Density Regression and Uncertainty Quantification with Bayesian Deep Noise Neural Networks: Supplementary Materials

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S1   METHOD DETAILS

S1.1 Details of Theoretical Results

S1.1.1 Details of Theorem 1

We define the variables in the posterior full-conditional distributions in Theorem 1.

Let \( \phi_N(\cdot \mid \mu, \sigma^2) \) and \( \Phi_N(\cdot \mid \mu, \sigma^2) \) be the PDF and CDF, respectively, of the normal distribution with mean \( \mu \) and variance \( \sigma^2 \).

For \( n \in 1, \ldots, N \), \( l \in 0, \ldots, L \), and \( k \in 1, \ldots, K_l \), let

\[
\omega_{l,k,j} = \left( \tau_{l,k}^{-2} + \alpha_{l,k,b_j}^2 \right)^{-1}
\]

\[
v_{l,k,j} = \tau_{l,k}^{-2} \omega_{l,k,j}
\]

\[
\psi_{l,k}^{(n)} = \gamma_{l,k} + \beta_l u_{l}^{(n)}
\]

\[
\tilde{\psi}_{l,k,j}^{(n)} = \left( \tilde{u}_{l+1,k} - b_j^{'} \right) \omega_{l,k,j}^{-1}
\]

\[
\lambda_{l,k,j}^{(n)} = v_{l,k,j} \psi_{l,k}^{(n)} + (1 - \tau_{l,k,j}^2) \tilde{\psi}_{l,k,j}^{(n)}
\]

\[
\zeta_{l,k,1} = 1
\]

\[
\zeta_{l,k,j} = \zeta_{l,k,j-1} \chi_{l,k,j}, \quad j \in 2, \ldots, J
\]

\[
\tilde{\zeta}_{l,k,j} = \frac{\tilde{\zeta}_{l,k,j-1}}{\tilde{\zeta}_{l,k,j-1}^{-1}}
\]

\[
\tilde{\kappa}_{l,k,j,j}^{(n)} = \phi_N\left( \tilde{u}_{l+1,k} \mid c_j, b_j^{'} + b_j^{'} \right)
\]

\[
\tilde{\tilde{\kappa}}_{l,k,j,j}^{(n)} = \phi_N\left( c_j^{'} \mid \lambda_{l,k,j}^{(n)}, \omega_{l,k,j}^2 \right)
\]

\[
\tilde{c}_{j,j}^{(n)} = (c_j^{'} - \lambda_{l,k,j}) \omega_{l,k,j}^{-1}
\]

\[
\tilde{\pi}_{l,k,j} = \Phi_N(\tilde{c}_{j,j} \mid 0, 1) - \Phi_N(\tilde{c}_{j,j-1} \mid 0, 1)
\]

\[
\pi_{l,k,j} \propto \tilde{\pi}_{l,k,j} \chi_{l,k,j}
\]

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We first derive the posterior full conditional distribution of $\phi_{l,k}$ as that of normal-normal priors with known variance.) Moreover, for some $\omega_{n,l,k,j}$ let
\[
\begin{align*}
\eta_{l,k} &= (\bar{u}_l^{\top} u_l^{(n)} + \tilde{B}_{l,k})^{-1} v_{l,k} u_l^{(n)} \\
B_{l,k} &= (\tau_{l,k}^{-2} u_l^{(n)} u_l^{(n)} + \tilde{B}_{l,k})^{-1}, \\
\bar{u}_l &= (u_l, 1), \\
\epsilon_{l,k} &= \omega_{n,l,k,j} - \tau_{l,k} u_l^{(n)} - \gamma_{l,k}.
\end{align*}
\]

Furthermore, let
\[
\begin{align*}
\eta_{l,k} &= (\bar{u}_l^{\top} u_l^{(n)} + \tilde{B}_{l,k})^{-1} v_{l,k} u_l^{(n)} \\
B_{l,k} &= (\tau_{l,k}^{-2} u_l^{(n)} u_l^{(n)} + \tilde{B}_{l,k})^{-1}, \\
\bar{u}_l &= (u_l, 1), \\
\epsilon_{l,k} &= \omega_{n,l,k,j} - \tau_{l,k} u_l^{(n)} - \gamma_{l,k}.
\end{align*}
\]

## S1.2 Proofs of Theoretical Results

### S1.2.1 Proof of Theorem 1

We first derive the posterior full conditional distribution of $\phi_{l,k}^{(n)}$ in Equation (9). Let
\[
\begin{align*}
\omega_{n,l,k,j}^{2} &= \left(\tau_{l,k}^{-2} + \sigma_{l+1,k}^{2} b_j^2\right)^{-1}, \\
\lambda_{n,l,k,j} &= \tau_{l,k}^{2} \omega_{n,l,k,j}^{2} \left(\gamma_{l,k} + \beta_l u_l^{(n)} + \sigma_{l+1,k}^{2} b_j \omega_{n,l,k,j}^{2} (u_{l+1,k} - b_j')\right).
\end{align*}
\]

