

# BNNs Hyperparameter Sampling: Comparing Gibbs vs. HMC (NUTS)

01/28/2021

Overview

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Prior Checks / Conformance

# Overview

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Three sampling techniques for parameters/hyperparameters:

- ▶ HMC (Centered Parametrization, NUTS for adaptation)
- ▶ HMC (Non-Centered Parametrization, NUTS for adaptation)
- ▶ FBM (Gibbs sampling for hyperparameters, HMC for all others)

## Centered vs. Non-Centered Parametrization

- ▶ Centered:

$$f(W|\mu, \tau) = \text{Normal}(\mu, \tau^{-0.5})$$

- ▶ Non-Centered:

$$W = \mu + \tau^{-0.5} W_{norm}, f(W_{norm}) = \text{Normal}(0, 1)$$

- ▶ Applies to all low-level weights and biases

# Global Assumptions

Architecture:

- ▶ 1 hidden layer, 8 hidden units
- ▶ tanh activation
- ▶ *parameter groups*: input-hidden weights, hidden-output weights, hidden biases, output bias
- ▶ variance of hidden-output weights scaled by number of units in hidden layer, to approach Gaussian Processes as number of units grows

Data:

- ▶ from FBM example
- ▶ input dimensions = 1, output dimensions = 1

Hyperparameter Priors (FBM Notation):

- ▶ input-hidden weights hyperparameter: 0.05:0.5
- ▶ hidden-output weights hyperparameter: 0.05:0.5
- ▶ hidden layer biases hyperparameter: 0.05:0.5
- ▶ output bias hyperparameter: 100

## Assumptions

Tuning Parameters for NUTS:

- ▶ adapt\_delta: 0.8 (default = 0.8)
- ▶ max\_treedepth: 10 (default = 10)
- ▶ adapt\_gamma: 0.05 (default = 0.05)

Initial Values:

- ▶ Weight Precision: 1
- ▶ Biases Precision: 1
- ▶ Target Noise Precision: 1
- ▶ Weights: 0
- ▶ Biases: 0

