Bayesian Neural Networks

General Principles

To model complex, non-linear relationships between variables, we can use multiple approaches including, splines, polynomials, gaussian processes, and neural networks. Here, we will focus on a Bayesian Neural Network (BNN). Think of a neural network as a highly flexible function made of interconnected layers of "neurons." Each connection between neurons has a *weight*, and each neuron has a *bias*. These *weights* and *biases* are like a vast set of adjustable knobs. In a standard network, the goal is to find the single best setting for all these knobs to map inputs to outputs. Unlike a standard neural network which learns a single set of optimal weights, a BNN learns distributions over its *weights* and *biases*. This allows it to capture not just the relationship in the data, but also its own uncertainty about that relationship. For this, we need to define:

1) **A Network Architecture**, which specifies the number of layers, the number of neurons in each layer, and the activation functions (e.g., ReLU, tanh) that introduce non-linearity. This defines the structure of our "knobs."

2) **Priors for Arrays of Weights and Biases**. In a simple model like linear regression, we define a prior for each individual parameter (e.g., one prior for the slope β). In a neural network, which can have thousands or millions of weights, we don't define a unique prior for every single one. Instead, we define a prior that acts as a template for an entire **array of parameters**. For example, we might declare that all weights in a specific layer are drawn from the same `Normal(0, 1)` distribution. This allows us to efficiently specify our beliefs about the entire set of network parameters.

3) **An Output Distribution (Likelihood)**, which defines the probability of the data given the network's predictions. For a continuous variable (regression), this is often a Normal distribution with a variance term σ that quantifies the data's noise around the model's predictions.

Considerations

Caution

- Like all Bayesian models, BNNs consider model parameter uncertainty . The parameters here are the network's **weights (W)** and **biases (b)**. We quantify our uncertainty about them through their posterior distribution . Therefore, we must declare prior distributions for all *weights* and *biases*, as well as for the output variance σ.

- Unlike in a linear regression where the coefficient β has a direct interpretation (e.g., the effect of weight on height), the individual *weights* and *biases* in a BNN are not directly interpretable. A single *weight*'s influence is entangled with thousands of other parameters through non-linear functions. Consequently, BNNs are best viewed as powerful **predictive tools** rather than explanatory ones. They excel at learning complex patterns and quantifying predictive uncertainty, but if the goal is to isolate and interpret the effect of a specific variable, a simpler model is often more appropriate.

- Prior distributions are built following these considerations:
  - As the data is typically scaled (see introduction), we can use a standard Normal distribution (mean 0, standard deviation 1) as a weakly-informative prior for all weights and biases. This acts as a form of regularization.
  - Since the output variance σ must be positive, we can use a positively-defined distribution, such as the Exponential or Half-Normal.

- BNNs can be used for both *regression* and *classification*. The final layer's activation and the chosen likelihood distribution depend on the task. For binary classification, a *sigmoid* activation is paired with a Bernoulli likelihood, which requires a link function (logit) to connect the linear output of the network to the probability space [0, 1]. For regression, the identity activation is often used with a Gaussian likelihood.

Example

Below is an example code snippet demonstrating a *Bayesian Neural Network* for regression using the Bayesian Inference (BI) package. Data consist of two continuous variables (height and weight), and the goal is to predict height from weight using a non-linear model.

