Informative Gaussian Scale Mixture Priors for Bayesian Neural Networks

Tianyu Cui
Department of Computer Science
Aalto University, Finland

Aki Havulinna
Finnish Institute for Health and Welfare (THL)
Helsinki, Finland

Pekka Marttinen*
Department of Computer Science
Aalto University, Finland

Samuel Kaski*
Department of Computer Science
Aalto University, Finland

Abstract

Encoding domain knowledge into the prior over the high-dimensional weight space is challenging in Bayesian neural networks. Two types of domain knowledge are commonly available in scientific applications: 1. feature sparsity (number of relevant features); 2. signal-to-noise ratio, quantified, for instance, as the proportion of variance explained (PVE). We show both types of domain knowledge can be encoded into the widely used Gaussian scale mixture priors with Automatic Relevance Determination. Specifically, we propose a new joint prior over the local (i.e., feature-specific) scale parameters to encode the knowledge about feature sparsity, and an algorithm to determine the global scale parameter (shared by all features) according to the PVE. Empirically, we show that the proposed informative prior improves prediction accuracy on publicly available datasets and in a genetics application.

1 Introduction

The Bayesian approach [Gelman et al., 2013] has been of interest because of its ability to incorporate domain knowledge into reasoning and to provide principled uncertainty estimates. Bayesian neural networks (BNNs) [Neal, 2012], however, are criticized for the difficulty of encoding domain knowledge into the prior over the high-dimensional weight space. This limits their use in applications where domain knowledge is important, e.g., when data are limited or signal is extremely weak and sparse. Applications in genetics often fall into the latter category and are used as motivating examples for the proposed methods.

Two types of domain knowledge are often available in scientific applications: ballpark figures on feature sparsity and the signal-to-noise ratio. Specifically, feature sparsity refers to the number of features expected to be used by the model. For example, in genomics less than 2% of the genome encodes for genes. A prior on the signal-to-noise ratio may encode the amount of variance of the target expected to be explained by the chosen features, and it can be measured as the proportion of variance explained (PVE) [Glantz et al., 1990]. For example, one gene may explain only a tiny fraction of the variance of a given phenotype, e.g., the PVE of the gene can be less than 1%.

Gaussian scale mixtures (GSMs) are commonly used sparse priors on the BNN weights, including, e.g., the horseshoe [Ghosh et al., 2018] and the spike-and-slab [Deng et al., 2019]. However, they are not flexible enough to encode all kinds of beliefs about sparsity, and it is not known how to encode information about the PVE into such a prior. Some recent works on functional BNNs encode domain knowledge into a functional prior, e.g., a Gaussian process [Flam-Shepherd et al., 2017, Sun et al., 2019], but it is not trivial to include sparsity in such priors.

We propose a new informative GSM prior for the weights to explicitly encode domain knowledge about feature sparsity and signal-to-noise ratio. Our main contributions are:

1. Propose a joint hyper-prior on the local scales that can model beliefs on the number of relevant features, which includes the spike-and-slab as a special case (Figure 1).
2. Derive the relation between PVE and the global scale parameter for BNNs with the ReLU activation function.
3. Develop a method to determine the global scale parameter of the GSM prior by using domain knowledge about the PVE, which circumvents heuristics employed in the commonly used approaches [Blundell et al., 2015] and computationally intensive cross-validation.

* Equal contributions
Variational inference can be used to approximate the intractable posterior distribution \( p(w | X, y) \) with a simpler distribution, \( q_\phi(w) \), by minimizing \( \text{KL}(q_\phi(w)) || p(w | X, y) \). This is equivalent to maximizing the ELBO

\[
\mathcal{L}(\phi) = \mathcal{H}(q_\phi(w)) + E_{q_\phi(w)}[\log p(y, w | X)]. 
\] (1)

The first term in Eq. 1 is the entropy of the approximated posterior, which can be calculated analytically for many choices of \( q_\phi(w) \). The second term can be estimated by the reparametrization trick [Kingma and Welling, 2013], which reparametrizes the approximated posterior \( q_\phi(w) \) by a deterministic and differentiable function \( w = g(\epsilon; \phi) \) with \( \epsilon \sim \mathcal{N}(0, 1) \), such that \( E_{q_\phi(w)}[\log p(y, w | X)] = E_{p(\epsilon)}[\log p(y, g(\epsilon; \phi) | X)] \).

2.2 Gaussian scale mixture priors

The Gaussian scale mixture [Andrews and Mallows, 1974] is defined to be a zero mean Gaussian conditional on its scale, and the distribution on the scale characterizes its statistical properties, e.g. sparsity. It has been combined with Automatic Relevance Determination (ARD)

\[
w_{i,j}^{(l)} | \lambda_i^{(l)}, \tau \sim \mathcal{N}(0, \tau^2 \lambda_i^{(l)2}); \quad \lambda_i^{(l)} \sim p(\lambda_i^{(l)}; \theta),
\] (2)

where \( \tau \) is the global scale shared by all of the NN weights.

2 Background

2.1 Bayesian neural networks

Bayesian neural networks [MacKay, 1992, Neal, 2012] are defined by placing a prior distribution on the weights \( w \) of a neural network. Then, instead of finding a point estimate of the weights by minimizing a cost function, a posterior distribution of the weights is calculated conditionally on the data. Let \( f(x; w) \) denote the output of a BNN and \( p(y | x, w) = p(y | f(x; w)) \) the likelihood. Then, given a dataset of inputs \( X = \{x^{(1)}, \ldots, x^{(N)}\} \) and outputs \( y = \{y^{(1)}, \ldots, y^{(N)}\} \), training a BNN means computing the posterior distribution \( p(w | X, y) \).

Variational inference can be used to approximate the intractable \( p(w | X, y) \) with a simpler distribution, \( q_\phi(w) \), by minimizing \( \text{KL}(q_\phi(w)) || p(w | X, y) \). This is equivalent to maximizing the ELBO

\[
\mathcal{L}(\phi) = \mathcal{H}(q_\phi(w)) + E_{q_\phi(w)}[\log p(y, w | X)]. 
\] (1)

The first term in Eq. 1 is the entropy of the approximated posterior, which can be calculated analytically for many choices of \( q_\phi(w) \). The second term can be estimated by the reparametrization trick [Kingma and Welling, 2013], which reparametrizes the approximated posterior \( q_\phi(w) \) by a deterministic and differentiable function \( w = g(\epsilon; \phi) \) with \( \epsilon \sim \mathcal{N}(0, 1) \), such that \( E_{q_\phi(w)}[\log p(y, w | X)] = E_{p(\epsilon)}[\log p(y, g(\epsilon; \phi) | X)] \).

Figure 1: Left: A spike-and-slab prior with slab probability \( p = 0.1 \) induces a binomial distribution on the number of relevant features. The proposed new prior can encode a spectrum of alternative beliefs, such as a discretized Gaussian or a ‘flattened’ Gaussian (for details see Section 3). Middle and right: the data (with PVE = 0.9 in its generating process) are more likely to be generated by a BNN when the PVE is set to be approximately correct (middle). The PVE of BNN can blow up easily (right). Colored lines are sample functions generated by the BNN. For detail, see Section 4.

Figure 2: Left: Non-centered parametrization of the GSM prior. We determine the distribution \( p(\lambda_i; \theta) \) (orange) by the prior knowledge about sparsity, and then determine the global scale parameter \( \tau \) (blue) by prior knowledge about the PVE. Right: A graphical model for encoding domain knowledge about the number of relevant features (sparsity) into the GSM prior. We introduce two intermediate random variables: the number of relevant features, \( m \), and an indicator variable for each feature \( I = \{I_i\}_{i=1}^D \), which will be marginalized out.
and \( p(\lambda_i^{(l)}; \theta) \) defines a hyper-prior on the local scales. The marginal distribution of \( w_i^{(l)} \) can be obtained by integrating out the local scales:
\[
p(w_i^{(l)}; \tau, \theta) = \int N(w_i^{(l)}; 0, \tau^2 \lambda_i^{(l)} \lambda_i^{(l)}) p(\lambda_i^{(l)}; \theta) d\lambda_i^{(l)}.
\]
(3)

Eq (2) can also be written in an equivalent non-centered parametrization [Papaspiliopoulos et al., 2007] form (Figure 2 left):
\[
w_i^{(l)} = \beta_i^{(l)} \lambda_i^{(l)}; \quad \beta_i^{(l)} \sim N(\beta_i^{(l)}; 0, \tau^2); \quad \lambda_i^{(l)} \sim p(\lambda_i^{(l)}; \theta),
\]
(4)

which has a better posterior geometry for inference [Bevan et al., 2015] than Eq (2). The non-centered parametrization form has been widely used in BNN literature [Louizos et al., 2017, Ghosh et al., 2018], and we also use this form in the rest of the paper.