**4 separate chains** were used with the same initializations but different random seeds.

## Results

# Predictive Uncertainty

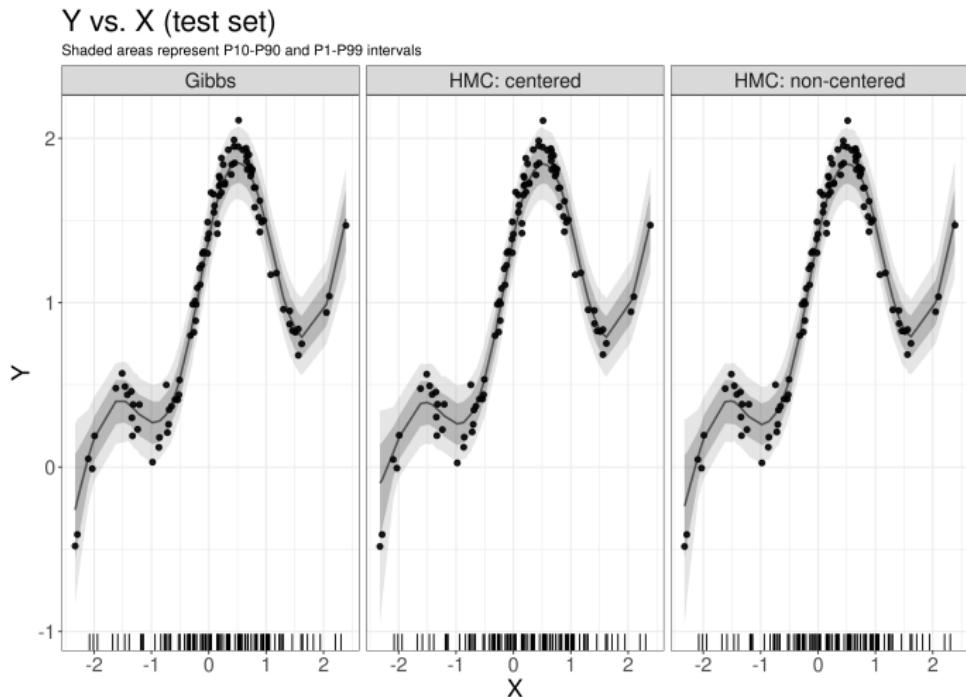


Figure 1: Predictive Quality

# Prediction Median

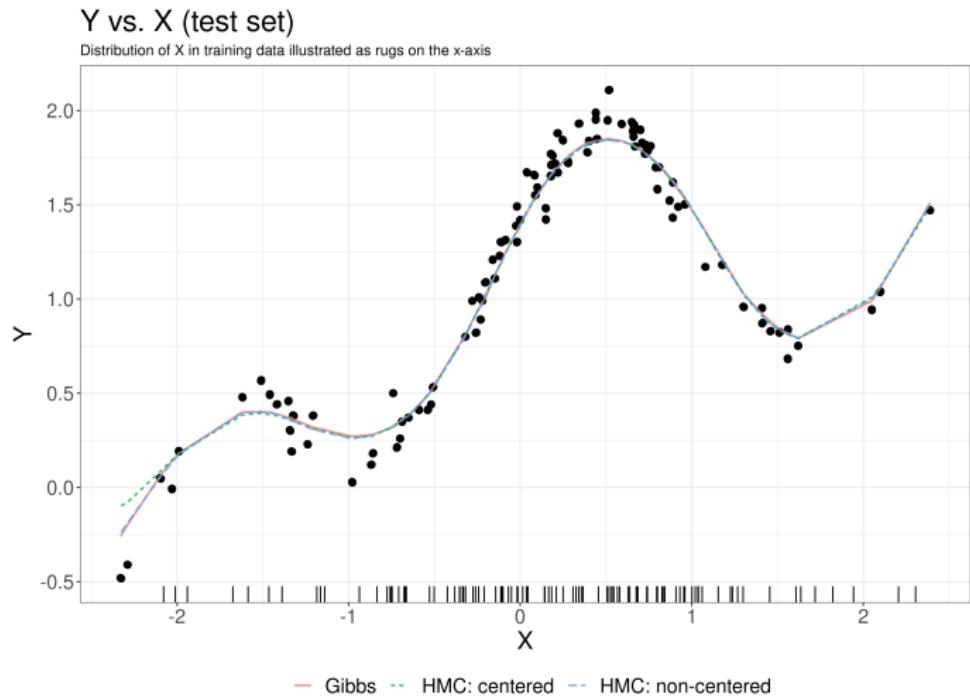


Figure 2: Predictive Median

# Hyperparameters: Measurement Noise - Standard Deviation

## Standard Deviation Hyperparameter: Target Noise

Vertical line indicates starting point of values used as representative samples. Four chains are used for consistent comparison.  
Every fifth sample shown.

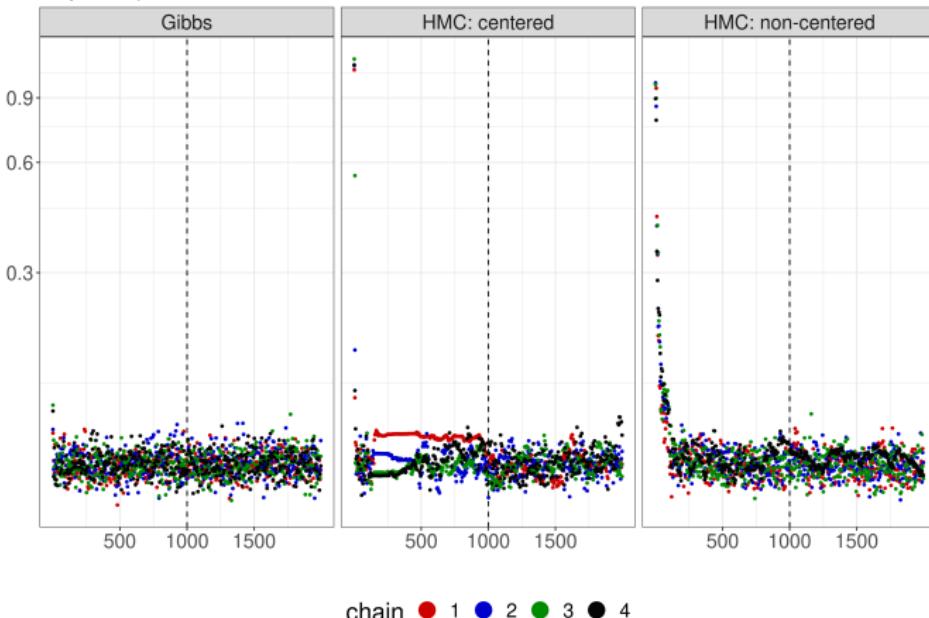


Figure 3: Target Noise Standard Deviation

# Hyperparameters: Inputs-to-Hidden Weights - Standard Deviation

## Standard Deviation Hyperparameter: Input-to-Hidden Weights

Vertical line indicates starting point of values used as representative samples. Four chains are used for consistent comparison.  
Every fifth sample shown.

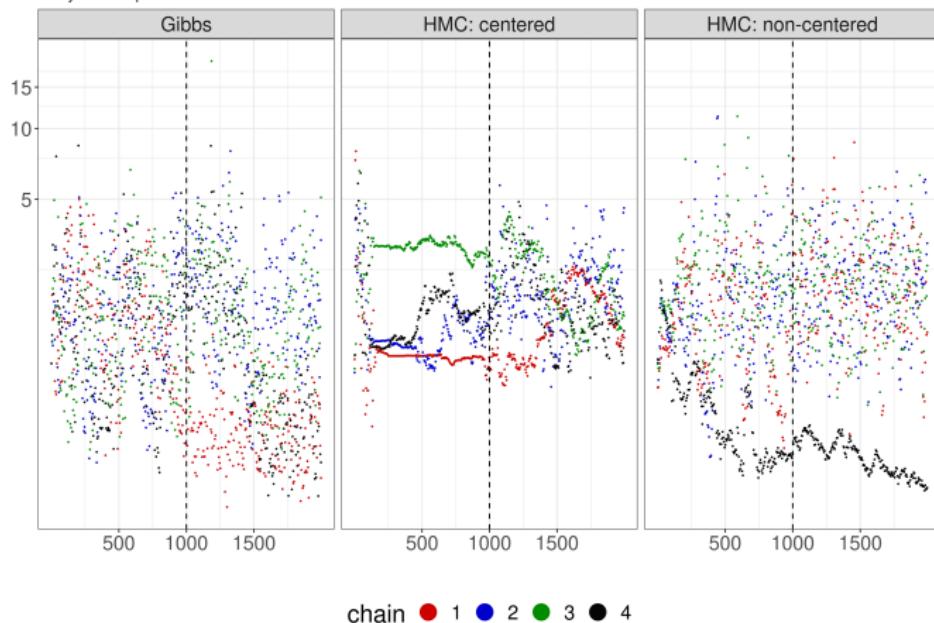


Figure 4: Inputs-to-Hidden Weights - Standard Deviation

# Hyperparameters: Hidden-to-Output Weights - Standard Deviation

## Standard Deviation Hyperparameter: Hidden-to-Output Weights

Vertical line indicates starting point of values used as representative samples. Four chains are used for consistent comparison. Every fifth sample shown.

