Variational Linearized Laplace Approximation for Bayesian Deep Learning

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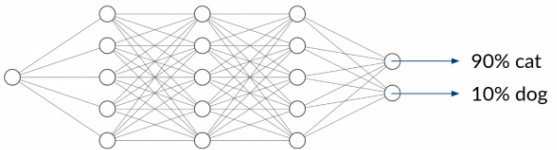
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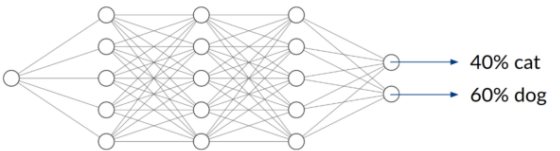
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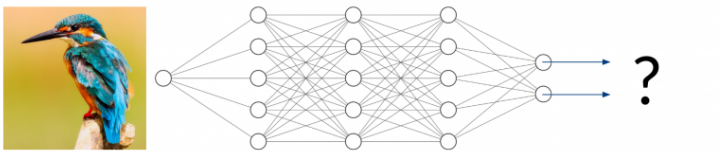
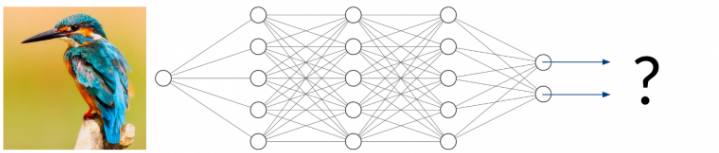
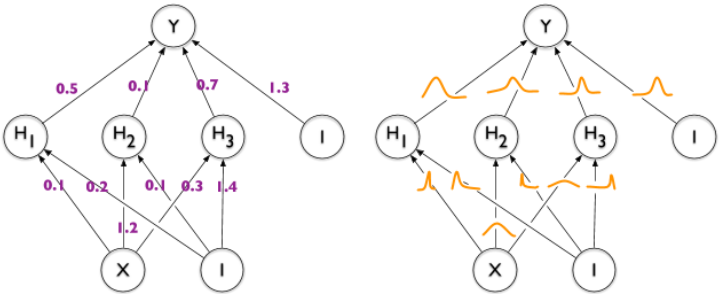




Deep learning methods are unable to quantify the uncertainty of their predictions!

Straight-forward solution: Using a Bayesian model.



Making predictions requires the posterior over the parameters of the model $\boldsymbol{\theta}$:

$$P(y^\star|\mathbf{x}^\star, \mathcal{D}) = \int P(y^\star|\mathbf{x}^\star, \boldsymbol{\theta}) P(\boldsymbol{\theta}|\mathcal{D}) \, d\boldsymbol{\theta}$$

where $P(\boldsymbol{\theta}|\mathcal{D})$ is **intractable for complex models**.

Approximate $P(\boldsymbol{\theta}|\mathcal{D})$ by something simpler $Q(\boldsymbol{\theta})$.

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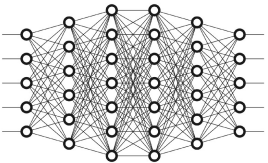
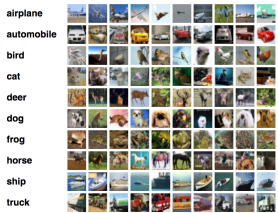
Poor performance of the model in many cases.

Laplace Approximation for Deep Learning

Deep Model



Dataset



Optimal parameter $\hat{\boldsymbol{\theta}}$ using deep learning techniques.

Given the optimal parameters $\hat{\boldsymbol{\theta}}$, we aim to make **uncertainty estimation** on the pre-trained model.

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Laplace approximation (LA) of $P(\boldsymbol{\theta}|\mathcal{D})$ centered on $\hat{\boldsymbol{\theta}}$ as

$$P(\boldsymbol{\theta}|\mathcal{D}) \approx Q(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}|\hat{\boldsymbol{\theta}}, \boldsymbol{\Sigma})$$

where

$$\boldsymbol{\Sigma}^{-1} = -\nabla^2_{\boldsymbol{\theta}\boldsymbol{\theta}} \log P(\boldsymbol{\theta}|\mathcal{D})_{|\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} = -\nabla^2_{\boldsymbol{\theta}\boldsymbol{\theta}} (\log P(\mathcal{D}|\boldsymbol{\theta}) + \log P(\boldsymbol{\theta}))_{|\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$$

