# A Bayesian Perspective of Neural Networks

Ethan Goan

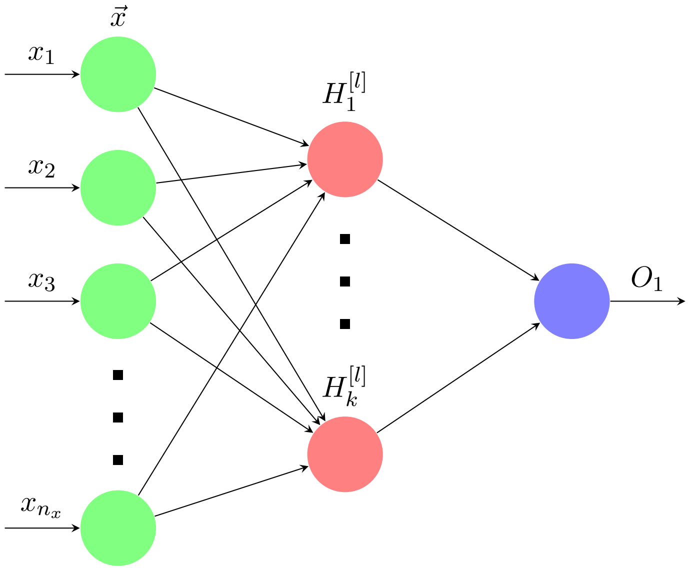
Supervised by
Prof. Clinton Fookes, Dr. Dimitri Perrin and Prof. Kerrie Mengersen

Queensland University of Technology

## Overview

- Introduce Neural Networks
- Some examples of neural networks applied to regression tasks
- Comparison to probabilistic models
- Recent research in the field of Bayesian Neural Networks

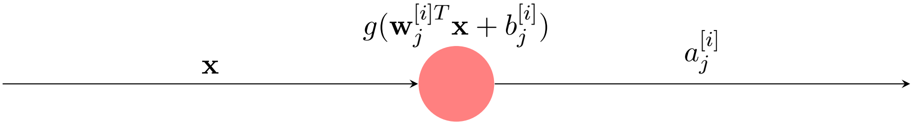
## Neural Network Graphical Model



## Inside a Neuron

Neuron consists of a linear mapping of the input, followed by a non-linear activation.

$$\begin{aligned}
a_j^{[i]} &= g(\mathbf{w}_j^{[i]T}\mathbf{x} + b_j^{[i]}) \\
\mathbf{w}_j^{[i]T} &= \text{ weight vector} \\
b_j^{[i]T} &= \text{ bias} \\
g(\cdot) &= \text{ non-linear activation function} \\
[i] &= \text{ layer number} \\
j &= \text{ node number within the } i^{th} \text{ layer}
\end{aligned}$$



## Vectorisation

Can implement the neural network model more efficiently by using matrix operations.

$$\mathbf{z}^{[1]} = W^{[1]}\mathbf{x} + \mathbf{b}^{[1]} = \begin{bmatrix} \cdots & w_1^{[1]T} & \cdots \\ \cdots & w_2^{[1]T} & \cdots \\ & \vdots & \\ \cdots & w_{k_l}^{[1]T} & \cdots \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n_x} \end{bmatrix} + \begin{bmatrix} b_1^{[1]} \\ b_2^{[1]} \\ \vdots \\ b_{k_l}^{[1]} \end{bmatrix}$$

$$\mathbf{a}^{[1]} = g(\mathbf{z}^{[1]})$$

## Further Vectorisation - Multiple Input Vectors

Can pass all (or as much as physically possible) into the network in a single iteration by storing the input vectors $\mathbf{x}_i$ as columns of a matrix $X$.

