Reparameterization invariance in approximate Bayesian inference

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Why linearised Laplace > regular Laplace

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Section 1: Laplace Approximation in BNNs

- Neural network $f_{\mathbf{w}} : \mathbb{R}^I \to \mathbb{R}^O$ with likelihood $p(\mathbf{y}|f_{\mathbf{w}}(\mathbf{x}))$ and prior $p(\mathbf{w})$

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- Approximate posterior as $p(\mathbf{w}|\mathbf{x}, \mathbf{y}) \approx \mathcal{N}(\mathbf{w}|\hat{\mathbf{w}}, -\mathbf{H}^{-1}_{\hat{\mathbf{w}}})$

- with Hessian matrix $\mathbf{H}_{\hat{\mathbf{w}}} = \nabla^2_{\mathbf{w}} \log p(\mathbf{x}, \mathbf{y}; \mathbf{w})|_{\hat{\mathbf{w}}}$

Linearised Laplace BNNs

- Linearise the NN at $\hat{\mathbf{w}}$

$$f_{\mathbf{w}}(\mathbf{x}) \approx f_{\hat{\mathbf{w}}}(\mathbf{x}) + \mathbf{J}_{\hat{\mathbf{w}}}(\mathbf{x})(\mathbf{w} - \hat{\mathbf{w}})$$

- using Jacobian $\mathbf{J}_{\hat{\mathbf{w}}}(\mathbf{x}) = \partial_{\mathbf{w}} f_{\mathbf{w}}(\mathbf{x})|_{\mathbf{w}=\hat{\mathbf{w}}} \in \mathbb{R}^{O \times D}$

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- Immer et al. (2021) argue that this choice implicitly linearises the BNN

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(If likelihood is gaussian, then $\mathbf{H}(\mathbf{x}) = \mathbb{I}_O$)

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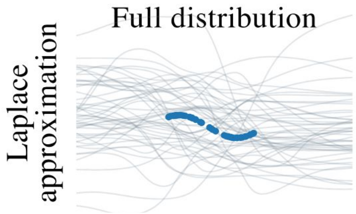
Predictive distributions

- Regular Laplace severely underfits

$$p(\mathbf{y}^*|\mathbf{x}^*, \mathcal{D}) = \mathbb{E}_{\mathbf{w}\sim q}[p(\mathbf{y}^*|f(\mathbf{w}, \mathbf{x}^*))] \approx \frac{1}{S}\sum_{i=1}^{S} p(\mathbf{y}^*|f(\mathbf{w}_i, \mathbf{x}^*)), \quad \mathbf{w}_i \sim q$$



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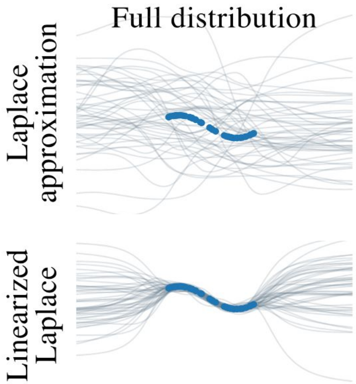

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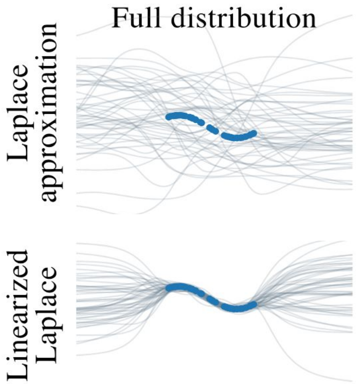

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- Why does adding another degree of approximation improve performance?

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- For any $\alpha > 0$, (w_1, w_2) and $({}^{w_1}/\alpha, \alpha w_2)$ are equivalent

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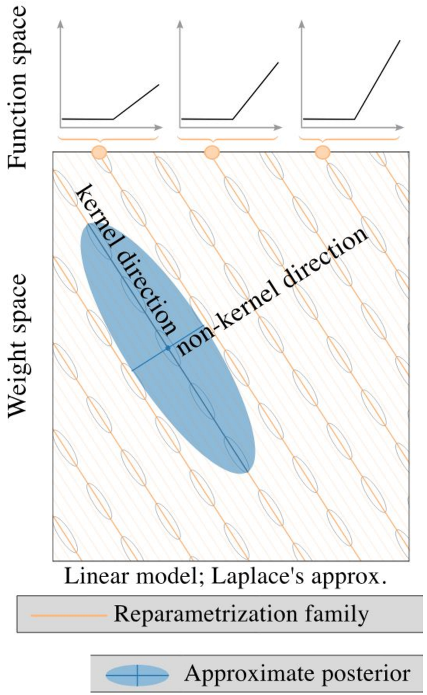

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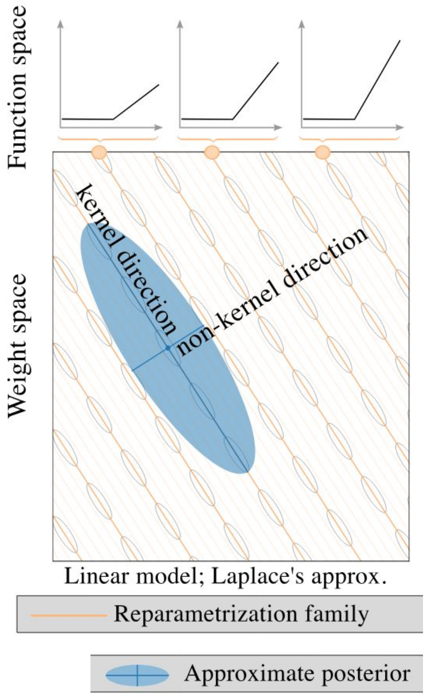
- The GGN covariance naturally aligns the linearised Laplace approx. post. with the reparameterisation (kernel) direction



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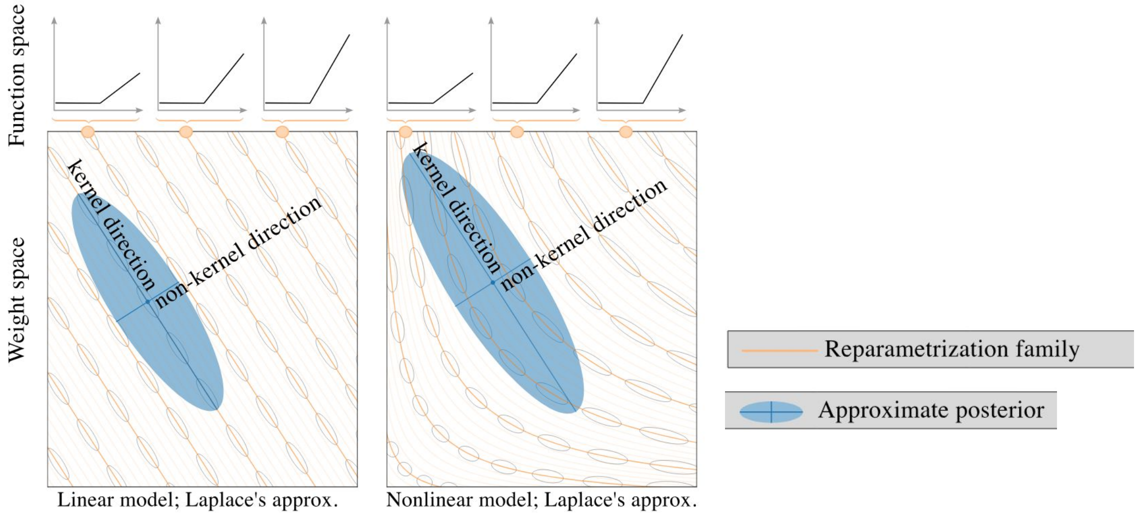
- The regular Laplace approximation puts a crude pdf over the space of (nonlinear) NN functions
  - Identical functions are given different masses (this also messes up marginal likelihood estimates)



