

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

01/27/2021

Overview

Results

Prior Checks / Conformance

Overview

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Three sampling techniques:

- ▶ HMC (Centered Parametrization, NUTS)
- ▶ HMC (Non-Centered Parametrization, NUTS)
- ▶ 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

For comparison of results, only **one chain** was used.

Results

Predictive Uncertainty

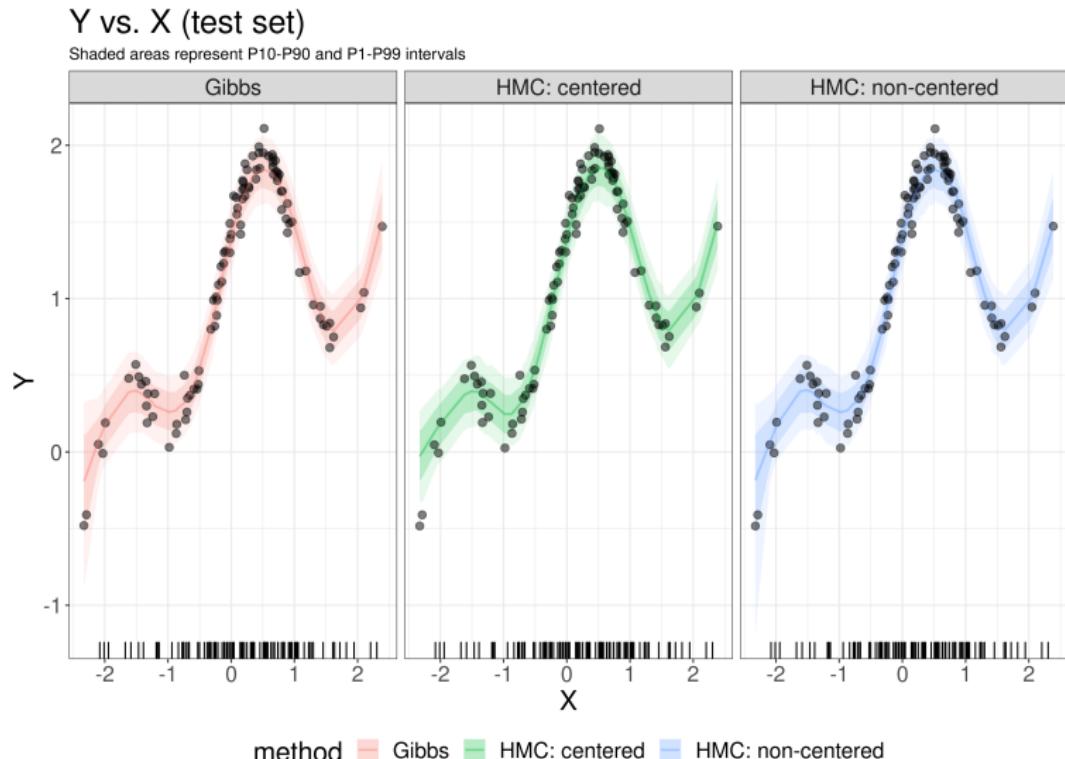