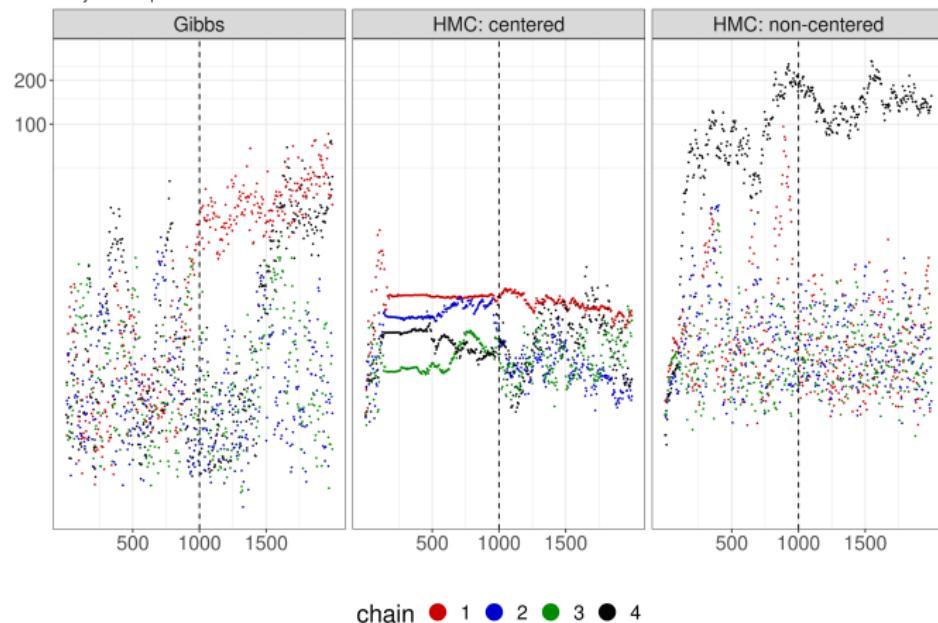


Figure 5: Hidden-to-Output Weights - Standard Deviation

# Hyperparameters: Hidden Unit Biases - Standard Deviation

## Standard Deviation Hyperparameter: Hidden Unit Biases

Vertical line indicates starting point of values used as representative samples. Four chains are used for consistent comparison.  
Every fifth sample shown.

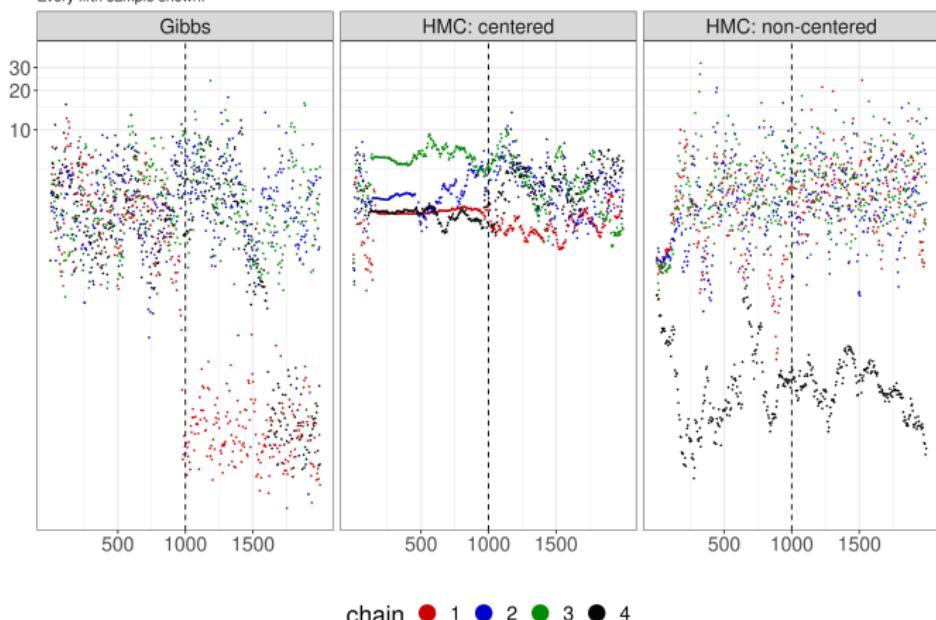


Figure 6: Hidden Unit Biases - Standard Deviation

# Parameters: Inputs-to-Hidden Weights

## Input-to-Hidden Weights

Vertical line indicates starting point of values used as representative samples. Four chains are used for consistent comparison.  
Every fifth sample shown.

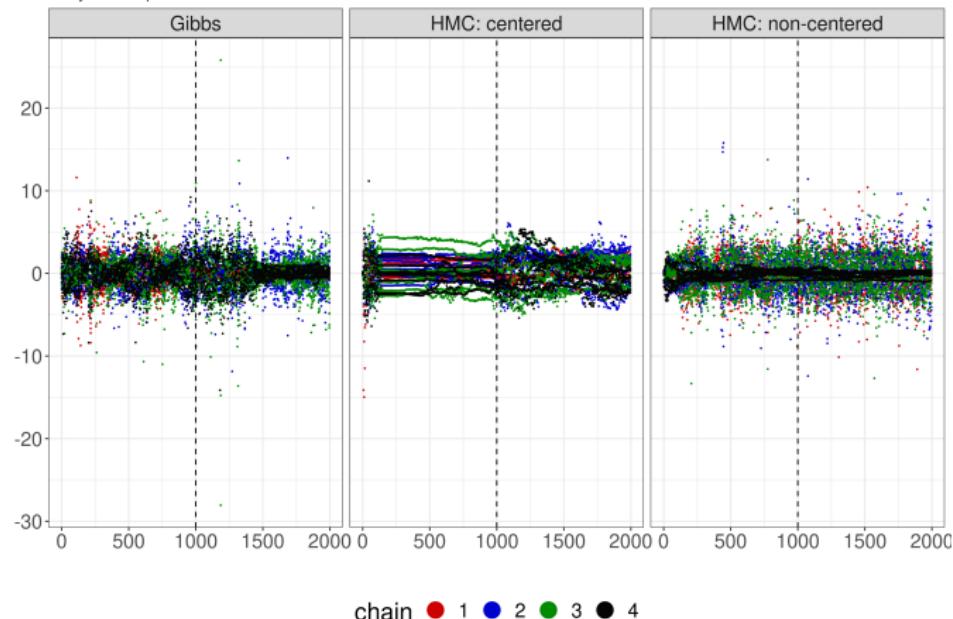


Figure 7: Inputs-to-Hidden Weights

# Parameters: Hidden-to-Output Weights

## Hidden-to-Output Unit Weights

Vertical line indicates starting point of values used as representative samples. Four chains are used for consistent comparison.  
Every fifth sample shown.

