Sampling and prior selection

2023

Model selection: coherent inference

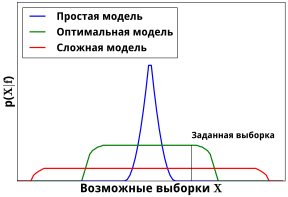
First level: select optimal parameters:

$$\mathbf{w} = \arg\max \frac{p(\mathfrak{D}|\mathbf{w})p(\mathbf{w}|\mathbf{h})}{p(\mathfrak{D}|\mathbf{h})},$$

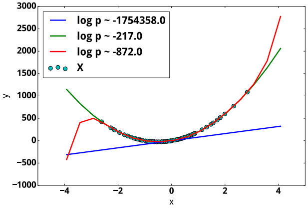
Second level: select optimal model (hyperparameters).

Evidence:

$$p(\mathfrak{D}|\mathbf{h}) = \int_{\mathbf{w}} p(\mathfrak{D}|\mathbf{w})p(\mathbf{w}|\mathbf{h})d\mathbf{w}.$$



Model selection scheme



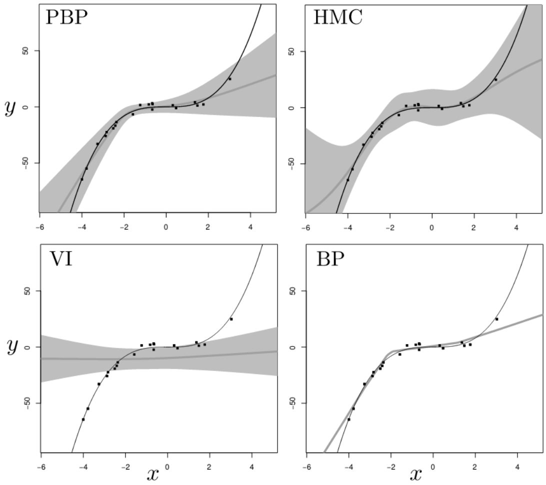
Example: polynoms

Evidence estimation

$$\mathsf{E}f = \int_{\mathrm{w}} f(\mathrm{w})p(\mathrm{w})d\mathrm{w}.$$

- Laplace approximation
  - Fixed form of approximation distribution
  - Poorly scales
- Variational inference
  - Well scales
  - Can use different forms of approximation distributions
  - Lower bound of evidence => biased
- MC
  - Can use different forms of approximation distributions
  - Approximates well
  - Slow

VI vs MC



Naive method

$$I = \mathrm{E}f = \int_w f(\mathrm{w})p(\mathrm{w})d\mathrm{w}.$$

Approximate:

$$\hat{I} = \frac{1}{N}\sum_{\mathrm{w}\sim p(\mathrm{w})} f(\mathrm{w}).$$

Properties

Integral estimation:

- strongly consistent : $\hat{I} \to^{\text{a.s.}} I$
- Unbiased: $\mathrm{E}\hat{I} = I$
- Assymptotically normal;
- $\mathrm{D}\hat{I} = O(\frac{1}{N})$.
- **Challenge:** we need to sample from p.

Why this does not work?

Inverse transform sampling

Let T be a invertible function from $u \sim \mathcal{U}(0,1)$ to some random variable distribution $p(w)$. Then

$$F_w(t) = p(w \leq t) = p(T(u) \leq t) = p(u \leq T^{-1}(t)) = T^{-1}(u).$$

Therefore $F_u^{-1} = T$.

Example

$$w = \lambda \exp(-\lambda t).$$

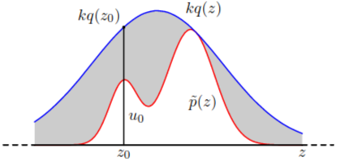
$$F_w(t) = 1 - \exp(-\lambda t).$$

$$F_w^{-1}(t') = -1\frac{1}{\lambda}\log(1 - t').$$

Rejection sampling

- Given $p(w)$ (up to normalizing constant)
- Set distribution q
- Set value k so that $kq(w) \geq p(z)$ for all z
- In a loop:
  - Sample $w_0 \sim q$
  - Sample $u \sim \mathcal{U}(0, kq(w_0))$
  - If $u \leq p(w_0)$, use it as a sample from $p(w)$

Core idea: sample u are uniform in a region limited by $p(w)$.



