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Uncertainty quantification in machine learning applications

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Introduction

We strive to popularize the usage of uncertainty quantification methods in machine learning through publications [Ste+22] and application in various projects covering diverse fields from regression and classification to instance segmentation. In addition, we employ domain shift detection techniques to tackle population-level out-of-distribution scenarios. In all cases, the goal is to assess model prediction validity given unseen test data.

Partners

CASUS CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

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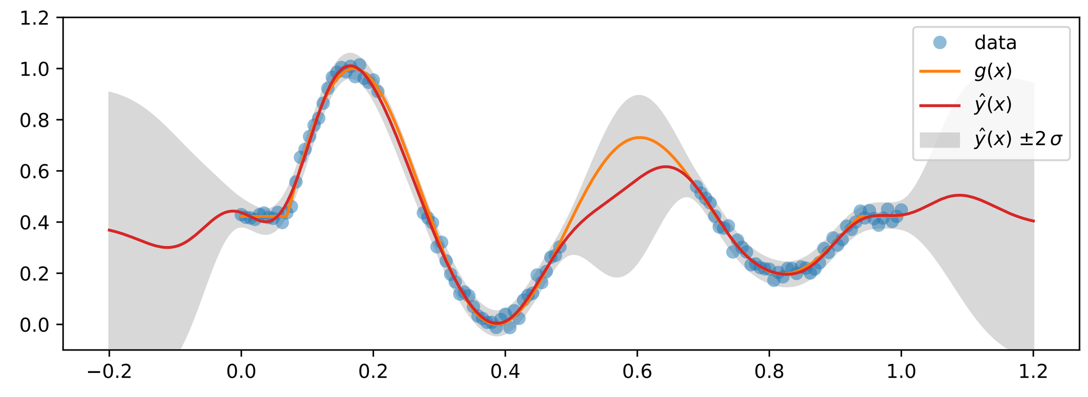
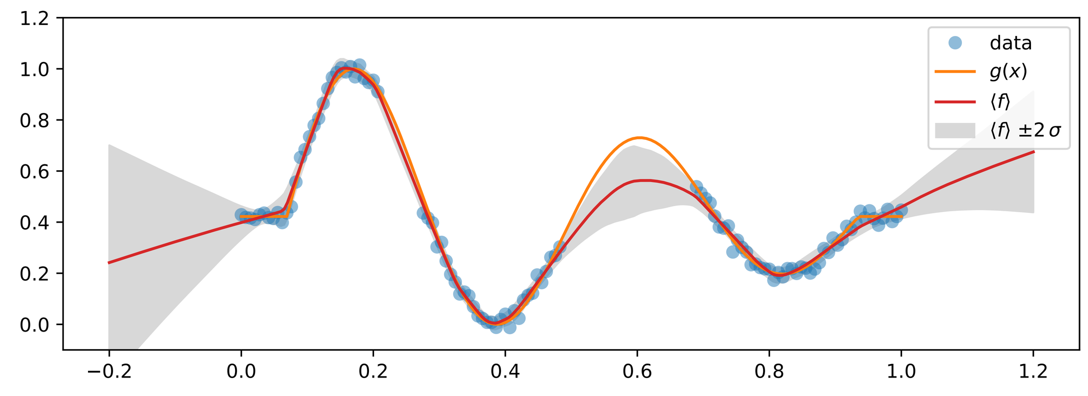
Regression (surrogate models)

