Foundations of Deep Learning, Winter Term 2021/22

Week 13: Uncertainty in Deep Learning

Uncertainty in Deep Learning

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Overview of Week 13

Lecture Overview

Foundations of Deep Learning, Winter Term 2021/22

Week 13: Uncertainty in Deep Learning

Why we Need Uncertainty in Neural Networks

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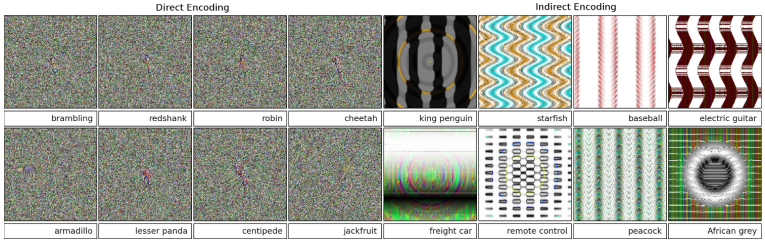
Motivation: Why Does Uncertainty Matter?

- Knowing model's uncertainty is crucial in safety-critical applications
  - Medical diagnosis
  - Autonomous driving
  - Operations in space
  - Household robotics
  - ...
- Decision theory = probability theory + utility theory

Uncertainty in Neural Networks for Classification

- Standard neural nets *do* output a probability distribution (softmax)
  - But this probability distribution is often not reliable
- Uncertainty should grow away from the typical data seen, but doesn't
  - E.g., for ReLU networks there are points far away from the training data for which the networks are arbitrarily certain [Hein et al., 2019]
  - E.g., deep neural nets can be overconfident for unrecognizable images:

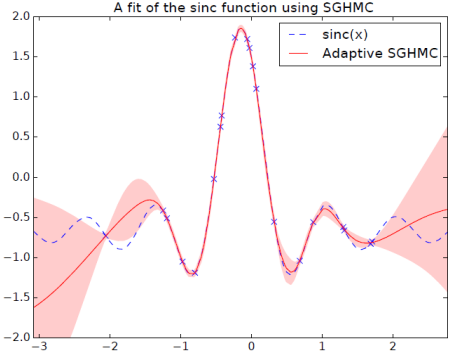


Evolved images that are classified with $\geq 99.6\%$ certainty to be a familiar object

[Image source: Nguyen et al., 2015]

Uncertainty in Neural Networks for Regression

- Standard NNs for regression only output a single value, no uncertainty
- Uncertainty should grow away from the typical data seen



[Image source: Springenberg et al., 2016]

Types of Uncertainty

- Aleatoric uncertainty
  - Intrincic observation noise; cannot be reduced
- Epistemic uncertainty
  - Uncertainty about the model
  - Relates to our knowledge of the world; can be reduced by more data
- We can express uncertainty about different quantities
  - Uncertainty about the true state of the world (epistemic)
  - Uncertainty about what we will measure (epistemic + aleatoric)

Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  In the case of classification, our standard softmax is already a probabilistic prediction. Why do we need more?
- Discussion:
  Can you think of an application area of neural networks where it is really important to quantify our uncertainty and "know when we don't know"?

Lecture Overview

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Week 13: Uncertainty in Deep Learning

Background: Properties of the Gaussian Distribution

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The Gaussian Distribution

The univariate form

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right)$$

Named after Carl Friedrich Gauss (1777-1855)

(Exposition follows Philipp Hennig's Gaussian process tutorial)

[Image source: Wikimedia Commons]

The Gaussian Distribution

The univariate form

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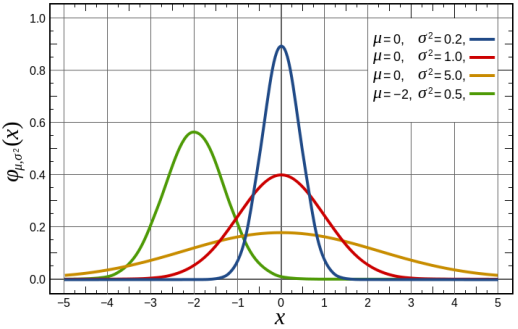


[Image source: Wikimedia Commons]

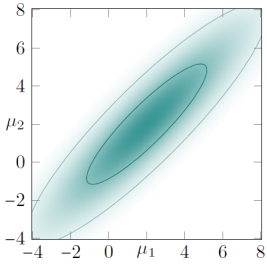
The Gaussian Distribution

The multivariate Gaussian (in N dimensions)

$$f(\boldsymbol{x}) = \frac{1}{(2\pi)^{N/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right)$$

- $\boldsymbol{x}$ and $\boldsymbol{\mu}$ are $N \times 1$ (column) vectors
- $\boldsymbol{\Sigma}$ is an $N \times N$ matrix

An example in 2 dimensions:



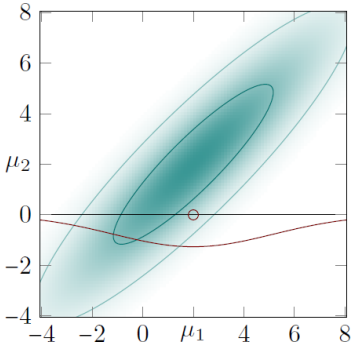
$$\boldsymbol{\mu} = \begin{pmatrix}\mu_1\\ \mu_2\end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix}\sigma_{11}^2 & \sigma_{12}^2\\ \sigma_{21}^2 & \sigma_{22}^2\end{pmatrix}$$

Property 1: Closure Under Marginalization

Gaussian distributions are closed under marginalization

Let $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ be jointly Gaussian distributed:

$$\begin{bmatrix}\boldsymbol{x}_1\\ \boldsymbol{x}_2\end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix}\boldsymbol{\mu}_1\\ \boldsymbol{\mu}_2\end{bmatrix}, \begin{bmatrix}\boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12}\\ \boldsymbol{\Sigma}_{12}^{\mathsf{T}} & \boldsymbol{\Sigma}_{22}\end{bmatrix}\right) \qquad \text{Then } \boldsymbol{x}_1 \sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11}).$$



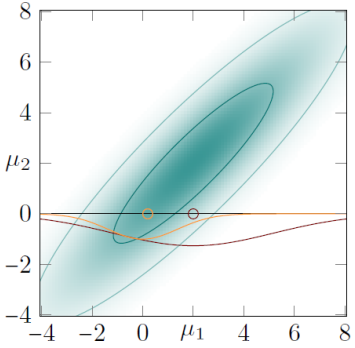
$$\boldsymbol{\mu} = \begin{pmatrix}\mu_1\\ \mu_2\end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix}\sigma_{11}^2 & \sigma_{12}^2\\ \sigma_{21}^2 & \sigma_{22}^2\end{pmatrix}$$

Property 2: Closure Under Conditioning

Gaussian distributions are closed under conditioning

Let $\boldsymbol{a}$ and $\boldsymbol{b}$ be jointly Gaussian distributed: $\begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix}, \begin{bmatrix} A & C \\ C^\intercal & B \end{bmatrix} \right)$

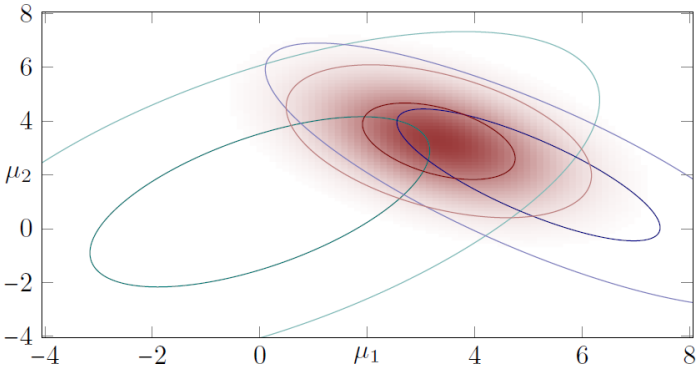
Then $\boldsymbol{b}|\boldsymbol{a} \sim \mathcal{N}\left(\boldsymbol{\mu}_b + C^\intercal A^{-1}(\boldsymbol{a} - \boldsymbol{\mu}_a), B - C^\intercal A^{-1} C\right)$.



Property 3: Closure Under Multiplication

$$\mathcal{N}(x; a, A)\mathcal{N}(x; b, B) \propto \mathcal{N}(x; c, C)$$

$$C := (A^{-1} + B^{-1})^{-1} \quad c := C(A^{-1}a + B^{-1}b)$$



Property 4: Closure Under Linear Maps

Gaussian distributions are closed under linear maps

- Let $\boldsymbol{w} \sim \mathcal{N}(\boldsymbol{\mu}_w, \boldsymbol{\Sigma}_w)$. Then, $\boldsymbol{x}^\mathsf{T}\boldsymbol{w} \sim \mathcal{N}(\boldsymbol{x}^\mathsf{T}\boldsymbol{\mu}_w, \boldsymbol{x}^\mathsf{T}\boldsymbol{\Sigma}_w\boldsymbol{x})$

Why Gaussians?

