Projected BNNs: Avoiding weight-space pathologies by learning latent representations of neural network weights

Melanie F. Pradier¹ Weiwei Pan¹ Jiayu Yao¹ Soumya Ghosh² Finale Doshi-Velez¹

Abstract

As machine learning systems get widely adopted for high-stake decisions, quantifying uncertainty over predictions becomes crucial. While modern neural networks are making remarkable gains in terms of predictive accuracy, characterizing uncertainty over the parameters of these models is challenging because of the high dimensionality and complex correlations of the network parameter space. This paper introduces a novel variational inference framework for Bayesian neural networks that (1) encodes complex distributions in highdimensional parameter space with representations in a low-dimensional latent space, and (2) performs inference efficiently on the lowdimensional representations. Across a large array of synthetic and real-world datasets, we show that our method improves uncertainty characterization and model generalization when compared with methods that work directly in the parameter space.

1. Introduction

Deep learning provides a flexible framework for function approximation that has been adopted across many domains including machine vision, natural language processing, speech recognition, bioinformatics, and game-playing (LeCun et al., 2015). Yet, deep models tend to overfit when the number of training examples is small (Su et al., 2019); furthermore, their primary focus in practice is often on computing point estimates of model parameters, and thus, these models do not provide uncertainties for their predictions – making them unsuitable for applications in critical domains such

This version was submitted to 36th International Conference on Machine Learning, Long Beach, California, PMLR 97, 2019. Copyright 2019 by the author(s).

as personalized medicine. Bayesian neural networks (BNN) promise to address these issues by modeling the uncertainty in the network weights, and correspondingly, the uncertainty in output predictions (MacKay, 1992b; Neal, 2012).

Unfortunately, characterizing uncertainty over parameters of modern neural networks in a Bayesian setting is challenging due to the high dimensionality of the weight space and complex patterns of dependencies among the weights. In these cases, Markov-chain Monte Carlo (MCMC) techniques for performing inference often fail to mix across the weight space, and standard variational approaches not only struggle to escape local optima, but also fail to capture dependencies between the weights.

A recent body of work has attempted to improve the quality of inference for Bayesian neural networks (BNNs) via improved approximate inference methods (Graves, 2011; Blundell et al., 2015; Hernández-Lobato et al., 2016), or by improving the flexibility of the variational approximation for variational inference (Louizos and Welling, 2017). In particular, variational families that explicitly model correlations between weights have been shown to be effective in approximate inference (Sun et al., 2017; Louizos and Welling, 2016; Gal and Ghahramani, 2016). However, many of these techniques only treat linear weight correlations while others face the challenge of performing inference over complex distributions over weights.

In this work, we introduce a novel inference approach in which we capture nonlinear latent structures amongst neural network parameters by learning a map of the weights onto a low-dimensional latent space. Our approach takes advantage of the following insight: learning (standard network) parameters is easier in the high-dimensional space, but characterizing (Bayesian) uncertainty is easier in the low-dimensional space. Low-dimensional spaces are generally easier to explore, if we have fewer correlations between dimensions, and can be better captured by standard variational approximations (e.g. mean field). At the same time, the non-linear transformation between latent space and weight space

¹School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA ²IBM Research, Cambridge, MA, USA. Correspondence to: Melanie F. Pradier <melanie.fpradier@gmail.com>, Weiwei Pan <weiweipan@g.harvard.edu>.

allows us to encode flexible approximating distributions for posteriors over the weights.

Our main contribution is an inference framework that is able to exploit nonlinear latent structures in weight space. We demonstrate, on synthetic datasets, the ability of our method to capture complex posterior distributions over weights by encoding them as distributions in latent space. We show that, as a result, our method is able to more accurately capture the uncertainty in the posterior predictive distribution. Finally, we demonstrate that, across a wide range of real-world data sets, our approach often produces more accurate predictions and higher quality predictive intervals compared to other state-of-the-art techniques.

2. Related Work

Classic work on Bayesian neural networks can be traced back to (Buntine and Weigend, 1991; MacKay, 1992a; Neal, 1993). (Neal, 1993) introduced Hamiltonian Monte Carlo (HMC) to explore the Bayesian neural network posterior. (MacKay, 1992a) and (Buntine and Weigend, 1991) instead relied on Laplace approximation to characterize the network posterior. While HMC remains the "gold standard" for posterior inference in BNNs, it does not scale well to modern architectures or large datasets. Similarly, vanilla application of the Laplace approximation has difficulty scaling to modern architectures with millions of parameters.

Structured Variational Approximations. Many recent works in variational inference have attempted to move beyond fully-factorized approximations of Bayesian neural network posteriors by modeling structured dependencies amongst BNN weights. Notably, matrix variate Gaussian distributions are proposed in (Louizos and Welling, 2016) to explicitly model the linear correlation between network weights. In a similar vein, our approach models non-linear dependencies and is most comparable to works that build flexible approximating families of weight distributions using auxiliary random variables, either through mixtures of simple distributions (Agakov and Barber, 2004; Maaløe et al., 2016; Ranganath et al., 2016; Salimans et al., 2013) or via (non)-linear transformations of simple distributions (Rezende and Mohamed, 2015; Kingma et al., 2016; Louizos and Welling, 2017).

Normalizing Flows and Transformations. In particular, Rezende and Mohamed (2015); Kingma et al. (2016) apply normalizing flows to increase flexibility of the variational family distribution. In the context of BNNs, (Louizos and Welling, 2017) assume normally distributed variational distributions for the weights

with *layer-wise* multiplicative noise that are *linearly* projected onto a latent space via normalizing flows. However, they still assume that the posterior factorizes layer wise. In contrast, our approach learns *non-linear* projections of the *entire* network weights onto a latent space. Furthermore, our construction allows us to optimize a tighter bound on the log evidence.

A number of recent works use the idea of hypernetworks, neural networks that output parameters of other networks, to parametrize the variational distribution (Krueger et al., 2017; Pawlowski et al., 2017). These works, however, do not model uncertainty in the latent projections. Moreover, they directly specify an implicit variational distribution over weights. Since, the implicit distribution's entropy is difficult to compute, authors have been forced to either use invertible projections thus trading off flexibility of the resulting distributions or otherwise approximate implicit weight densities potentially leading to severe local optima issues. In contrast, we incorporate uncertainty explicitly in both our generative and variational models and our approach of inference in the latent space avoids the challenges of dealing with implicit distributions.

In general, the vast majority of variational inference procedures for BNNs perform inference directly on the weight space (Sun et al., 2017; Louizos and Welling, 2016; Gal and Ghahramani, 2016) and face the challenge of working with complex distributions over high dimensional weights. In contrast, we perform inference in a lower dimensional latent space and thus solve an arguably easier problem.

Particle based inference Very recent work (Wang et al., 2019; Sun et al., 2019), building on ideas from Stein discrepancy (Liu et al., 2016; Liu and Wang, 2016), perform inference directly in the function space. However, these approaches still maintain either a variational distribution over the weights (Sun et al., 2019) or several particles in the weight space (Wang et al., 2019). Our work is orthogonal, where we model the weights via a lower dimensional latent space, similar ideas may prove useful for inference in function space.

Stochastic gradient MCMC (SG-MCMC) (Springenberg et al., 2016; Li et al., 2016) methods form the other popular class of BNN inference algorithms. While asymptotically exact, it is often difficult to determine when they have converged to their stationary distribution in the finite computation limit. Although, not our focus in the paper, SG-MCMC algorithms can be crafted for our projected BNN models.

