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Conference Paper

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Publication date:
2024-03-14

Permanent link:
https://doi.org/10.3929/ethz-b-000669553

Special Interest Group meeting
Thermal Issues
Eindhoven, The Netherlands, March 2024
www.euspen.eu

Model Uncertainty Estimation for Thermal Error Compensation in Machine Tools

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Abstract
This paper introduces a method to compensate for thermal errors in machine tools (MT) using LSTM neural networks, with a focus on addressing prediction uncertainties. It presents the application of Monte Carlo Dropout (MC-Dropout) to estimate the uncertainty of LSTM predictions using data generated in a simulated MT environment. MC-Dropout offers a practical, computationally efficient method to allow for effective thermal error compensation without repeated on-machine measurements. Incorporating uncertainty estimates can enhance decision-making, thus allowing more autonomous machine operations and improve the selection of training data for machine learning models, leading to greater overall prediction accuracy.

Monte Carlo Dropout, MC-Dropout, Uncertainty, LSTM, Machine Learning, Thermal error prediction, Simulation of machine tools

1. Introduction

Thermal errors in machine tools (MTs) can be compensated by measuring the temperature in and around the MT and using a properly trained machine learning model to predict temperature-induced tool centre point deviations. As the hysteresis of the thermal state is of high importance, such a compensation model should be able to consider the history in time series data. A model often used in this regard is the Long-Short-Term-Memory (LSTM) neural network [1, 2].
However, training data is often very limited and usually lacks coverage of large parts of the possible input space, which prevents the long-term robustness of compensation models. Using input data dissimilar to the training data can lead to inaccurate predictions despite high validation and test accuracy. Considering a running compensation on a MT, it is very inconvenient to check - through on-machine measurements - whether the predictions of the model are still accurate enough [3].
A possible way to estimate accuracy without direct monitoring is to check the model's certainty in predicting with the current inputs. However, the usual tools for regression and classification do not capture model uncertainty. In comparison, Bayesian models offer a mathematically grounded framework to reason about model uncertainty, but usually come with a prohibitive computational cost [4].
In this paper Monte Carlo (MC)-Dropout is used to cost-effectively estimate uncertainty in neural networks approximating Bayesian inference sacrificing neither computational complexity nor accuracy.

2. LSTM Modelling

The procedure is illustrated using an LSTM network optimized for the prediction of axis-specific thermal errors from temperature measurements around an MT similar to the work of Lang et al. [5]. This data is generated using a simulation of a DMG Mori NMV 5000 DCG shown in Figure 1. The basis of the simulation is implemented by Becerro [6].

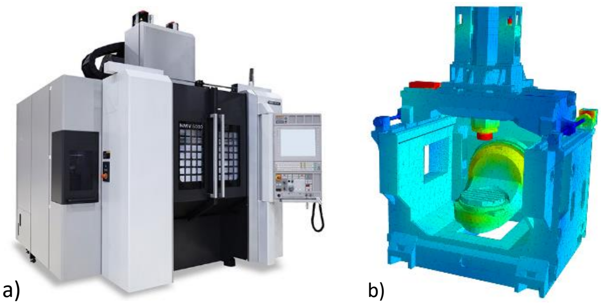

Figure 1. a) DMG Mori NMV 5000 DCG, a 5-axis MT. **b)** Simulation of the NMV 5000 in the MORe environment.

The optimized architecture of the LSTM is shown in Figure 2. The network takes 26 temperature values across 10 consecutive time steps – that is ten measurements over 66 minutes – as inputs. These are processed through two subsequent LSTM layers with 100 nodes, each followed by a dropout layer for regularization with dropout rate 0.05.

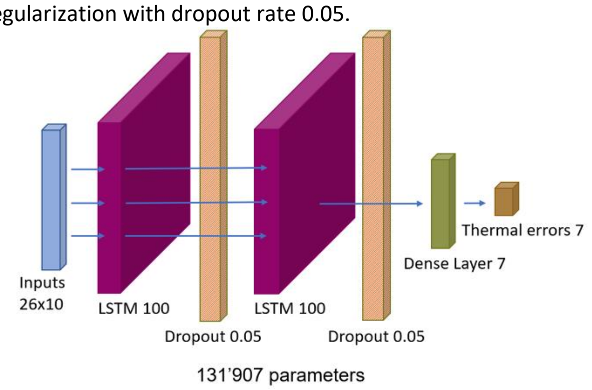

Figure 2. Architecture of neural network used for the estimation of measuring uncertainty.

The network is trained and then validated on 180 000 unique datapoints (corresponding pairs of temperature and TCP-deviations) and leads to a reduction of over 98 % of the volumetric error on a test set of 95 000 different datapoints.

Figure 3 displays the true and predicted volumetric errors and the remaining uncompensated volumetric error.