Bishop, 2006

Importance sampling

Consider the case when we cannot sample from $p(w)$, but we can estimate likelihood and want to estimate the integral

$$\mathsf{E}f = \int f(w)p(w)dz.$$

Let q be an auxilary distribution:

$$\mathsf{E}f = \int f(w)p(w)dw = \int f(w)\frac{p(w)}{q(w)}dz \approx \frac{1}{L}\sum_{l=1}^{L}\frac{p(w^l)}{q(w^l)}f(w^l).$$

MCMC

Basic idea: Sample similar to rejection sampling, but q is a Markov distribution with conditioning on the previous step.
We want the stationary (limiting) distribution to be equal to our $p(w)$.
Sufficient condition

$$p(w')T(w|w') = p(w)T(w'|w).$$

Metropolis-Hastings algorithm

- Sample new $w' \sim q(w|w^t)$.
- Accept with probability $A(w'|w^t) = \min\left(1, \frac{p(w')q(w^t|w')}{p(w^t)q(w'|w^t)}\right)$.
- If accepted: $w^{t+1} = w'$,
- Otherwise: $w^{t+1} = w^t$.

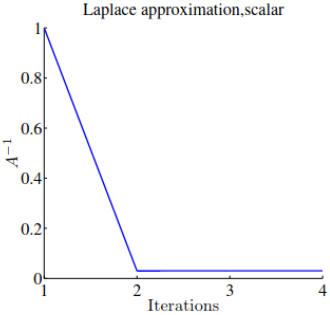
Sufficient condition is satisfied::

$$p(w')T(w|w') = p(w)T(w'|w) = p(w')T(w'|w^t) = p(w')q(w'|w^t)A(w'|w^t) =$$

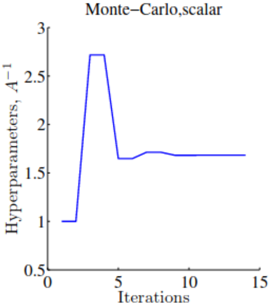
$$= p(w^t)q(w^t|w')A(w^t|w').$$

- Samples are correlated. We can decorrelate sample using each k sample.
- Works better in high-dimmensional settings than rejection sampling.
- Good choice of q is the main challenge for the algorithm.

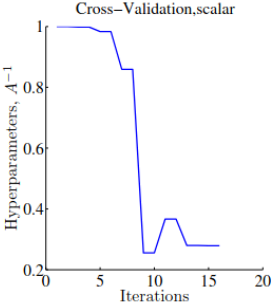
Hyperparameter selection for linear model



(a) Laplace approximation

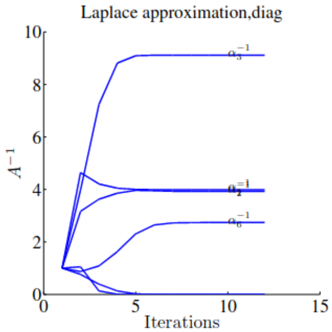


(b) Monte-Carlo

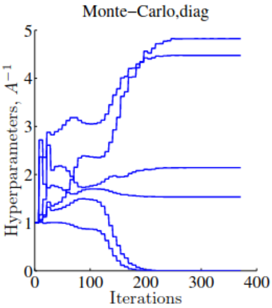


(c) Cross validation

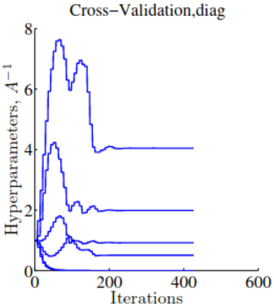
Hyperparameter selection for linear model



