A brief summary of Bayesian Deep Learning

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Overview

Linear Regression

- The simple LR, suppose data X is $1xn$, w is $nx1$, b is of size 1
- We have
  $Y = f(X, w, b)$
  $f(x, w, b) = x * w + b$
- w is the paratemeter we want
- Goal of linear regression is to find w such that,
  - $\|y - f(X, w, b)\|$ is minimized
  - Solution:

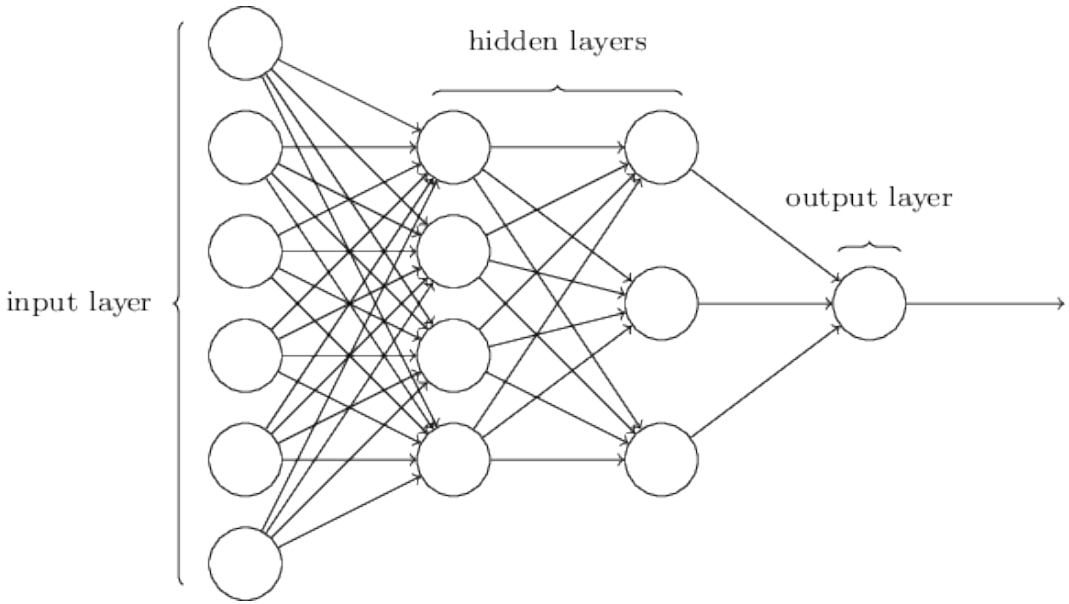
$$\begin{bmatrix} b \\ w \end{bmatrix} = (XX^T)^{-1}Xy$$

Logistic Regression

- Data X is $1xn$, w is $nx1$, b is of size 1
- We have
  $Z = f(X, w, b)$
  $Y = g(Z)$
  $g(x) = \frac{1}{1+e^{-x}}$
- Clip the output between $(0, 1)$

Neural Network

Data: $\mathcal{D} = \{(x_0, y_0), ..., (x_i, y_i), ..., (x_n, y_n)\} = \{X, Y\}$



- Neural Network is a parameterized fitting function.
- w and b are the weights of neural nets
- Fully Connected Nets

Neural Nets

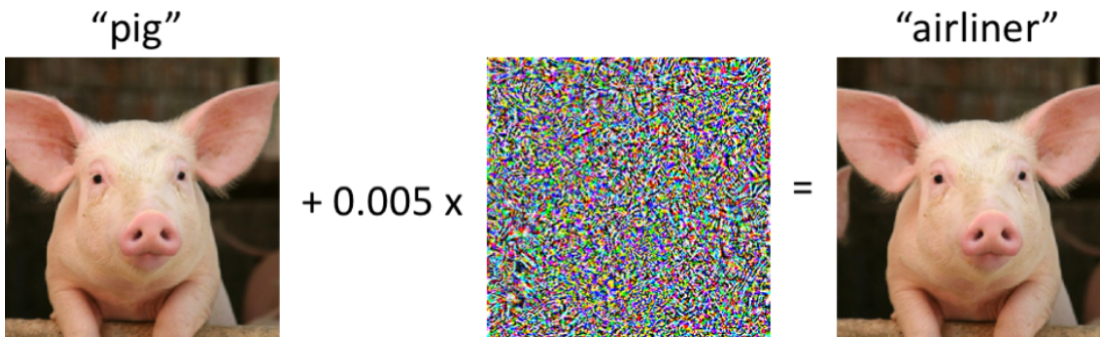
- Feedforward neural nets model $p(Y|X, w, b)$ as a composition of nonlinear functions(layers).
- $Z = \sigma(f(X, w_1, b_1))$
  $Y = ReLU(f(Z, w_2, b_2))$
- Relu, σ, Tanh are activation functions to introduce non-linearities into the network in case there are some non-linear complex functional mappings between the inputs and outputs.
- $ReLU(x) = max(x, 0)$
  $Tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$
  $\sigma(x) = \frac{1}{1+e^{-x}}$
- Usually trained to maximize likelihood using variants of stochastic gradient descent (SGD) optimization algorithms.