Figure 1: Predictive Quality

Prediction Median

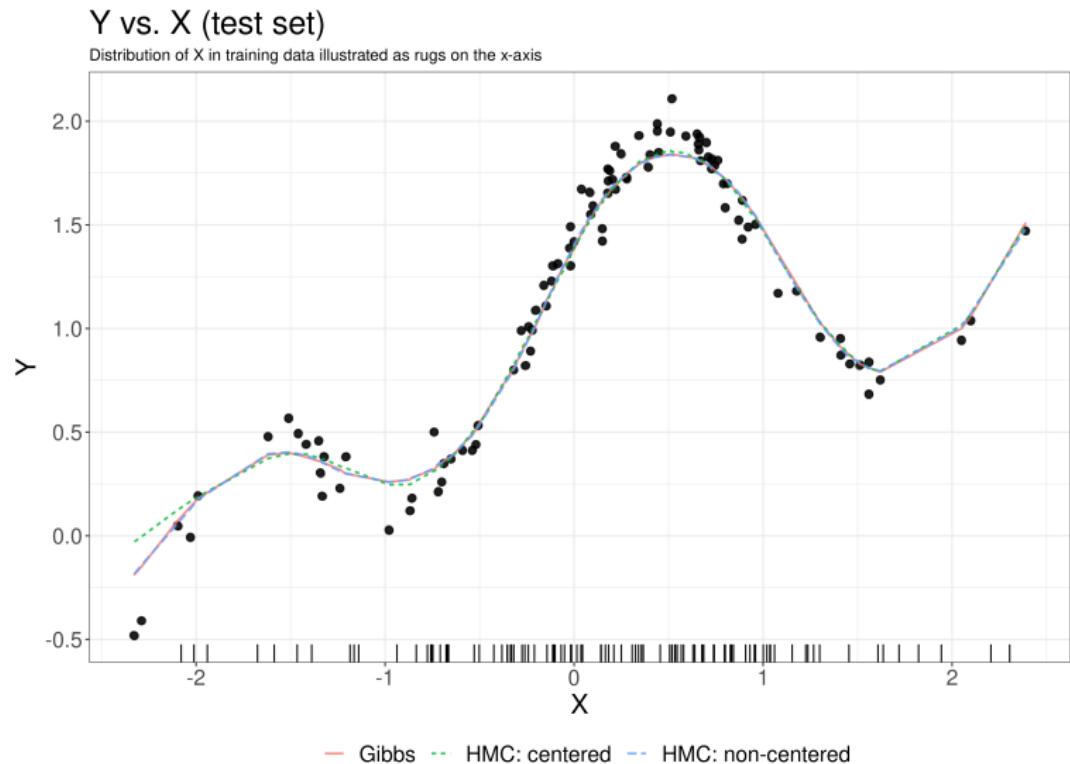


Figure 2: Predictive Quality

Hyperparameters: Measurement Noise - Precision

Target Noise: Precision Hyperparameter

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

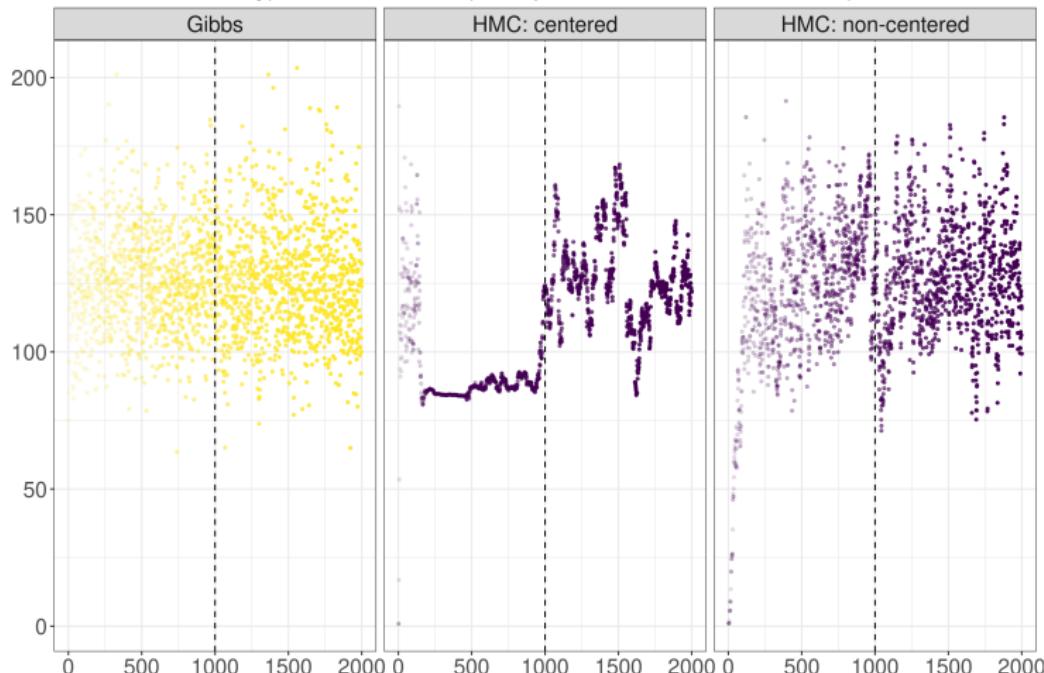


Figure 3: Target Noise Precision

Hyperparameters: Inputs-to-Hidden Weights - Precision

Input-to-Hidden Weights: Precision Hyperparameter

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