(a) Laplace approximation

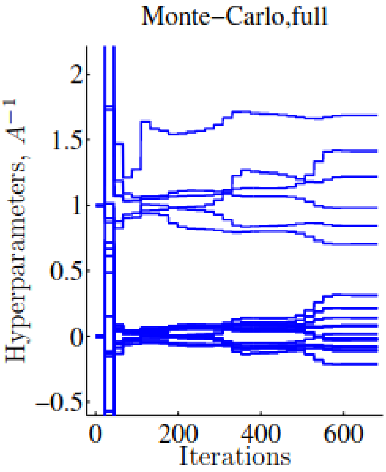


(b) Monte-Carlo

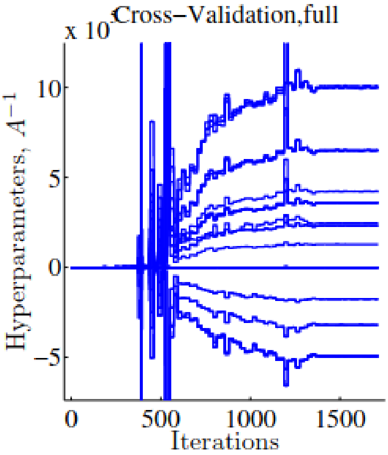


(c) Cross validation

Hyperparameter selection for linear model



(a) Monte-Carlo



(b) Cross validation

Stochastic gradient Langevin dynamics

A modification of SGD:

$$T = \mathrm{w} - \beta \nabla L + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \frac{\beta}{2})$$

where β changes with a number of iterations:

$$\sum_{\tau=1}^{\infty} \beta_\tau = \infty, \quad \sum_{\tau=1}^{\infty} \beta_\tau^2 < \infty.$$

Statement [Welling, 2011]. Distribution $q^\tau(\mathrm{w})$ converges to posterior distribution $p(\mathrm{w}|\mathrm{X}, \mathrm{f})$.
Entropy adjustment:

$$\hat{\mathrm{S}}(q^\tau(\mathrm{w})) \geq \frac{1}{2}|\mathrm{w}| \log(\exp(\frac{2\mathrm{S}(q^\tau(\mathrm{w}))}{|\mathrm{w}|}) + \exp(\frac{2\mathrm{S}(\epsilon)}{|\mathrm{w}|})).$$

Special case of Metropolis-Hastings

Precondition-matrix for SGLD

SGLD:

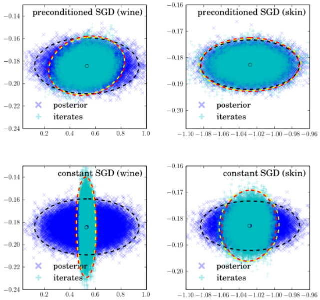
$$T = \mathrm{w} - \beta \nabla L + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \frac{\alpha}{2})$$

pSGLD:

$$T = \mathrm{w} - \beta \mathrm{M} \nabla L + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \frac{\alpha}{2}\mathrm{M}),$$

matrix M is optimized to make gradient step uniform for each direction (w.r.t. gradient variance).

Example for SGD, for SGLD the results are similar.



Gibbs sampling

Given a graphical model $w_1, \ldots, w_n$.
Then in a loop over variables:

$$\hat{w}_i \sim p(w_i | w_1, w_{i-1}, w_{i+1}, w_n), w_i := \hat{w}_i$$

Gibbs sampling is also a special case of MH.

Contrastive Divergence: idea

Energy-based model:

$$p(x|w) = \frac{\exp\left(-E_w(x)\right)}{Z(w)}, \quad Z = \int_x \exp\left(-E_w(x)\right),$$

$$\frac{\partial \log p(x|w)}{\partial w} = \mathrm{E}_{x' \sim p(x|\mathrm{w})} \frac{\partial E(x')}{\partial w} - \frac{\partial E(x)}{\partial w}$$

Algorithm for RBM:

- Take x from the dataset
- $h_0 \sim p(h_0|x)$
- $x_1 \sim p(x|h_0)$
- ...
- Obtain x_k
- $\frac{\partial \log p(x|w)}{\partial w} = \frac{\partial E(x_k)}{\partial w} - \frac{\partial E(x)}{\partial w}$

Autoencoder: generative model?

(Alain, Bengio 2012): consider regularized autoencoder:

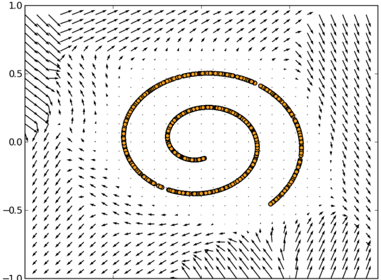
$$||\mathrm{f}(\mathrm{x}, \sigma) - \mathrm{x}||^2,$$

where σ is a noise level.