Different \( p(\lambda_i^{(l)}; \theta) \) define different marginal prior distributions on the weights according to Eq (3). For example, when \( \lambda_i^{(l)} \) is Bernoulli, each weight \( w_i^{(l)} \) follows a spike-and-slab prior distribution [Mitchell and Beauchamp, 1988]: when \( \lambda_i^{(l)} \) is the half-Cauchy distribution, the weights are horseshoe [Carvalho et al., 2009]. The parameter \( \theta \) is important in practice, especially for small data sets [Piironen and Vehtari, 2017], as it controls the shape of \( p(\lambda_i^{(l)}; \theta) \), and thus affects the sparsity level of \( w \) directly. If the distribution of \( \lambda_i^{(l)} \) concentrates at 0, a sparse model will be preferred, otherwise, a dense model will be learned instead.

### 2.3 Proportion of Variance Explained

Assume that the data generating process takes the form
\[
y = f(x; w) + \epsilon,
\]
(5)

where \( f(x; w) \) is the model, and \( \epsilon \) is the unexplainable noise. The Proportion of Variance Explained (PVE) [Glantz et al., 1990] of \( f(x; w) \) on dataset \( \{X, y\} \), also called the coefficient of determination (R^2) in linear regression, is then defined as:
\[
PVE(w) = 1 - \frac{\text{Var}(y - f(x; w))}{\text{Var}(y)} = \frac{\text{Var}(f(x; w))}{\text{Var}(y)},
\]
(6)

and it is commonly used to measure of the impact of features \( x \) on the prediction target \( y \), especially in genomics [Martinen et al., 2014]. In general, PVE should be less than 1, because the variance of the predicted values should not exceed that of the data. However, it may easily happen that this does not hold in non-linear models, such as neural networks, unless explicitly accounted for. For an example see Figure 1.

It is known that the scale parameter of mean-field (fully factorized) Gaussian priors on BNNs affects the variability of the functions drawn from the prior [Neal, 2012], and thus the PVE. As we will show in Section 3 for BNNs with the GSM prior defined in Eq (2) the global scale \( \tau \) and the local scales \( p(\lambda_i^{(l)}; \theta) \) jointly control the PVE, and the effect of \( \tau \) grows exponentially as the depth increases. This underlines the importance of setting \( \tau \) properly based on the expected PVE. When the scale parameter is set so that the corresponding PVE is close to the true value, the model is more likely to recover the true data generating function (demonstration in Figure 1).

### 3 Prior knowledge about sparsity

In this section, we propose a new hyper-prior for the local scales \( p(\lambda_i^{(l)}; \theta) \) according to the generative model shown in Figure 2 (right). The new prior generates the local scales conditionally on the number of relevant features, which allows us to explicitly express domain knowledge about the number of relevant features.

#### 3.1 Discrete informative scale priors

We first consider the case when each scale \( \lambda_i^{(l)} \) is a discrete random variable with domain \( \{0, 1\} \), such as the independent Bernoulli scale parameters in the spike-and-slab prior. We will then generalize this to the continuous scale in Section 3.2.

##### 3.1.1 Prior on the number of relevant features

We assume the prior beliefs about the number of relevant features \( m \) is defined as \( p_m(m; \theta) \), i.e., a probability mass function for \( m \), where \( 0 \leq m \leq D \) (dimension of the dataset). The prior \( p_m \) directly controls the model sparsity. Intuitively, if \( p_m \) concentrates on 0, a sparse model is preferred as it has a high prior probability to use a small number of features; if \( p_m \) puts a large probability mass on \( D \), all of the features are likely to be used instead. Hence, unlike other priors encouraging shrinkage, such as Laplace or horseshoe, our new prior is more interpretable about sparsity as it directly models the number of relevant features.

The modeler can choose \( p_m(m; \theta) \) based on the prior information available. When we have a good idea about the number of relevant features, a unimodal prior can be used, such as a discretized Gaussian:
\[
p_m(m; \mu, \tau_m) = c_m \exp \left( -\frac{\tau_m (m - \mu)^2}{2} \right),
\]
(7)
where \( \mu \) is the mode, \( \tau_m \) represents the precision as the inverse variance in the continuous Gaussian, and \( c_n \) is the normalization constant. Often we may only be able to specify an interval for the number of relevant features. Then we can use, for example, a ‘flattened’ Gaussian (Figure 1):

\[
p_m(m; \mu_-, \mu_+, \tau_m) = c_n \exp\left\{-\frac{\tau_m R^2(m; \mu_+, \mu_-)}{2}\right\},
\]

\[
R(m; \mu_-, \mu_+) = \max\{(m - \mu_+), (\mu_- - m), 0\},
\]

where \([\mu_-, \mu_+]\) defines the interval where the probability is uniform and reaches its maximum value, and \(c_n\) is the corresponding normalization constant. If there is no prior information about sparsity, a discrete uniform prior over \([0, D]\) is a plausible alternative.

### 3.1.2 Feature allocation

Given the prior distribution \( p_m(m; \theta) \), we specify how it affects which variables will be used first for a given \( m \), and then marginalize over \( m \). We introduce identity variables \( I_i \in \{0, 1\} \) to denote if feature \( i \) is used (\( I_i = 1 \)) or not (\( I_i = 0 \)); they should satisfy \( m = \sum_{i=1}^{D} I_i \). Assuming no prior knowledge about relative importance of features (this assumption can be easily replaced if needed), i.e., \{\( I_i \)\}_{i=1}^{D} has a jointly uniform distribution given \( m \), we have:

\[
p(I_{i}^{D}|m) = c_d \delta[m - \sum_{i=1}^{D} I_i],
\]

where the normalization constant is \( c_d = \frac{(D)^{-1}}{m} \).

Now we can calculate the joint distribution of \{\( I_i \)\}_{i=1}^{D} by marginalizing out \( m \):

\[
p(I_{i}^{D}; \theta) = \sum_{m=0}^{D} p_m(m; \theta)p(I_{i}^{D}|m),
\]

\[
= p_m\left(\sum_{i=1}^{D} I_i; \theta\right)\left(\sum_{i=1}^{D} I_i\right)^{-1}.
\]

For Bernoulli local scale variables \( \lambda_i^{(l)} \), the \( \lambda_i^{(l)} \) itself takes the role of the identity variable \( I_i \). Thus we obtain the joint distribution over discrete scale parameters \( \lambda_i \) as

\[
p_d(\lambda_1^{(l)}, \ldots, \lambda_D^{(l)}; \theta) = p_m(\sum_{i=1}^{D} \lambda_i^{(l)}; \theta)\left(\sum_{i=1}^{D} \lambda_i^{(l)}\right)^{-1},
\]

where the distribution \( p_m(\sum_{i=1}^{D} \lambda_i^{(l)}; \theta) \) encodes our domain knowledge of the number of relevant features.

Generally, the local scales \{\( \lambda_i^{(l)} \)\}_{i=1}^{D} are dependent. However, when \( p_m(m; \theta) \) is a Binomial distribution (or a Gaussian approximated by a Binomial), the joint distribution of the local scales \{\( \lambda_i^{(l)} \)\}_{i=1}^{D} becomes a product of independent Bernoullis in Eq.11 which corresponds to the spike-and-slab prior (Figure 1).

### 3.2 Informative prior on continuous local scales

When the local scales are continuous (\( \lambda_i^{(l)} \in [0, +\infty) \)), the number of relevant features \( m \) is not a sensible way to define sparsity, because the posterior probability of the event \{\( w_i^{(l)} = 0 \)\} is zero almost everywhere [Carvalho et al. 2009]. Thus \( m \) will always equal \( D \), unless heuristic pruning is used [Louizos et al. 2017].

