Master Presentation Marius Hobbhahn

Start: 14:30

Fast Predictive Uncertainty for Classification with Bayesian Deep Networks

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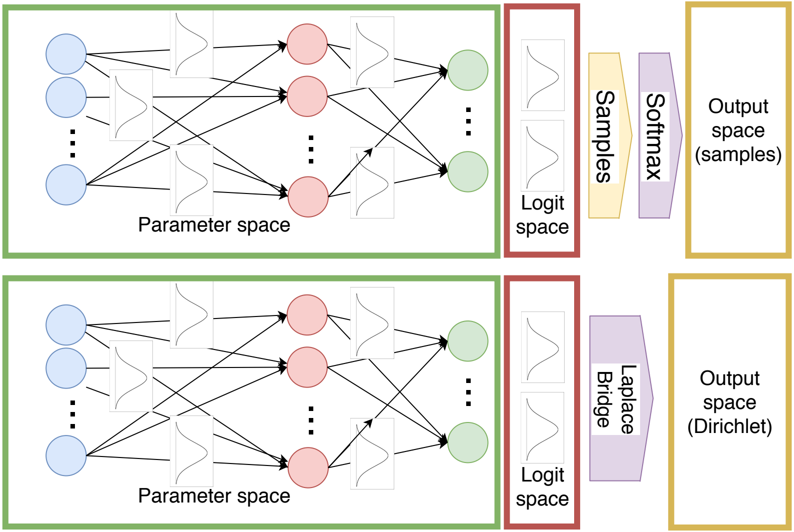
Motivation

Why do we need fast uncertainty in neural networks?

- safety-critical applications e.g. self-driving cars
- trade-off between accuracy and speed
- out-of-distribution detection

Context

What's our new contribution?



Theory

Let $\mathbf{x}$ be an n-dimensional continuous random variable with joint density function $p_{\mathbf{x}}$. If $\mathbf{y} = g(\mathbf{x})$, where g is a differentiable function, then $\mathbf{y}$ has density $p_{\mathbf{y}}$:

$$p_{\mathbf{y}}(\mathbf{y}) = p_{\mathbf{x}}\left(g^{-1}(\mathbf{y})\right) \left| \det \left[\frac{dg^{-1}(\mathbf{y})}{d\mathbf{y}} \right] \right| \tag{1}$$

where the differential is the Jacobian of the inverse of g evaluated at $\mathbf{y}$.

A new basis for the Dirichlet

The math

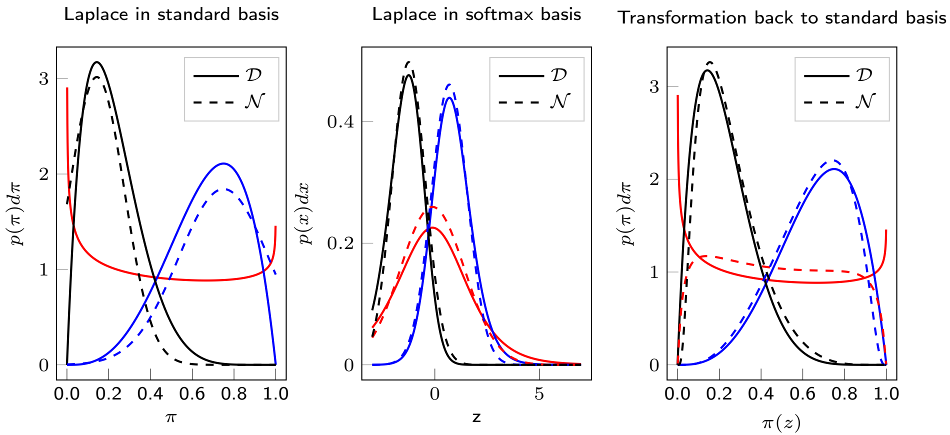
- $$\mathrm{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}) := \frac{1}{B(\alpha)} \prod_{k=1}^{K} \pi_k^{\alpha_k - 1} \tag{2}$$