Then

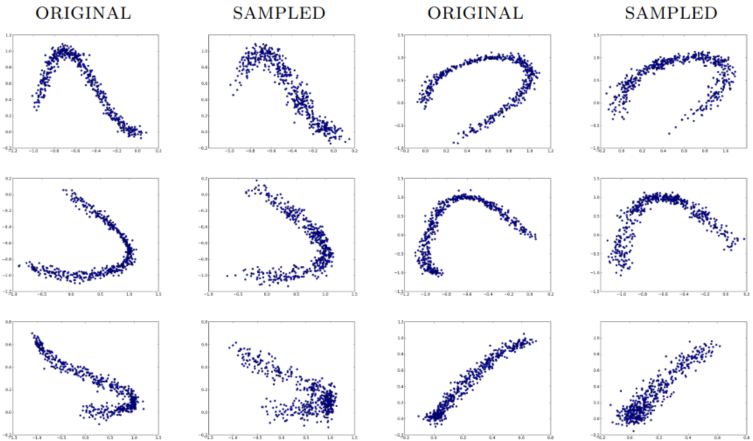
$$\frac{\partial \log p(x)}{\partial x} = \frac{||\mathrm{f}(\mathrm{x}, \sigma) - \mathrm{x}||^2}{\sigma^2} + o(1) \text{ при } \sigma \to 0.$$

Vector field induced by reconstruction error



Autoencoder for sampling

$$A = \frac{p(x^*)}{p(x)} = \exp\left(E(x) - E(x^*)\right) \approx \frac{\partial E(x)}{\partial x}^{\mathsf{T}}(x^* - x) + o(||x - x^*||).$$



Optimization of q

Distribution q can be set using neural networks.

- **Main requirements:** existance of $p(x|x'), p(x'|x) \rightarrow$ the distribution must be invertible.
- Neural network in a form of $\mathrm{f(x, w) = x + g(x, w)}$ is a flow and invertible.

Optimization variants:

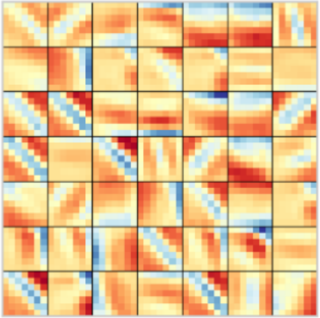
- Entropy * Acceptance rate (Li et al., 2020)
- GAN between empirical distribution and q (Song et al., 2017).

Informative prior vs Uninformative prior

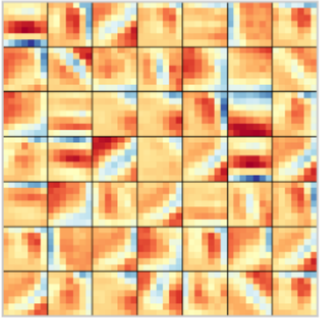
- Informative prior: corresponds to some expert knowledge
  - Example: air temperature in some region: Gaussian variable with known mean and variance estimated from previous observations.
  - Mistanke in informative prior estimation leads to poor models.
- Uninformative prior: corresponds to some basic knowledge
  - Example: air temperature in some region: uniform improper prior.
- Weakly-informative prior: somewhere in between
  - Example: air temperature in some region: uniform distribution in [-50, 50].

What if our prior and posterior are very close?

The deep weight prior: Atanov et al., 2019



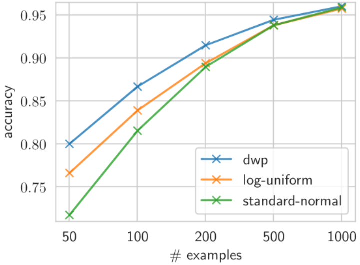
(b) Learned filters



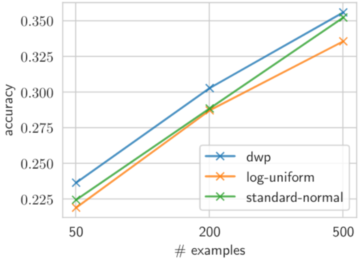
(c) Samples from DWP

The distribution can be modeled by complex models and can generate rather informative samples!