Weight embeddings/Modeling. In terms of modeling, our work is close in spirit to (Karaletsos et al.,

2018), where the authors represent nodes in a neural network by latent variables via a deterministic linear projection, drawing network weights conditioned on those representations. In contrast to their approach, we learn a distribution over non-linear projections, and find a latent representation for the weights directly rather than projecting the nodes.

Yet others (Garnelo et al., 2018), try to model flexible conditional distributions given arbitrary data instances. The resulting stochastic process termed Neural processes, are promising but may have difficulty scaling to even moderate dimensional data and have an orthogonal focus – on fast adaptation and meta-learning. In contrast, our goal is to perform improved inference for BNNs. In the appendix, we sketch out a variant of our model that is closely related to neural processes.

Ensembles of Neural Networks. Bayesian inference completely, another line of work relies on (non-Bayesian) neural network ensembles to estimate predictive uncertainty (Lakshminarayanan et al., 2017; Pearce et al., 2018). The idea is simple: each network in the ensemble will learn similar values close to the training data, and different ones in regions of the space far from the training data. Whereas (Lakshminarayanan et al., 2017) rely on multiple random restarts and adversarial training, (Pearce et al., 2018) introduce noise in the regularization term of each network, which directly relates to the randomized MAP sampling literature (Lu and Van Roy, 2017; Garipov et al., 2018). In (Pearce et al., 2018), the authors derive a parallelism between their ensemble sampling approach and Bayesian behavior, but this only holds for infinite single-layer neural networks.

Compression of Neural Network Weights. Finally, the dimensionality reduction aspect of our modeling is comparable to neural network compression. There are a number of non-Bayesian methods for compressing standard neural networks, all of which, to our knowledge, rely on linear dimensionality reduction techniques on the space of weights and or network nodes (Denil et al., 2013; Sainath et al., 2013; Xue et al., 2013; Nakkiran et al., 2015). In contrast, our work is focused on non-linear dimensionality reduction in a Bayesian setting with the aim to improve uncertainty quantification.

3. Background and Notation

Let $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1), \dots (\mathbf{x}_N, \mathbf{y}_N)\}$ be a dataset of N i.i.d observed input-output pairs. We model this data by $\mathbf{y} = f_{\mathbf{w}}(\mathbf{x}) + \epsilon$, where ϵ is a noise variable and

 \boldsymbol{w} refers to the weights of a neural network.¹. In the Bayesian setting, we assume some prior over the weights $\boldsymbol{w} \sim p(\boldsymbol{w})$. One common choice is to posit i.i.d normal priors over each network weight $w_i \sim \mathcal{N}\left(0, \sigma_w^2\right)$.

Our objective is to infer the posterior distribution over functions $p(f_{\boldsymbol{w}}|\mathcal{D})$, which is equivalent to inferring the posterior distribution over the weights $p(\boldsymbol{w}|\mathcal{D})$. Given the posterior distribution, we model predictions for new observations and their associated uncertainties through the posterior predictive distribution:

$$p(\mathbf{y}^{\star}|\mathbf{x}^{\star}, \mathcal{D}) = \int p(\mathbf{y}^{\star}|\mathbf{x}^{\star}, \boldsymbol{w}) p(\boldsymbol{w}|\mathcal{D}) d\boldsymbol{w}. \tag{1}$$

The posterior $p(\boldsymbol{w}|\mathcal{D}) \propto p(\mathcal{D}|\boldsymbol{w})p(\boldsymbol{w})$ generally does not have an analytic form due to the non-linearity of $f_{\boldsymbol{w}}$; thus, one must resort to approximate inference techniques. Variational inference, for example, attempts to find a distribution $q_{\boldsymbol{\lambda}}(\boldsymbol{w})$ that closely approximates the true posterior $p(\boldsymbol{w}|\mathcal{D})$. The measure of proximity is typically the KL-divergence:

$$D_{KL}(q_{\lambda}(\boldsymbol{w})||p(\boldsymbol{w}|\mathcal{D}))$$

$$= \int q_{\lambda}(\boldsymbol{w})[\log q_{\lambda}(\boldsymbol{w}) - \log p(\boldsymbol{w}|\mathcal{D})]d\boldsymbol{w}$$

$$= -\mathcal{H}(q) - \mathbb{E}_{q}[\log p(\mathcal{D}, \boldsymbol{w})] + \log p(\mathcal{D})$$

$$= -\mathcal{L}(\lambda) + \log p(\mathbf{y}|\mathbf{x}). \tag{2}$$

where $\mathcal{L}(\lambda) = \mathcal{H}(q) + \mathbb{E}_q[\log p(\mathcal{D}, \boldsymbol{w})]$ is the evidence lower bound (ELBO) on the marginal likelihood $\log p(\mathbf{y}|\mathbf{x})$. Approximate inference in this case can be cast as the problem of optimizing $\mathcal{L}(\lambda)$ with respect to λ , since minimizing the KL-divergence between $q_{\lambda}(\boldsymbol{w})$ and $p(\boldsymbol{w}|\mathcal{D})$ is equivalent to maximixing the lower bound $\mathcal{L}(\lambda)$, as shown in Eq. (2).

For BNNs, the posterior distribution $p(\boldsymbol{w}|\mathcal{D})$ often contains strong correlations, such that the optimization of $\boldsymbol{\lambda}$ is prone to get stuck in local optima. Moreover, simple variational families $q_{\boldsymbol{\lambda}}(\boldsymbol{w})$, such as mean field approximations, fail to capture those correlations.

4. Latent Projection BNN

4.1. Generative Model

In our approach, which we call *Projected Bayesian Neural Network (Proj-BNN)*, we posit that the neural network weights \boldsymbol{w} are generated from a latent space or *manifold* of much smaller dimensionality. That is, we assume the following generative model:

$$z \sim p(z), \, \phi \sim p(\phi), \, w = g_{\phi}(z), \, \mathbf{y} \sim \mathcal{N}(f_{w}(\mathbf{x}), \sigma_{y}^{2})$$
 (3)

 $^{^{1}}$ In this paper, w refers to both, network weights and biases, since each layer can be augmented with an extra input dimension containing 1's to account for the biases.

where \boldsymbol{w} lies in \mathbb{R}^{D_w} , the latent representation \boldsymbol{z} lie in a lower dimensional space \mathbb{R}^{D_z} , and $\boldsymbol{\phi}$ parametrizes the arbitrary projection function $g_{\boldsymbol{\phi}}: \mathbb{R}^{D_z} \to \mathbb{R}^{D_w}$. Given this generative model, our objective is to compute the joint posterior distribution $p(\boldsymbol{z}, \boldsymbol{\phi}|\mathbf{y}, \mathbf{x})$ over both the latent representation \boldsymbol{z} and the latent projection parameters $\boldsymbol{\phi}$.