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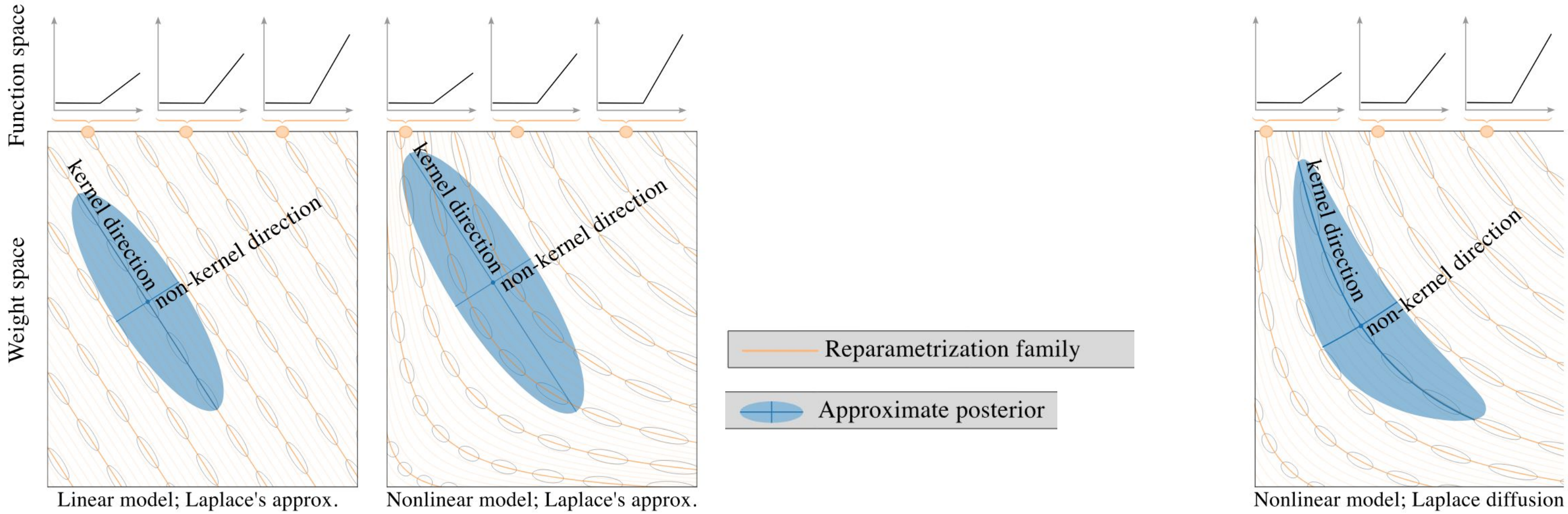

Section 2: Reparameterisation of linear functions

- Consider a linear function $f(\mathbf{w}) = \mathbf{A}\mathbf{w} + \mathbf{b}$

  and a reparameterisation $g : \mathbb{R}^D \to \mathbb{R}^D$ such that $f(g(\mathbf{w})) = f(\mathbf{w})$

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- Then $\mathbf{A}(g(\mathbf{w}) - \mathbf{w}) = \mathbf{0}$
- So the direction of movement between $\mathbf{w}$ and $g(\mathbf{w})$ lies in the kernel/nullspace of $\mathbf{A}$

$$g(\mathbf{w}) - \mathbf{w} \in \ker(\mathbf{A})$$

Find the kernel of the linearised NN (and avoid it!)

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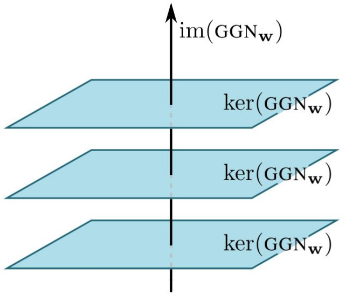

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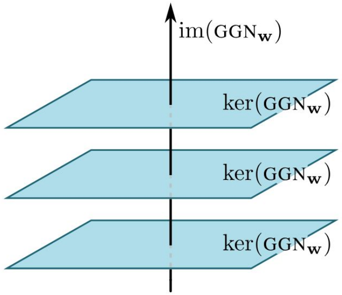
  - (ideally we'd just explore this)



Find the kernel of the linearised NN (and avoid it!)

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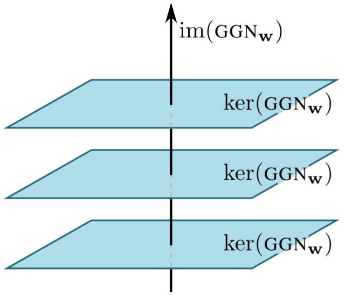
- $\ker(\text{GGN}_{\mathbf{w}})$ corresponds to the directions of reparameterisation



Laplace samples can be decomposed into image and kernel contributions

- Let $\mathbf{U}^T \mathbf{\Lambda} \mathbf{U}$ be the eigendecomposition of $\mathrm{GGN}_{\hat{\mathbf{w}}}$ with $\mathbf{U_1}$ and $\mathbf{U_2}$ corresponding to non-zero and zero eigenvalues respectively

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$$\Sigma = \left(\left[\frac{\mathbf{U_1}}{\mathbf{U_2}} \right]^T \left[\begin{array}{c|c} \tilde{\mathbf{\Lambda}} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array} \right] \left[\frac{\mathbf{U_1}}{\mathbf{U_2}} \right] + \alpha \mathbf{I} \right)^{-1} = \mathbf{U_1^T}(\tilde{\mathbf{\Lambda}} + \alpha \mathbf{I}_k)^{-1}\mathbf{U_1} + \alpha^{-1}\mathbf{U_2^T}\mathbf{U_2}$$

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(Note that all probability mass in the kernel comes from the prior)

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  - Adds ‘incorrect’ degrees of freedom to the approx. post.