The deep weight prior: Atanov et al., 2019

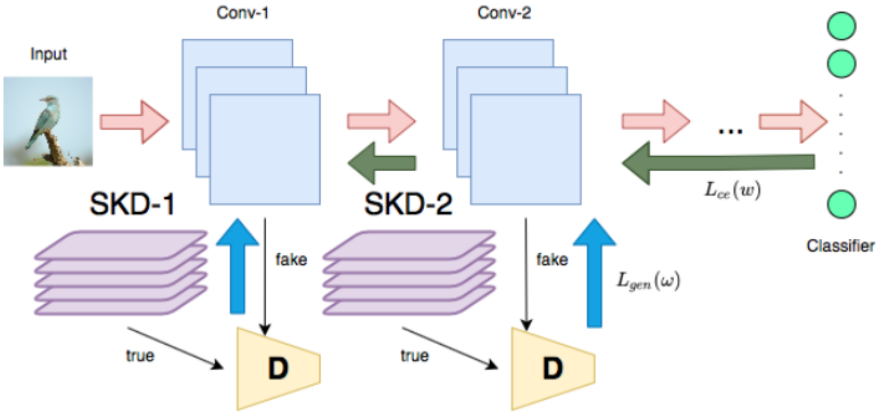


(a) Results for MNIST

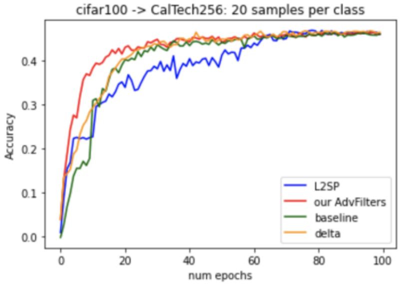


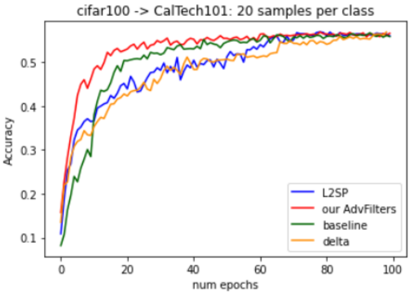
(b) Results for CIFAR-10

Deep weight prior for distillation, Kolesov 2022

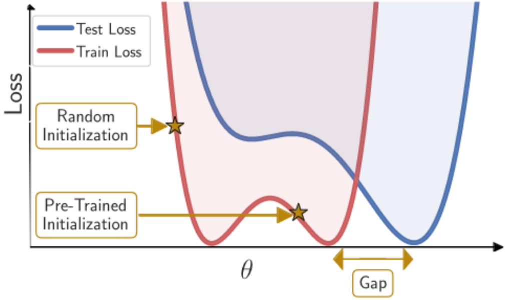


Deep weight prior for distillation, Kolesov 2022

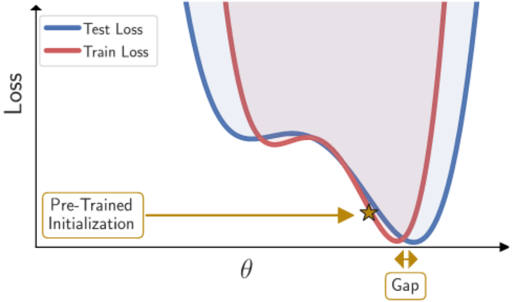




Pre-Train Your Loss: Easy Bayesian Transfer Learning with Informative Priors, 2022



(a) Standard Transfer Learning



(b) Transfer Learning with Learned Priors

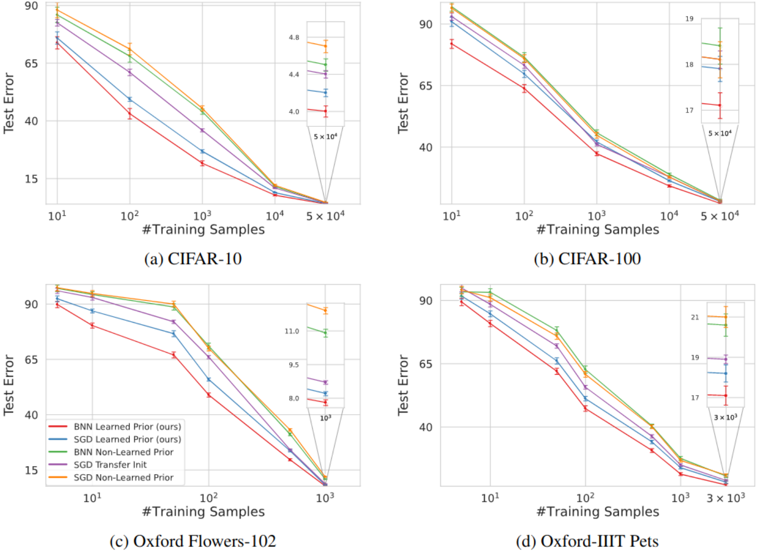
Pre-Train Your Loss: Easy Bayesian Transfer Learning with Informative Priors, 2022

