

Generalised Variational Inference Meets Bayesian Deep Learning

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joint work with Veit D. Wild (Oxford), Robert Hu (Amazon),
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Nanyang Technological University, Singapore
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Three Pillars of Trustworthy Machine Learning

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Thanks to:

PhD Students (Oxford):



Shahine Bouabid



Siu Lun Chau (now at
CISPA Saarbrücken)



Jake Fawkes



Robert Hu (now at
Amazon)



Jean-François Ton (now
at ByteDance AI Lab)



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Cambridge)



Yee Whye Teh
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DeepMind)



Krikamol Muandet
(CISPA Saarbrücken)



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(UC San Diego)

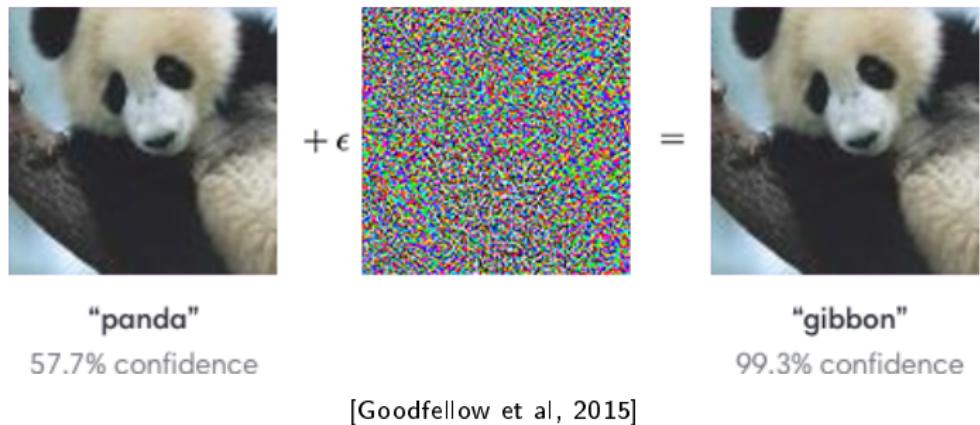


Russell Tsuchida
(Data61-CSIRO)

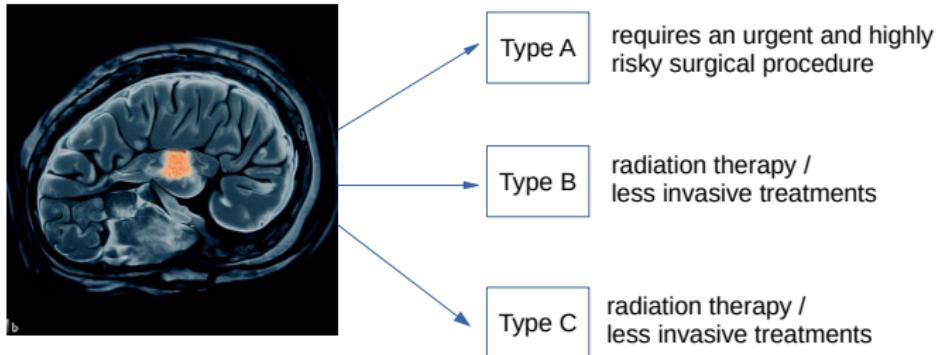


Cheng Soon Ong
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Uncertainty Calibration