4.2. Inference

Following the same structure in the generative model, we propose a variational distribution $q_{\lambda}(z, \phi) = q_{\lambda_z}(z)q_{\lambda_0}(\phi)$ such that:

$$z \sim q_{\lambda_z}(z), \ \phi \sim q_{\lambda_{\phi}}(\phi), \ w = g_{\phi}(z).$$
 (4)

In particular, we posit a mean-field posterior approximation for each independent term $q_{\lambda_z}(z) \doteq \mathcal{N}(\tilde{\mu}_z, \tilde{\sigma}_z \mathbf{I})$ and $q_{\lambda_{\phi}}(\phi) \doteq \mathcal{N}(\tilde{\mu}_{\phi}, \tilde{\sigma}_{\phi} \mathbf{I})$, where $\tilde{\mu}_z, \tilde{\mu}_{\phi}$ and $\tilde{\sigma}_{\phi}, \tilde{\sigma}_{\phi}$ refer to the mean and standard deviation vectors of each Normal variational distribution respectively, $\lambda_z = \{\tilde{\mu}_z, \tilde{\sigma}_z\}$, and $\lambda_{\phi} = \{\tilde{\mu}_{\phi}, \tilde{\sigma}_{\phi}\}$. Note that, although we adopt a fully factorized posterior approximation for z and z, the induced posterior approximation z, we over the network weights z can capture complex dependencies due to the non-linear transformation z.

Given such variational distribution, a straightforward inference algorithm is to use black-box variational inference (BBVI) (Ranganath et al., 2014) with the reparametrization trick (Kingma et al., 2015) to minimize the joint evidence lower bound (ELBO) $\mathcal{L}(\lambda)$ given by:

$$\mathcal{L}(\boldsymbol{\lambda}) = \mathbb{E}_q \Big[\log p \big(\mathbf{y} | \mathbf{x}, g_{\boldsymbol{\phi}}(\boldsymbol{z}) \big) \Big]$$

$$- D_{\mathrm{KL}} \big(q_{\boldsymbol{\lambda}_z}(\boldsymbol{z}) || p(\boldsymbol{z}) \big) - D_{\mathrm{KL}} \big(q_{\boldsymbol{\lambda}_{\boldsymbol{\phi}}}(\boldsymbol{\phi}) || p(\boldsymbol{\phi}) \big).$$
 (5)

However, jointly optimizing the projection parameters ϕ and latent representation z is often a hard optimization problem; direct optimization of the ELBO in Eq. (5) is prone to local minima and might lead to poor performance solutions. To alleviate this issue, we additionally come up with an intelligent initialization (no uncertainty) for ϕ , and then perform variational inference using BBVI. In the following, we describe the complete inference framework in three stages.

Characterize the space of plausible weights. First, we seek to gather a diverse set of weight parameters (without considering uncertainty), which will be used to learn a smart initialization of ϕ afterwards. As explained in Section 1, learning parameters in the high-dimensional \boldsymbol{w} -space is easy, the difficult part is to get accurate uncertainty estimations. More precisely, we collect multiple, high-quality candidate weight solutions $\{\mathbf{w_c}^{(r)}\}_{r=1}^R$ by training a non-Bayesian neural network

and sampling around the MAP solution, using Fast Geometric Ensembling (FGE) (Garipov et al., 2018; Izmailov et al., 2018). This is equivalent to training an ensemble of neural networks from multiple restarts, but in the time required to train a single model, and avoiding identifiability problems over the weight space. FGE allow us to recover a variety of weights which will lead to similar function values where there is training data, but different outputs otherwise. Although there exist methods in the literature to force diversity in the solutions of neural network ensembles, we opt for FGE for simplicity and computational efficiency.

Learn a point-estimate for the projection function. In order to find an intelligent initialization in the BBVI algorithm for the projection function g_{ϕ} , we perform dimensionality reduction on the previously collected sets of weights $\{\mathbf{w_c}^{(r)}\}_{r=1}^R$. We opt for an autoencoder to account for non-linear complex transformations, but other alternatives can also be applied. Let $f_{\theta}: D_w \to D_z$ and $g_{\phi}: D_z \to D_w$ denote the encoder and decoder, respectively, of the autoencoder $h_{\theta,\phi} = g_{\phi} \circ f_{\theta}$. Our aim is to find a point estimate for the parameters of the projection.

While we want to find latent projections that minimize the reconstruction error of the weights, at the same time, we also need to explicitly encourage for projections that will map into weights that yield high log likelihood values for our original training data \mathcal{D} . We find that, in practice, the explicit constraint on the predictive accuracy of reconstructed weights $\hat{\mathbf{w}}_{\mathbf{c}}^{(r)} = h_{\theta,\phi}\left(\mathbf{w}_{\mathbf{c}}^{(r)}\right)$ is required since weights that are "similar" in Euclidean norm may yield models of very different predictive qualities.³ This results in the following loss to minimize:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}) = \frac{1}{R} \sum_{r=1}^{R} \left(\mathbf{w_c}^{(r)} - h_{\boldsymbol{\theta}, \boldsymbol{\phi}} \left(\mathbf{w_c}^{(r)} \right) + \gamma^{(r)} \right)^2 + \beta \mathbb{E}_{(x, y) \sim \mathcal{D}} \left[\frac{1}{R} \sum_{r=1}^{R} \log p \left(y | x, h_{\boldsymbol{\theta}, \boldsymbol{\phi}} \left(\mathbf{w_c}^{(r)} \right) \right) \right],$$
(6)

where $\gamma^{(r)} \sim \mathcal{N}(0, 1)$ is an additional input noise term that makes training more robust. The first term in Eq. (6) corresponds to the average mean square error of each $\mathbf{w_c}^{(r)}$ and its reconstructed version $\hat{\mathbf{w}_c}^{(r)}$, while the second term accounts for the reconstruction error

 $^{^2}$ Solutions corresponding to weight permutations are naturally avoided by sampling close to the same local optimum.

³If we only optimize for minimum weight reconstruction, we find projections whose reconstructed weights have lower quality in terms of test log likelihood $p(\mathbf{y}|\mathbf{x}, \hat{\mathbf{w}}_{\mathbf{c}}^{(r)})$.

(in terms of log likelihood) of the original output data \mathbf{y} given \mathbf{x} and $\hat{\mathbf{w}}_{\mathbf{c}}^{(r)}$. We call this approach a *prediction-constrained* autoencoder. Prediction-constrained models have previously been introduced in the context of mixture and topic models (Hughes et al., 2017; 2018).

Learn the approximate posterior $q_{\lambda}(z,\phi)$. Given the point-estimate projection parameters ϕ^* from the previous stage, we can now initialize the mean variational parameters for $q_{\lambda}(z,\phi)$, and perform principled posterior approximation using black-box variational inference. For simplicity, we assume a mean-field structure $q_{\lambda}(z,\phi) = q_{\lambda_z}(z)q_{\lambda_\phi}(\phi)$ for the latent representation z and projection parameters ϕ . We optimize the variational parameters $\lambda = \{\lambda_z, \lambda_\phi\}$ to minimize the KL-divergence $D_{\text{KL}}(q_{\lambda}(z,\phi)||p(z,\phi|\mathbf{y},\mathbf{x}))$, which is equivalent to maximizing the evidence lower bound (ELBO) from Eq. (5). The expectation in Eq. (5) and gradient can be estimated using simple Monte Carlo integration along with the reparametrization trick (Kingma and Welling, 2014; Rezende et al., 2014):

$$\mathbb{E}_q\Big[\log p\big(\mathbf{y}|\mathbf{x}, g_{\boldsymbol{\phi}}(\boldsymbol{z})\big)\Big] \approx \frac{1}{S} \sum_{s=1}^{S} \log p\big(\mathbf{y}|\mathbf{x}, g_{\boldsymbol{\phi}^{(s)}}(\boldsymbol{z}^{(s)})\big),$$