Instead of using the number of relevant features to represent sparsity, we propose to use the effective number of features \( m_{eff} \) [Pirinen and Vehtari 2017], which is defined as

\[
m_{eff} = \sum_{i=1}^{D} \eta_i = \sum_{i=1}^{D} (1 - \kappa_i),
\]

where \( \kappa_i \) is the shrinkage factor [Carvalho et al. 2009] that can be defined for any GSM prior as follows: The \( \kappa_i \) reflects the proportion the feature \( i \) is shrunk compared to its maximum likelihood estimate, and it is defined as

\[
\kappa_i = \frac{c_s}{c_s + \lambda_i^{(l)}},
\]

where \( c_s \) is a small positive constant [Carvalho et al. 2009]. In our experiments we simply use \( c_s = 0.1 \) to apply this with BNNs. We assume that the user can give a prior belief \( p_{m_{eff}}(m_{eff}; \theta) \) about \( m_{eff} \) in a similar way as the number of relevant features \( m \) in Section 3.1.

Inspired by Eq.10 for the discrete case, we define the joint distribution on \( \eta_i \):

\[
p(\eta_1, \ldots, \eta_D; \theta) \propto p_{m_{eff}}(\sum_{i=1}^{D} \eta_i; \theta)\left(\sum_{i=1}^{D} \eta_i\right)^{-1},
\]

where \( p_{m_{eff}}(m_{eff}; \theta) \) is a continuous prior for the effective number of features, analogously to the discrete prior over the number of relevant features in Section 3.1. The Binomial coefficient in Eq.14 is calculated for the continuous \( \sum_{i=1}^{D} \eta_i \) using the Stirling’s approximation. Since the non-shrinkage factor \( \eta_i = 1 - \kappa_i \) increases monotonically\(^\text{1}\),

\([^\text{1}]:\) For example, \( c_s = \sigma^2 N^{-1} \tau^{-2} \) in Bayesian linear regression [Carvalho et al. 2009], where \( \sigma^2 \) is the variance of data, \( N \) is the size of data, and \( \tau \) is the global scale parameter.
A more concentrated \( m_{\text{eff}} \) induces a \( \lambda_i \) with a heavier tail. w.r.t. \( \lambda_i^{(l)} \), we get the joint density of the scale parameters using the law of change of variables:

\[
p_c(\lambda_1, \ldots, \lambda_D; \theta) \propto p_{m_{\text{eff}}} \left( \sum_{i=1}^{D} \eta(\lambda_i^{(l)}); \theta \right) \left( \sum_{i=1}^{D} \frac{1}{\eta(\lambda_i^{(l)})} \right)^{-1} \prod_{i=1}^{D} \frac{d\eta(\lambda_i^{(l)})}{d\lambda_i^{(l)}},
\]

where \( \eta(\lambda_i^{(l)}) = \eta_i = \frac{1}{\sqrt{c_i + \lambda_i^{(l)^2}}} \). We show the marginal distribution of \( \lambda_i \) for different \( p_{m_{\text{eff}}}(m_{\text{eff}}; \theta) \) in Figure 3. When \( p_{m_{\text{eff}}} \) concentrates more on 0, e.g., the \( N(0, 0.5) \) in Figure 3 (left), \( \lambda_i \) has a heavier tail (the blue line in Figure 3 right). We note that although the normalization constant is not analytically available in Eq (15) making inference with this prior is still feasible via variational inference and the reparameterization trick.

### 3.3 BNNs with informative priors

In BNNs, the number of features used by the model (sparsity) is determined by the weights in the input layer, unless all nodes of any hidden layer are jointly dropped, which is very unlikely in practice. Thus we encode the domain knowledge on sparsity in the informative prior of the input layer, i.e., \( l = 0 \) in Eq (11) and (15). For the other layers we use the spike-and-slab in our experiments (see Experiments). However, informative priors could also be used in higher layers. Because specifying domain knowledge about the number of hidden nodes would be difficult, \( p_m \) could be set to be uniform. This way one could potentially learn the optimal number of hidden nodes, and we leave this for future work.

To summarizing, according to Section 3.1 we use the following prior on the input layer:

\[
w^{(0)} = \beta^{(0)} \lambda^{(0)}; \quad \beta_{i,j}^{(0)} \sim N(\beta_{i,j}^{(0)}; 0, \tau^2),
\]

with the hyper-prior on the local scales following \( \lambda^{(0)} \sim p_d(\lambda^{(0)}; \theta) \) for discrete cases and \( \lambda^{(0)} \sim p_c(\lambda^{(0)}; \theta) \) for continuous cases. We use independent concrete Bernoulli distributions \([\text{Maddison et al.}, 2016]\) to approximate the posterior of \( \lambda^{(0)} \) in the discrete case and Log-normal in the continuous case, and independent Gaussian to approximate the posterior of \( \beta^{(0)} \) for both cases.

### 4 Prior knowledge about PVE

In this section, we introduce an approach for determining the global scale \( \tau \) for the GSM priors in Eq (4) according to domain knowledge about the expected PVE.

#### 4.1 PVE for Bayesian neural networks

According to the definition of PVE in Eq (6), when \( f(x; w) \) is a BNN, PVE\((w)\) has a distribution determined by the distribution of \( w \). In this paper, instead of analysing the distribution of PVE\((w)\), we analyse a summary statistic of the PVE commonly used in Bayesian linear model \([\text{Gelman et al.}, 2019]\). The statistic is the expected PVE\((w)\),

\[
\mu_{\text{PVE}} = \mathbb{E}_{p(w)}[\text{PVE}(w)],
\]

over functions drawn from the BNN. Consequently, instead of restricting PVE directly, we express the prior beliefs using \( \mu_{\text{PVE}} \), e.g., requiring it to be less than 1.

For BNNs with arbitrary activation functions or priors \( p(w) \), the analytical form of \( \mu_{\text{PVE}} \) is intractable. However, under certain assumptions, we have the following theorem (Proof in the Supplement):

**Theorem 1.** If the weights \( \{w_{i,j}^{(l)}\} \) in different layers \( l \geq 1 \) are independent, and priors \( \{w_{i,j}^{(l)}\} \) within any single layer \( l \) have a zero mean and the same second moment \( \sigma_{i,j}^{(l)^2} \), then the expected PVE of a ReLU BNN with \( L \) hidden layers and \( M_l \) units in layer \( l \) is given by

\[
\mu_{\text{PVE}} = \alpha \sigma^{(l)^2} \prod_{l=1}^{L} \sigma_{i,j}^{(l)^2} \sum_{i=1}^{D} \frac{\text{Var}(x_i)}{\text{Var}(y)},
\]

where \( \alpha \) is a constant independent of the priors of weights.

**Theorem 1** will be used to determine the global scale \( \tau \) according to the prior knowledge on \( \mu_{\text{PVE}} \) in Section 4.2. Note that **Theorem 1** is applicable to the commonly used priors, such as the fully factorized Gaussian or the spike-and-slab, as well as to the new proposed informative prior, as long as the second moment of the prior is finite.

#### 4.2 Determining \( \tau \) according to PVE

For any zero-mean GSM ARD prior for BNNs, the variance (second moment) of the weight \( w_{i,j}^{(l)} \) in Eq (4) equals:

\[
\sigma_{i,j}^{(l)^2} = \mathbb{E}[(\beta_{i,j}^{(l)})^2] \mathbb{E}[(\lambda_{i,j}^{(l)})^2] = \mathbb{E}[\lambda_{i,j}^{(l)^2}] \tau^2.
\]
In practice, we first set the hyper-priors on the local scales (the same for all nodes within a single layer), \( p(\alpha^{(l)}; \theta) \), by encoding the domain knowledge about sparsity, which determines \( E[\alpha^{(l)}_i] = E[\alpha^{(l)}_j] \). According to Theorem 1, the expected PVE can be simplified to

\[
\mu_{PVE} = \tilde{\alpha} \tau^{2L+2}
\]

where \( \tilde{\alpha} \) is a constant that depends on the variance of the data, model architecture, and pre-encoded sparsity, independent of \( \tau \). Hence, we see that when the factors affecting \( \tilde{\alpha} \) are kept constant, \( \mu_{PVE} \) is fully determined by the global scale \( \tau \) alone.