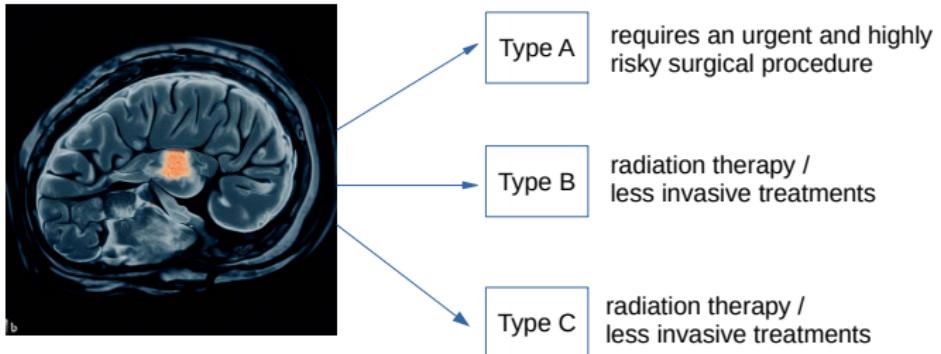


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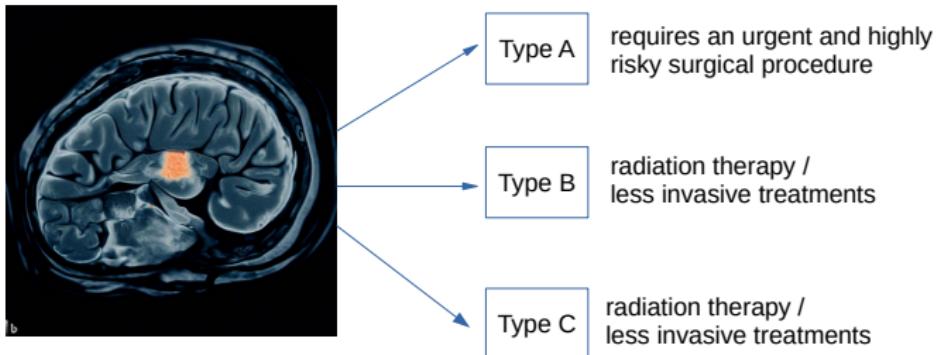
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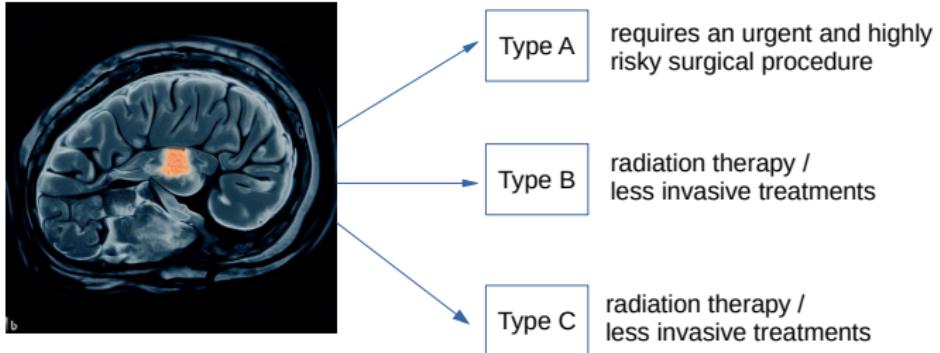
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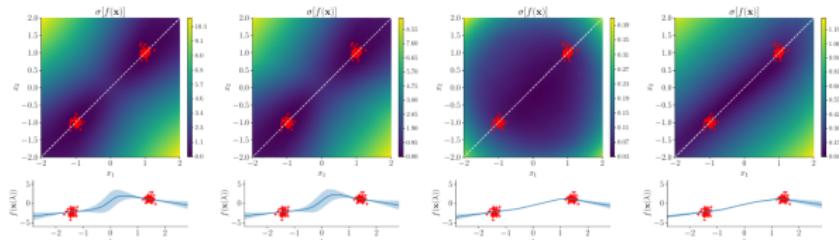
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- **A calibrated model:** among the inputs classified as having 90% chance of being Type A, 90% are indeed Type A.
- To assess whether a model is calibrated, we need to **compare two conditional probability distributions:** predicted distribution of Y given X to the actual distribution of Y given our prediction.
- **Kernel embeddings:** A state-of-the-art framework for representing and comparing distributions.

[Gretton et al, 2007; Gretton et al, 2012; DS et al, 2013; Muandet et al, 2017; Widmann et al, 2021]

Uncertainty Quantification: Bayesian Deep Learning

For a neural network $f(x; w)$ with parameters w , a traditional way to model uncertainty is to use **Bayesian learning** for w .

- The parameter space for w is **high-dimensional** and the posterior **multimodal**.
- **Many approximations needed:** do we still capture *enough of the true posterior* to justify being Bayesian?



[Foong et al, 2020]

- What priors on the function space are induced by the **prior on the neural network weights**?

An alternative:

Formulate a **generalized** Bayesian framework in the function space directly.