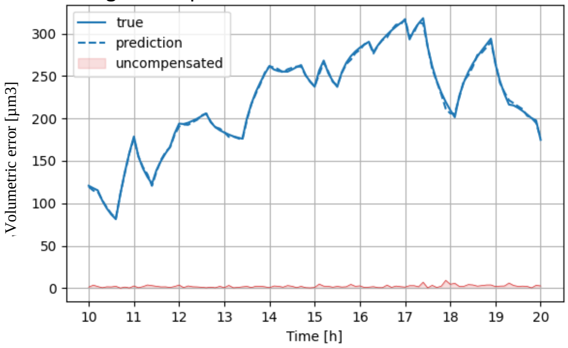

Figure 3. Compensation Accuracy of the presented LSTM network. Only 100 of 95'000 tested predictions are visualized for clarity.

3. Monte Carlo Dropout

To determine a measure for the uncertainty on dropout-featuring models, Gal et al. [4] propose the Monte Carlo-Dropout Method. By applying the dropout regularization technique in the inference phase, the prediction of the neural network will differ, depending on the influence of the dropped-out nodes. Through repeating this process times for the same input, a gaussian-like distribution emerges for the prediction of each output. The standard deviations of that distribution can be used to inform the uncertainty of the neural network for each output. This method approximates Bayesian inference in deep Gaussian processes without the usual computational cost involved [4].

This procedure is highlighted in Figure 4.

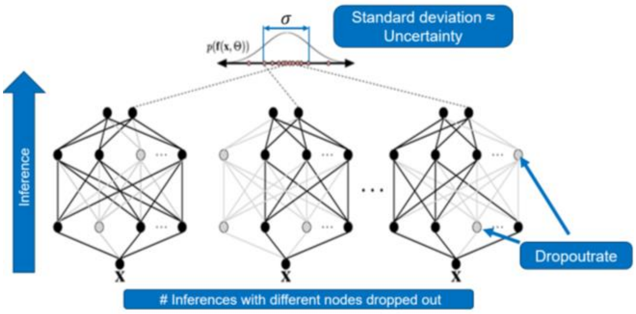

Figure 4. Illustration of Monte Carlo Dropout in neural networks to estimate uncertainty.

The framework used for computation of neural networks (TensorFlow) already features optimized inference using dropout layers, such that a single forward pass takes less than a second depending on model depth and hardware used.

The dropout rate used can be different from the one used during training of the model. Given a high enough number of inferences, it only scales the absolute standard deviation but not the relative standard deviation of the respective predictions.

4. Applied MC-Dropout

The uncertainty of the trained LSTM model is analysed using MC-Dropout over one hundred inferences with a dropout rate of 0.2 for each node of each of the two dropout layers in the presented LSTM network.

Figure 5 shows the spread of predictions of the different iterations via the boundaries of the minimum and maximum value (hatched area), the range of the standard deviation and the mean of all predictions for each input (dotted). This can be compared against the prediction without dropout (dashed) and the true value (solid).

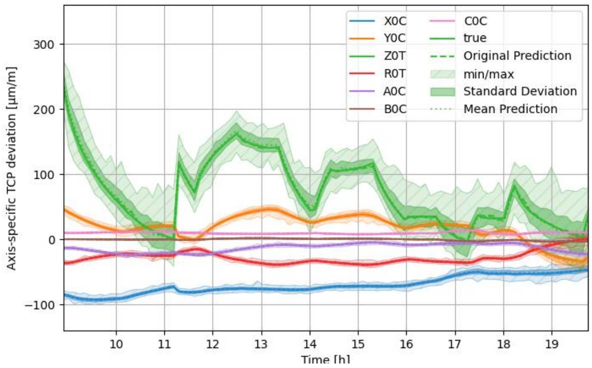

Figure 5. Displays the prediction of each axis-specific error including the uncertainty estimate resulting from MC-Dropout. Only an excerpt of the inferred inputs is visualized for clarity.

5. Conclusion and Outlook

Areas where the network shows high uncertainty or where the mean prediction is far off the original can be of special interest for further analysis or inform how to react to network prediction. In uncertain predictions, compensation can be paused, and parts can be labelled for post-treatment.

The main benefit of measuring model uncertainty is the ability to estimate prediction accuracy without the need for labelled data. As such it could be used to trigger a model update/retraining on a machine which is thermally compensated via a neural network, without requiring regular measurements to determine the model accuracy (TALC) [8].

Uncertainty can further be used to determine areas or sequences for which the network fails to predict with certainty/accuracy, which in turn is useful to inform which training data to create or label to increase model robustness and accuracy or to reduce the amount of training data required to achieve accurate predictions.

Acknowledgements

Co-financed by Innosuisse - Swiss Innovation Agency Project no. 27835.1 IP-ENG.

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