



Accelerated Linearized Laplace Approximation for Bayesian Deep Learning

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The issues of deterministic neural networks



Which model to select?

The issues of deterministic neural networks



["Benchmarking Bayesian Deep Learning with Diabetic Retinopathy Diagnosis" by Angelos Filos et al.]

Can we trust the prediction with such confidence?

Bayesian deep learning is helpful here



Bayesian neural networks Approximate Bayesian inference



Simple yet less flexible



Variational inference

Efficient yet without the guarantee of asymptotic consistency



Non-parametric and asymptotically exact yet typically with low convergence rate

Laplace approximation Adapts a pre-trained DNN to BNN



["Laplace Redux – Effortless Bayesian Deep Learning" by Daxberger et al.]

- I. Find the maximum a posteriori (MAP) solution (the mode of Bayesian posterior) $\hat{\theta} = \arg \max_{\theta} \log p(\mathcal{D}|\theta) + \log p(\theta)$
- 2. Construct a Gaussian approximation with the Hessian of log posterior $q(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}; \hat{\boldsymbol{\theta}}, \boldsymbol{\Sigma}) \qquad \boldsymbol{\Sigma}^{-1} = -\nabla_{\boldsymbol{\theta}\boldsymbol{\theta}}^2 (\log p(\mathcal{D}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta}))|_{\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}}$
- 3. Make prediction by marginalization

The generalized Gauss-Newton (GGN) approximation and linearized LA (LLA)

Let $g_{\theta}(x)$ denote the model and set an isotropic Gaussian prior. GGN approx. sets

$$oldsymbol{\Sigma}^{-1} = \sum_i J_{oldsymbol{\hat{ heta}}}(oldsymbol{x}_i)^ op \Lambda(oldsymbol{x}_i,oldsymbol{y}_i) J_{oldsymbol{\hat{ heta}}}(oldsymbol{x}_i) + \mathbf{I}_P/\sigma_0^2,$$

where $J_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) \triangleq \nabla_{\boldsymbol{\theta}} g_{\boldsymbol{\theta}}(\boldsymbol{x})|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$ and $\Lambda(\boldsymbol{x}, \boldsymbol{y}) \triangleq -\nabla_{\boldsymbol{g}\boldsymbol{g}}^2 \log p(\boldsymbol{y}|\boldsymbol{g})|_{\boldsymbol{g}=g_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x})}$

- LLA applies LA to the first-order approximation of the NN of concern $g^{\rm lin}_{\bm{\theta}}(\bm{x}) = g_{\hat{\bm{\theta}}}(\bm{x}) + J_{\hat{\bm{\theta}}}(\bm{x})(\bm{\theta} \hat{\bm{\theta}})$
- LLA is more sensible than LA in the presence of GGN approximation [Immer et al., 22]
- LLA can perform on par with or better than popular alternatives on various uncertainty quantification (UQ) tasks
- The Laplace library [Daxberger et al., 21] further substantially advances LLA's applicability

Further approximations are required in practice!

- The GGN matrix of size P×P is still unamenable in modern DL scenarios (P is the number of parameters)
- Further approximations sparsifying the GGN are introduced:
- Diagonal and KFAC [Martens & Grosse, 15] approximations



Concern only the last-layer inference



 However, these strategies sacrifice the fidelity of the learning outcomes as the approximation errors in these cases can hardly be theoretically measured

Further approximations are required in practice!

