Advances in Laplace Inference for Reliable and Interpretable Bayesian Deep Learning

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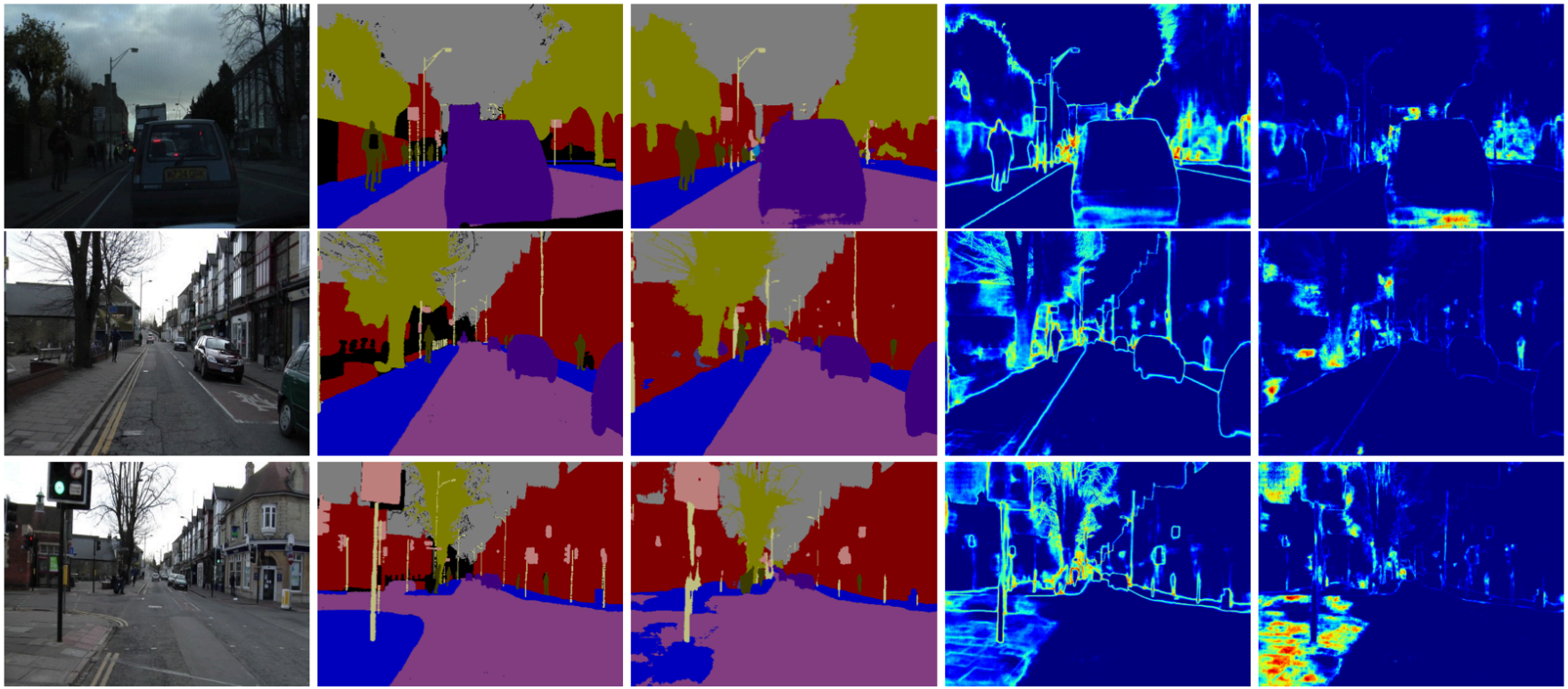
Motivation



(a) Input Image (b) Ground Truth (c) Semantic Segmentation (d) Aleatoric Uncertainty (e) Epistemic Uncertainty

Figure: Uncertainty for semantic segmentation. (Fig. 1 of *Kendall et al., 2017*)

Laplace approximation: Notation

We will be focusing on supervised learning over inputs $\boldsymbol{x}_{1:n}$ and labels $y_{1:n}$.

Neural network: Let $f_{\boldsymbol{\theta}} : \mathcal{X} \to \mathcal{Y}$ be a neural network with parameters $\boldsymbol{\theta}$.

$$f_{\boldsymbol{\theta}} \triangleq f^{(L)}_{\boldsymbol{\theta}^{(L)}} \circ \cdots \circ f^{(1)}_{\boldsymbol{\theta}^{(1)}}, \;\; \boldsymbol{\theta} \triangleq \texttt{Concat}\left[\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(L)}\right] \in \mathbb{R}^P, \;\; \boldsymbol{\theta}^{(\ell)} \in \mathbb{R}^{D_{\text{in}} \cdot D_{\text{out}}}$$

Probabilistic inference: Update our belief over $\boldsymbol{\theta}$ after seeing $\{\boldsymbol{x}_{1:n}, y_{1:n}\}$.

$$\underbrace{p(\boldsymbol{\theta} \mid \boldsymbol{x}_{1:n}, y_{1:n})}_{\text{posterior dist.}} = \frac{\overbrace{p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \boldsymbol{\theta})}^{\text{likelihood}} \overbrace{p(\boldsymbol{\theta})}^{\text{prior dist.}}}{\underbrace{\int p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \boldsymbol{\theta})\, p(\boldsymbol{\theta})\, d\boldsymbol{\theta}}_{\text{marginal likelihood}}}$$

Laplace approximation: VI and MAP estimation

Variational inference: Goal is to approximate the **posterior distribution**.

$$p(\boldsymbol{\theta} \mid \boldsymbol{x}_{1:n}, y_{1:n}) = \frac{p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \boldsymbol{\theta})\, p(\boldsymbol{\theta})}{\int p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \boldsymbol{\theta})\, p(\boldsymbol{\theta})\, d\boldsymbol{\theta}} \approx q(\boldsymbol{\theta} \mid \boldsymbol{\lambda}) \triangleq q_{\boldsymbol{\lambda}}(\boldsymbol{\theta})$$

MAP estimation: Rely on SGD to find a maximum *a posteriori* estimate.

$$\begin{aligned}
\hat{\boldsymbol{\theta}} &= \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta} \mid \boldsymbol{x}_{1:n}, y_{1:n}) \\
&= \arg\min_{\boldsymbol{\theta}} -\log p(\boldsymbol{\theta} \mid \boldsymbol{x}_{1:n}, y_{1:n}) \\
&= \arg\min_{\boldsymbol{\theta}} -\log p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \boldsymbol{\theta}) - \log p(\boldsymbol{\theta})
\end{aligned}$$

Laplace approximation: Taylor expansion

Laplace's method (*P.S. Laplace, 1774*): Let $\psi(\boldsymbol{\theta}) \triangleq \log p(\boldsymbol{\theta} \mid \boldsymbol{x}_{1:n}, y_{1:n})$.
Take the 2nd-order Taylor expansion of $\psi(\boldsymbol{\theta})$ around the MAP estimate $\hat{\boldsymbol{\theta}}$.

$$\psi(\boldsymbol{\theta}) \approx \psi(\hat{\boldsymbol{\theta}}) + (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) \cancel{\left[\ldots\right]} + \frac{1}{2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^\top \left[\nabla^2_{\boldsymbol{\theta}} \psi(\boldsymbol{\theta})\right]_{\hat{\boldsymbol{\theta}}} (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$$

Compare this to the log-p.d.f. of a multivariate Normal distribution (MVN).

$$\log \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{\theta} - \boldsymbol{\mu}) + \text{const.}$$

Laplace approximation: Mean and covariance

The **Laplace approximation** q of p is a MVN (mean $\hat{\boldsymbol{\theta}}$, cov. matrix $\hat{\boldsymbol{\Sigma}}$).