Both \( \alpha \) and \( \tilde{\alpha} \) in Eq (19) are only analytically tractable when all \( M_l \) are infinite (Shown in the Supplement), which is impractical. However, since we know the exact form of \( \mu_{PVE} \), we can obtain a very accurate estimation of \( \tilde{\alpha} \) by solving the linear regression problem

\[
\log \mu_{PVE} = \log \tilde{\alpha} + (2L + 2) \log \tau.
\]

We solve Eq (20) using data \( \{(\tau_k, \mu_{PVE})\}_{k=1}^K \) obtained by simulating from the BNN (with the pre-specified prior and data \( \{X, y\} \)) for multiple values of \( \tau_k \) to get a Monte-Carlo estimate of the corresponding \( \mu_{PVE} \), and in practice \( K = 20 \) is enough to make the \( R^2 \) of Eq (20) greater than 99.99%. See an algorithm and example in Supplementary.

After the constant \( \tilde{\alpha} \) has been estimated, \( \tau \) can be specified using domain knowledge about \( \mu_{PVE} \), according to Eq (19). We set the aleatoric uncertainty, i.e., \( \text{Var}(\epsilon) \) in Eq (5), to \( 1 - \mu_{PVE} \), so that the model Eq (5) is consistent with our prior knowledge. If we have no relevant knowledge, a non-informative prior on \( \mu_{PVE} \) can be used instead, such as the uniform distribution on \( [0, 1] \). According to the change of variable, the prior induced on \( \tau \) is given by

\[
p(\tau) = p(\mu_{PVE}) \left| \frac{d\mu_{PVE}}{d\tau} \right| = \tilde{\alpha}(2L + 2) \tau^{2L+1}. \tag{21}
\]

For some heavy-tailed priors, e.g. the horseshoe, whose second moments do not exist, \( \mu_{PVE} \) does not exist either, and Theorem 1 cannot be applied. However, other summary statistics of the PVE(w), such as the median, may be used to determine the global parameter for the horseshoe. We leave this for future work.

## 5 Related Work

BNNs with a fully factorized Gaussian prior and posterior were proposed by [Graves, 2011]. BNNs with a fully factorized Gaussian prior and a mixture of Dirac-delta posteriors can be interpreted as NNs with dropout [Gal and Ghahramani, 2016]. Nalisnick et al. [2019] extended these works, and showed that NNs with any multiplicative noise can be interpreted as BNNs with GSM ARD priors. Some priors have been proposed to induce sparsity, such as log-uniform priors [Louizos et al., 2017], horseshoe priors [Louizos et al., 2017, Ghosh et al., 2018], and Spike-and-slab priors [Deng et al., 2019]. However, none of the works has proposed how to encode domain knowledge explicitly.

Building informative priors for neural networks in the functional space has been widely studied. One common type of prior information concerns the behavior of the output with certain inputs. Noise contrastive priors (NCPs) [Hafner et al., 2018] were designed to encourage reliable high uncertainty for OOD (out-of-distribution) data points. Gaussian processes have been widely used as functional priors, because of their ability to encode rich functional structures. Flam-Shepherd et al. [2017] transformed a functional GP prior into a weight-space BNN prior, with which variational inference is performed. Functional BNNs [Sun et al., 2019], however, perform variational inference directly in the functional space, where meaningful functional GP priors can be specified. Pearce et al. [2019] used a combination of different BNN architectures to encode prior knowledge about the function. Although building functional priors can avoid uninterpretable high-dimensional weights, encoding sparsity information of features into the functional space is not trivial.

## 6 Experiments

We first apply BNNs with the new discrete informative prior on synthetic datasets, and compare the convergence rate with the ‘golden standard’ baseline: the spike-and-slab prior. We then apply our approach on 5 public UCI datasets with and without injected irrelevant features, and to a Genome-Wide Association Study (GWAS) dataset. We show that incorporating domain knowledge on both sparsity and PVE through our approach can improve the results. All data sets were standardized before training.

### Common model settings

We used BNNs with ARD spike-and-slab prior (SSBNN) as the baseline for discrete scales, where the slab probabilities \( p \) of input layers were determined based on knowledge about the number of relevant features, and the slab probabilities of hidden layers were set to 0.1. We consider the horseshoe prior on all layers (HSBNN) as the baseline for continuous scales, using the same hyper-parameters as in Ghosh et al. [2018]. For BNNs with informative priors on the input layers, we used the ‘flattened’ Gaussian (Eq (8)) to model the number of relevant features \( m \) for discrete cases (InfoD), and the effective number of features \( m_{eff} \) for continuous cases (InfoC). The hidden layers of InfoD are the same as in SSBNN, and InfoC are the same as in the corresponding HSBNN.
Figure 4: Experiments on synthetic datasets for different data sizes (300, 700, 1100). We compared the spike-and-slab prior (SSBNN) and discrete informative priors (InfoD) with 3 different types of information. The discrete informative priors have a better convergence when the prior belief about sparsity is tight and accurate (blue lines), especially in small datasets. InfoD can converge to the correct number of features (10, the green dotted lines), while SSBNN fails.

6.1 Synthetic data

Setup: We simulated datasets with 500 features, of which only 10 are used to compute the target with the model \( y = f(x_{1:10}; w) + \epsilon \). The model contains both main effects and interactions between the selected features (details in Supplementary). The noise \( \epsilon \) is Gaussian with zero mean and standard deviation equal to 3, so that the signal-to-noise ratio is 1. We generated 3 datasets of different sizes (300, 700, and 1100), and compared the convergence of both MSE and sparsity (number of features) with different priors for each dataset. We used the test MSE to determine convergence. The expected number of features included in the first layer, calculated using the feature inclusion probabilities, is used as the estimate for the number of relevant features for both the priors.

Parameter settings: We applied BNNs with two different types of ARD priors: spike-and-slab prior (SSBNN) and discrete informative prior (InfoD). The common global scale is \( \tau = 0.1 \) for all models. The slab probability of SSBNN on the first layer is set to 0.02, to reflect the expected number 10 of relevant features. We encoded three types of prior knowledge into InfoD by setting \( \mu_- \) and \( \mu_+ \) differently:

1. a strongly informative InfoD \( (\mu_- = 5, \mu_+ = 15) \);
2. a weakly informative InfoD \( (\mu_- = 0, \mu_+ = 150) \);
3. a wrong InfoD \( (\mu_- = 150, \mu_+ = 250) \).

We used a concrete Bernoulli with temperature 0.1 to approximate the posteriors of scales for both SS and InfoD priors, and set the learning rate of Adam to \( 10^{-2} \). The neural networks architecture that we used have 2 hidden layers of sizes 100 and 50 nodes.

Results: Figure 4 shows the convergence of test error and sparsity (the number of relevant features) with the different priors. For small datasets (300), when prior is more important, the InfoD prior with the wrong information converges to the same MSE and number of features as the SS prior, while the InfoD priors with correct information converge to a lower MSE and the correct number of features (10, the green dotted lines). When we increase the data size to 700, InfoD with the wrong information converges to the correct sparsity and the same MSE as the correct InfoD priors, but more slowly. For the largest dataset with 1100 data points, the converged MSEs for the different priors are similar. However, with the SS prior the number of features is overestimated even at convergence. The strongly informative InfoD prior always converges faster than the weakly informative InfoD prior, but the advantage diminishes when the size of the dataset increases.