- The central limit theorem tells us that means of large populations are distributed according to a Gaussian
- However, individual measurements are rarely Gaussian-distributed
  - So, this isn't really the main reason we use Gaussians
- The use of Gaussians is mostly a mathematical convenience that lets us solve integrals in closed form!

Questions to Answer for Yourself / Discuss with Friends

- Repetition: Write down the formula for a multivariate Gaussian.
- Repetition: List four operations under which Gaussians are closed.

Lecture Overview

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Week 13: Uncertainty in Deep Learning

Bayesian Linear Regression

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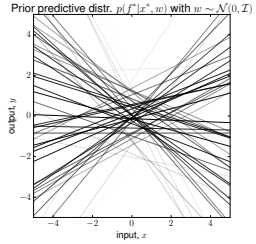
Principles of Bayesian Reasoning

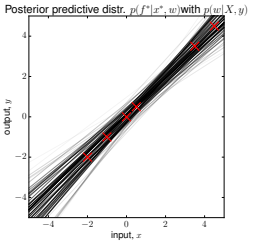
Don't select a single model, but acknowledge all sources of uncertainty

- Prior over possible models
- Likelihood of the data under these models, making certain models more likely
- Posterior over possible models

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}} \propto \text{likelihood} \times \text{prior}$$

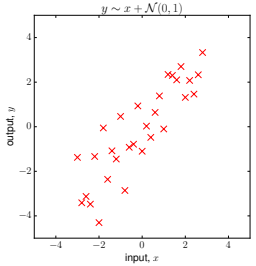


Prior over models (here: lines)



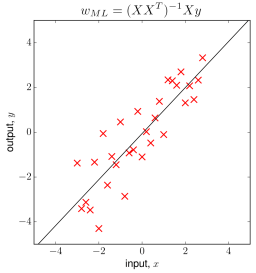
Posterior over models

Linear Regression



- We have a dataset of n observations, $\mathcal{D} = \{(\boldsymbol{x}_i, y_i) | i = 1, \ldots, n\}$
- Each $\boldsymbol{x}_i$ denotes a $D \times 1$ column vector and each y_i is a scalar output or target
- We collect all inputs $\boldsymbol{x}_i$ into the $D \times n$ design matrix $\boldsymbol{X} = [\boldsymbol{x}_1 \cdots \boldsymbol{x}_n]$ and the targets into the $n \times 1$ vector $\boldsymbol{y}$.
  - Note: here, we use the notation from the excellent book Gaussian processes for Machine Learning by Rasmussen & Williams so that you can read up on all derivations. (Note that $\boldsymbol{X}$ is transposed from our usual notation.)

Standard Linear Regression Model



$$f(\boldsymbol{x}) = \boldsymbol{x}^{\mathsf{T}}\boldsymbol{w}, \qquad y = f(\boldsymbol{x}) + \epsilon \tag{2.1}$$

$$\epsilon \sim \mathcal{N}(0, \sigma_n^2) \tag{2.2}$$

(all equation numbers from Chapter 2 of
Gaussian processes for Machine Learning by Rasmussen & Williams)

Maximum Likelihood Estimation of $\boldsymbol{w}$

The likelihood $p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})$ is then defined as:

$$\begin{aligned} p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w}) &= \prod_{i=1}^{n} p(y_i|\boldsymbol{x}_i, \boldsymbol{w}) \\ &= \prod_{i=1}^{n} \frac{1}{(\sqrt{2\pi}\sigma_n)} \exp\left(-\frac{(y_i - \boldsymbol{x}_i^\mathsf{T}\boldsymbol{w}_i)^2}{2\sigma_n^2}\right) \\ &= \frac{1}{(2\pi\sigma_n^2)^{n/2}} \exp\left(-\frac{1}{2\sigma_n^2}|\boldsymbol{y} - \boldsymbol{X}^\mathsf{T}\boldsymbol{w}|^2\right) \\ &= \mathcal{N}(\boldsymbol{y}; \boldsymbol{X}^\mathsf{T}\boldsymbol{w}, \sigma_n^2 I) \end{aligned} \tag{2.3}$$

Maximum likelihood estimation seeks to maximize this likelihood:

$$\Rightarrow \boldsymbol{w}_{\mathsf{ML}} = (\boldsymbol{X}\boldsymbol{X}^\mathsf{T})^{-1}\boldsymbol{X}\boldsymbol{y}$$

This is known as the normal equations.

The Bayesian Way of Setting $\boldsymbol{w}$

- Don't commit to a single $\boldsymbol{w}_{\mathsf{ML}}$,
  but rather integrate over an infinite number of possibilities

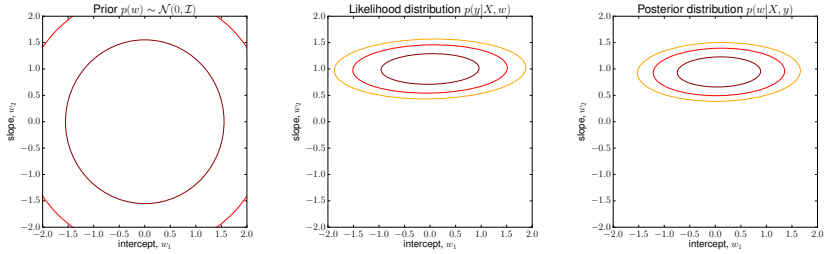
- Define a prior distribution $p(\boldsymbol{w})$ over $\boldsymbol{w}$ quantifying our expectations
- Compute the likelihood $p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})$ of the data under each model

- Compute posterior $p(\boldsymbol{w}|\boldsymbol{y}, \boldsymbol{X})$ by Bayes' rule: proportional to likelihood times prior.

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}$$

$$p(\boldsymbol{w}|\boldsymbol{y}, \boldsymbol{X}) = \frac{p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{y}|\boldsymbol{X})} \tag{2.5}$$

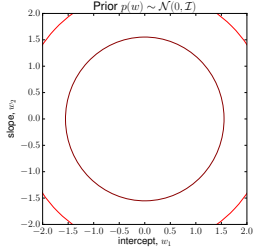
The Bayesian Way of Setting $\boldsymbol{w}$

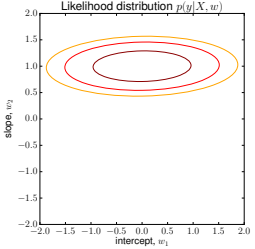


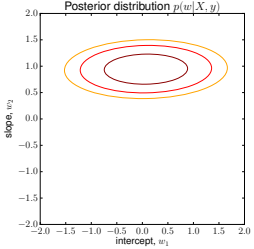
$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}$$

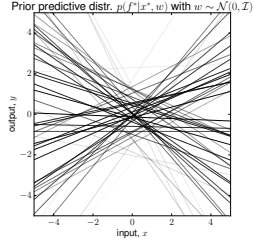
$$p(\boldsymbol{w}|\boldsymbol{y}, \boldsymbol{X}) = \frac{p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{y}|\boldsymbol{X})} \tag{2.5}$$

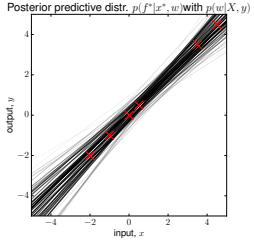
Weights Correspond to Functions











Computation of the Posterior Under a Gaussian Prior

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}$$

$$p(\boldsymbol{w}|\boldsymbol{y}, \boldsymbol{X}) = \frac{p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{y}|\boldsymbol{X})} \tag{2.5}$$

The denominator generally requires approximating a complicated integral $p(\boldsymbol{y}|\boldsymbol{X}) = \int p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})p(\boldsymbol{w})d\boldsymbol{w}$. But everything simplifies if we choose a prior that is conjugate to the likelihood; in this case another Gaussian:

$$\boldsymbol{w} \sim \mathcal{N}(0, \Sigma_p) \tag{2.4}$$

In that case, the posterior is Gaussian again:

$$p(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y}) \sim \mathcal{N}\left(\bar{\boldsymbol{w}} = \frac{1}{\sigma_n^2} A^{-1} \boldsymbol{X}\boldsymbol{y}, A^{-1}\right), \tag{2.7}$$

with A given by:

$$\mathsf{A} = \sigma_n^{-2} \boldsymbol{X}\boldsymbol{X}^\mathsf{T} + \Sigma_p^{-1}$$