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Linearised laplace automatically ignores $\mathbf{w}_{\text{ker}}$

$$f_{\text{lin}}^{\hat{\mathbf{w}}}(\hat{\mathbf{w}} + \mathbf{w}_{\text{ker}} + \mathbf{w}_{\text{im}}, \mathbf{x}) = f_{\text{lin}}^{\hat{\mathbf{w}}}(\hat{\mathbf{w}} + \mathbf{w}_{\text{im}}, \mathbf{x})$$

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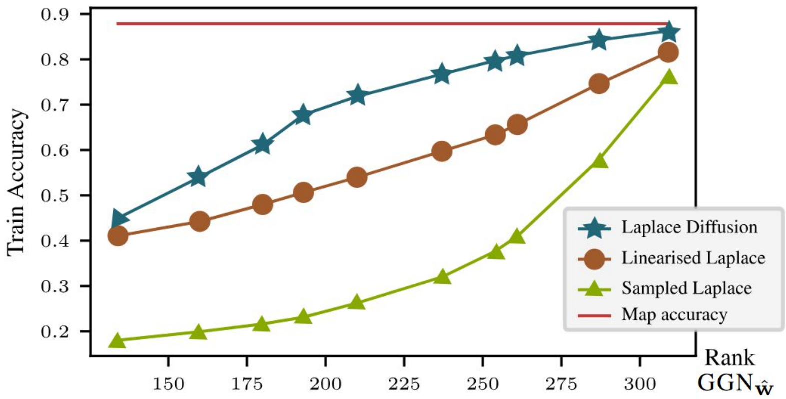
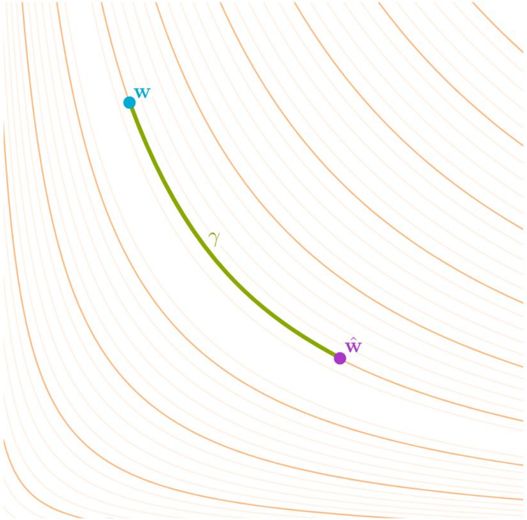


Small CNN on MNIST so GGN can be computed exactly – (rank increases with more data if we keep the same number of parameters)

Section 3: Reparameterisation of NNs

- They do the same analysis but for nonlinear models (e.g. regular NNs)



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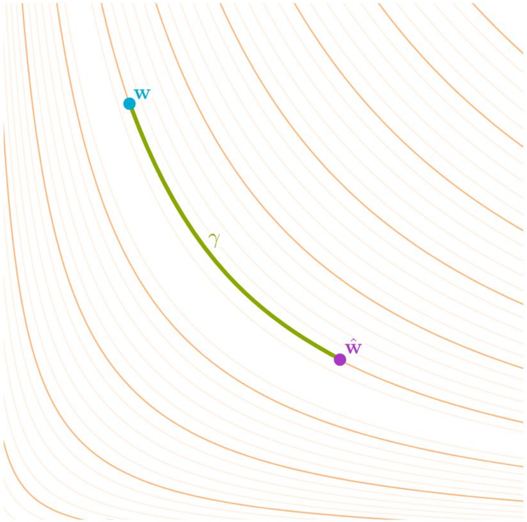

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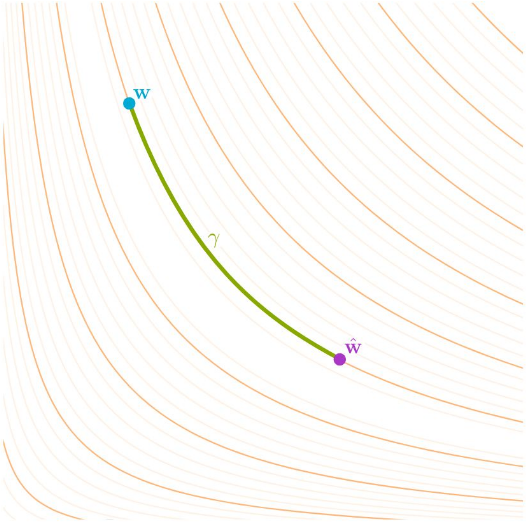

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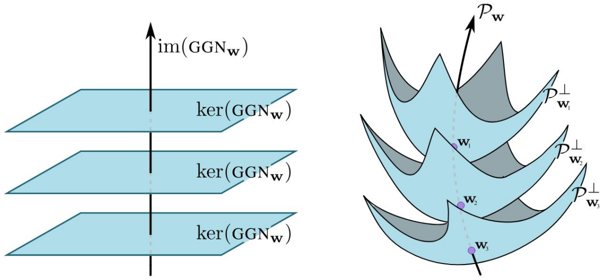

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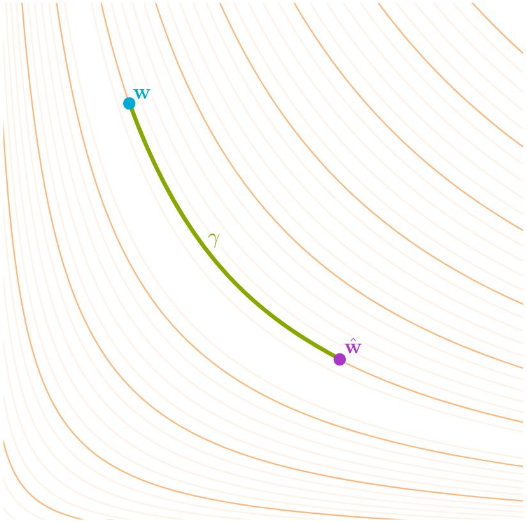

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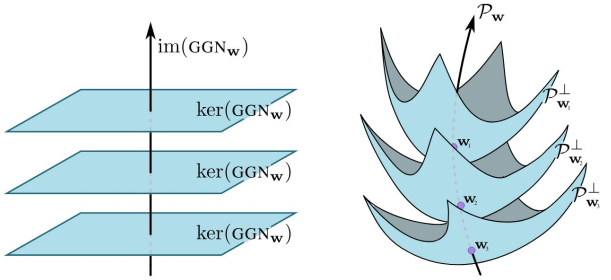
- We can similarly decompose Laplace samples into a combination of two manifolds embedded in $\mathbb{R}^D$, $(\mathcal{P}_\mathbf{w}, \mathfrak{m})$ and $(\mathcal{P}_\mathbf{w}^\perp, \mathfrak{m}^\perp)$, which act like $\mathrm{im}(\mathrm{GGN}_\mathbf{w})$ and $\ker(\mathrm{GGN}_\mathbf{w})$
- Then we can ignore the reparameterisation directions by only exploring $(\mathcal{P}_\mathbf{w}, \mathfrak{m})$ (*Laplace diffusion*)



Define Effective Parameter-Space as a Quotient Group

$\mathbf{w}_1 \sim \mathbf{w}_2$ iff there exists a smooth path between $\mathbf{w}_1$ and $\mathbf{w}_2$ such that

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Then we define the effective parameter space as the quotient group $\mathcal{P} = \mathbb{R}^D / \sim$

(i.e. only consider parameters that give us unique functions)

Define a Reparameterisation Distance and get a (Pseudo-)Riemannian manifold

We'd like to define a distance such that $\mathrm{dist}(\mathbf{w}_1, \mathbf{w}_2) = 0 \quad \Leftrightarrow \quad \mathbf{w}_1 \sim \mathbf{w}_2$

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NOTE:

1. GGN is rank-deficient (hence pseudo-riemannian)
2. $\mathbf{w}_1 \sim \mathbf{w}_2$ doesn't then necessarily mean $\mathrm{GGN}_{\mathbf{w}_1} = \mathrm{GGN}_{\mathbf{w}_2}$ (pseudo-metric might be different based on your Laplace centre/mode (... but infinitesimally that doesn't matter too much))

Equivalence of the manifold and the quotient group

Proposition 4.4. *There exists a bijection between* $(\mathbb{R}^D, \mathrm{GGN}_{\mathbf{w}})$ *and* $\mathcal{P}$.