[V. D. Wild, R. Hu, and DS, *Generalized Variational Inference in Function Spaces: Gaussian Measures meet Bayesian Deep Learning*, in NeurIPS, 2022.]

Deep Learning

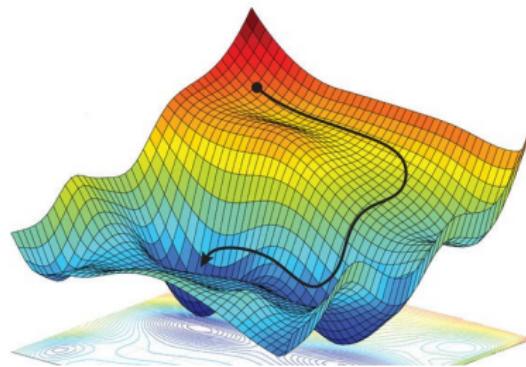
Observe data $\mathcal{D} := \{(x_n, y_n) \mid n = 1, \dots, N\}$.

- Likelihood is given by

$$p(\mathcal{D}|w) = \prod_{n=1}^N p(y_n|f(x_n; w)), \text{ where e.g. } y_n|f(x_n; w) \sim \mathcal{N}(f(x_n; w), \sigma^2),$$

and $f(\cdot; w)$ is a neural network with parameters w .

- Deep learning finds good optima of $\log p(\mathcal{D}|w)$.



Bayesian Deep Learning

Bayesian neural network:

Place a prior distribution $p(w)$ on the network weights. This results in a prior distribution on random functions, i.e. $f(x; W)$, $W \sim p(w)$. Find posterior $p(w|\mathcal{D})$.

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Why Bayesian Deep Learning?

- *Posterior predictive*: for any new $x^* \in \mathcal{X}$ averages over many individual neural networks – and these are weighted by their agreement with observed data.

$$\begin{aligned} p(y^*|\mathcal{D}) &= \int p(y^*|w)p(w|\mathcal{D}) dw \\ &= \int p(y^*|f(x^*; w))p(w|\mathcal{D}) dw \end{aligned}$$

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But: the posterior $p(w|\mathcal{D})$ is **intractable** – approximations are required.

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- **Variational inference**

- ▶ ...And its stochastic variants e.g. [Graves, 2011]

Weight-Space Variational Inference

Variational approximation:

Let $q(w) = q(w; \nu)$ be a class of distributions with (variational) parameters ν . We want $q(w; \nu)$ to approximate the true posterior $p(w|\mathcal{D})$. Learn ν by maximising the ELBO criterion *lower bound on the marginal likelihood*:

$$\mathcal{L}(\nu) := \mathbb{E}_{q(w)} [\log p(y|w)] - \mathbb{D}_{KL}(q(w)||p(w)), \quad (1)$$

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- What priors on the function space are induced by $p(w)$: how do we encode some sensible properties of functions via $p(w)$?

Generalised Variational Inference in Function Spaces

Gaussian Measures meet Bayesian Deep Learning

Veit D. Wild (Oxford), Robert Hu (Amazon), Dino Sejdinovic (Adelaide)

NeurIPS 2022, arXiv:2205.06342, github.com/MrHuff/GVI



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→ Is there another way?

GVI: Probabilistic Lifting + Convexification

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Posterior approximation uses a generalised criterion

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where:

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- ℓ is a loss function (not necessarily log-likelihood)
- D is a distance between probability measures (not necessarily KL)

Interpretation: Take any (non-convex) loss surface, and perform **probabilistic lifting** by averaging over q . Finally, the regularizer plays the role of **convexification**, making the objective in q strictly convex.

This work: GVI in Function Spaces

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- Idea: Use GVI in an infinite dimensional function space: we extend results of Knoblauch et al. [2022] to infinite dimensional parameter spaces.
- We can target

$$\mathcal{L} := -\mathbb{E}_{\mathbb{Q}}[\log p(y|F)] + \mathbb{D}(\mathbb{Q}^F, \mathbb{P}^F), \quad (3)$$

for inference where \mathbb{D} is an appropriate distance between probability measures on the function space.