Deep Learning

- The backprop paper first came out in 1986 when NNs are called *Connectionism*.
- The innovations of architectures and algorithms(e.g. ReLU, many layers, better initialization, learning rate decay, dropout, LSTMs,...)
- Availability of large dataset.
- Improvement of computational power (GPUs).
- Better autodiff software packages (Theano, Tensorflow, Torch).

Limitations

- Data hungry
- Computational-intensive
- Point estimate, poor at representing uncertainty
- Easily fooled by adversarial attacks
- Nontransparent black-boxes, difficult to trust



(Figures from https://medium.com/@smkirthishankar/the-unusual-effectiveness-of-adversarial-attacks-e1314d0fa4d3)

Being Bayesian

The key idea is to learn probability density over parameter space.

Bayesian Linear Regression

- Put a prior over the parameters, i.e. $w \sim N(0, \sigma)$
- Finding the posterior distribution is the goal of Bayesian method,

$$
\begin{aligned}
p(w|Y,X) &= \frac{p(Y|X,w)p(w)}{p(Y|X)} \\
&\propto \exp(\frac{1}{2\sigma_n^2}(y - X^T w)^T (y - X^T w)) \exp(-\frac{1}{2} w^T \sigma^{-1} w) \\
&\propto \exp(\frac{1}{2}(w - \bar{w})^T A (w - \bar{w}))
\end{aligned}
$$

  where $\bar{w} = \frac{1}{\sigma_n^2} A^{-1} X y$ and $A = (\frac{1}{\sigma_n^2} X X^T + \sigma^{-1})$

- Hence, $P(w|Y,X) = N(\bar{w}, A^{-1})$
- However the analytical form of posterior distribution is not always possible. The priors that can enable analytical posterior forms are called conjugate priors.

Bayesian Linear Regression

- The parameter that maximize the posterior distribution is called the maximum a posteriori (MAP) solution.

$$\bar{w}_{MAP} = \frac{1}{\sigma_n^2}(\frac{1}{\sigma_n^2}XX^T + \sigma^{-1})^{-1}Xy$$

- The solution that maximizes the likelihood distribution is called MLE (maximum likelihood estimation) solution,

$$\bar{w}_{MLE} = (XX^T)^{-1}Xy$$

- How about prediction?

Bayesian Linear Regression

Suppose we want to predict at the new input x_*, then the predictive distribution is,

$$p(y_*|x_*, X, Y) = \int p(y_*|x_*, w)p(w|X, Y)dw$$
$$= N(\frac{1}{\sigma_n^2}x_*^T A^{-1}Xy, x_*^T A^{-1}x_*)$$

where $A = (\frac{1}{\sigma_n^2}XX^T + \sigma^{-1})$
Here we apply the kernel trick, the distribution of y_* becomes,
$p(y_*|x_*, X, Y) \sim N(\mu_*, \sigma_*)$
where $\mu_* = k(x_*, X)(k(X, X) + \sigma_n^2 I)^{-1}y$ and
$\sigma_* = k(x_*, x_*) - k(x_*, X)(k(X, X) + \sigma_*^2 I)^{-1}k(X, x_*)$
This is also the weight space view of Gaussian process regression.

