Concrete Dropout

MLSALT4 Paper Replication Exercise

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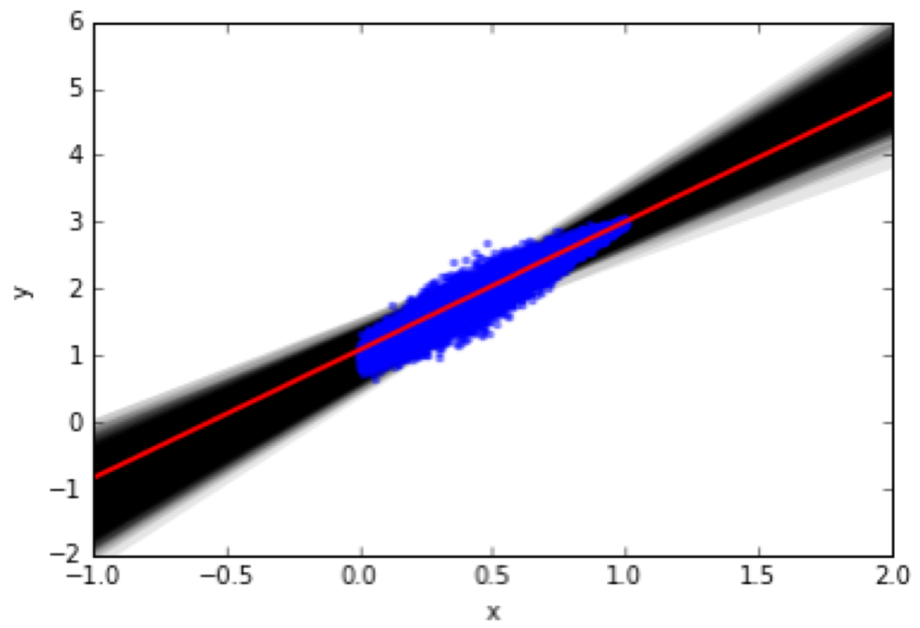
What is uncertainty?

Not knowing which line is the true model creates **epistemic uncertainty** in **y**

Inherent unpredictable noise creates **aleatoric uncertainty** in **y**



Dropout can measure uncertainty

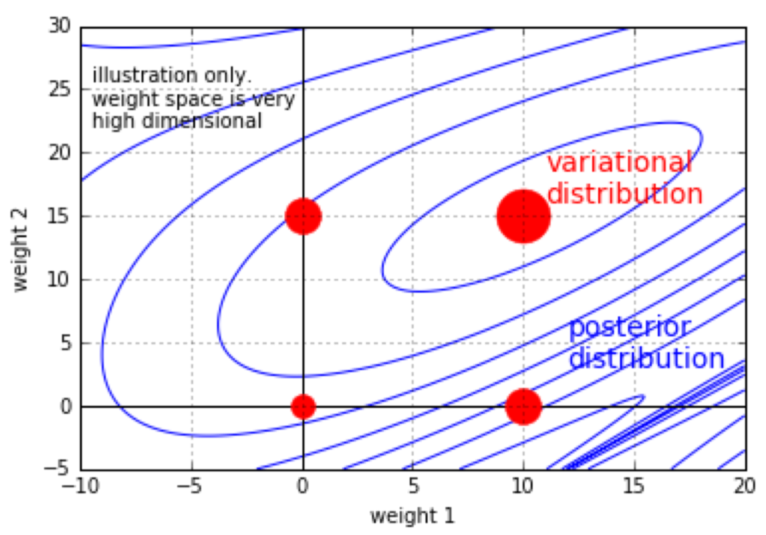
Gal and Ghahramani (2015) reinterpreted dropout regularisation as variational inference in BNNs

Posterior distribution $p(\omega|D)$ is approximated as

$$q_\theta(\omega) = \sum_{z \sim Bernoulli} p(z)\delta(\omega = W)$$

where

$$W = M \cdot diag(z)$$



Variational distribution is a hypercube of delta peaks in weight space. It is parameterised by furthest corner of cube from origin, M, and dropout probability, p. An optimal p is a proxy measure of **epistemic uncertainty**.