- $$\pi_k(\mathbf{z}) := \frac{\exp(z_k)}{\sum_{l=1}^{K} \exp(z_l)}\,, \tag{3}$$

- $$\mathrm{Dir}_{\mathbf{z}}(\boldsymbol{\pi}(\mathbf{z})|\boldsymbol{\alpha}) := \frac{1}{B(\alpha)} \prod_{k=1}^{K} \pi_k(\mathbf{z})^{\alpha_k}\,, \tag{4}$$

A new basis for the Dirichlet

In pictures



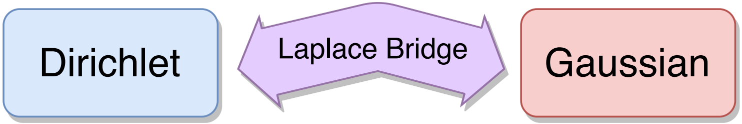
The Laplace Bridge

A bridge between the parameters of the Dirichlet and Gaussian

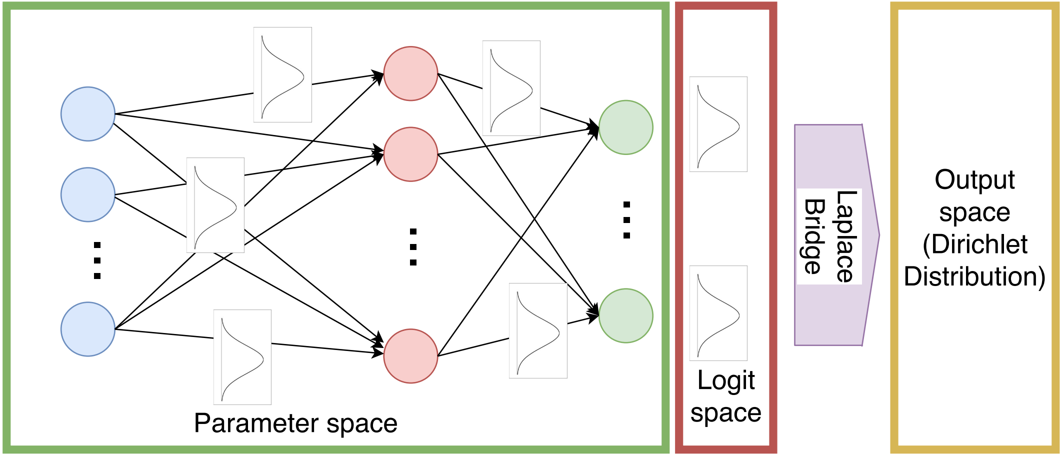
$$\alpha_k = \frac{1}{\Sigma_{kk}} \left(1 - \frac{2}{K} + \frac{e^{\mu_k}}{K^2} \sum_{l}^{K} e^{-\mu_l} \right) \tag{5}$$

$$\mu_k = \log \alpha_k - \frac{1}{K} \sum_{l=1}^{K} \log \alpha_l \tag{6}$$

$$\Sigma_{kl} = \delta_{kl} \frac{1}{\alpha_k} - \frac{1}{K} \left[\frac{1}{\alpha_k} + \frac{1}{\alpha_l} - \frac{1}{K} \sum_{u=1}^{K} \frac{1}{\alpha_u} \right] \tag{7}$$