MALA Materials Learning Algorithms

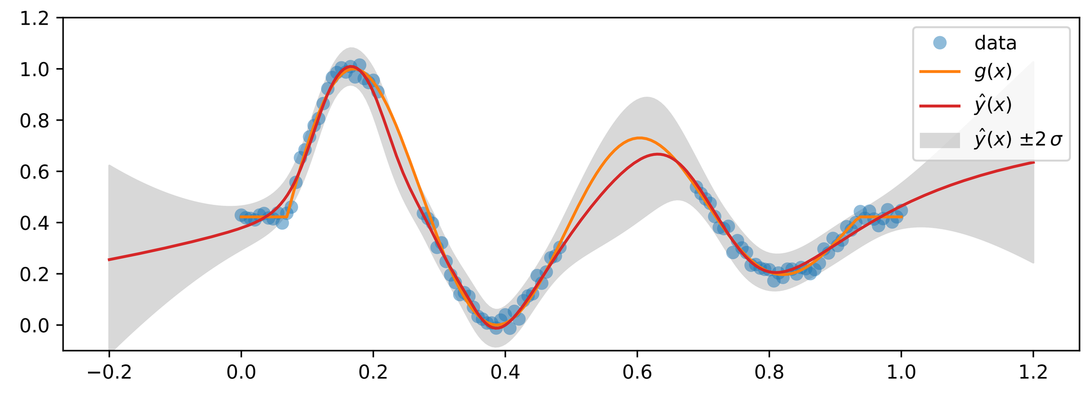
`https://github.com/mala-project/mala`



(a) Gaussian process base line



(b) Ensemble of neural networks



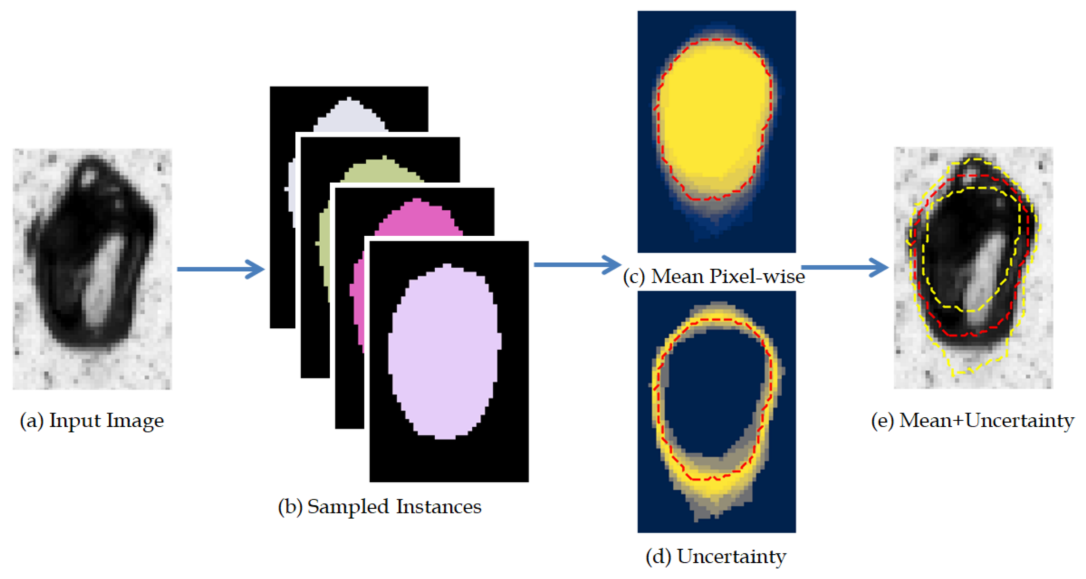
(c) Laplace approximation [Dax+21]

Figure 1: Study of various uncertainty quantification methods (S. Schmerler, S. Kulkarni, L. Fiedler, A. Cangi).