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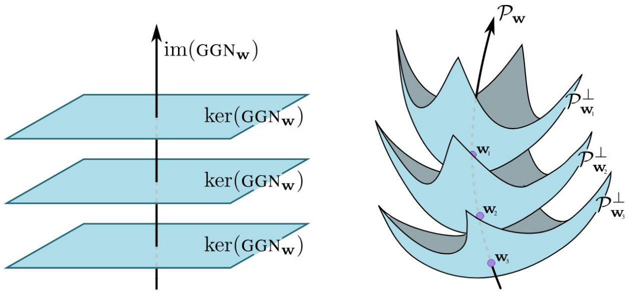
Problem: $(\mathbb{R}^D, \mathrm{GGN}_{\mathbf{w}})$ is only pseudo-Riemannian (GGN is rank-deficient)

Define two Riemannian manifolds which act as $\mathrm{im}(\mathrm{GGN}_{\mathbf{w}})$ and $\ker(\mathrm{GGN}_{\mathbf{w}})$



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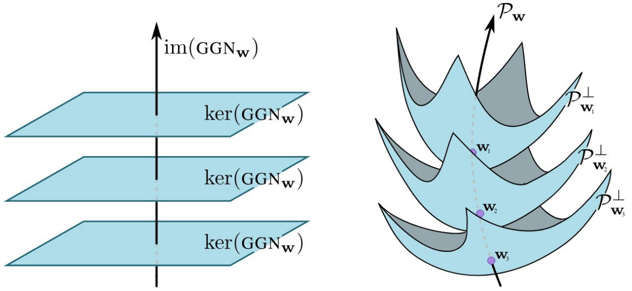

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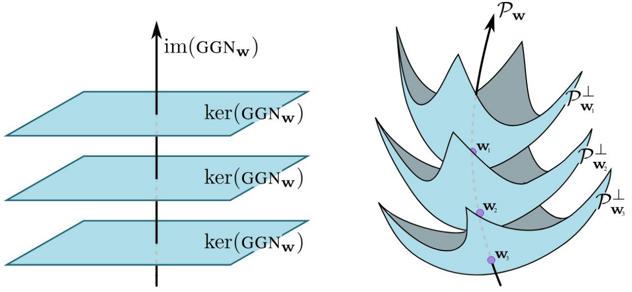

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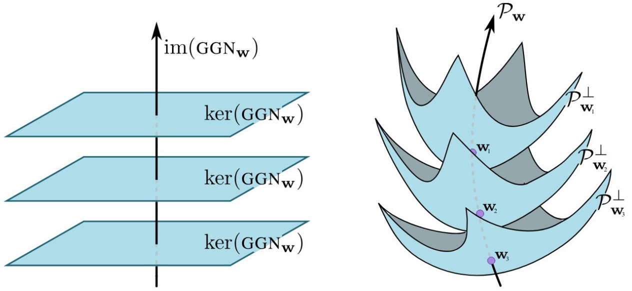

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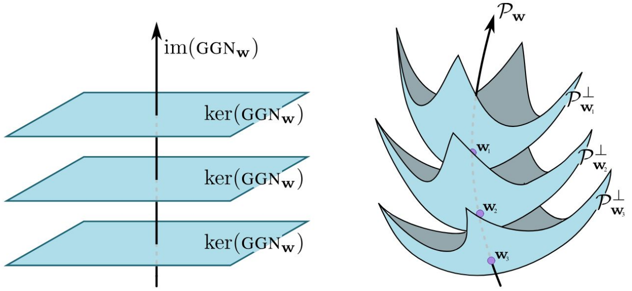

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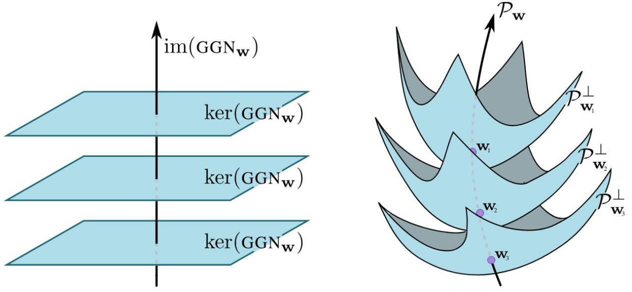

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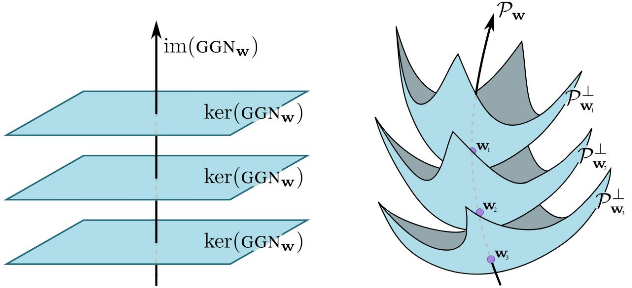
    - So contains only functions which are identical on the training set



Section 4: Diffusion on various manifolds

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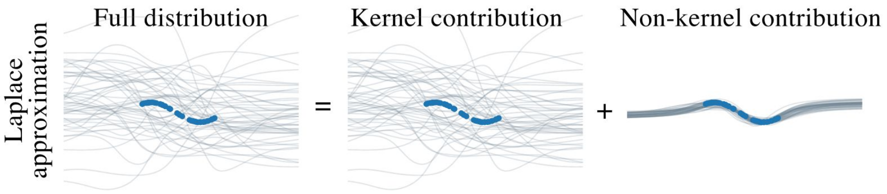

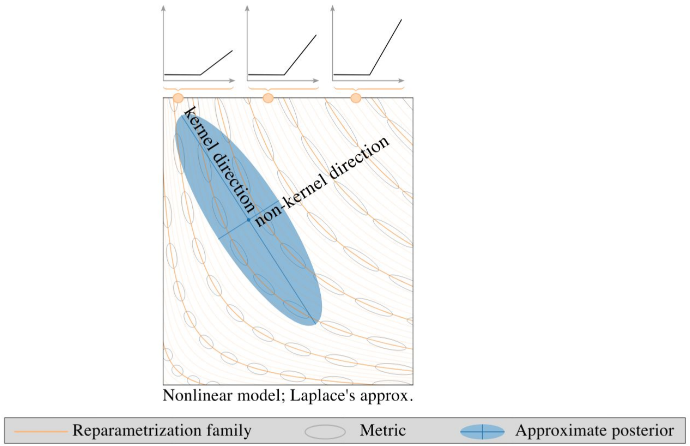

Nonlinear model; Laplace's approx.