By Equations (6) and (7), we have
\[
\begin{align*}
f \left( \phi^{(n)}_{l,k} \mid \text{rest} \right) &= f \left( \phi^{(n)}_{l,k} \mid u_l^{(n)}, \beta_l, \tau_{l,k}, u_{l+1,k}, \sigma_{l,k} \right) \\
&= C f \left( \phi^{(n)}_{l,k} \mid u_{l+1,k}^{(n)}, \tau_{l,k} \right) \\
&= C \lambda_{n,l,k,j} \omega_{n,l,k,j} \left(\gamma_{l,k} + \beta_l u_l^{(n)} + \sigma_{l+1,k}^{2} b_j \omega_{n,l,k,j}^{2} (u_{l+1,k} - b_j')\right) \\
&= \prod_{j=1}^{J} \left(\gamma_{l,k} + \beta_l u_l^{(n)} + \sigma_{l+1,k}^{2} b_j \omega_{n,l,k,j}^{2} (u_{l+1,k} - b_j')\right).
\end{align*}
\]

for some $\pi_{n,l,k,j} \in \mathbb{R}^+$ ($j = 1, \ldots, J$) with $\sum_{j=1}^{J} \pi_{n,l,k,j} = 1$. (The second last equation holds by the same argument as that of normal-normal priors with known variance.) Moreover, for $j = 2, \ldots, J$, we have
\[
\begin{align*}
\lim_{\phi_{l,k}^{(n)} \to c_{j-1}^{+}} f \left( \phi_{l,k}^{(n)} \mid \text{rest} \right) &= \lim_{\phi_{l,k}^{(n)} \to c_{j-1}^{+}} \prod_{j=1}^{J} \pi_{n,l,k,j} \phi_{l,k}^{(n)} \left(\gamma_{l,k} + \beta_l u_l^{(n)} + \sigma_{l+1,k}^{2} b_j \omega_{n,l,k,j}^{2} (u_{l+1,k} - b_j')\right) \\
&= \prod_{j=1}^{J} \pi_{n,l,k,j} \phi_{l,k}^{(n)} \left(\gamma_{l,k} + \beta_l u_l^{(n)} + \sigma_{l+1,k}^{2} b_j \omega_{n,l,k,j}^{2} (u_{l+1,k} - b_j')\right)
\end{align*}
\]
Then, which gives 

Moreover, by Equation (4),

Define 

Suppose 

Lemma S1.1. Suppose \( X \in \mathbb{R}^{K \times N} \) and \( y \in \mathbb{R}^{1 \times N} \). If \( \beta \in \mathbb{R}^{1 \times K} \) satisfies

for some \( \mu_0 \in \mathbb{R}^{1 \times K}, \Sigma_0 \in \mathbb{R}^{K \times K} \), and \( T \in \mathbb{R}^{N \times N} \), then the posterior distribution of \( \beta \) is

\[
\beta | y, X \sim \mathcal{N}(\mu_N, \Sigma_N), \quad \Sigma_N = (\Sigma_0^{-1} + XT^{-1}X^\top)^{-1}, \quad \mu_N = \Sigma_N(\mu_0\Sigma_0^{-1} + yT^{-1}X^\top).
\]
This formulation of the predictive density follows Equations (1) to (3) directly.

Lemma S1.2. Suppose $\sigma^2 \in \mathbb{R}_+$ and $x = \{x_i\}_{i=1}^N \in \mathbb{R}^N$ satisfy

$$
\sigma^2 \sim \mathcal{IG}(a_0, b_0), \quad x_i | \sigma^2 \overset{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)
$$

for some $a_0, b_0 \in \mathbb{R}_+$ and $\mu \in \mathbb{R}$. Then the posterior distribution of $\sigma^2$ is

$$
\sigma^2 | x \sim \mathcal{IG}(a_N, b_N), \quad a_N = a_0 + \frac{N}{2}, \quad b_N = b_0 + \frac{\|x - \mu\|^2}{2}
$$

Proof. This result is the widely known inverse gamma-normal conjugate priors for variance parameters with normally distributed observations and known mean (Wikipedia contributors, 2022b).

Then Equations (10) and (11) are immediate consequences of Lemma S1.1, while Equations (12) to (15) follow Lemma S1.2 directly.

S1.2.2 Proof of Theorem 2

This formulation of the predictive density follows Equations (1) to (3) directly.

S1.2.3 Proof of Theorem 3

Lemma S1.3. Suppose $W \in \mathbb{R}^K$ is a random vector and $t \in \mathbb{R}^K$ a constant vector. Let $\beta \in \mathbb{R}^{K' \times K}$, $\gamma \in \mathbb{R}^{K'}$, and define $f_{\beta, \gamma}(s) = \beta s + \gamma$. Moreover, let $\epsilon \in \mathbb{R}^K$ be a random vector with $\text{Cov}[\epsilon] = \text{diag}[\tau^2]$ and $\epsilon \perp W$, and define $f_{\tau^2}(s) = s + \epsilon$. Further, let $f_c : \mathbb{R} \to \mathbb{R}$ be a Lipschitz function with Lipschitz constant $c$, and let $f_c(s) = [f_c(s_1), \ldots, f_c(s_K)]$ for $s = [s_1, \ldots, s_K] \in \mathbb{R}^K$. Then

$$
\mathbb{E} \left[ \|f_{\beta, \gamma}(W) - f_{\beta, \gamma}(t)\|^2 \right] \leq \|\beta\|^2 \mathbb{E} \left[ \|W - t\|^2 \right]
$$

$$
\mathbb{E} \left[ \|f_{\tau^2}(W) - t\|^2 \right] \leq \mathbb{E} \left[ \|W - t\|^2 \right] + \text{sum}(\tau^2)
$$

$$
\mathbb{E} \left[ \|f_c(W) - f_c(t)\|^2 \right] \leq c^2 \mathbb{E} \left[ \|W - t\|^2 \right]
$$

Proof. These results follow directly from the definitions of $f_{\beta, \gamma}$, $f_{\tau^2}$, and $f_c$.