- ➊ How to define prior \mathbb{P}^F ?
- ➋ What distance should we use?
- ➌ How to parametrize variational measures \mathbb{Q}^F ?

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Write $F \sim \mathcal{N}(m, C)$ for a GRE with mean element $m \in H$ and covariance operator C . $\mathcal{N}(m, C)$ is called a **Gaussian measure** on H .

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For arbitrary $m \in H$ and arbitrary positive, self-adjoint and trace-class C , there exists a GRE such that $F \sim \mathcal{N}(m, C)$.

2. The choice of divergence: Wasserstein-2

Recall the generalised loss:

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- $E = L^2(\mathcal{X}, \rho, \mathbb{R}) := \{f : \mathcal{X} \rightarrow \mathbb{R} \mid \int |f(x)|^2 d\rho(x) < \infty\}$ with ρ input distribution on \mathcal{X}
- $P := \mathbb{P}^F \sim \mathcal{N}(m_P, C_P)$
- $Q := \mathbb{Q}^F \sim \mathcal{N}(m_Q, C_Q)$
- $\mathbb{D}(\cdot, \cdot) = W_2(\cdot, \cdot)$ with W_2 given as Wasserstein-distance

2. The choice of divergence: Wasserstein-2

Recall the generalised loss:

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with:

$$C_P g := \int k(\cdot, x') g(x') d\rho(x'), \quad C_Q g := \int r(\cdot, x') g(x') d\rho(x') \quad (5)$$

for all $g \in L^2(\mathcal{X}, \rho, \mathbb{R})$ where k and r are *trace-class kernels*.

2. The choice of divergence: Wasserstein-2

The Wasserstein distance between Gaussian measures on Hilbert spaces has a closed-form expression [Gelbrich, 1990]:

$$W_2^2(P, Q) = \|m_P - m_Q\|_2^2 + \text{tr}(C_P) + \text{tr}(C_Q) - 2 \cdot \text{tr}\left[\left(C_P^{1/2} C_Q C_P^{1/2}\right)^{1/2}\right], \quad (6)$$

where $\text{tr}(\cdot)$ denotes the trace of an operator and $C_P^{1/2}$ is the square root of the positive, self-adjoint operator C_P .

2. The choice of divergence: Wasserstein-2

Estimation of Wasserstein-2 for Gaussian measures:

$$\begin{aligned}\|m_P - m_Q\|_2^2 &= \int (m_P(x) - m_Q(x))^2 d\rho(x) \\ &\approx \frac{1}{N} \sum_{n=1}^N (m_P(x_n) - m_Q(x_n))^2\end{aligned}$$

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Further:

$$tr(C_P) = \int k(x, x) d\rho(x) \approx \frac{1}{N} \sum_{n=1}^N k(x_n, x_n),$$

$$tr(C_Q) = \int r(x, x) d\rho(x) \approx \frac{1}{N} \sum_{n=1}^N r(x_n, x_n).$$

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The last term poses some difficulties:

$$tr \left[(C_P^{1/2} C_Q C_P^{1/2})^{1/2} \right] \approx \frac{1}{\sqrt{NN_S}} \sum_{s=1}^{N_S} \sqrt{\lambda_s(r(X_S, X)k(X, X_S))}, \quad (7)$$

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where $X_S := (x_{S,1}, \dots, x_{S,N_S})$, $N_S \in \mathbb{N}$ with:

$$X_{S,1}, \dots, X_{S,N_S} \stackrel{\text{ind.}}{\sim} \hat{\rho} \quad (8)$$

$$r(X_S, X) := (r(x_{S,s}, x_n))_{s,n} \quad (9)$$

$$k(X, X_S) := (k(x_n, x_{S,s}))_{n,s} \quad (10)$$

and $\lambda_s(r(X_S, X) k(X, X_S))$ denotes the s -th eigenvalue of the matrix $r(X_S, X) k(X, X_S) \in \mathbb{R}^{N_S \times N_S}$.