- However, these strategies sacrifice the fidelity of the learning outcomes as the approximation errors in these cases can hardly be theoretically measured
- Our solution: accElerated Linearized Laplace Approximation (ELLA), which scales LLA up to make probabilistic predictions in a more assurable way

The inherent connections between Neural Tangent Kernels (NTKs) and LLA

• Integrating $q(\theta) = N(\theta; \theta^{2}, \Sigma)$ with the linear model $g_{\theta}^{lin}(x)$ actually gives rise to a function-space approximate posterior

 $\mathcal{GP}(f|g_{\hat{\theta}}(\boldsymbol{x}),\kappa_{\mathrm{LLA}}(\boldsymbol{x},\boldsymbol{x}')) \text{ with } \kappa_{\mathrm{LLA}}(\boldsymbol{x},\boldsymbol{x}') \triangleq J_{\hat{\theta}}(\boldsymbol{x})\boldsymbol{\Sigma}J_{\hat{\theta}}(\boldsymbol{x}')^{\top}$

- Doing some simple math, we have $\kappa_{\text{LLA}}(\boldsymbol{x}, \boldsymbol{x}') = \sigma_0^2 \Big(\kappa_{\text{NTK}}(\boldsymbol{x}, \boldsymbol{x}') - \kappa_{\text{NTK}}(\boldsymbol{x}, \mathbf{X}) [\boldsymbol{\Lambda}_{\mathbf{X}, \mathbf{Y}}^{-1} / \sigma_0^2 + \kappa_{\text{NTK}}(\mathbf{X}, \mathbf{X})]^{-1} \kappa_{\text{NTK}}(\mathbf{X}, \boldsymbol{x}') \Big)$ where $\kappa_{\text{NTK}}(\boldsymbol{x}, \boldsymbol{x}') \triangleq J_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) J_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}')^{\top}$
- The main challenge then turns into the computation and inversion of the gram matrix $\kappa_{NTK}(X, X)$ of size NC × NC

Kernel approximation of NTK enables the acceleration of LLA

• If we can approximate $\kappa_{\text{NTK}}(\mathbf{x}, \mathbf{x}')$ with the inner product of some explicit K-dim representations of the data, i.e., $\kappa_{\text{NTK}}(\mathbf{x}, \mathbf{x}') \approx \varphi(\mathbf{x}) \varphi(\mathbf{x}')^{\top}$,



then

$$\kappa_{\text{LLA}}(\boldsymbol{x}, \boldsymbol{x}') \approx \sigma_0^2 \Big(\varphi(\boldsymbol{x}) \varphi(\boldsymbol{x}')^\top - \varphi(\boldsymbol{x}) \varphi_{\mathbf{X}}^\top \Big[\mathbf{\Lambda}_{\mathbf{X}, \mathbf{Y}}^{-1} / \sigma_0^2 + \varphi_{\mathbf{X}} \varphi_{\mathbf{X}}^\top \Big]^{-1} \varphi_{\mathbf{X}} \varphi(\boldsymbol{x}')^\top \Big) \\ = \varphi(\boldsymbol{x}) \Big[\underbrace{\sum_i \varphi(\boldsymbol{x}_i)^\top \Lambda(\boldsymbol{x}_i, \boldsymbol{y}_i) \varphi(\boldsymbol{x}_i) + \mathbf{I}_K / \sigma_0^2}_{\mathbf{G}} \Big]^{-1} \varphi(\boldsymbol{x}')^\top \triangleq \kappa_{\text{ELLA}}(\boldsymbol{x}, \boldsymbol{x}') \\ \underbrace{\mathbf{G}}_{\mathbf{G}}$$

Kernel approximation Random features (RFs)





Figure 1: Approximation of the regular attention mechanism AV (before D^{-1} -renormalization) via (random) feature maps. Dashed-blocks indicate order of computation with corresponding time complexities attached.