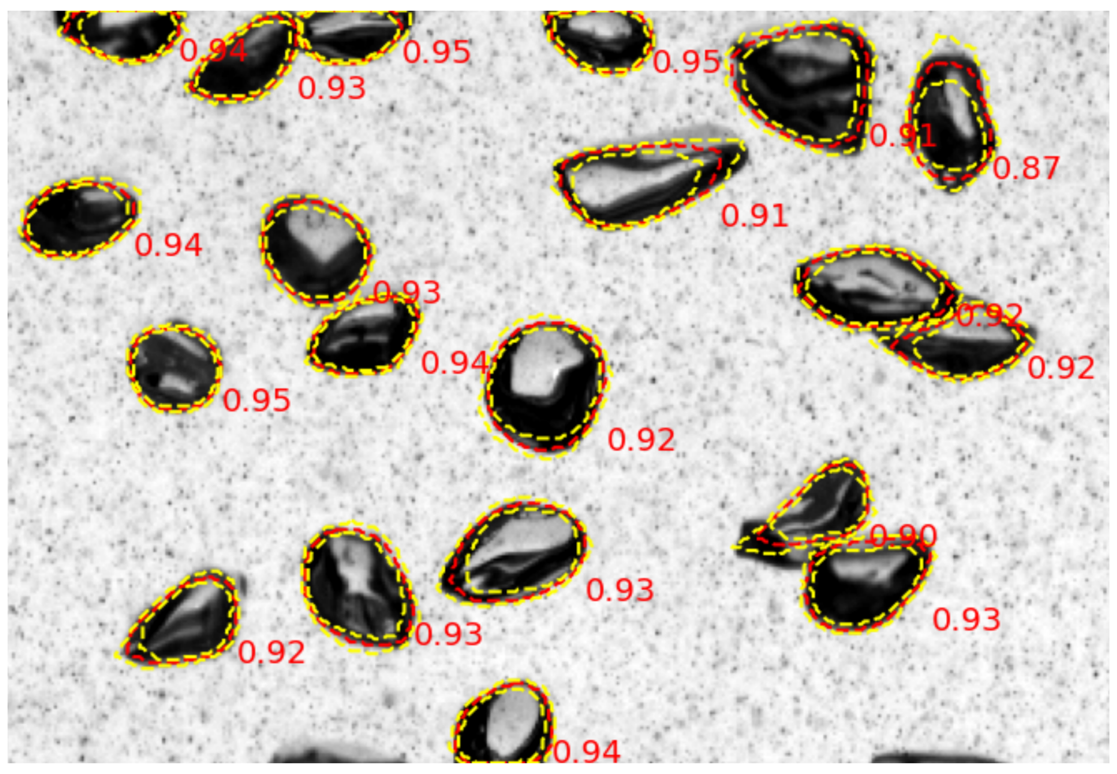
Instance Segmentation

StarDist

`https://github.com/stardist/stardist`



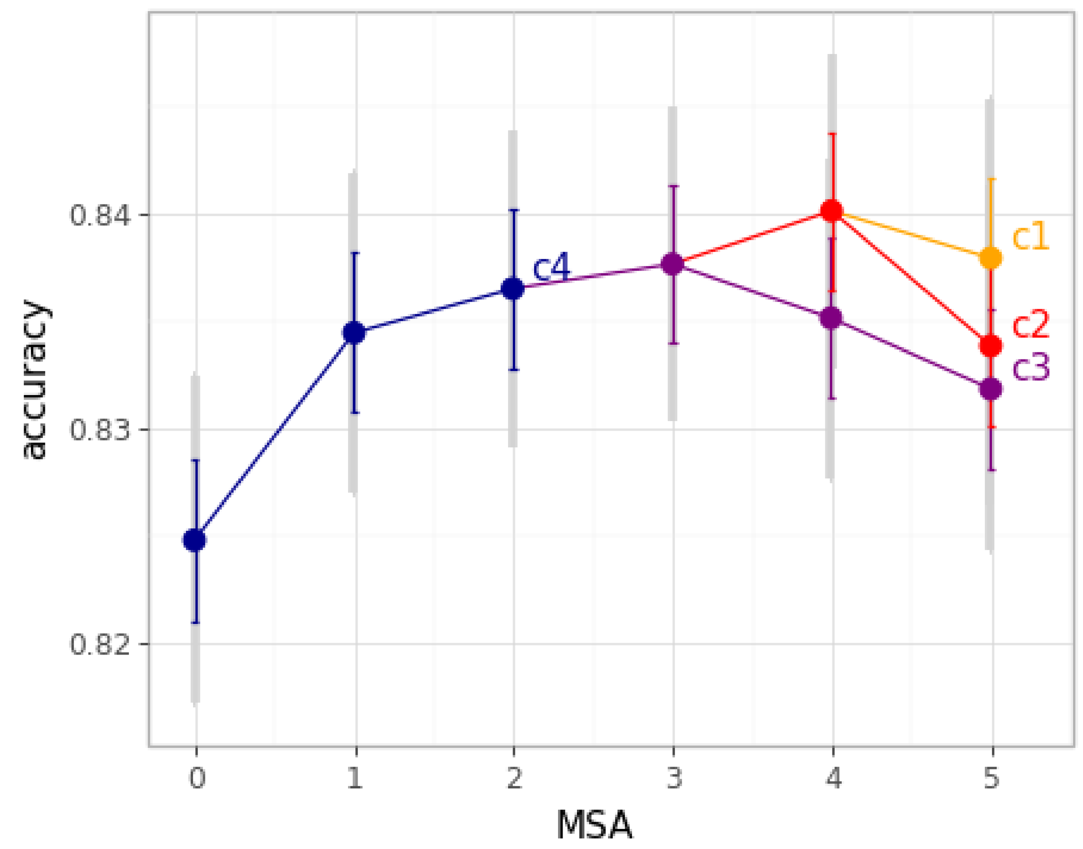
(a) StarDist [Sch+18] ensembles