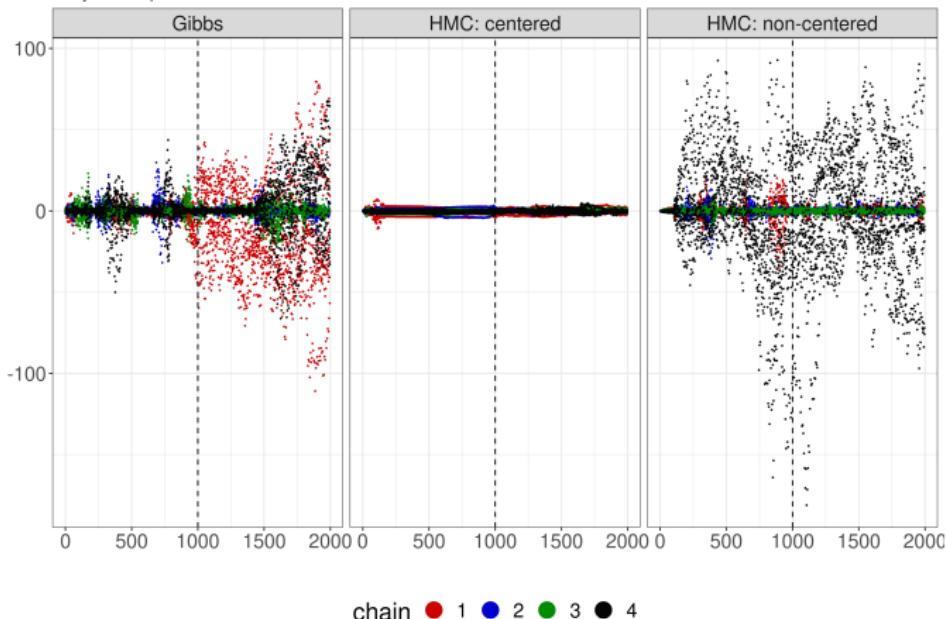


Figure 8: Hidden-to-Output Weights

# Parameters: Hidden Units Biases

## Hidden Unit Biases

Vertical line indicates starting point of values used as representative samples. Four chains are used for consistent comparison.  
Every fifth sample shown.

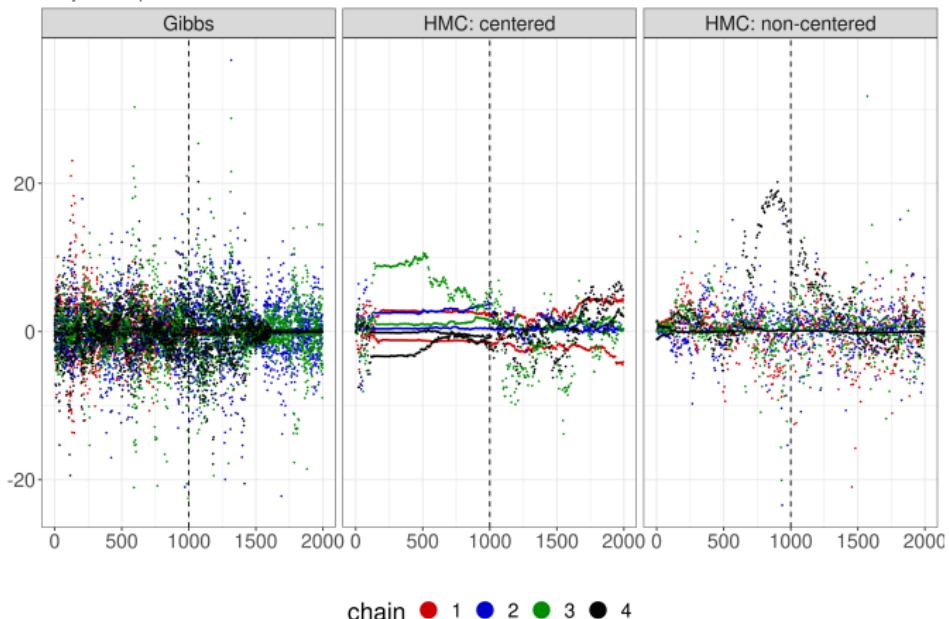


Figure 9: Hidden Units Biases

# Parameters: Output Unit Bias

## Output Unit Biases

Vertical line indicates starting point of values used as representative samples. Four chains are used for consistent comparison.  
Every fifth sample shown.

