Bayesian Neural Networks
for Text Classification and Regression

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Let's predict hate speech

Remember this exercise from week 2b?

Data We have a dataset of observations of the kind (x, y) where x is a relatively short piece of text and y is a binary flag that indicates the presence of hate speech.
Model $Y|\theta, x \sim \text{Bern}(f(x;\theta))$ where f is an NN
Problem It looks like sometimes the classifier makes mistakes. We are asked to provide the **model's uncertainty about its predictions**.

Options

1. We can report the probability $p(y|x, \theta)$ which can be easily obtained from our model. We are happy to have chosen a probabilistic approach!
2. Our model does not support a meaningful notion of uncertainty, it predicts probability distributions **deterministically** and therefore the probabilities themselves have no variance. We need another module from DL4NLP!

This may shock you, but $p(y|x, \theta)$ is not an uncertainty estimate.

Here is the source of confusion. A decision y, given x and θ, is not what the model predicts. The model predicts a probability value $p(y|x, \theta)$, or more generally, **a probability distribution** $Y|x, \theta$. This prediction is itself deterministic and therefore has no variance. In a strong sense, $f(x;\theta)$ is *absolutely certain* about the probability value it's predicted.

Intuition Would you take Donald Trump's word on his involvement in corruption? Would your answer change should Donald Trump say "Oh, I am 1000% sure I am not involved in corruption. And by the way, I bet you've never seen a probability so large, it is, it is so large, it's huge, seriously, best probability ever".

Uncertainty

A parameter, along with NN architectures and every assumption we make, **singles out a function** $f(x; \theta)$.

Deeper down it also specifies another function, namely, the probability mass/density function $p(y|x, \theta)$ that assigns likelihood to observations.

Perturbing the parameter, even just a little, may reveal that this function changes dramatically for certain x.

But why should we care about a perturbation in parameter space? After all, haven't we chosen our parameters for a reason?

For example, $|f(x; \theta + \epsilon) - f(x; \theta)|$ may be very large!

Some parameter estimation algorithm gives us θ, and it is pretty clear all throughout training that many different instances of θ can do just as well (under our criterion, say likelihood). So small perturbations in parameter around our solution should not be so frowned upon.

I'd actually stretch and say perturbations should not be frowned upon, no matter how tiny or large (something like Euclidean distance in parameter space is quite irrelevant here).

Uncertainty

But I want to make a strong argument. So, let's choose perturbed parameters **very** carefully. Say we have a stochastic process that only generates instances of θ that are *well-supported by our data* $\mathcal{D}$. This hypothetical process denoted $\Theta|\mathcal{D}$ sees data and narrows our parameter options to good parameters only.

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If $\text{Var}(Q)$ is large, the model knows very little about the probability of y_* given x_*. Think of it this way, our **very best** instances of θ, *those which are very likely given* $\mathcal{D}$, fail at assigning a reasonably consistent probability value to the data point.

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Uncertainty

A model's assessment of its own uncertainty is not the likelihood value $p(y|x,\theta)$, nor the related quantity $\text{Var}(Y|x,\theta)$.

Instead, it's the variance of that likelihood value for instances of θ that are likely given all data we have already observed.

Uncertainty is quantified by $\text{Var}(Y_*|x_*,\mathcal{D})$.

Variance of $Y|x,\mathcal{D}$ is about *uncertainty*, variance of $Y|x,\theta$ is just about *likelihood*.

For a moment, let me use $\mathcal{M}$ to explicitly denote all of our model assumptions (i.e., conditional independencies, parametric families, NN architectures). Then

- $\text{Var}(Y|X=x,\mathcal{D},\mathcal{M})$ is a measure of the uncertainty of a model $\mathcal{M}$ about Y given x taking into account all hypotheses supported by a set of observations $\mathcal{D}$;
- $\text{Var}(Y|X=x,\Theta=\theta,\mathcal{M})$ is the variance of the likelihood of Y given x under a specific hypothesis θ compatible with model $\mathcal{M}$; The data $\mathcal{D}$ plays no role here (except perhaps indirectly via an algorithm for picking θ).

Uncertainty requires a Bayesian view of the world. Luckily for us, Bayesian theory requires very little more than axiomatic probability theory (Bernardo and Smith, 2009). Well, and a bit of creativity to approximate some tough computations.