to obtain pixel uncertainty, from [Sid22].



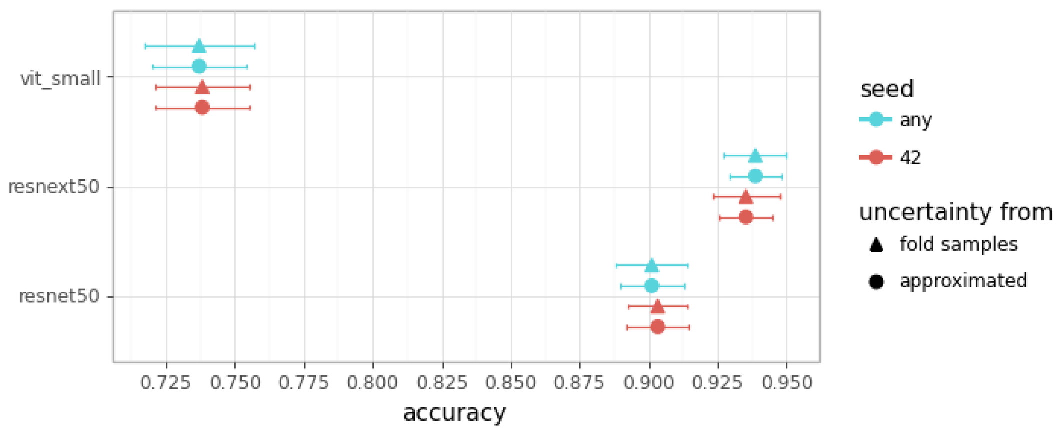
(b) Example application

Figure 2: StarDist segmentation mask uncertainty (S. Starke, Q. Siddiqui).