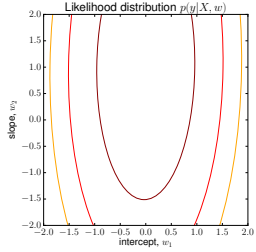
The Posterior Predictive Distribution

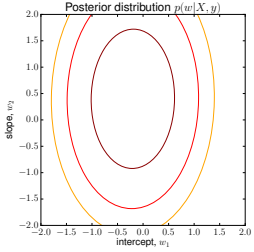
- Each weight vector $\boldsymbol{w}$ corresponds to a linear model
- For a new data point $\boldsymbol{x}_\star$, each weight vector $\boldsymbol{w}$ gives rise to a linear model prediction $f_\star = \boldsymbol{x}_\star^\mathsf{T}\boldsymbol{w}$
- We simply average the predictions of linear models with all possible $\boldsymbol{w}$, weighting each model by the posterior probability of its corresponding $\boldsymbol{w}$:

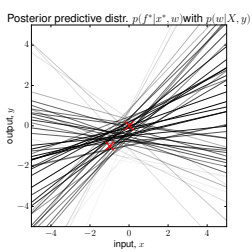
$$\begin{aligned} p(f_\star|\boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y}) &= \int p(f_\star|\boldsymbol{x}_\star, \boldsymbol{w}) p(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y}) d\boldsymbol{w} \\ &= \mathcal{N}(f_\star; \frac{1}{\sigma_n^2}\boldsymbol{x}_\star^\mathsf{T} A^{-1}\boldsymbol{X}\boldsymbol{y}, \boldsymbol{x}_\star^\mathsf{T} A^{-1}\boldsymbol{x}_\star) \end{aligned} \tag{2.9}$$

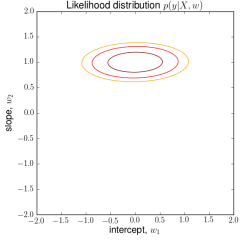
$\rightarrow$ This is a Gaussian because Gaussians are closed under linear maps and marginalization.

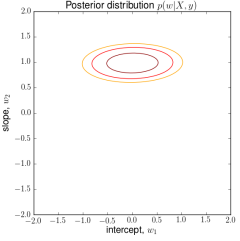
Enough Data Overwhelms the Prior

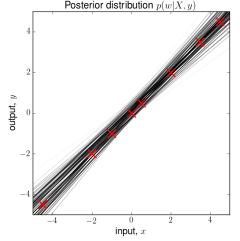












Bayesian Linear Regression With Basis Functions

The same analysis goes through if we replace $\boldsymbol{x}$ with some so-called basis functions $\phi(\boldsymbol{x})$ of $\boldsymbol{x}$, e.g., powers of x

$$\phi(x) = (1, x, x^2, x^3, \ldots)^\mathsf{T}$$

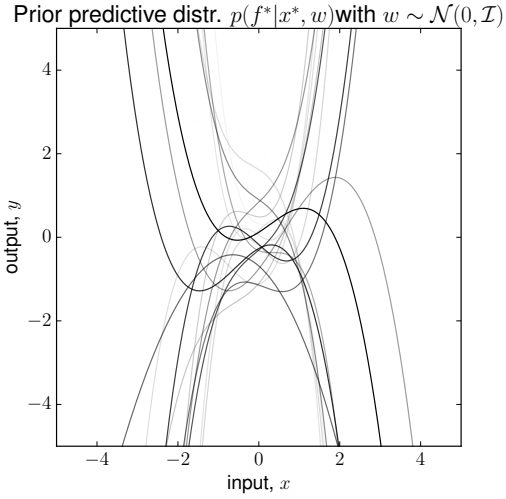
Basis function linear regression is then:

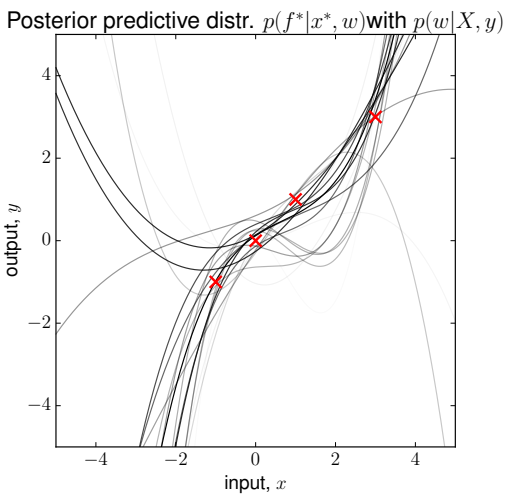
$$f(\boldsymbol{x}) = \phi(\boldsymbol{x})^\mathsf{T}\boldsymbol{w} \tag{2.10}$$

And the equivalent of 2.9 is:

$$f_\star|\boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y} \sim \mathcal{N}\left(\frac{1}{\sigma_n^2}\phi(\boldsymbol{x}_\star)^\mathsf{T}A^{-1}\Phi\boldsymbol{y}, \phi(\boldsymbol{x}_\star)^\mathsf{T}A^{-1}\phi(\boldsymbol{x}_\star)\right) \tag{2.11}$$
$$\text{with } \Phi = \phi(\boldsymbol{X}) \text{ and } A = \sigma_n^{-2}\Phi\Phi^\mathsf{T} + \Sigma_p^{-1}$$

Bayesian Cubic Regression





. . . and you can do the same based on learned features from the last layer of a neural network

Summary of Bayesian Linear Regression

- General Bayesian principle: we hedge our bets, integrate over infinitely many models
- In the special case of Bayesian linear regression, we can do this in closed form:
  - We use a Gaussian prior $p(\boldsymbol{w})$ that quantifies our expectations
  - We use a Gaussian likelihood $p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})$
  - This results in a Gaussian posterior $p(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y})$
  - This also results in a Gaussian predictive distribution $p(f_\star|\boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y})$
- Bayesian linear regression still works with basis functions $\phi(\boldsymbol{x})$ instead of $\boldsymbol{x}$ itself
  - These basis functions can also be nonlinear
  - The computation just needs to be linear in $\boldsymbol{w}$

Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  Write down the formula for the posterior $p(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y})$ in terms of the prior $p(\boldsymbol{w})$ and the likelihood $p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})$
- Repetition:
  In Bayesian cubic regression, which components dominate if all weights have a uniform weight in the prior?

Lecture Overview

Foundations of Deep Learning, Winter Term 2021/22

Week 13: Uncertainty in Deep Learning

Being Bayesian about Neural Networks

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What Does it Mean to be Bayesian About Neural Nets?

- Dealing with all sources of parameter uncertainty:
  - More than one weight vector can explain the observed data
  - Take into account all possible explanations

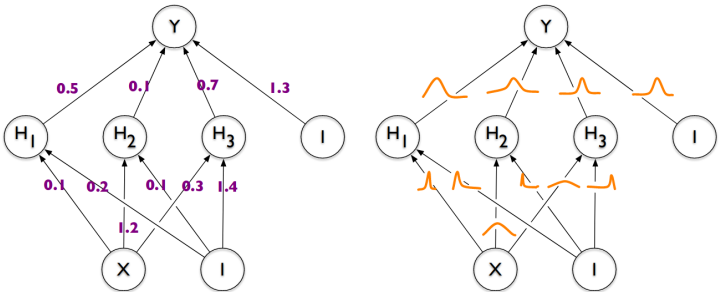

Figure: *Left*: Standard NN with parameter point estimates. *Right*: Bayesian NN with parameter distributions.