Optimal variational distribution found by minimising

$$\mathcal{L}(M,p) = KL[q_{M,p}(\omega)||p(\omega|D)]$$

$$= \underbrace{KL[q_{M,p}(\omega)||p(\omega)]}_{\textbf{Regulariser}} - \underbrace{\mathbb{E}_{q(\omega)}[\log p(D|\omega)] + \log p(D)}_{\textbf{MLE Loss}}$$

In a single layer of size K, for a Gaussian prior with variance l^{-2}, the regulariser is approximated as:

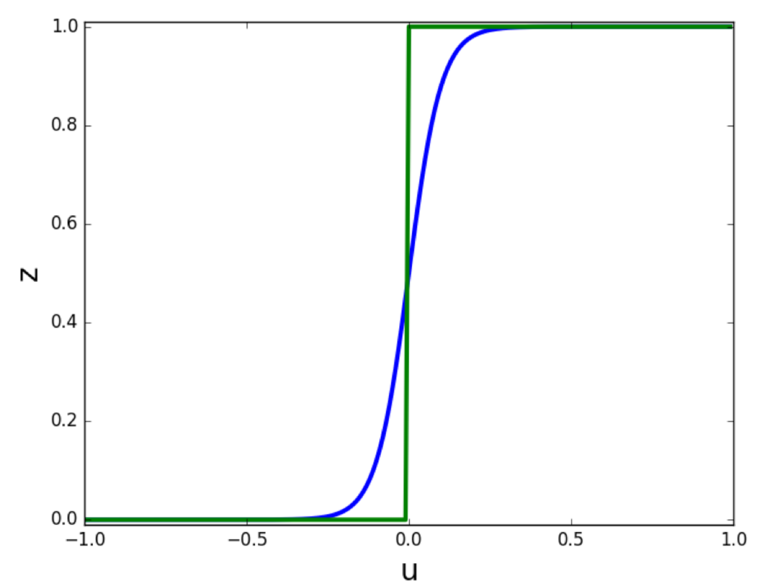
$$KL[q_{M,p}(\omega)||p(\omega)] \approx \frac{l^2(1-p)}{2}||M||^2 - KH(p)$$

Problems with tuning dropout p

Grid search over dropout probability is expensive:

- Wastes computing resources and experimental time
- Exponential increase in number of dropout configurations with number of NN layers
- In RL, dropout p should decrease as more data becomes available

Learning dropout probabilities



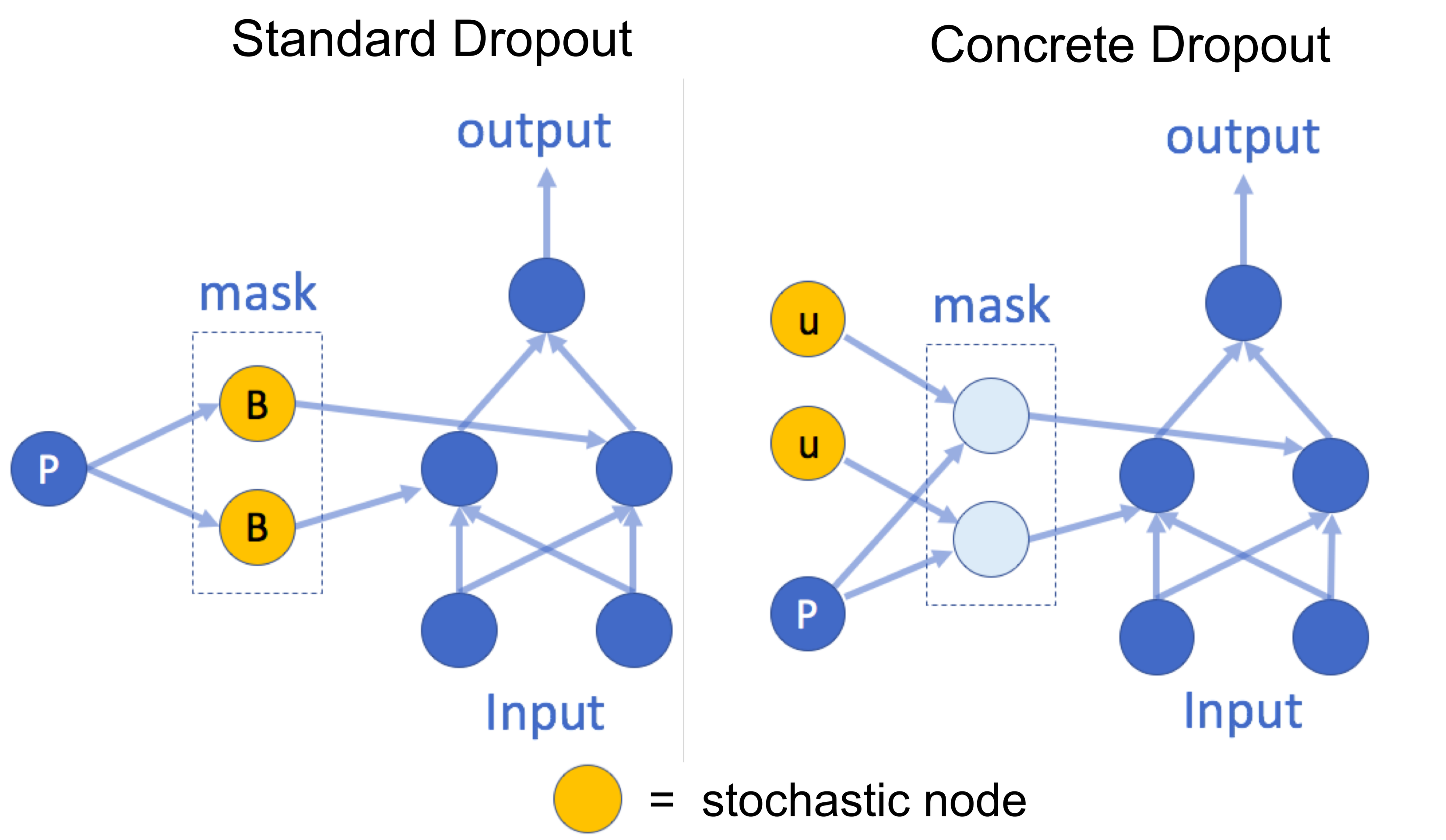
The **concrete distribution** is a relaxation of a categorical distribution onto the simplex.