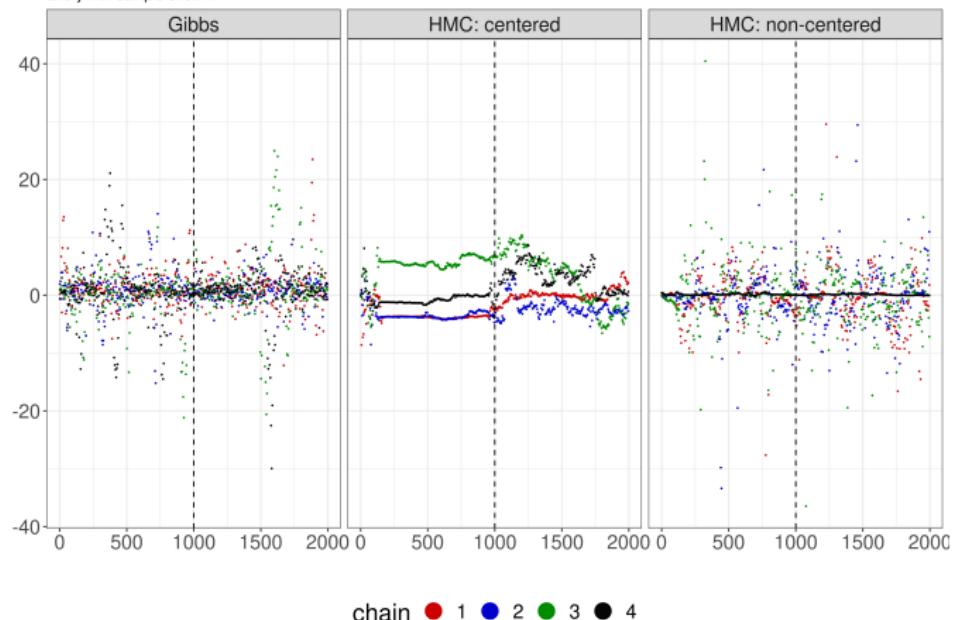


Figure 10: Output Unit Bias

# Stepsize Comparison

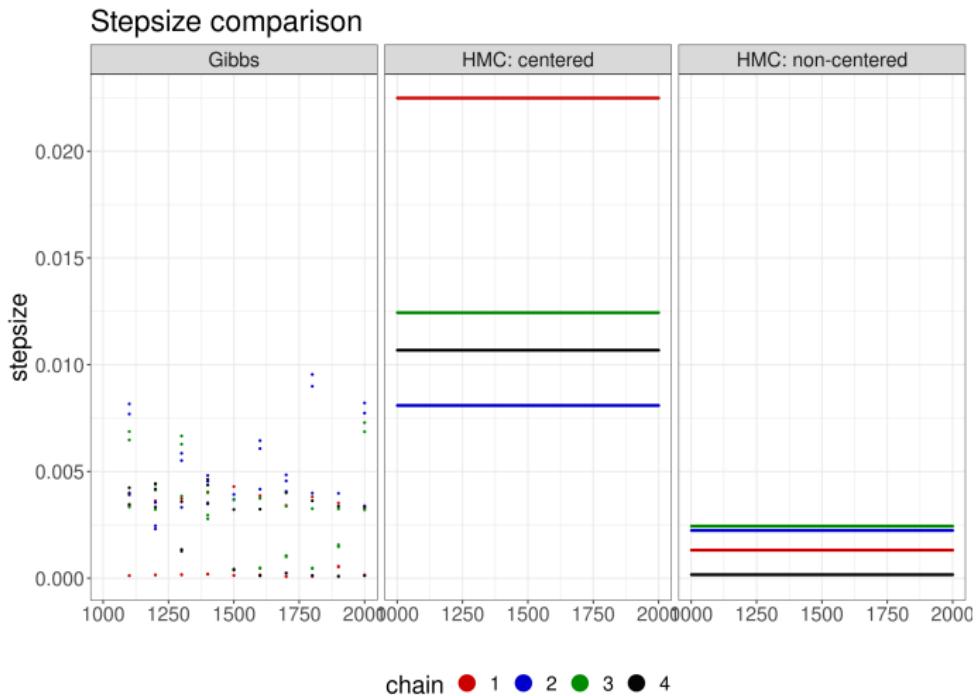


Figure 11: Step Size Comparison

## Prior Checks / Conformance

# Predictive Uncertainty

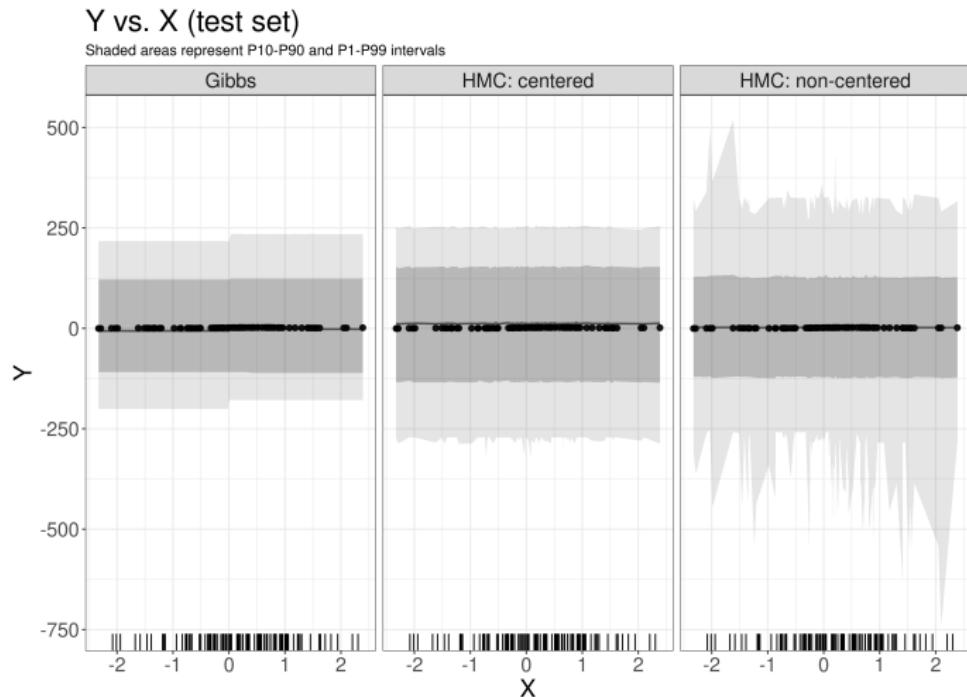


Figure 12: Predictive Quality