$$Z^{[1]} = W^{[1]}X + \mathbf{b}^{[1]} = \begin{bmatrix} \cdots & w_1^{[1]T} & \cdots \\ \cdots & w_2^{[1]T} & \cdots \\ & \vdots & \\ \cdots & w_{k_l}^{[1]T} & \cdots \end{bmatrix} \begin{bmatrix} \vdots & \vdots & & \vdots \\ \mathbf{x}^{(1)} & \mathbf{x}^{(2)} & \cdots & \mathbf{x}^{(m)} \\ \vdots & \vdots & & \vdots \end{bmatrix} + \begin{bmatrix} b_1^{[1]} \\ b_2^{[1]} \\ \vdots \\ b_{k_l}^{[1]} \end{bmatrix}$$

$$A^{[1]} = g(Z^{[1]})$$

## Training - Gradient Descent

Forward Propagation in a 2 layer network (1 hidden layer)

$$
\begin{aligned}
Z^{[1]} &= W^{[1]}X + b^{[1]} \\
A^{[1]} &= g(Z^{[1]}) \\
Z^{[2]} &= W^{[2]}A^{[1]} + b^{[2]} \\
A^{[2]} &= g(Z^{[2]}) = \hat{y}
\end{aligned}
$$

To perform gradient descent, first need to define an objective to minimise.

$$\mathcal{L}(\hat{y}, y) = -\Big(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y})\Big)$$

$$J(w, b) = \frac{1}{m} \Sigma_{i=1}^{m} \mathcal{L}(\hat{y}_i, y_i)$$

## Training - Gradient Descent

With our cost objective to minimise,

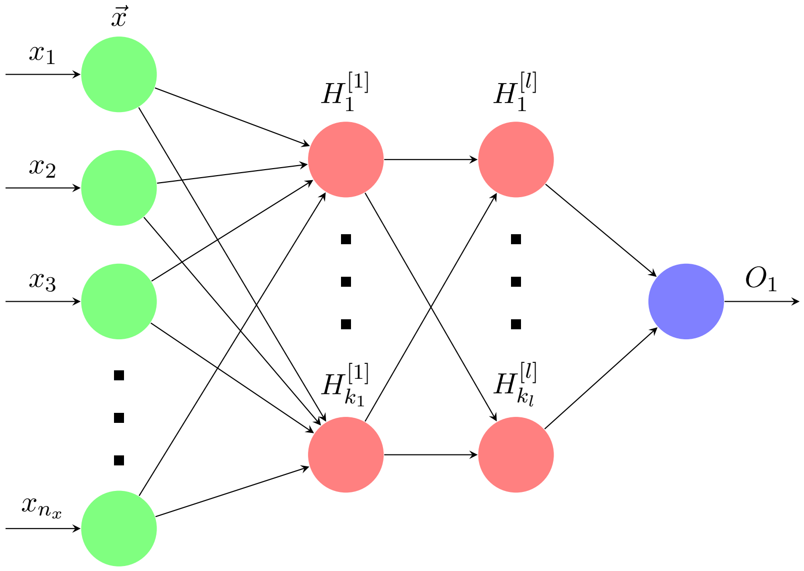
$$J(w, b) = \frac{1}{m} \Sigma_{i=1}^{m} \mathcal{L}(\hat{y}_i, y_i)$$

we can find the partial derivative of this objective and use it to update out network parameters.

$$\theta = \theta - \alpha \frac{\partial J}{\partial \theta}$$

where $\alpha$ is our learning rate, and $\theta$ is any of our model weights $W^{[l]}$ or bias' $\mathbf{b}^{[l]}$.

