Technische Universität Braunschweig

Regression With Uncertainties

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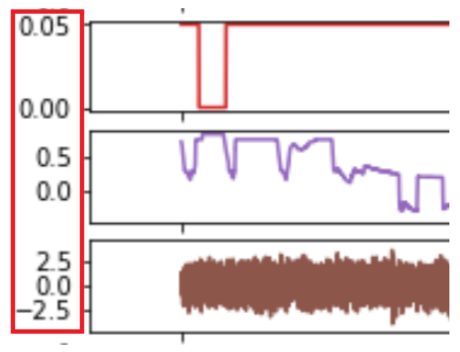
Data Visualization

The range of input values vary significantly, hence they are min-max normalized wrt. the training data



Network Architecture

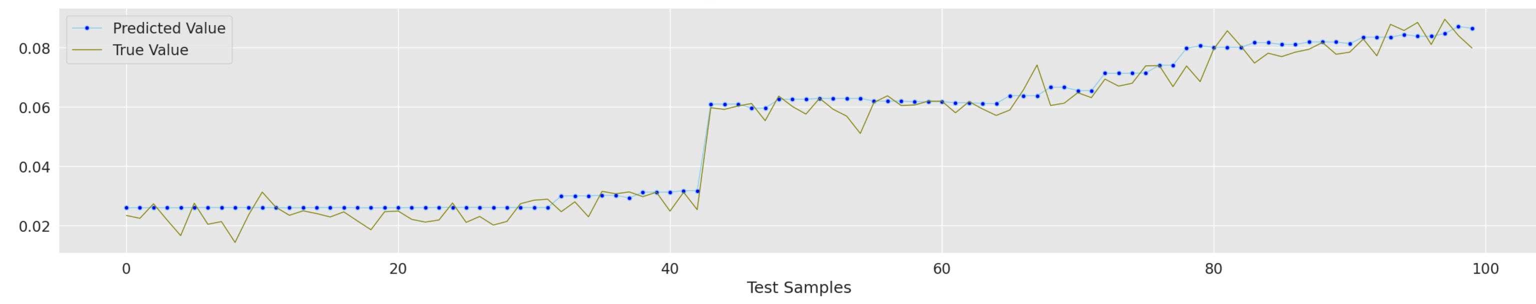
Layer details	Input layer	Hidden layer	Output layer
Units	128	64	1 / 2
Activation	ReLU	ReLU	Linear

In the case of MC-Dropout, there are also three additional dropout layers in between the above-mentioned layers, starting from before the input layer.

Model 1: Mean Squared Error Loss

Loss: $\frac{1}{N}\sum_{i=1}^{i=N}(y_i - \hat{y}_i)^2$, y_i is the target value, $\hat{y}_i$ is the predicted value.

Motivation: To penalise predictions based on the squares of their difference compared ot the target values.



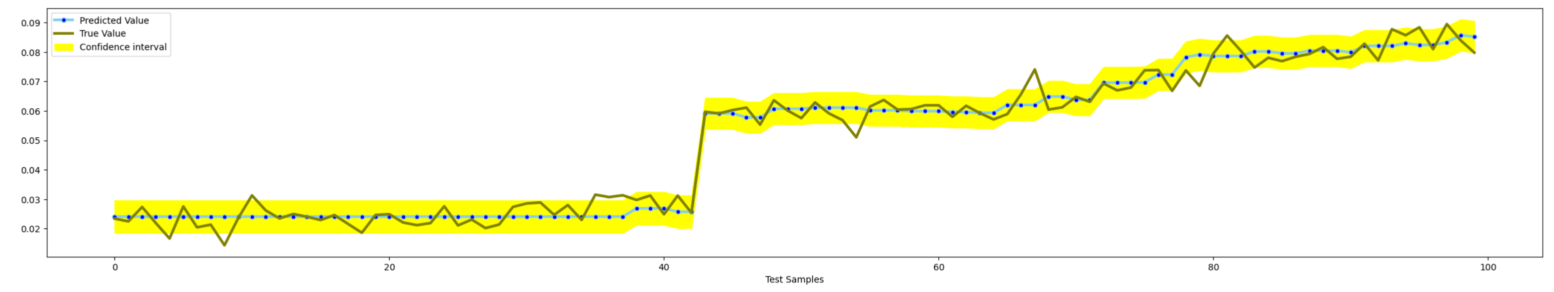
Model MSE: 3.1255e-05

Model MAE: 4.2321e-03

Model 2: Negative Log Loss

Loss: $\frac{1}{N}\sum_{i=1}^{i=N}\left(\frac{(y_i-\hat{y}_i)^2}{2\sigma_i^2} + 2ln(\sigma_i)\right)$, y_i is the target value, $\hat{y}_i$ is the predicted value, $\sigma_i = \exp v_i$, v_i is an additional output of the model.