[Image source: Blundell et al., 2015]

The DNGO Model: Being Bayesian At Least About the Output Layer

1. Fit a standard neural network to the data
2. Use the representation in the last hidden layer as basis functions $\phi(\boldsymbol{x})$ of the input $\boldsymbol{x}$
3. Use Bayesian linear regression for the output layer

$\rightsquigarrow$ Successfully used as a probabilistic model for Bayesian optimization [Snoek et al., 2015]

Frequentist Approach: MLE and MAP Estimates

- Data: $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^N = (\boldsymbol{X}, \boldsymbol{y})$
- Parameters $\boldsymbol{\theta}$: (all) weights of the neural network
- Prior: $p(\boldsymbol{\theta})$
- Likelihood: $p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta})$
- Posterior: $p(\boldsymbol{\theta}|\mathcal{D}) \equiv p(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{y})$
  - MAP estimation:

$$\begin{aligned}\boldsymbol{\theta}^{MAP} &= \arg\max_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{y}) \\ &= \arg\max_{\boldsymbol{\theta}} \log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\end{aligned}$$

    → if prior $p(\boldsymbol{\theta})$ is Gaussian (Laplacian), this is L_2 (L_1) regularization
  - Maximum Likelihood Estimation (MLE):

$$\boldsymbol{\theta}^{MLE} = \arg\max_{\boldsymbol{\theta}} \log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta})$$

    → corresponds to a uniform prior $p(\boldsymbol{\theta})$

Bayesian Neural Networks

- Data: $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^N = (\boldsymbol{X}, \boldsymbol{y})$
- Parameters $\boldsymbol{\theta}$: (all) weights of the neural network
- Prior: $p(\boldsymbol{\theta})$
- Likelihood: $p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta})$
- Posterior: $p(\boldsymbol{\theta}|\mathcal{D}) \equiv p(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\boldsymbol{y}|\boldsymbol{X})} = \frac{p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$
  - Problem: $p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta})$ is not as simple as in linear models
    - E.g., its mean is not a linear function of $\boldsymbol{\theta}$
  - The posterior is therefore not a Gaussian anymore
    - One possibility: approximate $p(\boldsymbol{\theta}|\mathcal{D})$ with a simple distribution (e.g., a Gaussian again) $\rightarrow$ variational inference
    - Another possibility: sample from $p(\boldsymbol{\theta}|\mathcal{D})$ $\rightarrow$ MCMC
- Prediction (inference): $p(y'|\mathcal{D}, \boldsymbol{x}') = \int p(\boldsymbol{y}'|\boldsymbol{x}', \boldsymbol{\theta})p(\boldsymbol{\theta}|\mathcal{D})d\boldsymbol{\theta}$
  - Equivalent to averaging predictions from an ensemble of an infinite number of NNs (weighted by the posterior probabilities of $\boldsymbol{\theta}$)

Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  How can you use Bayesian linear regression to at least be Bayesian about the output layer of a neural network for regression?
- Repetition:
  Why can't we use Bayesian linear regression to be Bayesian about all the parameters $\boldsymbol{\theta}$ of a neural network?

Lecture Overview

Foundations of Deep Learning, Winter Term 2021/22

Week 13: Uncertainty in Deep Learning

Variational Inference

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Variational Inference

- Goal: approx. an intractable posterior distribution $p(\boldsymbol{\theta}|\mathcal{D})$ by a simpler distribution $q_\phi(\boldsymbol{\theta})$
- Approach: pick a model family $q_\phi(\boldsymbol{\theta})$ and optimize its parameters ϕ to make $q_\phi(\boldsymbol{\theta})$ as close as possible to $p(\boldsymbol{\theta}|\mathcal{D})$
  - Unfortunately, $p(\boldsymbol{\theta}|\mathcal{D})$ is intractable, so we also can't compute $KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D}))$
  - But we can implicitly minimize this KL divergence by rewriting it:

$$
\begin{aligned}
KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D})) &= \int q_\phi(\boldsymbol{\theta}) \log \frac{q_\phi(\boldsymbol{\theta})}{p(\boldsymbol{\theta}|\mathcal{D})} d\boldsymbol{\theta} \\
&= \mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log \frac{q_\phi(\boldsymbol{\theta})}{p(\boldsymbol{\theta}|\mathcal{D})}\right] = \mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log \frac{q_\phi(\boldsymbol{\theta})}{p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})} p(\mathcal{D})\right] \\
&= \mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log q_\phi(\boldsymbol{\theta}) - \log p(\mathcal{D}|\boldsymbol{\theta}) - \log p(\boldsymbol{\theta}) + \log p(\mathcal{D})\right] \\
&= \mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log q_\phi(\boldsymbol{\theta}) - \log p(\mathcal{D}|\boldsymbol{\theta}) - \log p(\boldsymbol{\theta})\right] + \log p(\mathcal{D}) \\
&= \mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log q_\phi(\boldsymbol{\theta}) - \log p(\mathcal{D}|\boldsymbol{\theta}) - \log p(\boldsymbol{\theta})\right] + \log p(\mathcal{D}) \\
&= KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta})) - \mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log p(\mathcal{D}|\boldsymbol{\theta})\right] + \log p(\mathcal{D})
\end{aligned}
$$

Evidence Lower Bound (ELBO)

$$KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D})) = KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta})) - \mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log p(\mathcal{D}|\boldsymbol{\theta})\right] + \log p(\mathcal{D})$$

$$\Rightarrow$$

$$KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D})) + \underbrace{\mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log p(\mathcal{D}|\boldsymbol{\theta})\right] - KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}))}_{\text{evidence lower bound (ELBO)}} = \log p(\mathcal{D})$$

- In order to minimize $KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D}))$ w.r.t. $\boldsymbol{\theta}$, we only need to maximize ELBO since $p(\mathcal{D})$ is a constant (it does not depend on θ)
- ELBO embodies a trade-off between satisfying the complexity of the data and satisfying the simplicity of the prior
  - $\mathbb{E}_{q_\phi(\boldsymbol{\theta})}\left[\log p(\mathcal{D}|\boldsymbol{\theta})\right] \rightarrow$ data likelihood: data dependent (max!)
  - $KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta})) \rightarrow$ difference from true prior: prior dependent (min!)
- Since $KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D})) \geq 0$, ELBO is a lower bound on $\log p(\mathcal{D})$
- For an appropriate choice of q, ELBO is tractable to compute.

Variational inference is a very active field of research

- ELBO is very popular
  - Approximates the true posterior with the variational posterior and therefore replaces the difficult integral
  - Wide range of applications
- Summary of ongoing research efforts on variational inference
  - ELBO requires calculations over the whole dataset
    - Circumvented by Monte Carlo estimates (Stochastic VI)
    - Methods for reducing variance in the gradients
  - The choice of $q_\phi(\boldsymbol{\theta})$ is important; need to trade off:
    + Expressive power
    + Computational feasibility: memory cost and speed

Questions to Answer for Yourself / Discuss with Friends

- Repetition: Why does it make sense to replace computing one KL divergence $KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D}))$ with a computation that involves another KL-divergence $KL(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}))$?
- Repetition: Which two terms does ELBO consist of?
- Repetition: Derive the fact that ELBO is a lower bound to $\log p(\mathcal{D})$.

Lecture Overview

Foundations of Deep Learning, Winter Term 2021/22

Week 13: Uncertainty in Deep Learning

Markov Chain Monte Carlo

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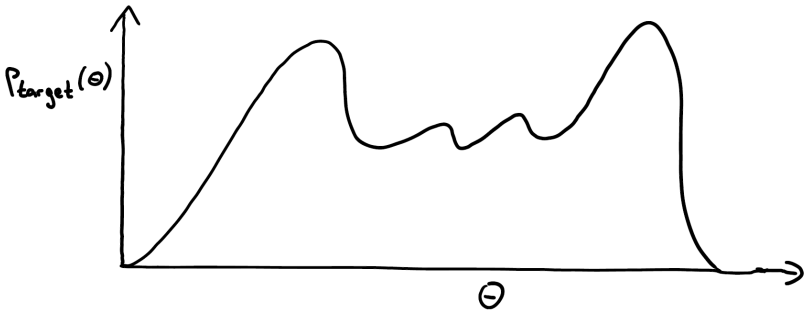
Markov Chain Monte Carlo (MCMC) Sampling: Intuition

- Problem: given a probability distribution $p_{target}(\boldsymbol{\theta})$ that we can evaluate up to a normalization constant, draw samples according to $p_{target}(\boldsymbol{\theta})$
  - In our case $p_{target}(\boldsymbol{\theta}) = p(\boldsymbol{\theta}|\mathcal{D})$



- Move along a chain according to a proposal distribution
- Accept improving moves
- Only accept worsening moves with a certain probability
- Keep a history (the "chain") of visited states

Markov Chain Monte Carlo (MCMC) Sampling: Key Idea

- Key idea: a chain that samples $\boldsymbol{\theta}^{(t)} \rightarrow \boldsymbol{\theta}^{(t+1)} \rightarrow \boldsymbol{\theta}^{(t+2)} \rightarrow \ldots$
  - such that the samples converge to the target distribution $p_{target}(\boldsymbol{\theta})$

- We use every t-th sample $\boldsymbol{\theta}^{(k+it)}$ to approximate samples from $p_{target}(\boldsymbol{\theta})$
  - E.g., with $k = 50$ and $t = 10$, our sample sequence is $\boldsymbol{\theta}^{(50)}$, $\boldsymbol{\theta}^{(60)}$, $\boldsymbol{\theta}^{(70)}$, $\boldsymbol{\theta}^{(80)}$, $\ldots$
  - A histogram of this sequence then approximates $p_{target}(\boldsymbol{\theta})$
  - The sequence can also be used to approximate expectations of a function $f(\boldsymbol{\theta})$ under $p_{target}(\boldsymbol{\theta})$:

$$\mathbb{E}_{p_{target}}(f) \approx \frac{1}{M} \sum_{i=1}^{M} f(\boldsymbol{\theta}^{(k+it)})$$