where $\mathbf{z}^{(s)} = \boldsymbol{\epsilon}_z^{(s)} \, \tilde{\boldsymbol{\sigma}}_z + \tilde{\boldsymbol{\mu}}_z, \, \boldsymbol{\lambda}_z = \{\tilde{\boldsymbol{\mu}}_z, \tilde{\boldsymbol{\sigma}}_z\}$ are the variational parameters of the distribution $q_{\boldsymbol{\lambda}_z}(z), \, \boldsymbol{\phi}^{(s)} = \boldsymbol{\epsilon}_{\phi}^{(s)} \, \tilde{\boldsymbol{\sigma}}_{\phi} + \tilde{\boldsymbol{\mu}}_{\phi}, \, \boldsymbol{\lambda}_{\phi} = \{\tilde{\boldsymbol{\mu}}_{\phi}, \tilde{\boldsymbol{\sigma}}_{\phi}\}$ are the variational parameters of the distribution $q_{\boldsymbol{\lambda}_{\phi}}(\phi)$, and $\boldsymbol{\epsilon}_z^{(s)}, \, \boldsymbol{\epsilon}_{\phi}^{(s)} \sim \mathcal{N}(0, \mathrm{I})$ are the auxiliary noise variables for the reparametrization trick. The KL-divergence terms in Eq. (5) can be computed in closed form, as all distributions p(z), $p(\phi), \, q_{\boldsymbol{\lambda}_z}(z)$, and $q_{\boldsymbol{\lambda}_{\phi}}(\phi)$ are normal-distributed.

The variational parameters $\tilde{\boldsymbol{\mu}}_{\phi}$ are initialized to the point-estimate ϕ^{\star} computed in the previous stage, whereas the variational parameters $\boldsymbol{\lambda}_z$ and $\tilde{\boldsymbol{\sigma}}_{\phi}$ are initialized randomly.⁴ Algorithm 1 summarizes the three-step framework for tractable inference.

5. Results

This section contains results on synthetic and real-world datasets to illustrate the performance and potentials of the proposed approach (Proj-BNN). We show that Proj-BNN provides flexible posterior approximations, resulting in better uncertainty estimations, and improved model generalization in terms of held-out test log likelihood across multiple datasets.

We compare Proj-BNN to the following baselines: Bayes by Back Prop (BbB) (Blundell et al., 2015),

Algorithm 1 Inference for Proj-BNN

Input: observations $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$

- 1. Gather multiple sets of weights $\{\mathbf{w_c}^{(r)}\}_{r=1}^R$ via Fast Geometric Ensembling (Garipov et al., 2018).
- 2. Train a prediction-constrained autoencoder $h_{\theta,\phi}$ using $\{\mathbf{w_c}^{(r)}\}_{r=1}^R$ as input data to minimize the loss function described in Eq. (6).
- 3. Perform BBVI to learn an approximate posterior distribution over latent representations z and projection parameters ϕ .
 - Initialize mean variational parameters $\tilde{\mu}_{\phi}$ for ϕ with the autoencoder solution.
 - Optimize ELBO $\mathcal{L}(\lambda)$ in Eq. (5) to obtain $q_{\lambda}(z, \phi)$ closest to $p(z, \phi|\mathbf{y}, \mathbf{x})$ in terms of KL-divergence.

Result: Approximate posterior $q_{\lambda}(z, \phi)$

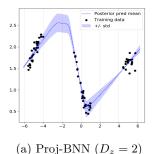
Multiplicative Normalizing Flow (MNF) (Louizos and Welling, 2017), Matrix Variate Gaussian Posteriors (MVG) (Louizos and Welling, 2016), Bayesian Hypernetworks (BbH) (Pawlowski et al., 2017), and Fast Geometric Ensembling (FGE) (Garipov et al., 2018).

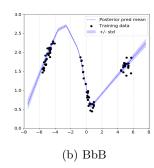
5.1. Synthetic Data

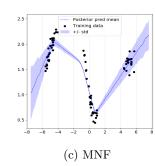
First, we demonstrate on synthetic data that, by performing approximate inference on \boldsymbol{z} , we can better capture uncertainty in the posterior predictive. Furthermore, we show that when the space of plausible weights for a regression model is complex, capturing this geometry in approximate inference is difficult; in contrast, performing inference in a simpler latent space allows for better exploration of the solution set in the weight space of the regression model.

Better estimates of uncertainty. Figure 1 compares the posterior predictive distributions obtained by Proj-BNN against BbB, MNF, and MVG. The data is generated by sampling points non-uniformly from a function represented by a feedforward network (with 1 hidden layer, 20 hidden nodes and RBF activation centered at 0 with length scale 1) whose weights are obtained by applying a fixed linear transform to a fixed latent vector \boldsymbol{z} . We observe that our method is able to obtain a mean posterior predictive that fits the data and is furthermore able to capture more uncertainty in the posterior predictive. Notably, baseline methods tend to underestimate predictive uncertainty, especially in places with few observations, and thus produces over-confident predictions.

⁴In practice, initializing $\tilde{\sigma}_{\phi}$ to small values gave better performance, i.e., $\log \tilde{\sigma}_{\phi} \sim \mathcal{N}(-9, 0.1)$.







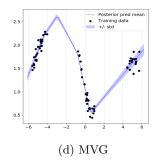


Figure 1: Inferred predictive posterior distribution for a toy data set drawn from a NN with 1-hidden layer, 20 hidden nodes and RBF activation functions. **Proj-BNN** is able to learn a plausible predictive mean and better capture predictive uncertainties.

Capturing complex geometries in w-space. We argue that the reason for the observed improvement in the quality of posterior predictive obtained by our method is often due to the fact that it is difficult to approximate complex geometries of the solution set in the weight space of sophisticated regression models. Mapping the solution set onto a simpler region in a lower dimensional latent space allows for more efficient approximations. In Figure 2a, we visualize samples of plausible weights for a feedforward network (with a single hidden layer, three nodes and RBF activation function) fitted to a data set with four modes. We see that the solution set in the weight space for this model is naturally bimodal, where each mode corresponds to functions that fit a particular choice of three of the four modes in the data.

Figure 2 shows that direct variational approximation of the posterior over weights is only able to capture one of the modes in the solution set, while approximating the posterior over z's using our method captures both modes. For the latter, we trained a decoder $g_{\phi}(\cdot)$ that maps an isotropic 2-D Gaussian to weights that we sampled from the solution set. As a result, the posterior predictive mean obtained by our method is able to approximate the four modes, while the predictive mean obtained from directly approximating the posterior over w can approximate only three of the four modes.

5.2. Real Data

Simulation settings. We perform nonlinear regression on eight UCI datasets, listed in Figure 3. In all the following experiments, we use a random train-test-validation split of 80-10-10. All datasets are normalized

in a preprocessing step to have zero mean and unit standard deviation. For all inference methods, We train a Bayesian neural network with one layer of 50 nodes and Rectified Linear Units (ReLU) activations, and fix the observational noise to $\sigma_y = 0.1$. Across all models, we assume the same priors $p(\boldsymbol{w}) = p(\boldsymbol{z}) = p(\boldsymbol{\phi}) \doteq \mathcal{N}(0,0.1)$. We perform cross-validation of the step size $\lambda_1 \in \{0.1,0.01,0.001,0.0001\}$ and fix the batch-size to 128. We use Adam (Kingma and Ba, 2014) as the optimizer and the joint unnormalized posterior distribution $p(\boldsymbol{w}|\mathcal{D}_{train})$ as the objective function.