6.2 UCI datasets

Setup: We analyze 5 publicly available datasets (Table 1): Bike sharing, California housing prices, Energy efficiency, Concrete compressive strength, and Yacht hydrodynamics. We carry out two types of experiments: 1. analyze the original datasets as such, in which case the domain knowledge about sparsity is unknown; 2. concatenate 100 irrelevant features with the original features, which allows us to specify informative priors about sparsity (the number of relevant features is at most the number of original features). We examine whether the performance can be improved by encoding the extra knowledge about the PVE and sparsity into the prior. We use 60% of data for training, 20% for validation, and 20% for testing. We consider three evaluation metrics: negative log-likelihood (NLL),
Table 1: NLL with \( \text{mean-field} \) and ARD priors; 3. continuous GSM ARD priors. The best result on each row has been boldfaced. The dimension \( (P) \) and size \( (N) \) of each dataset are shown in the second column. We see that informative priors (InfoD and InfoC) perform better both in discrete and continuous cases, especially when prior information is available (on extended datasets), and the knowledge of PVE improves the performance constantly.

| Datasets               | \( D/N \) | \text{mean-field} | SSBNN | SSBNN+PVE | InfoD | InfoD+PVE | HSBNN | InfoC |
|------------------------|-----------|------------------|-------|-----------|-------|-----------|-------|-------|
| Bike                   | 13, 17k   | .270 ± .001      | .271 ± .011 | .265 ± .006 | .261 ± .005 | .259 ± .003 | .256 ± .003 | .261 ± .002 |
| California             | 9, 20k    | .406 ± .002      | .396 ± .003 | .396 ± .001 | .395 ± .003 | .395 ± .002 | .383 ± .003 | .383 ± .002 |
| Energy                 | 8, 0.7k   | .418 ± .010      | .397 ± .017 | .360 ± .010 | .375 ± .008 | .359 ± .006 | .343 ± .001 | .341 ± .009 |
| Concrete               | 8, 1k     | .475 ± .006      | .410 ± .013 | .406 ± .006 | .404 ± .007 | .399 ± .005 | .399 ± .005 | .403 ± .005 |
| Yacht                  | 6, 0.3k   | .393 ± .006      | .255 ± .009 | .256 ± .007 | .254 ± .009 | .244 ± .008 | .285 ± .012 | .271 ± .011 |

For the original datasets, we see that setting the global scale \( \tau \) according to \( \mu_{\text{PVE}} \) (SSBNN+PVE and InfoD+PVE) increases the data likelihood, which reflects both the quality of predictive uncertainty and prediction accuracy. The new proposed informative priors (InfoD and InfoC) can also slightly improve the performance for the smaller datasets although we have no prior information about sparsity to encode. Horseshoe (HSBNN) has a comparable performance even without explicitly encoded information.

In the extended datasets with 100 extra irrelevant features, knowledge of both PVE and sparsity improve the performance significantly in discrete-scale cases. For most datasets, SSBNNs even with the correct level of sparsity are not good enough to produce reasonable results. We find that for the large datasets, the discrete-scale priors are better than the continuous ones, and for small datasets, continuous-scale priors have better performance, although they cannot include information about the PVE. We also find that non-sparsity-inducing priors (mean-field Gaussian) work comparably on some original datasets with large \( N \), but work poorly on most datasets.

The results with \( \mu_{\text{PVE}} = 0.7/0.9 \) (Supplementary) show that the conclusions are not sensitive to the specific value of PVE assumed.

6.3 GWAS application

**Motivation:** The goal of a Genome-Wide Association Study (GWAS) is to learn associations between genetic variants called SNPs (input features) and phenotypes (targets). Ultimately, the goal is to predict the phenotype given the SNPs of an individual. This task is extremely challenging because 1. the input features are very high-dimensional and strongly correlated and 2. they may
explain only a tiny fraction of the variance of the phenotype, e.g., less than 1%. Thus, most approaches employ several heuristic but crucial preprocessing steps to reduce the input dimension and correlation. There exists strong domain knowledge about sparsity and the amount of variance explained by the SNPs, and we show that by incorporating this knowledge into informative priors we can accurately predict where alternatives fail.

Dataset: The FINRISKI dataset contains SNPs and 228 different metabolites as phenotypes for 4620 individuals. We selected 6 genes that have previously been associated with the metabolites [Kettunen et al., 2016]. We use the SNPs of each gene to predict the corresponding most correlated metabolite, resulting in 6 different experiments.

Parameter settings: We train BNNs with 1 hidden layer consisting of 100 hidden nodes. We consider 3 different priors: mean-field Gaussian, spike-and-slab (SSBNN), and the discrete informative prior (InfoD). We make predictions using the posterior mean and evaluate the performance by the PVE (higher is better) on test data. We use 50% of data for training and 50% for testing, and we repeat this 50 times for each of the 6 experiments (i.e. genes), allowing us to assess experiment specific variability due to the random split and training.

The slab probability \( p \) of SSBNN is fixed to 0.1, and we use \( \mu_+ = 0 \) and \( \mu_- = 0.2D \) in InfoD, where \( D \) is the number of SNPs in the chosen gene. This reflects the prior belief that less than 20% of the SNPs in the gene actually affect the phenotype. The global scale \( \tau \) of each prior is either fixed to 1 (without prior information about PVE), or calculated by setting \( \mu_{PVE} \) to previous findings [Kettunen et al., 2016] according to Section 4.

Results: Figure 5 shows results for the 6 experiments. We see that setting the \( \tau \) according to the prior knowledge on the PVE always improves accuracy and reduces uncertainty for all priors (purple bars). Without using the prior knowledge on the PVE, learning with all priors can overfit seriously (blue bars, negative test PVE). The novel informative discrete GSM prior has the highest accuracy with the smallest standard deviation in all experiments, both with PVE and without PVE.

7 Conclusion

We proposed a new informative Gaussian scale mixture prior on BNN weights, whose global and local scale parameters are specified using domain knowledge about expected signal-to-noise ratio and sparsity. We demonstrated the utility of the prior on simulated data, publicly available datasets, and in a GWAS application, where they outperformed strong commonly used baselines. The informative hyper-prior over the local scales can be generalized to all scale mixture distributions, not just the Gaussian scale mixture, such as the Strawderman-Berger prior. Possible future work includes encoding PVE into heavy-tailed distributions, such as the horseshoe, and extending the results to hierarchical priors (hyper-prior over the global scale).
References

D. F. Andrews and C. L. Mallows. Scale mixtures of normal distributions. *Journal of the Royal Statistical Society: Series B (Methodological)*, 36(1):99–102, 1974.

M. Betancourt and M. Girolami. Hamiltonian Monte Carlo for hierarchical models. *Current Trends in Bayesian Methodology with Applications*, 79:30, 2015.

C. Blundell, J. Cornebise, K. Kavukcuoglu, and D. Wierstra. Weight uncertainty in neural networks. *arXiv preprint arXiv:1505.05424*, 2015.

C. M. Carvalho, N. G. Polson, and J. G. Scott. Handling sparsity via the horseshoe. In *Artificial Intelligence and Statistics*, pages 73–80, 2009.

W. Deng, X. Zhang, F. Liang, and G. Lin. An adaptive empirical Bayesian method for sparse deep learning. In *Advances in Neural Information Processing Systems*, pages 5564–5574, 2019.

D. Flam-Shepherd, J. Requeima, and D. Duvenaud. Mapping Gaussian process priors to Bayesian neural networks. In *NIPS Bayesian deep learning workshop*, 2017.

Y. Gal and Z. Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In *International Conference on Machine Learning*, pages 1050–1059, 2016.

A. Gelman, J. B. Carlin, H. S. Stern, D. B. Dunson, A. Vehtari, and D. B. Rubin. *Bayesian Data Analysis*. Chapman and Hall/CRC, 2013.

A. Gelman, B. Goodrich, J. Gabry, and A. Vehtari. R-squared for Bayesian regression models. *The American Statistician*, pages 1–7, 2019.

S. Ghosh, J. Yao, and F. Doshi-Velez. Structured variational learning of Bayesian neural networks with horseshoe priors. In *International Conference on Machine Learning*, pages 1739–1748, 2018.

S. A. Glantz, B. K. Slinker, and T. B. Neilands. *Primer of applied regression and analysis of variance*, volume 309. McGraw-Hill New York, 1990.

A. Graves. Practical variational inference for neural networks. In *Advances in Neural Information Processing Systems*, pages 2348–2356, 2011.

D. Hafner, D. Tran, T. Lillicrap, A. Irpan, and J. Davidson. Noise contrastive priors for functional uncertainty. *arXiv preprint arXiv:1807.09289*, 2018.

