradicts the increasing property of quantiles. Since the effect of crossing quantiles is aggravated when estimating multiple quantile levels separately (Takeuchi et al., 2006), we did not observe this effect when performing simultaneous quantile regression with moderate sample sizes. However, one alternative to further avoid crossing quantiles and enforce monotonicity outside the training data, is to add a regularization term to the pinball loss objective:

\[
\mathbb{E}_x \left[ \mathbb{I} \left[ f(x, \tau + \epsilon) - f(x, \tau) < 0 \right] \right]
\]

where \(\epsilon \approx 10^{-3}\) is a small number. Figure 2 illustrates the effect of this regularizer in regions outside the training distribution when performing simultaneous quantile regression on a small sample from Figure 1.

Second, since it is common practice to shift and scale every feature to zero-mean and unit-variance and our quantile randomization follows an \(U[0, 1]\) distribution, we subtract \(\frac{1}{2}\) and multiply by 12 the quantile level \(\tau\) before passing it to the model; however, we do not apply this scaling when passing the quantile level to the pinball loss function.

As an illustration, the gray shade in Figure 1 estimates the aleatoric uncertainty in a simple example using Eq (2).

**What about multivariate targets?** Quantile regression is applicable to learning problems where the target variable takes values with a natural order, such as one-dimensional regression and classification tasks. When dealing with multivariate regression tasks, it is possible to apply one simultaneous quantile regression per target coordinate. When dealing with multivariate (categorical) classification it is possible to proceed similarly, or employ specific calibration methods (Guo et al., 2017) in order to interpret softmax scores as aleatoric uncertainty estimates.

### 3. Orthonormal Certificates for Epistemic Uncertainty

Next, we describe a novel way to estimate epistemic uncertainty, the type of uncertainty related to unexplored regions of the feature space.

To this end, consider a thought experiment in binary classification, discriminating between a positive distribution \(P\) and a negative distribution \(Q\). Construct the optimal binary classifier \(c\), mapping samples from \(P\) to zero, and mapping samples from \(Q\) to one. The classifier \(c\) is determined by the positions of \(P\) and \(Q\). Thus, if we consider a second binary classification problem between the same positive distribution \(P\) and a different negative distribution \(Q'\), the new optimal classifier \(c'\) may differ significantly from \(c\). However, both classifiers \(c\) and \(c'\) have one treat in common: they map samples from the positive distribution \(P\) to zero.

This thought experiment illustrates the difficulty of estimating epistemic uncertainty when learning from a positive distribution \(P\) without any reference to a negative, “out-of-domain” distribution \(Q\). That is, we are interested not only in one binary classifier mapping samples from \(P\) to zero, but in the infinite collection of such classifiers. Considering the infinite collection of classifiers mapping samples from the positive distribution \(P\) to zero, the upper tail of their class-probabilities should depart significantly from zero at
samples not from $P$, signaling high epistemic uncertainty. This intuition motivates our epistemic uncertainty estimate, orthonormal certificates.

To describe the construction of the certificates, consider a deep model $y = f(\phi(x))$ trained on feature-target samples drawn from the joint distribution $P(X, Y)$. Here, $\phi$ is a deep feature extractor extracting high-level representations from data, and $f$ is a shallow classifier grouping such representations into classes. Construct the dataset of high-level representations of training examples, denoted by $\Phi = \{\phi(x_i)\}_{i=1}^n$. Second, train a collection of certificates $c_1, \ldots, c_k$. Each training certificate $c_j$ is a simple neural network trained to map the dataset $\Phi$ to zero, by minimizing a loss function $\ell_c$. Finally, we define our estimate of epistemic uncertainty as:

$$u_c(x^*) := \frac{1}{k} \sum_{j=1}^k (c_j^T \phi(x^*))^2$$

Due to the smoothness of $\phi$, the average certificate $c_j$ should evaluate to zero near the training distribution. Conversely, for inputs distinct from those appearing in the training distribution, $c_j$ should depart from zero and signal high epistemic uncertainty. A threshold to declare a new input “out-of-distribution” can be obtained by computing the 95% percentile of the response across in-domain data.

