BNN for Multiclass Classification

General Principles

Building upon the Binary Classification BNN, the **BNN Multiclass Classification** model can handle dependent variables with $K > 2$ discrete categories.

Instead of the final layer returning a single output, the final layer in a multiclass BNN returns a K-dimensional vector of scores (logits) for each observation. To transform these continuous scores into valid probabilities that sum to 1 across all K classes, we apply the **softmax** activation function. Finally, the categorized predictions are evaluated using a **Categorical** likelihood.

Considerations

> **Note**
>
> - **Output Layer Dimensions**: While binary classification network predictions can be compressed to a single output logit per observation, multiclass networks MUST output exactly K dimensions in their final layer, matching the number of target classes.
> - **The Softmax Simplex**: Applying the softmax function across the final layer's logits guarantees that the resulting outputs form a probability simplex . This is biologically similar to independent Poisson rates strictly normalizing to fixed categorical ratios.
> - **Likelihood Function**: After calculating the probabilities with softmax, we use a `Categorical` distribution as the final likelihood, matching the integer index of the observed category.
> - **Improved Calibration**: Multiclass BNNs greatly reduce out-of-distribution overconfidence. Standard deep learning cross-entropy models will often assign >99% probability to an unseen class purely due to the exponential nature of softmax. In a BNN, exploring the posterior width of the parameters yields "flat" unconfident probability profiles over K classes when the input is outside the training distribu-

tion.

Example

Below is an example code snippet demonstrating a *Bayesian Neural Network for multiclass classification* using the BayesForge (**BF**) package. This example generates a synthetic $K = 3$ cluster dataset.

Python

```python
from BayesForge import bf
import jax.numpy as jnp
import jax

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

# Generate Synthetic Data ------------------------------------
# 3 classes based on a random normal distribution split
key = jax.random.PRNGKey(42)
X = jax.random.normal(key, (300, 2))
# Rule: Q1=Class 0, Q2/Q3=Class 1, Q4=Class 2
Y = jnp.where(X[:, 0] > 0, jnp.where(X[:, 1] > 0, 0, 1), 2)

m.data_on_model = dict(X=X, Y=Y)

# Define model -----------------------------------------------
def model(X, Y, D_H1=5, K=3):
    N, D_X = X.shape

    # First hidden layer: 2 input features -> 5 hidden units
    w1 = m.bnn.layer_linear(
        X,
        dist=m.dist.normal(0, 1, name='w1_weight', shape=(D_X, D_H1)),
        activation='tanh'
    )

    # Final output layer: 5 hidden units -> K output units
    # Note: No activation is applied automatically inside the layer function here
    w2 = m.bnn.layer_linear(
```

```python
        w1,
        dist=m.dist.normal(0, 1, name='w2_weight', shape=(D_H1, K))
    )

    # Apply Softmax across the K dimension (axis=-1) to yield probabilities
    p = jax.nn.softmax(w2, axis=-1)

    # Categorical Likelihood matching indices in Y
    m.dist.categorical(probs=p, obs=Y)

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

# Predictions from the model ------------------------------------------------
import matplotlib.pyplot as plt

# Create a grid to evaluate the model
n_grid = 50
x0 = jnp.linspace(X[:, 0].min() - 0.5, X[:, 0].max() + 0.5, n_grid)
x1 = jnp.linspace(X[:, 1].min() - 0.5, X[:, 1].max() + 0.5, n_grid)
xx0, xx1 = jnp.meshgrid(x0, x1)
X_grid = jnp.c_[xx0.ravel(), xx1.ravel()]

# Swap data on model temporarily to predict on the grid
m.data_on_model = dict(X=X_grid, Y=jnp.zeros(X_grid.shape[0], dtype=jnp.int32))
pred = m.sample(data = m.data_on_model)['x']
p_mean = jnp.mean(pred, axis=0)

# Plotting the posterior predictive mean (categorical blending)
fig, ax = plt.subplots(figsize=(8, 6), constrained_layout=True)
contour = ax.contourf(xx0, xx1, p_mean.reshape(n_grid, n_grid), cmap="viridis", alpha=0.6)
scatter = ax.scatter(X[:, 0], X[:, 1], c=Y, cmap="viridis", edgecolors='k')
ax.set(title="Posterior Predictive Mean", xlabel="Feature 1", ylabel="Feature 2")
fig.colorbar(contour, ax=ax)
```

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bf v 0.0.48 package loaded
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Sample's batch dimension size 4000 is different from the provided 1 num_samples argument. De

