Bayesian Neural Networks for Text Classification and Regression

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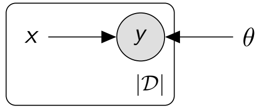
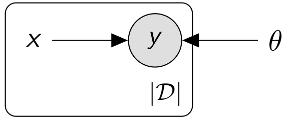
Probabilistic models parameterised by NNs

The typical text classifier or regressor consists of



- some text input x which we observe but do not model
  i.e. we do not attempt to estimate $p(x)$
- some random, though *observed*, target or response y
  e.g. a scalar in regression, a category in classification
- a deterministic mapping from input x and parameters θ
  to the *likelihood* $p(y|x, \theta)$
- mappings realised with the help of *NN architectures*

Example: Regression



$$Y|\theta, x \sim \mathcal{N}(\underbrace{\mu(x;\theta)}_{=u}, \underbrace{\sigma(x;\theta)}_{=s}^2)$$

$$p(y|x,\theta) = \frac{1}{\sqrt{2\pi s^2}} \exp\left(-\frac{(x-u)^2}{2s^2}\right)$$

- $\mu(\cdot;\theta)$ maps x to a location in $\mathbb{R}$
- $\sigma(\cdot;\theta)$ maps x to a scale in $\mathbb{R}_{>0}$
- θ denotes parameters of our NN blocks;

affine$_d(\cdot)$ maps its input to $\mathbb{R}^d$ via an affine transformation

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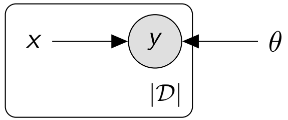

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Example architecture:

$$\mathbf{e}_i = \text{emb}(x_i) \qquad \mu(x;\theta) = \text{affine}_1(\mathbf{h})$$
$$\mathbf{h} = \text{rnn}(\mathbf{e}_1^n) \qquad \sigma(x;\theta) = \text{softplus}(\text{affine}_1(\mathbf{h}))$$

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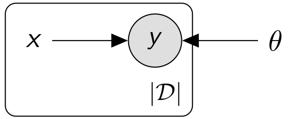
Example: Classification



$$Y|\theta, x \sim \mathrm{Cat}(\pi(x;\theta))$$
$$p(y|x,\theta) = \pi_y(x;\theta)$$

- $\pi(\cdot;\theta)$ maps x to a K-dimensional probability vector
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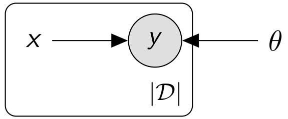

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Example architecture:

$$\begin{aligned} \mathbf{e}_i &= \mathrm{emb}(x_i) \\ \mathbf{h} &= \mathrm{rnn}(\mathbf{e}_1^n) \\ \pi(x;\theta) &= \mathrm{softmax}(\mathrm{affine}_K(\mathbf{h})) \end{aligned}$$

Parameter Estimation

Choose θ that maximises the log-likelihood function

$$\mathcal{L}(\theta|\mathcal{D}) = \sum_{\langle x,y\rangle\in\mathcal{D}} \log p(y|x,\theta)$$

aka *maximum likelihood estimation* (MLE)

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Search for θ using gradient-based methods
i.e. look for a solution to

$$\nabla_\theta \mathcal{L}(\theta|\mathcal{D}) = \mathbf{0}$$

- backpropagation automates differentiation
- unbiased gradient estimates suffice
  i.e. $\theta^{(t+1)} = \theta^{(t)} + \gamma_t \mathbb{E}_{\mathcal{S}\sim\mathcal{D}}\left[\nabla_{\theta^{(t)}} \mathcal{L}(\theta^{(t)}|\mathcal{S})\right]$

Outline

1 Bayes: what and why?

2 Choosing a prior

3 Posterior Inference for BNNs

4 Bayesian Dropout

Bayes: what and why?

- What is a Bayesian neural net (BNN)?

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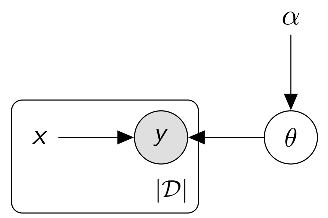
- What is a Bayesian neural net (BNN)?
- Why should we care about them?

What's a BNN?

BNN



Regression

$$Y|\theta, x \sim \mathcal{N}(\mu(x;\theta), \sigma(x;\theta)^2)$$

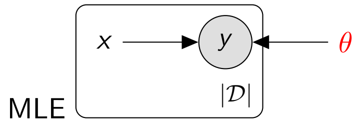
Classification

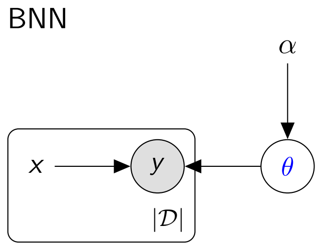
$$Y|\theta, x \sim \mathrm{Cat}(\pi(x;\theta))$$

with for example $\theta \sim \mathcal{N}(\underbrace{0, I}_{\alpha})$

- as before, NNs power the mapping from x and θ to $p(y|x,\theta)$
- though now θ is a *random variable* distributed according to a prior $p(\theta|\alpha)$

NNs and BNNs side by side





- MLE: assumes θ to be **given**
- BNN: all variables are treated alike, that is, they are random variables whether or not we call them *parameters*

BNNs also have deterministic parameters (e.g α)
we call those *hyperparameters* and they are ideally *fixed*

Optimising α, say using MLE, makes you an *Empirical Bayesian*, more on that later!

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For the theory, including philosophical, mathematical, and statistical perspectives see (Bernardo and Smith, 2009)

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Though there are philosophical reasons for adopting the Bayesian paradigm, I concentrate on practical ones.

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Then I ask

- how do we know we can trust $p(y|x, \theta)$ for any pair $\langle x, y \rangle$?

The importance of knowing what we don't know

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- the likelihood is itself a prediction
- one that's based on a particular instance of the model (θ)
- it tells us that this model supports our data, but does our data support this model?

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The posterior $p(\theta|\mathcal{D})$.

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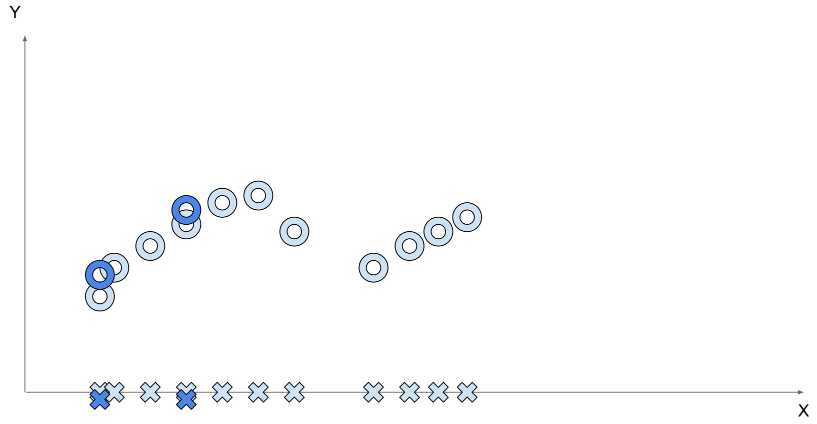
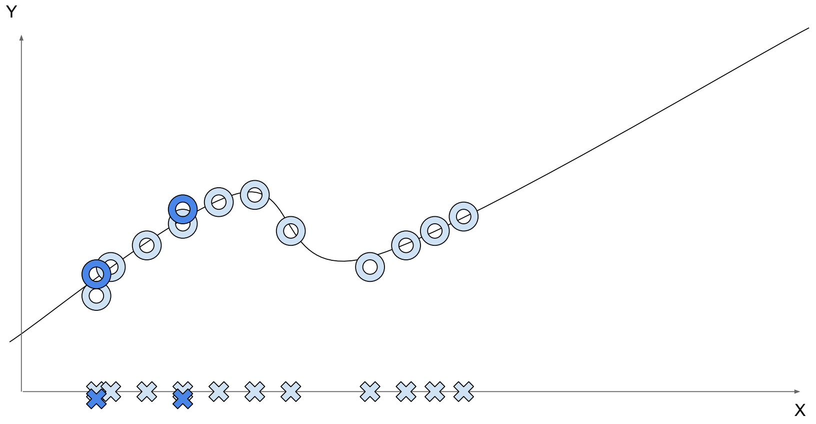
Uncertainty illustrated



Suppose a regression problem for which we have observations

Uncertainty illustrated



Let's approach with the help of NNs, i.e. $y = \mathrm{NN}(x; \theta)$

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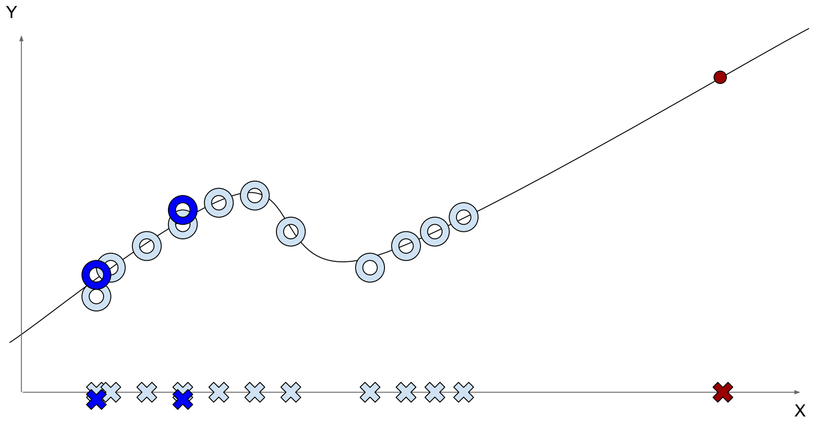

By design, it extrapolates predictions to unseen inputs, e.g. x_*

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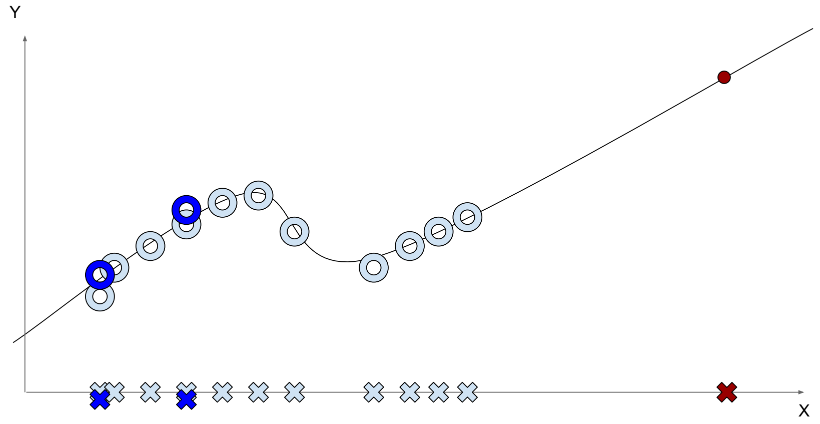

Can we trust our model given x_* is far from observations?