When using the mean squared error loss for $\ell_c$, certificates can be seen as a generalization of distance-based estimators of epistemic uncertainty:

$$u_d(x^*) = \min_{i=1, \ldots, n} \|\phi(x_i) - \phi(x^*)\|_2^2$$

$$= \min_{i=1, \ldots, n} \|\phi(x_i)\|_2^2 - 2\phi(x_i)^T \phi(x^*)$$

$$= \max_{i=1, \ldots, n} 2\phi(x_i)^T \phi(x^*) - \|\phi(x_i)\|_2^2$$

which is a set of $n$ linear certificates $c_i(x^*) = a_i^T x^* + b_i$ with coefficients fixed by the feature representation of each training example.

To handle high-dimensional datasets, certificates are applied at the last layer representation $\phi(x)$ of deep models. The rationale behind this choice follows from the manifold hypothesis (Bengio et al., 2013; Alain & Bengio, 2016; Ferman et al., 2016), which states that natural data lives in low-dimensional manifolds, and deep learning models attempt to find this manifold to linearly separate the data. More specifically, we implement $k$ certificates on top of a $h$-dimensional representation as a single $c \times k$ linear layer, trained to predict the $k$-vector "0" under some loss $\ell_c$. Since we want diverse, non-constant (at zero) certificates, we impose an orthogonality constraint between certificates. The orthogonality constraint encourages diversity among certificates, while enforcing a Lipschitz-1 smoothness condition on each of them. The overall objective function for the orthonormal certificates is:

$$\hat{c} = \arg \min \frac{1}{n} \sum_{i=1}^n \ell_c(c_i^T \phi(x_i), 0) + \lambda \cdot ||c^T c - I_k||.$$  (4)

The use of non-linear certificates is also possible. In this case, the Lipschitz condition for each certificate can be controlled using a gradient penalty (Gulrajani et al., 2017), and their diversity can be enforced by measuring explicitly the variance of predictions around zero.

Orthonormal certificates are applicable to both regression and classification problems. The choice of the loss function $\ell_c$ depends on the particular learning problem under study. As a rule of thumb we suggest training the certificates using cross entropy or mean squared error loss depending on the initial networks’ task, classification or regression respectively. When using the mean-squared error, linear orthonormal certificates seek the directions in the data with the least amount of variance. This leads to an interesting interpretation in terms of Principal Component Analysis (PCA). In particular, linear orthonormal certificates minimized by mean squared error estimate the null-space of the training features, the “least-variant components”, the principal components associated to the smallest singular values of the training features.

As an illustration, the pink shade in Figure 1 estimates the epistemic uncertainty in a simple example using Eq (3).

### 4. Experiments

In this section, we conduct a variety of experiments to analyze the performance of simultaneous quantile regression for the estimation of aleatoric uncertainty (Section 4.1), and orthonormal certificates for epistemic uncertainty (Section 4.2).

#### 4.1. Aleatoric uncertainty

We evaluate the ability of simultaneous quantile regression to estimate aleatoric uncertainty across three different tasks: estimation of predictive intervals, discovery of causal relations, and estimation of heterogeneous treatment effect.

##### 4.1.1. ESTIMATION OF PREDICTIVE INTERVALS

First, we evaluate our aleatoric uncertainty estimate based on simultaneous quantile regression (2) to construct $(1 - \alpha)$ Prediction Intervals (PIs). These are intervals containing the true value about some target variable, given the values for some feature variable, with at least $(1 - \alpha)\%$ probability. The quality of prediction intervals is measured by two competing objectives, namely their:

- Prediction Interval Coverage Probability (PICP), that
is, the number of true observations falling inside the estimated prediction interval;

- **Mean Prediction Interval Width (MPIW)**, that is, the average width of the prediction intervals.

We are interested in calibrated prediction intervals (PICP = 1 − α) that are narrow (in terms of MPIW). For sensitive applications, having well calibrated predictive intervals is more important than their size.

In the following, we call our aleatoric uncertainty estimate **ConditionalQuantile**, and compare it to three popular alternatives:

- **ConditionalGaussian** (Lakshminarayanan et al., 2017) employs a conditional Gaussian distribution and maximum likelihood to estimate the conditional variance of the target variable given values for the feature variable. Predictive intervals are computed using such variance.

- **Dropout** (Gal & Ghahramani, 2016) uses dropout (Hinton et al., 2012) at testing time to obtain multiple predictions about the target variable given a single value for the feature variable. Predictive intervals are computed empirically from the obtained sample.