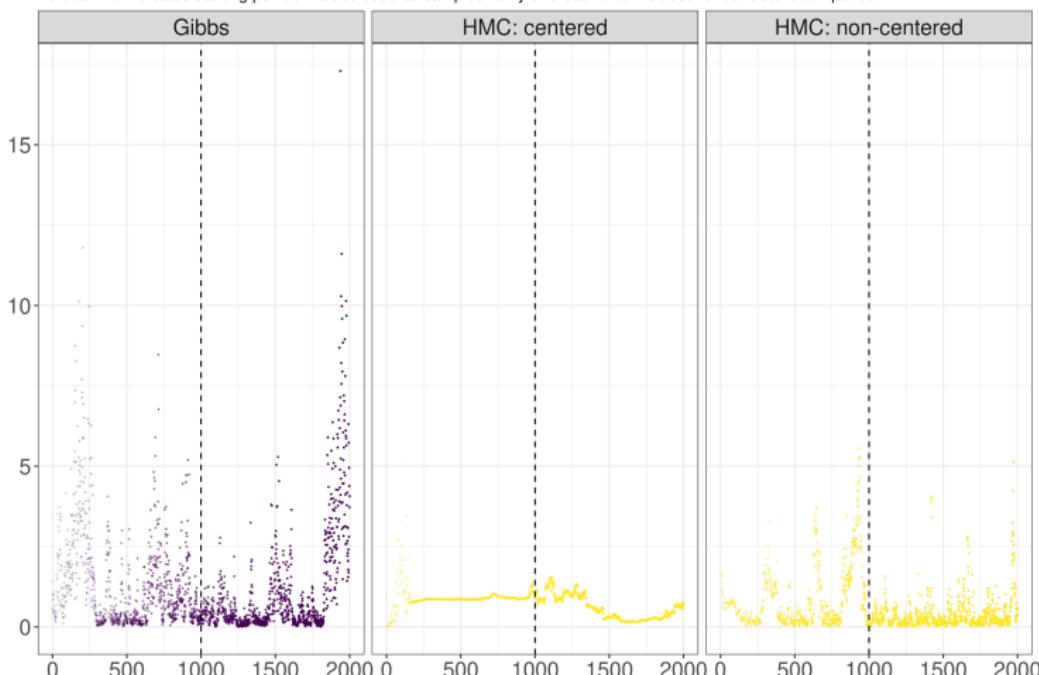


Figure 4: Inputs-to-Hidden Weights - Precision

Hyperparameters: Hidden-to-Output Weights - Precision

Hidden-to-Output Weights: Precision Hyperparameter

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

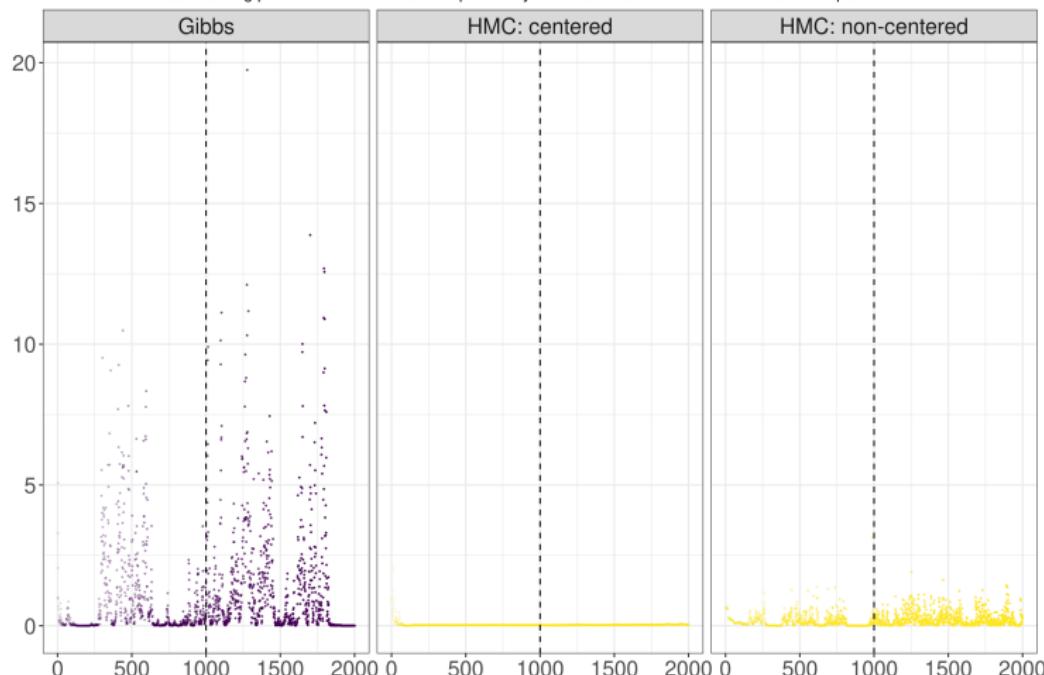


Figure 5: Hidden-to-Output Weights - Precision

Hyperparameters: Hidden Biases - Precision

Hidden Unit Biases: Precision Hyperparameter

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

