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Dropout as a Bayesian Approximation

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Applied Machine Learning (AML) seeks to cover the issues that may arise in the practical application of machine learning in real-world problems. Deep learning architectures such as neural networks (NNs), convolutional neural networks and others are extensively used in AML. However, when it comes to model uncertainty, such tools for regression and classification do not capture it. In comparison, Bayesian models offer a mathematically grounded framework to reason about model uncertainty, but usually come with a prohibitive computational cost. The importance of uncertainty can be considered using the following examples: In the case of classification, a model might return a result with high uncertainty and it may lead to make a decision of passing the input to a human for classification. Model uncertainty is important in such an area of machine learning as reinforcement learning as well. With uncertainty information an agent can make the decision when to exploit and when to explore its environment. Overall, understanding if a model is under-confident or falsely over-confident can help get better performance out of it.

We consider a new theoretical framework casting dropout training in deep neural networks as approximate Bayesian inference in deep Gaussian processes. The theory's direct result gives the tools to model uncertainty with dropout NNs — extracting information from existing models that has been thrown away so far. Accordingly, even without sacrificing either computational complexity or test accuracy, the problem of representing uncertainty in deep learning is decreasing. We perform an extensive study of the properties of dropout's uncertainty. Various network architectures and nonlinearities are assessed on tasks of regression and classification, using MNIST [1] as an example. We show a considerable improvement in predictive log-likelihood and root-mean-square-error compared to existing state-of-the-art methods, and finish by using dropout's uncertainty in deep reinforcement learning [2].

[1] Ya. LeCun, C. Cortes, C. J. C. Burges, *The MNIST Database of handwritten digits.* http://yann.lecun.com/exdb/mnist/
[2] Y. Gal, Z. Ghahramani, *Dropout as a Bayesian approximation: Representing model uncertainty in deep learning*, 2015.

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