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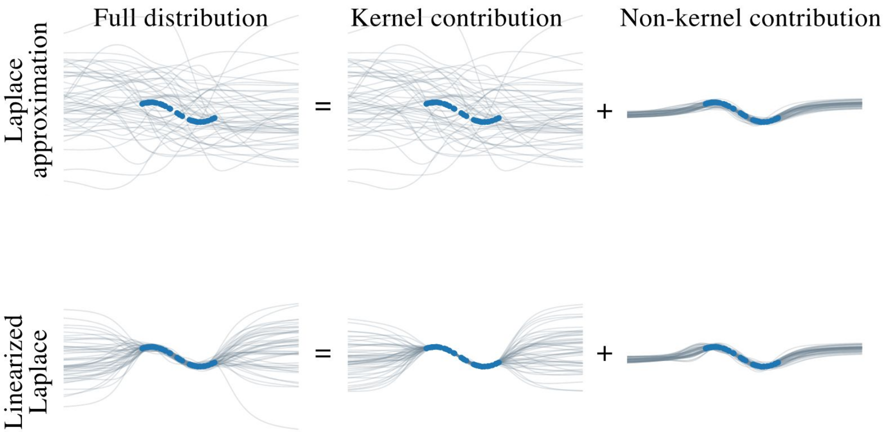

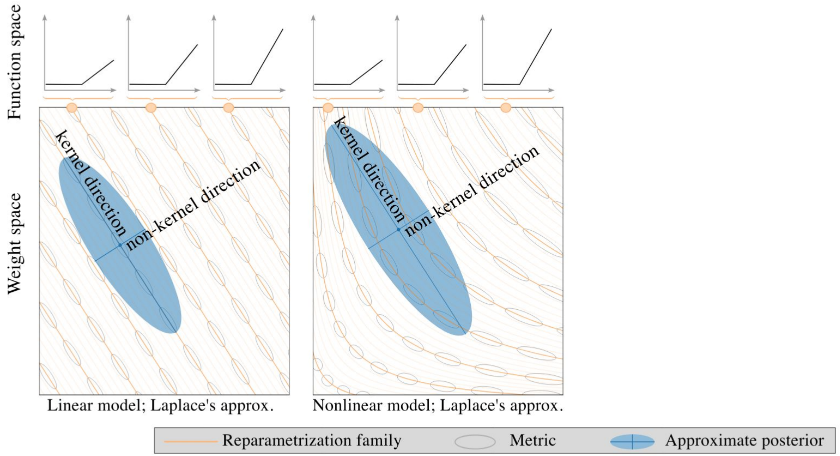

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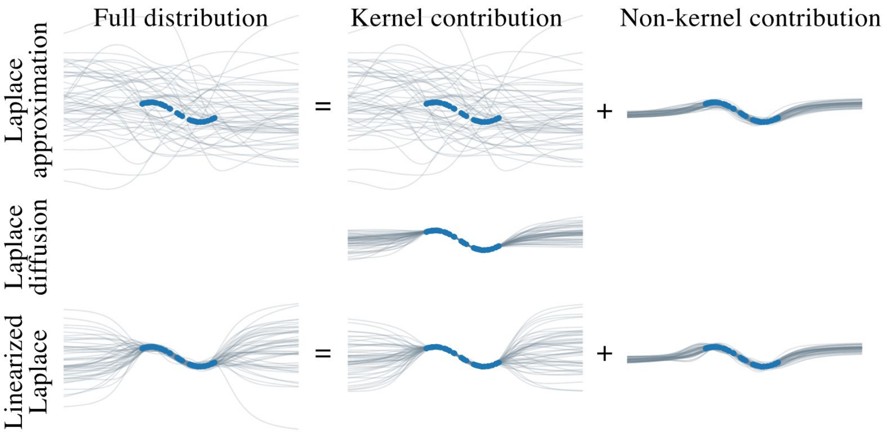

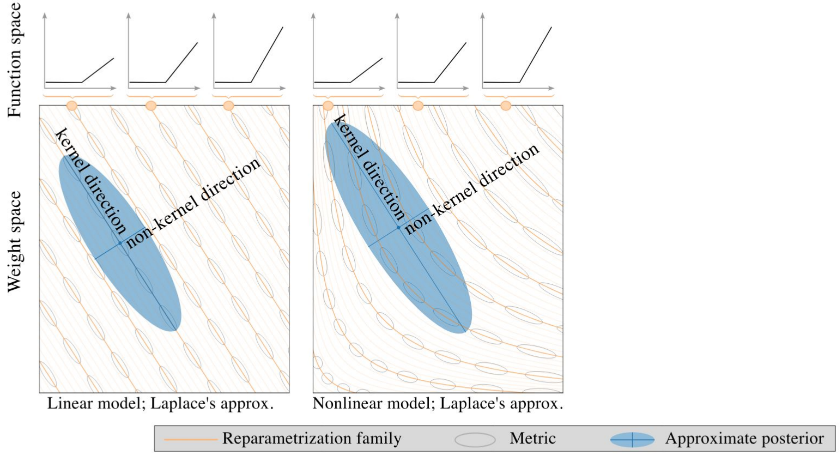

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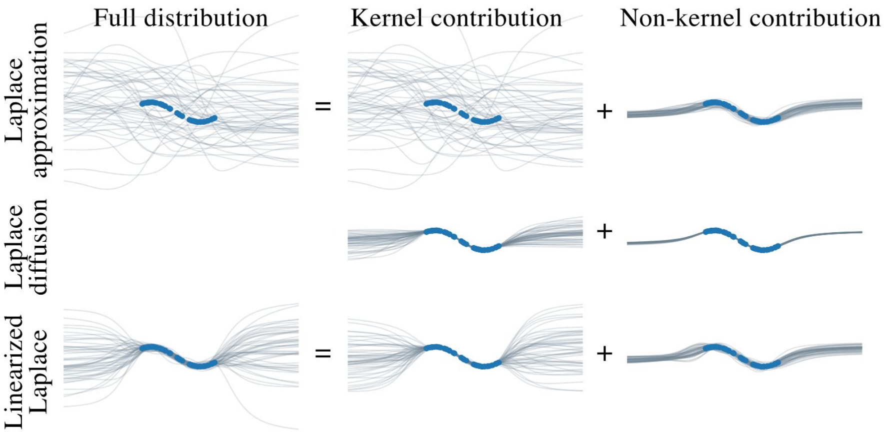