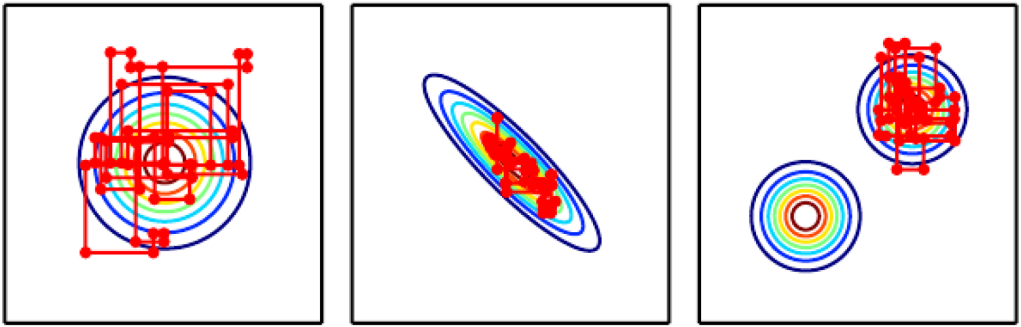
Markov Chain Monte Carlo (MCMC) Sampling: Theory

- Ingredients
  - A state space $\boldsymbol{\Theta}$
  - A transition distribution $p(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1)$ for $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \in \boldsymbol{\Theta}$
    - For all $\boldsymbol{\theta}_1 \in \boldsymbol{\Theta}$: $\sum_{\boldsymbol{\theta}_2 \in \boldsymbol{\Theta}} p(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1) = 1$
    - For $\boldsymbol{\theta}_2 \neq \boldsymbol{\theta}_1$, $p(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1) = g(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1)A(\boldsymbol{\theta}_2, \boldsymbol{\theta}_1)$
- We want the chain to sample from a stationary distribution π
  - For all $\boldsymbol{\theta}_2 \in \boldsymbol{\Theta}$: $\sum_{\boldsymbol{\theta}_1 \in \boldsymbol{\Theta}} \pi(\boldsymbol{\theta}_1) p(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1) = \pi(\boldsymbol{\theta}_2)$
  - This stationary distribution $\pi(\boldsymbol{\theta})$ should be $\pi(\boldsymbol{\theta}) \equiv p_{target}(\boldsymbol{\theta})$
- Sufficient condition for a stationary distribution to exist: detailed balance
  - For any $\boldsymbol{\theta}, \boldsymbol{\theta}' \in \boldsymbol{\Theta}$: probability for being in $\boldsymbol{\theta}$ and transitioning to $\boldsymbol{\theta}'$ must be same as for being in $\boldsymbol{\theta}'$ and transitioning to $\boldsymbol{\theta}$
  - Formally: $\pi(\boldsymbol{\theta})p(\boldsymbol{\theta}'|\boldsymbol{\theta}) = \pi(\boldsymbol{\theta}')p(\boldsymbol{\theta}|\boldsymbol{\theta}')$

Markov Chain Monte Carlo (MCMC) Sampling: Practice

- Even if we satisfy detailed balance, it may take a while until we sample from the stationary distribution
  - This time is called the mixing time
  - Intuitively, the time until the chain forgot where it started
- In practice, the mixing time is not known
  - We only start taking samples from the chain after a burning in phase (the length of this is a hyperparameter)

The Mixing Time Depends on the Distribution



[Image source: Goodfellow et al., 2016 (Figure 17.1)]

Famous MCMC Algorithm (from 1953): Metropolis-Hastings

- Proposal distribution: $g(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1)$ for generating new states
- Acceptance ratio $A(\boldsymbol{\theta}_2, \boldsymbol{\theta}_1)$
- Transition probability is then: $p(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1) = g(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1) \cdot A(\boldsymbol{\theta}_2, \boldsymbol{\theta}_1)$
- Acceptance ratio selected to always satisfy detailed balance:

$$A(\boldsymbol{\theta}_2, \boldsymbol{\theta}_1) = \min(1, \frac{p_{target(\boldsymbol{\theta}_2)}}{p_{target(\boldsymbol{\theta}_1)}} \frac{g(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2)}{g(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1)})$$

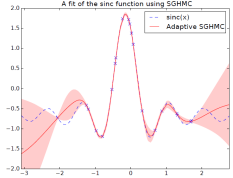
Full algorithm:

- Pick an initial $\boldsymbol{\theta}_0$ (e.g., at random); set $t = 0$
- For $t = 0, \ldots, T$:
  - Generate a next candidate state $\boldsymbol{\theta}' \sim g(\boldsymbol{\theta}'|\boldsymbol{\theta}_t)$
  - Accept with probability $\min(1, \frac{p_{target(\boldsymbol{\theta}_1)}}{p_{target(\boldsymbol{\theta}_2)}} \frac{g(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1)}{g(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2)})$

MCMC Can Be Sped Up By Gradients

- Gradient-based updates of $\boldsymbol{\theta}$ are much faster than sampling following a simpler proposal distribution
  - Hamiltonian Monte Carlo (HMC) takes into account gradients
  - Special case: Langevin Dynamics: $\Delta\boldsymbol{\theta}_t = \frac{\epsilon_t}{2}\left(\nabla \log p(\boldsymbol{\theta}_t) + \nabla \log p(\mathcal{D}|\boldsymbol{\theta}_t)\right) + \eta_t$, with $\eta_t \sim \mathcal{N}(0, \epsilon)$
- $p(\mathcal{D}|\boldsymbol{\theta})$ depends on the full data, like batch gradient descent
  - Can be sped up by considering mini batches of n data points: $p(\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n|\boldsymbol{\theta})$ $\rightsquigarrow$ Stochastic Gradient Langevin Dynamics (SGLD) [Welling Teh, 2011]
  - SGLD is almost identical to SGD, just adds $\eta_t \sim \mathcal{N}(0, \epsilon)$
- General HMC can also work with mini-batches

  $\rightarrow$ SGHMC [Chen et al, 2014]
  - We've also extended SGHMC for Bayesian optimization with Bayesian neural networks [Springenberg et al., 2016]



[Image source: Springenberg et al., 2016]

Questions to Answer for Yourself / Discuss with Friends

- Repetition: Explain MCMC in your own words.
- Repetition: What is the condition for a "stationary distribution"?
- Repetition: What is the relation between the mixing time and the length of the burning in phase?

Lecture Overview

Foundations of Deep Learning, Winter Term 2021/22

Week 13: Uncertainty in Deep Learning

Prior-Fitted Networks for Bayesian Inference

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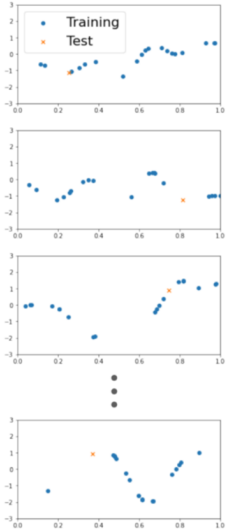
Motivation for Prior-Fitted Networks (PFNs) [Müller et al, 2022]

- So far, we estimated $p(\boldsymbol{\theta}|\mathcal{D}_{train})$ via variational inference or MCMC
- To make predictions for a new data point $\boldsymbol{x}_{test}$, we would then compute the predictive distribution as:

$$p(y_{test}|\boldsymbol{x}_{test}, \mathcal{D}_{train}) = \int_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathcal{D}_{train}) p(y_{test}|\boldsymbol{x}_{test}, \boldsymbol{\theta}) d\boldsymbol{\theta}$$

- In prior-fitted networks, we will directly approximate $p(y_{test}|\boldsymbol{x}_{test}, \mathcal{D}_{train})$
  - We will assume that we can sample datasets $\mathcal{D}^{(i)} \sim p(\mathcal{D})$
  - We will draw many datasets $\mathcal{D}^{(i)}$ and split each into $\mathcal{D}^{(i)}_{train}$ and $\mathcal{D}^{(i)}_{test} = \{\boldsymbol{x}^{(i)}_{test}, y^{(i)}_{test}\}$
  - We will then learn a model that predicts $y^{(i)}_{test}$ from $\langle \boldsymbol{x}^{(i)}_{test}, \mathcal{D}^{(i)}_{train} \rangle$
  - This model has then learned to predict $p(y_{test}|\boldsymbol{x}_{test}, \mathcal{D})$ in a single forward pass
  - PFNs might be a disruptive alternative to variational inference and MCMC

Illustration of Prior-Fitted Networks (PFNs)