A picture: GPs, Regressions, SVMs

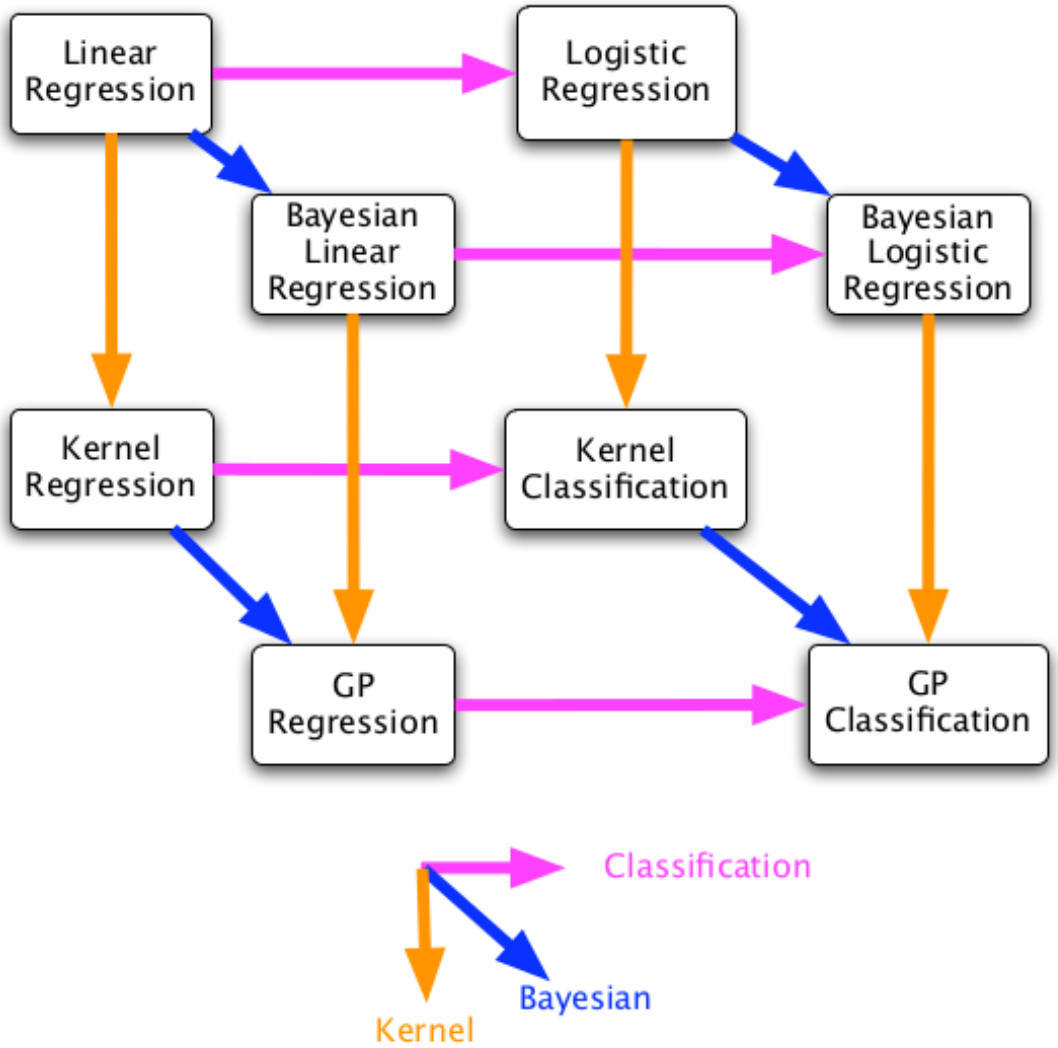
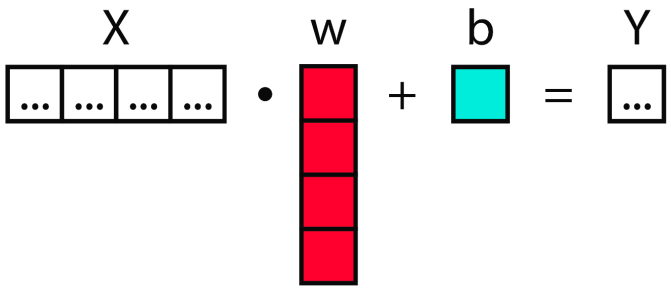


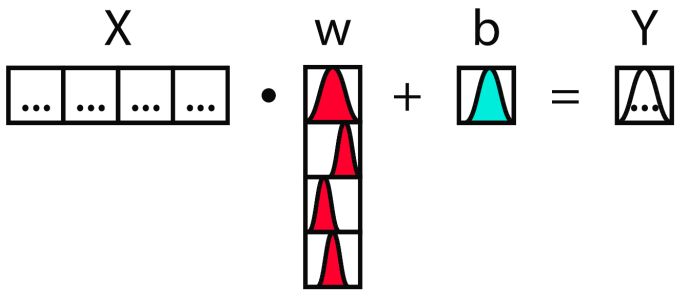
Figure from Zoubin Ghahramani's talk *"A history of Bayesian neural networks"* on NIPS 2016

