Improving Regression Uncertainty Estimates with an Empirical Prior

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Abstract

While machine learning models capable of producing uncertainty estimates are becoming widespread, uncalibrated uncertainty estimates are often overconfident, and often assume predetermined probability distributions over the error which do not match the empirical calibration error. Most work on calibrating uncertainty estimates focuses on classification rather than regression, which introduces novel challenges. We present a calibration method referred to as Calibrating Regression Uncertainty Distributions Empirically (CRUDE) that does not assume a fixed uncertainty distribution, instead making the weaker assumption that error distributions have a constant shape across the output space, shifted by predicted mean and scaled by predicted standard deviation. CRUDE requires no training of the calibration estimator aside from a parameter to account for consistent bias in the predicted mean. Our method is distribution-agnostic and provides sharper and more accurate uncertainty estimates than state of the art techniques, as demonstrated by calibration and sharpness measures across many datasets.

1. Introduction and Related Work

Uncertainty estimates are important across a wide range of applications, from medical diagnosis to weather forecasting to autonomous driving. Accurately assessing confidence in a prediction, and specifying the underlying distribution of potential errors, is a cornerstone of reliable and interpretable models in any high stakes scenario. For example, having good confidence intervals when forecasting solar power production in the near future allow utilities to better account for fluctuations (Murata et al., 2018). Similarly, having good uncertainty estimates on a model meant to assess tumor size is important, as those metrics may be used to assess a variety of other clinical aspects (Kourou et al., 2015).

While uncertainty calibration for classification is a fairly well-developed research area, uncertainty calibration for regression has remained relatively less explored (Kuleshov et al., 2018). Notably, previous work has indicated that the models which perform best on the regression tasks that they are trained on will rarely be calibrated, and early stopping to guarantee calibration on a calibration dataset will usually hinder model performance overall (Laves et al., 2020).

Kuleshov et al. (2018) authored one of the most influential papers on this topic, which proposed training an auxiliary model to calibrate uncertainty metrics by minimizing a calibration loss. Levi et al. (2019) aimed to highlight theoretical issues with this work, namely that it tends to overfit and allows for a calibration model to be regarded as calibrated even when the calibrated uncertainties are uncorrelated with the true uncertainties. Levi et al. proposed a simpler calibration model that sidestepped such assumptions. Laves et al. (2020) built on the Levi et al. method to incorporate epistemic uncertainty in addition to aleatoric uncertainty.

Figure 1. Comparison between the calibration curve for different calibrations applied to a neural network with a Monte Carlo dropout-derived uncertainty estimate. We show CRUDE (ours), the method from Kuleshov et al., and a Gaussian MLE calibration corresponding to Levi et al., for a neural network trained on the Forest Fires dataset (Cortez & Morais, 2007). Note that the dotted line $x = y$ corresponds to perfect calibration.
Improving Regression Uncertainty Estimates with an Empirical Prior

Figure 2. Visualization of the assumption made about the relationship between the underlying uncertainty distribution function and the observed errors: errors, scaled by sigma, can be seen as samples from this underlying distribution function.

However, one of the challenges that the Kuleshov et al. paper set out to solve was addressing situations where error distributions are not truly Gaussian, which may be inevitable if the underlying distribution is skewed or multimodal and the model is unable to completely disentangle these factors. In addition, the criticism of the calibration metric as allowing any distribution to be calibrated neglects the distinction between calibration and sharpness in calibration literature: calibration evaluates the probabilistic accuracy of an uncertainty distribution, while sharpness is the metric by which calibrated uncertainty estimates are compared (Gneiting et al., 2007). Calibrated uncertainties that are well-correlated with errors will be sharper than those that are not. Sharpness has other compelling features too, as it is a metric that permits performance comparison across calibrated models.

Yet, many of the Levi et al. concerns about the Kuleshov et al. method are well-founded: because it recalibrates on the aggregate calibration curve\(^1\), there exist probability distributions unrelated to the underlying distribution that can be found that correspond to “perfect” calibration regardless of the true uncertainty distributions. However, we show this leads to less-sharp estimates of uncertainty. We also note that the definition in Kuleshov et al. requires an invertible calibration curve, something that is often missing from sufficiently overconfident models, which degrades the performance of the method. It may be possible to somewhat ameliorate this by preprocessing the uncertainty distribution, but this is not part of the method, and likely would not resolve the underlying disregard for sharpness.

In theory, there are many transformations that lead to a calibrated distribution, but ideally we would like the one that results in the sharpest possible uncertainty estimates.