For the proposed approach proj-BNN, we gather 150 weight samples with FGE to train the prediction-constrained autoencoder. The architecture of the projection function is cross-validated between either 1 layer of 20 nodes, or 2 layers of 10 nodes. Open source code is available in the public repository: *Anonymized*. Further details on the experimental setup and baselines can be found in the Appendix.

Generalization in benchmark datasets. Figure 3 shows that inference in latent space can improve model generalization. On datasets where ground truth distributions are not available for comparison and the inferred distributions are not easily visualized, we argue that the higher quality posterior and posterior predictive potentially obtained from Proj-BNN can be observed through an improvement in the generalizability in the models we obtain. We compare the generalization performance, measured in terms of marginal test likelihood, of Proj-BNN with the three baseline models, BBB, MNF and MVG. In Figure 3, we see that Proj-BNN performs competitively, if not better than baseline models, on all but one dataset.

⁵The true sampled weights are obtained by fitting the data multiple times from random weight initializations.

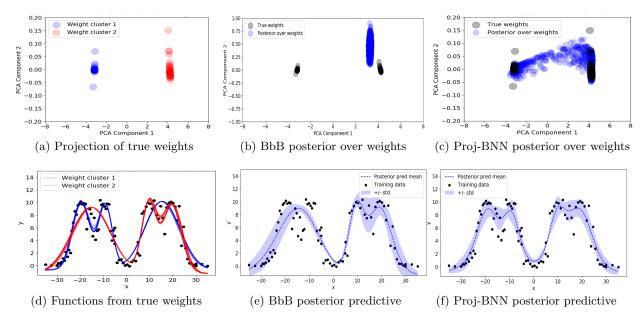


Figure 2: Learning a variational posterior over z captures both modes in the weight space. (a) PCA projection of sampled true weights of the feedforward network. (b) Variational posterior over weights learned by performing inference directly on w, using Bayes by Back Prop (BbB); only one mode captured. (c) Variational posterior over weights, w, obtained by transforming the variational posterior over z. (d) Examples of functions corresponding to weights sampled from each weight cluster. (e) Posterior predictive using BBB; only three modes captured. (f) Posterior predictive using Proj-BNN; all four modes captured.

6. Discussion

The geometry of weight posteriors impacts the quality of variational approximations. Experimental results on the synthetic data demonstrates the advantage of Proj-BNN in cases where the geometry of the true posterior over weights is complex, e.g. multimodal or highly non-convex. Here, traditional mean field variational inference will tend to capture only a small part of the true posterior, e.g. a single mode or a small convex region, due to the zero-forcing nature of KL-divergence minimization. Furthermore, in these cases, we find that optimization for variational inference tend to be easily trapped in undesirable local optima. In contrast, provided with a robust non-linear projection onto a low dimensional latent space, we are able to drastically reduce the complexity of the optimization problem, e.g. by reducing the number of parameters to be optimized. As a result, the posterior predictive distributions obtained by Proj-BNN often capture more uncertainty, whereas comparable methods that perform inference directly on weights tend to underestimate uncertainty and, thus, can produce over-confident predictions.

On real datasets, Proj-BNN outperforms or remains competitive, in terms of model generalization, with comparable baseline methods while working with representations of significantly smaller dimensionality. This is again evidence that performing inference in lower dimensional latent space can better capture complex posterior distributions in weight space. In cases where Proj-BNN underperforms in comparison to the baselines, we conjecture that the shortcoming may be due to insufficient sampling of the weight space during the first stage of training with fast geometric ensembling.

The quality of the non-linear latent projection impacts the quality of variational inference. The quality of the variational approximations obtained by Proj-BNN relies on 1) the ability to characterize the set of plausible neural network weights given a data set and 2) the ability to learn informative transformations between latent space and weight space. The former requires us to sample intelligently from the weight space. We currently use Fast Geometric Ensembling which is sample-efficient, but we see opportunities for future research to incorporate training objectives that explicitly encourage diversity of the samples we obtain. For condition 2), we note that learning transformations that are able to reconstruct weights from their latent representations is not necessarily helpful for inference, as the reconstructed weights might encode to models that suffer from a drastic decrease in predictive accuracy.

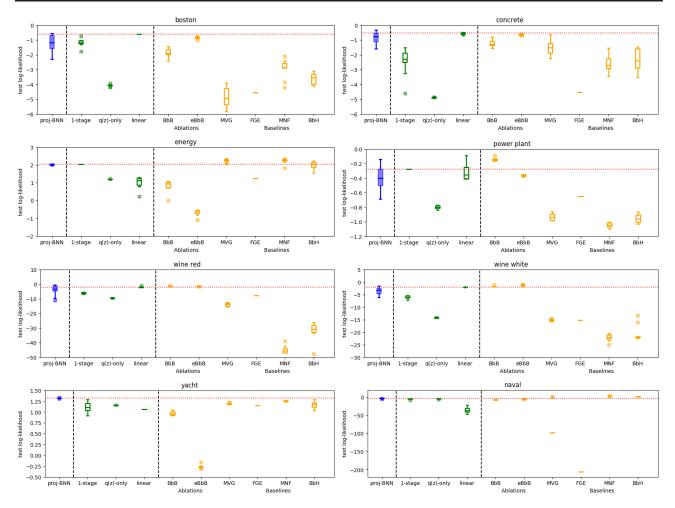


Figure 3: Test log-likelihood for UCI benchmark datasets for best dimensionality of z-space. Red dotted horizontal line corresponds to Proj-BNN performance (our approach) or one of its variants. Baselines methods: 1) BbB: mean field (Blundell, et.al 2015); 2) eBbB: extended BbB, with 1 layer of 3000 nodes; 3) MVG: multivariate Gaussian prior BNN (Louizos et.al, 2016); 4) FGE Fast Geometric Ensembling (Gastarov et.al, 2018); 5) MNF: multiplicative normalizing flow (Louizos et.al, 2017); 6) BbH: Bayesian hypernetworks (Pawlowski et.al, 2017). Ablations of Proj-BNN are: Proj-BNN with linear projections (linear), Proj-BNN without training the autoencoder, i.e., only stage 3 in Alg. 1 (1-stage), Proj-BNN modeling uncertainty only in z (q(z)-only).

We address this by adding a predictive-constrained autoencoder for learning the transformations. Additional constraints may be incorporated here to further improve inference in the latent space.

7. Conclusion

In this paper, we have presented a framework, Proj-BNN, for performing approximate inference for Bayesian Neural Networks that avoid many of the optimization problems of traditional inference methods. In particular, we are able to better capture the geometry of the posterior over weights by learning a probability distribution over non-linear transformations of the

weight space onto a simpler latent space and perform mean-field variational inference in the latent space.

Using synthetic data sets, we show that, in cases where the posterior over weights exhibits complex geometry (e.g. is multimodal), variational inference performed on weights space will often become trapped in local optima, whereas variational distributions in latent space can more easily capture the shape of the true posterior through a non-linear transformation. We compare Proj-BNN with five relevant baselines, each of which is an enrichment of the standard variational approach for BNN inference, and show that Proj-BNN is able to better capture posterior predictive uncertainty (without compromising predictive accuracy) on synthetic data.