Outline

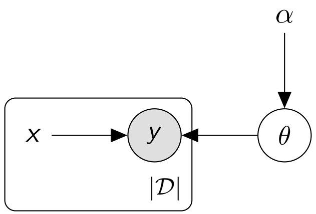
Bayes: what and why?

In this section we aim to answer

- 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 $p(\theta|\alpha)$

Just a joint distribution!

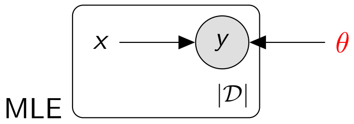
Observations are rvs, and *parameters* are rvs.

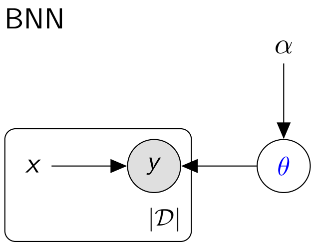
In a Bayesian model, data and parameters are no different. They are all given random treatment. The only substantial difference, being observed or not, has no effect in the theory. Read it this way: the set of principles is the same (axiomatic probability theory), there is no need for context-dependent patches.

In a Bayesian model, the prior parameter α, sometimes called a hyper-parameter, is typically fixed (or itself governed by a distribution, whose parameter is fixed (or, itself governed by a distribution, whose parameter is fixed (or ...))).

A BNN is a Bayesian model with NN-parameterised likelihood.

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*

Let's recap

- we have a **likelihood** $p(x|\theta)$, with which we can assign probability $p(\mathcal{D}|\theta)$ to data $\mathcal{D}$
- we have a **prior** $p(\theta|\alpha)$, it restricts the 'possible worlds' to some worlds that are plausible *a priori* (that is, before we look at this particular data $\mathcal{D}$)
- together they induce a **joint distribution** $p(\mathcal{D}, \theta|\alpha)$
- whose marginal $p(\mathcal{D}|\alpha) = \int p(\theta|\alpha)p(\mathcal{D}|\theta)\mathrm{d}\theta$ we also call **evidence**

NNs: parameters θ are known and given, which means, we need to find them somewhere. This view is so widespread that is common to think that optimisation and learning are the same thing.

BNNs: parameters θ are random and sampled from a prior. There's no search, there's no need for searching. Every single query of interest takes nothing but probability calculus. Here learning dispenses with optimisation.

Some Bayesians do optimise hyperparameters α, say using maximum (marginal) likelihood estimation $\arg\max_\alpha \log p(\mathcal{D}|\theta)$. Those Bayesians are known as *Empirical Bayesians*. There's something funny about this term, it makes it look like being Bayesian precludes empirical considerations. There's nothing *un-empirical* about Bayes.

Bayes

Being *Bayesian* seems to require specifying a prior distribution over parameters, though it's more than that

- it's about acknowledging that most quantities are *unknown*
- and proceeding to reason probabilistically under uncertainty
- priors are a means to this end, they specify what kinds of values are reasonable and with what expectation
- as we will see, acknowledging uncertainty and treating it seriously requires probabilistic inference

Why am I emphasising this? You will find arguments of the kind *"this regularisation is equivalent to that prior"*. The connection between a regulariser and a prior does not confer any Bayesian-type credibility to a non-Bayesian algorithm. These claims are usually made *asymptotically*, under the assumption that you have infinite data and access to global optima. Are these assumptions reasonable enough to justify some weak connection to Bayes? What's the purpose of the connection anyway? For example, remarking a connection for it inspires changes to the algorithm could be a good reason. Attempting to impose a perception of principledness is far less useful. In ML we have to compromise here and there *all* the time, there should be no shame in that. Still, motivating our compromises matters, it informs our peers, and we should make careful use of superficially powerful claims, after all, our goals include communicating research clearly.

Why do we call it a theory? Isn't it just a tool? A type of probability calculus? The motivations for the Bayesian paradigm are rooted in *a theory of rational decision making under uncertainty*, and in that sense it does go beyond probability calculus: it adds a semantic layer to it with philosophical implications (Bernardo and Smith, 2009). If you want to concentrate on statistical and practical data analysis implications, a textbook like BDA3 (Gelman et al., 2013) is more appropriate though.

