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 Bayesian Inference (**BI**) package. This example generates a synthetic $K = 3$ cluster dataset.

Python

```
from BI import bi
import jax.numpy as jnp
import jax

# Setup device--------------------------------------------------
m = bi(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(
```

```
        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)
```

```
/home/sosa/work/3.12venv/lib/python3.10/site-packages/tqdm/auto.py:21: TqdmWarning:

IProgress not found. Please update jupyter and ipywidgets. See https://ipywidgets.readthedocs

BI v 0.0.46 package loaded
jax.local_device_count 32
```

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Running chain 3:   0%|          | 0/2000 [00:01<?, ?it/s]

Running chain 2:   5%|         | 100/2000 [00:01<00:08, 232.10it/s]Running chain 0:   5%|
Running chain 1:   5%|         | 100/2000 [00:01<00:09, 210.75it/s]


Running chain 3:   5%|         | 100/2000 [00:01<00:09, 197.42it/s]Running chain 0:  10%|

Running chain 2:  10%|         | 200/2000 [00:02<00:09, 191.34it/s]


Running chain 3:  10%|         | 200/2000 [00:02<00:09, 186.39it/s]
Running chain 1:  10%|         | 200/2000 [00:02<00:11, 151.66it/s]Running chain 0:  15%|
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Running chain 3:  15%|          | 300/2000 [00:02<00:08, 196.52it/s]

Running chain 2:  15%|          | 300/2000 [00:02<00:08, 190.56it/s]
Running chain 1:  15%|          | 300/2000 [00:02<00:09, 180.84it/s]

Running chain 2:  20%|          | 400/2000 [00:02<00:07, 216.48it/s]Running chain 0:  20%|


Running chain 3:  20%|          | 400/2000 [00:03<00:07, 214.67it/s]
Running chain 1:  20%|          | 400/2000 [00:03<00:07, 203.58it/s]


Running chain 3:  25%|          | 500/2000 [00:03<00:06, 237.90it/s]Running chain 0:  25%|

Running chain 2:  25%|          | 500/2000 [00:03<00:07, 212.58it/s]
Running chain 1:  25%|          | 500/2000 [00:03<00:06, 222.40it/s]


Running chain 3:  30%|          | 600/2000 [00:03<00:05, 251.40it/s]Running chain 0:  30%|

Running chain 2:  30%|          | 600/2000 [00:03<00:06, 229.74it/s]
Running chain 1:  30%|          | 600/2000 [00:03<00:05, 241.48it/s]


Running chain 3:  35%|          | 700/2000 [00:04<00:04, 266.37it/s]

Running chain 2:  35%|          | 700/2000 [00:04<00:05, 252.78it/s]Running chain 0:  35%|
Running chain 1:  35%|          | 700/2000 [00:04<00:05, 259.14it/s]


Running chain 3:  40%|          | 800/2000 [00:04<00:04, 279.70it/s]

Running chain 2:  40%|          | 800/2000 [00:04<00:04, 276.93it/s]Running chain 0:  40%|
Running chain 1:  40%|          | 800/2000 [00:04<00:04, 270.11it/s]


Running chain 3:  45%|          | 900/2000 [00:04<00:03, 302.54it/s]
Running chain 1:  45%|          | 900/2000 [00:04<00:03, 312.69it/s]Running chain 0:  45%|

Running chain 2:  45%|          | 900/2000 [00:04<00:03, 278.49it/s]
```

```
Running chain 3:  50%|        | 1000/2000 [00:04<00:03, 295.72it/s]
Running chain 1:  50%|        | 1000/2000 [00:05<00:03, 299.00it/s]Running chain 0:  50%|

Running chain 2:  50%|        | 1000/2000 [00:05<00:03, 260.21it/s]


Running chain 3:  55%|        | 1100/2000 [00:05<00:03, 283.07it/s]
Running chain 1:  55%|        | 1100/2000 [00:05<00:03, 271.76it/s]Running chain 0:  55%|


Running chain 3:  60%|        | 1200/2000 [00:05<00:02, 283.50it/s]

Running chain 2:  55%|        | 1100/2000 [00:05<00:03, 231.44it/s]
Running chain 1:  60%|        | 1200/2000 [00:05<00:03, 262.96it/s]Running chain 0:  60%|


Running chain 3:  65%|        | 1300/2000 [00:06<00:02, 284.19it/s]

Running chain 2:  60%|        | 1200/2000 [00:06<00:03, 226.25it/s]
Running chain 1:  65%|        | 1300/2000 [00:06<00:02, 266.98it/s]Running chain 0:  65%|


Running chain 3:  70%|        | 1400/2000 [00:06<00:02, 291.83it/s]

Running chain 2:  65%|        | 1300/2000 [00:06<00:03, 223.70it/s]
Running chain 1:  70%|        | 1400/2000 [00:06<00:02, 262.71it/s]


Running chain 3:  75%|        | 1500/2000 [00:06<00:01, 292.14it/s]Running chain 0:  70%|


Running chain 3:  80%|        | 1600/2000 [00:07<00:01, 286.14it/s]
Running chain 1:  75%|        | 1500/2000 [00:07<00:01, 261.98it/s]Running chain 0:  75%|

Running chain 2:  70%|        | 1400/2000 [00:07<00:02, 219.98it/s]