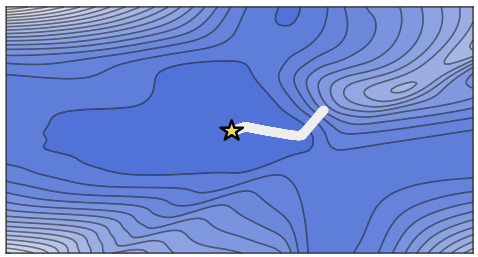
$$q(\boldsymbol{\theta}) \triangleq \mathcal{N}(\boldsymbol{\theta}; \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\Sigma}}) \quad \hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \psi(\boldsymbol{\theta}) \quad \hat{\boldsymbol{\Sigma}} = -\left[\nabla^2_{\boldsymbol{\theta}} \psi(\boldsymbol{\theta})\right]^{-1}_{\hat{\boldsymbol{\theta}}}$$

- Beware! $\hat{\boldsymbol{\Sigma}}$ needs to be *symmetric* and *positive semi-definite*.
- However $\psi(\boldsymbol{\theta})$ being twice continuously diff. around $\hat{\boldsymbol{\theta}}$ is sufficient:
  - Symmetric: Order of differentiation does not matter.
  - Positive semi-definite: Hessian taken at $\hat{\boldsymbol{\theta}}$ is negative semi-definite.

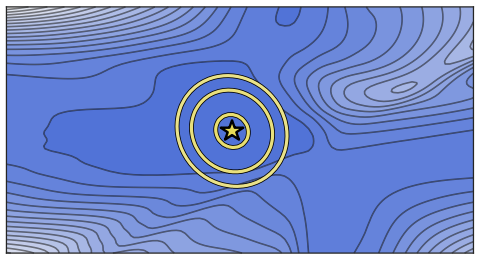
Laplace approximation: Predictive posterior

How do we make predictions using our Laplace approximation?

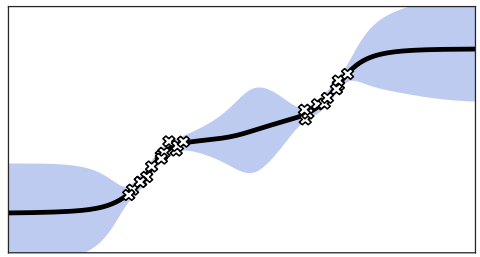
$$
\begin{aligned}
p(y^\star \mid \boldsymbol{x}^\star, \boldsymbol{x}_{1:n}, y_{1:n}) &= \int p(y^\star \mid \boldsymbol{x}^\star, \boldsymbol{\theta})\, p(\boldsymbol{\theta} \mid \boldsymbol{x}_{1:n}, y_{1:n})\, d\boldsymbol{\theta} \\
&\approx \int p(y^\star \mid \boldsymbol{x}^\star, \boldsymbol{\theta})\, q(\boldsymbol{\theta})\, d\boldsymbol{\theta} \\
&= \mathop{\mathbb{E}}_{\boldsymbol{\theta} \sim q} \Big[p(y^\star \mid \boldsymbol{x}^\star, \boldsymbol{\theta}) \Big]
\end{aligned}
$$



(a) Step 1: Find MAP



(b) Step 2: Fit approx.



(c) Step 3: Predict!

Figure: Fig. 1 of (*Daxberger et al., 2021*)

Laplace approximation: Bayesian neural networks?

LA hinges on inverting Hessian of the log-**posterior distribution** w.r.t. $\boldsymbol{\theta}$

$$\hat{\boldsymbol{\Sigma}} = -\left[\nabla^2_{\boldsymbol{\theta}} \psi(\boldsymbol{\theta})\right]^{-1}_{\hat{\boldsymbol{\theta}}} = -\left[\nabla^2_{\boldsymbol{\theta}} \log p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \boldsymbol{\theta}) + \nabla^2_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta})\right]^{-1}_{\hat{\boldsymbol{\theta}}}$$

- Known to work with small neural networks. (*D.J.C. MacKay, 1992*)
- However the Hessian quickly becomes problematic as P grows.
  - Auto-diff. frameworks help but Hessian still needs $\mathcal{O}(P^2)$ storage.
  - Inversion can also be difficult. (compute & numerical instability)
  - Not guaranteed to be negative semi-definite! (e.g. saddle points)

Hessian approximation: Fisher information matrix

Fisher information: Avoid 2^{nd}-order differentiation and focus on the score.

$$\hat{\boldsymbol{\Sigma}} \approx \boldsymbol{\Sigma}_{\text{Fish.}}, \quad \boldsymbol{\Sigma}_{\text{Fish.}} \triangleq - \left[\sum_{i=1}^{n} \mathop{\mathbb{E}}_{y \sim p(\dots)} \left[\left[\nabla_{\boldsymbol{\theta}} \log p(y \mid \boldsymbol{x}_i, \boldsymbol{\theta}) \right]_{\hat{\boldsymbol{\theta}}}^{2} \right] + \dots \right]^{-1}$$

Note: Guaranteed positive semi-definite. (cf. info. geometry, natural grad.)

Hessian approximation: Gen. Gauss-Newton matrix

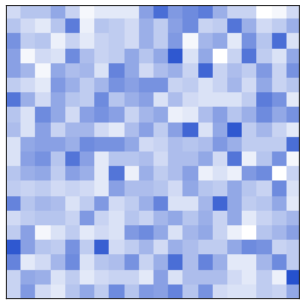
Gen. Gauss-Newton (GGN): Let $\mathcal{J}_{\boldsymbol{\theta}}(\boldsymbol{x}) \triangleq \left[\nabla_{\boldsymbol{\theta}} f_{\boldsymbol{\theta}}(\boldsymbol{x})\right]_{\hat{\boldsymbol{\theta}}}$ denote Jacobian.

$$\hat{\boldsymbol{\Sigma}} \approx \boldsymbol{\Sigma}_{\text{GGN}},\ \boldsymbol{\Sigma}_{\text{GGN}} \triangleq -\left[\sum_{i=1}^{n} \mathcal{J}_{\boldsymbol{\theta}}(\boldsymbol{x}_i) \left[\nabla_f^2 \log p(y_i \mid f)\right]_{\hat{f}} \mathcal{J}_{\boldsymbol{\theta}}(\boldsymbol{x}_i)^\top + \dots\right]^{-1}$$

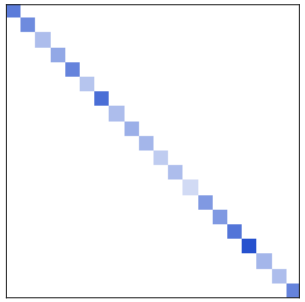
Note: Equivalent to the Fisher for most common log-likelihoods.

Hessian approximation: Matrix factorization

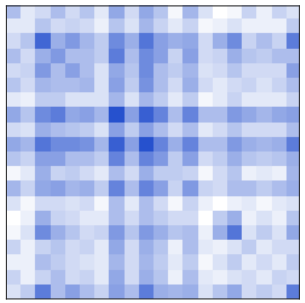
The full covariance matrices $\mathbf{\Sigma}_{\text{Fish.}}$ and $\mathbf{\Sigma}_{\text{GGN}}$ are still quadratic in the number of parameters P, making them difficult to store and difficult to invert.



Diagonal factorization: Keep the matrix diagonal and ignore the off-diagonal elements. Lightweight but highest tradeoff in approximation fidelity.

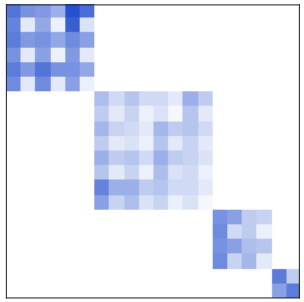


Low-rank factorization: Use a low-rank approximation, such as truncated singular value decomposition (SVD). Can be combined with the diagonal factorization.



Hessian approximation: Kronecker factorization

Block-diagonal factorization: Factorize across neural network layers by approximating diagonal blocks for each layer ℓ, i.e. making the assumption of layer independence.