Why Bayes?

A fairly practical reason for Bayes stems from a question such as? How can we quantify the model's uncertainty about a *prediction*?

Wouldn't it be useful to shed light onto

- when do we know we can trust the model for a given pair $\langle x, y \rangle$?

When I say *prediction*, does anyone still think of the following?

$$y_* = \arg\max_y \; p(y|x_*, \theta)$$

If so, let's agree on some terminology. This is a decision rule (it is not even the only one possible) and it relies on the likelihood $p(y|x_*, \theta)$

- think of the likelihood as a prediction on its own right
- an NN parameterised by θ has predicted this value from x_*

When Bayes? This is not like choosing your favourite cake, you *can* be objective about this. In ML we should be that kind of flexible. If Bayesian computations posed no challenging, I'd feel more like telling you *always Bayes*, at least, whenever your data are outcomes of random experiments. But that's not reality. So, learn about Bayes and decide when it's worth the trouble. That applies to all of our tools, doesn't it? Sometimes an NN is not worth the trouble: the time you save in feature engineering you waste in silly numerical instability and fighting overfitting with extremely limited theoretical guidance.

The importance of knowing what we don't know

If $p(y_*|x_*, \theta)$ **is not** about uncertainty, then what is?

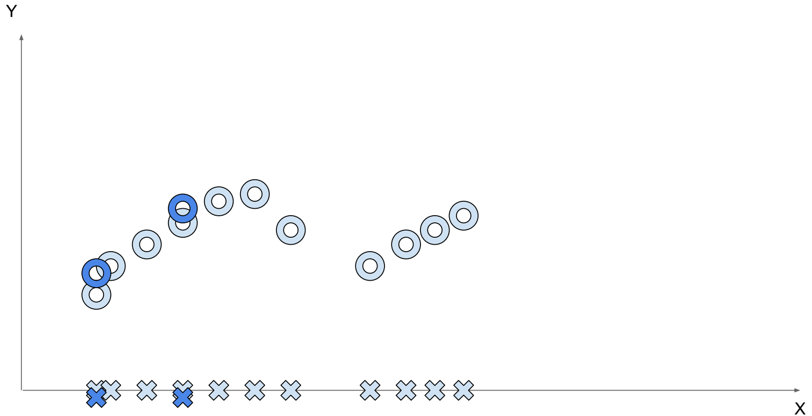
When a data point is well supported by θ, that is, $p(y_*|x_*, \theta)$ is high, we should ask ourselves, is θ even supported by the evidence we have?

In other words, what are interested in the posterior distribution $\Theta|\mathcal{D}, \alpha$:

$$p(\theta|\mathcal{D}, \alpha) = \frac{p(\theta, \mathcal{D}|\alpha)}{p(\mathcal{D}|\alpha)}$$

"The importance of knowing what we don't know" (Gal, 2016, Chapter 1).

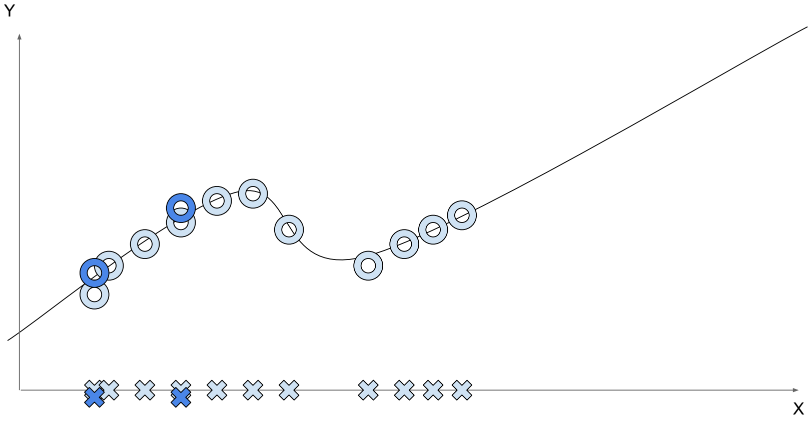
Uncertainty illustrated



Suppose a regression problem for which we have observations

Here we have data points for some regression problem which we could use to fit an NN (let's say we start with MSE).

