Uncertainty Quantification Using Bayesian Neural Networks

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Abstract

Uncertainty quantification (UQ) is crucial to attest the decision-making [1]. We here propose to quantify uncertainty using Bayesian Neural Networks (BNN), see [2, 3, 4]. The deterministic parameters of the NN are replaced by probability distributions with Gaussian prior, and the parameters of these distributions are learned. Once trained, the NN outputs can be evaluated multiple times to obtain the output distribution. When using BNN, the difficulty is related to the posterior distribution that is intractable. We propose to use the method proposed in [5] called Bayes by backprop, which applies variational approximation to get the posterior distribution. Many samples of the NN weights are then generated to get an uncertainty measure in addition to the class prediction. The method is applied to FMNIST data for classification. The UQ is evaluated using Shannon Entropy (SE) and the Brier Score (BS). SE measures the model's confidence level, while the BS assesses the precision of predictions. An evaluation using out of domain (OOD) data is also proposed, i.e. the algorithm is trained on FMNIST data and tested on MNIST ones. Results attest to the relevance the proposed approach. Fig. 1 shows that the SE and BS increases for test data OOD, indicating high uncertainty. In Fig. 2 (right) we observe a high fluctuation in the predicted class suggests that the algorithm is not sure and the prediction may not be accurate. As future work, the approach will be applied on mammograms images.

References

[1] Gawlikowski. J, C.R.N. Tassi, A. Mohsin, J. Lee, M.Humt, J. Feng, A. Kruspe, R. Triebel, Peter P. Jung, R. Roscherand S. Muhammad, W. Yang, R. Bamler, and X.X. Zhu, "A survey of uncertainty in deep neural networks," *Artif. Intell. Rev.*, vol. 56, no. Suppl 1, pp. 1513–1589, jul 2023.

[2] D J C. MacKay, "A practical bayesian framework for back-propagation networks.neural computation," *Neural computation*, vol. 4, no. 3, 1992.

[3] Radford M Neal, *Bayesian learning for neural networks*, vol. 118, Springer Science & Business Media, 2012.

[4] A. Graves, "Practical variational inference for neural networks," *Neural Information Processing Systems NIPS*, vol. 24, 2011.

[5] C. Blundell, J. Cornebise, K. Kavukcuoglu, and D. Wierstra, "Weight uncertainty in neural networks," *Proceedings of the 32nd International Conference on Machine Learning, PMLR*, vol. 37, pp. 1613–1622, 2015.

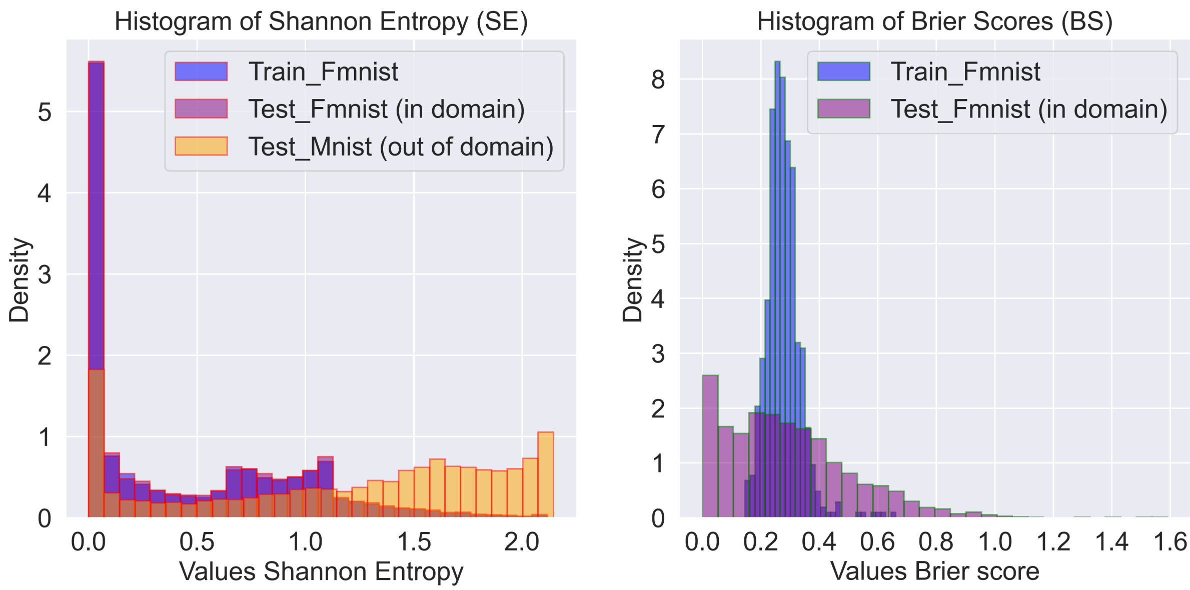

Figure 1: Histograms of SE (left) and BS (right).

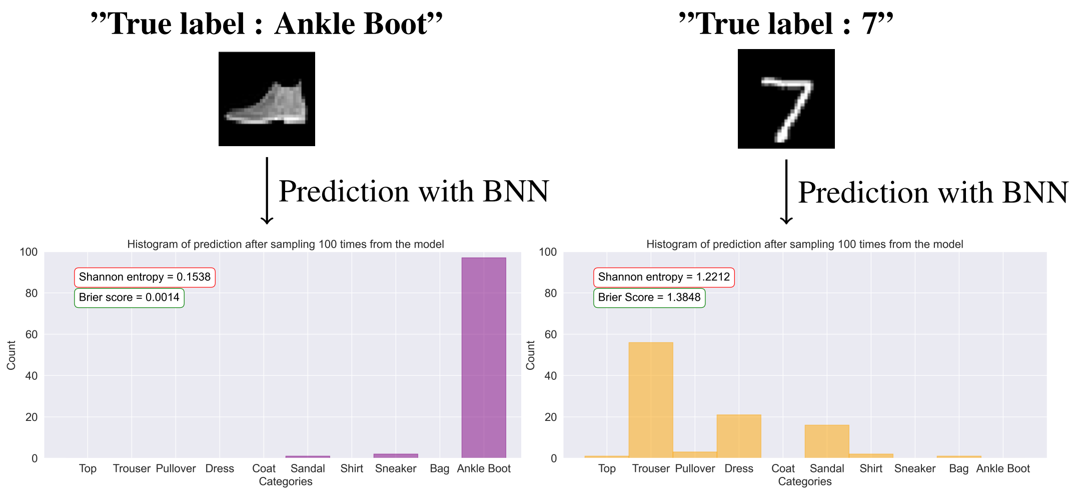

Figure 2: Comparison of FMNIST (in domain) and MNIST (out of domain) images with their prediction histograms after sampling 100 times.