Kronecker factorization (*Ritter et al., 2018*)**:** The approximate blocks for a single data point can be formulated as a Kronecker product (K-FAC).

$$
\begin{aligned}
-\left[\mathbf{\Sigma}_{\text{GGN}}^{(\ell)}\right]^{-1} &= \sum_{i=1}^{n} \left[\mathbf{A}_i^{(\ell)} \otimes \mathbf{B}_i^{(\ell)}\right] \\
&\approx \left[\sum_{i=1}^{n} \mathbf{A}_i^{(\ell)}\right] \otimes \left[\sum_{i=1}^{n} \mathbf{B}_i^{(\ell)}\right] \triangleq \mathbf{A}^{(\ell)} \otimes \mathbf{B}^{(\ell)}
\end{aligned}
$$

Note: $\mathbf{A}^{(\ell)} \in \mathbb{R}^{D_{\text{out}}^{(\ell)} \times D_{\text{out}}^{(\ell)}}$, $\mathbf{B}^{(\ell)} \in \mathbb{R}^{D_{\text{in}}^{(\ell)} \times D_{\text{in}}^{(\ell)}}$ and both are pos. semi. definite.

Hessian approximation: Predictive misspecification

Misspecification? Used the GGN but now the predictive is underfitting?

① Data $\mathcal{D}$ and model

Prior: $p\left(\begin{bmatrix} w \\ b \end{bmatrix}\right) = \mathcal{N}(\mathbf{0}, \mathbf{I}_2)$

Model:

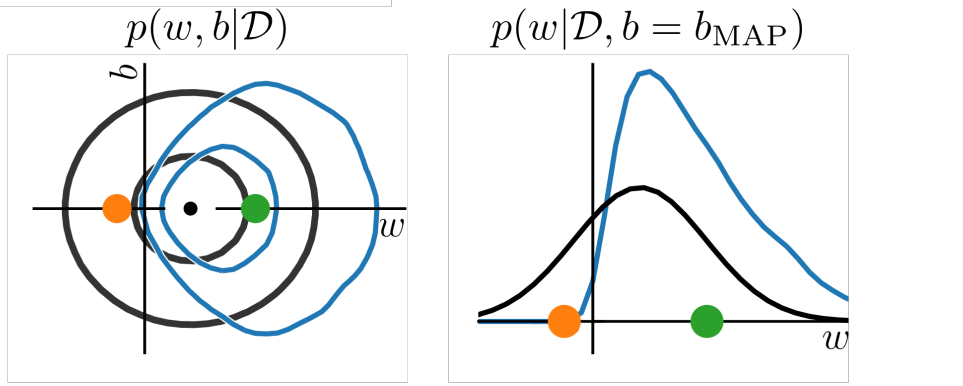
$f(x; w, b) = 5 \tanh(wx + b)$

Likelihood:

$p([y = 1] \mid f) = \texttt{sigmoid}(f)$

The BNN underfits because some samples can give extremely wrong predictions (e.g. sample shown in orange). How do we correct this?

② Posterior inference



③ Posterior predictive distribution

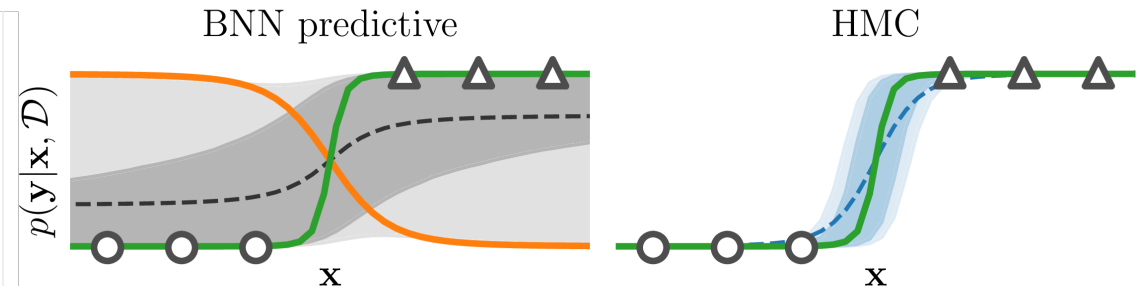


Figure: Fig. 3 of (*Immer et al., 2021a*)

Linearized Laplace: Linearization of $f_{\boldsymbol{\theta}}$

Recall that $\hat{\boldsymbol{\Sigma}}$ depends on the Hessian of the log-**posterior dist.** w.r.t. $\boldsymbol{\theta}$.

$$\hat{\boldsymbol{\Sigma}} = -\left[\nabla^2_{\boldsymbol{\theta}} \log p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \boldsymbol{\theta}) + \nabla^2_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta})\right]^{-1}_{\hat{\boldsymbol{\theta}}}$$

Focus on the log-**likelihood**. Let $\mathcal{H}_{\boldsymbol{\theta}}(\boldsymbol{x}) \triangleq \left[\nabla^2_{\boldsymbol{\theta}} f_{\boldsymbol{\theta}}(x)\right]$ denote Hessian.

$$\nabla_{\boldsymbol{\theta}} \log p(y_i \mid \boldsymbol{x}_i, \boldsymbol{\theta}) = \mathcal{J}_{\boldsymbol{\theta}}(\boldsymbol{x}_i)^\top \left[\nabla_f \log p(y_i \mid f)\right]$$

$$\nabla^2_{\boldsymbol{\theta}} \log p(y_i \mid \boldsymbol{x}_i, \boldsymbol{\theta}) = \mathcal{H}_{\boldsymbol{\theta}}(\boldsymbol{x}_i)^\top \left[\nabla_f \log p(y_i \mid f)\right] \underbrace{-\mathcal{J}_{\boldsymbol{\theta}}(\boldsymbol{x}_i) \left[\nabla^2_f p(y_i \mid f)\right]_{\hat{f}} \mathcal{J}_{\boldsymbol{\theta}}(\boldsymbol{x}_i)^\top}_{\text{GGN approximation!}}$$

Linearized Laplace: Linearization of $f_{\boldsymbol{\theta}}$

GGN approx. makes the assumption that $\mathcal{H}_{\boldsymbol{\theta}}(\boldsymbol{x}_i)^\top \left[\nabla_f \log p(y_i \mid f)\right]$ is zero.

Condition 1: The *residual* $\left[\nabla_f \log p(y_i \mid f)\right]$ vanishes for all data points. This is not desired, as it would indicate overfitting, nor is it very realistic.

Condition 2: The Hessian $\mathcal{H}_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$ vanishes for all input points. This is true for linear networks, and we can enforce it by linearizing our network!

Local linearization of $f_{\boldsymbol{\theta}}$ (*Immer et al., 2021a*)**:** Applying GGN approx. to the Hessian of the likelihood turns underlying model from BNN to GLM.

$$f_{\boldsymbol{\theta}}^{\text{lin.}}(\boldsymbol{x}) = f_{\boldsymbol{\theta}}(\boldsymbol{x}) + (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})\mathcal{J}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x})$$

Linearized Laplace: GP formulation

Function-space equivalence (*Immer et al., 2021a*): This linearized model in weight-space is equivalent to a Gaussian process (GP) in function-space.

$$
\begin{aligned}
m(\boldsymbol{x}) &= \mathop{\mathbb{E}}_{\boldsymbol{\theta}}\left[f_{\boldsymbol{\theta}}^{\text{lin.}}(\boldsymbol{x})\right] = f_{\hat{\boldsymbol{\theta}}}^{\text{lin.}}(\boldsymbol{x}) \\
k(\boldsymbol{x}, \boldsymbol{x}') &= \mathrm{Cov}_{\boldsymbol{\theta}}\left[f_{\boldsymbol{\theta}}^{\text{lin.}}(\boldsymbol{x}),\, f_{\boldsymbol{\theta}}^{\text{lin.}}(\boldsymbol{x}')\right] \\
&= \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) \boldsymbol{\Sigma}_{\text{GGN}} \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x})^{\top}
\end{aligned}
$$