Uncertainty illustrated



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

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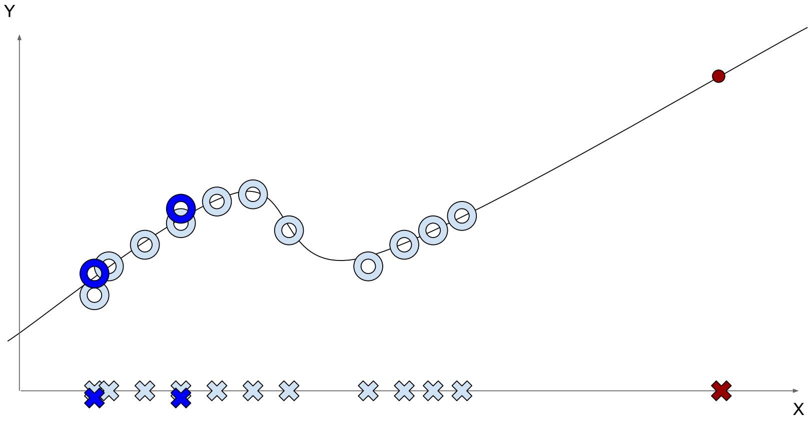

By design, it extrapolates predictions to unseen inputs, e.g. x_*

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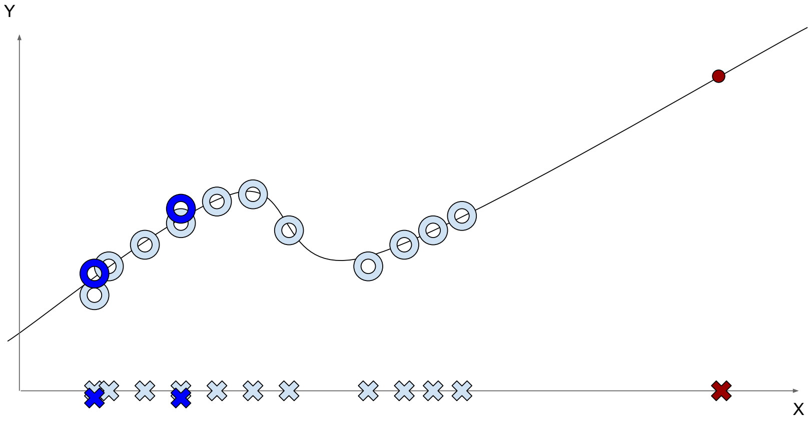

Can we trust our model given x_* is far from observations?

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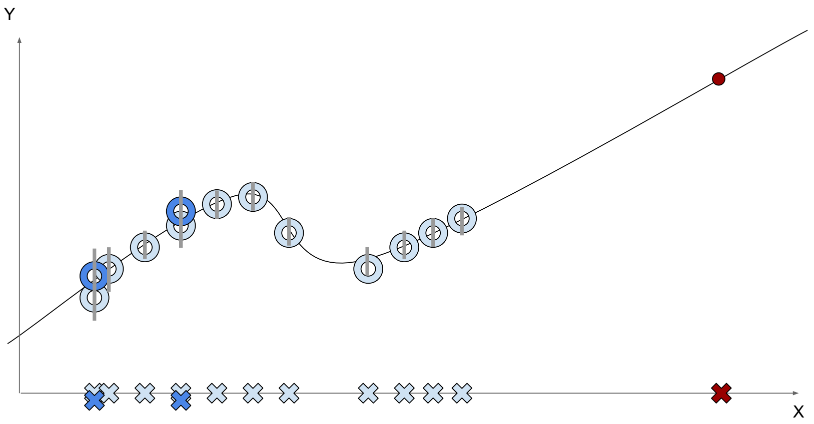

Let's fit Gaussians, i.e. $\mathcal{N}(\mu(x;\theta), \sigma(x;\theta)^2)$, around targets