Running chain 3:  85%|        | 1700/2000 [00:07<00:01, 290.15it/s]
Running chain 1:  80%|        | 1600/2000 [00:07<00:01, 256.56it/s]Running chain 0:  80%|

Running chain 2:  75%|        | 1500/2000 [00:07<00:02, 217.02it/s]
```

```
Running chain 3:  90%|      | 1800/2000 [00:07<00:00, 292.58it/s]
Running chain 1:  85%|      | 1700/2000 [00:07<00:01, 252.27it/s]Running chain 0:  85%|


Running chain 3:  95%|     | 1900/2000 [00:08<00:00, 288.06it/s]

Running chain 2:  80%|      | 1600/2000 [00:08<00:01, 209.16it/s]
Running chain 1:  90%|      | 1800/2000 [00:08<00:00, 258.51it/s]Running chain 0:  90%|


Running chain 3: 100%|     | 2000/2000 [00:08<00:00, 297.91it/s]Running chain 3: 100%|      |


Running chain 2:  85%|      | 1700/2000 [00:08<00:01, 212.81it/s]Running chain 0:  95%|
Running chain 1:  95%|     | 1900/2000 [00:08<00:00, 257.39it/s]Running chain 0: 100%|      |


Running chain 2:  90%|      | 1800/2000 [00:09<00:00, 220.52it/s]
Running chain 1: 100%|     | 2000/2000 [00:09<00:00, 262.78it/s]Running chain 1: 100%|      |


Running chain 2:  95%|     | 1900/2000 [00:09<00:00, 213.67it/s]

Running chain 2: 100%|     | 2000/2000 [00:09<00:00, 216.46it/s]Running chain 2: 100%|      |
/home/sosa/work/BI/BI/Main/main.py:666: UserWarning:

Sample's batch dimension size 4000 is different from the provided 1 num_samples argument. De

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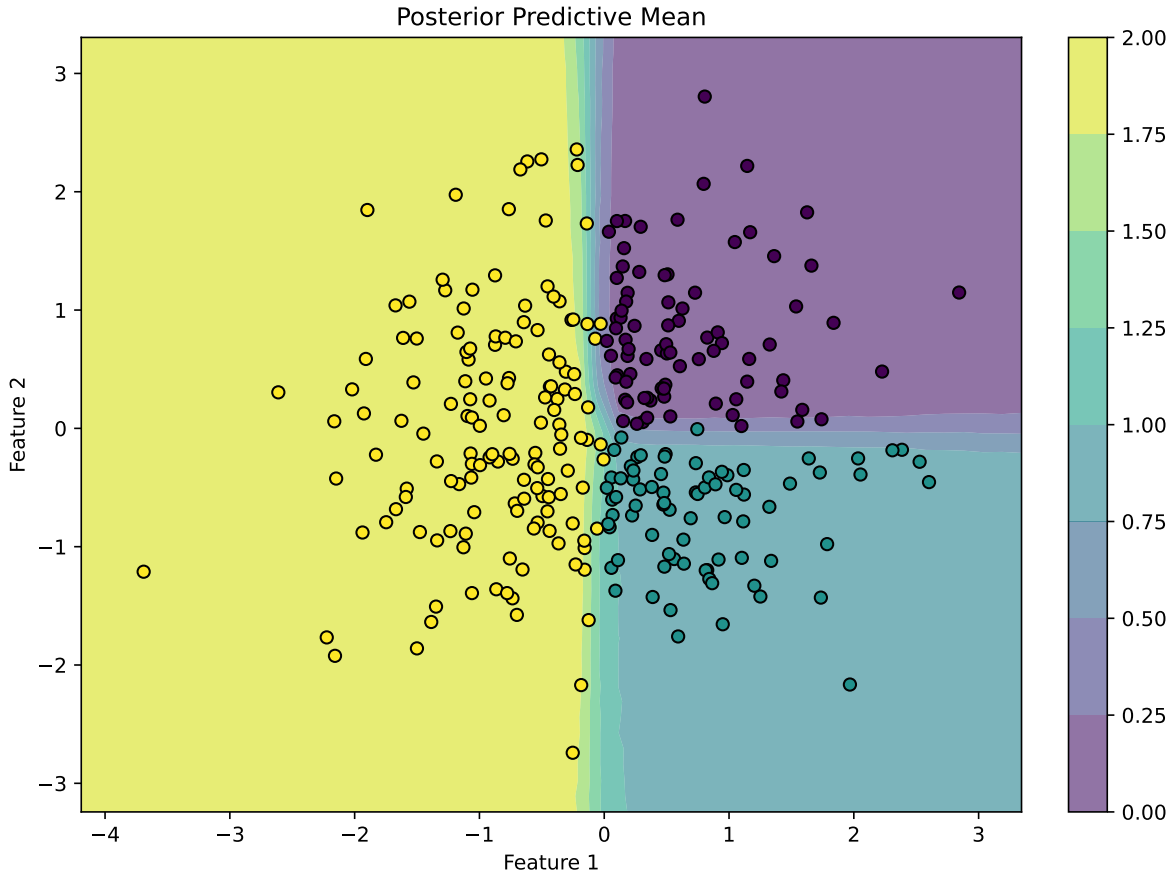
```



Julia

```julia
using BayesianInference
using PythonCall

# Setup device-----------------------------------------------
m = importBI(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 ------------------------------------------------
@BI 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