Let $S^2_\ell = \sum_{k=1}^{K_\ell} \sigma^2_{\ell k}$ and $R^2_\ell = \sum_{k=1}^{K_\ell} \tau^2_{\ell k}$. Define $g_0(x|\Gamma_0) = \beta_0 x + \gamma_0$ and $g_L(x|\Gamma_L) = \beta_L h(g_{L-1}(x|\Gamma_{L-1})) + \gamma_L$. Moreover, by definition $y = v_L$ and $v_l = \beta_l [h(v_{l-1}) + \delta_{l-1}] + \gamma_l + \epsilon_l$ for $l > 0$. We use induction to show

$$
\mathbb{E} \left[ \|y - g_L(x, \Gamma_L)\|^2 \bigg| x, \Theta_\ell \right] \leq \sum_{l=0}^{L} \left[ d^2_0 S^2_{\ell-1} + T^2_{l} \prod_{l'=l+1}^{L} d^2_{l'} \right] C^2_{n}(L-l)
$$

all $L \geq 0$. For $L = 0$, we have

$$
\mathbb{E} \left[ \|y - g_0(x, \Gamma_0)\|^2 \bigg| x, \Theta_0 \right] = \mathbb{E} \left[ \|\epsilon_0\|^2 \bigg| x, \Theta_0 \right] = T^2_0 = \sum_{l=0}^{0} \left[ d^2_0 S^2_{\ell-1} + T^2_{l} \prod_{l'=l+1}^{0} d^2_{l'} \right] C^2_{n}(0-l).
$$
For $L > 0$, we have

\[
\mathbb{E} \left\{ \| y - g_L(x, \Gamma_L) \|^2 \mid x, \Theta_L \right\} = \mathbb{E} \left\{ \| \beta_L [h(v_{L-1}) + \delta_{L-1}] + \gamma_L + \epsilon_L - [\beta_L h(g_{L-1}(x|\Gamma_{L-1}))+\gamma_L] \|^2 \mid x, \Theta_L \right\} \\
\quad \leq \mathbb{E} \left\{ \| \beta_L [h(v_{L-1}) + \delta_{L-1}] + \gamma_L - [\beta_L h(g_{L-1}(x|\Gamma_{L-1}))+\gamma_L] \|^2 \mid x, \Theta_L \right\} + \text{sum}(\tau^2_L) \\
\quad \leq d^2_L \mathbb{E} \left\{ \| h(v_{L-1}) + \delta_{L-1} - h(g_{L-1}(x|\Gamma_{L-1})) \|^2 \mid x, \Theta_L \right\} + \text{sum}(\tau^2_L) \\
\quad \leq d^2_L \mathbb{E} \left\{ \| h(v_{L-1}) - h(g_{L-1}(x|\Gamma_{L-1})) \|^2 \mid x, \Theta_L \right\} + \text{sum}(\tau^2_L) + d^2_L \text{sum}(\sigma^2_{L-1}) \\
\quad \leq d^2_L C^2_h \mathbb{E} \left\{ \| v_{L-1} - g_{L-1}(x|\Gamma_{L-1}) \|^2 \mid x, \Theta_L \right\} + \text{sum}(\tau^2_L) + d^2_L \text{sum}(\sigma^2_{L-1}) \\
\quad = d^2_L C^2_h \mathbb{E} \left\{ \| v_{L-1} - g_{L-1}(x|\Gamma_{L-1}) \|^2 \mid x, \Theta_L \right\} + T^2_L + d^2_L S^2_{L-1} \\
\quad \leq \left\{ \sum_{l=0}^{L-1} \left[ d^2_l S^2_{l+1} + T^2_l \right] \left[ \prod_{l'=l+1}^{L} d^2_{l'} \right] C^2_h^{2(L-l)} \right\} + T^2_L + d^2_L S^2_{L-1} \\
\quad = \left\{ \sum_{l=0}^{L-1} \left[ d^2_l S^2_{l+1} + T^2_l \right] \left[ \prod_{l'=l+1}^{L} d^2_{l'} \right] C^2_h^{2(L-l)} \right\} + \sum_{l=L}^{L} \left[ d^2_l S^2_{l+1} + T^2_l \right] \left[ \prod_{l'=l+1}^{L} d^2_{l'} \right] C^2_h^{2(L-l)} \\
\quad = \left\{ \sum_{l=0}^{L} \left[ d^2_l S^2_{l+1} + T^2_l \right] \left[ \prod_{l'=l+1}^{L} d^2_{l'} \right] C^2_h^{2(L-l)} \right\} ,
\]

where the inequalities hold by Lemma S1.3 and the inductive hypothesis.