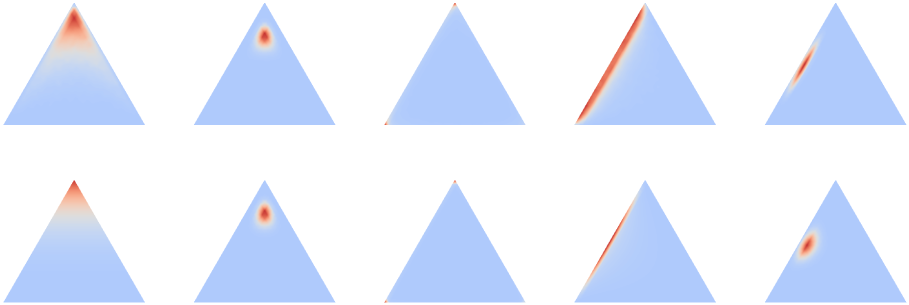
- The Dirichlet in the inverse softmax basis approximates a Gaussian
- Via the Laplace approximation in the transformed basis we can create a closed-form transformation $\alpha \to (\mu, \Sigma)$.
- We can also construct an inverse of this transformation $(\mu, \Sigma) \to \alpha$
- In total, we have a **fast** way to transform between the parameters of a Dirichlet and a Gaussian


Parameter space
Logit space
Laplace Bridge
Output space (Dirichlet Distribution)