The final objective

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$$\widehat{W}^2 := \frac{1}{N} \sum_{n=1}^N (m_P(x_n) - m_Q(x_n))^2 + \frac{1}{N} \sum_{n=1}^N k(x_n, x_n) \quad (13)$$

$$+ \frac{1}{N} \sum_{n=1}^N r(x_n, x_n) - \frac{2}{\sqrt{NN_S}} \sum_{s=1}^{N_S} \sqrt{\lambda_s(r(X_S, X)k(X, X_S))}, \quad (14)$$

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3. How to parametrize the variational family?

- Stochastic Variational Gaussian processes (SVGP) [Titsias, 2009]:

$$m_Q(x) := m_P(x) + \sum_{m=1}^M \beta_m k(x, z_m) \quad (15)$$

$$r(x, x') := k(x, x') - k_Z(x)^T k(Z, Z)^{-1} k_Z(x) + k_Z(x)^T \Sigma k_Z(x), \quad (16)$$

where $\beta = (\beta_1, \dots, \beta_M) \in \mathbb{R}^M$ and $\Sigma \in \mathbb{R}^{M \times M}$ are variational parameters.
 $Z = (Z_1, \dots, Z_M)$ can be a data subsample or also included as variational parameters.

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GVI-net m_Q : Use a deep neural net as the parametrization of the variational posterior mean.

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GWI-net m_Q : Use a deep neural net as the parametrization of the variational posterior mean.

GWI-net C_Q : Use the covariance parametrization of SVGP.

In a nutshell

- Deep neural network is our model and network weights are the model parameters.

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- Our model is defined directly on the function space and deep neural network weights are the variational parameters.

Toy Examples: GWI-net on 1-D data

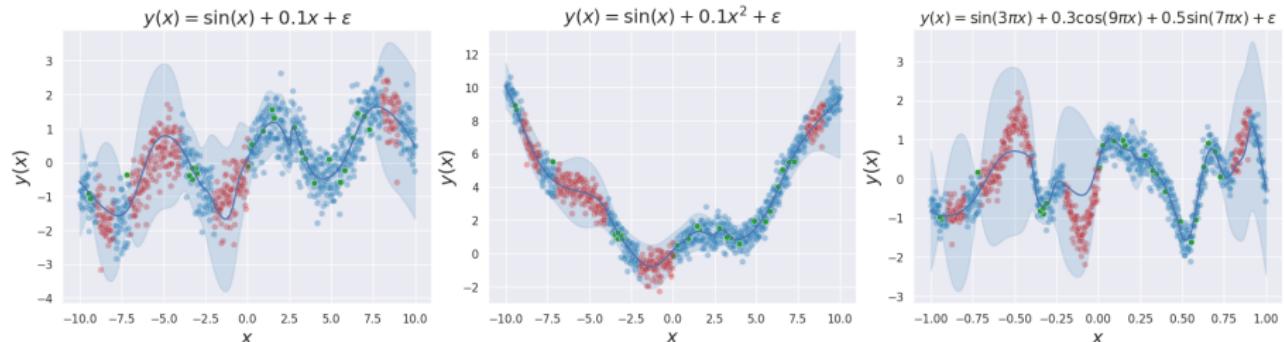


Figure: ■ : Training data ■ : Unseen data ■ : Inducing points

We use $N = 1000$ equidistant points and add white noise with $\varepsilon \sim \mathcal{N}(0, 0.5^2)$.

The plot shows $m_Q(x) \pm 1.96\sqrt{\mathbb{V}[Y^*(x)|Y]}$ where $\mathbb{V}[Y^*(x)|Y]$ is the posterior predictive variance given as $r(x,x) + \sigma^2$.