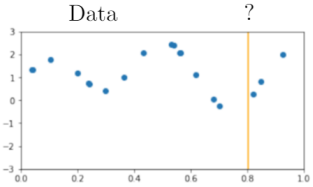


Samples from the prior

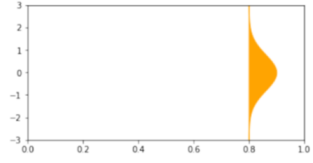
Learn a model to predict test from train

We call this model a prior-fitted network(PFN)

We have thus meta-learned to approximate Bayesian inference, purely by supervised learning with set-valued inputs

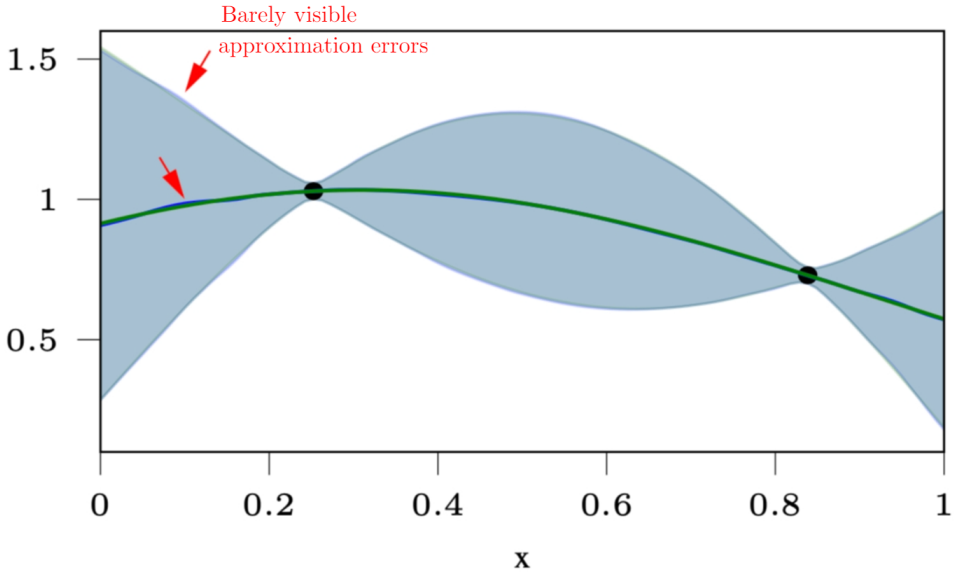


Perform a forward pass with the PFN

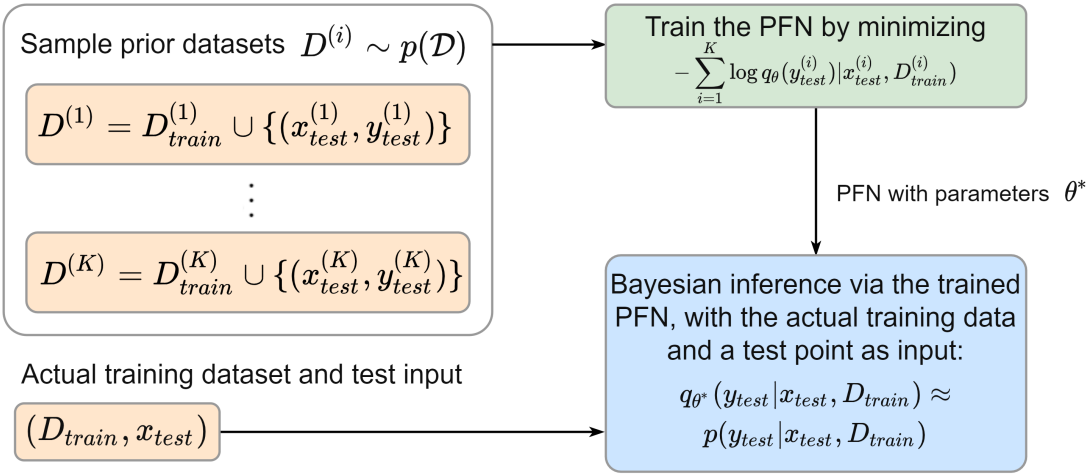


Posterior predictive distribution

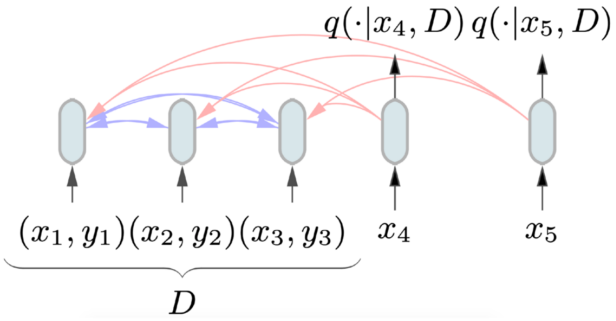
Gaussian Process Approximation



Some Details for Prior-Fitted Networks (PFNs)

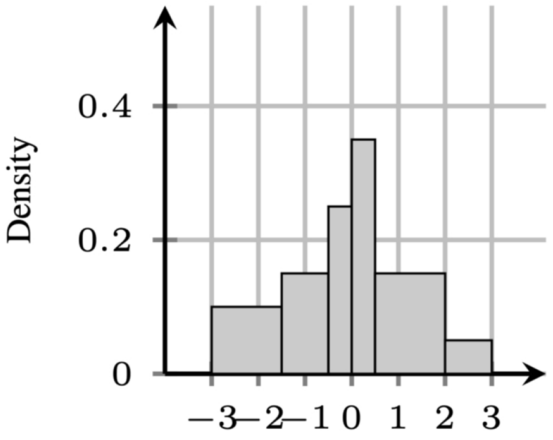


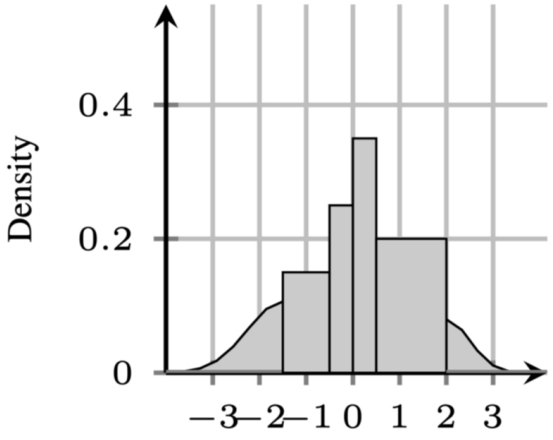
The Model We Use for PFNs: a Permutation-Invariant Transformer



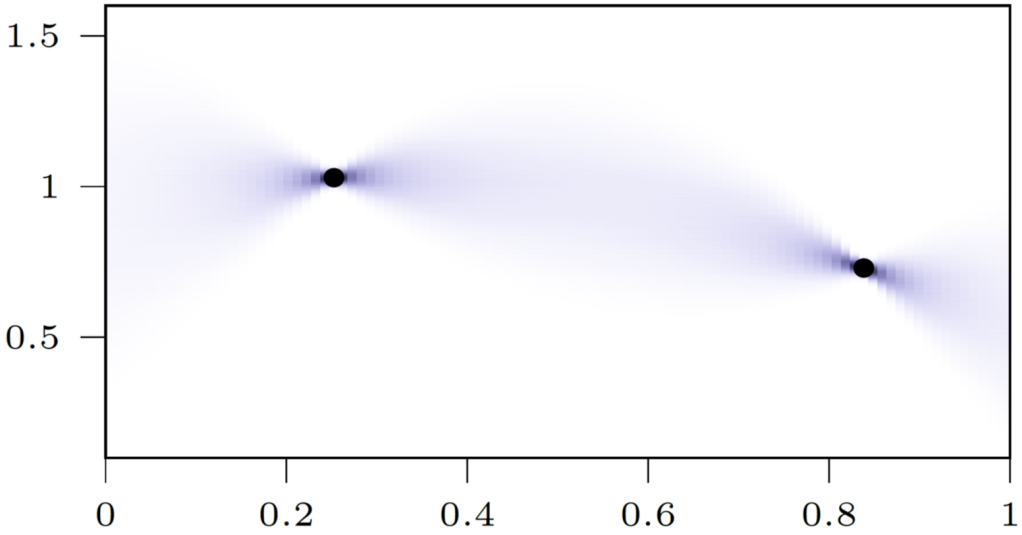
- We simply drop the positional embedding to obtain permutation invariance
- We do not model correlations between outputs
- To draw joint samples, we would draw one at a time and then include it in the input