Bayesian Linear Regression

BLR is as simple as changing from,



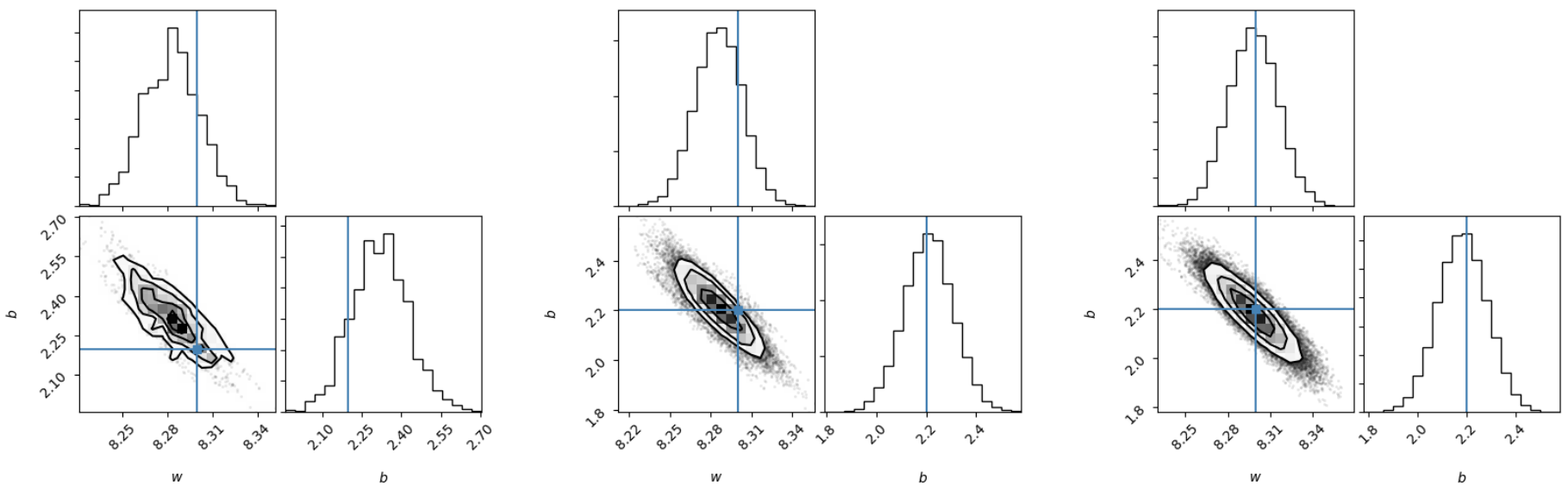
to



(Figures from Eric J. Ma's talk "*An Attempt At Demystifying Bayesian Deep Learning*" at PyData NYC, 2017)

BLR Demo with TensorFlow-probability

- The model, $y(x, w, b) = x * w + b$, assume $w \sim N(0, 10)$, $b \sim U(-10, 10)$
- Noise is added in the training data by $\epsilon \sim N(0, 1)$
- The likelihood function is equal to the joint probability distribution of the random sample evaluated at the given observations
- Sampled with Hamiltonian Monte Carlo



Num of Samples: 2000, 20000, 40000(left to right)

Models vs Algorithms

- Models:
  - HMMs, Boltzmann machines
  - CNNS, RNNs
  - GPs
- Algorithms:
  - Stochastic Gradient Descent
  - MCMC
  - Variational Bayes
  - Conjugate gradients
- "Bayesian" belongs in the Algorithms category, not the Models category. Any well defined model can be treated in a Bayesian manner. (Zoubin, 2016)

What about Bayesian Deep Learning?

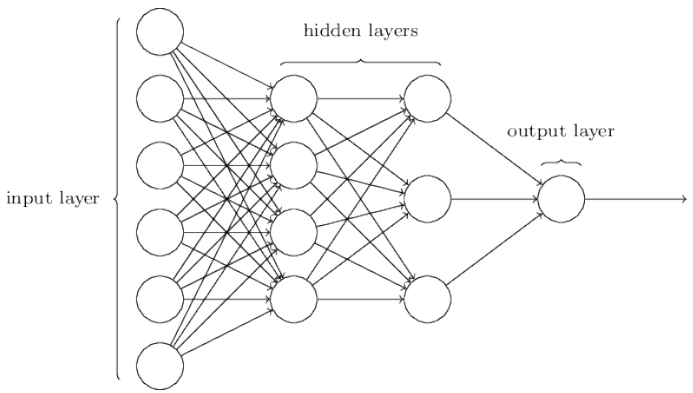
Bayesian Deep Learning

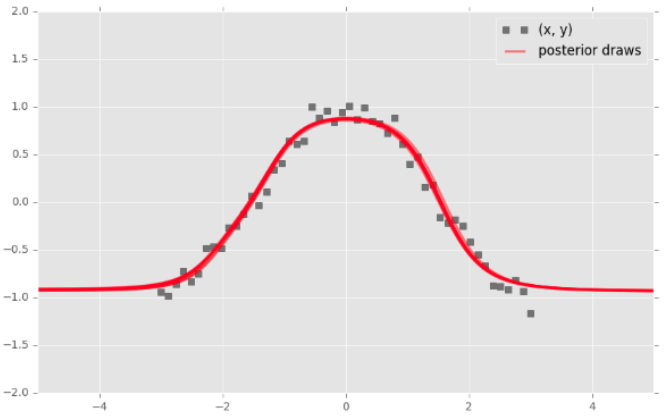
- Posterior

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

- Inference

$$p(Y|X) = \int p(Y|X,W)p(W|X,Y)dW$$





- A neural network with one hidden layer, infinitely many hidden units and Gaussian priors on the weights $\rightarrow$ *aGP*(*Neal*, 1994).

Reviews: *Minimizing the Description Length*

Geoffrey E Hinton and Drew Van Camp. Keeping the neural networks simple by minimizing the description length of the weights. In COLT, pages 5-13. ACM, 1993.

- A more complex model is always better to fit the training data.
- The best model is defined that minimizes the combined cost of describing the model and describing the misfit between the model and the data.
- In simple words,
  - There is a sender who can see both the input and the output.
  - There is a receiver who can only see the input.
- The sender first fits a NN to the entire training dataset and then send the weights to the receiver.
- By adding the discrepancy to the output of the network, the receiver can generate exactly the correct output.
- Total cost = coding the data misfits + coding the weights

Reviews: *Ensemble Learning in Neural Network*

David Barber and Christopher M Bishop. Ensemble learning in Bayesian neural networks. In Generalization in Neural Networks and Machine Learning Springer Verlag, 215-238, 1998.

- This method is called the variational inference nowadays.
- This paper introduce a variational distribution q(w) that approximates the posterior.
- Main contribution of this paper is to find the efficient update rule for optimizing q(w) by using full covariance Gaussian variational approximation to weights.

