Probabilistic Machine Learning
Lecture 17
Probabilistic Deep Learning

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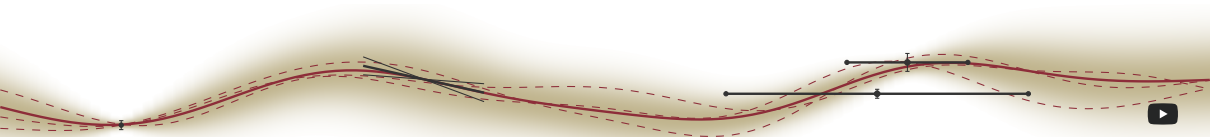


For our purposes, a **deep neural network** is a function

$$f(\boldsymbol{x}, \boldsymbol{\theta}) : \mathbb{X} \times \mathbb{R}^D \to \mathbb{R}^F$$

parametrized by *parameters* $\boldsymbol{\theta} \in \mathbb{R}^D$ and mapping inputs $\boldsymbol{x} \in \mathbb{X}$ to outputs $f(\boldsymbol{x}, \boldsymbol{\theta}) \in \mathbb{R}^F$. The network is trained by **empirical risk minimization** (ERM), to find parameters $\boldsymbol{\theta}_*$ on a training set $\mathcal{D} = [(x_i, y_i)]_{i=1,\dots,N}$

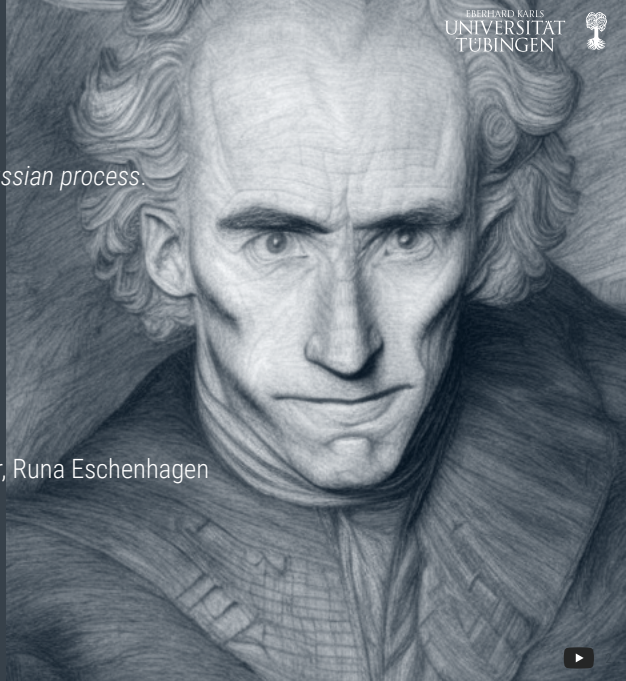
$$\boldsymbol{\theta}_* = \arg\min_{\boldsymbol{\theta} \in \mathbb{R}^D} \underbrace{\mathcal{L}(\boldsymbol{\theta})}_{\text{Loss}} = \arg\min_{\boldsymbol{\theta} \in \mathbb{R}^D} \left(\frac{1}{N} \sum_{i=1}^{N} \underbrace{\ell(y_i; \overbrace{f(x_i, \boldsymbol{\theta})}^{\text{deep net}})}_{\text{empirical risk}} + \underbrace{r(\boldsymbol{\theta})}_{\text{regularizer}} \right).$$

Today:

How to turn *any* deep network into a *Gaussian process*.

Courtesy of

- Pierre-Simon, Marquis de Laplace, 1810
- David JC MacKay, 1998
- Emtiyaz Khan, 2019
- Agustinus Kristiadi, 2020
- Alex Immer, 2021
- Matthias Bauer, Vincent Fortuin, Eric Daxberger, Runa Eschenhagen
- and many others whose papers I missed



Deep networks *are* GPs

1. Realise that the loss is a **negative log-posterior**

$$\mathcal{L}(\boldsymbol{\theta}) = \left(\frac{1}{N} \sum_{i=1}^{N} \underbrace{\ell(y_i; \overbrace{f(x_i, \boldsymbol{\theta})}^{\text{deep net}})}_{\text{empirical risk}} + \underbrace{r(\boldsymbol{\theta})}_{\text{regularizer}} \right) = -\sum_{i=1}^{N} \log p(\boldsymbol{y} \mid \boldsymbol{\theta}) - \log p(\boldsymbol{\theta}) = -\log p(\boldsymbol{\theta} \mid \boldsymbol{y}) + \text{const.}$$