**S1.2.4 Proof of Corollary 4**

First, observe that the activation functions in the statement of Corollary 4 are all Lipschitz functions with Lipschitz function $C_h \leq 1$. Then by applying the global bounds to Corollary 4, we have

\[
\mathbb{E} \left\{ \| y - g_L(x, \Gamma_L) \|^2 \mid x, \Theta_L \right\} \leq \sum_{l=0}^{L} \left( d^2 K \sigma^2 + K \tau^2 \right) d^2(L-l) C^2_h^{2(L-l)} \\
\quad = K \left( d^2 \sigma^2 + \tau^2 \right) \sum_{l=0}^{L} d^2(L-l) C^2_h^{2(L-l)} \\
\quad \leq K \left( d^2 \sigma^2 + \tau^2 \right) \sum_{l=0}^{L} d^2(L-l) \\
\quad \leq K (d^2 + 1) (\sigma^2 + \tau^2) \sum_{l=0}^{L} d^{2l} \\
\quad = K(d^2 + 1) (\sigma^2 + \tau^2) \sum_{l=0}^{L} (d^{2L} + 1) \\
\quad \leq K(d^2 + 1) (\sigma^2 + \tau^2) \sum_{l=0}^{L} (d^{2(L+1)} + 1) \\
\quad \leq 3KL(d^{2L+1} + 1)(\sigma^2 + \tau^2),
\]

which completes the proof.
S2 Synthetic data experiments

S2.1 Experiment setup

S2.1.1 Data simulation

We simulated synthetic data with different conditional distribution patterns to evaluate each method’s ability of learning the density. We sampled one-dimensional input value from $U[-1, 1]$ or $0.9U[-1, 0] + 0.1U[0, 1]$. For the output value, we generated it by $y = m(x) + \eta(x)$, where $m(x)$ is a deterministic median function and $\eta(x)$ is the random variable of the noise, such that $\text{median}[\eta(x)] = 0$ for all $x$. We fix the median of $y$ to the piecewise linear function $m(x) = (x + 1)I[x \leq -0.5] - xI[-0.5 < x < 0] + xI[x > 0]$ and simulated three different types of noise by using uniform distributions or their mixtures:

1. Heteroscedastic noise:
   \[ \eta(x) \sim \begin{cases} U[-0.5, 0.5], & \text{if } x \in [-0.85, -0.65] \cup [-0.35, -0.15] \cup [0.35, 0.65] \\ U[-0.1, 0.1], & \text{otherwise} \end{cases} \]

2. Skewed noise:
   \[ \eta(x) \sim \begin{cases} 0.5U[-0.1, 0] + 0.5U[0, 0.8], & \text{if } x \in [-0.5, 0] \\ 0.5U[-0.8, 0] + 0.5U[0, 0.1], & \text{otherwise} \end{cases} \]

3. Multimodal noise:
   \[ \eta(x) \sim \begin{cases} 0.3U[-0.5, -0.4] + 0.4U[-0.4, 0.4] + 0.3U[0.4, 0.5], & \text{if } x \in [-0.5, 0.5] \\ U[-0.125, 0.125], & \text{otherwise} \end{cases} \]

The training sample size varied among 1000, 2000, 4000, and the testing size was 10% of the training size. We randomly generated 20 datasets for each noise type and sample size.

S2.1.2 Model setup

Model setups were the same as those in the UCI data experiments (Section S3.1.2), except for DMC, which did not give meaningful predictions and used a virtually constant function with very large predictive variance to fit all the datasets.

S2.1.3 Evaluation criteria

To evaluate the accuracy of the estimated predictive distribution, we computed its difference from the true predictive distribution. We used a grid of 100 values of $x$ on $[-1, 1]$. For every $x$, we computed the empirical $0.025, 0.075, \ldots, 0.925, 0.975$ quantiles of the estimated predictive distribution and the true distribution. Then we computed the average absolute difference between the estimated and true quantiles, which is equivalent to numerically computing the $L_1$ distance between the inverse CDFs of the estimated and true predictive distributions, and averaged them across all the grid points of $x$.

S2.2 Additional results

The estimated predictive density of baseline methods not included in Figure 1 are displayed in Figure S1.
S3 UCI data experiments

S3.1 Experiment setup

S3.1.1 Dataset curation

We downloaded the nine UCI datasets from https://github.com/yaringal/DropoutUncertaintyExps, including the indices of the random splits. See the repository and (Gal and Ghahramani, 2016) for details.

S3.1.2 Model setup

B-DeepNoise. We assigned $\mathcal{IG}(0.001, 0.001)$ as weakly informative priors to the variance parameters. The network included 4 hidden layers with 50 hidden nodes per layer. The activation function was the hard tanh function $h(x) = \min(1, \max(-1, x))$. The parameters were initialized by stochastic gradient descent, and 500
posterior samples were drawn. The input and output were centered at 0 and scaled to 1, where the centers
and scales were computed by using the training samples only.

All the baseline methods had the same architecture, activation, and normalization as B-DeepNoise. For
GPU computation, we used an NVIDIA Quadro P6000.

Dropout Monte Carlo (DMC). We used the implementation by the original authors (Gal and Ghahra-
man, 2016), including their hyperparameter tuning procedures. See https://github.com/yaringal/
DropoutUncertaintyExps. for details.