Reviews: *Practical Variational Inference*

Taken from Introduction:

- "In the eighteen years since variational inference was first proposed for neural networks (Hinton and Camp, 1993) it has not seen widespread use."
- "We believe this is largely due to the difficulty of deriving analytical solutions to the required integrals over the variational posteriors."
- "The approach taken here is to forget about analytical solutions and search instead for variational distributions whose expectation values (and derivatives thereof) can be efficiently approximated with numerical integration."

Reviews: *Practical Variational Inference*

- This paper is the first paper to formally use a variational inference on Bayesian neural networks.
- This paper assumes that the posterior distribution is a Gaussian distribution where the covariance matrix is diagonal and presented efficient gradients for optimizing the mean and variance.

Reviews: *Bayes by backprop*

Weight Uncertainty in Neural Networks

- All weights in the neural networks are represented by probability distributions over possible values, rather than having a single fixed value.
- Instead of training a single network, the proposed method trains an ensemble of networks, where each network has its weights sampled from a learnt probability distribution.
- This paper also changes the optimization objective

Summary of BNN

- The goal of a Bayesian Neural Network(BNN) is to find a posterior distribution:

  $p(W|X, Y) \propto p(Y|X, W)p(W)$

  where X and Y are the input and output training data and W is a set of network weights.

- Once we have $p(W|X, Y)$, the output y_* at unseen x_* is predicted through Bayesian inference:

  $p(y_*|x_*) = \int p(y|x_*, W)p(W|X, Y)dW$

- In practice, none if them is tractable.

Summary of BNN

- Variational Inference is used to handle this issue.
- Instead of finding $p(W|X, Y)$, optimize a variational distribution $q(\theta)$ by minimizing

$$KL(q_\theta(W)\|p(W|X, Y)) = \int q_\theta(W) log \frac{q_\theta(W)}{p(W|X, Y)} dW$$

- Variational inference is used to approximate the (intractable) posterior distribution with (tractable) variational distribution with respect to the KL divergence.
- But $KL(q_\theta(W)\|p(W|X, Y))$ is not tractable as well.
- We choose to compute the lower-bound called evidance lower-bound(ELBO) instead.

$$ELBO = \int q_\theta(W) log p(Y|X, W) dW - KL(q_\theta(W)\|p(W))$$

Summary of BNN

- In computing ELBO, we do not need to know $p(W|X, Y)$.

$$ELBO = \int q_\theta(W) log p(Y|X, W) dW - KL(q_\theta(W)||p(W))$$

- All we need is
  - prior: $p(W)$
  - variational distribution: $q_\theta(W)$
  - likelihood: $p(Y|X, W)$
- Minimizing the KL divergence is equivalent to maximizing the evidence lower bound (ELBO) which also contains the integral with respect to the distribution over latent variables.

Summary of BNN

- In computing ELBO, we do not need to know $p(W|X, Y)$.

$$ELBO = \int q_\theta(W) log p(Y|X, W) dW - KL(q_\theta(W) \| p(W))$$

- All we need is
  - prior: $p(W)$
  - variational distribution: $q_\theta(W)$
  - likelihood: $p(Y|X, W)$
- How to define a likelihood function?

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- All we need is
  - prior: $p(W)$
  - variational distribution: $q_\theta(W)$
  - likelihood: $p(Y|X, W)$
- How to define a likelihood function?
- If we could recall BLR, the solution is GP approximation again!

Summary of BNN

Gaussian process approximation

$$\mathbf{K}(\mathbf{x},\mathbf{y}) = \int p(\mathbf{w})p(b)\sigma(\mathbf{w}^T\mathbf{x}+b)\sigma(\mathbf{w}^T\mathbf{y}+b)\mathrm{d}\mathbf{w}\mathrm{d}b$$

↓ MC approximation

$$\widehat{\mathbf{K}}(\mathbf{x},\mathbf{y}) = \frac{1}{K}\sum_{k=1}^{K}\sigma(\mathbf{w}_k^T\mathbf{x}+b_k)\sigma(\mathbf{w}_k^T\mathbf{y}+b_k)$$

↓ Apply to Gaussian processes

$$\mathbf{w}_k \sim p(\mathbf{w}),\ b_k \sim p(b),$$
$$\mathbf{W}_1 = [\mathbf{w}_k]_{k=1}^K, \mathbf{b} = [b_k]_{k=1}^K$$
$$\widehat{\mathbf{K}}(\mathbf{x},\mathbf{y}) = \frac{1}{K}\sum_{k=1}^{K}\sigma(\mathbf{w}_k^T\mathbf{x}+b_k)\sigma(\mathbf{w}_k^T\mathbf{y}+b_k)$$
$$\mathbf{F} \mid \mathbf{X}, \mathbf{W}_1, \mathbf{b} \sim \mathcal{N}(\mathbf{0}, \widehat{\mathbf{K}}(\mathbf{X},\mathbf{X}))$$
$$\mathbf{Y} \mid \mathbf{F} \sim \mathcal{N}(\mathbf{F}, \tau^{-1}\mathbf{I}_N),$$

↓ GP Marginal likelihood

$$p(\mathbf{Y}|\mathbf{X}) = \int p(\mathbf{Y}|\mathbf{X},\mathbf{W}_1,\mathbf{W}_2,\mathbf{b})p(\mathbf{W}_1)p(\mathbf{W}_2)p(\mathbf{b})$$