**Contribution:** We propose a calibration method, Calibrating Regression Uncertainty Distributions Empirically (CRUDE), based on Levi et al. and Kuleshov et al. that assumes less about the underlying error distribution, does not require an auxiliary calibration model, and has a consistent prior, improving calibration and sharpness over both the Levi et al. and Kuleshov et al. approaches on many datasets.

## 2. Derivation

A calibration problem is formulated as follows: we take as input a trained model that outputs mean and variance estimates for any given input set\(^2\), and a calibration set of data that is independent of the training set. We aim to produce a probability distribution over the output space of the model that best corresponds to our calibration dataset.

The essential assumption we make is that the true error measures\(^3\), linearly scaled down by the predicted standard deviation, are independent and identically distributed. Mathematically, we assume that there is some underlying probability distribution \(\mathcal{D}\) such that for all \(x\):

\[
p(y|x; \hat{\mu}(x), \hat{\sigma}^2(x)) = \mathcal{D}\left(\frac{\hat{\mu}(x) - y}{\hat{\sigma}(x)}\right)
\]

We can treat each uncertainty-scaled error divided by the predicted uncertainty, \(\frac{\hat{\mu}(x) - y}{\hat{\sigma}(x)}\), as an unbiased sample from the underlying error distribution. Then, we can use the

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\(1\)The concept of the calibration curve is elaborated on in Section 2

\(2\)We generally neglect any other assertions the model makes about the shape of output distributions.

\(3\)That is, the signed empirical distance of the observation to the predicted mean.
quantile function directly on the scaled-errors observed on a held-out calibration dataset (or alternatively, as observed over some number of folds).

Thus, in order to predict an uncertainty interval from an uncertainty estimate, we scale the uncertainty interval calculated on the error-scaled distribution by the uncertainty estimate. That is, for a given prediction \( \hat{y} \) and its uncertainty \( \sigma \), and for the calibration set predicted means \( \hat{M} \), predicted uncertainties \( \hat{\Sigma} \), and observed values \( Y \), we define our guiding equation: the quantile (or percent-point function) of the error density distribution \( D \) can be expressed as:

\[
\text{cdf}^{-1}(D)(\hat{y}; \hat{\Sigma}, \hat{\sigma}) = \bar{y} + \hat{\sigma} \cdot \text{quantile} \left( \frac{\hat{M} - Y}{\hat{\Sigma}}, \hat{\sigma} \right)
\]

Put simply, the sampled quantile of the underlying distribution is re-scaled by the predicted mean and variance given the specific input to create the final distribution.

### 3. Evaluating Calibration and Sharpness

#### 3.1. Calibration

Because we can associate each error with a probability in a regression prediction with uncertainty, we can evaluate the relationship between the expected and observed confidence levels. That is, for a calibrated model, the errors that it predicts will be in the 30th percentile of its distribution, should be above the true errors 30% of the time. This is known as the probability integral transform (PIT) value and a well-calibrated model should have a uniform distribution over the percentiles associated with errors (Gneiting et al., 2007).

Ideally, each expected confidence percentile should match the fraction of values observed below the predictions of that percentile. To measure proximity to this, we replicate the Kuleshov et al. calibration metric, which utilizes the RMSE between the expected confidence levels and the observed confidence levels. We initialize values of \( p \) in the range \([0,1]\) with a step size of 0.01, and for each \( p_j \), we calculate the empirical frequency, \( \hat{p}_j \):

\[
\hat{p}_j = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}[\hat{y}^{(i)} < \text{cdf}^{-1}(D)(p_j; \hat{y}^{(i)}, \hat{\sigma}^{(i)})]
\]

We can then calculate the calibration, \( \text{cal}(\text{cdf}(D)) : \)

\[
\text{cal}(\text{cdf}(D)) = \frac{1}{n} \sum_{i=1}^{n} \left( \hat{p}_j - p_j \right)^2
\]

#### 3.2. Sharpness

Calibration does not show us the full picture: a calibration’s efficacy on a dataset is also based on the resulting sharpness (which is related to the degree to which the uncertainties
are correlated with the true error) (Kuleshov et al., 2018; Gneiting et al., 2007; Levi et al., 2019; Laves et al., 2020). In order to evaluate sharpness, we can use the mean calibrated predicted variance on the validation set (Gneiting et al., 2007), but we take the square root of this value to match the dimensionality of the error.