The Model Head: Regression as Classification

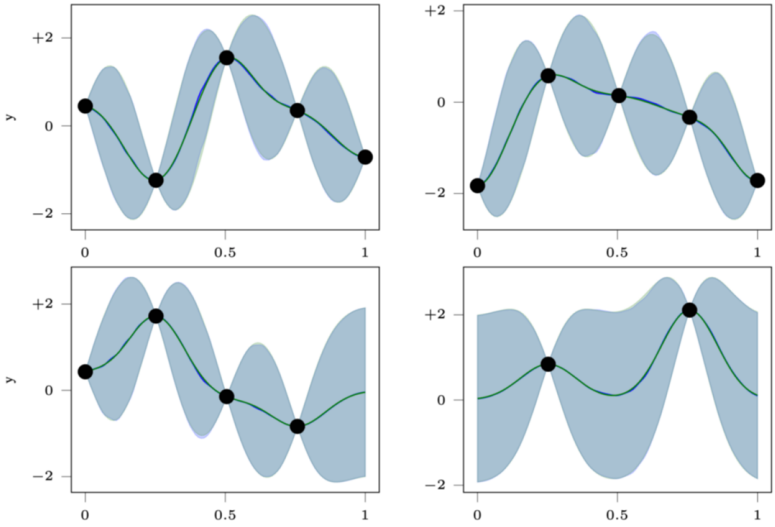




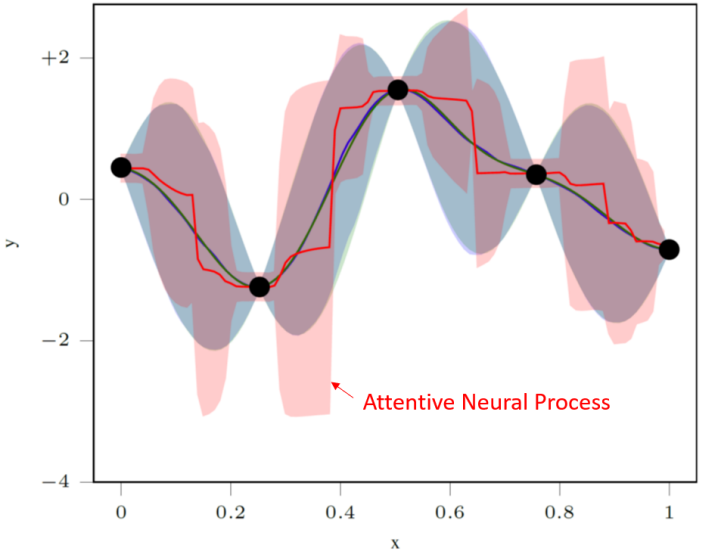
Regression as Classification



Results: Gaussian Process (GP) Approximation

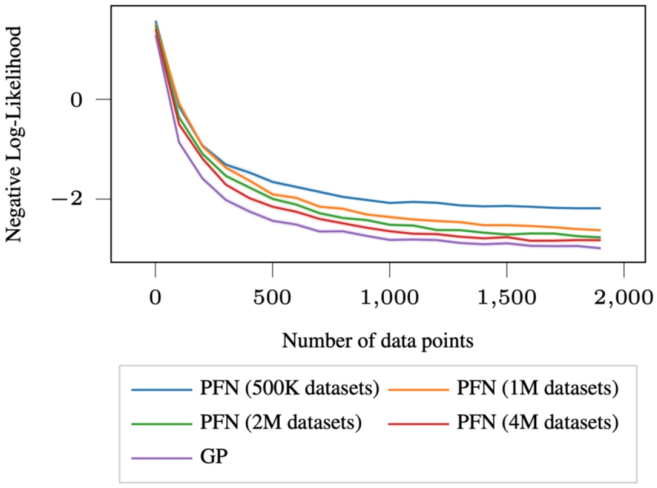


Results: Comparison to Attentive Neural Processes

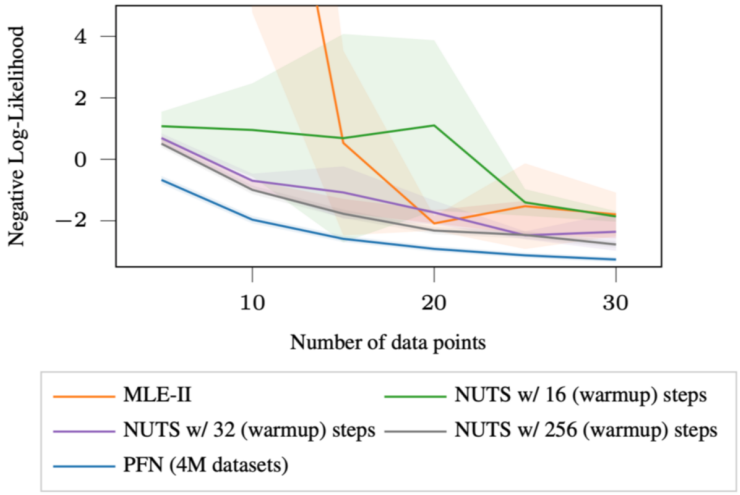


Results: Scalability

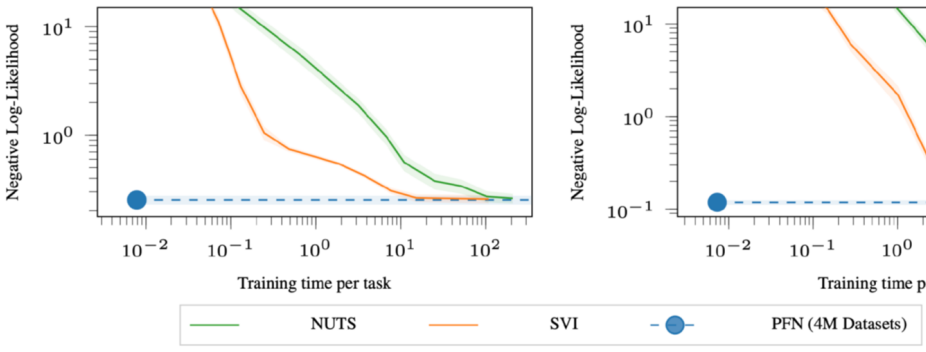
- Longer training (=seeing more datasets sampled from the prior) improves the approximation
- Direct scalability to about 4000 data points; more would need Transformer efficiency tricks



Results: GP Approximation with Unknown Hyperparameters



Results: Bayesian Neural Networks Approximation



- Results for two different network architectures
- (a) a BNN with 3 features, 2 layers and a hidden dimensionality of 5 and
- (b) a BNN with 8 features, 2 layers and a hidden dimensionality of 64.

Application to Binary Classification in Tabular Datasets

Experiment setup

- Binary, balanced classification
- 20 datasets from OpenML
- 30 training data points, 70 test
- Up to 60 features

Prior for generating D synthetic bin. class. datasets:

- Sample a neural architecture
- Sample all its weights from $N(0,1)$
- Sample entries of input matrix $Xi.i.d$ from $N(0,1)$
- Forwardprop X to obtain logits
- Binarize: set y to 1 for top 50% logits, to 0 for others

This is the first time real data enters the picture

Learn a PFN to minimize

$$\sum_{i=1:D} p(y_{31}^{(i)},\ldots,y_{100}^{(i)}|(x_1^{(i)},y_1^{(i)}),\ldots,(x_{30}^{(i)},y_{30}^{(i)}),x_{31}^{(i)},\ldots,x_{100}^{(i)})$$

Real training dataset & test x values

$$(x_1,y_1),\ldots,(x_{30},y_{30}),x_{31},\ldots,x_{100})$$

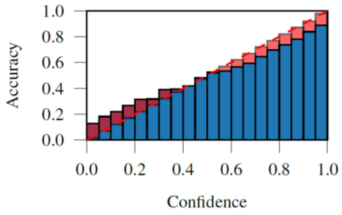
Perform a forward pass with the PFN

$$p(y_{31},\ldots,y_{100}|(x_1,y_1),\ldots,(x_{30},y_{30}),x_{31},\ldots,x_{100})$$

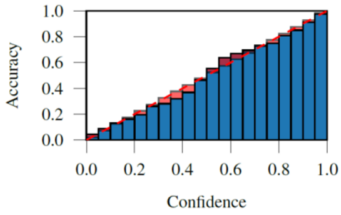
PFNs Outperform all the Baselines, with a Single Forward Prop

Metric	PFN-BNN	PFN-GP	Log. Reg.	GP	KNN	BNN	Catboost	XGB
Mean rank ROC AUC	**2.786**	3.833	4.690	5.286	6.214	5.000	4.833	3.357
Loss/Tie/Win vs PFN-BNN	–	14/1/6	16/1/4	17/0/4	17/1/3	17/1/3	13/1/7	12/2/7
Wilcoxon p. vs PFN-BNN	–	3.6e-13	3.6e-13	3.9e-13	3.6e-13	3.6e-13	1.9e-12	1.6e-06
Expected Calibration Error	**0.025**	0.067	0.157	0.095	0.093	0.089	0.157	0.066
Benchmark Time	GPU: **0:00:13** CPU: 0:04:23		0:09:56	0:24:30	0:00:34	12:04:41	2:05:20	20:59:46

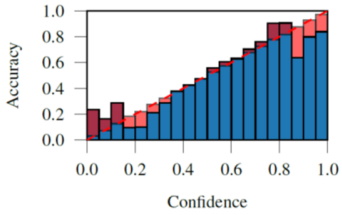
(a) Bayesian Neural Network



(b) PFN-BNN



(c) XGBoost



Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  Can you explain the idea of PFNs in your own words?
- Repetition:
  Why are PFNs permutation-invariant?
- Transfer:
  If you wanted a PFN to behave like a random forest, how would you define the prior?