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where applying the generalized Gauss-Newton matrix approximation

$$\boldsymbol{\Sigma}^{-1} \approx \tilde{\boldsymbol{\Sigma}}^{-1} = \sum_{n=1}^{N} \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{x}_n) \Lambda(\mathbf{x}_n, y_n) \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{x}_n)^T + \frac{1}{\sigma_0^2} \boldsymbol{I}_P \,.$$

with

$$\mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{x}_n) = \nabla_{\boldsymbol{\theta}} g(\mathbf{x}_n, \boldsymbol{\theta})_{|\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} \quad \Lambda(\mathbf{x}_n, y_n) = -\nabla^2_{\mathbf{gg}} \log P(y_n|\mathbf{g})_{|\mathbf{g}=g(\mathbf{x}_n,\hat{\boldsymbol{\theta}})}$$

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$$\Downarrow$$

There is a shift between the posterior and the predictive distribution.

$$Q(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}|\hat{\boldsymbol{\theta}}, \tilde{\boldsymbol{\Sigma}}) \quad P(y^\star|\mathbf{x}^\star, \mathcal{D}) \approx \mathbb{E}_{Q(\boldsymbol{\theta})}\left[P(y^\star|g(\mathbf{x}^\star, \boldsymbol{\theta}))\right]$$

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The GGN approximation, is the true posterior of a linearized model

$$g^{lin}(\mathbf{x}, \boldsymbol{\theta}) = g(\mathbf{x}, \hat{\boldsymbol{\theta}}) + \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{x}_n)^T(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$$

Which means, that predictions should be made over the linearized model:

$$P(y^\star|\mathbf{x}^\star, \mathcal{D}) \approx \mathbb{E}_{Q(\boldsymbol{\theta})}\left[P(y^\star|g^{lin}(\mathbf{x}^\star, \boldsymbol{\theta}))\right]$$

The **linearized Laplace approximation** (LLA) is equivalent to a **Gaussian Process**.

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Prior distribution

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Gaussian Process

$$m(\mathbf{x}) = g^{lin}(\mathbf{x}, \boldsymbol{m})$$
$$K(\mathbf{x}, \mathbf{x}') = \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{x})^T \boldsymbol{S} \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{x}')$$

Using LLA approximate posterior

$$Q(\boldsymbol{\theta}) = \mathcal{N}(\hat{\boldsymbol{\theta}}, \tilde{\boldsymbol{\Sigma}})$$

$$\Downarrow$$

Gaussian Process

$$m^\star(\mathbf{x}) = g^{lin}(\mathbf{x}, \hat{\boldsymbol{\theta}})$$

$$K^\star(\mathbf{x}, \mathbf{x}') = \sigma_0^2 \left(\kappa(\mathbf{x}, \mathbf{x}') - \kappa(\mathbf{x}, \mathbf{X}) \left(\frac{1}{\sigma_0^2} \boldsymbol{\Lambda}_{\mathbf{X},\mathbf{y}}^{-1} + \kappa(\mathbf{X}, \mathbf{X}) \right)^{-1} \kappa(\mathbf{X}, \mathbf{x}') \right).$$

where $\kappa(\mathbf{x}, \mathbf{x}') = \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{x})^T \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{x}')$.

Main idea: Approximate the exact GP posterior using a sparse approach with inducing points.

Main inconvenience: Using a sparse GP **changes the predictive mean**, loosing the pre-trained solution.

Solution: Use a Generalized Sparse GP in the RKHS.

Dual representation of Gaussian Processes

An RKHS $\mathcal{H}$ is a Hilbert space of functions satisfying the reproducing property: $\forall \mathbf{x} \in \mathcal{X}\ \exists \phi_{\mathbf{x}} \in \mathcal{H}$ such that $\forall f \in \mathcal{H}, f(\mathbf{x}) = \langle \phi_{\mathbf{x}}, f \rangle$.

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A **Gaussian process** $\mathcal{GP}(m, K)$ has a dual representation in a RKHS as: there exists $\mu \in \mathcal{H}$ and a linear semi-definite positive operator $\Sigma : \mathcal{H} \to \mathcal{H}$ such that, for any $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$, $\exists \phi_{\mathbf{x}}, \phi_{\mathbf{x}'}$, verifying

$$m(\mathbf{x}) = \langle \phi_{\mathbf{x}}, \mu \rangle \,, \quad K(\mathbf{x}, \mathbf{x}') = \langle \phi_{\mathbf{x}}, \Sigma(\phi_{\mathbf{x}'}) \rangle$$

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As an abuse of notation, we write $f \sim \mathcal{N}(\mu, \Sigma)$, which is a Gaussian measure in the RKHS.