- **QualityDriven** (Pearce et al., 2018) is a state-of-the art model to estimate high-quality prediction intervals in deep learning models, which minimizes a smooth surrogate of the PICP/MPIW metrics. Predictive intervals are returned directly by this model.

Following common practice in the literature about (aleatoric) uncertainty (Hernández-Lobato & Adams, 2015; Lakshminarayanan et al., 2017; Pearce et al., 2018), we evaluate all methods across a variety of regression datasets (Asuncion & Newman, 2007). We use the same neural network architecture for all methods, cross-validate the learning rate and weight decay parameters for the Adam optimizer (Kingma & Ba, 2014), and try 20 random seeds.

Figure 3 summarizes our results on constructing 95% prediction intervals for 10 different datasets. Here, each marker is a different experiment (value of learning rate, weight decay, and random seed). The markers in bold are those that would be selected using cross-validation for that particular seed. Thus, each method is associated to 20 bold markers associated to their final cross-validated result for 20 random data splits. Overall, our proposed method ConditionalQuantile provides the best calibration results (their PICP value on the x-axis is closest to the dotted y-line indicating the target width 95%), while being amongst the narrowest prediction intervals (their MPIW value on the y-axis is small). Other methods such as Dropout are not able to achieve the target coverage PICP = 0.95, while ConditionalGaussian achieves the desired coverage at the expense of very wide predictive intervals.

### 4.1.2. Causal Discovery

We consider the problem of bivariate causal discovery: given a sample from the joint distribution \( P(X, Y) \), determine whether \( X \) causes \( Y \) (\( X \rightarrow Y \)), or \( Y \) causes \( X \) (\( X \leftarrow Y \)). The problem of causal discovery is one where the shape of the conditional distribution of the effect given the cause plays a major role (Mooij et al., 2016). Indeed, many causal discovery methods can be understood as preferring the “simplest” factorization of the joint distribution (amongst \( P(X, Y) = P(Y|X)P(X) \)) indicating \( X \rightarrow Y \).
and \( P(X, Y) = P(X|Y)P(Y) \) indicating \( X \leftarrow Y \) as the causal explanation \cite{mooij2016}. Here, simplest is measured in terms of some measure such as the Kolmogorov complexity \cite{janzing2010}. Recently, \cite{tagasovska2018} showed that the pinball loss can be used as a proxy to estimate the Kolmogorov complexity of a probability distribution. Thus, we may interpret the regression model with lower overall pinball loss (amongst the one mapping \( X \) to \( Y \), and the one mapping \( Y \) to \( X \)) as the causal model.

Table 1 shows our Simultaneous Quantile Regression (SQR, Equation 1) achieves competitive performance at the task of detecting the causal relationship between two variables. Our evaluation is performed across multiple datasets, including the well-known real-world benchmark from Tübingen \cite{mooij2016}. The other datasets are generated according to \cite{tagasovska2018} Section 4), including datasets generated from Additive Noise (AN-), Multiplicative Noise (MN-) and Location-Scale (LS-)

<table>
<thead>
<tr>
<th>Method</th>
<th>AN</th>
<th>AN-S</th>
<th>LS</th>
<th>LS-S</th>
<th>MN-U</th>
<th>Tubingen</th>
</tr>
</thead>
<tbody>
<tr>
<td>LINGAM</td>
<td>0.00</td>
<td>0.04</td>
<td>0.07</td>
<td>0.03</td>
<td>0.00</td>
<td>0.42</td>
</tr>
<tr>
<td>GR-AN</td>
<td>0.05</td>
<td>0.15</td>
<td>0.11</td>
<td>0.20</td>
<td>0.50</td>
<td>0.50</td>
</tr>
<tr>
<td>biCAM</td>
<td>1.00</td>
<td>1.00</td>
<td>0.62</td>
<td>0.09</td>
<td>0.03</td>
<td>0.59</td>
</tr>
<tr>
<td>ANM</td>
<td>0.95</td>
<td>0.11</td>
<td>0.91</td>
<td>0.54</td>
<td>0.90</td>
<td>0.63</td>
</tr>
<tr>
<td>GPI</td>
<td>0.98</td>
<td>0.98</td>
<td>0.99</td>
<td>0.99</td>
<td>0.74</td>
<td>0.64</td>
</tr>
<tr>
<td>IGCI-g</td>
<td>0.36</td>
<td>0.33</td>
<td>0.60</td>
<td>0.42</td>
<td>0.83</td>
<td>0.68</td>
</tr>
<tr>
<td>EMD</td>
<td>0.41</td>
<td>0.27</td>
<td>0.63</td>
<td>0.37</td>
<td>0.07</td>
<td>0.72</td>
</tr>
<tr>
<td>IGCI-u</td>
<td>0.96</td>
<td>0.63</td>
<td>0.91</td>
<td>0.44</td>
<td>0.66</td>
<td>0.73</td>
</tr>
</tbody>
</table>