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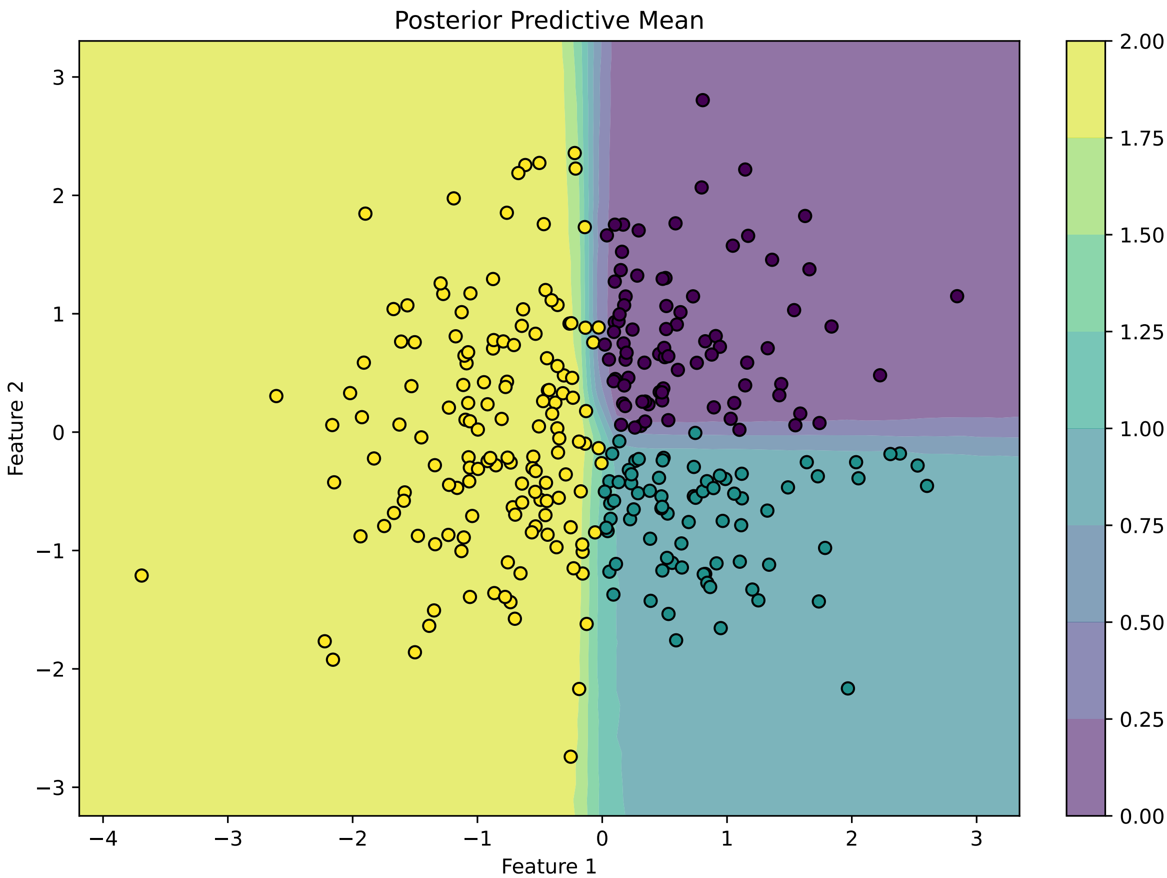
```



Julia

```
using BayesForge
using PythonCall

# Setup device-------------------------------------------------
m = importBF(platform="cpu")

# Generate Synthetic Data ------------------------------------
np = pyimport("numpy")
jax_random = pyimport("jax.random")
jnp = pyimport("jax.numpy")

key = jax_random.PRNGKey(42)
X = jax_random.normal(key, (300, 2))
```

```
# Simple rule to partition into K=3 classes
Y = jnp.where(X[:, 0] > 0, jnp.where(X[:, 1] > 0, 0, 1), 2)

m.data_on_model["X"] = X
m.data_on_model["Y"] = Y

# Define model ------------------------------------------------
@BF function model(X, Y)
    N, D_X = size(X)
    D_H1 = 5
    K = 3

    # First hidden layer
    w1 = m.bnn.layer_linear(
        X,
        dist=m.dist.normal(0, 1, name="w1_weight", shape=(D_X, D_H1)),
        activation="tanh"
    )

    # Final output layer
    w2 = m.bnn.layer_linear(
        w1,
        dist=m.dist.normal(0, 1, name="w2_weight", shape=(D_H1, K))
    )

    # Softmax conversion to probability simplex
    p = jax.nn.softmax(w2, axis=-1)

    # Categorical Likelihood
    m.dist.categorical(probs=p, obs=Y)
end

# Run mcmc ------------------------------------------------
m.fit(model, num_samples=500, progress_bar=false)
```

Mathematical Details

Bayesian Formulation

For a multiclass classification task spanning N observations and K mutually exclusive classes, we model the probability vector θ_i that the response $Y_i \in \{0, 1, ..., K-1\}$ falls into each respective class.

Using a single hidden layer with a hyperbolic tangent (tanh) activation function, the model is structured as:

$$
\begin{aligned}
Y_i &\sim \text{Categorical}(\theta_i) \\
\theta_i &= \text{Softmax}(\phi_i) \\
\phi_i &= H_i \Theta_2 \\
H_i &= \tanh(X_i \Theta_1) \\
\Theta_1 &\sim \text{Normal}(0, 1) \\
\Theta_2 &\sim \text{Normal}(0, 1)
\end{aligned}
$$

where:

- Y_i is the observed class index for the i-th observation ($Y_i \in \{0, 1, ..., K-1\}$).
- θ_i is the predicted probability vector for the i-th observation.
- ϕ_i are the K-dimensional logits.
- X_i is the input row vector for the i-th observation, with features length $D_X = 2$.
- H_i is the hidden layer representation vector for the i-th observation. It has length $D_H = 5$.
- Θ_1 is the weight matrix of the first hidden layer (2×5).
- Θ_2 is the final layer weight matrix mapping the hidden features to the logits for the $K = 3$ classes (5×3).
- All elements within the weight matrices Θ_1 and Θ_2 are assigned independent standard Normal priors.

Notes

> **Note**
>
> - For large outputs where $K > 100$, computing the exact softmax normalization scalar (the denominator term combining all exponentiated logits) can become computationally expensive over thousands of MCMC posterior evaluations.
> - Neural networks configured with a standard Cross-Entropy loss mapping to one-hot vectors conceptually perform exactly this sequence: dot product of final weights $\rightarrow$ Softmax $\rightarrow$ Categorical Likelihood.

Reference(s)

1. PyData Berlin 2025: Introduction to Stochastic Variational Inference with NumPyro