Function-space predictive (*Immer et al., 2021a*): Leads to a closed form for sampling from the network. Use Monte-Carlo simulation for predictive.

$$
\begin{aligned}
p(f^{\star} \mid \boldsymbol{x}^{\star}, \boldsymbol{x}_{1:n}, y_{1:n}) &= \mathcal{N}(f^{\star}; f_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}^{\star}), \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}^{\star}) \boldsymbol{\Sigma}_{\text{GGN}} \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}^{\star})^{\top}) \\
p(y^{\star} \mid \boldsymbol{x}^{\star}, \boldsymbol{x}_{1:n}, y_{1:n}) &= \mathop{\mathbb{E}}_{f^{\star}}\left[p(y^{\star} | f^{\star})\right]
\end{aligned}
$$

Linearized Laplace: Demonstration

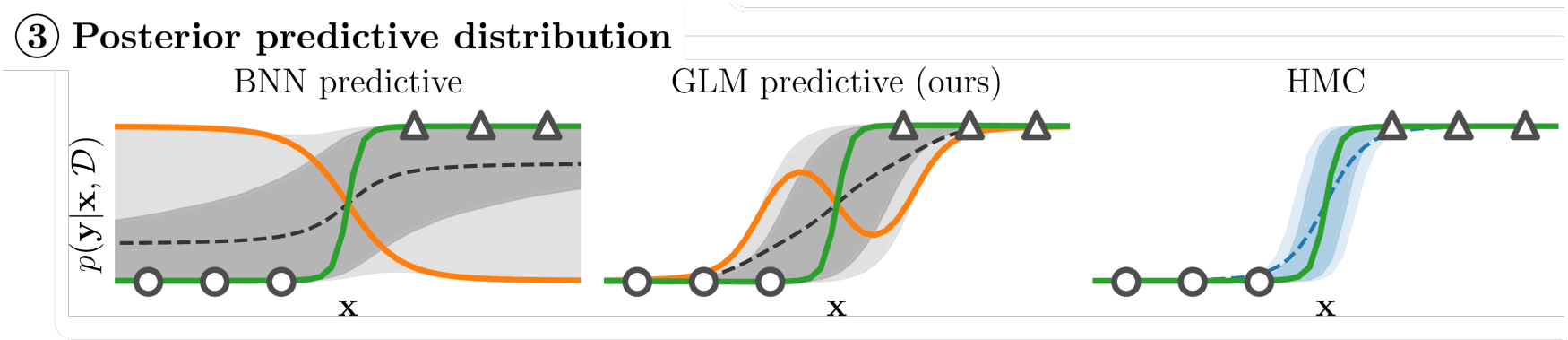


Figure: Using GLM as the underlying model. (Fig. 3 of *Immer et al., 2021a*)

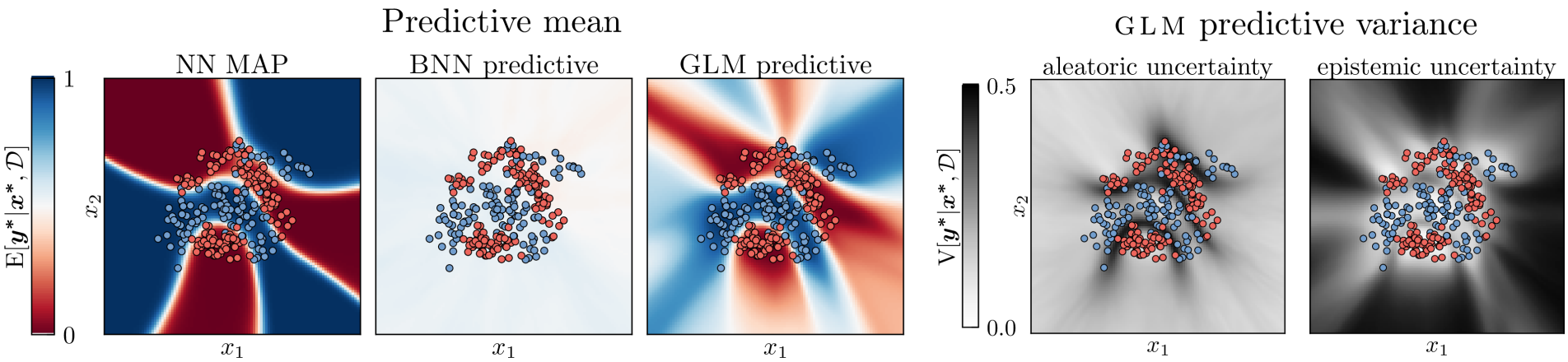


Figure: Mean and uncertainty on banana dataset. (Fig. 4 of *Immer et al., 2021a*)

Linearized Laplace: Model selection

Marginal likelihood (*Immer et al., 2021b*) **:** Likelihood of model $\mathcal{M}$.
Overly simple or complex models have low-probability (Occam's razor).

$$\log p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \mathcal{M}) = \int \log p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta} \mid \mathcal{M})\, d\boldsymbol{\theta}$$

$$\approx \log p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \hat{\boldsymbol{\theta}}) + \log p(\hat{\boldsymbol{\theta}} \mid \mathcal{M}) - \frac{1}{2} \log \left| \frac{1}{2\pi} \boldsymbol{\Sigma}^{-1} \right|$$

Note: Model $\mathcal{M}$ can be choice of architecture, hyper-parameters, etc.

Linearized Laplace: Model selection

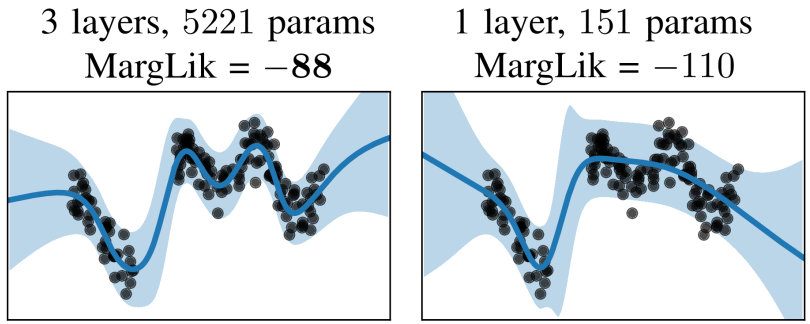


Figure: Marginal likelihood on toy regression. (Fig. 1 of *Immer et al., 2021b*)

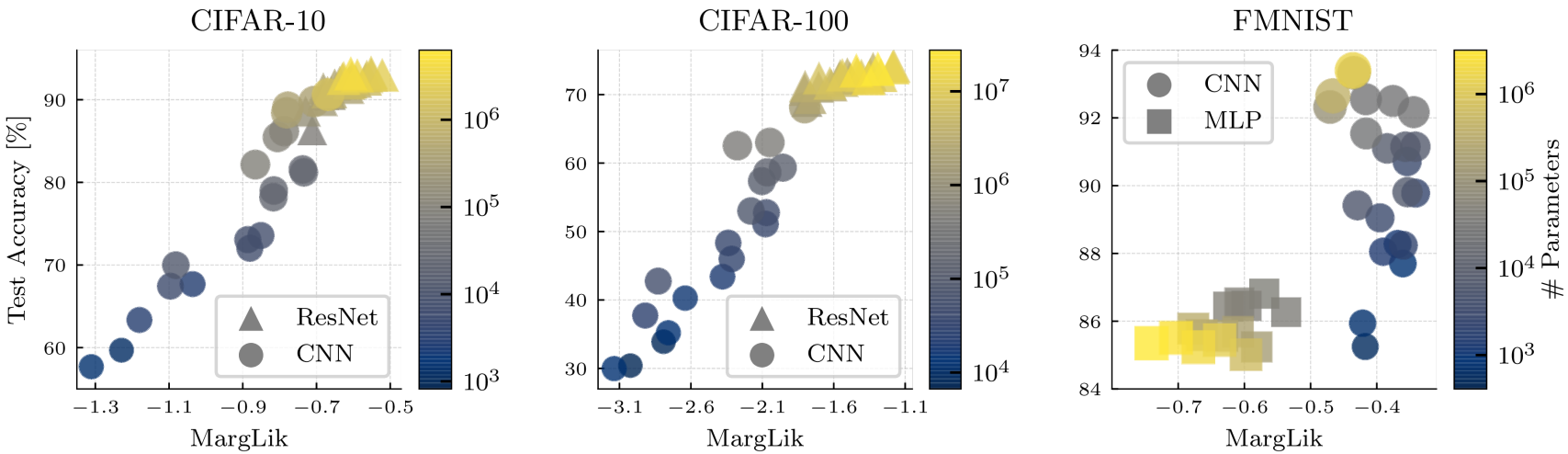


Figure: Marginal likelihood and test accuracy (Fig. 2 of *Immer et al., 2021b*)