SQR (m=1) | 0.99 | 0.51 | 0.98 | 0.78 | 0.62 | 0.75     |
SQR (m=3) | 0.99 | 0.73 | 1.00 | 0.85 | 1.00 | 0.75     |
SQR (m=5) | 0.99 | 0.76 | 1.00 | 0.82 | 1.00 | 0.77     |

Figure 4 showcases such application for the Student-Teacher Achievement Ratio dataset \cite{achilles2008}, where we estimate the effect of “class size” (treatment) over the “exam scores” (effect) of students, while considering additional individual features from both the students and the teachers (individual covariates). As independently confirmed by other studies \cite{qu2015}, we can also notice the heterogeneity in the treatment effect, namely that the variable “class size” has a larger causal effect for students associated to a larger “exam scores” variable. This shows that uncertainty quantification has a role in policy design.

### 4.2. Epistemic uncertainty

We evaluate the ability of orthonormal certificates \cite{3} to estimate epistemic uncertainty in the task of out-of-distribution example detection.

#### 4.2.1. OUT-OF-DISTRIBUTION EXAMPLES

We configure the task of detecting out-of-distribution examples as follows. First, we consider four different classification datasets with ten classes: MNIST, CIFAR-10, Fashion-MNIST, and SVHN. Second, we split each of these datasets at random into five “in-domain” classes and five “out-of-domain” classes. Third, we train a PreActResNet18 model \cite{he2016} \cite{liu2018} on the training split of the in-domain classes. Fourth, we use a measure of epistemic uncertainty on top of the last layer features to distinguish between the testing split of the in-domain classes and the testing split of the out-of-domain classes. These two splits are roughly the same size in all datasets, so we measure the performance of different epistemic uncertainty estimates at the task of distinguishing in- versus out-of- test instances using the ROC AUC statistic.

We note that our experimental setup is much more challenging than the usual considered in one-class classification (where one is interested in a single in-domain class) or out-
Table 2. ROC AUC means and standard deviations of out-of-distribution detection experiments for all methods (rows) and datasets (columns).