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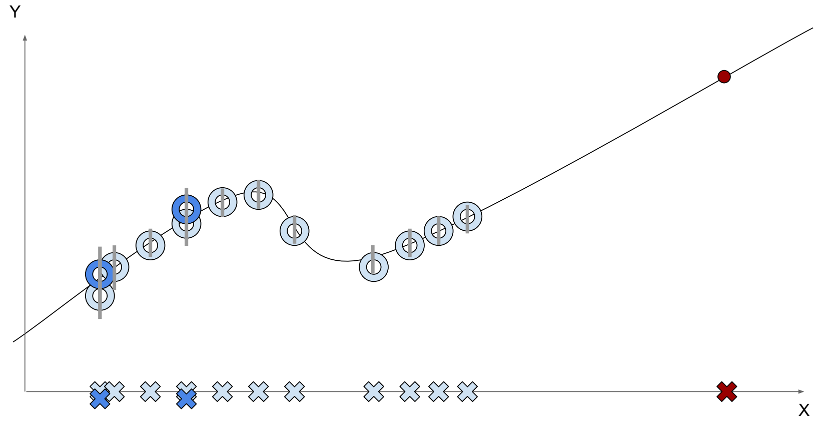
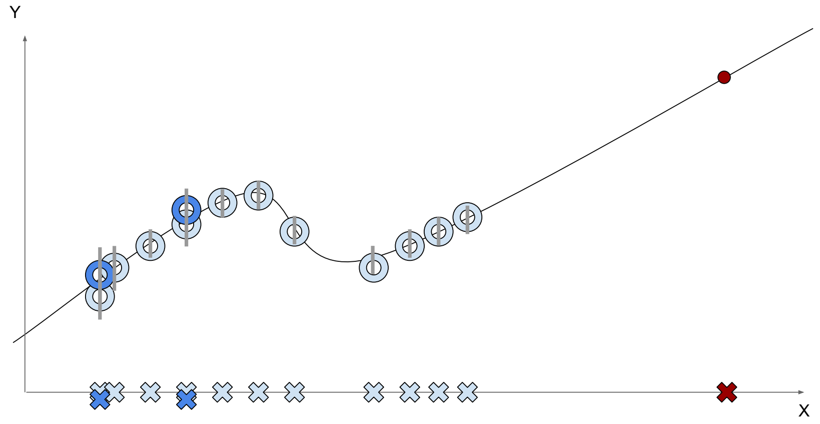


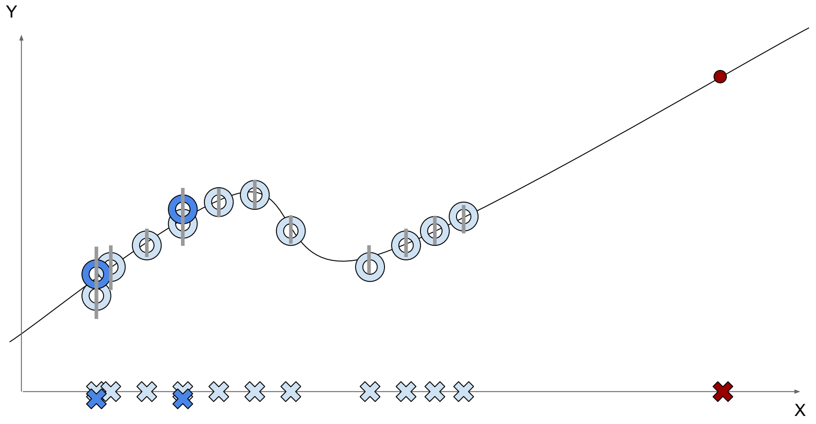
Let's fit Gaussians, i.e. $\mathcal{N}(\mu(x;\theta), \sigma(x;\theta)^2)$, around targets

Uncertainty illustrated



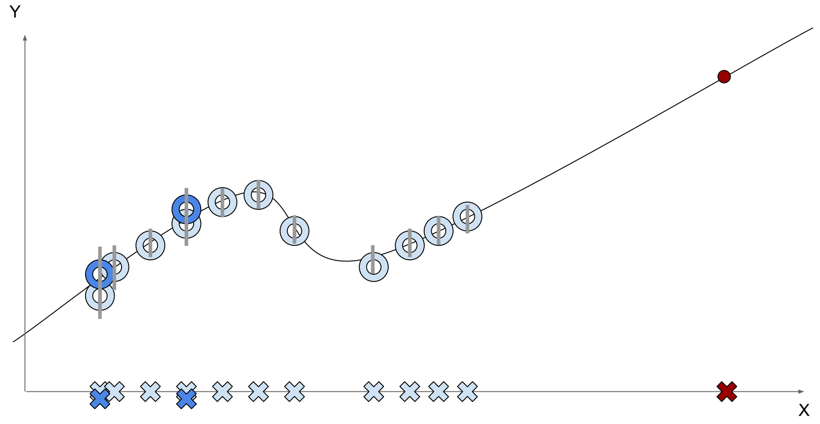
Note that we never observe much variability for a given input x

Uncertainty illustrated



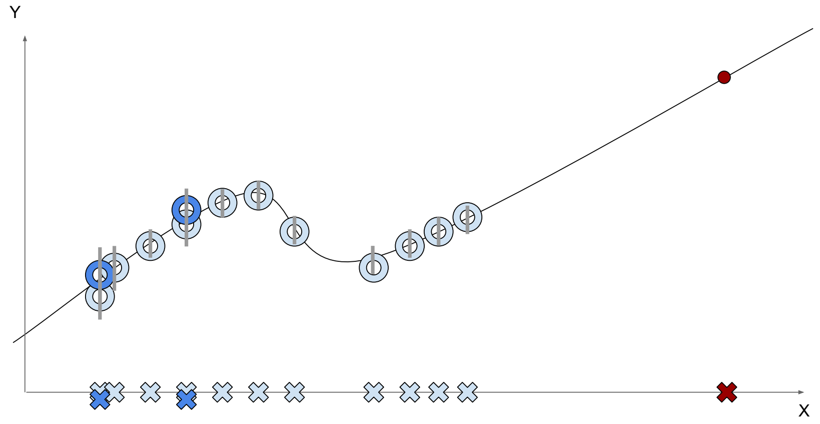
$\mu(x;\theta)$ learns to be on average close to every response for x

Uncertainty illustrated



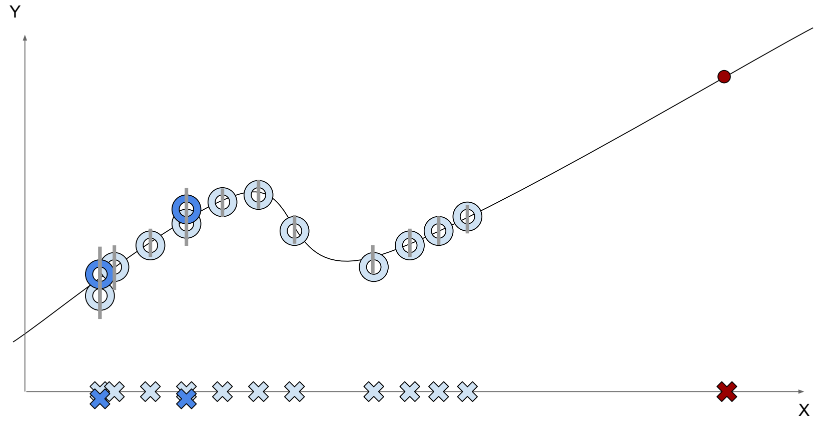
$\sigma(x;\theta)$ instead learns to cover all responses for x, but no more

Uncertainty illustrated



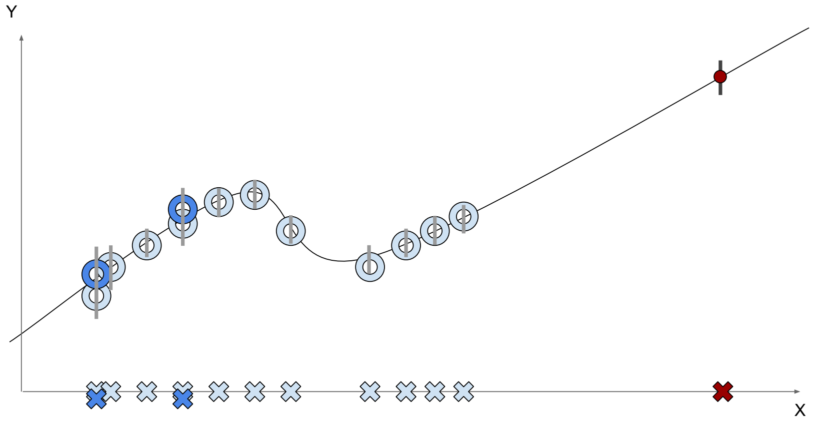
for MLE does not like covering more than observed responses

Uncertainty illustrated



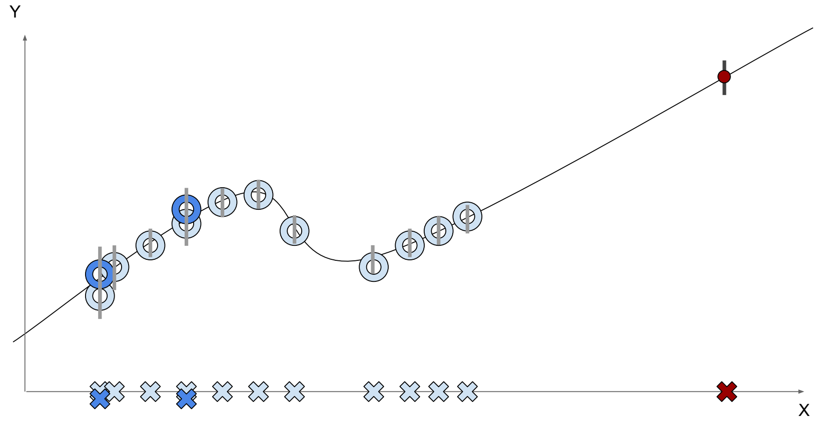
What is our expectation for $\sigma(x_*; \theta)$?