# Hyperparameters: Measurement Noise - Standard Deviation

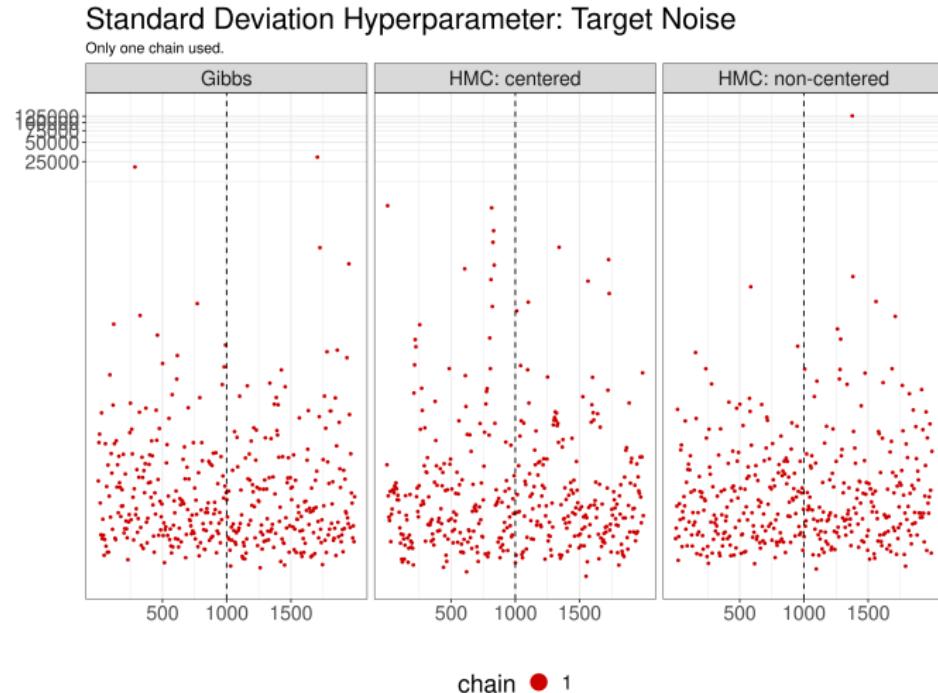


Figure 13: Target Noise Standard Deviation

# Hyperparameters: Inputs-to-Hidden Weights - Standard Deviation

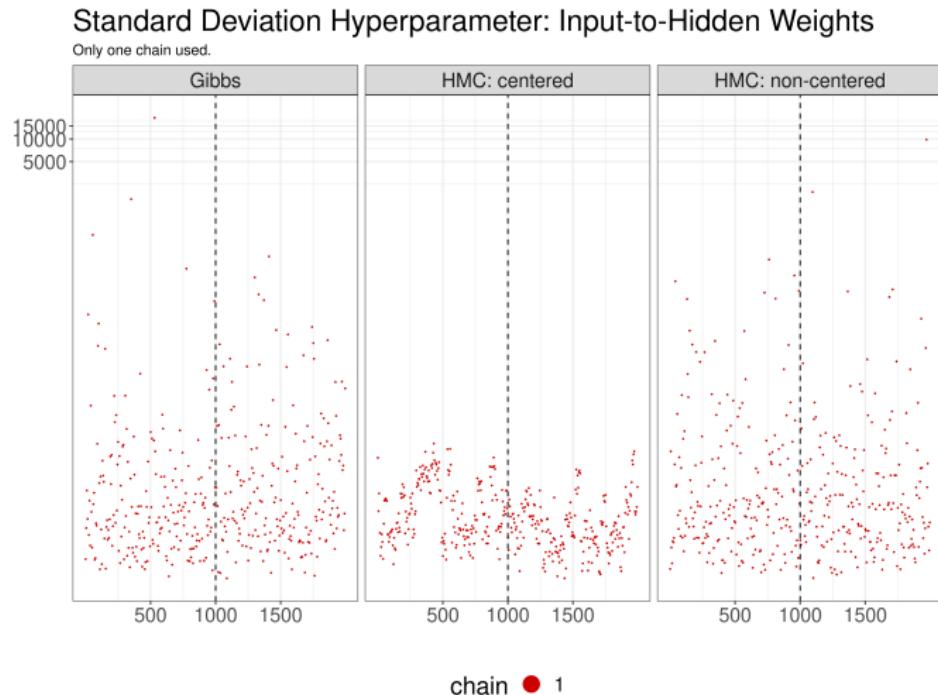


Figure 14: Inputs-to-Hidden Weights - Standard Deviation

# Hyperparameters: Hidden-to-Output Weights - Standard Deviation

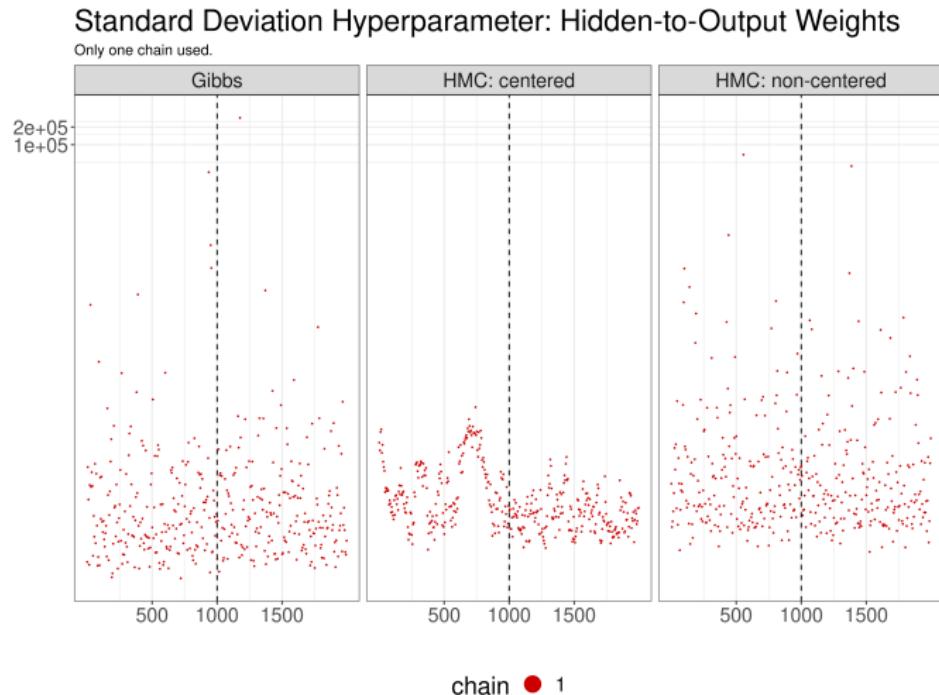