2. **Train the deep net *as usual*** to find $\boldsymbol{\theta}_* = \arg\max_{\boldsymbol{\theta} \in \mathbb{R}^D} p(\boldsymbol{\theta} \mid \boldsymbol{y})$
3. At $\boldsymbol{\theta}_*$, compute a **Laplace approximation** of the log-posterior, with $\Psi := -\nabla\nabla^\intercal \log p(\boldsymbol{\theta}_* \mid \boldsymbol{y})$

$$\log p(\boldsymbol{\theta} \mid \boldsymbol{y}) + \text{const.} = \mathcal{L}(\boldsymbol{\theta}) \approx \mathcal{L}(\boldsymbol{\theta}_*) + 1/2(\boldsymbol{\theta} - \boldsymbol{\theta}_*)^\intercal \Psi (\boldsymbol{\theta} - \boldsymbol{\theta}_*) = \log \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\theta}_*, -\Psi^{-1})$$

4. **Linearize** $f(\boldsymbol{x}, \boldsymbol{\theta})$ around θ_*, with $[J(\boldsymbol{x})]_{ij} = \frac{\partial f_i(\boldsymbol{x}, \boldsymbol{\theta}_*)}{\partial \theta_j}$ as $f(\boldsymbol{x}, \boldsymbol{\theta}) \approx f(\boldsymbol{x}, \boldsymbol{\theta}_*) + J(\boldsymbol{x}, \boldsymbol{\theta}_*)(\boldsymbol{\theta} - \boldsymbol{\theta}_*)$

$$\text{thus } p(f(\bullet) \mid \mathcal{D}) = \int p(f \mid w)\, dp(w) \approx \mathcal{GP}(f(\bullet); f(\bullet, \boldsymbol{\theta}_*), -J(\bullet)\Psi^{-1}J(\circ)) \quad \text{with}$$

$$\mathbb{E}(f(\bullet)) = f(\bullet, \boldsymbol{\theta}_*) \qquad \text{the trained net as the mean function}$$

$$\text{cov}(f(\bullet), f(\circ)) = -J(\bullet)\Psi^{-1}J(\circ)^\intercal \qquad \text{the Laplace tangent kernel as the covariance function}$$

Another Look

What are the computational steps necessary?

$$p(f(\bullet) \mid \mathcal{D}) = \mathcal{GP}(f(\bullet);\ \underbrace{f(\bullet, \boldsymbol{\theta}_*)}_{\text{trained network}},\ \underbrace{-J(\bullet)\Psi^{-1}J(\circ)^\intercal}_{\text{Laplace tangent kernel}})$$

Overhead:

- At **Train Time**: After training is completed, compute

$$\Psi \in \mathbb{R}^{D\times D} = \nabla_\theta \nabla_\theta^\intercal \mathcal{L} = \nabla_\theta \nabla_\theta \left(\frac{1}{N} \sum_{i=1}^{N} \ell(y_i; f(x_i, \boldsymbol{\theta})) + r(\boldsymbol{\theta}) \right)$$

  and its matrix-decomposition.

- At **Test Time**: For a new input $\boldsymbol{x}$, compute *backward pass* in addition to forward pass, to get

$$J(\boldsymbol{x}) = \nabla_\theta f(\boldsymbol{x}, \boldsymbol{\theta}_*)$$

Code

Laplace Approximations for Deep Learning

What's to like?

If you are a deep learning person…

- you get to keep your beloved point estimate $f(\bullet, \boldsymbol{\theta}_*)$
- you get to keep your beloved training procedure. Laplace is constructed *post-hoc*, even for pre-trained networks downloaded from the net (assuming model, data, and loss are available)
- you need only *auto-diff* and *numerical linear algebra*. No sampling, no stochasticity, no ensembles
- But the result is a GP, with all the trimmings (evidence, sampling, sparse decompositions, etc.)!

Laplace Approximations for Deep Learning

Challenges

- Hessian decomposition is $\mathcal{O}(D^3)$. But there are approximations. It's linear algebra!
- Laplace approximations are local. They can be "arbitrarily wrong" to the full posterior.
  - but they're still better than a point estimate!
  - and the loss functions of deep learning where never constructed to be good generative models in the first place!

The Laplace Tangent kernel

Some context

Whence the name?

- Jacot, Gabriel, Hongler, NeurIPS 219 introduce the *Neural tangent kernel*

$$k(\bullet, \circ) = J_{\theta_0}(\bullet) J_{\theta_0}^\intercal(\circ) = \sum_{d=1}^{D} \frac{\partial f_i(\bullet, \theta_0)}{\partial [\theta_0]_d} \frac{\partial f_j(\bullet, \theta_0)}{\partial [\theta_0]_d}$$

But they *do not make any connection to manifolds or tangents!* Their paper is a theoretical analysis of the flow of gradient descent, it does not yield meaningful uncertainty quantification.

Laplace approximations for Deep learning:

- Laplace approximations turn (nearly) *any* deep neural network into a Gaussian process
- they involve only *auto-diff* and *linear algebra*, both of which are robust and scalable
- Deep nets thus approximately inherit the probabilistic functionality
- for large-scale deep networks, care must be taken to find *approximate* solutions to the Hessian decomposition

Please cite this course, as

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    series = {Lecture Notes
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