Classification



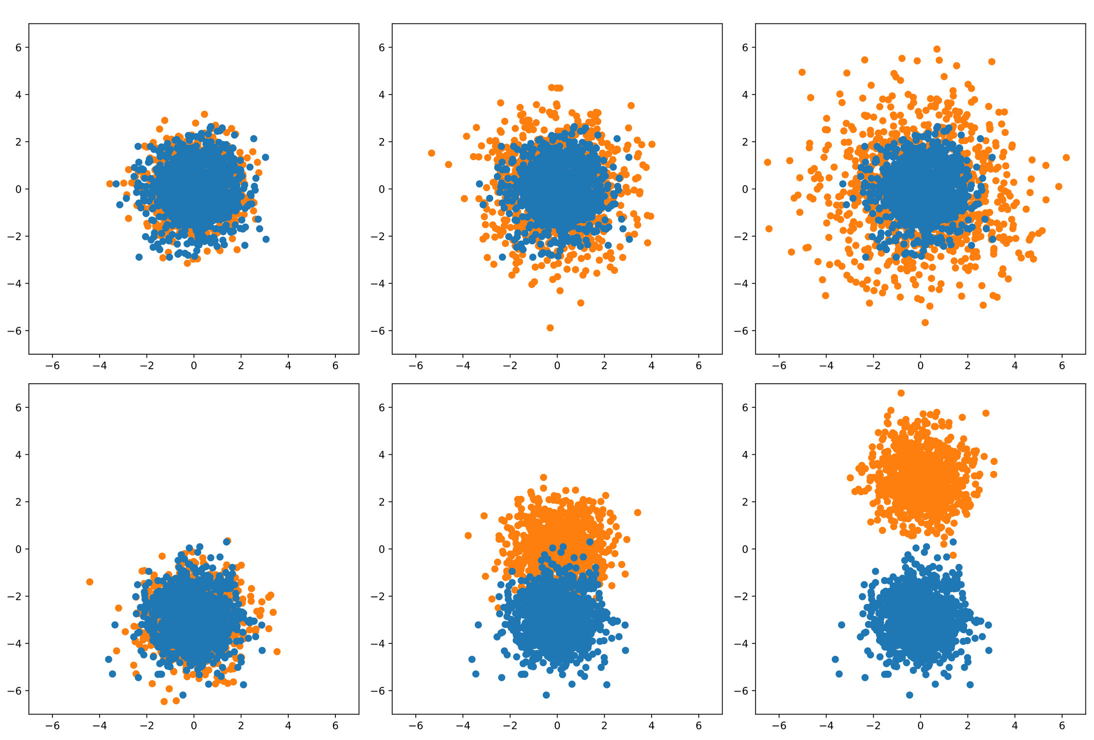
(a) Approximate uncertainty estimates for classification accuracies.



(b) Comparison of the approximate method of [Ras18] to more costly ensemble type base lines.

Figure 3: In [Ste+22] we provide a practical example of how authors can apply at least approximate uncertainty methods and by that motivate the adoption of those techniques in the community.

Upcoming: domain shifts



(a) Synthetic domain shift data

Figure 4: Domain shift/data set similarity testing by using a variant of C2ST [LO17] (`https://github.com/psteinb/c2st`) (S. Schmerler, P. Steinbach, S. Starke).

References

[Ste+22] P. Steinbach et al. "Machine Learning State-of-the-Art with Uncertainties". In: *ICLR* (2022). URL: `http://arxiv.org/abs/2204.05173`.

[Dax+21] E. Daxberger et al. *Laplace Redux – Effortless Bayesian Deep Learning*. 2021. URL: `http://arxiv.org/abs/2106.14806`.

[Sch+18] U. Schmidt et al. "Cell Detection with Star-Convex Polygons". In: *Medical Image Computing and Computer Assisted Intervention - MICCAI*. 2018, pp. 265–273.

[Sid22] Q. M. K. Siddiqui. "Estimating uncertainties in deep learning based instance segmentation models". MA thesis. TU Dresden, 2022.

[Ras18] S. Raschka. *Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning*. 2018. URL: `http://arxiv.org/abs/1811.12808`.

[LO17] D. Lopez-Paz et al. "Revisiting Classifier Two-Sample Tests". In: *5th International Conference on Learning Representations, ICLR*. 2017. URL: `http://arxiv.org/abs/1610.06545`.