Uncertainty illustrated



For all we know, $\sigma(\cdot;\theta)$ likes to predict small values

Uncertainty illustrated



$\sigma(\cdot;\theta)$ seriously underestimates uncertainty for x_*

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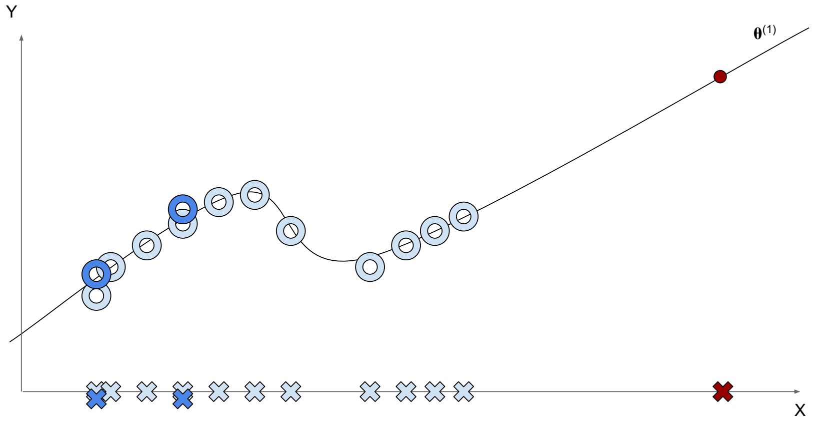
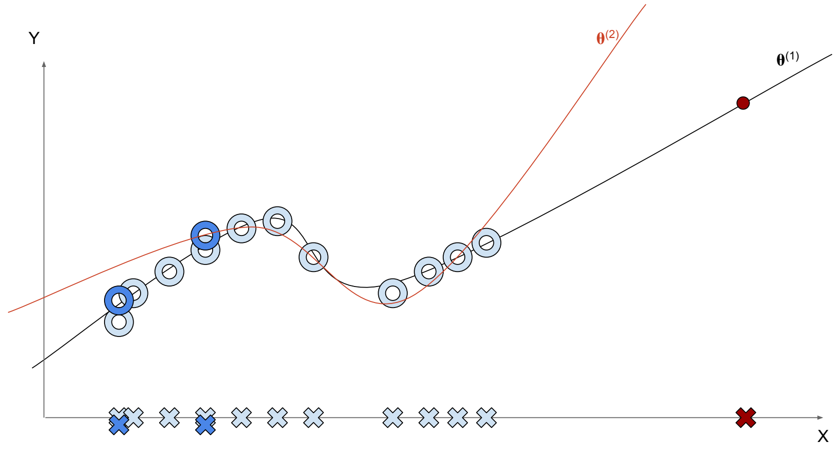


but what if, with probability $p(\theta^{(1)}|\mathcal{D})$, we consulted $\mu(x;\theta^{(1)})$?

Uncertainty illustrated



and $\mu(x; \theta^{(2)})$, with probability $p(\theta^{(2)}|\mathcal{D})$

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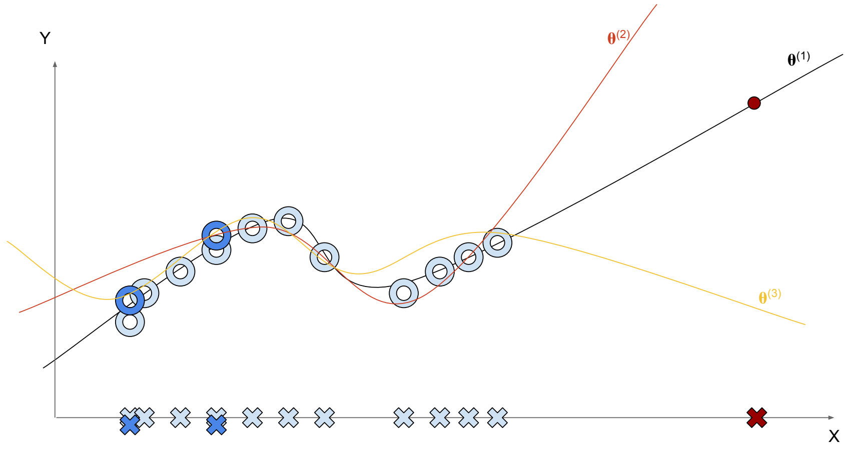
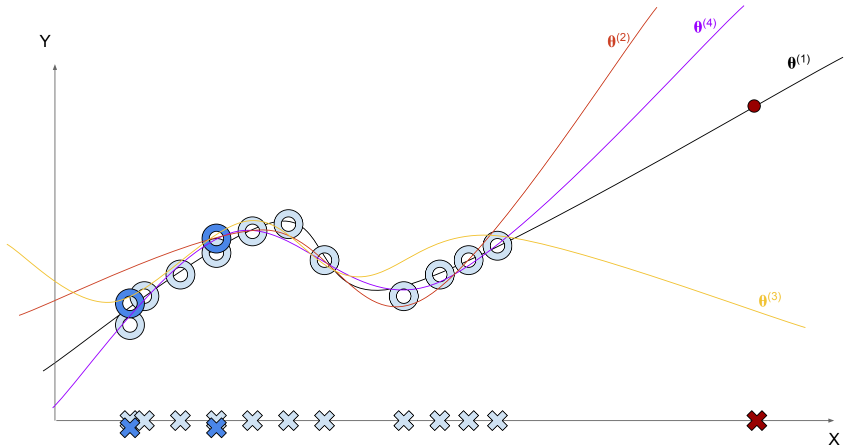


and $\mu(x;\theta^{(3)})$, with probability $p(\theta^{(3)}|\mathcal{D})$

Uncertainty illustrated



and $\mu(x; \theta^{(4)})$, with probability $p(\theta^{(4)}|\mathcal{D})$

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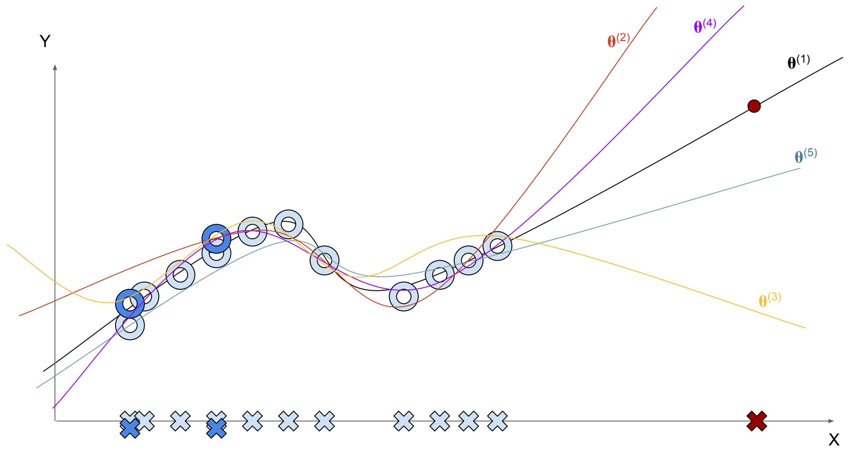

and $\mu(x; \theta^{(5)})$, with probability $p(\theta^{(5)}|\mathcal{D})$

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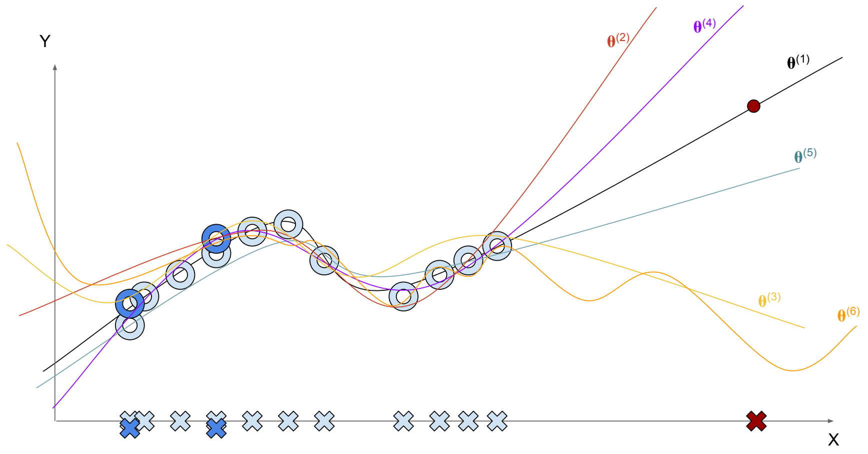

and $\mu(x;\theta^{(6)})$, with probability $p(\theta^{(6)}|\mathcal{D})$?