Variational Inference (VI). We used the implementation by (Ritter and Karaletsos, 2022). The batch
size was 100, and the model was trained for 2000 epochs with a learning rate of 0.001.

Deep ensemble (DE). We followed the recommendations of the original authors (Lakshminarayanan
et al., 2016) and used 5 independent networks. The predictive MSE was optimized by Adam (Kingma and
Ba, 2014) with a learning rate of 0.1. The model was trained for 40 epochs.

Backpropagation (BP). We used two feed-forward neural networks, where the second network included
a softplus layer on the output layer. The first network outputs the predictive mean, while the second
network outputs the predictive variance. The Gaussian NLL was used as the loss function. The training
hyperparameters were the same as those for DE.

Bayesian Neural Network (BNN). We used a BNN with learnable predictive variance, i.e. the model
outputs two parameters, one for the predictive mean and the other for the predictive variance. The Gaussian
NLL was used as the loss function. We used standard normal distributions as priors for all the weight and
bias parameters except for those connected to the log predictive variance, which used \(N(0, 0.25I)\) as priors.

To reduce the computation cost, parameters were initialized by stochastic gradient decent. The posterior
distribution was simulated by Hamiltonian Monte Carlo (Duane et al., 1987). Each HMC iteration involved
10 leapfrog steps. The step size was initialized to 0.01 and dynamically adjusted to achieve an acceptance
rate of 0.75 Andrieu and Thoms (2008).

S3.1.3 Evaluation criteria

In this section, we compare the calibrated prediction intervals (CPI) with the uncalibrated prediction
intervals (UPI). Conceptually, the average width of the 95\% calibrated prediction intervals (WCPI-95) is
the miscalibration-adjusted version of the 95\% uncalibrated prediction intervals (WUPI-95). WUPI-95 is a
popular metric for evaluating uncertainty quantification (UQ) efficiency. However, a major flaw of WUPI-95
is that when a method is overconfident about the testing data and underestimate the predictive uncertainty,
its WUPI-95 can be very small and does not reflect the actual inaccuracy. Thus if a method has a small
WUPI-95, the cause could be 1) that the method is both well-calibrated and efficient in UQ, or 2) that the
method is miscalibrated in UQ. One has to look up the empirical coverage rates of the UPIs on the testing
data to check the accuracy of UQ and differentiate the two situations. In other words, it is unfair to compare
the widths of the 95\% UPIs of two methods if one method empirically covers a much smaller percentage
of the testing samples compared to the other method.

Therefore, in order to use a single metric that systematically measures UQ efficiency and is invariant to
mis-calibration, we propose the WCPI-95. The WCPI-95 of a method is defined to be the WUPI-x, where x
is the smallest positive number such that the x\% UPIs cover no less than 95\% of the outcomes on the testing
data. Computationally, we iterate through the 1\% UPIs, 2\% UPIs, ..., 99\% UPIs, 100\% UPIs until at least
95\% of the testing samples are covered (say we are at the x\% UPIs at this step), and then we find the average
width of the x\% UPIs, which gives us the WCPI-95. For example, suppose Method A is over-confident in its
predictions, where its 95\% UPIs cover less than 95\% of the testing samples in average, and its 99\% UPIs
actually cover 95\% of the testing samples in average. In that case, the WCPI-95 of Method A is equal to its
WUPI-99, which is larger than its WUPI-95 and thus corrects for its over-confidence. On the other hand, if
Method B is under-confident, its WCPI-95 will be less than its WUPI-95. Finally, if method C is perfectly


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calibrated such that its 95% UPIs cover exactly 95% of the observations on the testing data, then its WCPI-95 is equal to its WUPI-95. Then by comparing the WCPI-95 of Methods A, B, and C, we can evaluate the UQ efficiency of the three methods fairly without having to worry that any of the methods may “hack” the theoretical predictive interval width by being consistently over-confident.

S3.2 Additional results

In addition to the RMSE, NLL, and WCPI-95 (Table 2), we also computed the average coverage rate of the 95% prediction intervals on the testing data. The results are reported in Table S1.

Table S1: Additional UCI experiment results on testing data for B-DeepNoise and baseline methods.

| Dataset           | BP       | VI       | BNN      | DMC      | DE       | B-DeepNoise |
|-------------------|----------|----------|----------|----------|----------|-------------|
| Yacht Hydrodynamics | 0.92 ±0.06 | 1.00 ±0.00 | 1.00 ±0.00 | 0.81 ±0.08 | 0.97 ±0.04 | 0.96 ±0.03  |
| Boston Housing    | 0.85 ±0.06 | 0.97 ±0.02 | 0.94 ±0.00 | 0.86 ±0.04 | 0.90 ±0.05 | 0.92 ±0.04  |
| Energy Efficiency | 0.92 ±0.05 | 1.00 ±0.01 | 0.99 ±0.00 | 0.94 ±0.03 | 0.98 ±0.02 | 0.96 ±0.05  |
| Concrete Strength | 0.86 ±0.05 | 0.89 ±0.03 | 0.97 ±0.02 | 0.88 ±0.02 | 0.92 ±0.03 | 0.93 ±0.03  |
| Wine Quality      | 0.85 ±0.04 | 0.62 ±0.05 | 0.91 ±0.06 | 0.61 ±0.04 | 0.91 ±0.02 | 0.92 ±0.03  |
| Kin8nm            | 0.86 ±0.04 | 0.55 ±0.02 | 0.94 ±0.04 | 1.00 ±0.00 | 0.95 ±0.01 | 0.96 ±0.01  |
| Power Plant       | 0.94 ±0.01 | 0.87 ±0.01 | 0.97 ±0.01 | 0.73 ±0.02 | 0.95 ±0.01 | 0.95 ±0.01  |
| Naval Propulsion  | 0.94 ±0.14 | 0.95 ±0.02 | 1.00 ±0.00 | 1.00 ±0.00 | 1.00 ±0.96 | 1.00 ±0.00  |
| Protein Structure | 0.93 ±0.01 | 0.83 ±0.01 | 0.98 ±0.01 | 0.57 ±0.02 | 0.96 ±0.00 | 0.93 ±0.00  |