Theorem (Cheng and Boots, 2016). Using a sparse GP approximation with variational distribution $q(\mathbf{f}, \mathbf{u}) = p(\mathbf{f}|\mathbf{u})q(\mathbf{u})$ is equivalent to restricting the mean and covariance functions of the dual representation in the RKHS to

$$\tilde{\mu} = \Phi_{\mathbf{Z}}(\boldsymbol{a}) \quad \text{and} \quad \tilde{\Sigma} = I + \Phi_{\mathbf{Z}} \boldsymbol{A} \Phi_{\mathbf{Z}}^T ,$$

where $\Phi_{\mathbf{Z}} : \mathbb{R}^M \to \mathcal{H}$ is defined as $\Phi_{\mathbf{Z}}(\boldsymbol{a}) = \sum_{m=1}^M a_m \phi_{\mathbf{z}_m}$, $\boldsymbol{a} \in \mathbb{R}^M$ and $\Phi_{\mathbf{Z}} \boldsymbol{A} \Phi_{\mathbf{Z}}^T = \sum_{i=1}^M \sum_{j=1}^M \phi_{\mathbf{z}_i} A_{i,j} \phi_{\mathbf{z}_j}^T$, $\boldsymbol{A} \in \mathbb{R}^{M \times M}$ such that $\tilde{\Sigma} \geq 0$.

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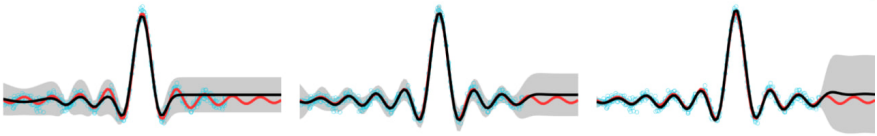

(a) $M = 10$ (b) $M_\alpha = 100, M_\beta = 10$ (c) $M = 100$

Comparison between models with shared and decoupled basis.

- (a)(c) denote the models with shared basis of size M.
- (b) denotes the model of decoupled basis with size (M_α, M_β).

For any function $t \in \mathcal{H}$, and $\epsilon > 0$, there exists a set of points $\mathbf{Z}_\alpha \subset \mathcal{X}$ and coefficients $\boldsymbol{a}$, such that

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We can fit the mean of the posterior distribution of the sparse decoupled GP to any function in the Hilbert space ($g(\cdot, \hat{\boldsymbol{\theta}})$).

If $g(\cdot, \hat{\boldsymbol{\theta}}) \notin \mathcal{H}$, we can use that $\mathcal{H}$ is dense in the span of the Gaussian Process.

Proposition. If $g(\cdot, \hat{\boldsymbol{\theta}}) \in \mathcal{H}$, $\forall \epsilon > 0$, there exists a set of M_α inducing points $\mathbf{Z}_\alpha \subset \mathcal{X}$ and $\boldsymbol{a} \in \mathbb{R}^{M_\alpha}$ such that the dual representation in the RKHS of the corresponding sparse Gaussian process defined by

$$\tilde{\mu} = \Phi_{\mathbf{Z}_\alpha}(\boldsymbol{a}) \quad \text{and} \quad \tilde{\Sigma} = (I + \Phi_{\mathbf{Z}_\beta} \boldsymbol{A} \Phi_{\mathbf{Z}_\beta}^T)^{-1} \,,$$

corresponds to a posterior approximation $\mathcal{GP}(m^\star, K^\star)$ with mean and covariance functions defined as

$$\begin{aligned} m^\star(\mathbf{x}) &= h_\epsilon(\mathbf{x}) \,, \\ K^\star(\mathbf{x}, \mathbf{x}') &= K(\mathbf{x}, \mathbf{x}') - K_{\mathbf{x}, \mathbf{Z}_\beta} (\boldsymbol{A}^{-1} + K_{\mathbf{Z}_\beta})^{-1} K_{\mathbf{Z}_\beta, \mathbf{x}'} \,, \end{aligned}$$

where $\mathbf{Z}_\beta \subset \mathcal{X}$ is a set of M_β inducing points, $\boldsymbol{A} \in \mathbb{R}^{M_\beta \times M_\beta}$ such that $\tilde{\Sigma} \geq 0$ and h_ϵ verifies $d_{\mathcal{H}}(g(\cdot, \hat{\boldsymbol{\theta}}), h_\epsilon) \leq \epsilon$.