Linearized Laplace: Hyperparam. optimization

Hyperparam. optimization (*Immer et al., 2021*): Diff. hyperparams $\mathcal{M}^{\partial}$. Alternate between optimizing params. $\boldsymbol{\theta}$ and hyperparams. $\mathcal{M}^{\partial}$ online.

$$\mathcal{M}^{\partial}_{t+1} \leftarrow \mathcal{M}^{\partial}_{t} + \gamma \nabla_{\mathcal{M}^{\partial}} \log q(y_{1:n} \mid \boldsymbol{x}_{1:n}, \mathcal{M})$$

Note: a.k.a. empirical Bayes or type-II maximum likelihood estimation.

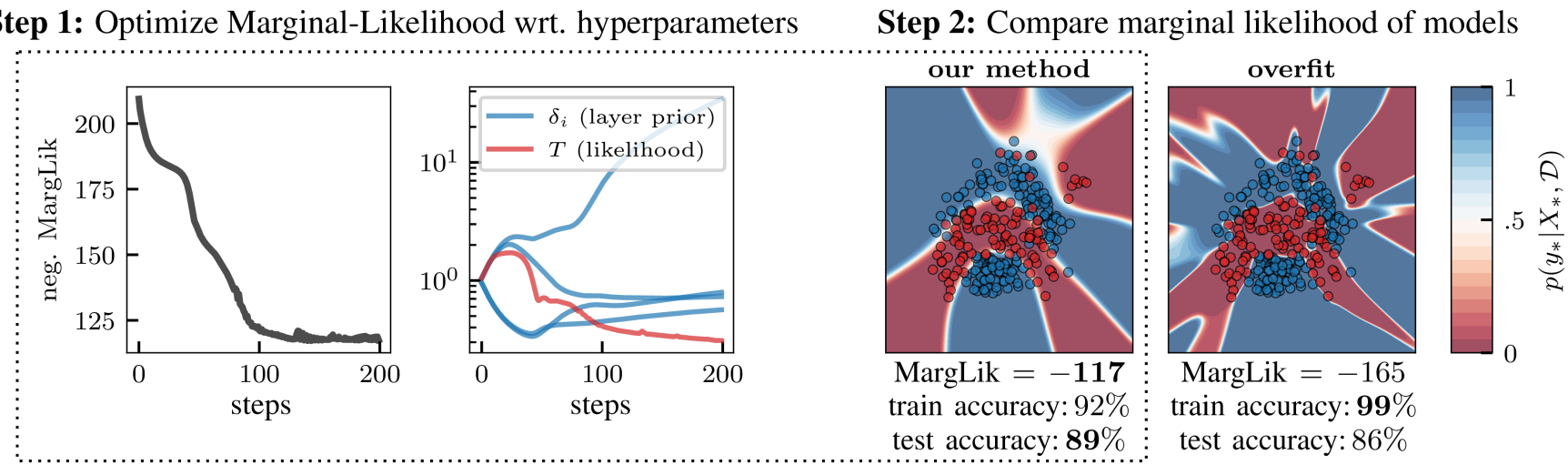


Figure: Optimizing marg. lik. in banana dataset. (Fig. 3 of *Immer et al., 2021b*)

Linearized Laplace: PyTorch package

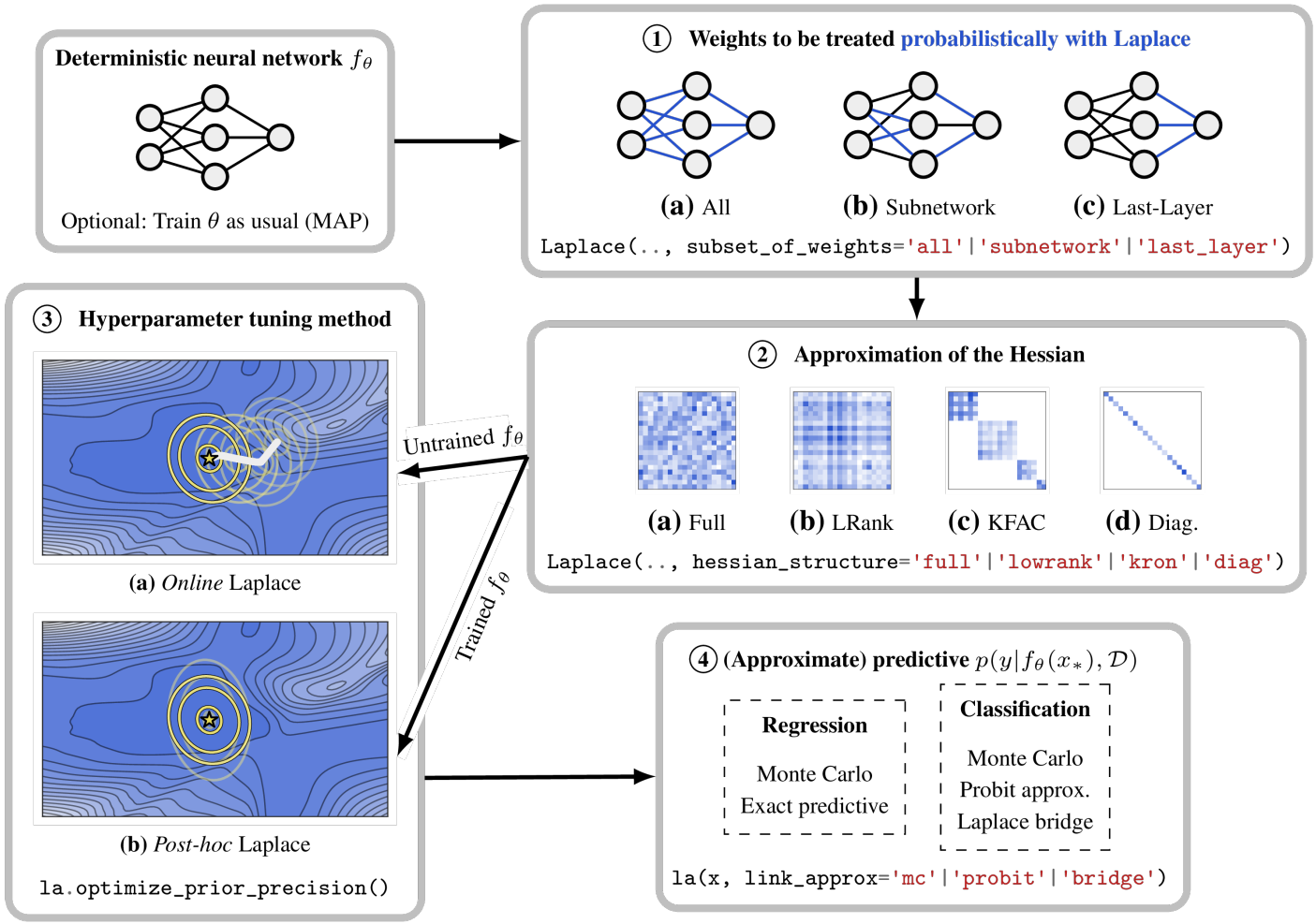


Figure: Overview of `laplace-torch`. (Fig. 2 of *Daxberger et al., 2021*)

Laplace-approximated NAMs: Introduction

Focus on tabular data, d columns of numer. or categ. features $x_1, \ldots, x_d$.