Kernel approximation Nystrom method

• Given $\mathbf{X}_{tr} = \{ \boldsymbol{x}_1, ..., \boldsymbol{x}_N \}$ from q, perform MC integration:

$$\frac{1}{N}\sum_{n'=1}^{N}\kappa(\boldsymbol{x},\boldsymbol{x}_{n'})\psi_j(\boldsymbol{x}_{n'}) = \mu_j\psi_j(\boldsymbol{x}), \forall j \ge 1$$

- Eigendecompose $\kappa(\mathbf{X}_{\mathrm{tr}}, \mathbf{X}_{\mathrm{tr}})$ and get $\{(\hat{\mu}_j, [\hat{\psi}_j(\boldsymbol{x}_1), ..., \hat{\psi}_j(\boldsymbol{x}_N)]^{\top})\}_{j=1}^k$
- Kernelized solutions:

$$\hat{\psi}_j(\boldsymbol{x}) = \frac{1}{N\hat{\mu}_j} \sum_{n'=1}^N \kappa(\boldsymbol{x}, \boldsymbol{x}_{n'}) \hat{\psi}_j(\boldsymbol{x}_{n'}), \ j = 1, ..., k$$

Adapt Nyström method to approximate the NTKs of multi-output NNs

• Rewrite $\kappa_{NTK}(x, x')$ as a scalar-valued kernel

 $\kappa_{ ext{NTK}}\left((oldsymbol{x},i),(oldsymbol{x}',i')
ight) \,=\, J_{\hat{oldsymbol{ heta}}}(oldsymbol{x},i) J_{\hat{oldsymbol{ heta}}}(oldsymbol{x}',i')^ op$

By definition, the eigenfunctions can represent the spectral information of the kernel:

$$\int \kappa_{\text{NTK}}\left((\boldsymbol{x},i),(\boldsymbol{x}',i')\right)\psi_k(\boldsymbol{x}',i')q(\boldsymbol{x}',i')=\mu_k\psi_k(\boldsymbol{x},i),\forall k\geq 1,$$

while being orthonormal under q:

$$\int \psi_k(\boldsymbol{x},i)\psi_{k'}(\boldsymbol{x},i)q(\boldsymbol{x},i) = \mathbb{1}[k=k'], \forall k,k' \geq 1.$$

By Monte Carlo estimation

$$\frac{1}{M}\sum_{m=1}^{M}\kappa_{\text{NTK}}\left((\boldsymbol{x},i),(\boldsymbol{x}_{m},i_{m})\right)\psi_{k}(\boldsymbol{x}_{m},i_{m})=\mu_{k}\psi_{k}(\boldsymbol{x},i),\forall k\in[K]$$

Adapt Nyström method to approximate the NTKs of multi-output NNs

• Applying this equation to the above samples gives rise to

$$\frac{1}{M}\sum_{m=1}^{M}\kappa_{\text{NTK}}\left((\boldsymbol{x}_{m'}, i_{m'}), (\boldsymbol{x}_{m}, i_{m})\right)\psi_{k}(\boldsymbol{x}_{m}, i_{m}) = \mu_{k}\psi_{k}(\boldsymbol{x}_{m'}, i_{m'}), \forall k \in [K], m' \in [M]$$

then we arrive at

$$rac{1}{M} \mathbf{K} oldsymbol{\psi}_k pprox \mu_k oldsymbol{\psi}_k, k \in [K]$$

• We compute the top-K eigenvalues λ_1 , ..., λ_K of matrix K and record the corresponding orthonormal eigenvectors u_1 , ..., u_K . Then it is easy to get the Nyström approximation of the top-K eigenfunctions:

$$\hat{\psi}_k(\boldsymbol{x}, i) = \frac{\sqrt{M}}{\lambda_k} \sum_{m=1}^M \boldsymbol{u}_k^{(m)} \kappa_{\text{NTK}}\left((\boldsymbol{x}, i), (\boldsymbol{x}_m, i_m)\right) = \frac{\sqrt{M}}{\lambda_k} J_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}, i) \mathbf{J}_{\hat{\boldsymbol{\theta}}, \tilde{\mathbf{X}}}^\top \boldsymbol{u}_k$$

• Finally, we have

$$arphi(oldsymbol{x}) = [J_{oldsymbol{\hat{ heta}}}(oldsymbol{x})oldsymbol{v}_{1},...,J_{oldsymbol{\hat{ heta}}}(oldsymbol{x})oldsymbol{v}_{K}] ext{ with }oldsymbol{v}_{k} = \mathbf{J}_{oldsymbol{\hat{ heta}}, ilde{\mathbf{X}}}^{ op}oldsymbol{u}_{k}/\sqrt{\lambda_{k}}$$