J. Kettunen, A. Demirkan, P. Würtz, H. H. Draisma, T. Haller, R. Rawal, A. Vaarhorst, A. J. Kangas, L.-P. Lyttikäinen, M. Pirinen, et al. Genome-wide study for circulating metabolites identifies 62 loci and reveals novel systemic effects of Lpa. *Nature Communications*, 7(1):1–9, 2016.

D. P. Kingma and M. Welling. Auto-encoding variational bayes. *arXiv preprint arXiv:1312.6114*, 2013.

C. Louizos, K. Ullrich, and M. Welling. Bayesian compression for deep learning. In *Advances in Neural Information Processing Systems*, pages 3288–3298, 2017.

D. J. MacKay. A practical Bayesian framework for backpropagation networks. *Neural Computation*, 4(3):448–472, 1992.

D. J. MacKay. Bayesian non-linear modeling for the prediction competition. In *Maximum Entropy and Bayesian Methods*, pages 221–234. Springer, 1996.

C. J. Maddison, A. Mnih, and Y. W. Teh. The concrete distribution: A continuous relaxation of discrete random variables. *arXiv preprint arXiv:1611.00712*, 2016.

P. Marttinen, M. Pirinen, A.-P. Sarin, J. Gillberg, J. Kettunen, I. Surakka, A. J. Kangas, P. Soininen, P. O’Reilly, M. Kaakinen, et al. Assessing multivariate gene-metabolome associations with rare variants using Bayesian reduced rank regression. *Bioinformatics*, 30(14):2026–2034, 2014.

T. J. Mitchell and J. J. Beauchamp. Bayesian variable selection in linear regression. *Journal of the American Statistical Association*, 83(404):1023–1032, 1988.

E. Nalisnick, J. M. Hernandez-Lobato, and P. Smyth. Dropout as a structured shrinkage prior. In *International Conference on Machine Learning*, pages 4712–4722, 2019.

R. M. Neal. *Bayesian learning for neural networks*, volume 118. Springer Science & Business Media, 2012.

O. Papaspiliopoulos, G. O. Roberts, and M. Sköld. A general framework for the parametrization of hierarchical models. *Statistical Science*, pages 59–73, 2007.

T. Pearce, M. Zaki, A. Brintrup, and A. Neely. Expressive priors in Bayesian neural networks: Kernel combinations and periodic functions. *arXiv preprint arXiv:1905.06076*, 2019.

J. Piironen and A. Vehtari. On the hyperprior choice for the global shrinkage parameter in the horseshoe prior. In *Artificial Intelligence and Statistics*, pages 905–913, 2017.

S. Sun, G. Zhang, J. Shi, and R. Grosse. Functional variational Bayesian neural networks. *arXiv preprint arXiv:1903.05779*, 2019.

F. Wenzel, K. Roth, B. S. Veeling, J. Swiatkowski, L. Tran, S. Mandt, J. Snoek, T. Salimans, R. Jena
ton, and S. Nowozin. How good is the bayes posterior in deep neural networks really? *arXiv preprint arXiv:2002.02405*, 2020.
Supplementary

8 Proof of Theorem 1

8.1 Introduction

We first introduce the notation and some well known results from probability theory.

Figure 6: A fully connected neural network.

Notations: We denote $a^{(l)}_i$ to be any one of the nodes in $l$th hidden layer before activation function $\phi(\cdot)$, and $h^{(l)}_i$ is the node after the activation. We use $w^{(l)}$ to represent all the weights from layer 0 (input layer) to layer $l$. The weights from layer $l$ to layer $l+1$ are independent. We use the subscript $i$, such as $a^{(l)}_i$ to denote, the $i$th node in a layer. The output of the neural network is $\hat{y} = f(x; w)$, where $x$ is the input. All the activation functions are ReLU. We assume in the prior distribution, weights $w^{(l)}$ in different layers are independent. We use $w^{(0)}$ denotes all the weights from layer 0 (input layer) to layer 1. The weights from same layer $l$ have the same prior with mean 0 and variance $\sigma_l^2$. When the $M_l$ are large, nodes follow Gaussian distribution according to central limit theorem. We assume all weights $w$ are independent with nodes, and there is no bias term in each layer. Features $x^{(l)}$ are also independent with each other.

Targets: We derive the form of

$$\mu_{pve} = E_{p(w)}[\frac{\text{Var}_x(f(X; w))}{\text{Var}_y(y)}]$$

(22)

where we normalize $y$ to have unit variance.

Probability results: We have following results based on above assumptions.

When $w_{j,i}^{(l)}$ is not considered as a random variable:

$$E[a^{(l)}_i] = \sum_j w_{j,i}^{(l-1)} E[h_j^{(l-1)}],$$

$$\text{Var}(a^{(l)}_i) = \sum_j w_{j,i}^{(l-1)2} \text{Var}(h_j^{(l-1)}) + \sum_{k,j \neq k} w_{j,i}^{(l-1)} \text{Cov}(h_j^{(l-1)}, h_k^{(l-1)}) w_{k,i}^{(l-1)}.$$  (23)

If Gaussian random variable $a$ has mean $\mu_a$ and variance $\sigma_a^2$, the first two moment of $a$ after ReLU activation $h = \phi(a)$ are:

$$E[h] = \int_{0}^{+\infty} a \frac{1}{\sqrt{2\pi}\sigma_a} e^{-\frac{(a-\mu_a)^2}{2\sigma_a^2}} da = \sigma_a SR(\mu_a);$$

$$E[h^2] = \int_{0}^{+\infty} a^2 \frac{1}{\sqrt{2\pi}\sigma_a} e^{-\frac{(a-\mu_a)^2}{2\sigma_a^2}} da = \sigma_a^2 [\mu_a \psi(\mu_a) + (1 + \mu_a^2)\Psi(\mu_a)],$$

where $\mu_a = \frac{\mu_a}{\sigma_a}$, $SR(x) = \psi(x) + x \Psi(x)$, $\psi(x)$ and $\Psi(x)$ are the PDF and CDF of standard Gaussian [Wu et al., 2018].

8.2 Proof of Theorem 1

According to Eq[24] we have following recursion:

$$E_{p(w^{(1:1-1)})}[\text{Var}_X(h^{(1)}_i)]$$

$$= E[E[h^2] - E[h_i]^2]$$

$$= E[\text{Var}_X(a^{(l)}_i)\mu_a^{(l)} \psi(\mu_a^{(l)}) + (1 + \mu_a^{(2)}(l))\Psi(\mu_a^{(l)})] - \text{Var}(a^{(l)})SR^2(\mu_a^{(l)})]$$

$$= E_{p(w^{(1:1-1)})}[\text{Var}_X(a^{(l)}_i)\beta(\mu_a^{(l)})],$$

(25)

where $\beta(\mu_a^{(l)}) = \mu_a^{(l)} \psi(\mu_a^{(l)}) + (1 + \mu_a^{(2)}(l))\Psi(\mu_a^{(l)}) - SR^2(\mu_a^{(l)})$ is the variance shrinkage factor of layer $l$, i.e., how much the variance will be shrunk by passing through a ReLU activation, and we use $\beta_l = \beta(\mu_a^{(l)})$ for simplicity. We first prove that $\beta(\mu_a^{(l)})$ is a constant for infinitely wide neural networks, and we then show $\beta_l$ is independent of $p(w)$ empirically for any finite neural network.

Lemma 2. The variance shrinkage factor of $l$th ReLU layer $\beta_l$ is a constant for any infinitely wide neural network, and it can be calculated by:

$$\beta_l = \beta(0) = \frac{\pi - 1}{2\pi},$$

where $\beta(\cdot)$ is mentioned in Eq[25].
Proof. We denote that $\mu_h^{(l)}$ and $\sigma_h^{2(l)}$ are the mean and variance of $h_i^{(l)}$. According to Eq 23, we know that:

$$
\begin{align*}
\mu_{a_l}^{(l)} &= \sum_j w_{j,i}^{(l-1)} \mu_{h_i}^{(l-1)}, \\
\sigma_{a_l}^{2(l)} &= \sum_j w_{j,i}^{(l-1)2} \sigma_{h_i}^{2(l-1)} + \sum_{k,j \neq k} w_{j,i}^{(l-1)} \text{Cov}(h_j^{(l-1)}, h_k^{(l-1)}) w_{k,i}^{(l-1)}.
\end{align*}
$$

(26)

Based on the symmetry of the hidden nodes, the covariance between two different hidden nodes in the same layer, Cov$(h_j^{(l-1)}, h_k^{(l-1)})$, are the same. And the mean $\mu_{h_j}^{(l-1)}$ for different hidden node in layer $l-1$ is also the same, i.e., $\mu_{h_j}^{(l-1)} = \mu_{h_k}^{(l-1)}$.