Table S2: Runtime (sec) for UCI data experiments.

| Dataset           | BP    | VI    | BNN   | DMC   | DE    | B-DeepNoise |
|-------------------|-------|-------|-------|-------|-------|-------------|
| Yacht Hydrodynamics | 4    | 133   | 772   | 3482  | 8     | 534         |
| Boston Housing    | 4    | 180   | 1090  | 3523  | 11    | 570         |
| Energy Efficiency | 5    | 247   | 1204  | 4456  | 12    | 625         |
| Concrete Strength | 7    | 331   | 1407  | 4551  | 19    | 837         |
| Wine Quality      | 7    | 580   | 1046  | 4599  | 19    | 837         |
| Kin8nm            | 25   | 3195  | 2042  | 7801  | 77    | 1266        |
| Power Plant       | 29   | 3657  | 2514  | 6101  | 88    | 2028        |
| Naval Propulsion  | 33   | 3586  | 2875  | 8876  | 83    | 3270        |
| Protein Structure | 127  | 11948 | 12518 | 12112 | 859   | 5700        |

S4 ABCD data analysis

S4.1 Experiment setup

S4.1.1 Data overview

The ABCD study aims at identifying the associations between brain development and cognitive behaviors. A total of 11,800 children aged between 9 and 10 participated in the study. In our experiments, we used Release 1.1, which consisted of minimally preprocessed fMRI data from 21 imaging sites (Hagler Jr et al., 2019). The images we analyzed was the 2-back task-based contrast map. The 2-back task engages brain regions associated with cognitive functions and memory regulation processes. The imaging resolution was 2mm, with each image containing $61 \times 73 \times 61$ voxels. The outcome variable was general intelligence score (g-score) (Sripada et al., 2020). The non-imaging features included 2-back task score, general psychopathology factor, age, sex, highest parental education level, household marital status, household income bracket, and self-identified racial and
ethnic memberships. Categorical variables were coded as multiple binary dummy variables. For the imaging features, we divided the brain into 90 AAL regions and extracted the average imaging value inside each region as a feature. The 90 imaging features were concatenated with the non-imaging features to form the input variables. After removing incomplete observations, the dataset contained 1191 subjects.

S4.1.2 Model setup
The settings of B-DeepNoise were the same as that in the UCI data experiments (Section S3.1.2).

S4.2 Additional results
In addition to Figure 3, we also computed the influence of brain regions on the predictive variance, as visualized in Figure S3. The magnitudes of influence of the top five most influential features on both the predictive mean and variance are reported in Table S3.

![Figure S3: Influence of brain regions on the predictive variance of the g-score.](image)

Table S3: Most influential features on the predictive mean and variance of g-score.

| Predictive Mean      | Predictive Variance    |
|----------------------|------------------------|
| feature              | influence              | feature              | influence              |
| CorrectRate2bk       | 1.3235                 | CorrectRate2bk       | 0.0659                 |
| Calcarine.R          | 0.6269                 | Calcarine.R          | 0.0327                 |
| Putamen.R            | 0.6012                 | Paracentral.Lobule.R | 0.0312                 |
| Paracentral.Lobule.R | 0.5786                 | Putamen.R            | 0.0309                 |
| Rectus.R             | 0.4770                 | Occipital.Inf.R      | 0.0275                 |

S5 DISCUSSION OF CLASSIFICATION TASKS

S5.1 Theoretical Comparison of Stochastic and Deterministic Models for Classification
In this section, we demonstrate that for categorical outcomes, stochastic models do not have theoretical advantage over deterministic models that are sufficiently flexible. Consider a standard classification model, where the \( K \)-class outcome variable is coded as a one-hot vector \( Y \in \{0,1\}^K \) and, given input features \( x \), is modeled as \( Y \sim \text{Categorical}(\text{softmax}(g(x))) \), where \( g(x) \) is a deterministic function, and \( E[Y] = \text{softmax}(g(x)) \) is the conditional expected value of the outcome, which is a probability vector. If we replace \( g(x) \) with a stochastic function \( \tilde{g}(x,Z) \), where \( Z \) is a random seed with density function \( f(z) \), then the outcome variable follows

\[
Y \sim \text{Categorical}(\text{softmax}(\tilde{g}(x,Z))), \quad Z \sim f.
\]

In this case, by the law of total expectation, the conditional expected value of the outcome is

\[
E[Y|x] = E[E[Y|Z,x]] = E[\text{softmax}(\tilde{g}(x,Z))] = \int_z \text{softmax}(\tilde{g}(x,z))f(z)dz.
\]
Define \( \tilde{p}(x) = \int \text{softmax}(\tilde{g}(x, z))f(z)dz \), which is a deterministic function that maps the input features to a probability vector. Since a categorical distribution is completely determined by its expected value, the derivation above implies that if \( g(x) \) is flexible enough such that \( \text{softmax}(g(x)) \) can approximate \( \tilde{p}(x) \) with arbitrary precision then the predictive distribution of the deterministic model can approximate the predictive distribution of the stochastic model with arbitrary precision.