<table>
<thead>
<tr>
<th>Method</th>
<th>cifar</th>
<th>fashion</th>
<th>mmist</th>
<th>svhn</th>
</tr>
</thead>
<tbody>
<tr>
<td>covariance</td>
<td>0.64 ± 0.00</td>
<td>0.71 ± 0.13</td>
<td>0.81 ± 0.00</td>
<td>0.56 ± 0.00</td>
</tr>
<tr>
<td>distance</td>
<td>0.60 ± 0.11</td>
<td>0.73 ± 0.10</td>
<td>0.74 ± 0.10</td>
<td>0.64 ± 0.13</td>
</tr>
<tr>
<td>distillation</td>
<td>0.53 ± 0.01</td>
<td>0.62 ± 0.03</td>
<td>0.71 ± 0.05</td>
<td>0.56 ± 0.03</td>
</tr>
<tr>
<td>entropy</td>
<td>0.80 ± 0.01</td>
<td>0.86 ± 0.01</td>
<td>0.91 ± 0.01</td>
<td>0.93 ± 0.01</td>
</tr>
<tr>
<td>functional</td>
<td>0.79 ± 0.00</td>
<td>0.87 ± 0.02</td>
<td>0.92 ± 0.01</td>
<td>0.92 ± 0.00</td>
</tr>
<tr>
<td>geometrical</td>
<td>0.70 ± 0.11</td>
<td>0.66 ± 0.07</td>
<td>0.75 ± 0.10</td>
<td>0.77 ± 0.13</td>
</tr>
<tr>
<td>largest</td>
<td>0.78 ± 0.02</td>
<td>0.85 ± 0.02</td>
<td>0.89 ± 0.01</td>
<td>0.93 ± 0.01</td>
</tr>
<tr>
<td>odin</td>
<td>0.74 ± 0.09</td>
<td>0.84 ± 0.00</td>
<td>0.89 ± 0.00</td>
<td>0.88 ± 0.08</td>
</tr>
<tr>
<td>pca</td>
<td>0.60 ± 0.09</td>
<td>0.57 ± 0.07</td>
<td>0.64 ± 0.06</td>
<td>0.55 ± 0.03</td>
</tr>
<tr>
<td>random</td>
<td>0.50 ± 0.00</td>
<td>0.51 ± 0.00</td>
<td>0.51 ± 0.00</td>
<td>0.50 ± 0.00</td>
</tr>
<tr>
<td>svdd</td>
<td>0.52 ± 0.01</td>
<td>0.54 ± 0.03</td>
<td>0.59 ± 0.03</td>
<td>0.51 ± 0.01</td>
</tr>
<tr>
<td>certificates</td>
<td>0.83 ± 0.00</td>
<td>0.92 ± 0.00</td>
<td>0.95 ± 0.00</td>
<td>0.91 ± 0.00</td>
</tr>
<tr>
<td>oracle</td>
<td>0.94 ± 0.00</td>
<td>1.00 ± 0.00</td>
<td>1.00 ± 0.00</td>
<td>0.99 ± 0.00</td>
</tr>
</tbody>
</table>

5. Related work

Most of the prior art focuses on measuring either aleatoric or epistemic uncertainty alone. Since quantifying uncertainty is of essential importance across domains (Begoli et al., 2019), the vast body of research can be structured even further by considering different (levels of) applications. Here we summarize the works most relevant to our contributions.

5.1. Aleatoric uncertainty

Capturing aleatoric uncertainty is learning about the conditional distribution of a target variable given values of a feature variable. One classical strategy to achieve this goal is to assume that such conditional distribution is Gaussian at all feature locations. Then, one can dedicate one output of the neural network to estimate the conditional variance via maximum likelihood estimation (Nix & Weigend, 1993), Kendall & Gal (2017), Lakshminarayanan et al. (2017). While simple, this strategy is restricted to model Gaussian aleatoric uncertainties, which are symmetric and unimodal. These methods can be understood as the neural network, heteroskedastic version of the aleatoric uncertainty estimates provided by Gaussian processes (Rasmussen, 2004).

A second strategy, implemented by (Pearce et al., 2018), is to use quality metrics for predictive intervals (such as PICP/MPIW) as a learning objective. This strategy leads to well-calibrated prediction intervals. Other Bayesian methods (Hafner et al., 2018) predict other uncertainty scalar statistics (such as conditional entropy) to model aleatoric uncertainty. However, these estimates summarize conditional distributions into scalar values, and are thus unable to distinguish between unimodal and multimodal uncertainty profiles, for instance.

In order to capture complex (multimodal, asymmetric) aleatoric uncertainties, a third strategy is to use implicit generative models (Mohamed & Lakshminarayanan, 2016). These are predictors that accept a noise vector as an additional input, to provide multiple predictions at any given location. These are trained to minimize the divergence between the conditional distribution of their multiple predictions and the one of the available data, based on samples. The multiple predictions can later be used as an empirical distribution of the aleatoric uncertainty. Some of these models are conditional generative adversarial networks (Mirza & Osindero, 2014) and DiscoNets (Bouchacourt et al., 2016). However, these models are difficult to train, and suffer from problems such as “mode collapse” (Goodfellow, 2016), which would lead to wrong prediction intervals.

When dealing categorical targets (such as in multiclass classification problems), the concept of aleatoric uncertainty is tightly related to the one of calibration: a neural network is well calibrated if examples a softmax score of $p$ are correctly classified $100p\%$ of the times (Guo et al., 2017).

Most related to our SQR, there are few examples on using the pinball loss to train neural networks for quantile regres-
sion. These considered the estimation of individual quantile levels (White 1992; Taylor 2000), or unconditional quantile estimates with no applications to uncertainty estimation (Dabney et al. 2018; Ostrovski et al. 2018).