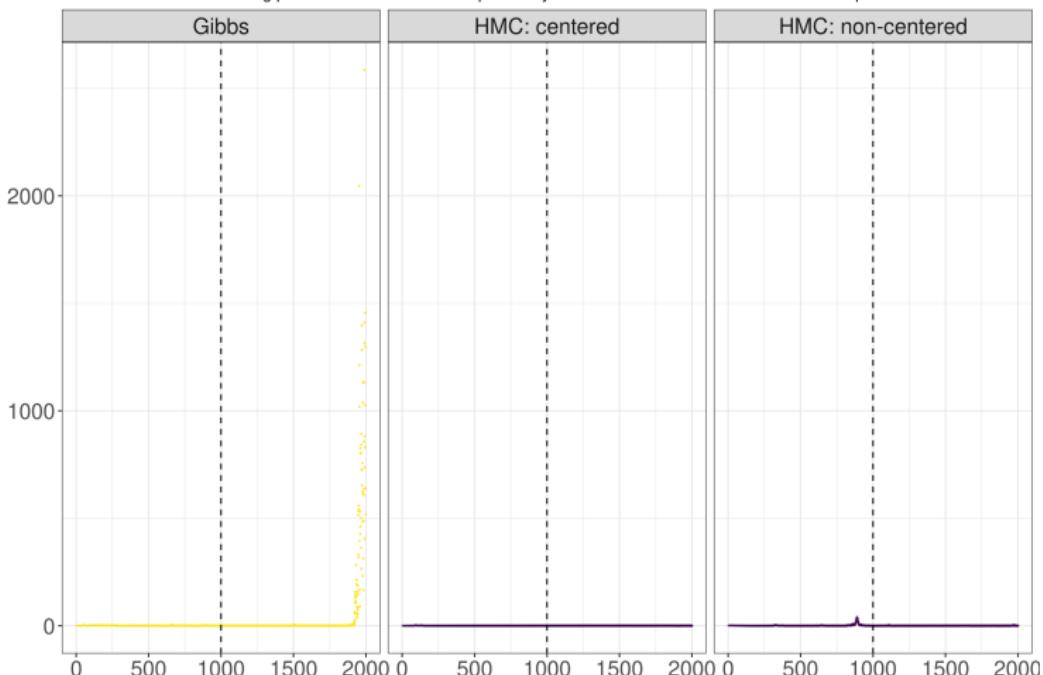


Figure 6: Hidden Biases - Precision

Parameters: Inputs-to-Hidden Weights

Input-to-Hidden Weights

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

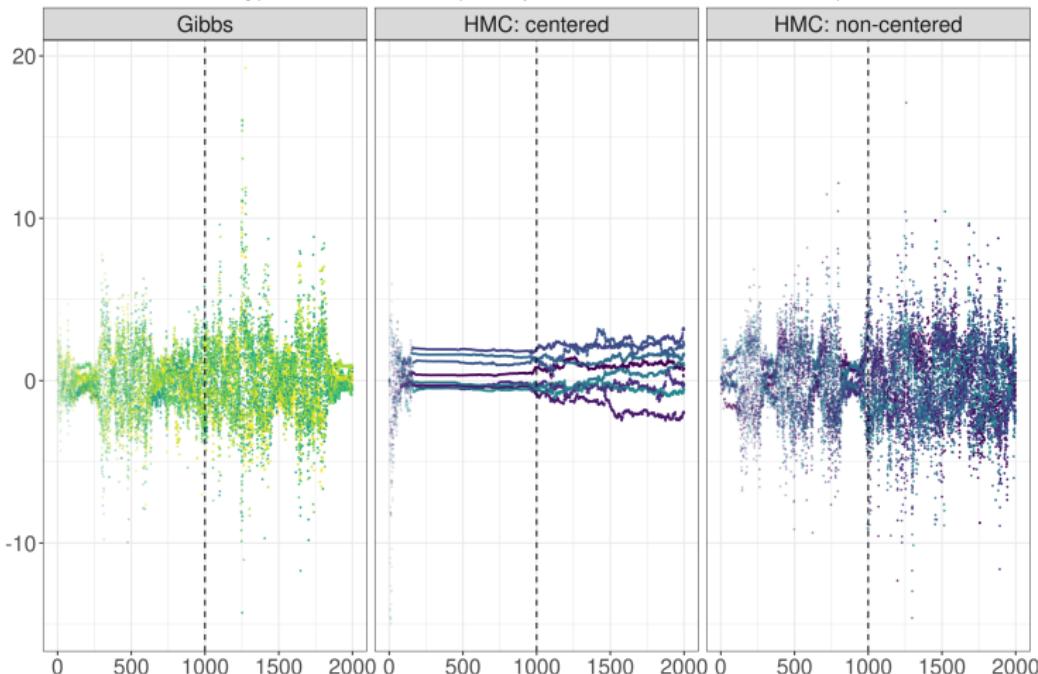


Figure 7: Inputs-to-Hidden Weights

Parameters: Hidden-to-Output Weights

Hidden-to-Output Unit Weights

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

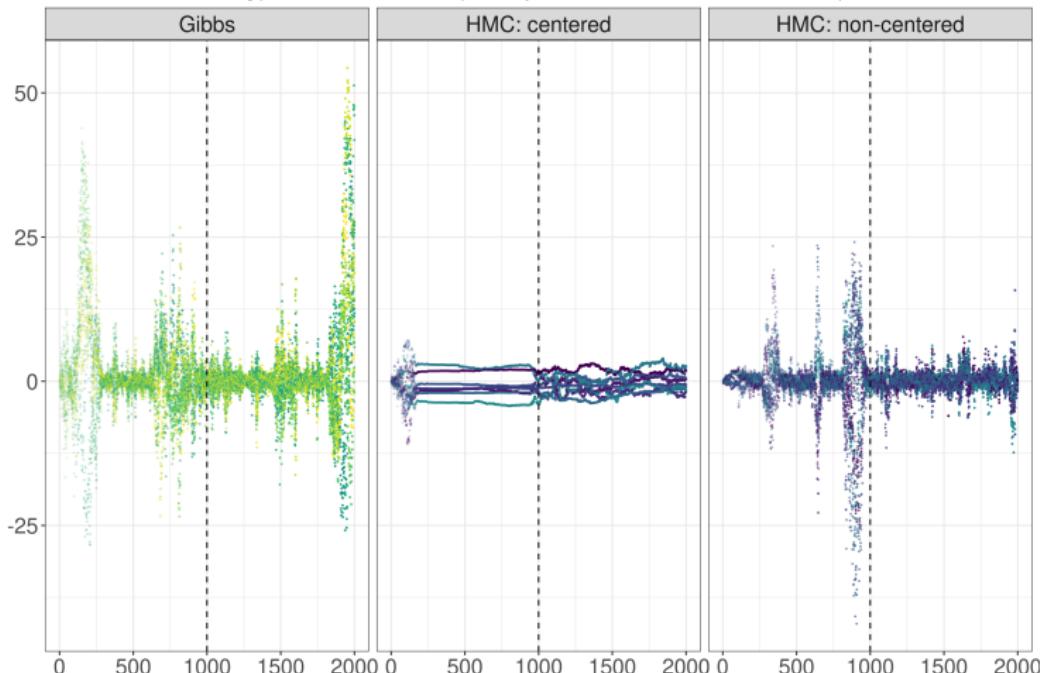


Figure 8: Hidden-to-Output Weights

Parameters: Hidden Unit Biases