- Decompose model into feature extractor and classifier
- Learn feature extractor's posterior on the source task using SWAG
- Consider target prior to be similar to source posterior:

$$p(\mathrm{w}) = \mathcal{N}(\boldsymbol{\mu}, h\mathrm{A}^{-1}),$$

  where $h \in \mathbb{R}$ is calibrated on the target task.
- Learn prior for the classifier on the target task

Pre-Train Your Loss: Easy Bayesian Transfer Learning with Informative Priors, 2022



(a) CIFAR-10 (b) CIFAR-100

(c) Oxford Flowers-102 (d) Oxford-IIIT Pets

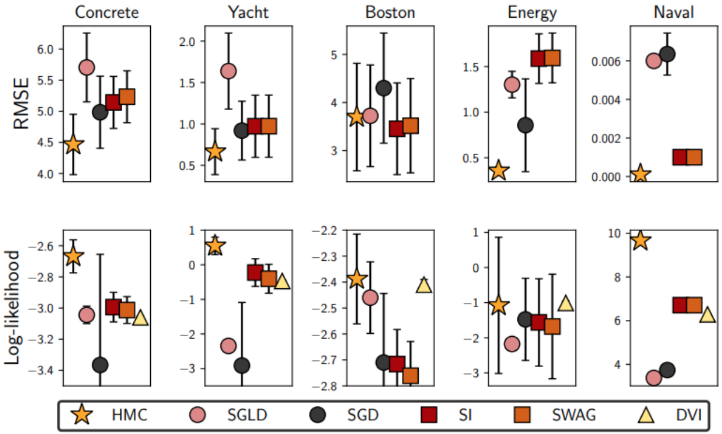
What Are Bayesian Neural Network Posteriors Really Like?

Izmailov et al., 2021:

- HMC for posterior distribuition estimation for deep models on some standard datasets.
- Resources: 512 TPU

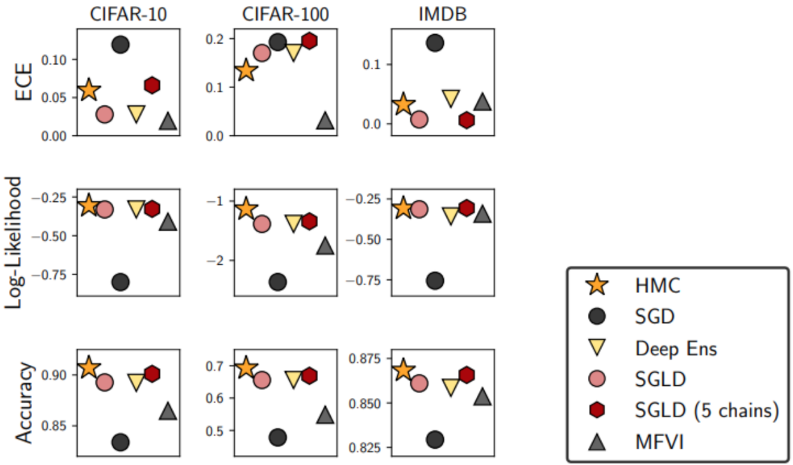
What Are Bayesian Neural Network Posteriors Really Like?

BNN evaluation: UCI



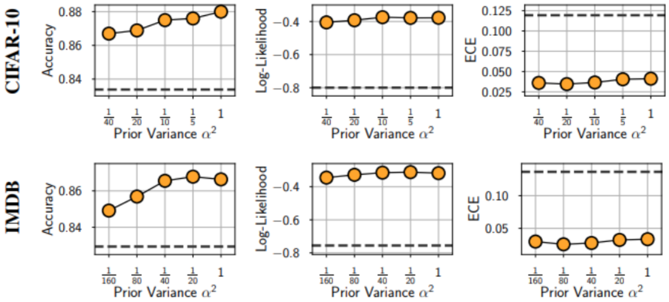
What Are Bayesian Neural Network Posteriors Really Like?

BNN evaluation: CIFAR and IMDB



What Are Bayesian Neural Network Posteriors Really Like?

Effect of priors



HMC BNNs are fairly robust to Gaussian prior variance.

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