Figure from Sungjoon Choi's presentation slides *Uncertainties in Deep Learning in a nutshell*

Summary of BNN

- Then apply the re-parametrization trick ($\tilde{W} = g(W + \epsilon_W)$ where $\epsilon_W(\epsilon)$) is a random variable) to the GP approximation result and get the re-parametrized ELBO

$$\int p(\epsilon) logp(Y|X, \tilde{W}) d\epsilon - KL(q_\theta(W) \| p(W))$$

- Then approximate the integral with MC integration, we have

$$\mathcal{L}_{GP\_MC} = \sum_{n=1}^{N} logp(y_n|x_n, \tilde{W}) + KL(q_\theta(W) \| p(W))$$

- With Gaussian prior on the parameters W, we have

$$\mathcal{L}_{GP\_MC} = \sum_{n=1}^{N} logp(y_n|x_n, \tilde{W}) + \sum_{m=1}^{M} \lambda_m \| W_m \|^2$$

- Where n is the number of data and m is the number of parameters.

Summary of BNN

- Once we have the paramaters W, predictive mean and variance can be approximated as:

$$E_q(y_*) = \int y_* q(y_*|x_*) dy_*$$
$$\approx \frac{1}{T} \sum_{t=1}^{T} y_*(x_*, \tilde{W}^t)$$
$$Var_q(y_*) \approx \tau^{-1} I + \frac{1}{T} \sum_{t=1}^{T} y_*(x_*, \tilde{W}^t)^T y_*(x_*, W^t) - E_q(y_*)^T E_q(y_*)$$

where τ is called model precision hyper-parameter.

Y.Gal *Uncertainty in Deep Learning*, 2016

Uncertainty in Deep Learning

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This dissertation is submitted for the degree of
Doctor of Philosophy

Gonville and Caius College September 2016

Review: Dropout as Bayesian Approximation

Algorithm 2 Optimisation of a neural network with dropout

1: Given dataset $\mathbf{X}, \mathbf{Y}$,
2: Define learning rate schedule η,
3: Initialise parameters θ randomly.
4: **repeat**
5: Sample M random variables $\widehat{\boldsymbol{\epsilon}}_i \sim p(\boldsymbol{\epsilon})$, S a random subset of $\{1, .., N\}$ of size M.
6: Calculate derivative w.r.t. θ:

$$\widehat{\Delta\theta} \leftarrow -\frac{1}{M\tau}\sum_{i\in S}\frac{\partial}{\partial\theta}\log p(\mathbf{y}_i|\mathbf{f}^{g(\theta,\widehat{\boldsymbol{\epsilon}}_i)}(\mathbf{x})) + \frac{\partial}{\partial\theta}\left(\lambda_1||\mathbf{M}_1||^2 + \lambda_2||\mathbf{M}_2||^2 + \lambda_3||\mathbf{b}||^2\right).$$

7: Update θ:
$\theta \leftarrow \theta + \eta\widehat{\Delta\theta}$.
8: **until** θ has converged.

Review: Dropout as Bayesian Approximation

- Gal Ghahramani: Approximate ELBO and Dropout NN objectives are identical.
- Optimising any neural network with dropout is equivalent to a form a apprimate Bayesian inference
- A network trained with dropout is already a BNN.
- However, MC Dropout requires applying dropout at every weight layer and averaging over T forward passes during testing.

Other approximation methods

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

$$p(Y|X) = \int p(Y|X,W)p(W|X,Y)dW$$

Other approximation methods for posterior and marginal likelihood estimation,

- Variational approximations
- Markov chain Monte Carlo methods (MCMC)
- Sequential Monte Carlo (SMC)
- Exact Sampling
- Bayesian Information Criterion (BIC)

Tools

The Python probabilistic programming packages provides:

- Statistical distributions
- Sampling algorithms
- Inference methods

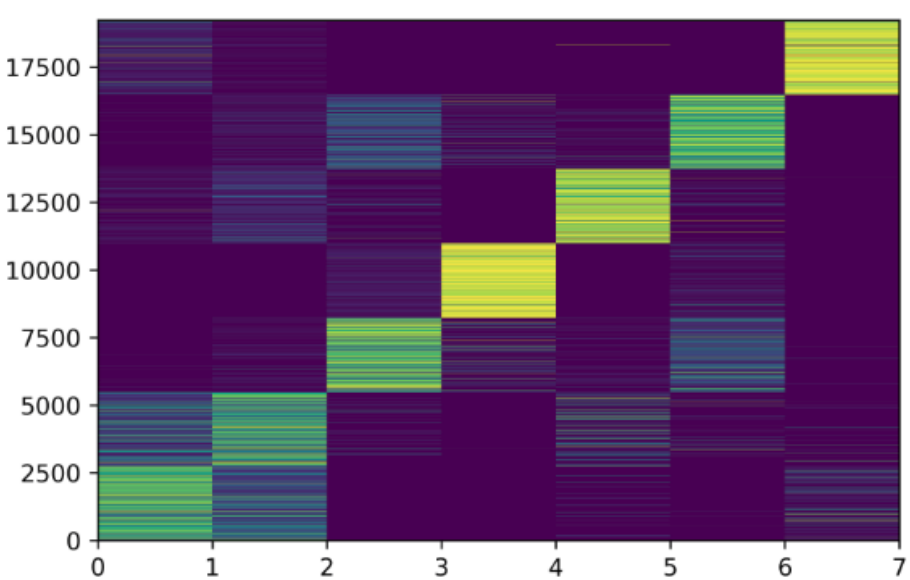
List of packages,

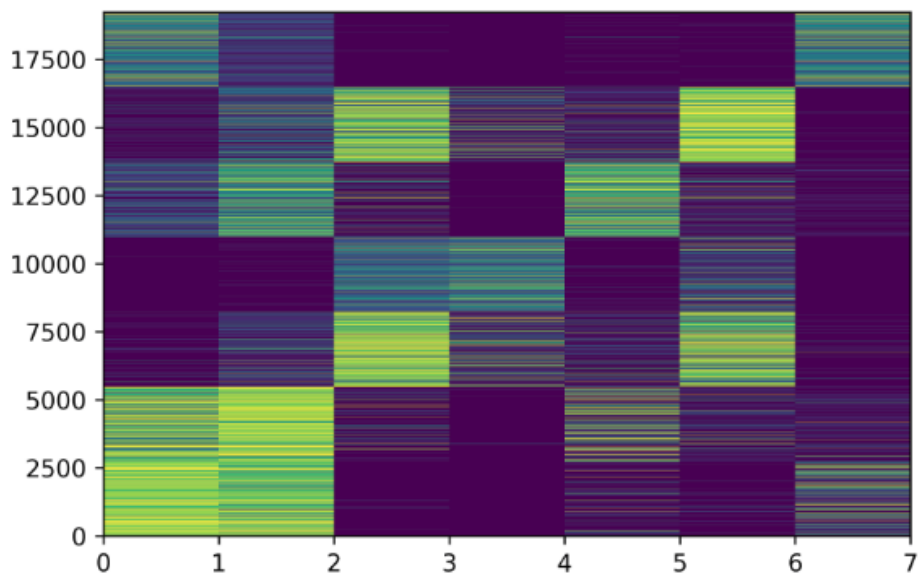
- Tensorflow-probability(tfp)
  - Edward: Dustin Tran, merging into tfp as Edward2
  - Zhusuan: TsingHua University, not officially released in pip
  - Sonnet: Deepmind
- PyMC3/4: Based on Theano but trying to move into tfp in PyMC4
- Pyro: Uber Lab, based on Torch

Demo: BNN Classification

Predict Forest Cover Type with PyMC3

- Toy Dataset: Covertype Dataset from UCI ML Repository
- Input: 66 categorical features
- Output: 7 forest cover types
- $W \sim N(0, 1)$
- Two hidden layers with 20 units each