Motivation: To assume that the target values follow a normal distribution, and get a model prediction and standard deviation that resembles that of the target values with uncertainty bounds of $\pm 2\sigma$



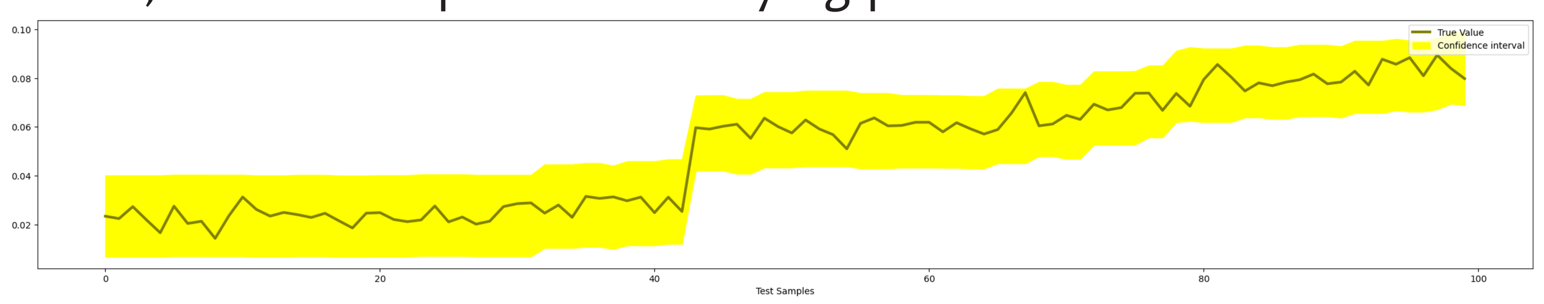
Model MSE: 3.0391e-05

Model MAE: 4.1574e-03

Model 3: Interval Loss

Loss: $\frac{1}{N}\sum_{i=1}^{i=N}\left[max(y_i - \bar{y}_i, 0)^2 + max(\underline{y_i} - y_i, 0)^2 + \beta(\bar{y}_i - \underline{y_i})\right]$, y_i is the target value, $\bar{y}_i$ is the upper limit of the confidence interval, $\underline{y_i}$ is the lower limit and $\bar{y}_i \geq \underline{y_i}$. Constant $\beta = 1e-4$

Motivation: To generate an interval which encompasses the target values, with the help of an underlying prediction network.



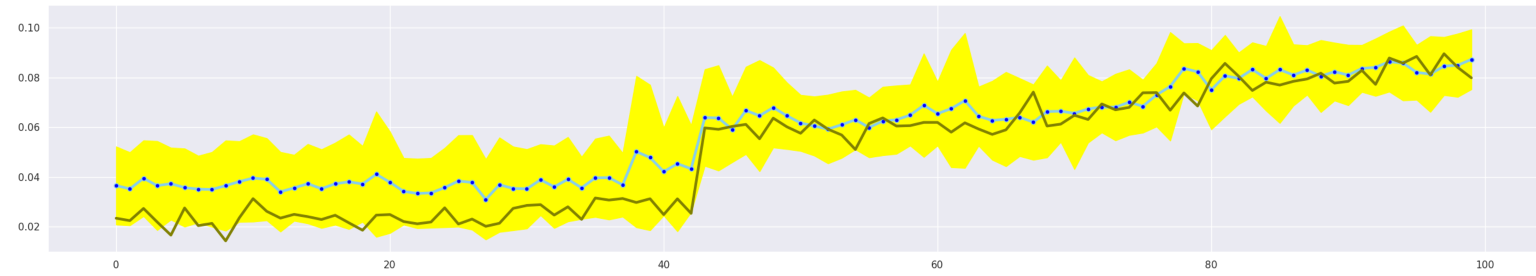
Model MSE for $\bar{y}$: 2.9754e-04 **Model MSE for $\underline{y}$:** 4.5315e-04

Model MAE for $\bar{y}$: 0.0151 **Model MAE for $\underline{y}$:** 0.0199

Model 4: Monte Carlo Dropout

Loss: Mean squared error loss, identical to model 2

Motivation: Treating dropout as a Bayesian approximation of a Gaussian process, multiple models are trained with different dropout masks. The mean and variance of the model outputs provides an ensemble prediction with a predicted value and its uncertainty



Model MSE: 2.6882e-04

Model MAE: 0.0146

Observations

Training effort: MSE < Interval Loss < NLL < MC Dropout

Application in Safety Critical Functions:

The afore-mentioned models and loss functions are not suitable for substituting safety critical functions, since there is uncertainty involved. Though the model accuracies on the training data and predictions can be improved, there is still the chance that an exception occurs which cannot be predicted accurately.

A suitable alternatives would be to utilize the quantified uncertainty in prompting human intervention fo handling exceptions, or treat the model predictions as a precursor to failure where possible and provide relevant warning signals