4. Implementation

To calibrate a model, for a given calibration dataset, we store the observed model errors divided element-wise by the model’s predicted uncertainty, $\frac{\hat{M} - Y}{\Sigma}$. Then, to return the calibrated percentile point function at a percentile $p$, given an estimate from the same model with $\hat{y}$, the calibration method returns $\hat{y} + \hat{\sigma} \cdot \text{quantile}\left(\frac{\hat{M} - Y}{\Sigma}, p\right)$. In order to calculate a 90th percentile interval range for a given prediction, we could plug in $p = 0.05$ and $p = 0.95$. In order to maximize the efficiency of the quantile lookup, we can sort the scaled errors given the calibration data, allowing this method to run in constant ($O(1)$) time with respect to the size of the calibration dataset with an $O(n \log n)$ preprocessing cost.

While our algorithm’s guiding equation is free of hyperparameters, in practice, to allow adaptability for a variety of models as well as decrease error due to variations in the shape of the underlying distribution, we introduce a parameter in our implementation. Before applying the formula for the derivation of the underlying cumulative distribution function, we consider a shift to all predicted means such that $\hat{M}' = \hat{M} + b$. We use Powell’s method (Powell, 2007) in order to find the shift that maximizes our calibration score on the calibration dataset.

5. Experiments

5.1. Models and Calibration Methods

We evaluate each calibration method on multiple predictive models with uncertainty which have shown good performance on numerous tasks, including two flavors of Bayesian neural networks, Gaussian processes\(^4\), and a recent model known as Natural Gradient Boosting (Duan et al., 2019). Specifically, the two neural network approaches that we consider include one using Monte Carlo dropout as described in Gal & Ghahramani (2015) as well as one which separately

\(^4\)Optimized using GPytorch (Gardner et al., 2018)
Improving Regression Uncertainty Estimates with an Empirical Prior

predicts a mean and variance (Papadopoulos et al., 2001), both with hyperparameters similar to those described in Gal & Ghahramani (2015). We compare no calibration, a Gaussian maximum likelihood estimate (including shift) inspired by the Levi et al. (2019) method, the Kuleshov et al. (2018) method, and CRUDE.

5.2. Datasets

We evaluate our model on 12 datasets, primarily from the freely available Machine Learning Repository from the University of California, Irvine. The datasets used have large variety across both applications and technical features, including input dimensionality and dataset size.

5.3. Evaluation

For each model on each dataset, we run 20 trials with the dataset shuffled and split repeatedly, with a \((0.5, 0.4, 0.1)\) split between training, calibration, and test data. For each trial, we score every calibration method for calibration and sharpness. We use the metrics discussed in Section 3 for calibration and sharpness.

Note that we do not use the calibration metrics proposed in Levi et al. (2019); Laves et al. (2020), as they do not consider the uncertainty distribution associated with a given uncertainty estimate, instead using mean absolute error as a metric. Moreover, as highlighted in the appendix of Laves et al., this may correspond to an implicit Laplacian prior.

6. Analysis and Results

We find that on the majority of tasks and models, our calibration method outperforms the alternative methods in both calibration and sharpness. While the degree of improvement varies, on several models and tasks it is greater than 50\%.

There is no model that is consistently the sharpest across all datasets when calibrated, though the dropout neural network and NGBoost are disproportionately represented among the sharpest solutions.

We also notice that the Kuleshov et al. method has the greatest likelihood of outperforming CRUDE in terms of calibration as the datasets are larger. However, in almost all cases where the Kuleshov et al. method results in improved calibration, there is a substantial sacrifice of sharpness. As highlighted by Levi et al., Kuleshov et al. will be able to calibrate any distribution with enough data, but it will often do so at the expense of sharpness. Another issue with the Kuleshov et al. method is that it is unable to recalibrate a sufficiently overconfident model, as it relies on the calibration curve being defined for the entire range of expected confidence levels.

Figure 4 shows an example scaled error distribution on the Power dataset, indicating that its skew may explain this improvement (Tüfekci, 2014).

Note that while it is possible to use CRUDE as a parameter-free calibration technique by setting the shift parameter to 0, this often decreases performance when a model’s training
Improving Regression Uncertainty Estimates with an Empirical Prior

prior is far from the empirical error distribution. One striking example of this is on the UCI Forest Fires Dataset where the task is forest fire area prediction from meteorological data as highlighted in Figure 5 (Cortez & Morais, 2007).

7. Conclusion and Future Work

CRUDE offers substantial improvements over existing regression calibration techniques, especially for datasets where the error distribution has a nonstandard shape. However, there are many meaningful avenues left to explore.

For most datasets, the assumption of a fixed uncertainty distribution, whether Gaussian or empirical, is incorrect to varying degrees. There are many ways to extend CRUDE to account for uncertainty distributions varying with respect to inputs, such as by performing it only on a given input’s nearest neighbors. Also, it may be possible to leverage the richer distributional information provided by Monte Carlo dropout. Ultimately, CRUDE opens the door to many improved regression calibration methods.

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