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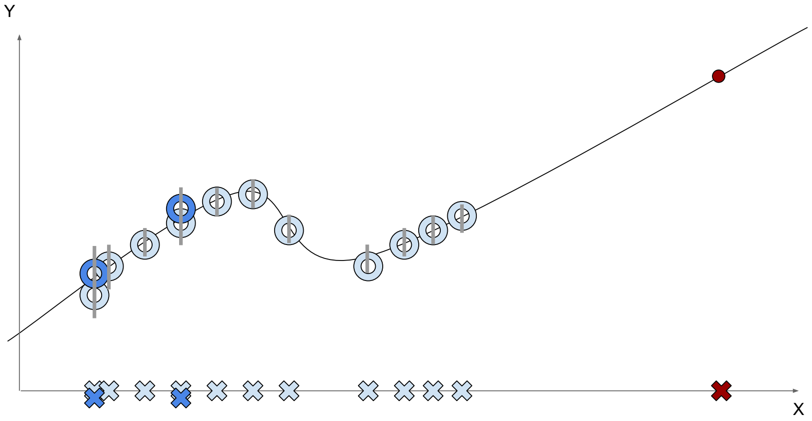

Note that we never observe much variability for a given input x

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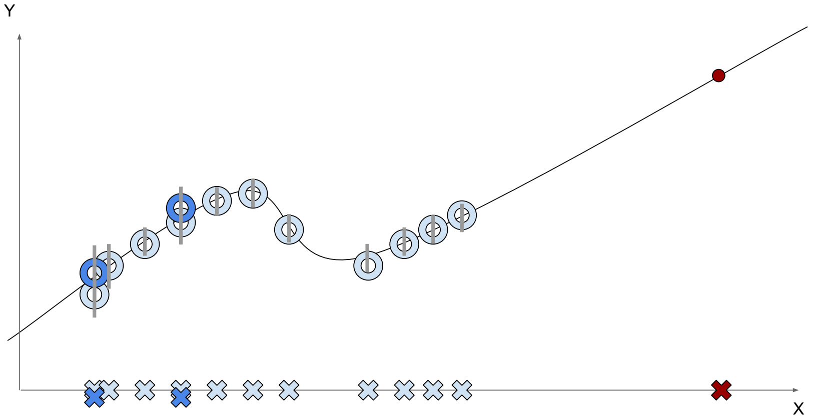

$\mu(x;\theta)$ learns to be on average close to every response for x

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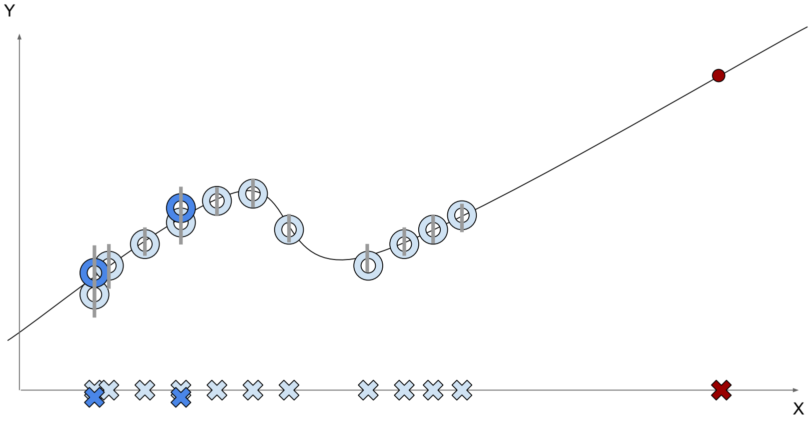

$\sigma(x;\theta)$ instead learns to cover all responses for x, but no more

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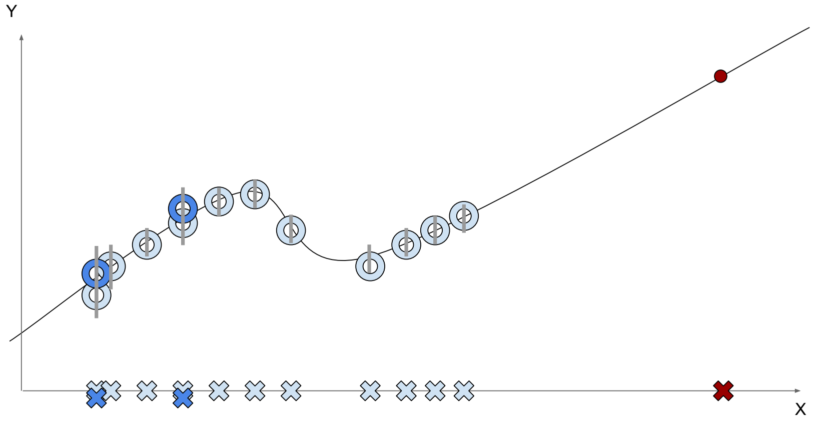

for MLE does not like covering more than observed responses

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- The Gaussian model looks better than MSE, but only where we have data.