In 1D, $z{\sim}Bernoulli(1-p)$ becomes

$$z \sim Sigmoid\left(\frac{\log\left(\frac{p}{1-p}\right)+\log\left(\frac{u}{1-u}\right)}{T}\right)$$

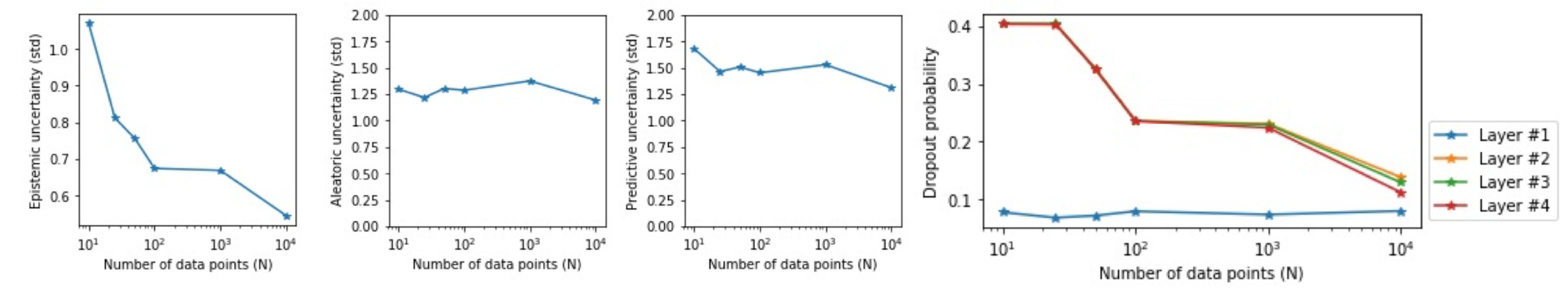
where $u \sim Uniform\,(0,1)$

- Dropout mask is now a **smooth deterministic function** of p and u
- Stochasticity is moved from the mask to uniform noise
- Gradient can freely flow through the network during backprop
- This is also called the "Reparameterisation Trick"