5.2. Epistemic uncertainty

Capturing epistemic uncertainty is learning about what regions of the input space are unexplored by the training data. As we review in this section, most estimates of epistemic uncertainty are based on measuring the discrepancy between different predictors trained on the same data. These include the seminal works on bootstrapping (Efron & Tibshirani 1994), and bagging (Breiman 1996) from statistics. Recent neural network methods to estimate epistemic uncertainty follow this principle (Lakshminarayanan et al. 2017).

Although the previous references follow a frequentist approach, the strategy of ensembling models is a natural fit for Bayesian methods, since these could measure the discrepancy between the (possibly infinitely) many amount of hypotheses contained in a posterior distribution. Since exact Bayesian inference is intractable for deep neural networks, recent years have witnessed a big effort in developing approximate alternatives. First, some works (Blundell et al. 2015; Hernandez-Lobato & Adams 2015) place an independent Gaussian prior for each weight in a neural network, and then learn the means and variances of these Gaussians using backpropagation. After training, the weight variances can be used to sample diverse networks, used to obtain diverse predictions and the corresponding estimate of epistemic uncertainty. A second line of work (Gal & Ghahramani 2016; Gal 2016; Kendall & Gal 2017) employs dropout (Hinton et al. 2012) during the training and evaluation of a neural network as an alternative way to obtain an ensemble of predictions. Since dropout has been replaced to a large extent by batch normalization (Ioffe & Szegedy 2015; He et al. 2016; Teye et al. 2018) showed how to use batch normalization to obtain ensembles of predictions from a single neural network.

A second strategy to obtain estimates for epistemic uncertainties is to use the available data as a starting point to construct “negative examples”. These negative examples resemble realistic input configurations that would lay outside the data distribution. Then, a predictor to distinguish between original training points and negative examples may be used to measure epistemic uncertainty. Examples of these strategy include noise-contrastive estimation (Gutmann & Hyvärinen 2010), noise-contrastive priors (Hafner et al. 2018), and GANs (Goodfellow et al. 2014).

In machine learning literature, the estimation of epistemic uncertainty is often motivated in terms of detecting out-of-distribution examples (Shafaei et al. 2018). However, it is worth recalling that the often ignored literature on anomaly/outlier detection and one-class classification can also be seen as an effort to estimate epistemic uncertainty (Pimentel et al. 2014). Even though one-class classification methods are implemented mostly in terms of kernel methods (Schölkopf et al. 2000; 2001), there are recent extensions to leverage deep neural networks (Ruff et al. 2018).

Most related to our orthonormal certificates, the method deep Support Vector Data Description (Ruff et al. 2018; SVDD) also trains a function to map all in-domain examples to a constant value. However, their evaluation is restricted to the task of one-class classification, and our experiments showcase that their performance is drastically reduced when the in-domain data is more diverse (contains more classes). Also, our orthonormal certificates do not require learning a deep model end-to-end, but can be applied to the last layer representation of any pre-trained network. Finally, we found that our proposed diversity regularizer (4) was crucial to obtain a diverse, well-performing set of certificates.

6. Conclusion

Motivated by the importance of quantifying confidence in the predictions of deep models, we propose simple, yet effective tools to measure both aleatoric (noise) and epistemic (model) uncertainty. To capture the inherent noise in the data, we showed an estimator based on simultaneous quantile regression, implemented efficiently through randomization of the pinball loss function. Such estimator shows state-of-art results in providing well-calibrated prediction intervals and high accuracy in causal discovery. The epistemic uncertainty, or the ability to “understand” for which data points the models’ predictions should not be trusted, can be captured by simple orthonormal certificates that recognize out-of-distribution samples with fidelity.

Further extensions could go in a number of directions: certificates could be used in active learning scenarios or detecting adversarial samples, while a unified quantile-based uncertainty framework is an interesting direction to explore. Both estimates being intuitive and easily applicable to a variety of tasks, could additionally contribute to increased confidence and easier adaptation of deep models in sensitive domains (such as medicine and policy) where the trustworthiness of the decision-making systems is of immense importance.

References


Frequentist Uncertainty Estimates for Deep Learning


