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Estimation of prediction uncertainty of machine learning models for metrology problems

Paweł Majewski[1,*], Kacper Marciniak[2], and Jacek Reiner[2]

[1]*Faculty of Information and Communication Technology, Wrocław University of Science and Technology, Janiszewskiego 11/17, 50-372 Wrocław, Poland;*
[2]*Faculty of Mechanical Engineering, Wroclaw University of Science and Technology, Łukasiewicza 5/7, 50-370 Wrocław, Poland;*
[*]*corresponding author: pawel.majewski@pwr.edu.pl*

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Introduction

Machine learning (ML) methods are becoming increasingly popular in more areas of engineering applications, including metrology [1]. The inference performance of ML models depends on many factors, including (a) the type of model architecture used, (b) the data used to train the model and its similarity to the test data, (c) the choice of operating point for the model (e.g. confidence score threshold), and (d) the process of training the model itself. Undoubtedly, the partial non-determinism for ML solutions causes some researchers to refer to them as a 'black box' [2], questioning the reliability of the results obtained in this way. Estimation of prediction uncertainty is something that can significantly increase user trust in ML-based solutions. This work proposes a method to estimate the prediction uncertainty for the problem of dimensioning the teeth of broaches.

Materials and methods

The problem addressed concerned determining the length and width of the broach tooth. The proposed solution was based on an object detection model (YOLOv8n [3]) to determine the bounding box for each image containing one broach tooth (as shown in Fig. 1). The obtained lengths of the sides of the bounding boxes, together with the known resolution (2 µm/pix), made it possible to determine the measured length and width further. The experiments used 3648 images (4000 pix x 3000 pix) of individual broach teeth collected using a dedicated machine vision system. The dataset of images was divided into a training-validation (3100 samples) part and a test part (548 samples). Estimating prediction uncertainty was performed using model ensemble mode inference, with each model trained on a different subset of samples from the original dataset. Subsets of training samples were determined according to general bootstrapping assumptions and for 70% of common samples between the original set and the subsets. The mean absolute error (MAE) metric was used to validate dimensioning accuracy. For uncertainty estimation, the prediction uncertainty interval (from -3σ to 3σ) was determined using previously calculated standard deviation σ of predictions. The evaluation checked the percentage of true dimension values included in the estimated uncertainty interval.

Results and discussion

The results of the conducted experiment are shown in Fig. 1.

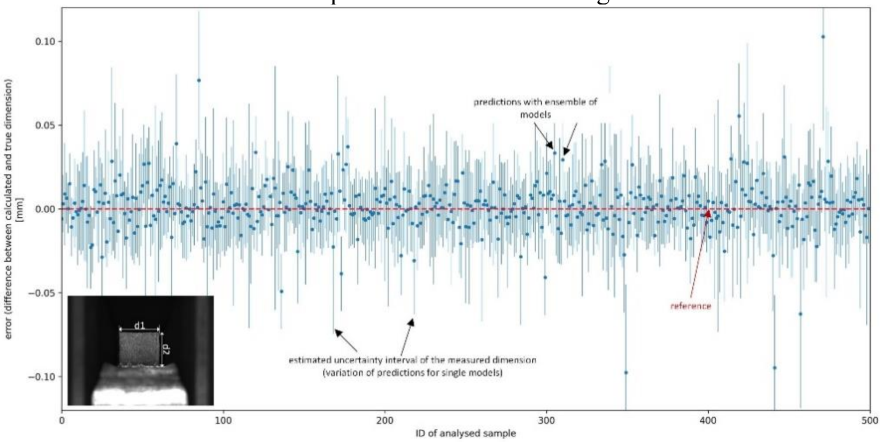

Fig. 1. Prediction errors of tooth dimensions with estimated uncertainty interval.

Summarising the results, MAE=10 µm was obtained for ensemble inference (20 single models in an ensemble), which was an improvement over the single model approach (MAE=12 µm). 93.4% of the true dimension values were within the estimated uncertainty interval. The average size of uncertainty interval was 55 µm.

Conclusions

The proposed method enabled the estimation of the prediction uncertainty while increasing the accuracy and reliability of the proposed solution. The flexibility of the approach and its applicability to other metrology problems should also be noted.

References

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