UCI Regression

Dataset	N	D	GWI		FVI	VIP-BNN	VIP-NP	BBB	VDO	$\alpha = 0.5$	FBNN	EXACT GP
			SVGP	DNN-SVGP								
BOSTON	506	13	2.8±0.31	2.27±0.06	2.33±0.04	2.45±0.04	2.45±0.03	2.76±0.04	2.63±0.10	2.45±0.02	2.30±0.10	2.46±0.04
CONCRETE	1030	8	3.24±0.09	2.64±0.06	2.88±0.06	3.02±0.02	3.13±0.02	3.28±0.01	3.23±0.01	3.06±0.03	3.09±0.01	3.05±0.02
ENERGY	768	8	1.81±0.19	0.91±0.12	0.58±0.05	0.56±0.04	0.60±0.03	2.17±0.02	1.13±0.02	0.95±0.09	0.68±0.02	0.54±0.02
KIN8NM	8192	8	-0.86±0.38	-1.2±0.03	-1.15±0.01	-1.12±0.01	-1.05±0.00	-0.81±0.01	-0.83±0.01	-0.92±0.02	N/A±0.00	N/A±0.00
POWER	9568	4	3.35±0.22	2.74±0.02	2.69±0.00	2.92±0.00	2.90±0.00	2.83±0.01	2.88±0.00	2.81±0.00	N/A±0.00	N/A±0.00
PROTEIN	45730	9	2.84±0.04	2.87±0.00	2.85±0.00	2.87±0.00	2.96±0.02	3.00±0.00	2.99±0.00	2.90±0.00	N/A±0.00	N/A±0.00
RED WINE	1588	11	0.97±0.02	0.76±0.08	0.97±0.06	0.97±0.02	1.20±0.04	1.01±0.02	0.97±0.02	1.01±0.02	1.04±0.01	0.26±0.03
YACHT	308	6	2.37±0.55	0.29±0.1	0.59±0.11	-0.02±0.07	0.59±0.13	1.11±0.04	1.22±0.18	0.79±0.11	1.03±0.03	0.10±0.05
NAVAL	11934	16	-7.25±0.08	-6.76±0.1	-7.21±0.06	-5.62±0.04	-4.11±0.00	-2.80±0.00	-2.80±0.00	-2.97±0.14	-7.13±0.02	N/A±0.00
Mean Rank			5.5	2.06	2.22	3.33	4.94	7	6.11	4.83		

Table: The table shows the average test NLL on several UCI regression datasets. We train on random 90% of the data and predict on 10%. This is repeated 10 times and we report mean and standard deviation. The results for our competitors are taken from Ma and Hernández-Lobato [2021].

Classification

Model	FMNIST			CIFAR 10		
	Accuracy	NLL	OOD-AUC	Accuracy	NLL	OOD-AUC
GWI-net	93.25 ±0.09	0.250 ±0.00	0.959 ±0.01	83.82 ±0.00	0.553 ±0.00	0.618 ±0.00
FVI	91.60±0.14	0.254±0.05	0.956±0.06	77.69±0.64	0.675±0.03	0.883±0.04
MFVI	91.20±0.10	0.343±0.01	0.782±0.02	76.40±0.52	1.372±0.02	0.589±0.01
MAP	91.39±0.11	0.258±0.00	0.864±0.00	77.41±0.06	0.690±0.00	0.809±0.01
KFAC-LAPLACE	84.42±0.12	0.942±0.01	0.945±0.00	72.49±0.20	1.274±0.01	0.548±0.01
RITTER et al.	91.20±0.07	0.265±0.00	0.947±0.00	77.38±0.06	0.661±0.00	0.796±0.00

Table: We report average accuracy, NLL and OOD-AUC on test data for 10 different train/test splits.

Summary

- Deep Neural Networks are good prediction models. Let's make them Bayesian.

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- Deep Neural Networks are good prediction models. Let's make them Bayesian.
- Deep Neural Networks are a good parametrization of the variational posterior for function space models.

A Rigorous Link between Deep Ensembles and (Variational) Bayesian Methods

Veit D. Wild (Oxford), Sahra Ghalebikesabi (Oxford),
Dino Sejdinovic (Adelaide), Jeremias Knoblauch (UCL)

NeurIPS 2023, arXiv:2305.15027, github.com/sghalebikesabi/GVI-WGF



GVI: Probabilistic Lifting + Convexification

Generalised Variational Inference [Knoblauch et al., 2022]:

Posterior approximation uses a generalised criterion

$$Q^*(\theta) := \operatorname{argmin}_{Q \in \mathcal{Q}} \underbrace{\left\{ \mathbb{E}_{Q(\theta)} \left[\sum_{n=1}^N \ell(y_n, \theta) \right] + D(Q(\theta), P(\theta)) \right\}}_{L(Q)},$$

where:

- \mathcal{Q} is a set of tractable distributions
- ℓ is a loss function (not necessarily log-likelihood)
- D is a distance between probability measures (not necessarily KL)

Interpretation: Take any (non-convex) loss surface, and perform **probabilistic lifting** by averaging over q . Finally, the regularizer plays the role of **convexification**, making the objective in q strictly convex.