Lecture Overview

Foundations of Deep Learning, Winter Term 2021/22

Week 13: Uncertainty in Deep Learning

Alternative Treatments of Uncertainty in Neural Networks

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Empirical Uncertainty Estimates via Ensembling

1. Construct an ensemble of M neural networks on the training data
   - More on how to do this on the next slides
2. For each test data point $\mathbf{x}$, predict with each of the M networks
   - Let $f_i(\mathbf{x})$ denote the output of the i-th network
3. Combine outputs of the M networks to obtain probabilistic predictions
   - For classification: average probabilistic (softmax) outputs $f_i(\mathbf{x})$:

$$f(\mathbf{x}) = \frac{1}{M} \sum_{i=1}^{M} f_i(\mathbf{x})$$

   - For regression: compute empirical mean and variance across the point predictions $f_i(\mathbf{x})$:

$$\begin{aligned} \boldsymbol{\mu}_{\mathbf{x}} &= \frac{1}{M} \sum_{i=1}^{M} f_i(\mathbf{x}) \\ \boldsymbol{\sigma}^2_{\mathbf{x}} &= \frac{1}{M} \sum_{i=1}^{M} (f_i(\mathbf{x}) - \boldsymbol{\mu}_{\mathbf{x}})^2 \end{aligned}$$

Different Ways to Construct Ensembles of M Neural Networks

- Via dropout $\rightarrow$ MC-DropOut [Gal Ghahramani, 2015]
  - Very popular, since training does not change at all
  - To obtain M networks, simply sample M random dropout masks
  - No overhead at training time; of course, still M-fold cost at test time
- Via Markov Chain Monte Carlo (MCMC)
- Via different random seeds for initialization and SGD [Lakshminarayanan et al., 2017]
  - These deep ensembles are surprisingly effective: state-of-the-art performance in 2019 [Ovadia et al, 2019]
  - Only disadvantage: M-fold overhead at training time
- Snapshot ensemble obtained via SGD with restarts (SGDR) [Huang et al., 2017]
  - No overhead at training time; of course, still M-fold cost at test time

Different Ways to Construct Ensembles of M Neural Networks

- Via different hyperparameter settings for the training pipeline
  - Hyperdeep ensembles [Wenzel et al., 2020]
  - Can directly reuse the hyperparameter evaluations from HPO [Feurer et al., 2015]

- Via different architectures
  - Recall that we said the Bayesian spirit is to deal with all sources of uncertainty
  - Different architectures often yield very different predictions
  - Neural ensemble search [Zaidi et al, 2020]

Predictive Uncertainty Estimates for Regression Tasks via Parametric Output Distributions

- We can train a network (with weights $\boldsymbol{\theta}$) to output the parameters $\mathbf{w}$ of a parametric model $p(\mathbf{y}|\mathbf{x}, \mathbf{w})$
  - Most common: Gaussian $\mathcal{N}(\mu, \sigma^2)$ ($\mathbf{w}$ parameterizes μ and σ^2)
  - For robustness: rather have network output μ and $\log(\sigma^2)$

- Simply maximize the log-likelihood w.r.t. network weights $\boldsymbol{\theta}$:

$$\log p(\mathcal{D} \mid \boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \log p(\mathbf{y}_i \mid \mathbf{w}(\mathbf{x}_i, \boldsymbol{\theta}))$$

- The predictive distribution for an input $\mathbf{x}$ is then defined as:

$$p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}) \equiv p(\mathbf{y} \mid \mathbf{w}(\mathbf{x}, \boldsymbol{\theta})).$$

Combining Predictive and Empirical Uncertainty Estimates

- We can combine predictive uncertainties with ensembling
- Each network i with weights $\boldsymbol{\theta}_i$ predicts a probability distribution

$$p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}_i) \equiv p(\mathbf{y} \mid \mathbf{w}(\mathbf{x}, \boldsymbol{\theta}_i))$$

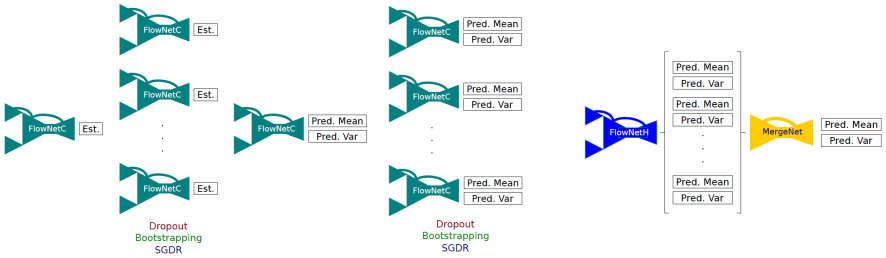
  with mean $\boldsymbol{\mu}_{\mathbf{x},i}$ and variance $\boldsymbol{\sigma}^2_{\mathbf{x},i}$

- We can combine these predictions in a mixture distribution
  - Intuitively, we need to combine the uncertainty of each network and the disagreement between networks
  - We use the law of total variance to compute the mean $\boldsymbol{\mu}_{\mathbf{x}}$ and variance $\boldsymbol{\sigma}^2_{\mathbf{x}}$ of the mixture distribution as:

$$\boldsymbol{\mu}_{\mathbf{x}} = \frac{1}{M}\sum_{i=1}^{M} \boldsymbol{\mu}_{\mathbf{x},i} \qquad \boldsymbol{\sigma}^2_{\mathbf{x}} = \frac{1}{M}\sum_{i=1}^{M} \left((\boldsymbol{\mu}_{\mathbf{x},i} - \boldsymbol{\mu}_{\mathbf{x}})^2 + \boldsymbol{\sigma}^2_{\mathbf{x},i} \right)$$

Overview of Alternatives + an Alternative in a Single Net

- Application: optical flow (thus the name FlowNet)
  - Collaboration between our CV + ML labs, ECCV 2018

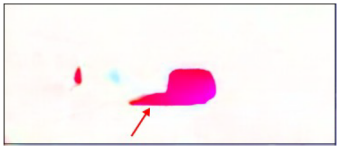


Standard | ensemble | predictive | predictive + ensembles | predictive + ensembles in a single net

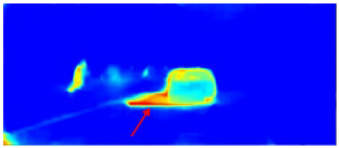
[Image source: Ilg et al, 2018]

As Desired, Large Uncertainty in Regions of Large Error

Image from KITTI dataset



Estimated optical flow



Estimated uncertainty

Also see the video

No network will ever be perfect,
but especially in safety-critical applications
it helps to know when we don't know

[Image source: Ilg et al, 2018]

Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  How can you obtain a predictive distribution from an ensemble of networks?
- Repetition:
  Name four ways to construct an ensemble of networks
- Repetition:
  How can you construct a network that outputs a predictive distribution for a regression task?

Lecture Overview

Foundations of Deep Learning, Winter Term 2021/22

Week 13: Uncertainty in Deep Learning

Summary, Further Reading, References

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Summary by learning goals

Having heard this lecture, you can now ...

- motivate the study of uncertainty in deep learning
- list some properties of Gaussian distributions
- derive Bayesian linear regression
- describe variational inference and derive the evidence lower bound
- describe MCMC and some MCMC algorithms
- explain prior-fitted networks and how they provide an alternative to variational inference and MCMC
- describe alternative methods to handle uncertainty in deep learning

Acknowledgement of Sources

Main sources for this lecture:

- Bayesian linear regression:
  - Chapter 2 of the excellent book Gaussian processes for Machine Learning
  - Philipp Hennig's Gaussian process tutorials
- MCMC: Chapter 17 of the Deep Learning book
- Prior-fitted networks: the original paper [Müller et al, 2022]

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