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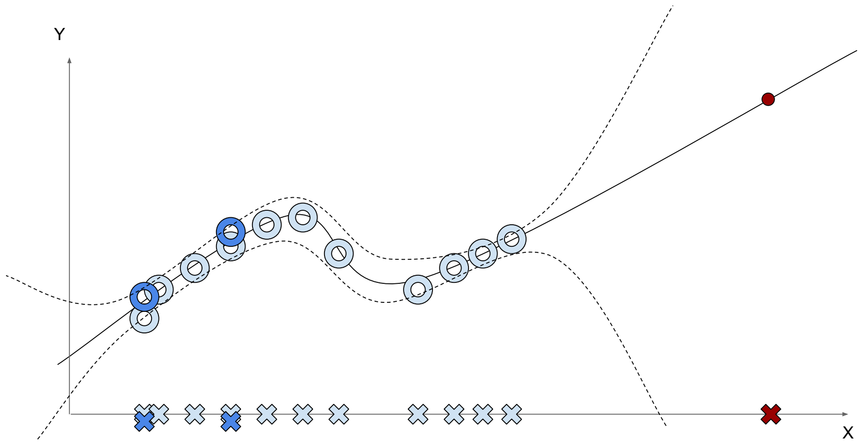

Suddenly, we are a lot less certain about predictions for x_*

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Ensembles reduce sensitivity of a prediction to initial conditions via average, i.e. $\hat{\mu}(x_*) = \frac{1}{S}\sum_{i=1}^{S} \mu(x_*; \theta^{(i)})$ for $\theta^{(i)} \sim \text{init}(\theta)$

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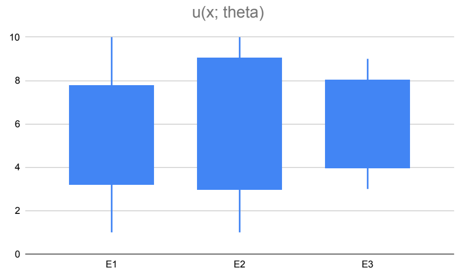
Note that eventually, it disregards the actual spread of $\mu(x_*;\theta)$



Bayesian Reasoning

Reasoning with *parametric BNNs* involves averaging over parameters

- in a Bayesian sense a *model* is a set of assumptions
  e.g. conditional independences, choice of prior, choice of likelihood, architecture blocks, hyperparameters
- formally we should write $p(\mathcal{D}, \theta|\mathcal{M})$ where $\mathcal{M}$ is the model assumptions — we omit $\mathcal{M}$ for brevity

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- uncertainty estimates are based on this posterior probability

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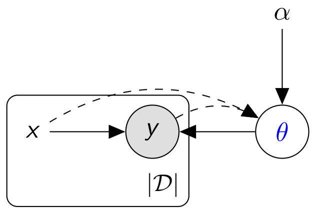
We will discuss *nonparametric Bayesian models* later and will see that uncertainty estimates are based on yet more robust model assumptions.

Bayesian Inference

Posterior inference



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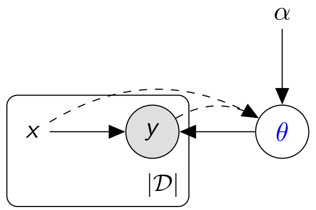

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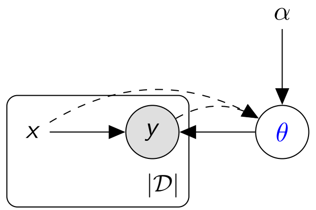

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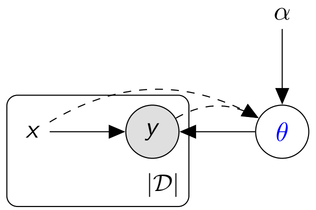

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$$p(\mathcal{D}) = \int p(\theta)p(\mathcal{D}|\theta)\mathrm{d}\theta$$

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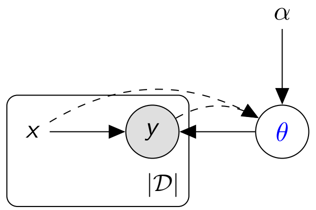

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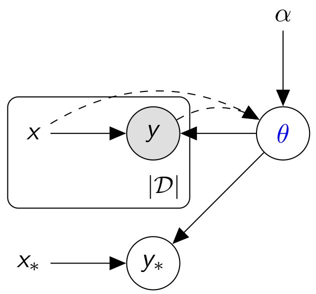
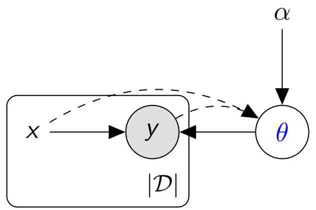
Posterior predictive distribution



$$p(y_*|x_*,\mathcal{D}) =$$

Bayesian Inference

Posterior inference



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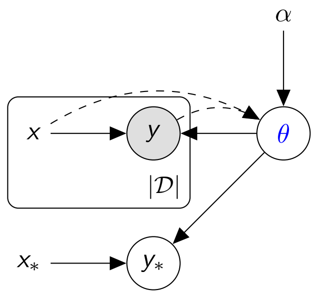

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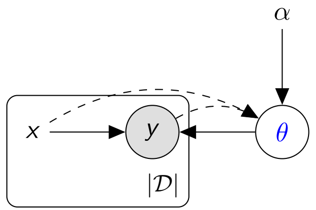

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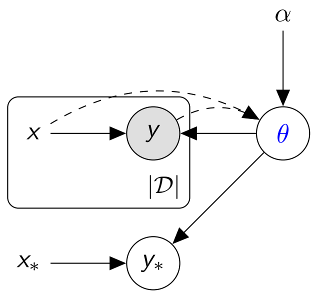

$$\begin{aligned} p(y_*|x_*,\mathcal{D}) &= \int p(y_*,\theta|\mathcal{D},x_*)\mathrm{d}\theta \\ &= \int p(\theta|\mathcal{D})p(y_*|x_*,\theta)\mathrm{d}\theta \end{aligned}$$

Conditional independence
$Y_* \perp \mathcal{D} \mid \theta$

Terminology

Prior	$p(\theta)$
Likelihood	$p(\mathcal{D}\|\theta)$
Posterior	$p(\theta\|\mathcal{D})$
Evidence (aka Marginal Likelihood)	$p(\mathcal{D})$
Posterior predictive distribution	$p(y_*\|x_*, \mathcal{D})$
Probabilistic inference	marginalisation/expectation

(remark: in DL the word *inference* is used differently)

Summary

BNNs are NNs with priors over parameters

The goal is to take uncertainty seriously

Uncertainty estimates help make decisions, e.g.

- model comparison and selection
- when a human should intervene

Other uses include

- reinforcement learning
- active learning
- meta-learning
- learn from streaming data

Bayesian reasoning requires probabilistic inference

Literature

BDA3 Gelman et al. (2013, Chapter 1)

Outline

1. Bayes: what and why?
2. Choosing a prior
3. Posterior Inference for BNNs
4. Bayesian Dropout

How does one choose a prior?

A prior is meant to capture our beliefs about the phenomenon we are modelling – in this case the relationship between x and y

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Let's first consider a simple example: mixture model

$$Z|\pi \sim \mathrm{Cat}(\pi)$$
$$X|\theta, z \sim \mathrm{Cat}(\theta^{(z)})$$

We first select a discrete mixture component z, this component then selects a Categorical distribution from which we generate a data point x

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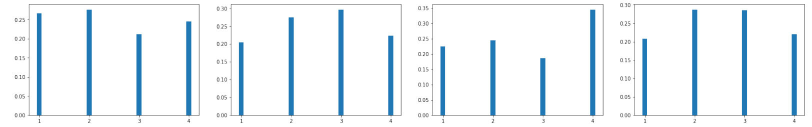
Bayes

$$\pi|\alpha \sim \text{Dir}(\alpha \mathbf{1}_K)$$
$$\theta^{(k)}|\beta \sim \text{Dir}(\beta \mathbf{1}_V)$$

What makes good mixing coefficients?

Say we have $K = 4$ components, I show a few samples for $\pi \sim \mathrm{Dir}(10 \times \mathbf{1}_K)$



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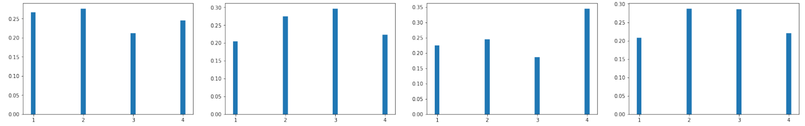

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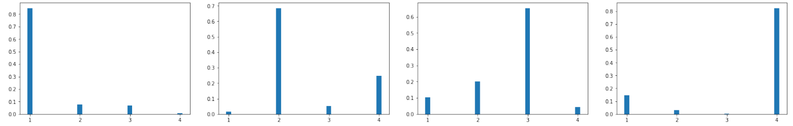

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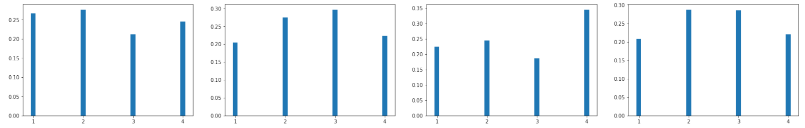

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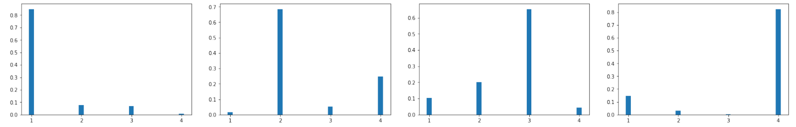

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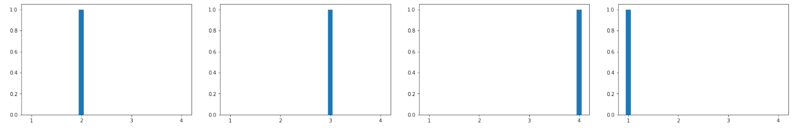

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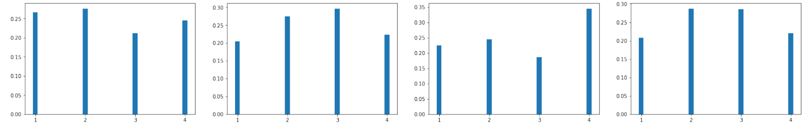

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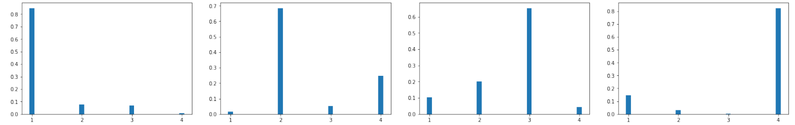