On 8 real datasets, we show that, in terms of test likelihood, Proj-BNN is able to perform competitively if not better than several baselines, working in latent dimensions that are much smaller than the dimensions of the weight space.

References

- Felix V Agakov and David Barber. An auxiliary variational method. In *International Conference on Neural Information Processing*, pages 561–566, 2004.
- Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, and Daan Wierstra. Weight uncertainty in neural networks. In *ICML*, 2015.
- Wray L Buntine and Andreas S Weigend. Bayesian back-propagation. *Complex systems*, 5(6):603–643, 1991.
- Misha Denil, Babak Shakibi, Laurent Dinh, Nando De Freitas, et al. Predicting parameters in deep learning. In Advances in neural information processing systems, 2013.
- Yarin Gal and Zoubin Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In *International Conference* on Machine Learning, pages 1050–1059, 2016.
- Timur Garipov, Pavel Izmailov, Dmitrii Podoprikhin, Dmitry P Vetrov, and Andrew Gordon Wilson. Loss surfaces, mode connectivity, and fast ensembling of dnns. arXiv preprint arXiv:1802.10026, 2018.
- Marta Garnelo, Jonathan Schwarz, Dan Rosenbaum, Fabio Viola, Danilo J Rezende, SM Eslami, and Yee Whye Teh. Neural processes. arXiv preprint arXiv:1807.01622, 2018.
- Alex Graves. Practical variational inference for neural networks. In *Advances in neural information processing systems*, pages 2348–2356, 2011.
- José Miguel Hernández-Lobato, Yingzhen Li, Mark Rowland, Daniel Hernández-Lobato, Thang Bui, and Richard Eric Turner. Black-box α -divergence minimization. 2016.
- Michael C Hughes, Gabriel Hope, Leah Weiner, Thomas H McCoy, Roy H Perlis, Erik B Sudderth, and Finale Doshi-Velez. Prediction-constrained topic models for antidepressant recommendation. arXiv preprint arXiv:1712.00499, 2017.
- Michael C Hughes, Gabriel Hope, Leah Weiner, Thomas H McCoy Jr, Roy H Perlis, Erik B Sudderth,

- and Finale Doshi-Velez. Semi-supervised prediction-constrained topic models. In AISTATS, pages 1067–1076, 2018.
- Pavel Izmailov, Dmitrii Podoprikhin, Timur Garipov, Dmitry Vetrov, and Andrew Gordon Wilson. Averaging weights leads to wider optima and better generalization. arXiv preprint arXiv:1803.05407, 2018.
- Theofanis Karaletsos, Peter Dayan, and Zoubin Ghahramani. Probabilistic Meta-Representations Of Neural Networks. October 2018. arXiv: 1810.00555.
- Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980, 2014.
- Diederik P. Kingma and Max Welling. Auto-Encoding Variational Bayes. December 2014. ICLR.
- Diederik P Kingma, Tim Salimans, and Max Welling. Variational dropout and the local reparameterization trick. In Advances in Neural Information Processing Systems, pages 2575–2583, 2015.
- Diederik P Kingma, Tim Salimans, Rafal Jozefowicz, Xi Chen, Ilya Sutskever, and Max Welling. Improved variational inference with inverse autoregressive flow. In *Advances in Neural Information Processing Systems*, pages 4743–4751, 2016.
- David Krueger, Chin-Wei Huang, Riashat Islam, Ryan Turner, Alexandre Lacoste, and Aaron Courville. Bayesian hypernetworks. arXiv preprint arXiv:1710.04759, 2017.
- Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. Simple and scalable predictive uncertainty estimation using deep ensembles. In Advances in Neural Information Processing Systems, pages 6402–6413, 2017.
- Yann LeCun, Yoshua Bengio, and Geoffrey Hinton. Deep learning. *nature*, 521(7553):436, 2015.
- Chunyuan Li, Changyou Chen, David Carlson, and Lawrence Carin. Preconditioned stochastic gradient langevin dynamics for deep neural networks. In AAAI, 2016.
- Qiang Liu and Dilin Wang. Stein variational gradient descent: A general purpose bayesian inference algorithm. In *Advances In Neural Information Processing Systems*, pages 2378–2386, 2016.
- Qiang Liu, Jason Lee, and Michael Jordan. A kernelized stein discrepancy for goodness-of-fit tests. In *International Conference on Machine Learning*, pages 276–284, 2016.

- Christos Louizos and Max Welling. Structured and efficient variational deep learning with matrix gaussian posteriors. In *International Conference on Machine Learning*, pages 1708–1716, 2016.
- Christos Louizos and Max Welling. Multiplicative normalizing flows for variational bayesian neural networks. In *International Conference on Machine Learning*, pages 2218–2227, 2017.
- Xiuyuan Lu and Benjamin Van Roy. Ensemble Sampling. arXiv:1705.07347 [cs, stat], May 2017. URL http://arxiv.org/abs/1705.07347. arXiv: 1705.07347.
- Lars Maaløe, Casper Kaae Sønderby, Søren Kaae Sønderby, and Ole Winther. Auxiliary deep generative models. In ICML, 2016.
- David JC MacKay. A practical Bayesian framework for backpropagation networks. *Neural computation*, 4(3):448–472, 1992a.
- David JC MacKay. A practical bayesian framework for backpropagation networks. *Neural computation*, 4 (3):448–472, 1992b.
- Preetum Nakkiran, Raziel Alvarez, Rohit Prabhavalkar, and Carolina Parada. Compressing Deep Neural Networks using a Rank-Constrained Topology, 2015.
- Radford M Neal. Bayesian learning via stochastic dynamics. In *NIPS*, 1993.
- Radford M Neal. Bayesian learning for neural networks, volume 118. Springer Science & Business Media, 2012.
- Nick Pawlowski, Martin Rajchl, and Ben Glocker. Implicit weight uncertainty in neural networks. arXiv preprint arXiv:1711.01297, 2017.
- Tim Pearce, Mohamed Zaki, Alexandra Brintrup, and Andy Neel. Uncertainty in neural networks: Bayesian ensembling. arXiv preprint arXiv:1810.05546, 2018.
- Rajesh Ranganath, Sean Gerrish, and David Blei. Black box variational inference. In *Artificial Intelligence* and *Statistics*, pages 814–822, 2014.
- Rajesh Ranganath, Dustin Tran, and David Blei. Hierarchical variational models. In *International Conference on Machine Learning*, pages 324–333, 2016.
- Danilo Jimenez Rezende and Shakir Mohamed. Variational inference with normalizing flows. In *ICML*, 2015.