According to the central limit theorem, the summation $\sum_{k,j \neq k} w_{j,i}^{(l-1)} w_{k,i}^{(l-1)} = 0$ and $\sum_j w_{j,i}^{(l-1)} = 0$, when the number of hidden units go to infinity. Thus Eq 26 can be rewritten as:

$$
\begin{align*}
\mu_{a_l}^{(l)} &= 0, \\
\sigma_{a_l}^{2(l)} &= \sum_j w_{j,i}^{(l-1)2} \sigma_{h_i}^{2(l-1)},
\end{align*}
$$

(27)

which implies that

$$\mu_{a_l}^{(l)} = 0.$$

(28)

Thus the variance shrinkage factor for any layer $l$ is

$$\beta_l = \beta(0) = \frac{\pi - 1}{2\pi},$$

which is the Lemma 2.

Then Eq 25 can be rewritten as:

$$
\begin{align*}
\mathbb{E}_{p(w)} [\text{Var}_X (h_j^{(l)})] &= \beta_l \mathbb{E}_{p(w)} [\text{Var}_X (a_l^{(l)})],
\end{align*}
$$

(29)

according to Lemma 2. Note that although theoretically Eq 29 only holds for infinitely wide neural networks, however, empirically (Figure 7), we find that Eq 29 still holds for neural networks with finite hidden nodes.

In prediction tasks, the final layer is $f(X;w) = \sum_{j=1}^{M_L} w_j^{(L)} h_j^{(L)}$, so we have:

$$
\begin{align*}
\mathbb{E}_{p(w)} [\text{Var}_X (f(X;w))] &= \mathbb{E}_{p(w)} [\sum_j w_j^{(L)2} \mathbb{E}_{p(w)} (h_j^{(L)})] \\
&= M_L \sigma (L)^2 \mathbb{E}_{p(w)} [\text{Var}_X (h_j^{(L)})]
\end{align*}
$$

(30)

According to Eq 23 we have following recursive equation:

$$
\begin{align*}
\beta_l \mathbb{E}_{p(w)} [\text{Var}_X (a_l^{(l)})] &= \beta_l \mathbb{E}_{p(w)} [\sum_j w_j^{(l-1)2} \text{Var}_X (h_j^{(l-1)})] \\
&+ \sum_{j,k,j \neq k} w_j^{(l-1)} \text{Cov}(h_j^{(l-1)}, h_k^{(l-1)}) w_k^{(l-1)} \\
&= \beta_l \mathbb{E}_{p(w)} [\sum_j w_j^{(l-1)2} \mathbb{E}_{p(w)} (h_j^{(l-2)})] \text{Var}_X (h_j^{(l-1)}) \\
&+ \beta_l M_l \sigma (l)^2 \mathbb{E}_{p(w)} [\text{Var}_X (h_j^{(l-1)})].
\end{align*}
$$

(31)

Also, for the first layer, by assuming all the features are independent, we have:

$$
\begin{align*}
\mathbb{E}_{p(w)} [\text{Var}_X (a_l^{(1)})] &= \mathbb{E}_{p(w)} [\sum_j w_j^{(0)2} \text{Var}_X (x_j)] \\
&+ \mathbb{E}_{p(w)} [\sum_{j,k,j \neq k} w_j^{(0)} \text{Cov}(x_j, x_k) w_k^{(0)}] \\
&= \sigma (0)^2 \sum_j \text{Var}_X (x_j).
\end{align*}
$$

(32)

From eq 29, 32, we can conclude that:

$$
\mu_{\text{PVE}} = \sigma (0)^2 \prod_{l=1}^{L} \beta_l M_l \sigma_l^{(l)^2} \sum_{i=1}^{D} \frac{\text{Var}_X (x_i)}{\text{Var}_Y (y)},
$$

where $\alpha = \prod_{l=1}^{L} \beta_l$. When the number of hidden nodes of each layer goes to infinity, $\alpha = \left( \frac{\pi - 1}{2\pi} \right)^L$.

9 Estimating $\bar{\alpha}$ through linear regression

We provide a simple algorithm to estimate $\bar{\alpha}$ by solving the linear regression problem.
Phospholipids in medium HDL

Phospholipids in very small VLDL

Concentration of chylomicrons and extremely large VLDL

Triglycerides in IDL

Figure 7: The empirical shrinkage factor $\beta_l$ for layer $l$ of a neural network with finite number of units. We can find that $\beta_l$ is almost constant for a wide range of scales $\tau \in [0, 10]$, which induces PVE from 0 to $8 \times 10^{-21}$. We used a neural network with 5 hidden layers which consisting 100 nodes for each layer. The priors of all weights are the same fully factorized Gaussian with mean 0 and scale $\tau$.

**Algorithm 1** Estimate the constant $\hat{\alpha}$ by linear regression

**Input:** Dataset: $(X, y)$; BNN: $f(x; w), w \sim p(w; \tau)$.

**Output:** Constant $\hat{\theta}$

1. Select $K$ global scales $\{\tau_k\}_{k=1}^K$.
2. For each $\tau_k$ do
3. for $m \leftarrow 1$ to $M$ do
4. Draw sample: $w_k^{(m)} \sim p(w; \tau_k)$
5. Forward passing: $\hat{y}_k^{(m)} = f(x; w_k^{(m)})$
6. Compute $\text{PVE}(w_k^{(m)}) = \frac{\text{Var}(f(X; w_k^{(m)}))}{\text{Var}(y)}$.
7. end for
8. Compute $\mu_{\text{PVE}}$ based on $M$ samples.
9. end for
10. Fit a linear regression model on $K$ pairs of simulated data: $\{(\log \tau_k, \log \mu_{\text{PVE}}(k))\}_{k=1}^K$, such that $\log \mu_{\text{PVE}}(k) = a \log \tau_k + b$.
11. return $\hat{\theta} = \exp(b)$

In above algorithm, a small $K = 20$ and $M = 100$ can produce a very accurate estimation ($R^2$ is higher than 99.99%), as shown in Figure 8.

10 Experiments settings and results

10.1 Synthetic data

We simulate the data using model:

$$y_i = \sum_{j=1}^{500} w_j^m x_j + \sum_{k=1}^5 w_k^l h_k(x_{2k-1}, x_{2k}) + \epsilon,$$  \hspace{1cm} (33)

where $w_j^m = 0$ for $j > 10$. The simulator contains both main effect and feature interactions, and the total number of features used in this model is 10. Features $x$ are sampled from a standard Gaussian, and $\epsilon$ is from $N(0, 3)$, so that the signal to noise ratio is 1.

The 5 interactions used in Eq. (33) are:

$$h_1 = h_1(x_1, x_2) = x_1x_2;$$
$$h_2 = h_2(x_3, x_4) = x_3e^{x_4};$$
$$h_3 = h_3(x_5, x_6) = x_5e^{x_6};$$
$$h_4 = h_4(x_7, x_8) = x_7x_8;$$
$$h_5 = h_5(x_9, x_{10}) = x_9e^{x_{10}}.$$  \hspace{1cm} (34)

10.2 GWAS

A description of each target that used is shown in Table 2.

**Table 2:** A description of each target in GWAS.

| Target | Description                    |
|--------|--------------------------------|
| ID: TG5 | Triglycerides in HDL           |
| XXS:VLDL:PL | Phospholipids in very small VLDL |
| XXL:VLDL:PL | Concentration of chylomicrons and extremely large VLDL |
| M:HD:PL   | Phospholipids in medium HDL    |
10.3 UCI sensitivity analysis

We tested how sensitive are the informative prior (InfoD) and SSBNN w.r.t the $\mu_{PVE}$ that we choose to encode. The results are shown in Table 3.