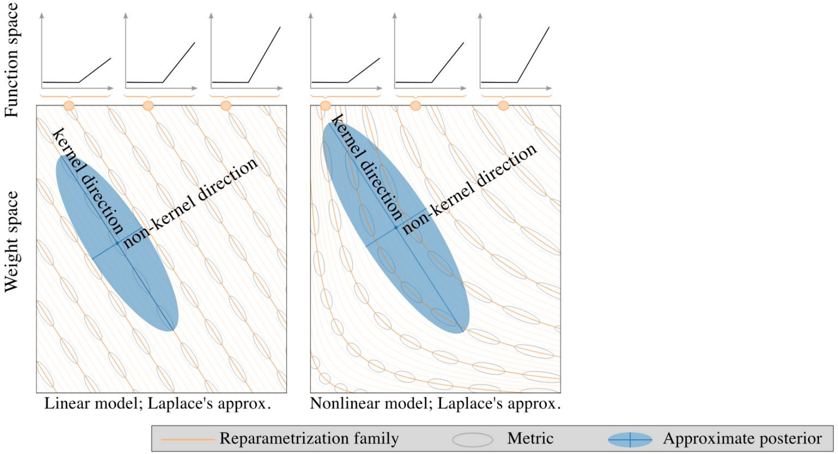

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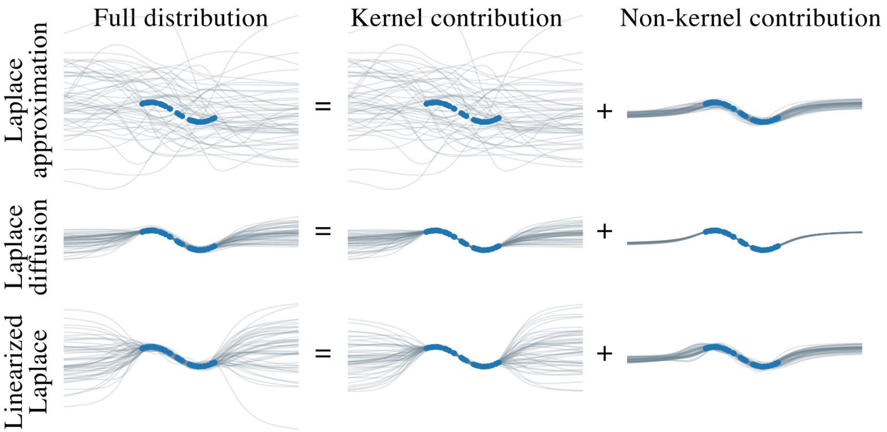
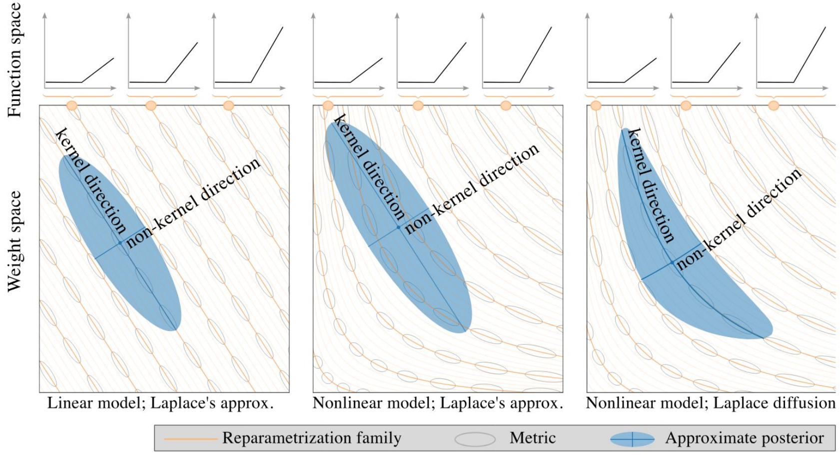
4. Alternate between the two





Results

Table 1: In-distribution performance across methods trained on MNIST, FMNIST and CIFAR-10.

		Conf. (↑)	NLL (↓)	Acc. (↑)	Brier (↓)	ECE (↓)	MCE (↓)
MNIST	Laplace Diffusion (ours)	**0.988±0.001**	**0.042±0.007**	**0.987±0.002**	**0.022±0.003**	**0.137±0.019**	**0.775±0.043**
	Sampled Laplace	0.589±0.008	3.812±0.284	0.146±0.032	1.176±0.046	0.443±0.026	0.985±0.002
	Linearised Laplace	0.968±0.004	0.306±0.041	0.926±0.008	0.117±0.012	0.251±0.034	0.855±0.041
FMNIST	Laplace Diffusion (ours)	**0.900±0.001**	**0.001±0.000**	**0.906±0.007**	**0.141±0.006**	**0.108±0.015**	**0.729±0.092**
	Sampled Laplace	0.618±0.021	4.507±0.000	0.098±0.010	1.295±0.014	0.518±0.013	0.986±0.001
	Linearised Laplace	0.897±0.003	0.423±0.000	0.862±0.005	0.207±0.006	0.147±0.017	0.756±0.048
CIFAR-10	Laplace Diffusion (ours)	**0.952±0.007**	**0.345±0.062**	**0.905±0.007**	**0.155±0.019**	0.259±0.008	0.870±0.021
	Sampled Laplace	0.843±0.004	0.997±0.222	0.717±0.049	0.422±0.081	**0.221±0.047**	0.804±0.080
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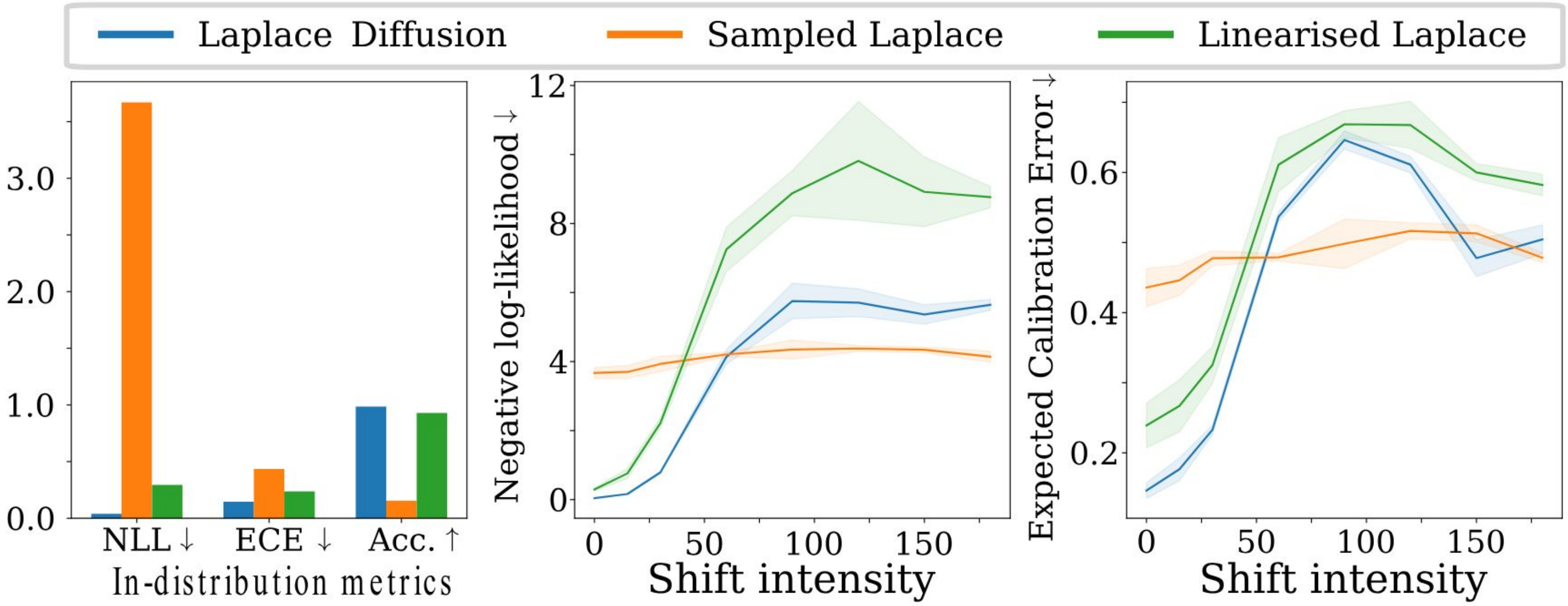
Table 2: Out-of-distribution AUROC (↑) performance for MNIST, FMNIST and CIFAR-10.