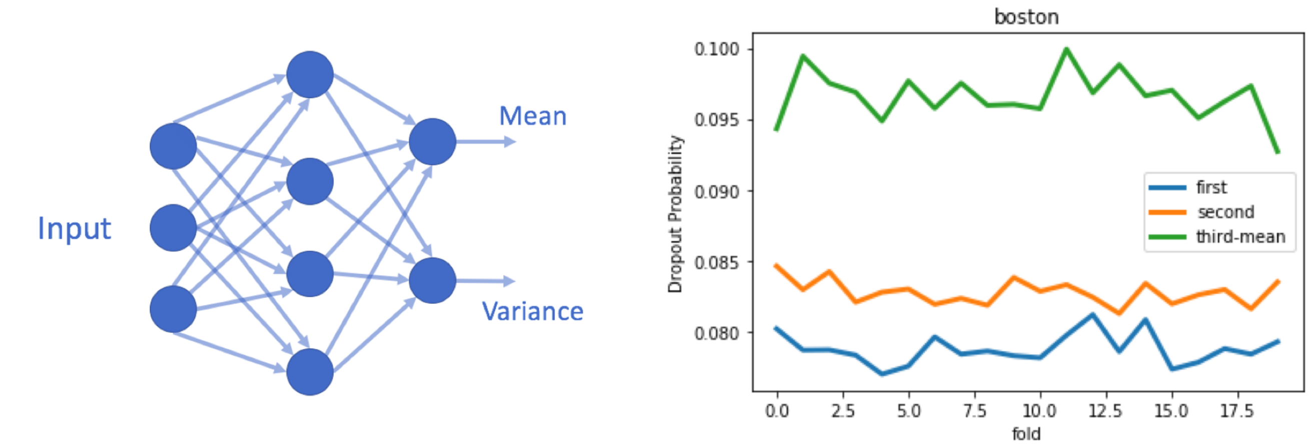


Experimental results

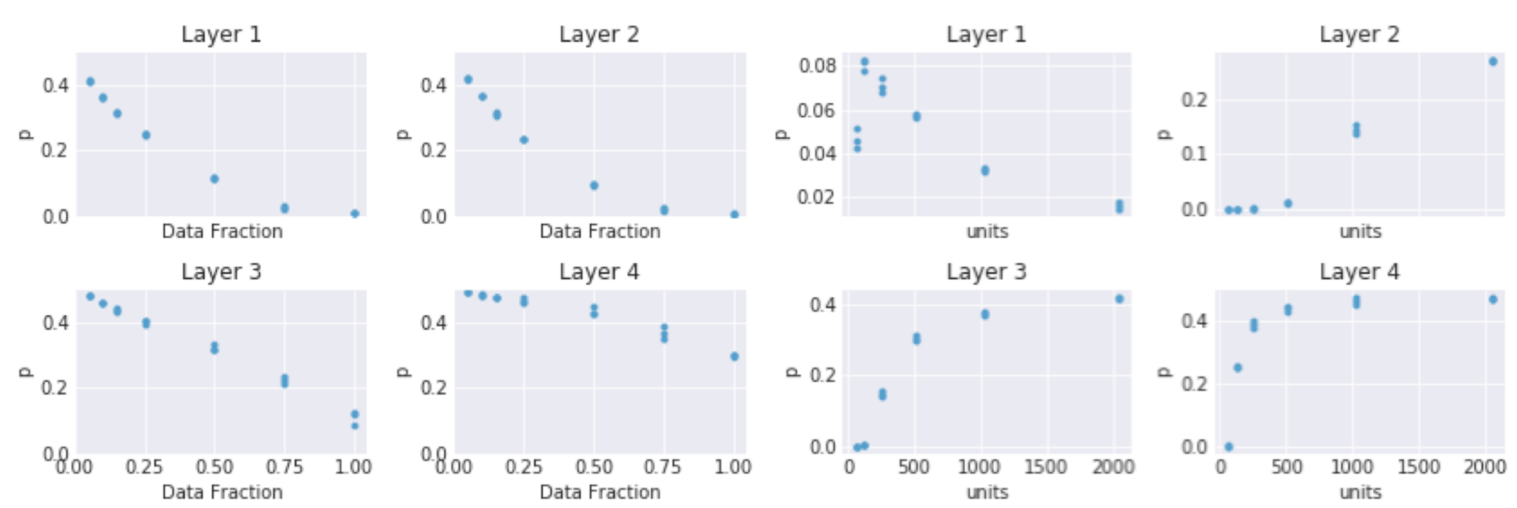
- Synthetic Data
  - 1-D linear regression model: $y = 2x + 8 + \epsilon$
  - Dropout probability decreases with more data points



- UCI Datasets
  - Dropout probability increases with depth



- MNIST
  - Dropout probability as a function of training set size (left; 3x512 MLP) and number of hidden units (right)



Proposed extensions

- Dropout can **reduce overfitting in RNNs**
- We propose applying concrete dropout to LSTMs/GRUs
- Possible architectures include input layer dropout, recurrent layer dropout, and combining the two

Gal, Y., Hron, J., & Kendall, A. (2017). Concrete dropout. In *Advances in Neural Information Processing Systems* (pp. 3584-3593).

Gal, Y., & Ghahramani, Z. (2015). Dropout as a Bayesian approximation: Insights and applications. In *Deep Learning Workshop, ICML* (Vol. 1, p. 2).