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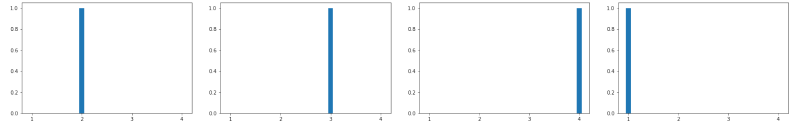
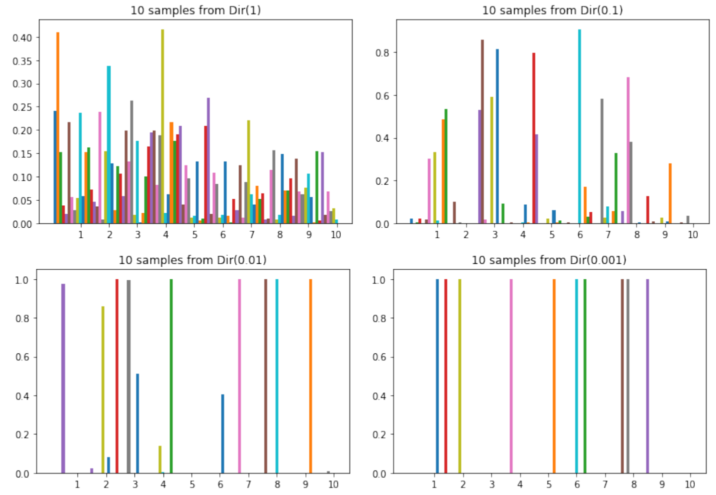


Can you make any assumptions before observing data?

What makes a good conditional?

Say we have $V = 10$ types of data points, I show samples $\theta^{(k)}|\beta \sim \text{Dir}(\beta)$



Mixture Models are Simple to Understand

The unobservable random variables π and $\theta^{(k)}$ are rather interpretable

- it's clear that we want assignments to be unambiguous
  sparse mixing weights
- it's clear that we want components to be rather selective
  sparse conditionals
- it's clear that we don't know the identify of clusters
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Meaning of weights in NNs are quite obscure!
Who can tell what aspect of a classifier any of the LSTM parameters controls?

Learning Functions

We are essentially using NNs to learn some unknown function that maps from data to probabilities — which then support decisions

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Fair, but how about this,

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- *How about the fact that we employ convex optimisers?*

It's hard to talk about what functions we can learn when the most important factors are *amount of data* and the *success of a local optimiser*

Random functions

Let's consider what happens when our parameters are random following a given prior.

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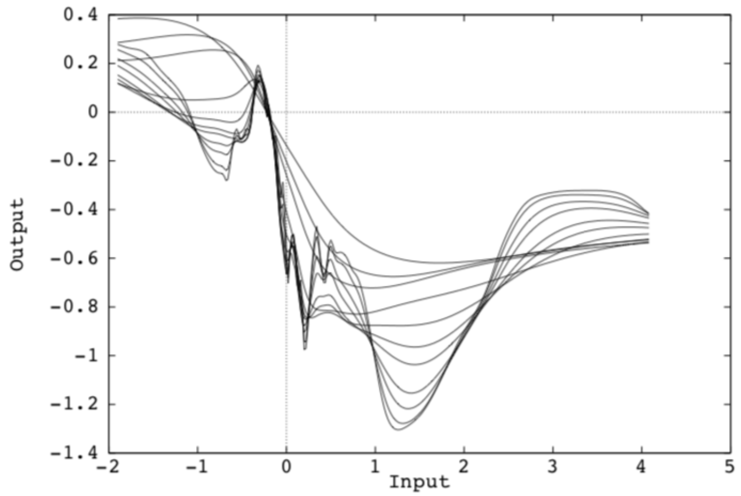
Sampling from these priors and performing forward passes with the network will expose a range of functions

- some might have specific properties
  e.g. smoothness, periodicity
- some will be preferred over others
- some may be impossible
  e.g. Brownian functions vs infinitely smooth functions

Draws



Example from MacKay (1998)

Priors

Priors are not about making things random for no reason
they are about encoding assumptions, or inductive biases!

Let's turn to known priors over functions!

Gaussian Processes

Consider the case of regression, where $y = f(x) + \epsilon$ for some $\epsilon \sim \mathcal{N}(0, \tau^{-1})$

- this implies $Y|f(x) \sim \mathcal{N}(f(x), \tau^{-1})$
- let's design a prior for $f(x)$
  Note that a parametric way to do so is to say $f(x) = w^\top \phi(x)$ for some fixed feature function $\phi(x)$ and impose a prior on w, but then again, what are the properties of such a prior?

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The probability distribution of a function $f(x)$ is a Gaussian process (GP) if for any finite selection of points $x^{(1)}, \ldots, x^{(N)}$ the density $p(f(x^{(1)}), \ldots, f(x^{(N)}))$ is a Gaussian.

A function represents an infinite object, but in ML we typically only reason over finite datasets!

GP prior

I'll employ boldfacing to denote a collection of N datapoints, e.g. $\mathbf{x} = \{x^{(1)}, \ldots, x^{(N)}\}$ and $\mathbf{y} = \{y^{(1)}, \ldots, y^{(N)}\}$, indexing returns an element, e.g. $x_i \overset{\text{def}}{=} x^{(i)}$.

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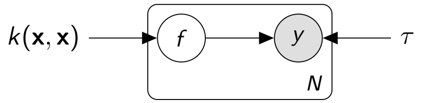
GP prior

$$\mathbf{F} | \mathbf{x} \sim \mathcal{N}(\mathbf{0}, k(\mathbf{x}, \mathbf{x}))$$
$$\mathbf{Y} | \mathbf{f} \sim \mathcal{N}(\mathbf{f}, \tau^{-1} \mathbf{I}_N)$$



The covariance matrix is defined by a kernel function $k(x, x')$

- I abuse notation and use $k(\mathbf{x}, \mathbf{x})$ to denote the $N \times N$ matrix $\mathbf{K}$ of kernel assessments, i.e. $K_{i,j} = k(x_i, x_j)$
- $k(x', \mathbf{x})$ denotes a row-vector of kernel assessments

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GP Inference

Given a collection $\mathbf{y}, \mathbf{f} | \mathbf{x}$ of jointly Gaussian variables, what's the family of the marginal?

$$p(\mathbf{y}|\mathbf{x}) = \int p(\mathbf{y}, \mathbf{f}|\mathbf{x}) \mathrm{d}\mathbf{f} =$$

Bishop (2006, Chapter 2) for operations with Multivariate Gaussians

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Recall: marginals of a multivariate Gaussian are Gaussians!

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Thus what's the family of the posterior?

$$p(\mathbf{f}|\mathbf{x}, \mathbf{y}) = \frac{p(\mathbf{y}, \mathbf{f}|\mathbf{x})}{p(\mathbf{y}|\mathbf{x})}$$

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$$p(\mathbf{f}|\mathbf{x}, \mathbf{y}) = \frac{p(\mathbf{y}, \mathbf{f}|\mathbf{x})}{p(\mathbf{y}|\mathbf{x})}$$

Recall: conditioning on a subset of a multivariate Gaussian yields a multivariate Guassian

Bishop (2006, Chapter 2) for operations with Multivariate Gaussians

Exact Inference with GPs

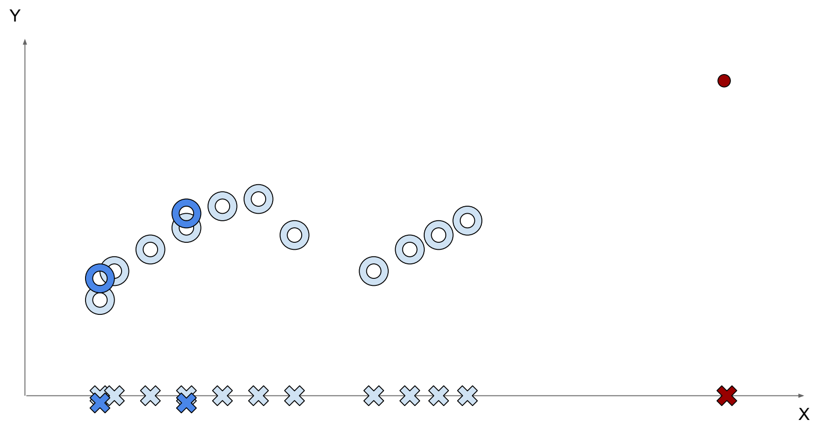
Posterior

$$\begin{aligned}\mathbf{F}|\mathbf{x},\mathbf{y} &\sim \mathcal{N}(\mathbf{m}_{\text{post}},\mathbf{K}_{\text{post}})\\ \mathbf{m}_{\text{post}} &= \mathbf{K}(\mathbf{K}+\tau^{-1}\mathbf{I}_N)^{-1}\mathbf{y}\\ \mathbf{K}_{\text{post}} &= \mathbf{K}-\mathbf{K}(\mathbf{K}+\tau^{-1}\mathbf{I}_N)^{-1}\mathbf{K}^\top\end{aligned}$$

Posterior predictive distribution:

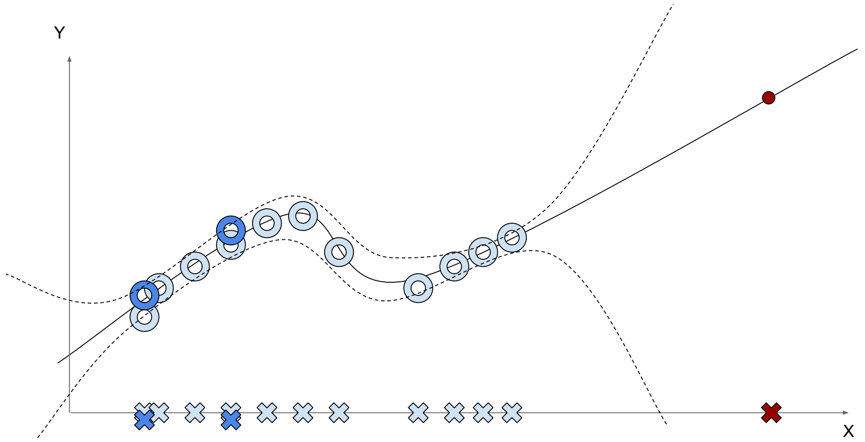
$$\begin{aligned}Y_*|x_*,\mathbf{x},\mathbf{y} \sim \mathcal{N}(&k(x_*,\mathbf{x})(\mathbf{K}+\tau^{-1}\mathbf{I}_N)^{-1}\mathbf{y},\\ &k(x_*,x_*)+\tau^{-1}-k(x_*,\mathbf{x})(\mathbf{K}+\tau^{-1}\mathbf{I}_N)^{-1}k(x_*,\mathbf{x})^\top)\end{aligned}$$