Trained on	MNIST			FMNIST			CIFAR-10	
Tested on	FMNIST	EMNIST	KMNIST	MNIST	EMNIST	KMNIST	CIFAR-100	SVHN
Laplace Diffusion (ours)	**0.909±0.033**	**0.625±0.018**	**0.929±0.008**	**0.759±0.045**	**0.741±0.010**	**0.749±0.023**	**0.851±0.002**	**0.862±0.010**
Sampled Laplace	0.500±0.026	0.494±0.006	0.482±0.013	0.495±0.037	0.503±0.036	0.493±0.033	0.687±0.033	0.599±0.038
Linearised Laplace	0.758±0.070	0.602±0.027	0.790±0.018	0.625±0.050	0.628±0.013	0.624±0.020	0.837±0.006	0.854±0.024

Rotated MNIST (shift = rotation angle)



Summary

- Linearised Laplace works better than full Laplace because it implicitly ignores the reparameterisation issues of BNNs

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- In practice, we often use an approximation of the GGN (e.g. KFAC), which would break the motivation behind their new method

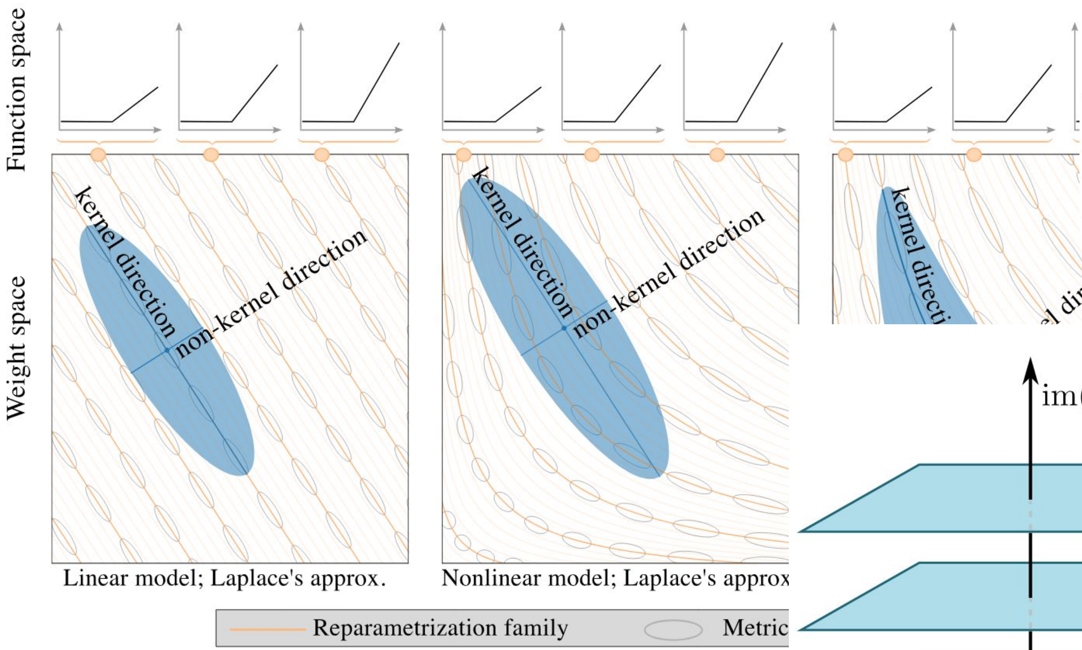
Links

Paper: https://arxiv.org/pdf/2406.03334

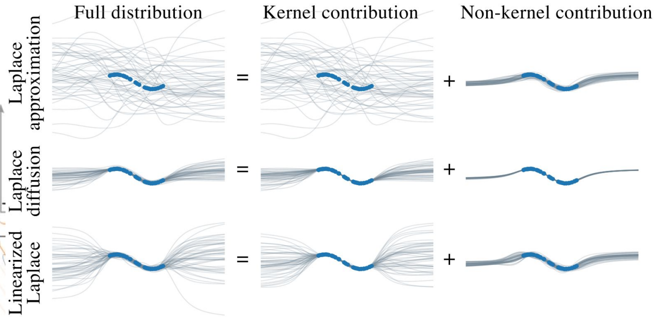
Slides from a talk by one of the authors:
https://www2.compute.dtu.dk/~sohau//talks/2024_MTNS/

Immer et al. (2021): “ Improving predictions of Bayesian neural nets via local linearization,” Alexander Immer, Maciej Korzepa, Matthias Bauer. Proceedings of The 24th International Conference on Artificial Intelligence and Statistics, PMLR 130:703-711, 2021. https://proceedings.mlr.press/v130/immer21a.html

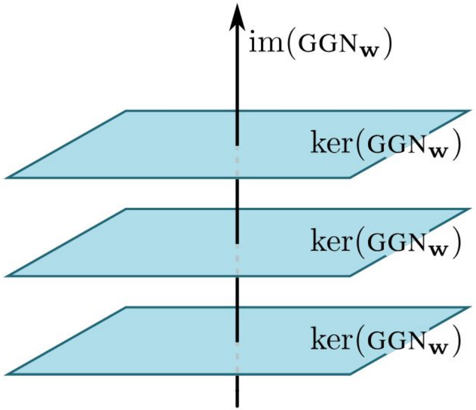
pics



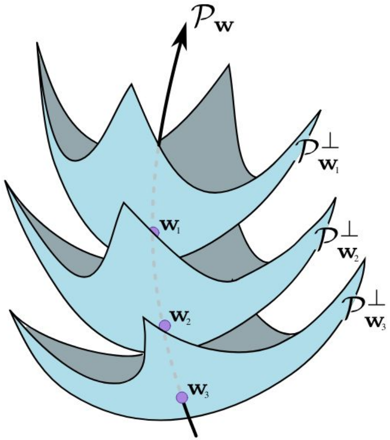
Function space
Weight space
kernel direction
non-kernel direction
kernel direction
non-kernel direction
kernel directi
l direction
Linear model; Laplace's approx.
Nonlinear model; Laplace's approx
Reparametrization family
Metric



Full distribution
Kernel contribution
Non-kernel contribution
Laplace approximation
Laplace diffusion
Linearized Laplace
=
+