Experiments

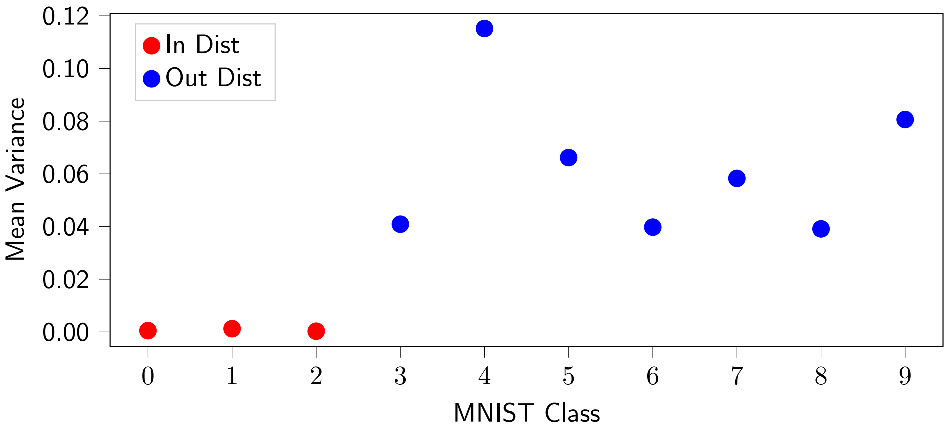
A sanity check

Samples from a 3D Gaussian + Softmax vs. Dirichlet



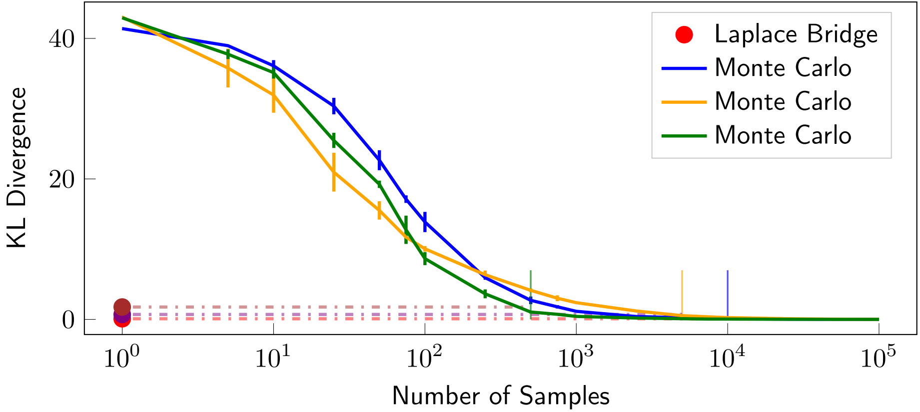
MNIST

Train on 0,1,2; test on 0-9



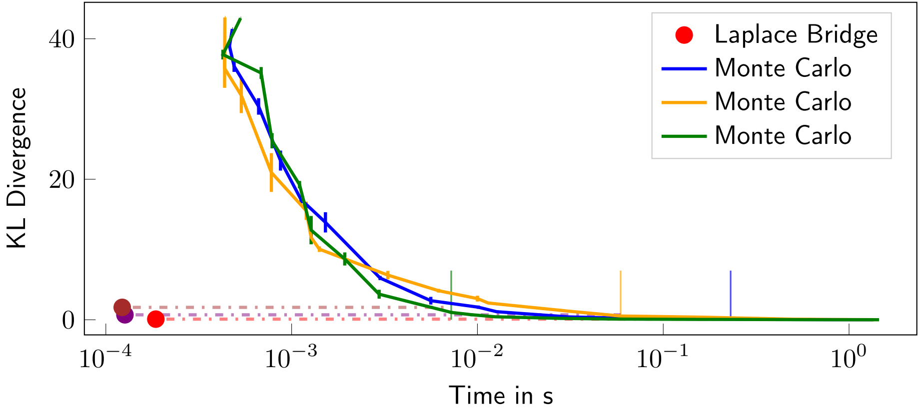
Speedtest - I

KL divergence vs. number of samples



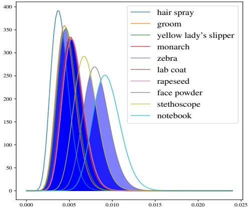
Speedtest - II

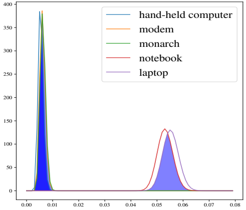
KL divergence vs. wall-clock time

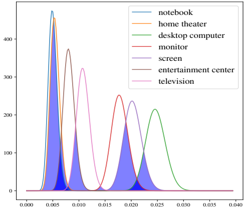


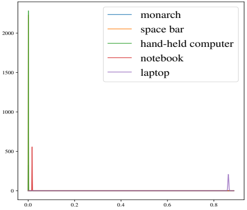
Imagenet

Using the properties of the Dirichlet - The marginal of a Dirichlet is a Dirichlet





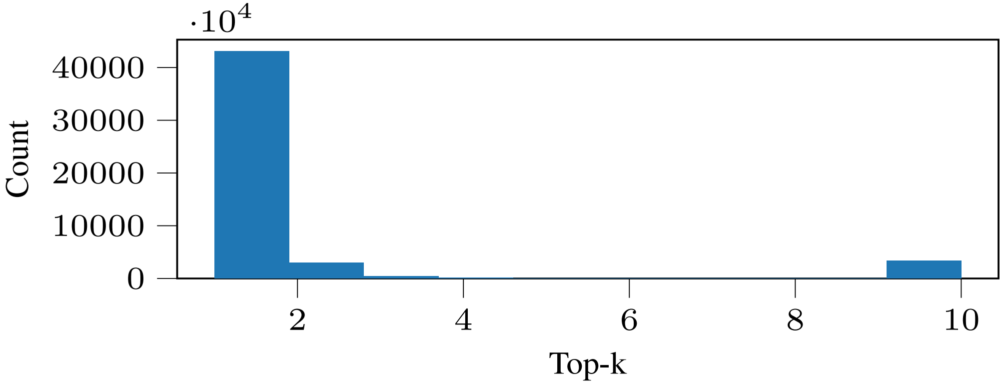




We can use the overlap of the distributions to create an uncertainty-aware top-k ranking.

Imagenet - II

How good is the flexible top-k ranking?



- The original top-1 accuracy of DenseNet on ImageNet is 0.744 and top-5 accuracy is 0.919
- The uncertainty-aware top-k accuracy is 0.797, where k is on average 1.688.

