Generalised Variational Inference Meets Bayesian Deep Learning

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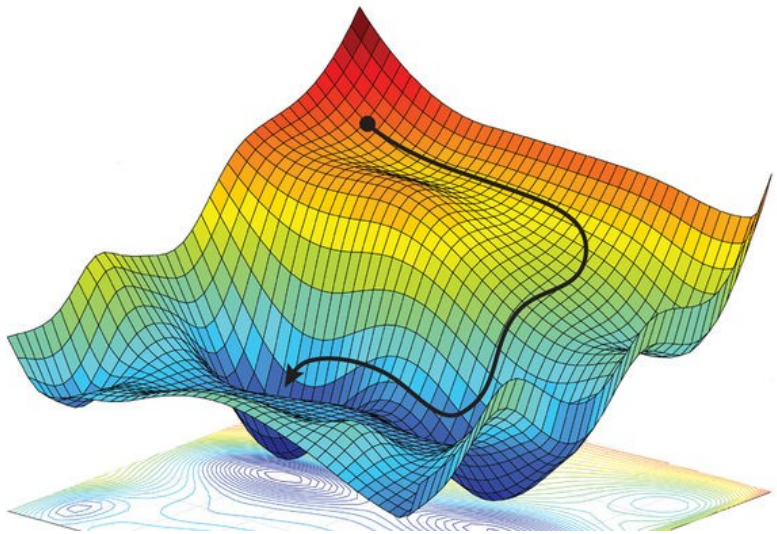
Deep Learning

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

- 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 $\log p(\mathcal{D}|w)$.



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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?

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

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

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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*:

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

which is (often) tractable, e.g. if $q(w)$ and $p(w)$ are normal.

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  $\longrightarrow$ Do we still capture *enough of the true posterior* to justify being Bayesian? [Foong et al., 2020]
  $\longrightarrow$ Is uncertainty calibrated? [Ovadia et al., 2019]
- 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/GWI

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  $\rightarrow$ Gaussian measures on Hilbert spaces (e.g. Gaussian processes)
- The KL-divergence is (in general) intractable in infinite dimensions and may be infinite [Burt et al., 2020].
  $\rightarrow$ Is there another way?

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where:

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- 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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- We can target

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

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

1. How to define prior $\mathbb{P}^F$?
2. What distance should we use?
3. How to parametrize variational measures $\mathbb{Q}^F$?

1. Prior: Gaussian Measures on Hilbert spaces

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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.
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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- $E = L^2(\mathcal{X}, \rho, \mathbb{R}) := \big\{f : \mathcal{X} \to \mathbb{R} \,|\, \int |f(x)|^2 \, d\rho(x) < \infty\big\}$ with ρ input distribution on $\mathcal{X}$

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with:

$$C_P g := \int k(\cdot, x')g(x') \, d\rho(x'), \qquad C_Q g := \int r(\cdot, x')g(x') \, d\rho(x') \tag{5}$$

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

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

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

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

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Estimation of Wasserstein-2 for Gaussian measures:

$$\|m_P - m_Q\|_2^2 = \int \left(m_P(x) - m_Q(x)\right)^2 d\rho(x)$$
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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:

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

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

$$X_{S,1}, \ldots, X_{S,N_S} \overset{\text{ind.}}{\sim} \hat{\rho} \tag{8}$$

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

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

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

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

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3. How to parametrize the variational family?

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

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

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

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

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GWI-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

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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