- Danilo Jimenez Rezende, Shakir Mohamed, and Daan Wierstra. Stochastic Backpropagation and Approximate Inference in Deep Generative Models. January 2014. arXiv: 1401.4082.
- Tara N. Sainath, Brian Kingsbury, Vikas Sindhwani, Ebru Arisoy, and Bhuvana Ramabhadran. Low-rank matrix factorization for Deep Neural Network training with high-dimensional output targets. pages 6655–6659. IEEE, May 2013.
- Tim Salimans, David A Knowles, et al. Fixed-form variational posterior approximation through stochastic linear regression. *Bayesian Analysis*, 8(4):837–882, 2013.
- Jost Tobias Springenberg, Aaron Klein, Stefan Falkner, and Frank Hutter. Bayesian optimization with robust bayesian neural networks. In *Advances in Neural Information Processing Systems*, pages 4134–4142, 2016.
- Jiawei Su, Danilo Vasconcellos Vargas, and Kouichi Sakurai. One pixel attack for fooling deep neural networks. *IEEE Transactions on Evolutionary Com*putation, 2019.
- Shengyang Sun, Changyou Chen, and Lawrence Carin. Learning structured weight uncertainty in bayesian neural networks. In *Artificial Intelligence and Statis*tics, pages 1283–1292, 2017.
- Shengyang Sun, Guodong Zhang, Jiaxin Shi, and Roger Grosse. Functional variational Bayesian neural networks. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=rkxacs0qY7.
- Ziyu Wang, Tongzheng Ren, Jun Zhu, and Bo Zhang. Function space particle optimization for bayesian neural networks. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=BkgtDsCckQ.
- Jian Xue, Jinyu Li, and Yifan Gong. Restructuring of deep neural network acoustic models with singular value decomposition. In *Interspeech*, pages 2365–2369, 2013.

Appendix A: Details on Experimental Setup

Generation of Toy Datasets

The data in Figure 1 was generated by sampling points non-uniformly from a function represented by a feedforward network (with 1 hidden layer, 20 hidden nodes and RBF activation centered at 0 with length scale 1) whose weights are obtained by applying a fixed linear transform to a fixed latent vector z.

The toy data in Figure 2 was generated by first sampling data points from the 4 modes shown in Figure 2d, and then fitting a feedforward network multiple times with a single hidden layer, three nodes and RBF activation function). Each cluster of weights corresponds to fitting a different set of three of the four modes in the data.

Baselines

- Bayes by Backprop (BbB): We implemented this algorithm ourselved. Note that proj-BNN can be reduced to BbB when the projection function is the identity. We perform cross-validation of the learning rate in the range: [0.0001, 0.005, 0.001, 0.01, 0.1].
- Fast Geometric Ensembling (FGE): this method is used both, as a baseline, and in the first stage of our inference framework to find a smart initialization for Proj-BNN. In both cases, we use the following hyperparameters: a step-size of 0.001 to first reach the MAP solution, and then a cyclic learning rate between 0.01 and 0.0001. Each cycle lasts for 10 epochs.
- Matrix Variate Gaussian Posteriors (MVG): we use the code in Tensorflow that is publicly available from the authors at: https://github.com/AMLab-Amsterdam/SEVDL_MGP. In their original formulation, the authors learn the observational noise: in order to allow for comparison across different baselines, for simplicity, we adapt their code to keep the observational noise fixed to $\sigma_y = 0.1$.
- Bayesian Hypernetworks (BbH): we use the code in Tensorflow from the authors that is publicly available at https://github.com/pawni/BayesByHypernet. For the architecture of the hypernetwork, we cross-validate across the architectures used in the authors'paper, namely: [[50], [64, 64], [128, 128]].
- Multiplicative Normalizing Flows (MNF): we use the code that is publicly available at https://github.com/AMLab-Amsterdam/MNF_VBNN. We keep all default hyperparameters, except the learning rate, which we cross-validate using a grid search [0.0005, 0.001, 0.005, 0.01].

Simulation Setup

For each data set, we gather R = 500 candidate weight solutions $\mathbf{w_c}$ using Fast Geometric Ensembling on the training set. We then keep the top best 150 sets of weights in terms of RMSE in validation set.

In all the experiments, we use a random train-test-validation split of 80-10-10. All datasets are normalized in a preprocessing step to have zero mean and unit standard deviation. For each optimization subtask in our inference framework, we perform cross-validation of the step size $\lambda_1 \in \{0.1, 0.01, 0.001, 0.0005, 0.0001\}$ and fix the batch-size to 128. We use Adam as the optimizer and the joint unnormalized posterior distribution $p(\boldsymbol{w}|\mathcal{D}_{train})$ as the objective function. Optimization is performed with L = 50,000 iterations and early stopping once the marginal log likelihood in validation set stop increasing after 30 iterations.

The proposed approach proj-BNN is implemented in Autograd, source code is publicly available at: Anonymized. For the prediction-constrained autoencoder (the projection function), we fix the architecture to either a single layer of 20 nodes or 10,10 with two hidden layers. We use RBF activation functions, and additional input noise with variance 1 for robustness. We cross-validate across the dimensionality of the latent space z in the range 2, 10, 50, 100. We use 20 samples for the reparametrization trick.

We evaluate by computing the marginal test log likelihood as:

$$\mathbb{E}_{p(\mathbf{x}^{\star}, \mathbf{y}^{\star})} \left[\log p(\mathbf{y}^{\star} | \mathbf{x}^{\star}, \mathcal{D}) \right] = \mathbb{E}_{p(\mathbf{x}^{\star}, \mathbf{y}^{\star})} \left[\log \int p(\mathbf{y}^{\star} | \mathbf{x}^{\star}, \boldsymbol{w}) p(\boldsymbol{w} | \mathcal{D}) d\boldsymbol{w} \right]$$
(7)

Appendix B: Further Results

Impact of dimensionality of latent space

Figure 4 shows the *point-wise* marginal test log-likelihood $p(\mathbf{Y}|\mathbf{X}, \boldsymbol{w}^{(s)})$ for 500 different samples $\boldsymbol{w}^{(s)} \sim q(\boldsymbol{w})$ of Proj-BNN for varying dimensionality of the latent space \boldsymbol{z} across the UCI benchmark datasets considered in the paper.

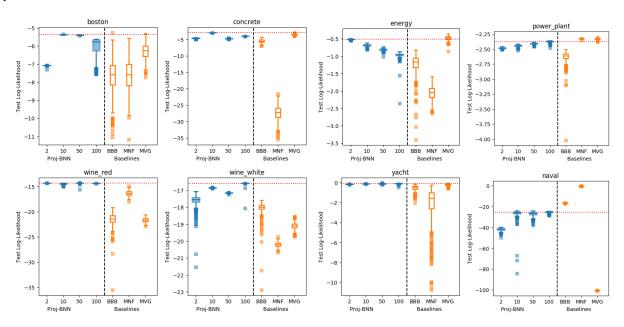


Figure 4: Test log-likelihood for UCI benchmark datasets for varying dimensionality of z-space. Each dot corresponds to $p(\mathbf{Y}|\mathbf{X}, \boldsymbol{w}^{(s)})$, where $\boldsymbol{w}^{(s)}$ is one sample from the optimized variational posterior $\boldsymbol{w}^{(s)} \sim q(\boldsymbol{w})$. Red dotted horizontal line corresponds to the best performance of our approach Proj-BNN. Baselines: a) BBB: Bayes By Backprop (Blundell, et.al 2015); b) MNF: multiplicative normalizing flow (Louizos et.al, 2017); c) MVG: multivariate Gaussian prior BNN (Louizos et.al, 2016).

Extrapolation and Interpolation Splits

In this Section, we repeat the simulations on the UCI benchmark datasets but perform a splitting of the data that tests the extrapolation and interpolation capacities of the models more precisely. In particular, we split the data according to the L2 norm of the observations. We create two datasets with 80% training, 10% validation, and 10% testing as follows: the extrapolation split is such that 5% of the observations with highest norm and 5% of the observations with lowest norm are kept in the test set; the interpolation split is the complementary to that one (that is, an inverted doughnut). Interestingly, BbB proves to be quite robust across all datasets. Overall, our approach is more robust to other structured variational inference techniques.