Implementation

 The estimation of φ on a data point x degenerates as K JVPs, which can be accomplished by invoking forward mode automatic differentiation (fwAD) for K times:

$$egin{pmatrix} egin{aligned} egin{aligned} egin{aligned} egin{aligned} egin{aligned} forward & & g_{eta}(oldsymbol{x}) \ oldsymbol{v}_k \end{pmatrix} & & \longrightarrow & g_{eta}(oldsymbol{x}) \ oldsymbol{J}_{eta}(oldsymbol{x}) oldsymbol{v}_k, \ k \in [K] \end{aligned}$$

where the model output $g_{\theta^{\uparrow}}(x)$ and the JVP $J_{\theta^{\uparrow}}(x)v_k$ are simultaneously computed in one single forward pass

• Prevalent DL libraries like PyTorch and Jax have already been armed with the capability for fwAD

Algorithms

Algorithm 1: Build the LLA posterior. # $g_{\hat{a}}$: NN pre-trained by MAP; (\mathbf{X}, \mathbf{Y}) : # training set; C: number of classes # M, K, σ_0^2 : hyper-parameters def estimate_G(φ ,X,Y,K, σ_0^2): $\mathbf{G} = \mathbf{zeros}(K, K)$ for (x, y) in (\mathbf{X}, \mathbf{Y}) : $q_x, \varphi_x = \varphi(x)$ $\Lambda_{x,y} = \text{hessian}(\text{nll}(g_x,y),g_x)$ $\mathbf{G} \mathrel{+}= \boldsymbol{\varphi}_{\boldsymbol{x}}^{\top} \boldsymbol{\Lambda}_{\boldsymbol{x},\boldsymbol{y}} \boldsymbol{\varphi}_{\boldsymbol{x}}$ return G+ eye(K) $/\sigma_0^2$ def _q_f(φ , G⁻¹, x) $q_x, \varphi_x = \varphi(x)$ $\boldsymbol{\kappa_{x,x}} = \boldsymbol{arphi_x} \mathbf{G}^{-1} \boldsymbol{arphi_x}^{ op}$ return $\mathcal{N}(\boldsymbol{q}_{\boldsymbol{x}},\boldsymbol{\kappa}_{\boldsymbol{x}|\boldsymbol{x}})$ $\varphi = \text{build}_{\varphi}(g_{\hat{\theta}}, \mathbf{X}, C, M, K)$ $\mathbf{G}^{-1} = \texttt{inv}(\texttt{estimate}_{\mathbf{G}}(\varphi, \mathbf{X}, \mathbf{Y}, K, \sigma_0^2))$ $q_f = partial(_q_f, \varphi, G^{-1})$