Figure 15: Hidden-to-Output Weights - Standard Deviation

# Hyperparameters: Hidden Unit Biases - Standard Deviation

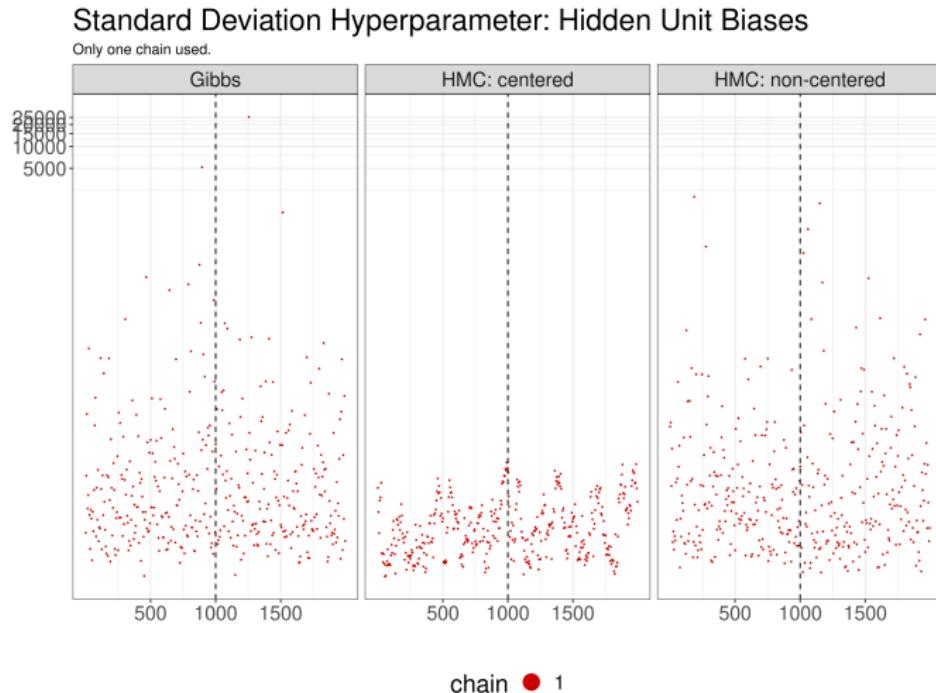


Figure 16: Hidden Unit Biases - Standard Deviation

# Parameters: Inputs-to-Hidden Weights

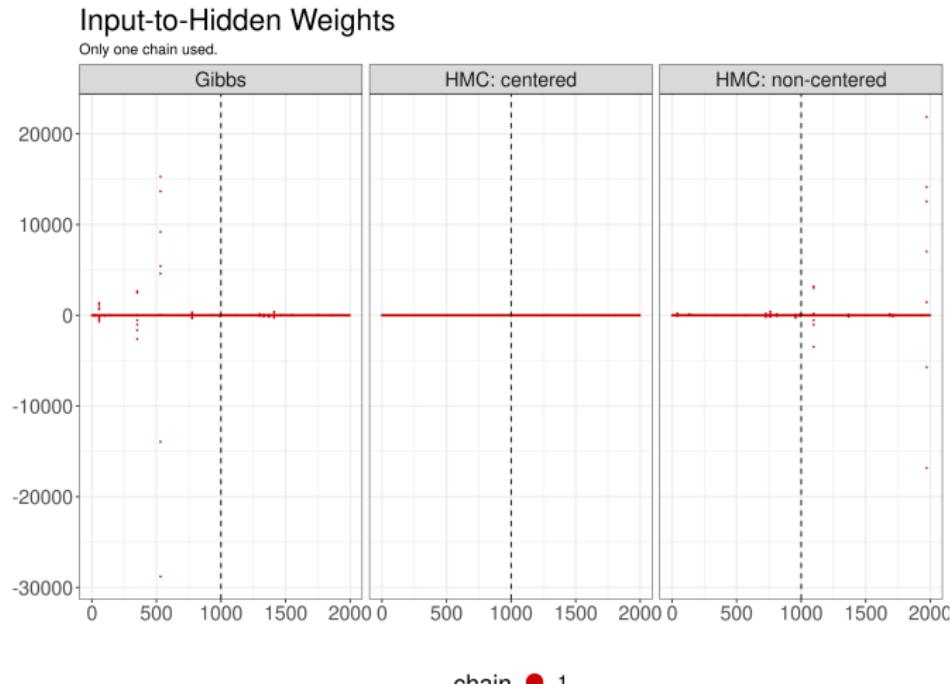


Figure 17: Inputs-to-Hidden Weights

