

# BNN for Regression

## General Principles

To model complex, non-linear relationships between variables, we can utilize various approaches, including [splines](#), [polynomials](#), [Gaussian processes](#), and neural networks. Here, we focus on the *Bayesian Neural Network (BNN)*. Think of a neural network as a highly flexible function composed of interconnected layers of neurons . Each connection possesses a *weight*, and each neuron has a *bias*. These *weights* and *biases* act as a vast set of adjustable knobs. In a standard neural network, the goal is to find the single best setting for these knobs to map inputs to outputs. Conversely, a BNN learns **distributions** over its *weights* and *biases* rather than single optimal values. This allows the model to capture not only the patterns in the data but also its own uncertainty regarding those patterns.

To construct a *BNN*, we must define:

- 1) **A Network Architecture:** This specifies the structural design—the number of layers, the number of neurons per layer , and the activation functions (e.g., ReLU, tanh) that introduce non-linearity. This defines the arrangement of our “knobs.”
- 2) **Priors for Arrays of Weights and Biases:** In simple models like linear regression, we define a prior for each individual parameter (e.g., the slope  $\beta$ ). However, neural networks often contain thousands or millions of parameters, making it impractical to define a unique prior for each one. Instead, we define priors that act as templates for entire **arrays of parameters**. For instance, we might specify that all weights in a given layer are drawn from the same  $\text{Normal}(0, 1)$  distribution. This allows us to efficiently quantify our beliefs about the entire set of network parameters.
- 3) **An Output Distribution (Likelihood):** This defines the probability of the observed data given the network’s predictions. For continuous variables (regression), this is typically a *Normal distribution* with a variance term  $\sigma$ , which quantifies the noise of the data around the model’s predictions.

## Considerations

## Caution

- **Uncertainty:** Like all Bayesian models, BNNs explicitly account for model parameter uncertainty . Here, the parameters are the network’s **weights (W)** and **biases (b)**. We quantify uncertainty through their posterior distribution . Consequently, we must declare prior distributions for all *weights* and *biases*, as well as for the output variance  $\sigma$ .
- **Interpretation:** Unlike in a linear regression where the coefficient  $\beta$  has a direct interpretation (e.g., the change in  $Y$  given a unit increase in  $X$ ), the individual *weights* and *biases* in a *BNN* are not directly interpretable. A single weight’s influence is entangled with thousands of others through non-linear functions. Therefore, BNNs should be viewed as powerful **predictive tools** rather than explanatory ones. They excel at learning complex topologies and quantifying predictive uncertainty, but if the goal is to isolate 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  $\sigma$  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.
- **Computational Scalability:** Strictly applying Bayes’ theorem to update the posterior distribution becomes computationally intractable for very large neural networks. Calculating the model evidence (the denominator in Bayes’ rule) requires integrating over a parameter space that may contain millions of dimensions. Furthermore, the posterior landscape in deep networks is often highly non-convex and multimodal. Consequently, sampling algorithms (such as MCMC) may suffer from poor mixing or become “stuck” in local modes, failing to explore the full posterior. In such high-dimensional scenarios, practitioners often must rely on approximate methods, such as Variational Inference or Stochastic Gradient MCMC , to ensure convergence.

## Example

Below is an example code snippet demonstrating a *Bayesian Neural Network* for regression using the BayesForge (BF) package. Simulated data consist of two continuous variables ( $Y$  and  $X$ ), and the goal is to predict  $X$  from  $Y$  using a non-linear model.

## Python

```
from BayesForge import bf
import json
import jax.numpy as jnp
import matplotlib.pyplot as plt

# Setup device-----
m = bf(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 second column is the slope
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 x 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, progress_bar=False) # Approximate posterior distributions for weights, biases

# 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")

```

bf v 0.0.48 package loaded

E0526 16:16:42.940964 1061732 cuda\_dnn.cc:523] Loaded runtime CuDNN library: 9.1.0 but source  
E0526 16:16:42.946182 1061732 cuda\_dnn.cc:523] Loaded runtime CuDNN library: 9.1.0 but source