Python

```python
from BI import bi
import json
import jax.numpy as jnp
import matplotlib.pyplot as plt

# Setup device------------------------------------------------
m = bi(platform='cpu')

# Import Data & Data Manipulation ------------------------------------------------

with open('BNN.json', 'r', encoding='utf-8') as file:
    # Load the JSON data into a Python dictionary
    data = json.load(file)
# X is already scaled
X = jnp.array(data['X']) # Note X shape = (N,2) where first column is the intercept and secon
Y = jnp.array(data['Y']) # Note Y shape = (N,1) where N is the number of observations

m.data_on_model = dict(X = X, Y = Y)
# Define model ------------------------------------------------
def model(X, Y,  D_H=5, D_Y=1):
    N, D_X = X.shape

    # First hidden layer: Transforms input to N × D_H (hidden units)
    w1 = m.bnn.layer_linear(
        X,
        dist=m.dist.normal(
            0, 1,  name='w1',shape=(D_X,D_H)
            ),
        activation='tanh'
        )

    # sample final layer of weights and neural network output
    # Final layer (z3) computes linear combination of second hidden layer
    w2 = m.bnn.layer_linear(
        X=w1,
        dist=m.dist.normal(0, 1,  name='w2',shape=(D_H,D_Y))
        )

    sigma = m.dist.exponential(1, name='sigma')
    m.dist.normal(w2, sigma, obs=Y,name='Y')

# Run mcmc ------------------------------------------------
m.fit(model, num_samples=500, progress_bar=False)   # Approximate posterior distributions fo

# Predictions from the model ------------------------------------------------
pred = m.sample(samples = 500)['Y']
pred = pred[..., 0]
mean_prediction = jnp.mean(pred, axis=0)
percentiles = jnp.percentile(pred, jnp.array([5.0, 95.0]), axis=0)
# make plots
fig, ax = plt.subplots(figsize=(8, 6), constrained_layout=True)
# plot training data
ax.plot(X[:, 1], Y[:, 0], "kx")
# plot 90% confidence level of predictions
ax.fill_between(
    X[:, 1], percentiles[0, :], percentiles[1, :], color="lightblue"
)
# plot mean prediction
ax.plot(X[:, 1], mean_prediction, "blue", ls="solid", lw=2.0)
ax.set(xlabel="X", ylabel="Y", title="Mean predictions with 90% CI")
```

```
jax.local_device_count 16
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```
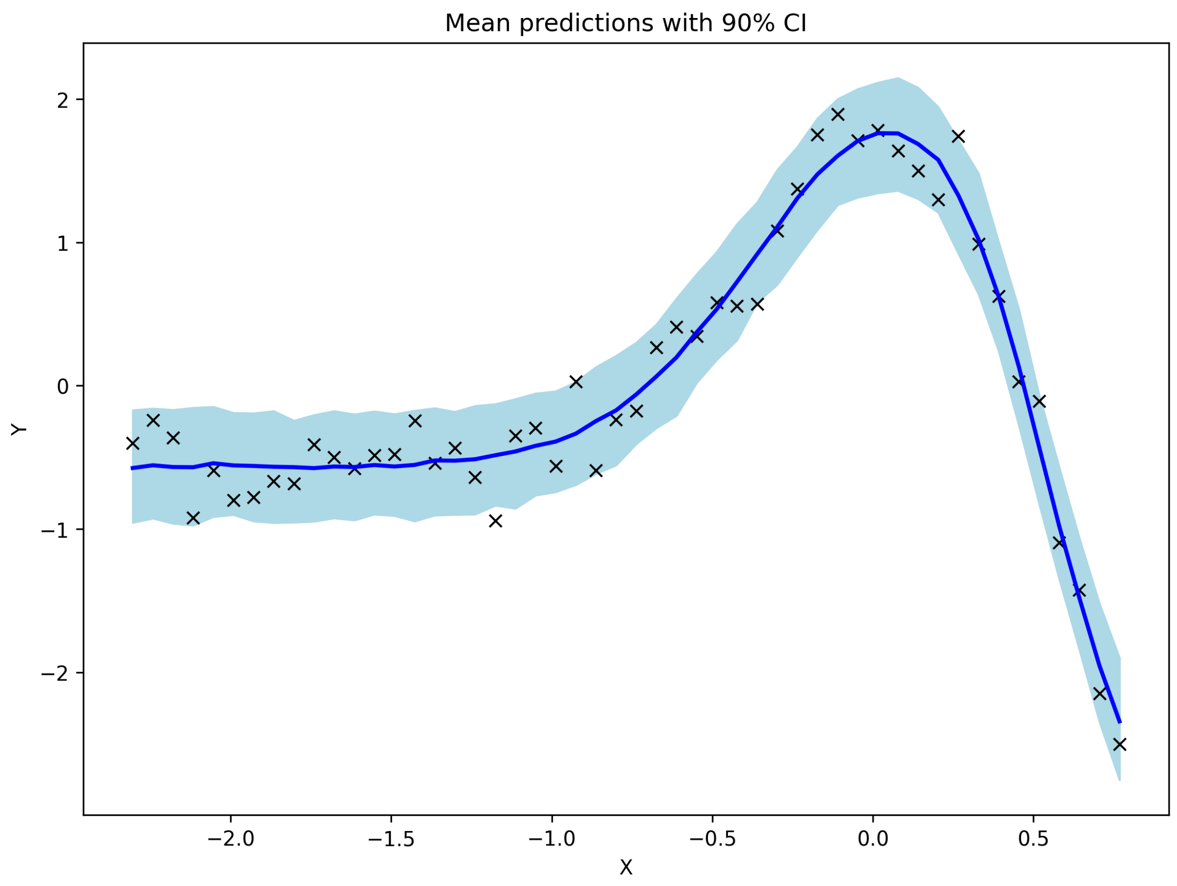

```
[Text(0.5, 0, 'X'),
 Text(0, 0.5, 'Y'),
 Text(0.5, 1.0, 'Mean predictions with 90% CI')]
```



R

```
library(BayesianInference)
m=importBI(platform='cpu')

# Load csv file
# Import data ---------------------------------------------------
path = normalizePath(paste(system.file(package = "BayesianInference"),"/data/BNN.json", sep =
data <- fromJSON(path)
m$data_on_model = list()
m$data_on_model$X = jnp$array(data$X)
m$data_on_model$Y = jnp$array(data$Y)

# Define model ------------------------------------------------
model <- function(X, Y, D_X = 2, D_H=5L, D_Y=1L){
  w1 <- m$bnn$layer_linear(X, dist=bi.dist.normal(0, 1,  name='w1',shape=c(D_X,D_H)), activa

  w2 <- m$bnn$layer_linear(
    w1,
    dist=bi.dist.normal(0, 1,  name='w2',shape=c(D_H,D_Y)),
    activation='tanh'
  )

  # Prior for the output standard deviation
  s = bi.dist.exponential(1, name = 's')

  # Likelihood
  bi.dist.normal(w2, s, obs = Y)
}

# Run mcmc ------------------------------------------------
m$fit(model) # Approximate posterior distributions
```

Mathematical Details

Notes

Note

- The primary difference between a *Frequentist* and *Bayesian* neural network lies in how parameters are treated. In the frequentist approach, weights and biases are point estimates found by minimizing a loss function (e.g., via gradient descent). Techniques like *Dropout* or *L2 regularization* are often used to prevent *overfitting*, which can be interpreted as approximations to a Bayesian treatment. In contrast, the *Bayesian* formulation does not seek a single best set of weights. Instead, it uses methods like MCMC or Variational Inference to approximate the entire posterior distribution for every *weight* and *bias*. This provides a principled and direct way to quantify model uncertainty.

- While present an example of non-linear regression, the Bayesian Neural Network can be used for linear regressions as well (keeping in mind that interpretation of the weights are impossible).

Reference(s)

(**neal1995bayesian?**)