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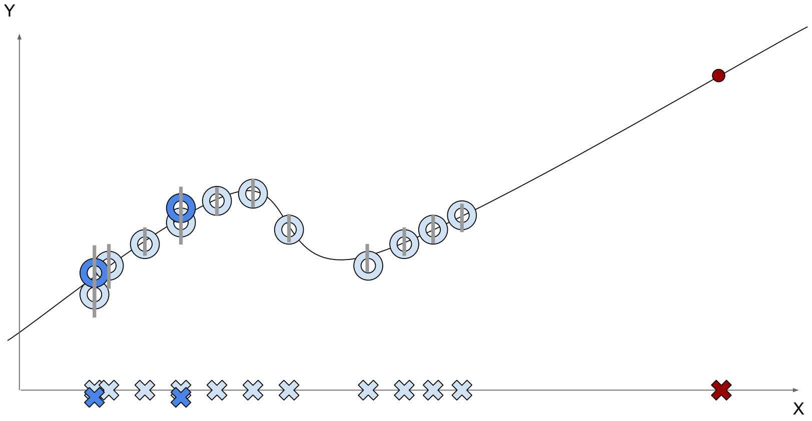

What is our expectation for $\sigma(x_*; \theta)$?

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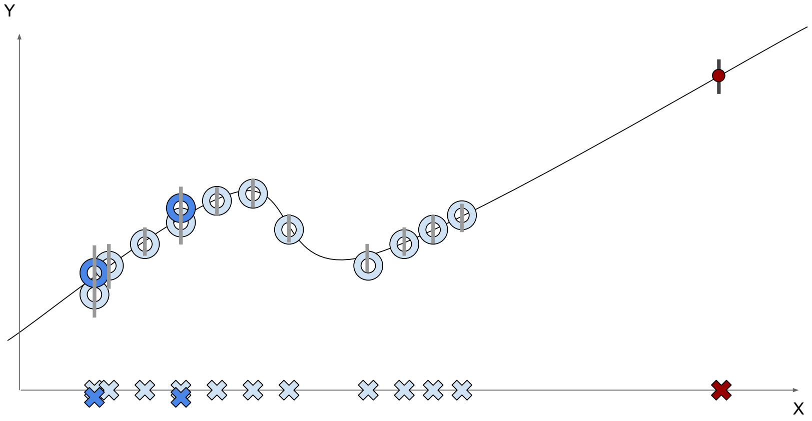

For all we know, $\sigma(\cdot;\theta)$ likes to predict small values

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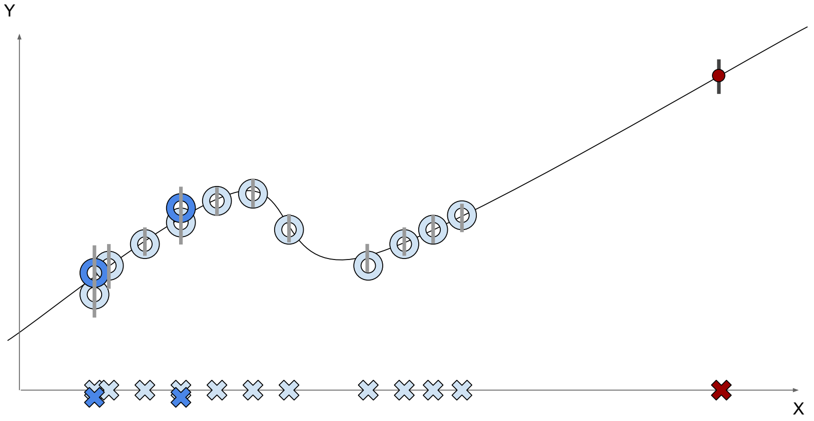