Algorithm 2: Build φ .

```
def build_\varphi(g_{\hat{\theta}}, \mathbf{X}, C, M, K):
          def _\varphi(q_{\hat{\rho}}, C, \{v_k\}_{k=1}^K, x):
                    \varphi_x = \operatorname{zeros}(C, K)
                    for k in range(K):
                              with fwAD.enable():
                                        oldsymbol{g}_{oldsymbol{x}},oldsymbol{j}oldsymbol{v}oldsymbol{p}=oldsymbol{g}_{(\hat{oldsymbol{	heta}},oldsymbol{v}_{k})}(oldsymbol{x})
                              \varphi_{\boldsymbol{x}}[:,k] = \boldsymbol{j}\boldsymbol{v}\boldsymbol{p}
                    \texttt{return} \, \boldsymbol{g_x}, \boldsymbol{\varphi_x}
         \mathbf{J}_{\hat{\boldsymbol{	heta}}, \tilde{\mathbf{X}}} = \operatorname{zeros}(M, \dim(\hat{\boldsymbol{	heta}}))
          for m in range(M):
                    x_m = uniform_sample(X)
                    i_m = uniform_sample([C])
                    \mathbf{J}_{\hat{\boldsymbol{	heta}} \ \tilde{\mathbf{X}}}[m] = \texttt{grad}(g_{\hat{\boldsymbol{	heta}}}(\boldsymbol{x}_m)[i_m], \hat{\boldsymbol{	heta}})
          \{\lambda_k, \boldsymbol{u}_k\}_{k=1}^K = \texttt{eig}(\mathbf{J}_{\hat{\boldsymbol{	heta}}, \tilde{\mathbf{X}}} \mathbf{J}_{\hat{\boldsymbol{	heta}}, \tilde{\mathbf{X}}}^{	op}, top = K)
          for k in range(K):
                    oldsymbol{v}_k = \mathbf{J}_{\hat{oldsymbol{	heta}}}^{	op} oldsymbol{u}_k / \sqrt{\lambda_k}
          return partial (_\varphi, g_{\hat{\theta}}, C, {v_k}_{k=1}^K)
```

Theoretical Analysis

 $\kappa_{\text{ELLA}} \text{ can be reformulated as follows (in the seek of theoretical analysis)} \\ \kappa_{\text{ELLA}}(\boldsymbol{x}, \boldsymbol{x}') = J_{\hat{\theta}}(\boldsymbol{x}) \underbrace{\mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{\top} \left[\mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}} \mathbf{J}_{\hat{\theta}, \mathbf{X}}^{\top} \mathbf{\Lambda}_{\mathbf{X}, \mathbf{Y}} \mathbf{J}_{\hat{\theta}, \mathbf{X}} \mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{\top} + \mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}} \mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{\top} J_{\hat{\theta}, \tilde{\mathbf{X}}}^{-1} \mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}}_{\mathbf{\Sigma}'} J_{\hat{\theta}}(\boldsymbol{x})^{\top} \underbrace{\mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{\top} \left[\mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{\top} \mathbf{J}_{\hat{\theta}, \mathbf{X}}^{\top} \mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{\top} + \mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{\top} \mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{\top} J_{\hat{\theta}, \tilde{\mathbf{X}}}^{-1} \mathbf{J}_{\hat{\theta}, \tilde{\mathbf{X}}}^{-1} \mathbf{$

Theorem 1 (Proof in Appendix A.4). Let c_{Λ} be a finite constant associated with Λ , and \mathcal{E}' the error of Nyström approximation $\|\mathbf{J}_{\hat{\theta},\mathbf{X}}\mathbf{J}_{\hat{\theta},\tilde{\mathbf{X}}}^{\top}(\mathbf{J}_{\hat{\theta},\tilde{\mathbf{X}}}\mathbf{J}_{\hat{\theta},\tilde{\mathbf{X}}}^{\top})^{-1}\mathbf{J}_{\hat{\theta},\tilde{\mathbf{X}}}\mathbf{J}_{\hat{\theta},\mathbf{X}}^{\top} - \mathbf{J}_{\hat{\theta},\mathbf{X}}\mathbf{J}_{\hat{\theta},\mathbf{X}}^{\top}\|$. It holds that $\mathcal{E} \leq \sigma_{0}^{4}c_{\Lambda}\mathcal{E}' + \sigma_{0}^{2}$.