The last condition holds for DNNs by their universal approximation property. Thus for classification tasks, any stochastic model can be replaced with a deterministic DNN model with arbitrary small difference in the predictive distribution. This theoretical result renders the flexible density learning capacity of B-DeepNoise unhelpful for classification tasks.

S5.2 B-DeepNoise for Categorical Outcomes

Although B-DeepNoise is not theoretically expected to have better uncertainty quantification accuracy than standard DNNs on classification tasks, (as demonstrated in Section S5.1) B-DeepNoise is still capable of learning the predictive distributions of categorical outcomes. This ability is achieved by adding a softmax activation function to the output layer. Then the posterior full-conditional distributions of the model parameters are the same except for those in the output layer, which we derive in this section.

Let \( y^{(n)} = [y_k^{(n)}]_{k=1}^K \in \mathbb{R}^K \) be a \( K \)-class categorical outcome variable, represented as a one-hot vector:

\[
y_k^{(n)} = \begin{cases} 
1, & \text{if } k \in \{1, \ldots, K\} \setminus \{ar{k}^{(n)}\}, \\
0, & \text{if } k = \bar{k}^{(n)}
\end{cases}
\]

where \( \bar{k}^{(n)} \) is the true category for \( y^{(n)} \). Using B-DeepNoise to model the distribution of the outcome given input features \( x^{(n)} \), we have

\[
\text{softmax}^{-1}\left\{ \mathbb{E}[y^{(n)}] \right\} = \epsilon_{L}^{(n)} + \gamma_{L} + \beta_{L}\left[\delta_{L}^{(n)} + h\left(\cdots \epsilon_{1}^{(n)} + \gamma_{1} + \beta_{1}\left[\delta_{0}^{(n)} + h\left(\epsilon_{0}^{(n)} + \gamma_{0} + \beta_{0}x^{(n)}\right)\right] \cdots\right)\right]
\]

where

\[
\text{softmax}(z_k) = \begin{cases} 
\frac{\exp(z_k)}{\sum_{k=1}^{K-1} \exp(z_k)+1}, & \text{if } k \in \{1, \ldots, K-1\} \\
\frac{1}{\exp(z_k)+1}, & \text{if } k = K
\end{cases}
\]

which we abbreviate as

\[
\text{softmax}(z) = \frac{[\exp(z), 1]}{\sum \exp(z) + 1}.
\]

Notice that the \( K \)th element in \( y^{(n)} \) by definition has logit equal to 0, so that the scale of \( z \) is identifiable. The task is to sample \( z^{(n)}|y^{(n)}, \mu^{(n)}, \tau^2 \) from the model

\[
z^{(n)} \overset{\text{iid}}{\sim} \mathcal{N}(\mu^{(n)}, \tau^2)
\]

\[
\pi^{(n)} = \frac{[\exp(z^{(n)}), 1]}{\sum \exp(z^{(n)}) + 1}
\]

\[
y^{(n)} \sim \text{Categorical}(\pi^{(n)}),
\]

where \( z^{(n)}, \mu^{(n)} \in \mathbb{R}^{K-1} \) and \( \tau^2 \in \mathbb{R} \). To do this, we update one element of \( z^{(n)} \) at a time while fixing the
other \( K - 2 \) elements. Then the joint log density for element \( k \) is

\[
- \log f \left( z_k^{(n)}, y^{(n)} | z_{-k}^{(n)}, \mu_k^{(n)}, \tau^2 \right) = - \log f \left( z_k^{(n)}, y^{(n)} | z_{-k}, \mu_k, \tau^2 \right) \\
= \frac{1}{2\tau^2} (z_k^{(n)} - \mu_k^{(n)})^2 + \log \left[ \frac{\exp (z_k^{(n)})}{\sum \exp (z_{-k}^{(n)})} + 1 \right] - z_{k(n)} + C_0 \\
= \frac{1}{2\tau^2} (z_k^{(n)} - \mu_k^{(n)})^2 + \log \left[ \frac{\exp (z_k^{(n)})}{\sum \exp (z_{-k}^{(n)})} + 1 \right] - z_{k(n)} + C_1 \\
= \frac{1}{2\tau^2} (z_k^{(n)} - \mu_k^{(n)})^2 + \log \left[ \frac{\exp (z_k^{(n)} - a_k^{(n)}) + 1}{\sum \exp (z_{-k}^{(n)})} \right] - z_{k(n)} + C_1 \\
= \frac{1}{2\tau^2} (z_k^{(n)} - \mu_k^{(n)})^2 + \log \left[ \exp \left\{ s_k^{(n)} (z_k^{(n)} - a_k^{(n)}) \right\} \right] + 1 + C_2
\]

where

\[
a_k^{(n)} = \log \left[ \sum \exp (z_{-k}^{(n)}) + 1 \right] \\
s_k^{(n)} = \begin{cases} 
-1, & \text{if } k = \bar{k}^{(n)}, \\
1, & \text{otherwise,}
\end{cases}
\]