We see that by increasing the $\mu_{PVE}$ to 0.9, most of the results can be improved, which makes sense, because all of these datasets have high signal-to-noise ratios and a neural network is expected to explain most of the variance. We can find a correct $\mu_{PVE}$ is more important for small datasets, where the prior plays an important role. We find that InfoD is less sensitive to the $\mu_{PVE}$ than SSBNN for most datasets, and InfoD is consistently better than SSBNN for most cases.

Table 3: Test $R^2$ of each method with different $\mu_{PVE}$ in priors. We can find that the performance dependents on the $\mu_{PVE}$ that we encode. And InfoD is less sensitive than SSBNN.

| Datasets      | BNNs $\mu_{PVE} = 0.7$ | $\mu_{PVE} = 0.8$ | $\mu_{PVE} = 0.9$ |
|---------------|-------------------------|-------------------|-------------------|
| **Original datasets (non-informative prior)** |
| Bike          | SSBNN+PVE 0.850          | 0.896             | 0.896             |
|               | InfoD+PVE 0.897          | 0.904             | 0.904             |
| California    | SSBNN+PVE 0.793          | 0.785             | 0.795             |
|               | InfoD+PVE 0.783          | 0.784             | 0.786             |
| Energy        | SSBNN+PVE 0.847          | 0.867             | 0.890             |
|               | InfoD+PVE 0.854          | 0.864             | 0.891             |
| Concrete      | SSBNN+PVE 0.771          | 0.792             | 0.802             |
|               | InfoD+PVE 0.791          | 0.801             | 0.801             |
| Yacht         | SSBNN+PVE 0.915          | 0.929             | 0.940             |
|               | InfoD+PVE 0.923          | 0.933             | 0.957             |
| **Extended datasets with irrelevant features (informative prior)** |
| Bike          | SSBNN+PVE 0.916          | 0.764             | 0.823             |
|               | InfoD+PVE 0.843          | 0.855             | 0.860             |
| California    | SSBNN+PVE 0.652          | 0.720             | 0.735             |
|               | InfoD+PVE 0.751          | 0.764             | 0.766             |
| Energy        | SSBNN+PVE 0.833          | 0.837             | 0.856             |
|               | InfoD+PVE 0.836          | 0.848             | 0.858             |
| Concrete      | SSBNN+PVE 0.690          | 0.726             | 0.736             |
|               | InfoD+PVE 0.742          | 0.767             | 0.783             |
| Yacht         | SSBNN+PVE 0.830          | 0.842             | 0.845             |
|               | InfoD+PVE 0.859          | 0.867             | 0.877             |

10.4 UCI extra results

The experiment results with MSE and $R^2$ on test set are shown in Table 4 and Table 5. Most of the results and conclusions are consistent with the main text. We can find neither continuous or discrete scales can have the best performance for all datasets, but the new informative prior (InfoD and InfoC) can always have a better performance on extended datasets, where extra information about number of relevant features is available. In discrete scale cases, encoding prior knowledge PVE is always a better choice than setting the global scale to 1.

References of Supplementary

Anqi Wu, Sebastian Nowozin, Edward Meeds, Richard E. Turner, José Miguel Hernández-Lobato, and Alexander L. Gaunt. Deterministic variational inference for robust Bayesian neural networks. *arXiv preprint arXiv:1810.03958*, 2018
### Table 4: Test MSE of each method on UCI datasets.

| Datasets    | (P, N) | Mean-field | SSBNN | SSBNN+PVE | InfoD | InfoD+PVE | HSBNN | InfoC |
|-------------|--------|------------|-------|-----------|-------|-----------|-------|-------|
| **Original datasets (non-informative prior)** |        |            |       |           |       |           |       |       |
| Bike        | (13, 17k) | .136 ± .002 | .136 ± .003 | .134 ± .002 | .134 ± .002 | .133 ± 002 | .133 ± .002 | .133 ± .002 |
| California  | (9, 20k)  | .362 ± .003 | .264 ± .001 | .264 ± .001 | .264 ± .001 | .264 ± .001 | .243 ± .001 | .242 ± .001 |
| Energy      | (8, 0.7k) | .155 ± .007 | .126 ± .003 | .120 ± .003 | .125 ± .002 | .120 ± .002 | .096 ± .007 | .100 ± .005 |
| Concrete    | (8, 1k)   | .233 ± .003 | .161 ± .002 | .160 ± .002 | .160 ± .002 | .158 ± .001 | .159 ± .003 | .160 ± .002 |
| Yacht       | (6, 0.3k) | .125 ± .004 | .093 ± .003 | .094 ± .002 | .093 ± .002 | .092 ± .003 | .110 ± .005 | .100 ± .004 |
| **Extended datasets with irrelevant features (informative prior)** | | | | | | | | |
| Bike        | (113, 17k) | .510 ± .015 | .365 ± .012 | .352 ± .014 | .276 ± .007 | .270 ± .008 | .402 ± .017 | .356 ± .011 |
| California  | (109, 20k) | .390 ± .003 | .352 ± .002 | .345 ± .002 | .326 ± .002 | .324 ± .001 | .366 ± .004 | .363 ± .003 |
| Energy      | (108, 0.7k) | .773 ± .116 | .187 ± .007 | .173 ± .005 | .175 ± .006 | .157 ± .005 | .159 ± .004 | .147 ± .002 |
| Concrete    | (108, 1k) | .708 ± .054 | .297 ± .008 | .287 ± .007 | .288 ± .005 | .280 ± .004 | .277 ± .003 | .255 ± .004 |
| Yacht       | (106, 0.3k) | .253 ± .069 | .495 ± .003 | .409 ± .020 | .280 ± .008 | .253 ± .008 | .291 ± .010 | .247 ± .012 |

### Table 5: Test $R^2$ of each method on UCI datasets.

| Datasets    | (P, N) | Mean-field | SSBNN | SSBNN+PVE | InfoD | InfoD+PVE | HSBNN | InfoC |
|-------------|--------|------------|-------|-----------|-------|-----------|-------|-------|
| **Original datasets (non-informative prior)** |        |            |       |           |       |           |       |       |
| Bike        | (13, 17k) | .895 ± .004 | .895 ± .004 | .896 ± .011 | .902 ± .004 | .904 ± .004 | .911 ± .001 | .910 ± .001 |
| California  | (9, 20k)  | .777 ± .006 | .785 ± .001 | .785 ± .002 | .785 ± .001 | .784 ± .001 | .795 ± .001 | .793 ± .001 |
| Energy      | (8, 0.7k) | .769 ± .004 | .835 ± .011 | .867 ± .008 | .854 ± .005 | .864 ± .006 | .887 ± .011 | .892 ± .007 |
| Concrete    | (8, 1k)   | .670 ± .002 | .790 ± .004 | .792 ± .004 | .793 ± .005 | .801 ± .004 | .798 ± .004 | .799 ± .003 |
| Yacht       | (6, 0.3k) | .726 ± .033 | .919 ± .004 | .929 ± .005 | .920 ± .004 | .933 ± .003 | .912 ± .008 | .920 ± .007 |
| **Extended datasets with irrelevant features (informative prior)** | | | | | | | | |
| Bike        | (113, 17k) | .491 ± .024 | .717 ± .026 | .764 ± .027 | .850 ± .006 | .855 ± .004 | .717 ± .023 | .777 ± .014 |
| California  | (109, 20k) | .641 ± .007 | .694 ± .008 | .720 ± .005 | .756 ± .003 | .674 ± .002 | .655 ± .005 | .659 ± .004 |
| Energy      | (108, 0.7k) | .619 ± .014 | .620 ± .012 | .837 ± .003 | .834 ± .002 | .848 ± .001 | .843 ± .002 | .852 ± .002 |
| Concrete    | (108, 1k) | .263 ± .089 | .731 ± .009 | .726 ± .009 | .742 ± .011 | .767 ± .010 | .741 ± .005 | .760 ± .007 |
| Yacht       | (106, 0.3k) | - .21 ± .114 | .785 ± .014 | .842 ± .007 | .857 ± .005 | .867 ± .006 | .848 ± .006 | .868 ± .007 |