## More Hidden Layers



# Comparison - Regression

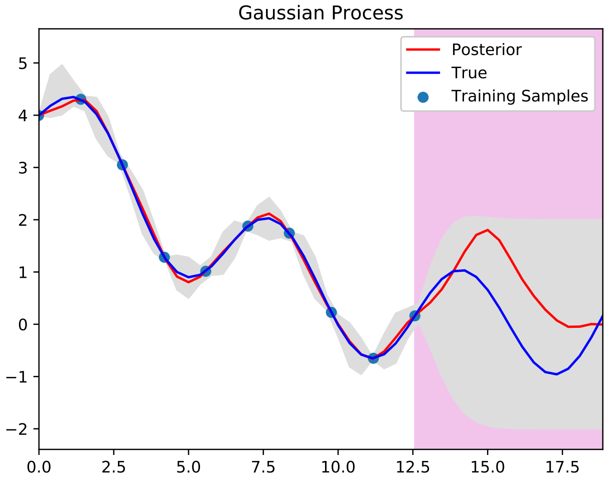


Figure: Regression using Gaussian Process

## Comparison - Regression

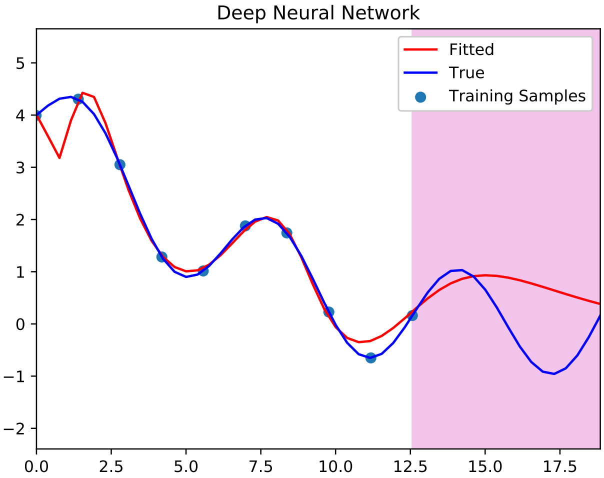


Figure: Regression using neural network with two hidden layers

## Stochastic Regularisation Techniques

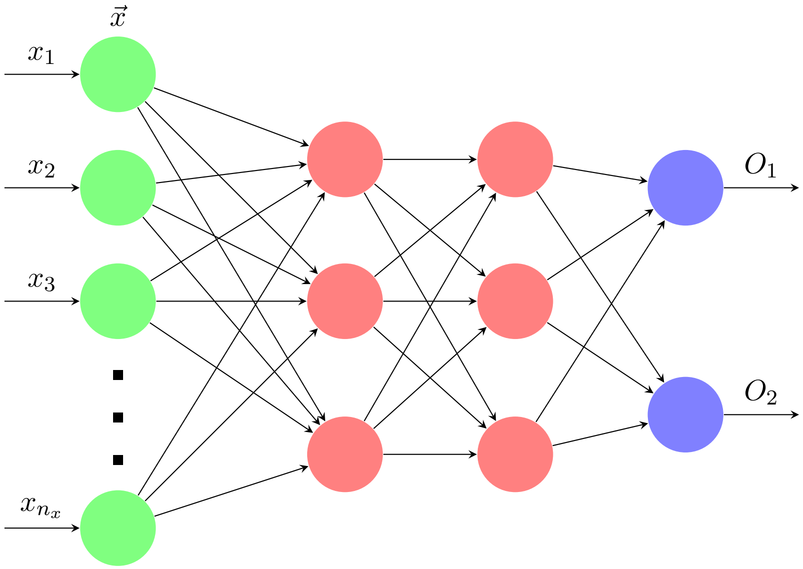
- Neural networks are prone to overfitting training data
- Stochastic Regularisation Techniques (SRTs) are introduced to combat this
- Most prominent technique is Dropout, where output of a unit is attenuated by multiplying element with a Bernoulli distributed RV Srivastava et al. (2014)