Neural additive models (*Agarwal et al., 2021*): Handle input columns indep. in separate sub-networks to observe the response as we vary inputs.

$$\mathbb{E}[g(y) \mid \boldsymbol{x}] = f_{\boldsymbol{\theta}}(\boldsymbol{x}) \triangleq f^{(1)}_{\boldsymbol{\theta}_1}(x_1) + f^{(2)}_{\boldsymbol{\theta}_2}(x_2) + \cdots + f^{(d)}_{\boldsymbol{\theta}_d}(x_d)$$

Laplace-approximated NAMs (*Bouchiat et al., 2024*): Swap the point estimates with Bayesian neural networks and use linearized Laplace approx.

$$f^{\text{lin.}}_{\boldsymbol{\theta}}(\boldsymbol{x}) \triangleq f^{(1),\,\text{lin.}}_{\boldsymbol{\theta}_1}(x_1) + f^{(2),\,\text{lin.}}_{\boldsymbol{\theta}_2}(x_2) + \cdots + f^{(d),\,\text{lin.}}_{\boldsymbol{\theta}_d}(x_d)$$
$$f^{(j),\,\text{lin.}}_{\boldsymbol{\theta}_j}(x_j) \triangleq f^{(j)}_{\hat{\boldsymbol{\theta}}_j}(x_j) + (\boldsymbol{\theta}_j - \hat{\boldsymbol{\theta}}_j)\mathcal{J}_{\hat{\boldsymbol{\theta}}_j}(x_j)$$

Laplace-approximated NAMs: Introduction

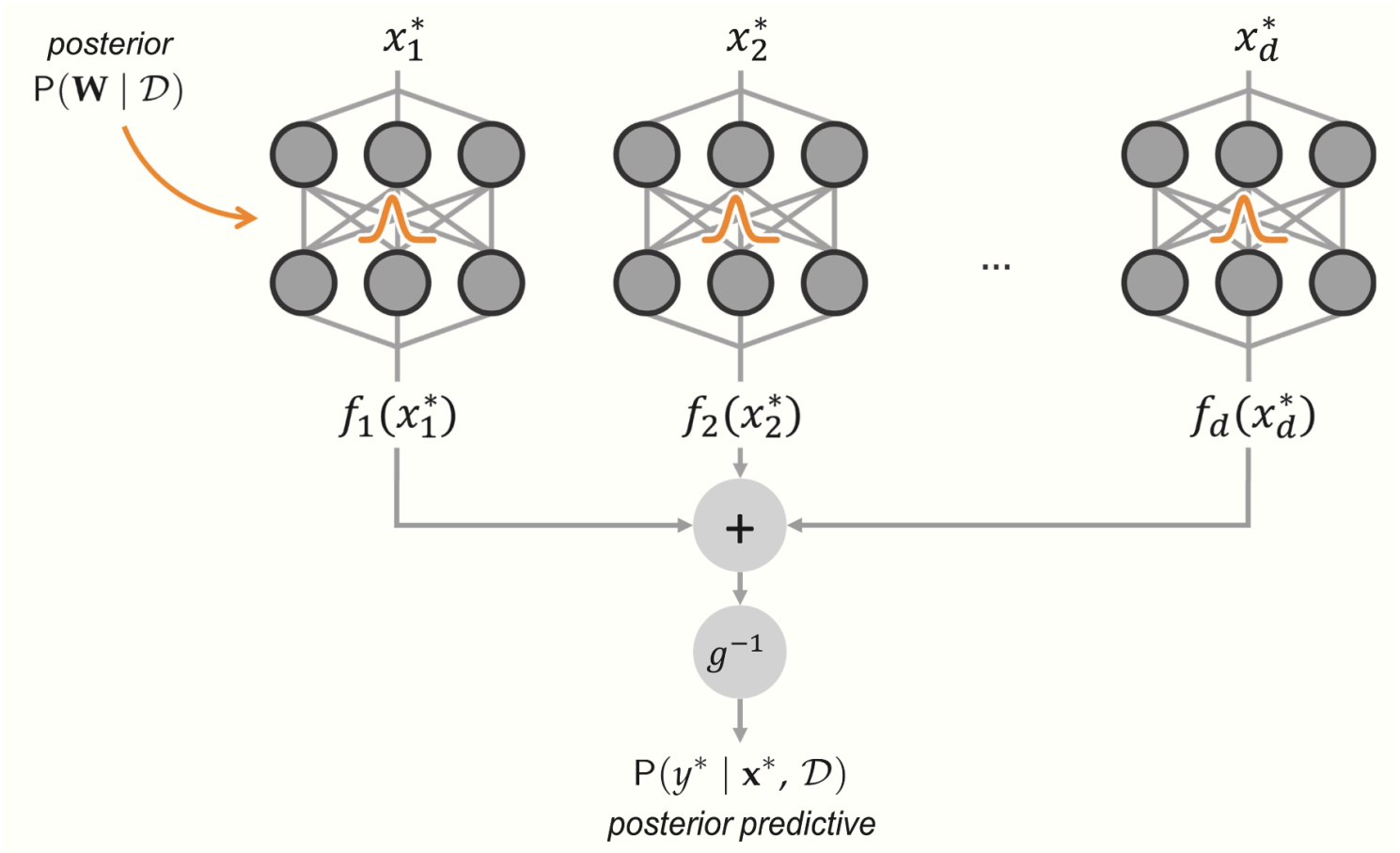


Figure: Diagram of LA-NAM architecture in (*Bouchiat et al., 2024*).

Laplace-approximated NAMs: Introduction

Laplace-approximated NAMs (*Bouchiat et al., 2024*): The independence of the subnetworks leads to factorized block-diagonal posterior covariance.

$$q(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}; \hat{\boldsymbol{\theta}}, \boldsymbol{\Sigma}_{\text{GGN}}), \quad \boldsymbol{\Sigma}_{\text{GGN}} = \begin{bmatrix} \boldsymbol{\Sigma}_{\text{GGN}}^{(1)} & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \cdots & \boldsymbol{\Sigma}_{\text{GGN}}^{(d)} \end{bmatrix}$$

Block factorization leads to factorized marg. lik. (*Immer et al., 2023*).

$$\begin{aligned} \log p(y_{1:n} \mid \boldsymbol{x}_{1:n}, \mathcal{M}) &\approx \log p(y_{1:n}, \hat{\boldsymbol{\theta}} \mid \boldsymbol{x}_{1:n}, \mathcal{M}) + \frac{1}{2} \left| \frac{1}{2\pi} \boldsymbol{\Sigma}_{\text{Full}}^{-1} \right| \\ &\geq \log p(y_{1:n}, \hat{\boldsymbol{\theta}} \mid \boldsymbol{x}_{1:n}, \mathcal{M}) + \frac{1}{2} \sum_j \left| \frac{1}{2\pi} \boldsymbol{\Sigma}_{\text{GGN}}^{(j)} \right| \end{aligned}$$

