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On Uncertainty-aware Deep Learning for Cytoarchitecture Classification

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High-resolution light-microscopic scans of histological brain sections allow identifying cytoarchitectonic areas. They are defined by the local characteristics of microstructural organization, which encompasses the size, type, shape, and distribution of neurons, as well as their distinct laminar and columnar organization. As established brain mapping methods relying on statistical image analysis are infeasible to handle the large size of high-resolution datasets acquired by high-throughput microscopic scanners, recent research focused on the development of automated cytoarchitecture classification methods based on deep learning. While the performance of these deep learning methods has steadily increased over the last years, they are unable to provide reliable estimates of prediction uncertainty. In particular, the softmax outputs of classification networks are generally not well suited to estimate a model's uncertainty. The lack of well-calibrated uncertainty estimates makes the interpretation of predictions challenging, in particular when dealing with out-of-distribution data.

To this end, we here studied the behavior of a state-of-the-art deep neural network for cytoarchitecture classification with respect to its uncertainty awareness. We compared it to two methods for uncertainty quantification: Dropout variational inference (DVI), which quantifies uncertainty based on the variance of multiple predictions acquired with inference-time dropout, and evidential deep learning (EDL), which is explicitly trained to output an informative uncertainty score. We apply both methods to in-distribution test data and out-of-distribution data from a brain not seen during training. We compare the models based on calibration metrics, uncertainty scores, and prediction entropy.

Our experiments revealed that the baseline model is generally overconfident, an often reported behavior of neural networks that manifests as high-prediction probability even for incorrectly classified samples. We observe similar behavior for out-of-distribution samples from a brain not included during training, where the model was unable to express its inability to make accurate predictions. In comparison to the baseline, both DVI and EDL resulted in considerably more plausible uncertainty measures. For example, we observed that the uncertainty scores obtained from models trained with EDL indicate high certainty in regions with highly distinct cytoarchitectonic properties, including the primary visual and motor cortex. While EDL outputs a single normalized uncertainty score per sample, DVI provides class-level uncertainty estimates based on per-class variance. This allows us to obtain localized uncertainty measures for specific brain regions. For example, we observed a low-certainty ribbon for the primary visual cortex at the transition between primary and secondary visual cortex, indicating cytoarchitectonic ambiguities at the boundary between the two regions. These ambiguities could be linked to the complex border phenomena that are characteristic of this region, the so-called border tuft and fringe area.

Our study revealed that predictions of existing models for cytoarchitecture classification are not well calibrated and lack the ability to express uncertainty. The investigated methods address these issues, providing complementary methods to assess uncertainty and improve model calibration. Future research will focus on the refinement of the training strategy and the involved hyperparameters. Finally, we plan to exploit the obtained uncertainty measures to identify high-certainty predictions for self-training approaches, which we expect to improve classification performance.

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