Hidden Unit Biases

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

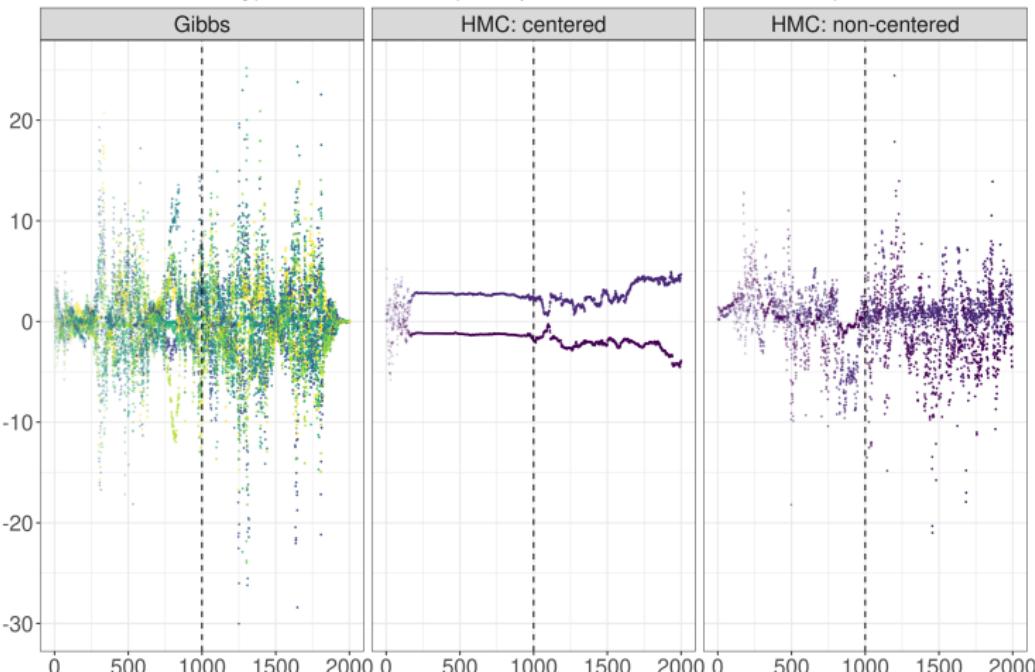


Figure 9: Hidden Unit Biases

Parameters: Output Unit Bias

Output Unit Biases

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

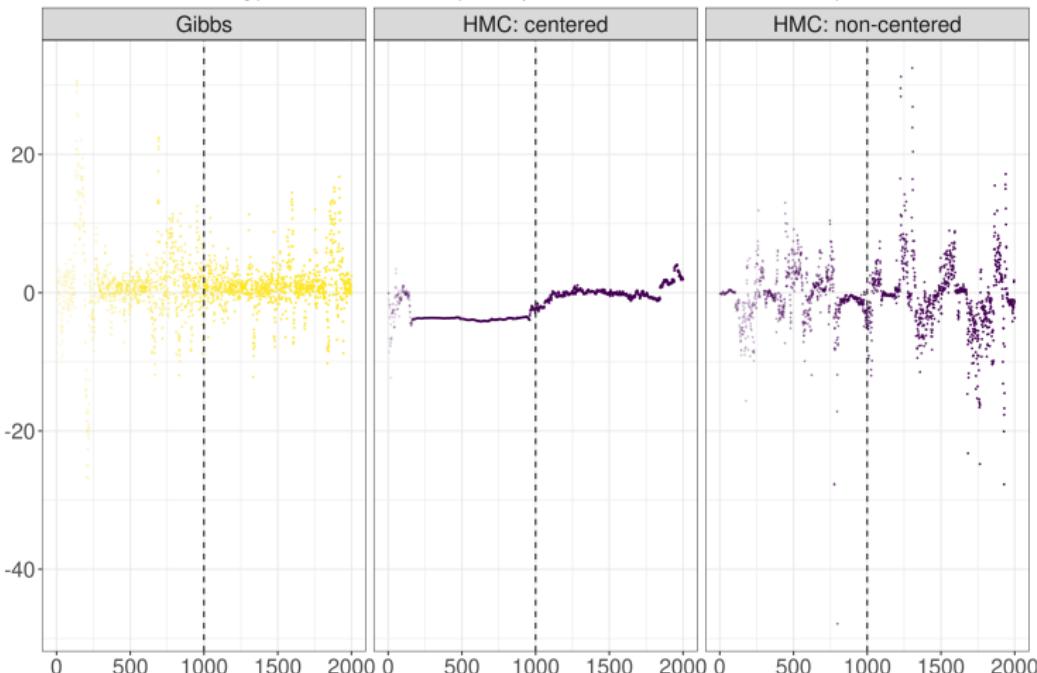


Figure 10: Output Unit Bias

Stepsize Comparison

Stepsize comparison

For HMC, all four chain's stepsizes are shown. For Gibbs, the different parameter group's step-sizes are shown.