Laplace-approximated NAMs: Toy example

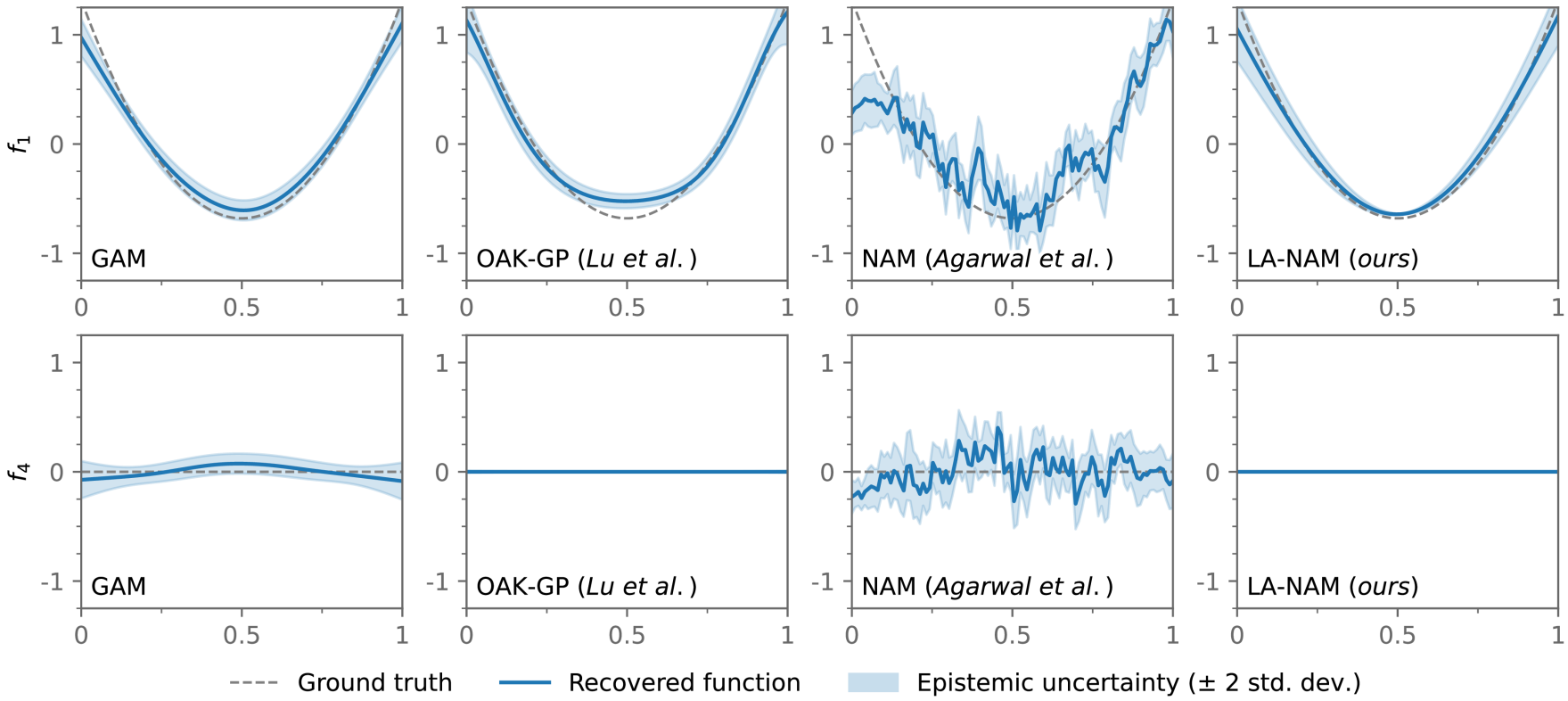


Figure: Demonstration on toy dataset. (Fig. 1 of *Bouchiat et al., 2024*)

Laplace-approximated NAMs: MIMIC-III dataset

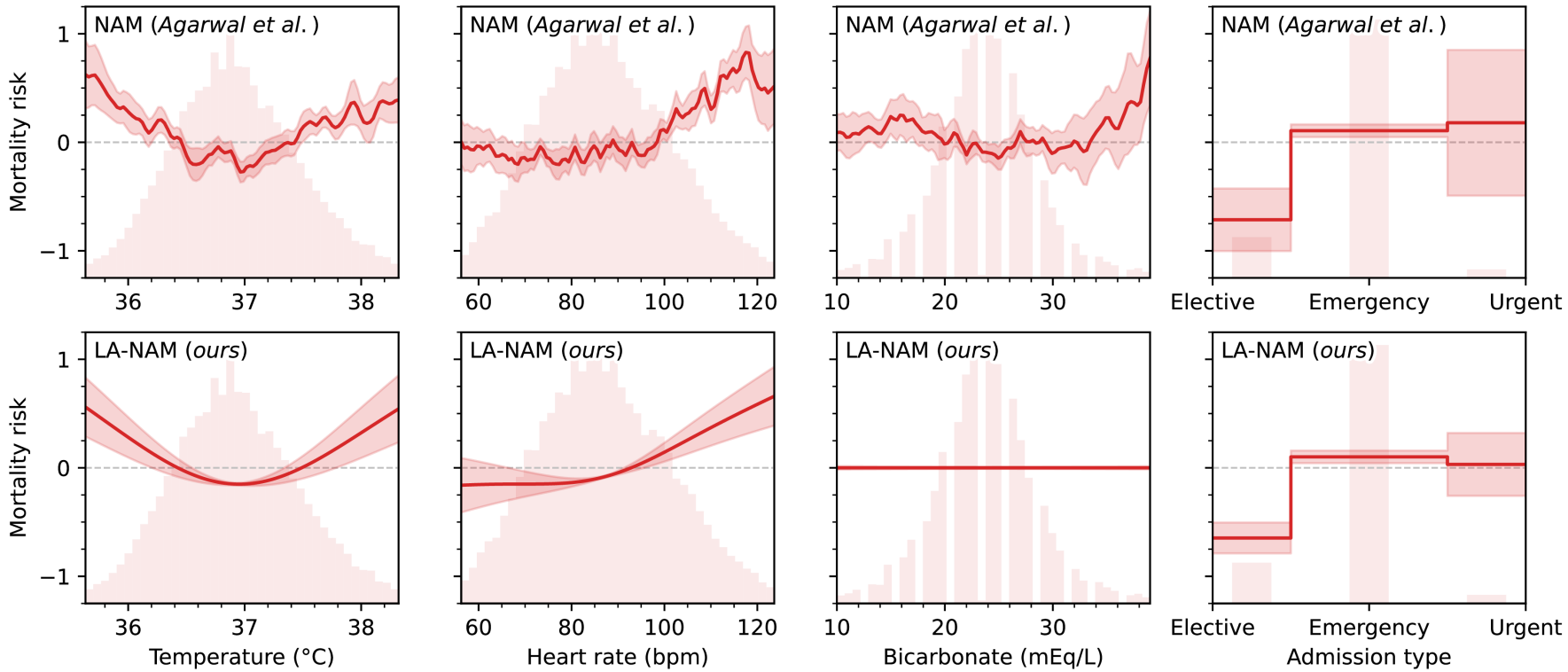
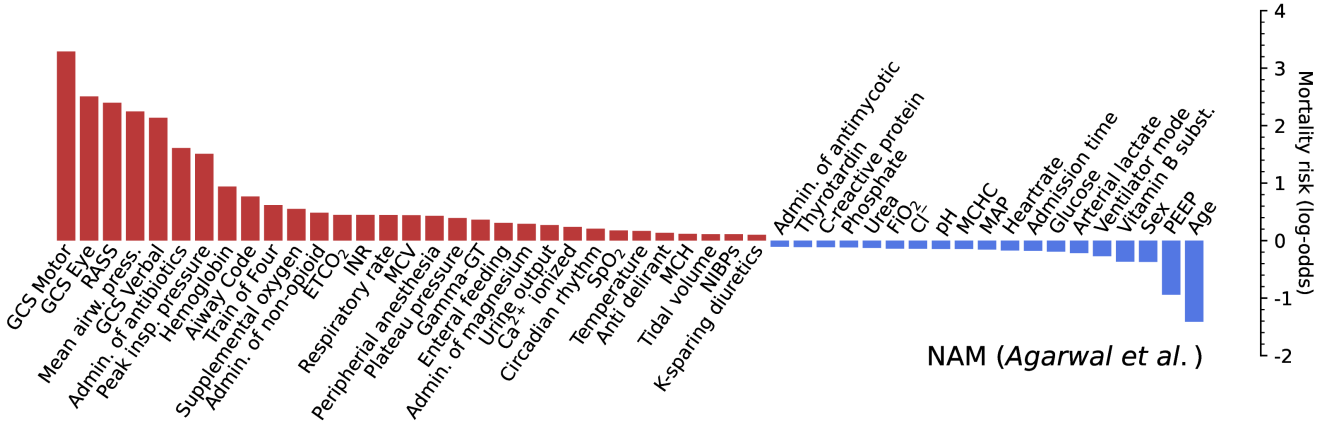
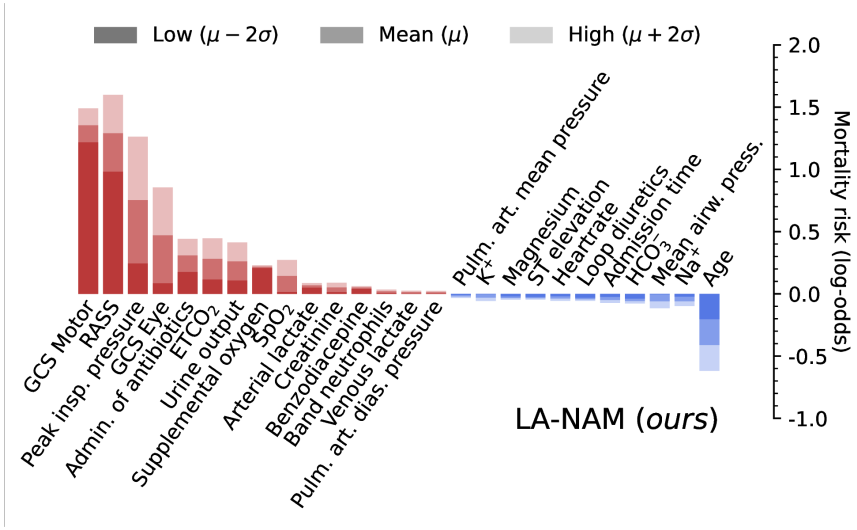