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where:

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Relaxing the variational family assumption?

Idea: formulate a gradient flow in the space of probability measures [Ambrosio et al., 2005] on the (generalized) variational objective $L(Q)$.

Parameter space

- Initialise: $\theta_0 \in \mathbb{R}^J$
- Gradient step:

$$\theta_{k+1} =$$

$$\arg \min_{\theta \in \mathbb{R}^J} \left\{ \ell(\theta) + \frac{1}{2\eta} \|\theta - \theta_k\|_2^2 \right\}.$$

Probability space

- Initialise: $Q_0 \in \mathcal{P}_2(\mathbb{R}^J)$
- Gradient step:

$$Q_{k+1} =$$

$$\arg \min_{Q \in \mathcal{P}_2(\mathbb{R}^J)} \left\{ L(Q) + \frac{1}{2\eta} W_2(Q, Q_k)^2 \right\}$$

with 2-Wasserstein metric

$$W_2(P, Q)^2 = \inf \left\{ \int \|\theta - \theta'\|_2^2 d\pi(\theta, \theta') : \pi \in \mathcal{C}(P, Q) \right\}.$$

A general form of objective

$$L(Q) := \int V(\theta) dQ(\theta) + \frac{\lambda_1}{2} \iint \kappa(\theta, \theta') dQ(\theta) dQ(\theta') + \lambda_2 \int \log q(\theta) q(\theta) d\theta,$$

The overall energy of a collection of particles sampled from Q is decomposed into three parts:

- the external potential $V(\theta)$ which acts on each particle individually
- the interaction energy defined via kernel $\kappa(\theta, \theta')$ describing pairwise interactions between particles,
- the overall entropy of the system.

This is precisely the GVI objective with regularizer that is a mixture of KL and MMD:

$$D(Q, P) = \lambda_1 MMD^2(Q, P) + \lambda_2 KL(Q, P)$$

Implementing the Wasserstein Gradient Flow

Interacting particles scheme:

- **Step 1:** Sample $N_E \in \mathbb{N}$ particles $\theta_1(0), \dots, \theta_{N_E}(0)$ independently from $Q_0 \in \mathcal{P}_2(\mathbb{R}^J)$.
- **Step 2:** Evolve the particle θ_n by following the stochastic differential equation (SDE)

$$d\theta_n(t) = -\left(\nabla V(\theta_n(t)) + \frac{\lambda_1}{N_E} \sum_{j=1}^{N_E} (\nabla_1 \kappa)(\theta_n(t), \theta_j(t))\right) dt + \sqrt{2\lambda_2} dB_n(t),$$

for $n = 1, \dots, N_E$, and $\{B_n(t)\}_{t>0}$ independent Brownian motions.

Cases:

- No regularizer, i.e. $\lambda_1 = \lambda_2 = 0$: deep ensemble [Lakshminarayanan et al., 2017], **No convergence to the global optimum**.
- Only KL regularizer, i.e. $\lambda_1 = 0$: deep Langevin ensemble (essentially Lakshminarayanan et al. [2017]+Welling and Teh [2011]), **Converges to the global optimum**.
- KL+MMD regularizer: deep repulsive Langevin ensemble (**new**), **Converges to the global optimum**

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Losses

For regression, $y \in \mathbb{R}$,

$$p(\mathcal{D}|F) = \prod_{n=1}^N p(y_n|F(x_n)) = \prod_{n=1}^N \mathcal{N}(y_n | F(x_n), \sigma^2), \quad (17)$$

where $\sigma^2 > 0$.

For classification, $y \in \{-1, +1\}$,

$$p(\mathcal{D}|F) = \prod_{n=1}^N p(y_n|F(x_n)) = \prod_{n=1}^N \sigma(y_n F(x_n)), \quad (18)$$

where $\sigma(t) = 1/(1 + e^{-t})$

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- typically $N_S, N_B \ll N$, e.g. $N_S = N_B = 100$