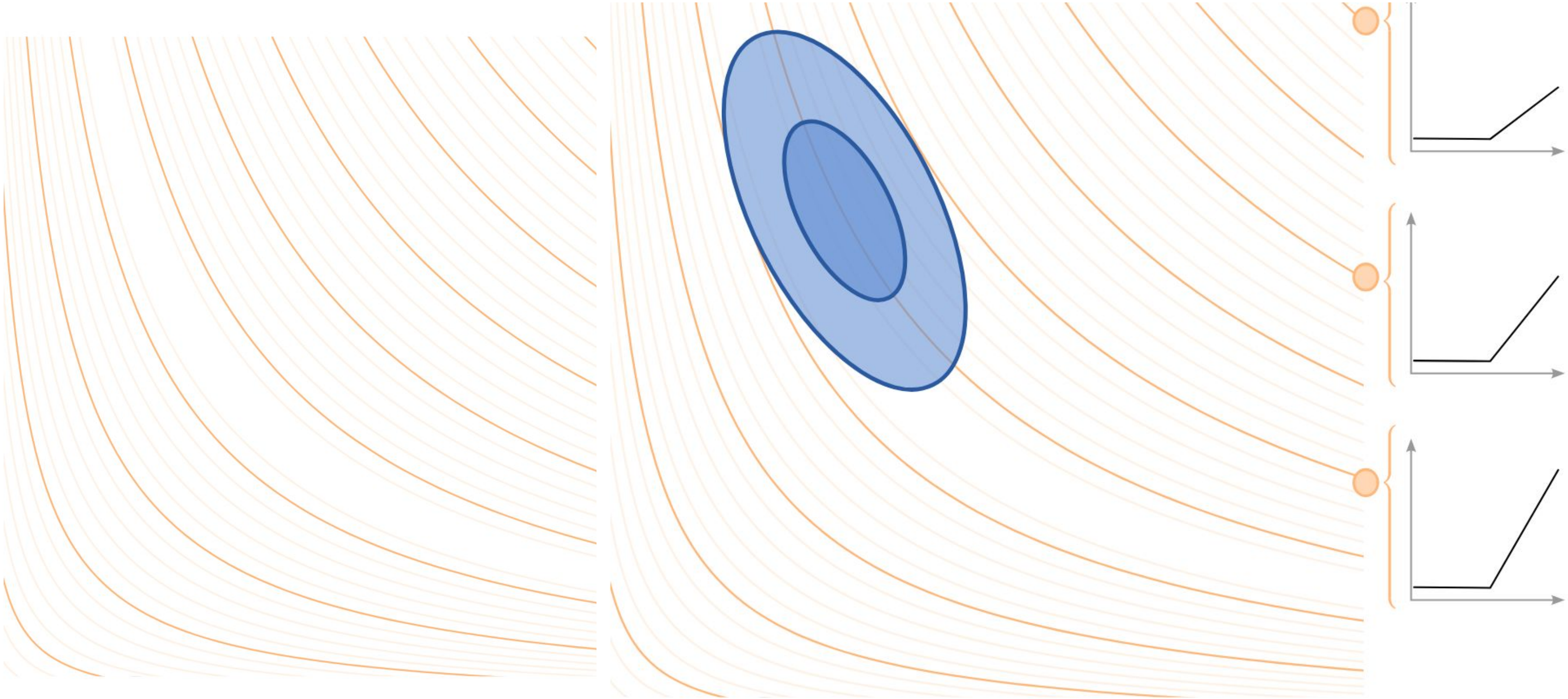


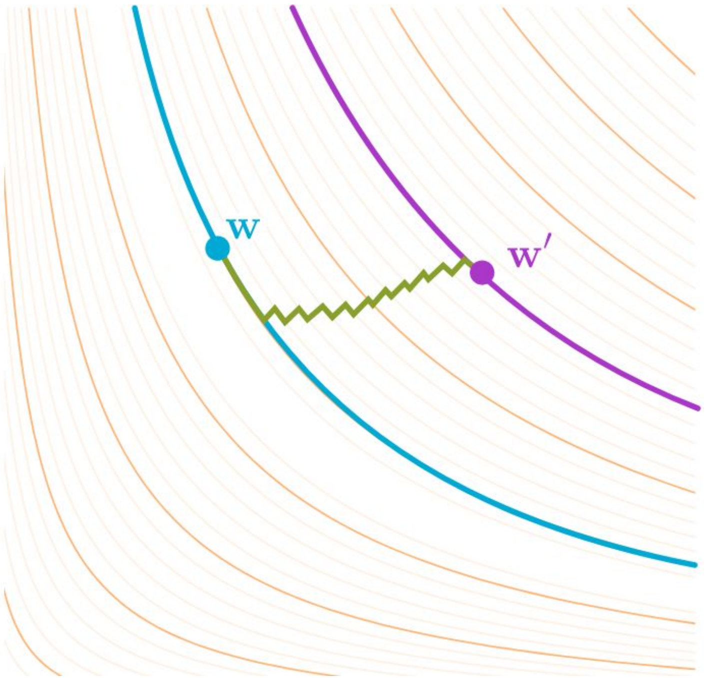
$\mathrm{im}(\mathrm{GGN}_{\mathbf{w}})$
$\ker(\mathrm{GGN}_{\mathbf{w}})$
$\ker(\mathrm{GGN}_{\mathbf{w}})$
$\ker(\mathrm{GGN}_{\mathbf{w}})$

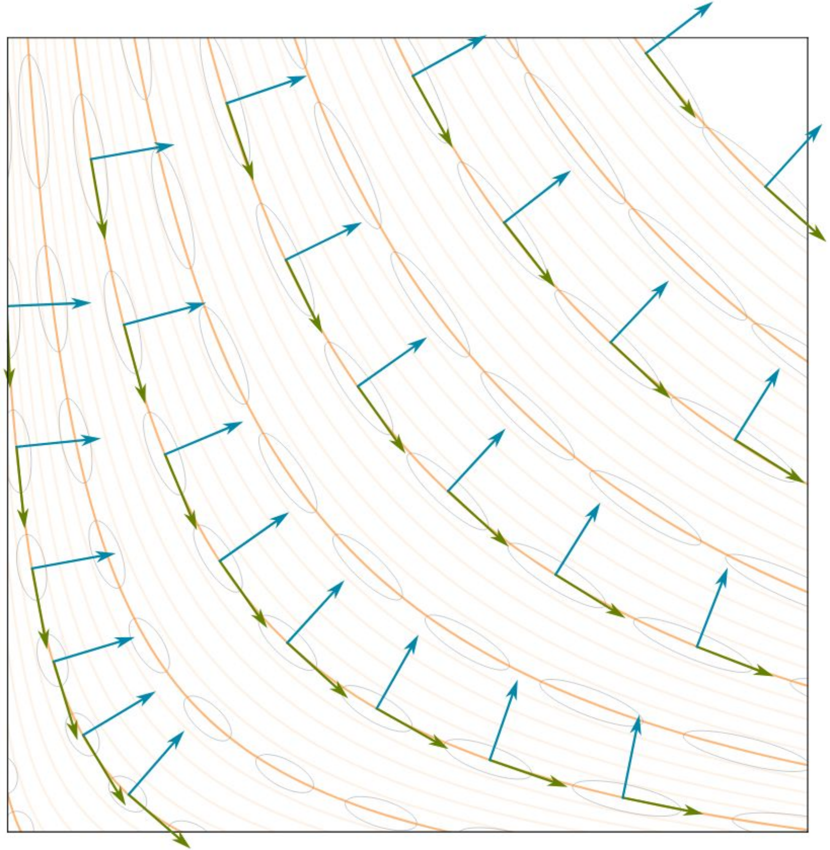


$\mathcal{P}_{\mathbf{w}}$
$\mathcal{P}^{\perp}_{\mathbf{w}_1}$
$\mathcal{P}^{\perp}_{\mathbf{w}_2}$
$\mathcal{P}^{\perp}_{\mathbf{w}_3}$
$\mathbf{w}_1$
$\mathbf{w}_2$
$\mathbf{w}_3$

From slides




w
w′



Section 4: They do diffusion

$$(\mathrm{M}, \mathbf{G})$$

$$\mathrm{d}\mathbf{w} = \sqrt{2\tau}\mathbf{G}(\mathbf{w})^{-\frac{1}{2}}\mathrm{d}W + \tau\Gamma\mathrm{d}t \qquad \text{where} \quad \Gamma_i(\mathbf{w}) = \sum_{j=1}^{D} \frac{\partial}{\partial \mathbf{w}_j}(\mathbf{G}(\mathbf{w})^{-1})_{i}$$

$$\mathbf{w}_{t+1} \;=\; \mathbf{w}_t + \sqrt{2h_t}\mathbf{G}(\mathbf{w}_t)^{-\frac{1}{2}}\boldsymbol{\epsilon}, \text{ where } \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$