## Dropout

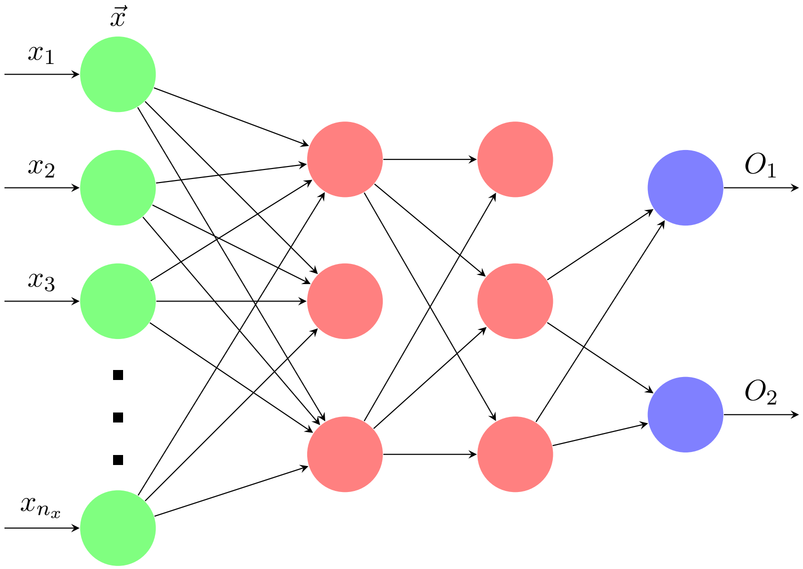
With dropout, the feedforward opertation becomes,

$$\begin{aligned}
r_j^{[i]} &\sim \text{Bernoulli}(p) \\
R^{[i]} &= \text{diag}(\epsilon) \\
\widetilde{A}^{[i-1]} &= R^{[i]} A^{[i-1]} \\
\widetilde{Z}^{[i]} &= W^{[i]} \widetilde{A}^{[i-1]} + b^{[i]} \\
\widetilde{A}^{[i]} &= g(\widetilde{Z}^{[i]})
\end{aligned}$$

## Before Applying Dropout



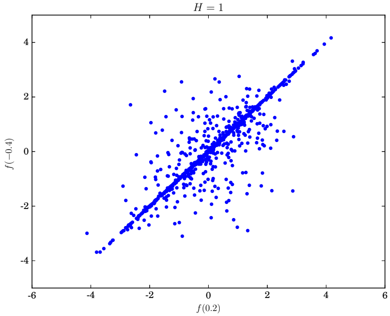
## Example After Applying Dropout



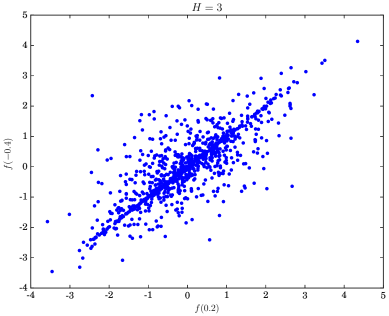
## A Bayesian Perspective

- Want to relate neural networks to probabilistic methods
- Development of Bayesian Neural Networks (BNN)
- BNN is a neural network with a prior placed over the network parameters $W^{[i]}, \mathbf{b}^{[\mathbf{i}]}$; Tishby, Levin, and Solla (1989); Neal (1996)
- Work in Neal (1996) showed how when a Gaussian prior is placed over network parameters for a single hidden layer network, the prior on the network output is a Gaussian Process

## Gaussian Process Prior

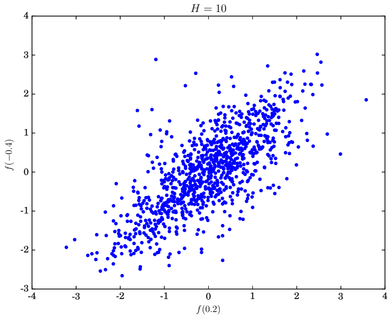


(a) 1 hidden units

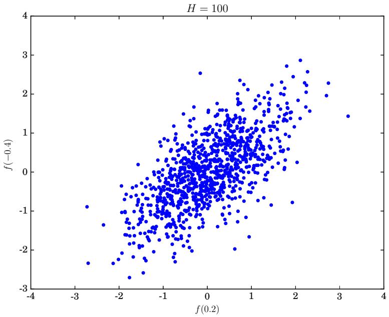


(b) 3 hidden units

# Gaussian Process Prior



(a) 10 hidden units



(b) 100 hidden units

## The Bayesian Way

Still looking for a for Bayesian treatment of Neural Networks

$$p(\omega|\mathbf{Y},\mathbf{X}) = \frac{p(\omega)p(\mathbf{Y}|\mathbf{X},\omega)}{p(\mathbf{Y}|\mathbf{X})}$$