Uncertainty illustrated (revisited)



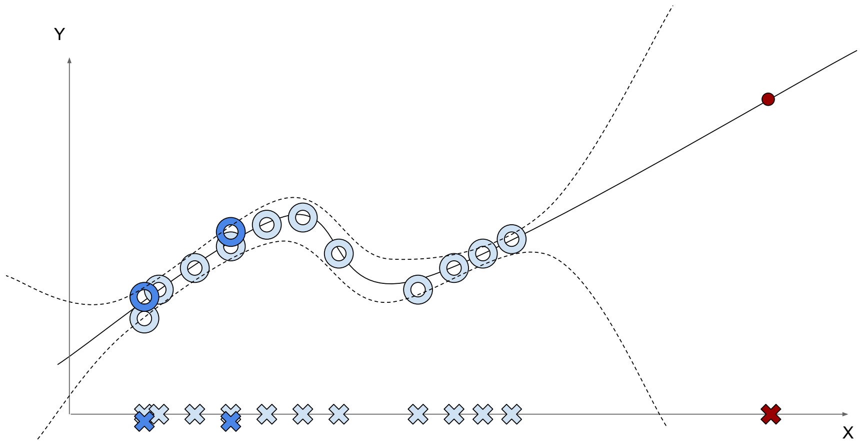
Let's get back to this

Uncertainty illustrated (revisited)



What if uncertainty depended on the distance to observations?

Uncertainty illustrated (revisited)



Kernels in GPs operationalise exactly this notion

Terminology

Random functions: latent treatment to $f(x)$

Kernel: $k : \mathcal{X} \times X \rightarrow \mathbb{R}$ such that $k(x, x')$ is the covariance between $f(x)$ and $f(x')$

Gaussian process prior: $F \sim \mathcal{G}P(0, k)$

GP inference: marginals and conditionals are Gaussians

Summary

Priors are as good as our understanding of what class of models they favour

NNs are meant to learn unknown functions

BNNs learn a distribution over functions by treating parameters as random variables

The effect of a parameter over the learned function is unclear

A prior over functions can be specified in a non-parametric way via specification of a covariance (kernel) function

A GP prior is a well-studied prior over functions

Literature

David MacKay's pioneering work	
Bayesian interpolation	MacKay (1992a)
or go all the way through his PhD thesis	MacKay (1992b)
Priors for Infinite Networks	Neal (1994, 1996)
Multivariate Gaussians	Bishop (2006, Chapter 2)
Introduction to GPs	MacKay (1998)

GP summer school classes by Neil Laurence

Kernel Cookbook by David Duvenaud

Neal (1994): `https://www.cs.toronto.edu/~radford/ftp/pin.pdf`

Outline

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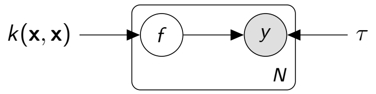
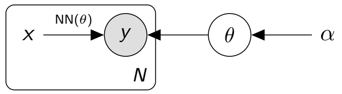
GPs vs BNNs

GP



BNN



GP's a non-parametric models

- the complexity (or capacity) of the model grows with the data
- posterior predictive is known and tractable
- we know a lot about the random functions we get

BNNs are parametric models

- the complexity (or capacity) is pre-specified
- posterior predictive is unknown and intractable
- we know little about the random functions we get

Why don't we always use GPs then?

Flexibility

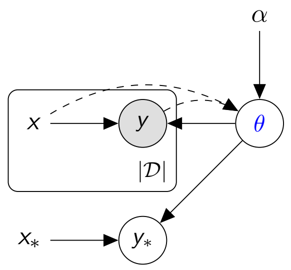
- kernels for text are fewer, less convenient, and less well-understood
- x can be very high-dimensional (and perhaps we have less intuitions to choose a kernel)

Computational complexity

- exact GP inference takes $O(N^3)$
- it's possible to scale them up, but that's an active research topic
- many solutions are specific to continuous inputs

Let’s then consider Bayesian inference for a BNN

This is essentially what we have to address



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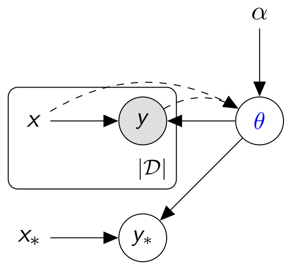

That is,

$$p(y_*, \theta|\mathcal{D}, x_*) = \int p(y_*, \theta|\mathcal{D})\mathrm{d}\theta = \int p(\theta|\mathcal{D})p(y_*|\theta, x_*)\mathrm{d}\theta$$

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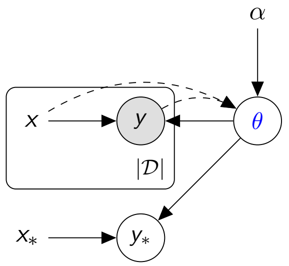

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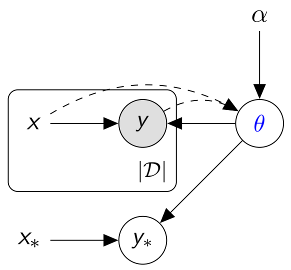
But $p(\theta|\mathcal{D}) = \int p(\theta|\alpha)p(\mathcal{D}|\theta)\mathrm{d}\theta$ is intractable

Let's then consider Bayesian inference for a BNN

This is essentially what we have to address



That is,

$$p(y_*, \theta|\mathcal{D}, x_*) = \int p(y_*, \theta|\mathcal{D})\mathrm{d}\theta = \int p(\theta|\mathcal{D})p(y_*|\theta, x_*)\mathrm{d}\theta$$

But $p(\theta|\mathcal{D}) = \int p(\theta|\alpha)p(\mathcal{D}|\theta)\mathrm{d}\theta$ is intractable
Let's learn a proxy $q(\theta|\lambda)$!

Variational Inference

Let's learn a proxy $q(\theta|\lambda)$ to $p(\theta|\mathcal{D})$ and solve

$$p(y_*, \theta|\mathcal{D}, x_*) = \int p(\theta|\mathcal{D}) p(y_*|\theta, x_*) \mathrm{d}\theta \approx \int q(\theta|\lambda) p(y_*|\theta, x_*) \mathrm{d}\theta$$

An alternative with guarantees is MCMC – as discussed in ML2. Example: MCMC for a mixture of Gaussians by David Blei.

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Principle: choose an approximation that minimises KL-divergence

$$\begin{aligned} &\arg\min_{q(\theta)} \; \mathrm{KL}(q(\theta)||p(\theta|\mathcal{D})) \\ &= \arg\min_{q(\theta)} \; \mathbb{E}_{q(\theta)}\left[\log \frac{q(\theta|\lambda)}{p(\theta|\mathcal{D})}\right] \quad \text{definition of KL} \end{aligned}$$

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Evidence Lowerbound (ELBO)

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All quantities are either tractable or easy to estimate by sampling!

ELBO continued

Parametric assumption

$$\begin{aligned}&\arg\max_{q(\theta)}\ \mathbb{E}_{q(\theta)}\left[\log p(\theta,\mathcal{D})\right]+\mathbb{H}(q(\theta))\\ &=\arg\max_{\lambda}\ \mathbb{E}_{q(\theta|\lambda)}\left[\log p(\theta,\mathcal{D})\right]+\mathbb{H}(q(\theta|\lambda))\end{aligned}$$

Recall

$$p(\theta,\mathcal{D})=p(\theta)\prod_{i=1}^{N}p(y^{(i)}|\theta,x^{(i)})$$

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And thus the ELBO evaluates to

$$\begin{aligned}&\mathbb{E}_{q(\theta|\lambda)}\left[\log p(\theta) + \sum_{i=1}^{N} \log p(y^{(i)}|\theta, x^{(i)})\right] + \mathbb{H}(q(\theta|\lambda))\\ &= \mathbb{E}_{q(\theta|\lambda)}\left[\sum_{i=1}^{N} \log p(y^{(i)}|\theta, x^{(i)})\right] - \mathrm{KL}(q(\theta|\lambda)||p(\theta))\end{aligned}$$

Mean Field Assumption

Let $\theta \in \mathbb{R}^D$. The simplest approximate posterior is

We can group parameters and assume independence of groups (e.g. layers).

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$$\mathrm{KL}(q(\theta|\lambda)||p(\theta)) = \sum_{d=1}^{D} \underbrace{\mathrm{KL}(q(\theta_d|\lambda)||p(\theta_d))}_{\text{closed form}}$$

is known in closed form.

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Choosing λ

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What's the workhorse of optimisation in deep learning?

Gradient-based optimisation for λ

We take steps in the direction that maximises the ELBO

$$\nabla_\lambda \,\mathrm{ELBO} = \nabla_\lambda \mathbb{E}_{q(\theta|\lambda)}\left[\sum_{i=1}^{N} \log p(y^{(i)}|\theta, x^{(i)})\right] - \nabla_\lambda \,\mathrm{KL}(q(\theta|\lambda)||p(\theta))$$

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$$\sum_{i=1}^{N} \log p(y^{(i)}|\theta, x^{(i)}) \quad \text{is certainly prohibitive!}$$

Stochastic gradients are allowed

Noisy, but unbiased, gradients:

$$\nabla_\lambda \mathbb{E}_{q(\theta|\lambda)}\left[\sum_{i=1}^{N} \log p(y^{(i)}|\theta, x^{(i)})\right]$$

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&\overset{\text{MC}}{\approx} \frac{N}{M} \sum_{i=1}^{M} \nabla_\lambda \mathbb{E}_{q(\theta|\lambda)}\left[\log p(y^{(i)}|\theta, x^{(i)})\right] && I \sim \mathcal{U}(1/N)
\end{aligned}
$$

Sample a batch, solve expected value under q, then take gradient.