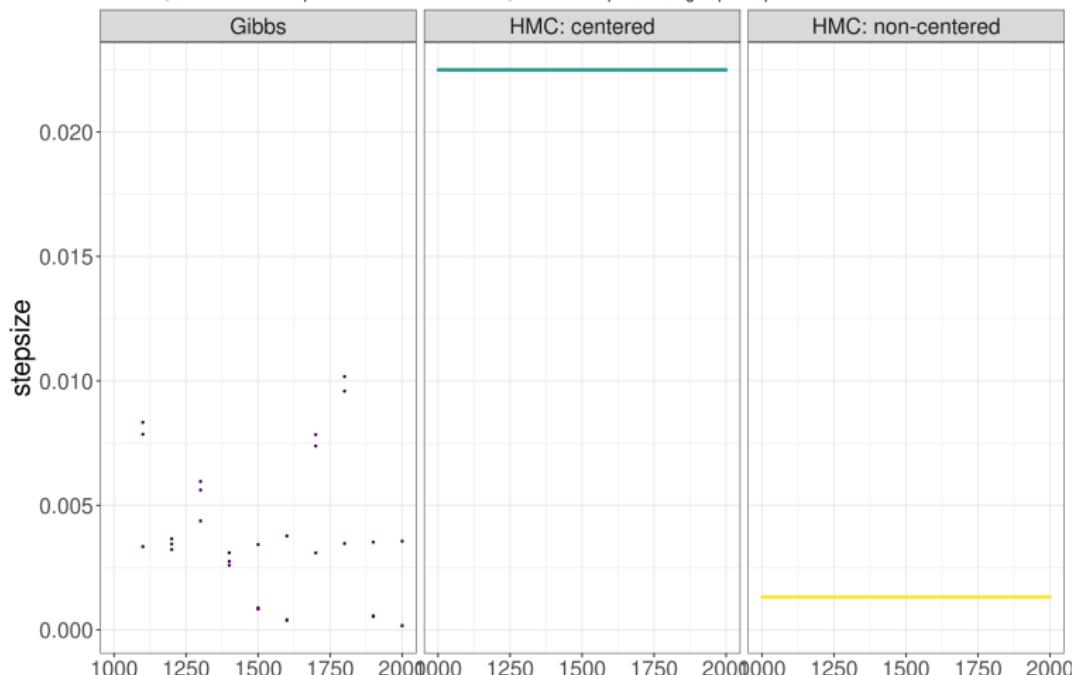


Figure 11: Output Unit Bias

Prior Checks / Conformance

Prior Checks

Y vs. X (test set)