$$p(\mathbf{y}^*|\mathbf{x}^*,\mathbf{Y},\mathbf{X},\omega) = \int p(\mathbf{y}^*|\mathbf{x}^*,\omega)p(\omega|\mathbf{Y},\mathbf{X})d\omega$$

But as expected, posterior for a deep neural network is intractable

## Current Research

- Preliminary work done in Neal (1996), MacKay (1992)
- Only recently resurfaced as a topic of interest
- Neural Networks are hard to perform inference on
- Recent work done in Graves (2011) is promising to address this issue
- How to use Bayesian methods to model uncertainty in our predictions Kingma, Salimans, and Welling (2015), Gal (2016)

## Variational Methods

Select an approximate posterior $q_\theta(\omega)$ and minimise KL Divergence between approximate and true posterior

$$\hat{\mathcal{L}}_{VI}(\theta) := -\int q_\theta(\omega) \log\Big(p(\mathbf{Y}|\mathbf{X},\omega)\Big) d\omega + \mathsf{KL}\Big(q_\theta(\omega)||p(\omega)\Big)$$

$$= -\sum_{i=1}^{n_x} \int q_\theta(\omega) \log\Big(p(\mathbf{y}_i|\mathbf{f}^\omega(\mathbf{x}_i))\Big) d\omega + \mathsf{KL}\Big(q_\theta(\omega)||p(\omega)\Big)$$

First term corresponds to expected log-liklihood

## Reparameterisation Trick

Expected log-liklihood term is of the form,

$$I(\theta) = \frac{\partial}{\partial\theta} \int f(x) p_\theta(x) dx$$

We can use the reparameterisation trick proposed in Kingma and Welling (2013), where the latent variable $\omega \sim q_\theta(\omega)$ is expressed as a deterministic function $g(\epsilon, \theta)$, with $\epsilon \sim p(\epsilon) = \Pi_{l,i} p(\epsilon_{l,i})$.

For example, if $\omega \sim \mathcal{N}(\mu, \sigma^2)$, can have $g(\theta, \epsilon) = \mu + \epsilon\sigma$, where $p(\epsilon) = \mathcal{N}(0, I)$

## Reparameterisation Trick

With this, we can rewrite our KL divergence term between the true and approximate posterior. In this way, our variational objective,

$$\hat{\mathcal{L}}_{VI}(\theta) := -\sum_{i=1}^{n_x} \int q_\theta(\omega) \log \Big( p(\mathbf{y}_i | \mathbf{f}^{\omega}(\mathbf{x}_i) \Big) d\omega + \mathsf{KL}\Big( q_\theta(\omega) || p(\omega) \Big)$$

becomes Gal (2016),

$$\hat{\mathcal{L}}_{VI}(\theta) := -\sum_{i=1}^{n_x} \int p(\epsilon) \log \Big( p(\mathbf{y}_i | \mathbf{f}^{g(\epsilon,\theta)}(\mathbf{x}_i) \Big) d\epsilon + \mathsf{KL}\Big( q_\theta(\omega) || p(\omega) \Big)$$

This expression can then be approximated using Monte Carlo methods to find our expression for the approximate posterior.