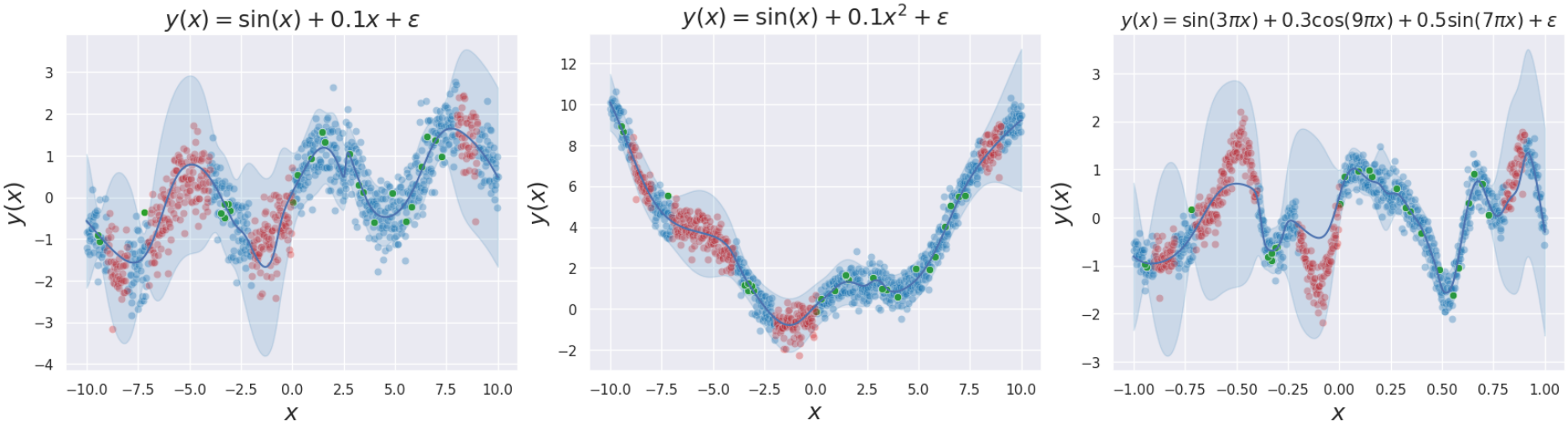

Figure: ■ : Training data ■ : Unseen data ■ : Inducing points

We use $N = 1000$ equidistant points and add white noise with $\epsilon \sim \mathcal{N}(0, 0.5^2)$. 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 SVGP	GWI DNN-SVGP	FVI	VIP-BNN	VIP-NP	BBB	VDO	$\alpha = 0.5$	FBNN	**EXACT GP**
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±0.0	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

	FMNIST			CIFAR 10		
Model	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.

- As a practical viewpoint: a different (generalized variational) objective for training your favourite deep neural net, which has extra parameters to quantify uncertainty.

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

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

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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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 $\theta_1(0), \ldots, \theta_{N_E}(0)$ 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)

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

  for $n = 1, \ldots, N_E$, 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

Number of particles N_E when many local minima are present

A uniform prior P and initialisation Q_0 and the loss $\ell(\theta) := -|\sin(\theta)|$, $\theta \in [-1000\pi, 1000\pi]$, which has 2000 local minima.

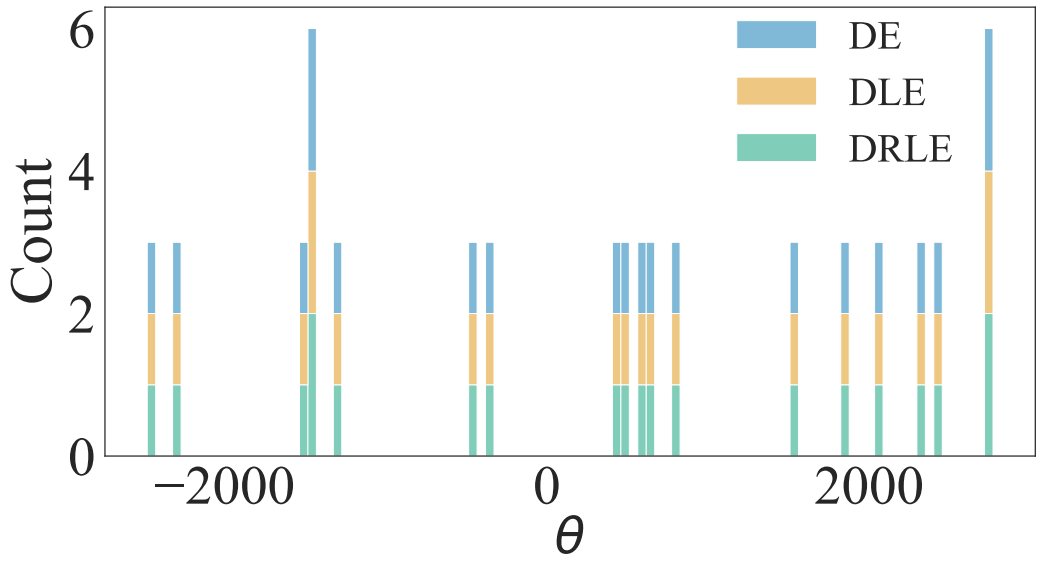

Figure: We generate $N_E = 20$ samples from the three ensemble methods. The x-axis shows the location of the particles after training. Since the same initialisation $\theta_n(0)$ is chosen for all methods, we observe that particles fall into the same local modes. Further, 16/20 particles are alone in their respective local modes and the location of the particles varies very little between the different methods.

Summary

- Gradient flows for GVI allow to unify a collection of existing algorithms under a common conceptual roof and plant the seeds for new deep ensemble algorithms.

Summary

- Gradient flows for GVI allow to unify a collection of existing algorithms under a common conceptual roof and plant the seeds for new deep ensemble algorithms.
- Performance difference between simple deep ensembles and more intricate schemes may not be numerically discernible for loss landscapes with many local minima.

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Losses

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

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

where $\sigma^2 > 0$.
For classification, $y \in \{-1, +1\}$,

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

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

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$\longrightarrow$ typically $N_S, N_B << N$, e.g. $N_S = N_B = 100$