Challenge

$\nabla_\lambda \text{ELBO} =$

$$\nabla_\lambda \mathbb{E}_{q(\theta|\lambda)} \left[\sum_{i=1}^{N} \log p(y^{(i)}|\theta, x^{(i)}) \right] - \nabla_\lambda \text{KL}(q(\theta|\lambda)||p(\theta))$$

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- we can compute KL and thus differentiate it
- mini-batching is allowed, so we can compute the first term for a few datapoints at a time
- but can we really solve $\mathbb{E}_{q(\theta|\lambda)}\left[\log p(y^{(i)}|\theta, x^{(i)})\right]$ for even a single instance?

Reparameterisation

Let there be a bijective transformation $t(\epsilon, \lambda)$, such that

$$\epsilon \sim \phi(\epsilon) \quad \Leftrightarrow \quad t(\epsilon, \lambda) \sim q(\theta|\lambda)$$

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Then it's clear that

- $\theta = t(\epsilon, \lambda)$ for $\epsilon \sim \phi(\cdot)$
- and $\epsilon = t^{-1}(\theta, \lambda)$ for $\theta \sim q(\cdot|\lambda)$

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Example: location-scale families such as the Normal distribution

$$\theta_d = \underbrace{\mu_d + \epsilon_d \sigma_d}_{=t(\epsilon_d, \lambda_d)} \qquad\qquad \epsilon_d = \frac{\theta_d - \mu_d}{\sigma_d} \sim \mathcal{N}(0, 1)$$

$$\lambda_d = (\mu_d, \sigma_d) \text{ and } \sigma_d > 0$$

Reparameterisation (cont.)

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Can you prove this law? Tip: use integration by substitution and change of density theorem.

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The *law of the unconscious statistician* says

$$\mathbb{E}_{q(\theta|\lambda)}\left[f(\theta)\right] = \mathbb{E}_{\phi(\epsilon)}\left[f(\theta = t(\epsilon, \lambda))\right]$$

Can you prove this law? Tip: use integration by substitution and change of density theorem.

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Assume we pick $q(\theta|\lambda)$ from a reparameterisable family
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Reparameterised Gradient Estimate

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$$\overset{\text{MC}}{\approx} \left(\frac{M}{NK}\sum_{k=1}^{K}\sum_{i=1}^{M}\nabla_\lambda \log p(y^{(i)}|\underbrace{t(\epsilon^{(k)},\lambda)}_{=\theta^{(k)}},x^{(i)})\right)$$

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- Sample parameters via deterministic reparameterisation
- Sample batch
- Compute likelihood and KL: forward
- Sampling parameters first allows for efficient parallel implementation

After training?

Training now gives you a point estimate for λ
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- it should prefer models that are likely after observing data $\mathcal{D}$ in light of whatever prior assumptions we made
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- $p(y_*|\mathcal{D}, x_*) \approx \int q(\theta|\lambda)p(y_*|\theta, x_*)\mathrm{d}\theta$
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We can also estimate $p(\mathcal{D})$ using q and the importance sampling

Terminology

Approximate posterior	$q(\theta\|\lambda)$
Variational inference	$\arg\min_{q(\theta)} \ \mathrm{KL}(q(\theta)\|\|p(\theta\|\mathcal{D}))$
ELBO	$\mathbb{E}_{q(\theta)}[\log p(\mathcal{D}\|\theta)] - \mathrm{KL}(q(\theta)\|\|p(\theta))$
Mean field assumption	$q(\theta\|\lambda) = \prod_{d=1}^{D} q(\theta_d\|\lambda_d)$

Reparameterised gradients

$$\nabla_\lambda \mathbb{E}_{q(\theta|\lambda)}\left[f(\theta)\right] = \mathbb{E}_{\phi(\epsilon)}\left[\nabla_\theta f(\theta) \nabla_\lambda t(\epsilon, \lambda)\right]$$

Posterior predictive distribution

$$p(y_*|\mathcal{D}, x_*) \approx \int q(\theta|\lambda) p(y_*|\theta, x_*) \mathrm{d}\theta$$

Summary

VI tuns inference into optimisation and gives you a proxy to $p(\theta|\mathcal{D})$

Estimates of posterior predictive mean and variance

- help you decide whether or not to make a decision
  - in classification: consider plotting precision and recall against predictive variance
  - in regression: interval in which you expect a response to be

Estimates of marginal likelihood

- help you compare models under different hyperparameters

Caveat: limited understanding about the impact of our priors

Literature

Variational inference	Blei et al. (2017)
Stochastic VI	Hoffman et al. (2013)
for nonconjugate inference	Titsias and Lázaro-Gredilla (2014)
Bayes by backprop	Blundell et al. (2015)
Model comparison	MacKay (1992a)

Outline

1 Bayes: what and why?

2 Choosing a prior

3 Posterior Inference for BNNs

4 Bayesian Dropout

Dropout

A **very** simple technique to make MLE more robust

- stochastic training: with probability $1 - p$, "drop" inputs to a fully connected layer
- possibly use L_2 regularisation (because why not?)
- deterministic test: disable "dropout" and scale weights by p

Srivastava et al. (2014)

Relate dropout to BNNs

BNNs come with a somewhat disappointing fact, that we have no clue what classes of random functions a given prior leads to

Many BNNs however can be seen as an approximation to a GP

- and the nonlinearities we employ correspond to a certain known kernel

Then let's see that variational inference for this model, using a pretty specific approximation $q(\theta|\lambda)$, turns dropout into approximate inference for an approximate GP.

The consequence is that we gain access to estimates of marginal likelihood and posterior predictive distribution

Notation

$\mathbf{w}$ is a C-dimensional column vector of parameters

$\mathbf{W} = [\mathbf{w}_r^\top]_{r=1}^R$ stacks row vectors into a $R \times C$ matrix

$\mathbf{x}$ is an I-dimensional input

$\mathbf{y}$ is an O-dimensional output

$\mathbf{x}_{1:N}, \mathbf{y}_{1:N}$ is a collection of input-output pairs

$\mathbf{y}_{:,d}$ gather the dth output of each observation

$\mathcal{N}(\mathbf{y}_{1:N}|\mathbf{m}_{1:N}, \mathbf{I}_N)$ denotes O independent multivariate Gaussians
i.e. $\prod_{d=1}^O \mathcal{N}(\mathbf{y}_{:,d}|\mathbf{m}_{:,d}, \mathbf{I}_N)$

A GP approximation

We specify a GP prior by specifying a kernel. Valid kernels can be composed into other valid kernels.

Formal properties of Kernels (Shawe-Taylor and Cristianini, 2004, Chapter 3)

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We specify a GP prior by specifying a kernel. Valid kernels can be composed into other valid kernels. For example:

$$k(\mathbf{x}, \mathbf{x}') = \int p(\mathbf{w}) p(b) \sigma(\mathbf{w}^\top \mathbf{x} + b) \sigma(\mathbf{w}^\top \mathbf{x}' + b) \mathrm{d}\mathbf{w} \mathrm{d}b$$

This particular kernel is not tractable to assess: we cannot solve the integral for general $p(\mathbf{w}, b)$ and nonlinearity $\sigma(\cdot)$.

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But we know MC estimation! For a fixed number of samples H

$$\hat{k}(\mathbf{x}, \mathbf{x}') = \frac{1}{H}\sum_{s=1}^{H} \sigma(\mathbf{w}_s^\top \mathbf{x} + b_s)\sigma(\mathbf{w}_s^\top \mathbf{x}' + b_s)$$

where $\mathbf{w}_s \sim p(\mathbf{w})$ and $b_s \sim p(b)$

Formal properties of Kernels (Shawe-Taylor and Cristianini, 2004, Chapter 3)

GP based on $\hat{k}$

We can immediately define a GP using this new kernel

$$
\begin{aligned}
b_s &\sim \mathcal{N}(0, l_0^{-2}) \\
\mathbf{b} &= [b_1, \ldots, b_H]^\top \\
\mathbf{w}_s &\sim \mathcal{N}(0, l^{-2}\mathbf{I}_I) \\
\mathbf{W}_1 &= [\mathbf{w}_s^\top]_{s=1}^H
\end{aligned}
$$

$$
\begin{aligned}
\hat{\mathbf{K}} &= \hat{k}(\mathbf{x}_{1:N}, \mathbf{x}_{1:N}) \\
\mathbf{F}|\mathbf{x}, \mathbf{W}_1, \mathbf{b} &\sim \mathcal{N}(\mathbf{0}, \hat{\mathbf{K}}) \\
\mathbf{Y}|\mathbf{f} &\sim \mathcal{N}(\mathbf{f}, \tau^{-1}\mathbf{I}_N)
\end{aligned}
$$

Recall that $\hat{K}_{ij} = \frac{1}{H}\sum_{s=1}^{H} \sigma(\mathbf{w}_s^\top \mathbf{x}_i + b)\sigma(\mathbf{w}_s^\top \mathbf{x}_j + b)$

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Note that we have essentially parameterised our kernel and imposed a prior on the kernel parameters.