Out-of-distribution Detection

Looking at the numbers

Train	Test	Diag Sampling MMC ↓	Diag Sampling AUROC ↑	Diag LB MMC ↓	Diag LB AUROC ↑	KFAC Sampling MMC ↓	KFAC Sampling AUROC ↑	KFAC LB MMC↓	KFAC LB AUROC ↑	Time in s ↓ Sampling	Time in s ↓ LB
MNIST	MNIST	0.942 ± 0.007	-	**0.987** ± 0.000	-	-	-	-	-	26.8	**0.062**
MNIST	FMNIST	0.397 ± 0.001	0.992 ± 0.000	**0.363** ± 0.000	**0.996** ± 0.000	-	-	-	-	26.8	**0.062**
MNIST	notMNIST	**0.543** ± 0.000	0.960 ± 0.000	0.649 ± 0.000	**0.961** ± 0.000	-	-	-	-	50.3	**0.117**
MNIST	KMNIST	**0.513** ± 0.001	**0.974** ± 0.000	0.637 ± 0.000	0.973 ± 0.000	-	-	-	-	26.9	**0.062**
CIFAR-10	CIFAR-10	0.948 ± 0.000	-	**0.966** ± 0.000	-	0.857 ± 0.003	-	**0.966** ± 0.000	-	6.58	**0.017**
CIFAR-10	CIFAR-100	**0.708** ± 0.000	**0.889** ± 0.000	0.742 ± 0.000	0.866 ± 0.000	**0.562** ± 0.003	**0.880** ± 0.012	0.741 ± 0.000	0.866 ± 0.000	6.59	**0.016**
CIFAR-10	SVHN	**0.643**± 0.000	0.933 ± 0.000	0.647 ± 0.000	**0.934** ± 0.000	**0.484** ± 0.004	**0.939** ± 0.001	0.648 ± 0.003	0.934 ± 0.001	17.0	**0.040**
SVHN	SVHN	0.986 ± 0.000	-	**0.993** ± 0.000	-	0.947 ± 0.002	-	**0.993** ± 0.000	-	17.1	**0.042**
SVHN	CIFAR-100	0.595 ± 0.000	0.984 ± 0.000	**0.526** ± 0.000	**0.985** ± 0.000	**0.460** ± 0.004	**0.986** ± 0.001	0.527 ± 0.002	0.985 ± 0.000	6.62	**0.017**
SVHN	CIFAR-10	0.593 ± 0.000	0.984 ± 0.000	**0.520** ± 0.000	**0.987** ± 0.000	**0.458** ± 0.004	0.986 ± 0.001	0.520 ± 0.002	**0.987** ± 0.000	6.62	**0.017**
CIFAR-100	CIFAR-100	**0.762** ± 0.000	-	0.590 ± 0.000	-	0.404 ± 0.000	-	**0.593** ± 0.000	-	6.76	**0.016**
CIFAR-100	CIFAR-10	0.467 ± 0.000	0.788 ± 0.000	**0.206** ± 0.000	**0.791** ± 0.000	0.213 ± 0.000	0.788 ± 0.000	**0.209** ± 0.000	**0.791** ± 0.000	6.71	**0.017**
CIFAR-100	SVHN	0.461 ± 0.000	0.795 ± 0.000	**0.170** ± 0.000	**0.815** ± 0.000	0.180 ± 0.001	**0.838** ± 0.001	**0.173** ± 0.000	0.815 ± 0.000	17.3	**0.041**

- The Laplace Bridge seems to be have better MMC and AUROC compared to sampling from a diagonal Gaussian approximation
- The Laplace Bridge is as good as a KFAC approximation
- The Laplace Bridge is around 400 times faster on average

Conclusions

What can or can't the Laplace Bridge achieve in the context of BNNs?

- The Laplace Bridge improves an important part of Bayesian Neural Network inference for classification (fast & non-invasive)
- The Dirichlet distribution has some additional interesting use cases (e.g. the top-k ranking)
- It will not revolutionize BNNs; it is just one piece in the larger puzzle

Questions?