Notice that \( \log \left[ \exp (z_k^{(n)} - a_k^{(n)}) + 1 \right] \) is the softplus function with respect to \( z_k^{(n)} \) centered at \( a_k^{(n)} \), which approaches the ReLU function \( \max(0, \cdot) \) when \( z_k^{(n)} \to \pm\infty \), and is convex around \( a_k^{(n)} \). Thus we can approximate it by breaking its domain into three parts:

\[
\log\{\exp[s(z-a)] + 1\} = \phi[s(z-a)] \approx \psi[s(z-a)] = \begin{cases} 
0 & \text{if } s(z-a) < -\frac{1}{2c} \\
\frac{1}{2}(z-a + \frac{s}{2c})^2 & \text{if } -\frac{1}{2c} \leq s(z-a) \leq \frac{1}{2c} \\
\phi[z(a)] & \text{if } s(z-a) > \frac{1}{2c} \\
\frac{z-1}{2}(z-a) & \text{if } z \in (-\infty, a - \frac{1}{2c}) \\
\frac{1}{2}(z-a + \frac{s}{2c})^2 & \text{if } z \in [a - \frac{1}{2c}, a + \frac{1}{2c}] \\
\frac{z+1}{2}(z-a) & \text{if } z \in (a + \frac{1}{2c}, \infty)
\end{cases}
\]

where \( c > 0 \) is a constant for approximating the logistic function with a hard sigmoid function

\[
\{\exp[s(z-a)] + 1\}^{-1} = \phi'[s(z-a)] \approx \psi'[s(z-a)] = \min[\max[0.5 + sc(z-a), 0], 1].
\]

For example, the first-order Taylor polynomial of \( \phi' \) at 0 sets \( c = 0.25 \), while TensorFlow and Theano sets \( c = 0.2 \), and PyTorch sets \( c = 1/6 \). (For the middle part, we may be tempted to use the Taylor polynomial of \( \phi \) centered at \( a \) (i.e. \( \log(2) + 0.5(z-a) + 0.125(z-a)^2 \)) or centered at one of the two boundary points, but that does not guarantee the overall function to be continuous.) Then the density function is broken into
three cases:

\[-\log f(z_k^{(n)}|y^{(n)}, z_k^{(n)}, \mu_k^{(n)}, \tau^2) = \frac{1}{2\tau^2} (z_k^{(n)} - \mu_k^{(n)})^2 + \log \left\{ \exp \left\{ \frac{z_k^{(n)} - a_k^{(n)}}{2\tau^2} \right\} + 1 \right\} + C_2\]

\[\approx \frac{1}{2\tau^2} (z_k^{(n)} - \mu_k^{(n)})^2 + \psi \left( a_k^{(n)} - z_k^{(n)} \right) \]

\[= \left\{ \begin{array}{ll}
\frac{1}{2\tau^2} (z_k^{(n)} - \mu_k^{(n)})^2 + C_2 & \text{if } s_k^{(n)} (z_k^{(n)} - a_k^{(n)}) < -\frac{1}{2\tau^2} \\
\frac{1}{2\tau^2} \left( z - \left( a - s_k^{(n)} \right) \right) + C_3 & \text{if } -\frac{1}{2\tau^2} \leq s_k^{(n)} (z_k^{(n)} - a_k^{(n)}) \leq \frac{1}{2\tau^2} \\
\frac{1}{2\tau^2} \left( a_k^{(n)} - s_k^{(n)} \right)^2 + C_4 & \text{if } s_k^{(n)} (z_k^{(n)} - a_k^{(n)}) > \frac{1}{2\tau^2} \\
\frac{1}{2\tau^2} \left( z_k^{(n)} - \mu_k^{(n)} - \frac{(n-1)^2}{2\tau^2} \right)^2 + C_4 & \text{if } z_k^{(n)} \in \left( -\infty, a_k^{(n)} - \frac{1}{2\tau^2} \right) \\
\frac{1}{2\tau^2} \left( z_k^{(n)} - \mu_k^{(n)} - \frac{(n-1)^2}{2\tau^2} \right)^2 + C_4 & \text{if } z_k^{(n)} \in \left( a_k^{(n)} - \frac{1}{2\tau^2}, a_k^{(n)} + \frac{1}{2\tau^2} \right) \\
\frac{1}{2\tau^2} \left( z_k^{(n)} - \mu_k^{(n)} - \frac{(n+1)^2}{2\tau^2} \right)^2 + C_4 & \text{if } z_k^{(n)} \in \left( a_k^{(n)} + \frac{1}{2\tau^2}, \infty \right)
\end{array} \right.\]

In all the cases the density has a quadratic form, and the density overall is continuous, which implies that the distribution is a three-component mixture of truncated normal distributions with adjacent truncation points.

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