Proj-BNNs as broad priors over functions

Proj-BNNs can be adapted to express broader priors over functions. In particular, consider a Proj-BNN variant where the auxiliary latent variable z is function specific. Given M functions where each function provides us with a set of training instances, $\{\mathbf{x}_m, \mathbf{y}_m\}_{m=1}^M$, for each task m,

$$\boldsymbol{z}_m \sim \mathcal{N}(\boldsymbol{z}_m \mid \boldsymbol{0}, \mathbf{I}), \, \boldsymbol{w}_m = g_{\boldsymbol{\phi}}(\boldsymbol{z}_m),$$
 (8)

$$\mathbf{y}_m \sim \mathcal{N}(f_{\boldsymbol{w}_m}(\mathbf{x}_m), \sigma_y^2), \tag{9}$$

with the projection parameters $\phi \sim p(\phi)$ shared across all functions. The function specific latent variables allow us to capture function specific variations while the share projection parameters allows for the sharing of statistical strength across functions.

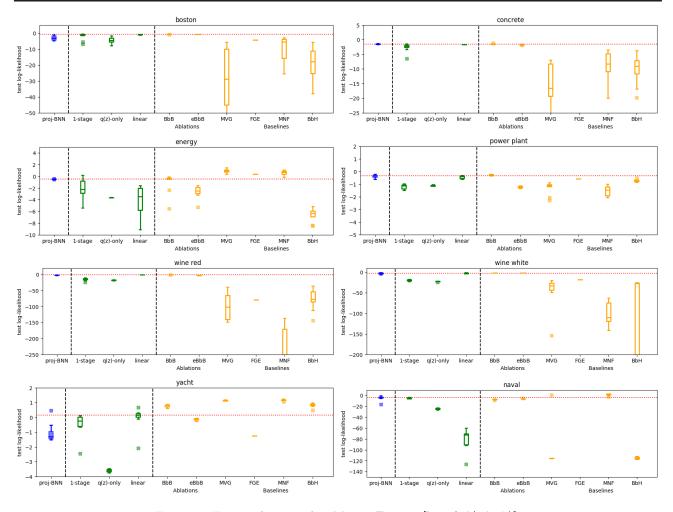


Figure 5: Extrapolation split. Metric $\mathbb{E}_{(\mathbf{x}^{\star},\mathbf{y}^{\star})} [\log p(\mathbf{y}_{n}^{\star}|\mathbf{x}_{n}^{\star},\mathcal{D})].$

To explore the effectiveness of such a model we created a toy 1-D regression dataset of sine functions, $y = a \times \sin(x+b)$, of varying amplitudes and phases. We sampled $a \sim \text{Unif}(-3,3)$ and varied b by selecting equally spaced points in the range $[0,2\pi]$. The set of training functions are shown in Figure 7. Given the diversity of functions, a shared BNN struggles to learn meaningful mappings. In contrast, the Proj-BNN described in Equation 9 with $D_z = 2$, and a 50 unit network with tanh activations, learns an intuitive representation of the entire space (Figure 9). Moreover, Proj-BNN decomposes uncertainty between z and ϕ (Figure 8). While z captures the structural differences between the functions, uncertainty in ϕ captures the uncertainty associated with a single function. These capabilities make Proj-BNN particularly attractive for multi-task and meta-learning applications, directions we plan to explore further in future work.

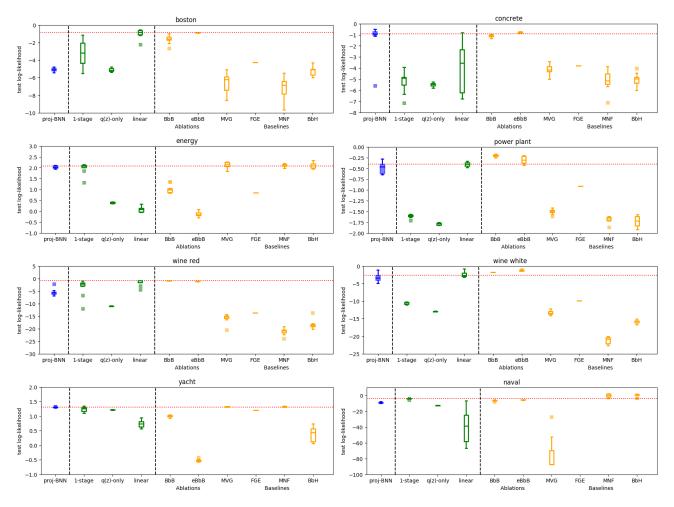


Figure 6: Interpolation split. Metric $\mathbb{E}_{(\mathbf{x}^{\star}, \mathbf{y}^{\star})} [\log p(\mathbf{y}_{n}^{\star} | \mathbf{x}_{n}^{\star}, \mathcal{D})].$

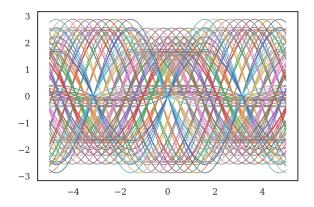


Figure 7: Visualization on training functions drawn from the family $y = a \times \sin(x + b)$.

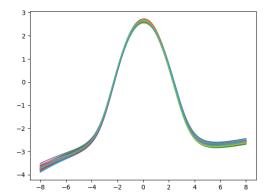


Figure 8: Visualization of variance captured in ϕ . Different colors correspond to different draws for a fixed z^s but varying samples of $\phi^s \sim q(\phi)$.

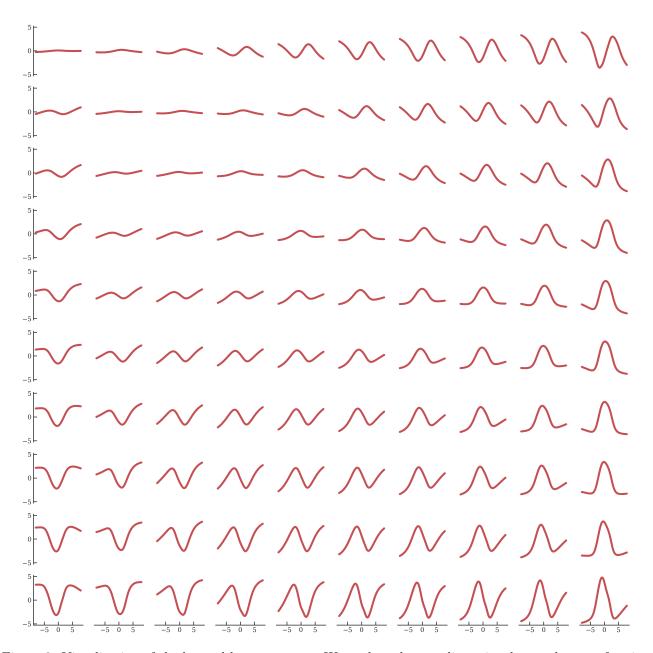


Figure 9: Visualization of the learned latent space z. We explore the two dimensional space by transforming linearly spaced coordinates on the unit square through the inverse CDF of a standard Gaussian to produce instantiations of z, z^s . Using the variational mean $\tilde{\mu}_{\phi}$, we plot $y = f_{w^s}(x)$, where $w^s = g_{\tilde{\mu}_{\phi}}(z^s)$.