Future

The generalized Laplace Bridge

Looking at the larger pattern

- Similar “Bridges” can be found for all exponential families.
- Develop a general theoretically grounded framework for the general Laplace Bridge
- Compute KL-divergences in the different basis

Implications: (with a small error)

- All exponential families can be transformed to Gaussians
- All exponential families can be transformed to each other
- All exponential families are conjugate priors for each other

Backup

Backup

Laplace approximations of a neural network

$$p(c|x) = \mathcal{N}(x; f(x, w_{\text{MAP}}), J(x)^T H^{-1} J(x)) \quad (8)$$

- $f(x; w_{\text{MAP}})$ is the network output induced by the MAP estimate w_{MAP}.
- $J(x) = \frac{\partial f(x, w_{\textbf{MAP}})}{\partial w} \in \mathbb{R}^{K \times P}$ is the Jacobian of the network
- $H_{ij} = \frac{\partial^2 \mathcal{L}(f(x), y)}{\partial w_i \partial w_j} \in \mathbb{R}^{P \times P}$ its Hessian.
- K, P are the number of classes and parameters of the network respectively.

Proposition

Let $\mathrm{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha})$ *be obtained via the Laplace Bridge from a Gaussian distribution* $\mathcal{N}(\mathbf{z}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ *over* $\mathbb{R}^K$. *Then, for each* $k = 1, \dots, K$, *letting* $\alpha_{\neq k} := \sum_{l \neq k} \alpha_l$, *if*

$$\alpha_k > \frac{1}{4}\left(\sqrt{9\alpha_{\neq k}^2 + 10\alpha_{\neq k} + 1} - \alpha_{\neq k} - 1\right),$$

then the variance $\mathrm{Var}(\pi_k|\boldsymbol{\alpha})$ *of the* k*-th component of* $\boldsymbol{\pi}$ *is increasing in* $\boldsymbol{\Sigma}_{kk}$.

First, we consider the special case where $\boldsymbol{\pi}$ is confined to a $I-1$ dimensional subspace satisfying $\sum_i \boldsymbol{\pi}_i = c$. In this subspace we can represent $\boldsymbol{\pi}$ by an $I-1$ dimensional vector $\mathbf{a}$ such that

$$\pi_i = a_i \quad i, ..., I-1 \tag{9}$$

$$\pi_I = c - \sum_i^{I-1} a_i \tag{10}$$

and similarly we can represent $\mathbf{z}$ by an $I-1$ dimensional vector $\boldsymbol{\varrho}$:

$$z_i = \varrho_i \quad i, ..., I-1 \tag{11}$$

$$z_I = 1 - \sum_i^{I-1} \varrho_i \tag{12}$$

then we can find the density over $\boldsymbol{\varrho}$ (which is proportional to the required density over z) from the density over $\boldsymbol{\pi}$ (which is proportional to the given density over $\boldsymbol{\pi}$) by finding the determinant of the $(I-1) \times (I-1)$ Jacobian $\mathbf{J}$ given by

$$J_{ik} = \frac{\partial \varrho_i}{\partial a_i} = \sum_{j}^{I} \frac{\partial z_i}{\partial \pi_j} \frac{\partial \pi_j}{\partial a_k} \tag{13}$$

$$= \delta_{ik}\mathbf{z}_i - \mathbf{z}_i\mathbf{z}_k + \mathbf{z}_i\mathbf{z}_I = \mathbf{z}_i(\delta_{ik} - (\mathbf{z}_k - \mathbf{z}_I)) \tag{14}$$

We define two additional $I-1$ dimensional helper vectors $\mathbf{z}_k^+ := \mathbf{z}_k - \mathbf{z}_I$ and $n_k := 1$, and use $\det(I - xy^T) = 1 - x \cdot y$ from linear algebra. It follows that

$$\det J = \prod_{i=1}^{I-1} \mathbf{z}_i \times \det[I - n{\mathbf{z}^+}^T] \tag{15}$$

$$= \prod_{i=1}^{I-1} \mathbf{z}_i \times (1 - n \cdot \mathbf{z}^+) \tag{16}$$

$$= \prod_{i=1}^{I-1} \mathbf{z}_i \times \left(1 - \sum_k \mathbf{z}_k^+\right) = I \prod_{i=1}^{I} \mathbf{z}_i \tag{17}$$