## Link to Dropout

$$\hat{\mathcal{L}}_{VI}(\theta) := -\sum_{i=1}^{n_x} \int p(\epsilon) \log \Big( p(\mathbf{y}_i | \mathbf{f}^{g(\epsilon,\theta)}(\mathbf{x}_i) \Big) d\epsilon + \mathsf{KL}\Big( q_\theta(\omega) || p(\omega) \Big)$$

In this expression, the term $\mathbf{f}^{g(\epsilon,\theta)}$ corresponds to the output of the network, with dropout described by $p(\epsilon)$ applied to the networks units. This expression can then be approximated using Monte Carlo methods to find our expression for the approximate posterior.

$$\hat{\mathcal{L}}_{MC}(\theta) := -\sum_{i=1}^{n_x} \log \Big( p(\mathbf{y}_i | \mathbf{f}^{g(\hat{\epsilon},\theta)}(\mathbf{x}_i) \Big) + \mathsf{KL}\Big( q_\theta(\omega) || p(\omega) \Big)$$

This expression can be optimised using gradient descent to optimal parameters $\theta$ for our approximate posterior $q_\theta(\omega)$.

## Predictive Posterior

$$
\begin{aligned}
\widetilde{\log}\Big(p(\mathbf{y}^*|\mathbf{x}^*, X, Y)\Big) &:= \log\Big(\frac{1}{T}\sum_{t=1}^{T} p(\mathbf{y}^*|\mathbf{x}^*, \omega_t)\Big) \\
&\xrightarrow[T\to\infty]{} \int p(\mathbf{y}^*|\mathbf{x}^*, \omega) q_\theta(\omega) d\omega \\
&\approx \int p(\mathbf{y}^*|\mathbf{x}^*, \omega) p(\omega|X, Y) d\omega
\end{aligned}
$$

Sampling from this approximate predictive distribution results in multiple forward passes during test time while including stochastic dropout variables Gal (2016).

## Topics of interest

- How can we better design neural networks with practical inference in mind
- Look at model design, ie. can we let a Bayesian method actually design our model
- Bayesian Domain Adaptation: how to use pretrained models as a prior?
- Can we incorporate output uncertainty in the training process?
- How to make decisions with uncertainty estimations?
- How good is our uncertainty estimations?
- Big one: How to use a Bayesian framework to better understand deep nets?

## References I

Gal, Yarin (2016). “Uncertainty in deep learning”. In: *University of Cambridge*.

Graves, Alex (2011). “Practical Variational Inference for Neural Networks”. In: *Advances in Neural Information Processing Systems 24*. Ed. by J. Shawe-Taylor et al. Curran Associates, Inc., pp. 2348–2356. URL: http://papers.nips.cc/paper/4329-practical-variational-inference-for-neural-networks.pdf.

Kingma, Diederik P, Tim Salimans, and Max Welling (2015). “Variational dropout and the local reparameterization trick”. In: *Advances in Neural Information Processing Systems*, pp. 2575–2583.

Kingma, Diederik P and Max Welling (2013). “Auto-encoding variational bayes”. In: *arXiv preprint arXiv:1312.6114*.

MacKay, David JC (1992). “A practical Bayesian framework for backpropagation networks”. In: *Neural computation* 4(3), pp. 448–472.

## References II

Neal, Radford M. (1996). *Bayesian Learning for Neural Networks*. Springer-Verlag New York, Inc.: Secaucus, NJ, USA. ISBN: 0387947248.

Srivastava, Nitish et al. (2014). “Dropout: A simple way to prevent neural networks from overfitting”. In: *The Journal of Machine Learning Research* 15(1), pp. 1929–1958.

Tishby, Naftali, Esther Levin, and Sara A Solla (1989). “Consistent inference of probabilities in layered networks: Predictions and generalization”. In: *IJCNN International Joint Conference on Neural Networks*. Vol. 2. IEEE New York, pp. 403–409.

## Code

Gaussian Process and Neural Network Regression
https://github.com/ethangoan/regression

Gaussian Prior over model parameters
https://github.com/ethangoan/bayesian_nn