# Parameters: Hidden-to-Output Weights

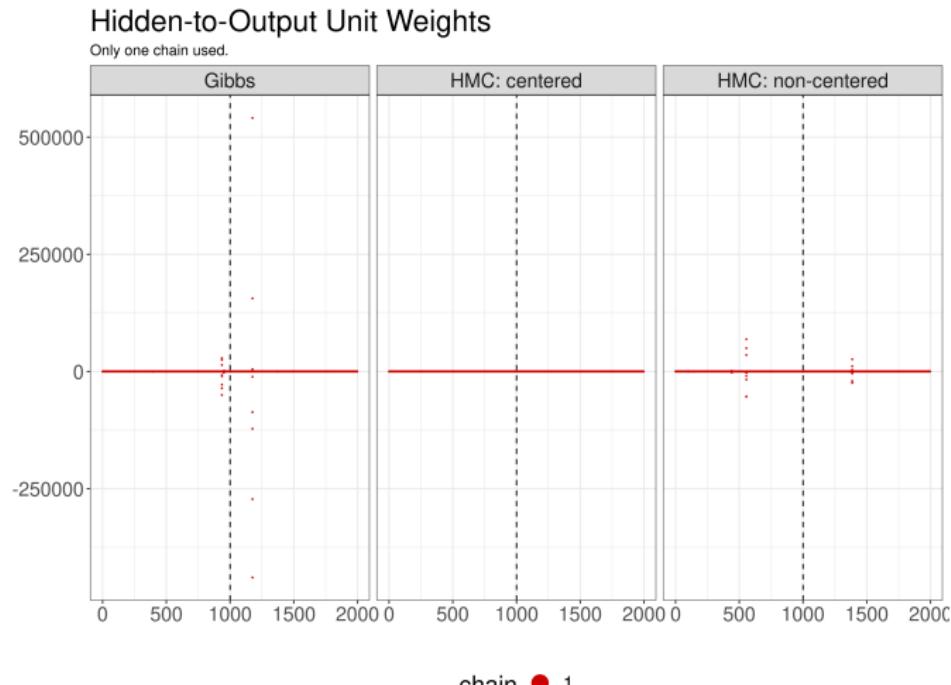


Figure 18: Hidden-to-Output Weights

# Parameters: Hidden Units Biases

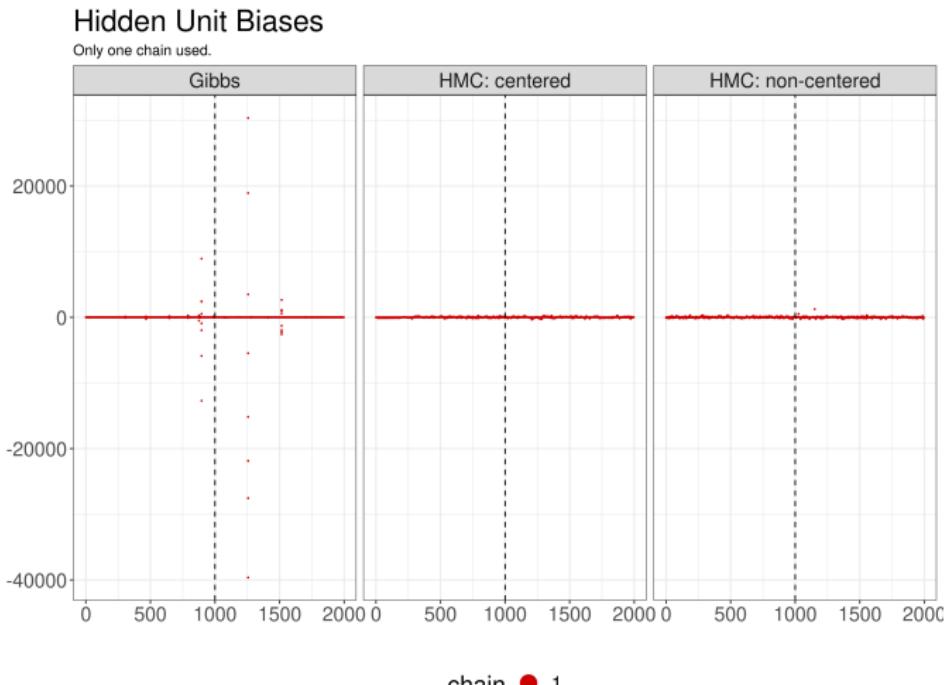


Figure 19: Hidden Units Biases

# Parameters: Output Unit Bias

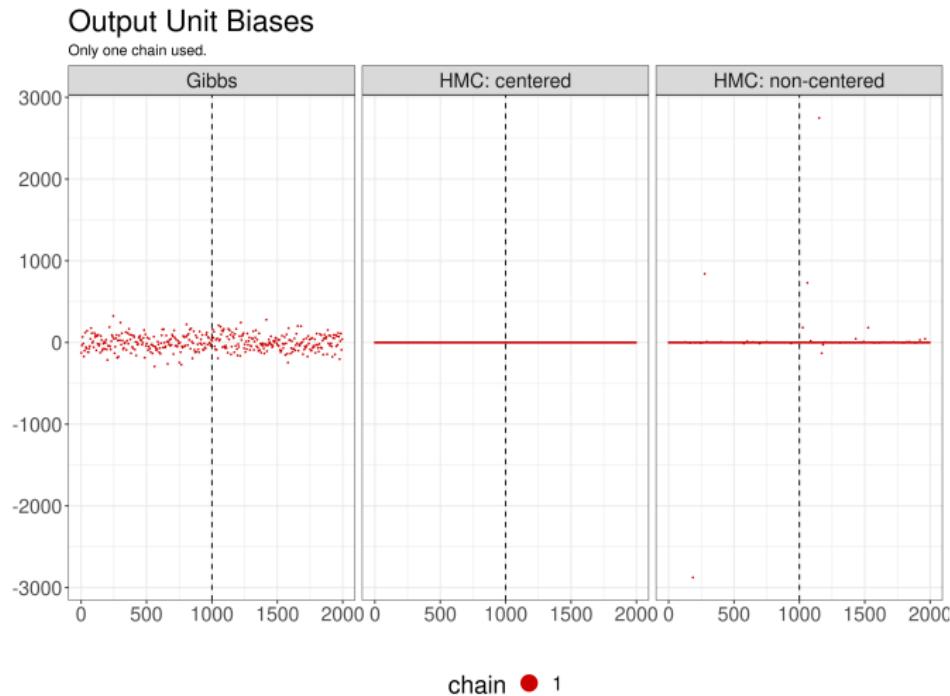


Figure 20: Output Unit Bias