Optimizing the ELBO in the Hilbert space:

$$\begin{aligned}\max_{q(f),\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{\theta}}(q(f)) &= \max_{q(f),\boldsymbol{\theta}} \int q(f) \log \frac{p_{\boldsymbol{\theta}}(y|f)p(f)}{q(f)} df \\ &= \max_{q(f),\boldsymbol{\theta}} \mathbb{E}_q \left[\log p_{\boldsymbol{\theta}}(y|f)\right] - \mathsf{KL}\left(q \mid p\right) \ .\end{aligned}$$

where

$$\mathsf{KL}\left(q \mid p\right) = \frac{1}{2}\boldsymbol{a}^T \boldsymbol{K}_\alpha \boldsymbol{a} + \frac{1}{2}\log|\boldsymbol{I} + \boldsymbol{K}_\beta \boldsymbol{A}| - \frac{1}{2}\mathrm{tr}\left(\boldsymbol{K}_\beta (\boldsymbol{A}^{-1} + \boldsymbol{K}_\beta)^{-1}\right)$$

Intuitive Recap

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1. The Linearized Laplace Approximation is equivalent to a GP.
2. Sparse approach based on inducing points to approximate the posterior GP.
3. Separate the inducing locations from the mean and covariance.
4. Use "*infinite*" inducing points for the mean. Fixing the mean to the pre-trained MAP solution.
5. The resulting method does scale with the number of parameters and the dataset size (mini-batch optimization).

ELLA

Another existing sparse approximation is ELLA.

1. Approximated the kernel matrix of the full dataset using a random subset of it.

$$\hat{\mathbf{X}} \subset \mathbf{X} \implies \hat{\boldsymbol{K}} = \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\hat{\mathbf{X}})\mathcal{J}_{\hat{\boldsymbol{\theta}}}(\hat{\mathbf{X}})^T \approx \boldsymbol{K} = \mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{X})\mathcal{J}_{\hat{\boldsymbol{\theta}}}(\mathbf{X})^T$$

2. Finds eigen-decomposition of $\hat{\boldsymbol{K}}$ to create lower-dimensional features $\phi(\mathbf{x})$.
3. Use these features to approximate the true covariance matrix $\boldsymbol{K}$.
4. Requires an unique iteration over the whole training dataset.

Preliminary results

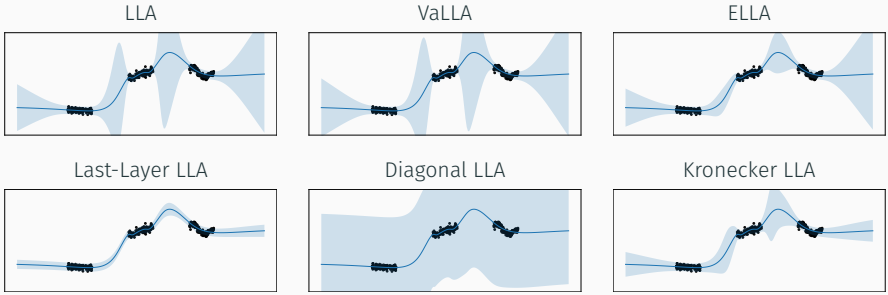
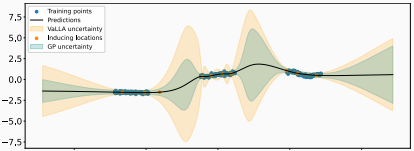


Figure 1: Predictive distribution (two times the standard deviation) on a toy 1D regression dataset with a 2 hidden layer MLP with 50 units.

VaLLA $M = 10$



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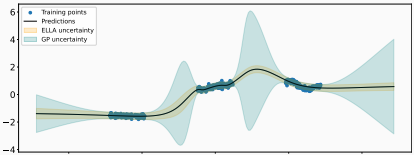
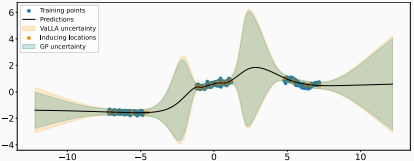
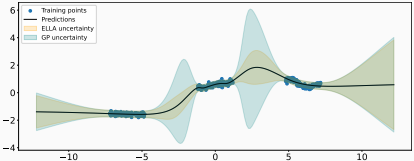


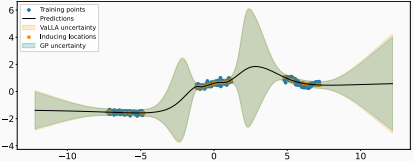
VaLLA $M = 20$



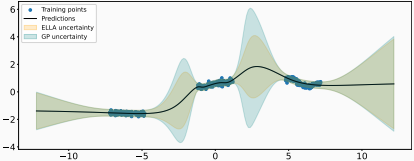
ELLA $M = 20$



VaLLA $M = 30$



ELLA $M = 30$



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2. The decoupled definition can be used to fix the mean of the GP to the pre-trained MAP solution.
3. Stochastic optimization can be employed to train the model.
4. As a result, VaLLA is scalable in both parameters and dataset size.
5. The obtained preliminary results show competitive uncertainty estimation compared to other LLA approximations.

Thank you for your attention!

- Cheng, Ching-An and Byron Boot (2017). “Variational inference for Gaussian process models with linear complexity”. In: *Advances in Neural Information Processing Systems* 30.
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