For any given parameter configuration $\mathbf{W}_1$ and $\mathbf{b}$, we get a GP:

$$p(\mathbf{y}_{1:N}|\mathbf{x}_{1:N}) = \int p(\mathbf{b})p(\mathbf{W}_1)p(\mathbf{y}_{1:N}|\mathbf{f}_{1:N})p(\mathbf{f}_{1:N}|\mathbf{W}_1, \mathbf{b}, \mathbf{x}_{1:N})\mathrm{d}\mathbf{f}_{1:N}\mathrm{d}\mathbf{W}_1\mathrm{d}\mathbf{b}$$

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Regression vs Classification

Regression

$$\mathbf{Y}|\mathbf{f} \sim \mathcal{N}(\mathbf{f}, \tau^{-1}\mathbf{I}_N)$$

Classification

$$\mathbf{Y}|\mathbf{f} \sim \mathcal{N}(\mathbf{f}, 0\mathbf{I}_N)$$
$$C|\mathbf{y} \sim \text{Cat}(\text{softmax}(\mathbf{y}))$$

- the GP is essentially inducing a distribution over logits
- note the change of notation (to be closer to Gal's), here **y** is not an observation, c is

Marginalise $\mathbf{f}$

We can marginalise $\mathbf{f}$ for an assignment of $\mathbf{W}_1$ and $\mathbf{b}$

Can you show that $\hat{\mathbf{K}} = \Phi\Phi^\top$?

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Note that $\hat{\mathbf{K}} = \Phi\Phi^\top$ for $\Phi = [\phi(\mathbf{x}_n, \mathbf{W}_1, \mathbf{b})^\top]_{n=1}^N$
with feature vectors $\phi(\mathbf{x}, \mathbf{W}_1, \mathbf{b}) = \sqrt{1/H}\sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b})$

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From marginalisation of a subset of jointly Gaussian variables

$$\begin{aligned} p(\mathbf{y}_{1:N}|\mathbf{x}_{1:N}) &= \int p(\mathbf{W}_1)p(\mathbf{b})p(\mathbf{y}_{1:N}|\mathbf{f}_{1:N})p(\mathbf{f}_{1:N}|\mathbf{W}_1, \mathbf{b}, \mathbf{x}_{1:N})\mathrm{d}\mathbf{f}_{1:N}\mathrm{d}\mathbf{W}_1\mathrm{d}\mathbf{b} \\ &= \int \mathcal{N}(\mathbf{y}_{1:N}|\mathbf{0}, \Phi\Phi^\top + \tau^{-1}\mathbf{I}_N)p(\mathbf{W}_1)p(\mathbf{b})\mathrm{d}\mathbf{W}_1\mathrm{d}\mathbf{b} \end{aligned}$$

We have "parameters", but note the model remains non-parametric
complexity (capacity) adjusts with data size

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Parametric assumption

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In particular, it's true that

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where $\mathbf{w}_d \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_H)$ is an H-dimensional auxiliary random vector

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We introduce O such vectors, $\mathbf{W}_2 = [\mathbf{w}_d^\top]_{d=1}^O$ each $\mathbf{w}_d \sim p(\mathbf{w})$

$$\begin{aligned} p(\mathbf{y}_{1:N}|\mathbf{x}_{1:N}) &= \int \mathcal{N}(\mathbf{y}_{1:N}|\mathbf{0}, \Phi\Phi^\top + \tau^{-1}\mathbf{I}_N)p(\mathbf{W}_1)p(\mathbf{b})\mathrm{d}\mathbf{W}_1\mathrm{d}\mathbf{b} \\ &= \int p(\mathbf{y}_{1:N}|\mathbf{x}_{1:N}, \mathbf{W}_1, \mathbf{W}_2, \mathbf{b})p(\mathbf{W}_1)p(\mathbf{b})p(\mathbf{W}_2)\mathrm{d}\mathbf{W}_2\mathrm{d}\mathbf{W}_1\mathrm{d}\mathbf{b} \end{aligned}$$

Digest

In the “first layer” we project inputs to H-dimensional *feature vectors* and apply a nonlinearity $\sigma(\cdot)$. This is a “hidden layer”.

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In the limit of an infinite hidden layer, marginalising over the stochastic parameters gives us a GP likelihood.

The induced kernel depends on the non-linearity $\sigma(\cdot)$

A parametric approximation to a GP

A BNN with Gaussian priors over parameters is a parametric approximation to a GP

$$p(\mathbf{y}_{1:N}|\mathbf{x}_{1:N}) = \int p(\mathbf{y}_{1:N}|\mathbf{x}_{1:N}, \mathbf{W}_1, \mathbf{W}_2, \mathbf{b})p(\mathbf{W}_1, \mathbf{W}_2, \mathbf{b})\mathrm{d}\mathbf{W}_2\mathrm{d}\mathbf{W}_1\mathrm{d}\mathbf{b}$$

Obviously the marginal is intractable, after all this is a BNN!

This is true for tanh, relu, step functions, sigmoid, for example.

VI

Recipe

- propose a parametric proxy $q(\theta|\lambda)$
  $\theta = \{\mathbf{W}_1, \mathbf{W}_2, \mathbf{b}\}$
- which you can reparameterise
- choose λ to maximise the ELBO via stochastic gradient-based optimisation
- now because we count on autodiff, make sure you use differentiable nonlinearities (step function is no longer an option)

Mean field

Independence across parameter groups

$$q(\mathbf{W}_1, \mathbf{W}_2, \mathbf{b}|\lambda) = q(\mathbf{W}_1|\lambda_1)q(\mathbf{W}_2|\lambda_2)q(\mathbf{b}|\lambda_b)$$

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$$q(\mathbf{b}|\lambda) = \mathcal{N}(\mathbf{b}|\mathbf{m}, \mathrm{diag}(\boldsymbol{\sigma}^2)) \quad \text{nicely reparameterisable!}$$

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Mixture of Gaussians posterior with $p \in (0, 1)$

$$q(\mathbf{w}_r|\lambda) = p\mathcal{N}(\mathbf{w}_r|\mathbf{m}_r, \mathrm{diag}(\boldsymbol{\sigma}^2)) + (1-p)\mathcal{N}(\mathbf{w}_r|\mathbf{0}, \mathrm{diag}(\boldsymbol{\sigma}^2))$$

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Can we reparameterise samples from this posterior?

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Can we reparameterise samples from this posterior?

- $\mathbf{w}_r = z(\mathbf{m}_r + \boldsymbol{\sigma} \odot \epsilon) + (1-z)\boldsymbol{\sigma} \odot \epsilon$
  for $Z \sim \mathrm{Bern}(p)$ and $\epsilon \sim \phi(\epsilon)$

Mixture of Deltas

Let $\boldsymbol{\sigma} \to \mathbf{0}$

- from mixture of Gaussians to mixture of Deltas

$$Z \sim \text{Bern}(p)$$

$$\mathbf{w}_r = \begin{cases} \mathbf{m}_r + \mathbf{0} \odot \epsilon & \text{if } z = 1 \\ (1 - z)\mathbf{0} \odot \epsilon & \text{if } z = 0 \end{cases}$$

$$= z\mathbf{m}_r$$

- biases are deterministic because $\boldsymbol{\sigma} \to \mathbf{0}$ the Gaussian tends to $\delta(\mathbf{m} - \mathbf{b})$

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The affine transform in fully connected layers becomes

$$([(z_s\mathbf{m}_s)^\top]_{s=1}^H)\mathbf{x} + \mathbf{m} = ([\mathbf{m}_s^\top]_{s=1}^H)(\mathbf{z} \odot x) + \mathbf{m}$$

with probability p, we essentially drop inputs
Same happens with $\mathbf{W}_2$ (weights of the second layer)

ELBO

Recall the ELBO

$$N\,\mathbb{E}_I\left[\mathbb{E}_Z\left[\log p(y^{(I)}|x^{(I)}, \theta = t(z,\lambda))\right]\right] - \mathrm{KL}(q(\theta|\lambda)||p(\theta))$$

where

- $\theta = \{\mathbf{W}_1, \mathbf{W}_2, \mathbf{b}\}$ and $\lambda = \{\mathbf{M}_1, \mathbf{M}_2, \mathbf{m}\}$
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We are only missing a KL term: which can be nicely approximated by L_2 on λ

KL approximation

In regression (recall τ is the prior precision for the likelihood $Y|f$)

$$\frac{p}{2\tau N}||\mathbf{M}_1||_2^2 + \frac{p}{2\tau N}||\mathbf{M}_2||_2^2 + \frac{1}{2\tau N}||\mathbf{m}||_2^2 \tag{1}$$

In classification (we assume a degenerate Gaussian for $Y|f$)

$$\frac{p}{2N}||\mathbf{M}_1||_2^2 + \frac{p}{2N}||\mathbf{M}_2||_2^2 + \frac{1}{2N}||\mathbf{m}||_2^2 \tag{2}$$

See Gal and Ghahramani (2016b)

Prior parameters

The prior length-scale is the inverse of the standard deviation of the distribution over the scaling weights in affine layers, it controls the rate of change of the sampled functions.

The prior precision (in regression) controls the observation noise, smaller precision leads to bigger error bars

In classification we let $\tau^{-1} \to 0$.

These are hyperparameters you have to search for. You can also relate them to the weight decay if your NN library offers weight decay out of the box.

Approximate posterior parameters

$\mathbf{M}_1$ variational mean for input-to-hidden, $\mathbf{m}$ variational mean of bias vector, $\mathbf{M}_2$ variational mean for hidden-to-output

- these are the only trainable parameters

In principle, we can have one Bernoulli parameter per layer, generally we don't because Bernoulli sampling is nondifferentiable and thus we have to tune the parameter by hand.

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- multiple forward passes, but a single trained model
- unlike in an ensemble, we are sampling from $q(\theta|\lambda)$, an approximation to $p(\theta|\mathcal{D})$

Extensions

Note a few things

- it was crucial to use a mixture of *deltas* as variational approximation
- this allowed us to sample parameters by having a mask over inputs (rather than over parameters)
- this trick seems general, but it does depend on the type of layer we deal with

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CNNs can be reformulated as a linear operation followed by a pooling non-linearity, in this view we need to drop outputs of the linear operation (a parameterised inner product) before pooling

Summary

Bayesian posterior inference for NNs with negligible training effort

Bayesian posterior predictive at linear cost (one forward pass per sample)

Future research

- better posterior approximations (more correlations)
- better handle on properties of kernels
- BNNs typically underestimate variance

Literature

Yarin Gal's thesis and blogpost Gal (2016)

Dropout as Bayesian approximation Gal and Ghahramani (2016b, esp appendix)

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