Figure: Application to MIMIC-III ICU mortality. (Fig. 2 of *Bouchiat et al., 2024*)

Laplace-approximated NAMs: MIMIC-III dataset



(a) Local predictions of NAM. (Fig. 3 of *Bouchiat et al., 2024*)



(b) Local predictions of LA-NAM. (Fig. 4 of *Bouchiat et al., 2024*)

Laplace-approximated NAMs: Feature interaction

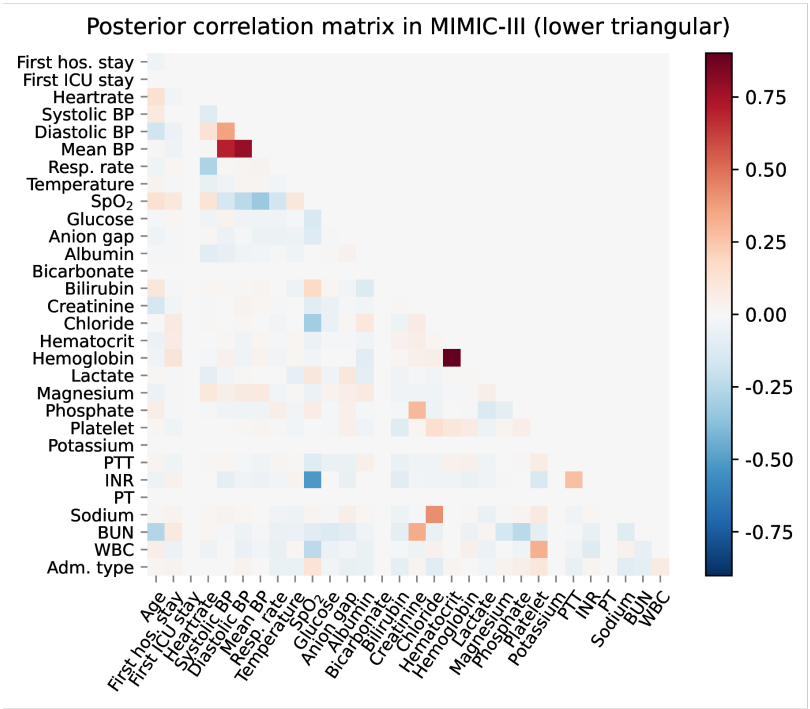
Laplace-approximated NAMs (*Bouchiat et al., 2024*): The subnetworks are not necessarily mutually independent in the true posterior distribution.

Determine mut. inf. using scalar marginal variances $\sigma_j^2, \sigma_{j'}^2$ and covariance $\sigma_{j,j'}^2$ with a last-layer Laplace approximation on output weights θ_j and $\theta_{j'}$.

$$\begin{aligned} \mathsf{I}(\boldsymbol{\theta}_j; \boldsymbol{\theta}_{j'}) &= \mathsf{H}(\boldsymbol{\theta}_j) + \mathsf{H}(\boldsymbol{\theta}_{j'}) - \mathsf{H}(\boldsymbol{\theta}_j, \boldsymbol{\theta}_{j'}) \\ &\approx \tfrac{1}{2} \log \left[\sigma_j^2 \sigma_{j'}^2 (\sigma_j^2 \sigma_{j'}^2 - \sigma_{j,j'}^2)^{-1} \right] \\ &= \tfrac{1}{2} \log \left[1 - \mathsf{Corr}(\theta_j, \theta_{j'})^2 \right]^{-1} \end{aligned}$$

Select top-k, append their $f_{\boldsymbol{\theta}_{j,j'}}^{(j,j')}(x_j, x_{j'})$ interaction subnetworks, fine-tune.

Laplace-approximated NAMs: Feature interaction



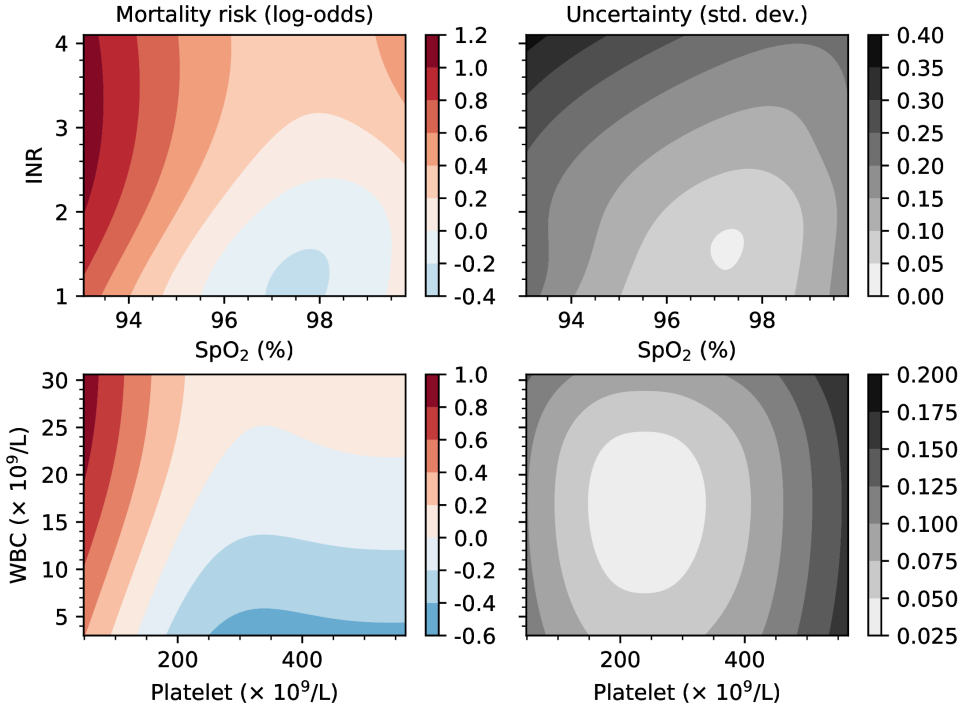


Figure: Feature interaction of LA-NAM. (Fig. 5 of *Bouchiat et al., 2024*)

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