Shaded areas represent P10-P90 and P1-P99 intervals

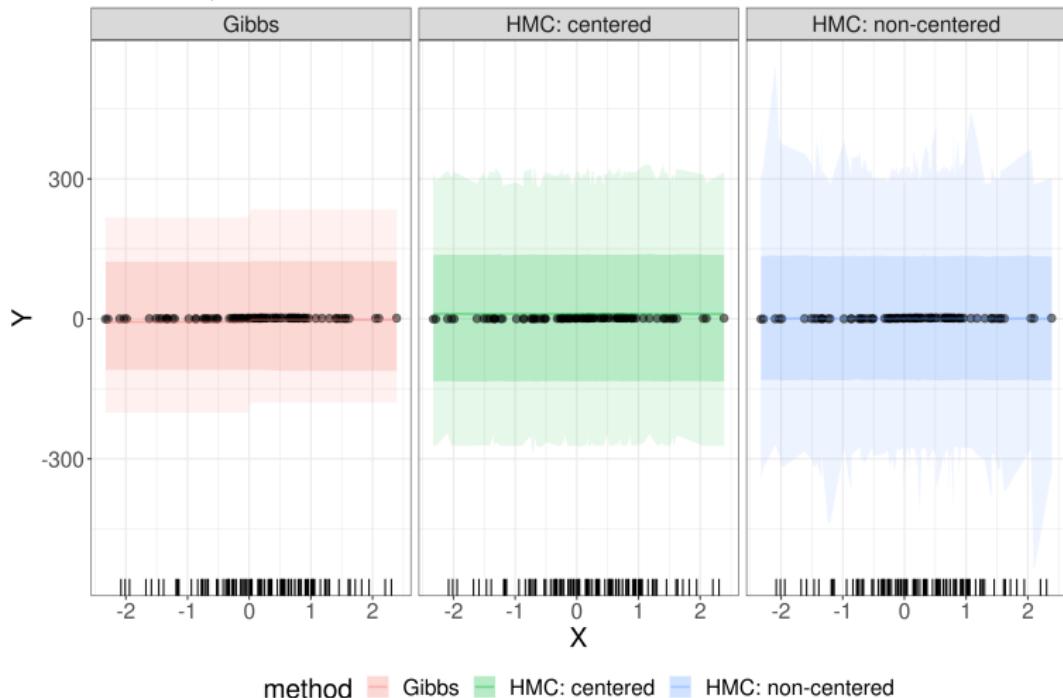


Figure 12: Predictive Quality

Prior Checks 2

Input-to-Hidden Weights: Precision Hyperparameter

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

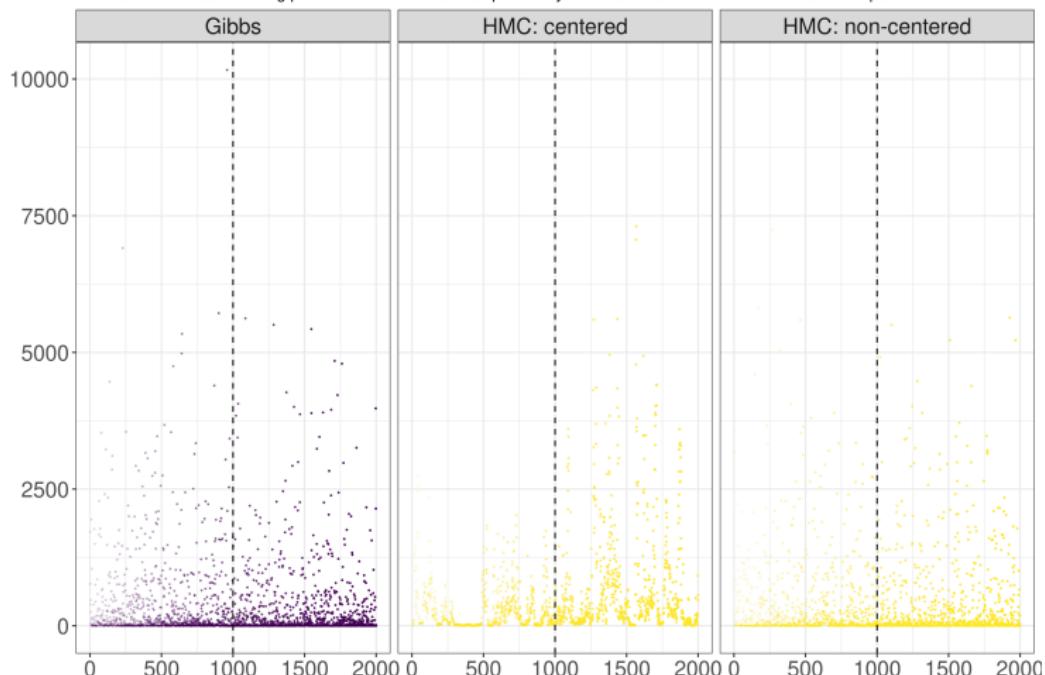


Figure 13: Input-to-hidden Weights Precision

Prior Checks 3

Input-to-Hidden Weights

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

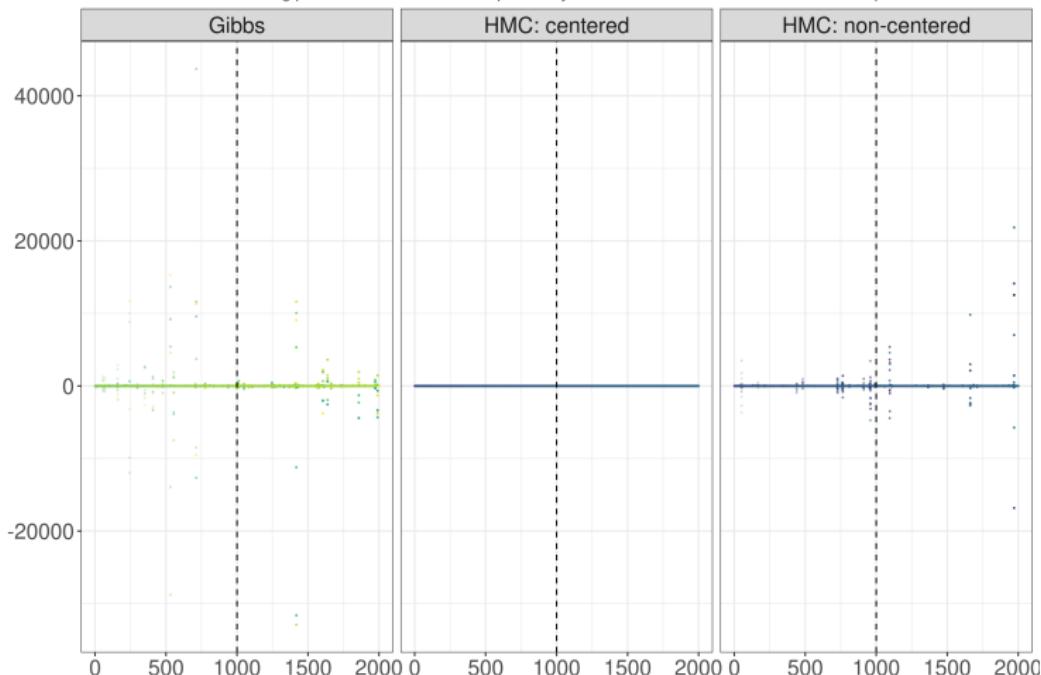


Figure 14: Inputs-to-hidden Weights

Prior Checks 4

Hidden-to-Output Weights: Precision Hyperparameter