jax.local\_device\_count 32

This function is still in development. Use it with caution.  
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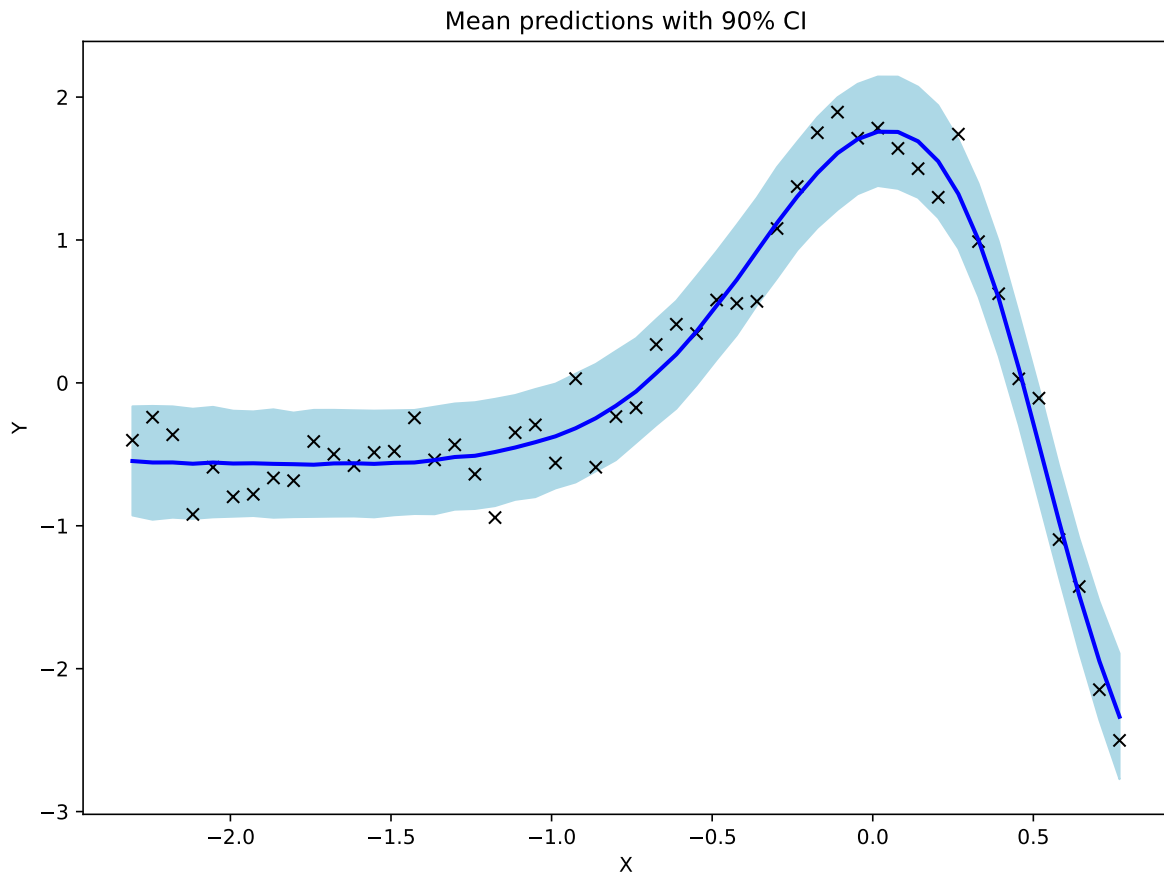
```
/home/sosa/work/BF/BayesForge/Main/main.py:674: UserWarning:
```

```
Sample's batch dimension size 4000 is different from the provided 500 num_samples argument. I
```

```
This function is still in development. Use it with caution.
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```
This function is still in development. Use it with caution.
```

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



**R**

```

library(BayesForge)
m=importBF(platform='cpu')

# Load csv file
# Import data -----
path = normalizePath(paste(system.file(package = "BayesForge"),"/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=bf.dist.normal(0, 1, name='w1',shape=c(D_X,D_H)), activation='tanh')

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

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

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

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

```

## Mathematical Details

In the Bayesian formulation, we place priors on all weights and biases and define a likelihood for the output. For a regression task with a  $K$ -hidden-layer BNN with  $J$  neurons per hidden layer and a  $D_X$ -vector of predictors and a  $D_Y$ -vector of outcomes we can run the model as below. For simplicity we consider a single hidden layer (as in the code example) with a hyperbolic tangent (tanh) activation function, mapped to a linear output layer. Because the input matrix  $X$  incorporates the intercept as its first column, the bias term is implicitly included in the layer's weights:

$$\begin{aligned}
Y_i &\sim \text{Normal}(\mu_i, \sigma) \\
H_i &= \tanh(X_i W_1) \\
\mu_i &= H_i W_2 \\
W_1 &\sim \text{Normal}(0, 1) \\
W_2 &\sim \text{Normal}(0, 1) \\
\sigma &\sim \text{Exponential}(1)
\end{aligned}$$

where:

- $Y_i$  is the observed outcome for the  $i$ -th observation.
- $\mu_i$  is the predicted mean output of the neural network for the  $i$ -th observation.
- $\sigma$  is the observation noise standard deviation.
- $X_i$  is the input row vector for the  $i$ -th observation, containing the intercept and the predictor variable. It has length  $D_X = 2$ .
- $H_i$  is the hidden layer representation vector for the  $i$ -th observation. It has length  $D_H = 5$ .
- $W_1$  is the weight matrix of the first hidden layer, with a shape of  $D_X \times D_H$  (i.e.,  $2 \times 5$ ).
- $W_2$  is the final layer weight matrix used to compute the linear combination of the hidden layer, with a shape of  $D_H \times D_Y$  (i.e.,  $5 \times 1$ ).
- All elements within the weight matrices  $W_1$  and  $W_2$  are assigned independent standard Normal priors.

## Notes

### **i** 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)

Phan, Pradhan, and Jankowiak (2019) [Bayesian Neural Networks](#) [Bayesian Neural Networks](#) [Numpyro Bayesian Neural Networks with Pyro](#)

Phan, Du, Neeraj Pradhan, and Martin Jankowiak. 2019. “Composable Effects for Flexible and Accelerated Probabilistic Programming in NumPyro.” *arXiv Preprint arXiv:1912.11554*.