Theorem 2 (Error bound of Nyström approximation). With probability at least $1 - \delta$, it holds that:

$$\mathcal{E}' \leq \tilde{\lambda}_{M+1} + \frac{NC}{\sqrt{M}} c_{\kappa} (2 + \log \frac{1}{\delta}).$$

Corollary 1. With probability at least $1 - \delta$, the following bound exists:

$$\mathcal{E} \leq \sigma_0^4 c_\Lambda (\tilde{\lambda}_{M+1} + rac{NC}{\sqrt{M}} c_\kappa (2 + \log rac{1}{\delta})) + \sigma_0^2.$$

 As desired, the upper bound of approximation error decreases along with the growing of the number of MC samples in Nystrom approximation

How the approximation errors vary w.r.t. K and M? (MNIST, CNNs)



The overfitting issue of ELLA and general LLA (Cifar-10, ResNets)

$$oldsymbol{\Sigma}^{-1} = \sum_i J_{\hat{oldsymbol{ heta}}}(oldsymbol{x}_i)^ op \Lambda(oldsymbol{x}_i,oldsymbol{y}_i) J_{\hat{oldsymbol{ heta}}}(oldsymbol{x}_i) + \mathbf{I}_P/\sigma_0^2$$

With more training data involved, the covariance in LA, LLA, and ELLA shrinks and the uncertainty dissipates.



Solution: early stopping

Illustrative Regression



Figure 1: 1-D regression on $y = \sin 2x + \epsilon$, $\epsilon \sim \mathcal{N}(0, 0.2)$. Red dots, central blue curves, and shaded regions refer to the training data, mean predictions, and uncertainty respectively. The model is a pretrained multilayer perceptron (MLP) with 3 hidden layers. As shown, the predictive uncertainty of ELLA is on par with or better than the competitors such as LLA with KFAC approximation (LLA-KFAC), LLA with diagonal approximation (LLA-Diag), and last-layer LLA (LLA^{*}).

Cifar-10 classification

Table 1: Comparison on test accuracy (%) \uparrow , NLL \downarrow , and ECE \downarrow on CIFAR-10. We report the average results over 5 random runs. As the accuracy values of most methods are close, we do not highlight the best.

Method	ResNet-20			ResNet-32			ResNet-44			ResNet-56		
	Acc.	NLL	ECE									
ELLA	92.5	0.233	0.009	93.5	0.215	0.008	93.9	0.204	0.007	94.4	0.187	0.007
MAP	92.6	0.282	0.039	93.5	0.292	0.041	94.0	0.275	0.039	94.4	0.252	0.037
MFVI-BF	92.7	0.231	0.016	93.5	0.222	0.020	93.9	0.206	0.018	94.4	0.188	0.016
LLA^*	92.6	0.269	0.034	93.5	0.259	0.033	94.0	0.237	0.028	94.4	0.213	0.022
LLA*-KFAC	92.6	0.271	0.035	93.5	0.260	0.033	94.0	0.232	0.028	94.4	0.202	0.024
LLA-Diag	92.2	0.728	0.404	92.7	0.755	0.430	92.8	0.778	0.445	92.9	0.843	0.480
LLA-KFAC	92.0	0.852	0.467	91.8	1.027	0.547	91.4	1.091	0.566	89.8	1.174	0.579



Figure 3: NLL (Left) and ECE (Right) on CIFAR-10 corruptions for models trained with ResNet-56 architecture. Each box corresponds to a summary of the results across 19 types of skew.

ImageNet classification

Table 2: Comparison on test accuracy (%) \uparrow , NLL \downarrow , and ECE \downarrow on ImageNet. We report the average results over 3 random runs.

Method	ResNet-18			ResNet-34			ResNet-50		
	Acc.	NLL	ECE	Acc.	NLL	ECE	Acc.	NLL	ECE
ELLA	69.8	1.243	0.015	73.3	1.072	0.018	76.2	0.948	0.018
MAP	69.8	1.247	0.026	73.3	1.081	0.035	76.2	0.962	0.037
MFVI-BF	70.3	1.218	0.042	73.7	1.043	0.033	76.1	0.945	0.030



Figure 5: NLL (Left) and ECE (Right) on ImageNet corruptions for models trained with ViT-B architecture. Each box corresponds to a summary of the results across 19 types of skew.

	Method	Acc.	NLL	ECE
Results on ViT	ELLA	81.6	0.695	0.022
	MAP	81.5	0.700	0.039





Thanks!