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

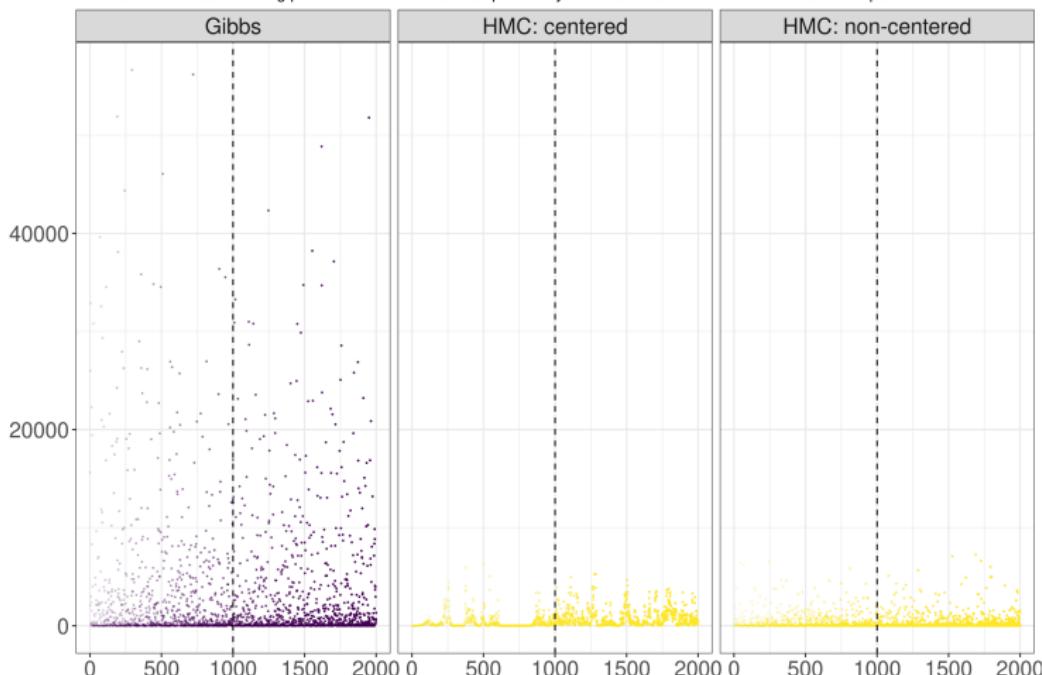


Figure 15: Hidden-to-output Weights Precision

Prior Checks 5

Hidden-to-Output Unit Weights

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

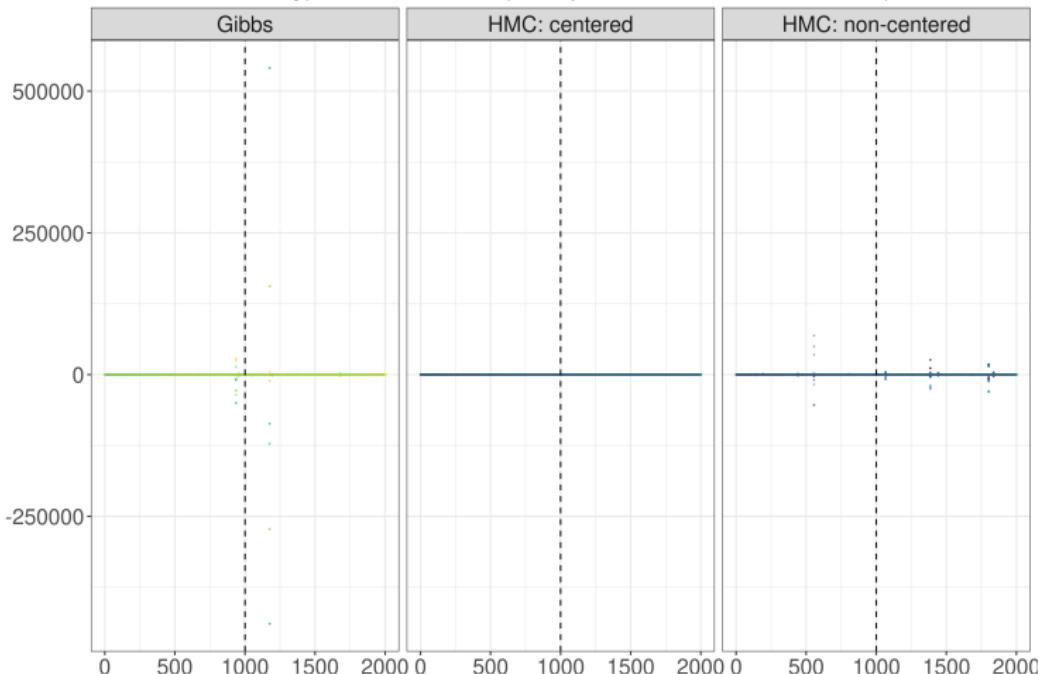


Figure 16: Hidden-to-output Weights

Prior Checks 6

Target Noise: Precision Hyperparameter

Vertical line indicates starting point of values used as samples. Only one Stan chain is used for consistent comparison.

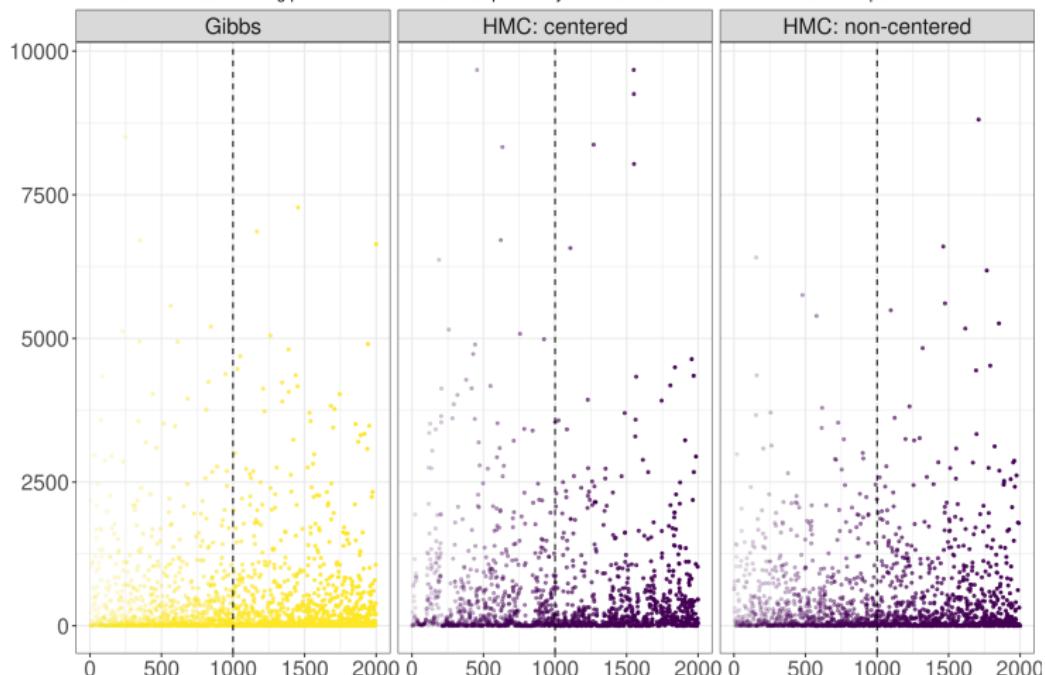


Figure 17: Target precision