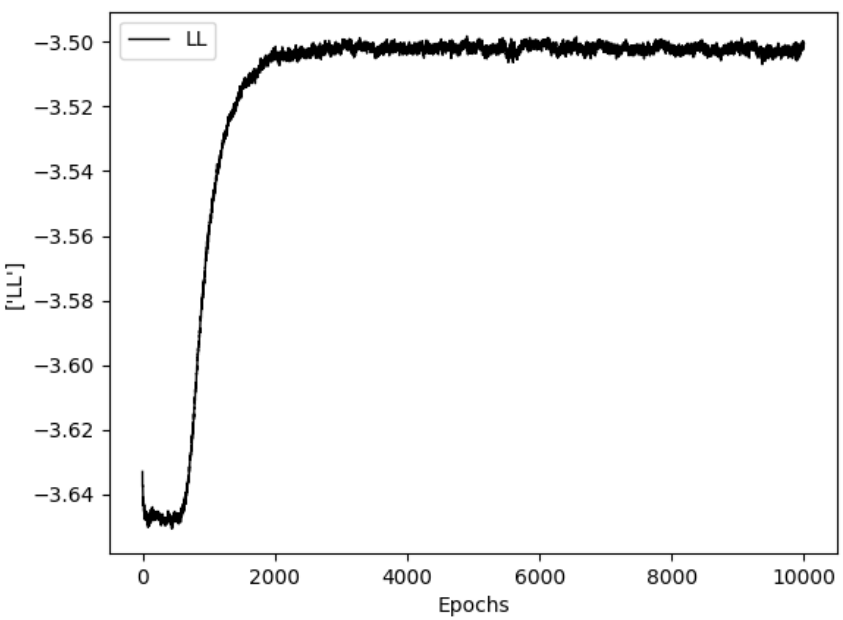


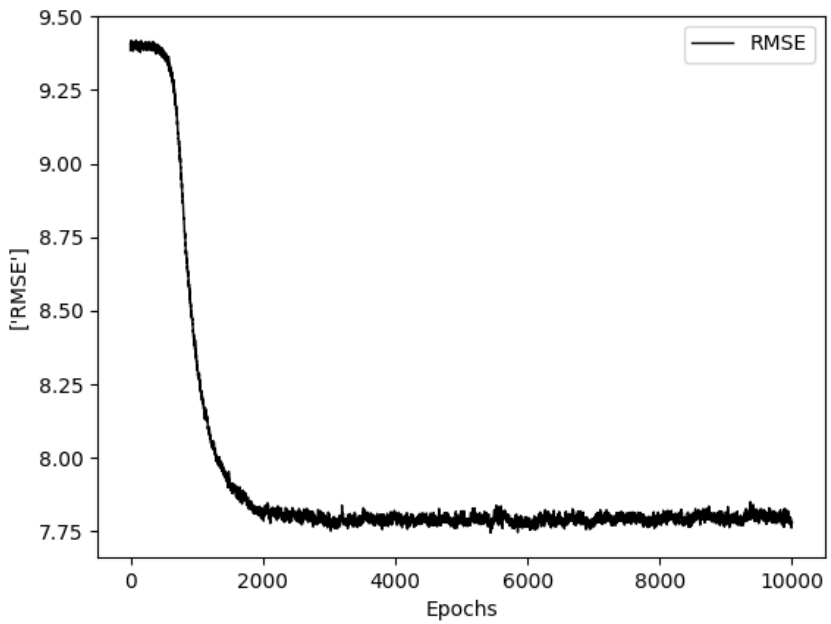
Left: μ *Right* : σ

Demo: BNN Regression

Predict Boston Housing data with Zhusuan

- Toy Dataset: Boston Housing Dataset from UCI ML Repository originally
- Input: 506 data points with 13 features
- Output: House price
- $W \sim N(0, 1)$
- Hidden layers: [32, 128, 32]

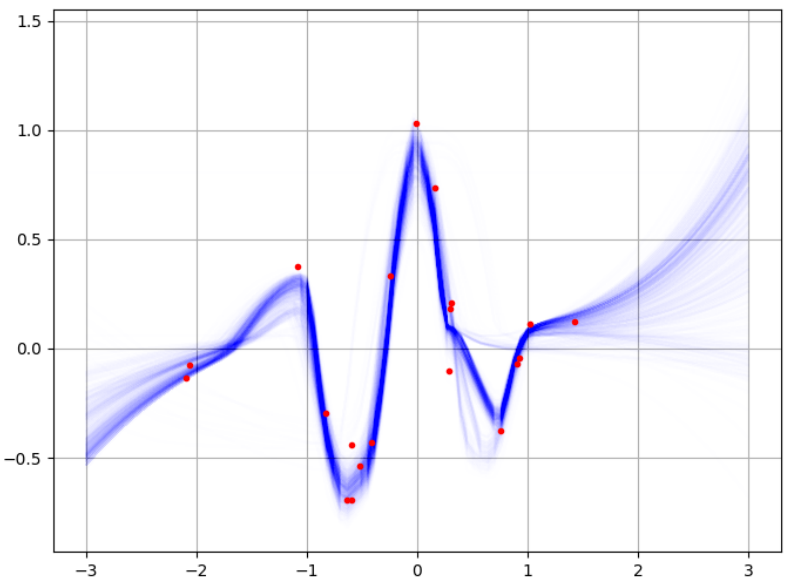


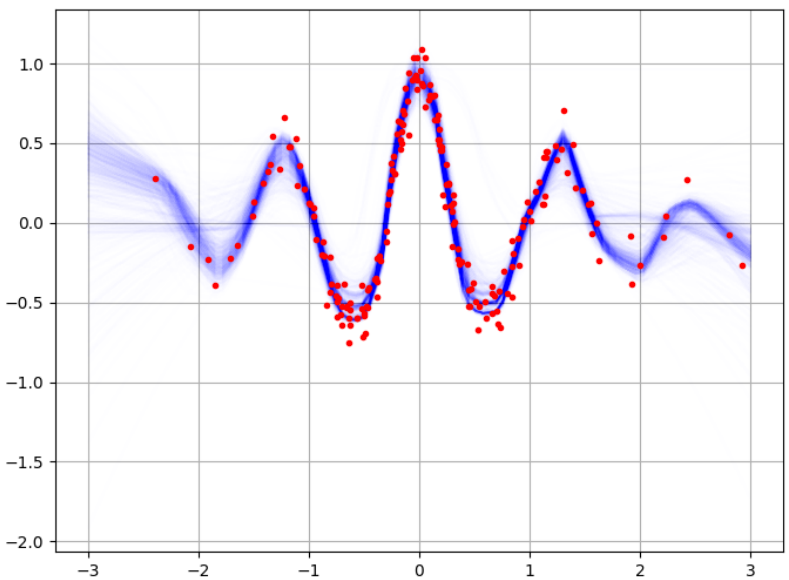


Demo:Dropout as Bayesian

Regression simple funtions with Tensorflow.distributions

- Implementation of Dropout as Bayesian
- Two hidden layers [100, 100]
- Data sampled from $N(\frac{cos(5x)}{|x|} + 1, 0.1)$
- Updated 1000 iterations





Left: 20 sample points Right: 200 sample points

Future Work

- The demo code is found online
- Computational Statistics knowledge
- Exploration

The End