$\sigma(\cdot;\theta)$ seriously underestimates uncertainty for x_*

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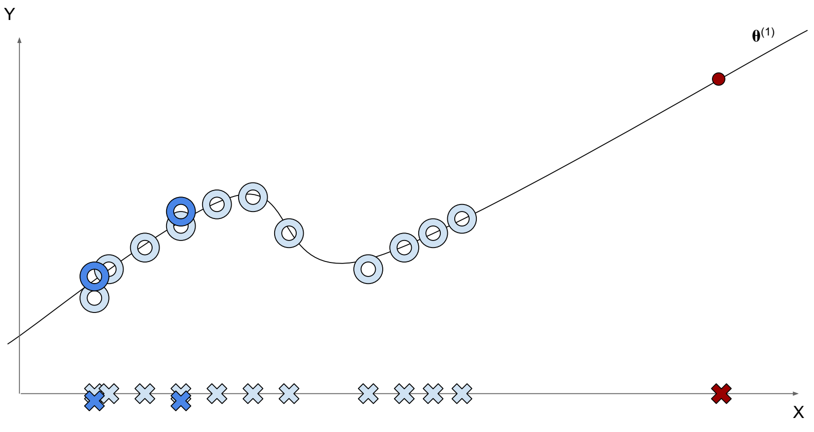

but what if, with probability $p(\theta^{(1)}|\mathcal{D})$, we consulted $\mu(x;\theta^{(1)})$?

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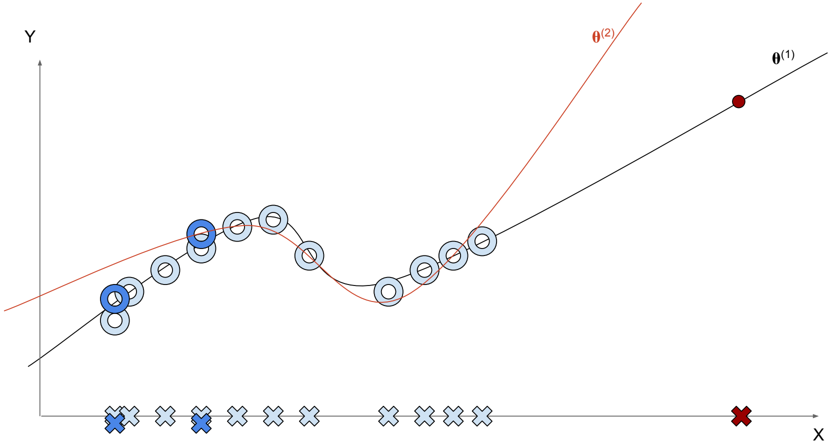
- The Gaussian model looks better than MSE, but only where we have data.
- Ditch the idea of prediction variance. Instead, we impose a prior on θ and infer a posterior distribution given all of our observed data. Now let's consult patterns that are likely **given** data.

Uncertainty illustrated



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

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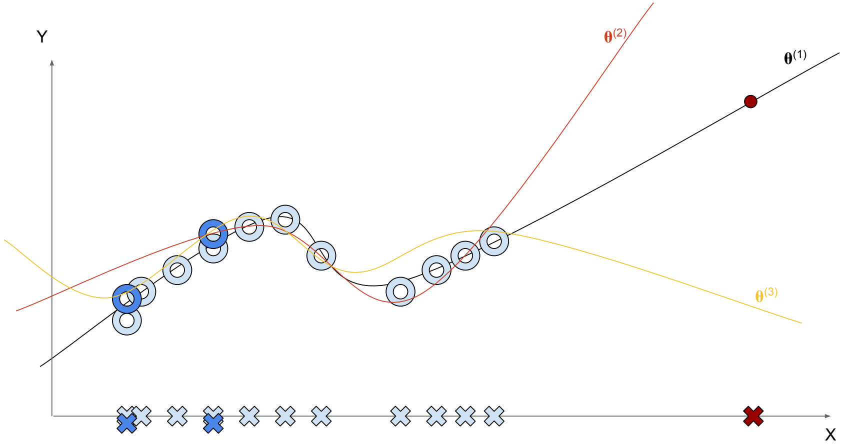
Uncertainty illustrated



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

Here we have data points for some regression problem which we could use to fit an NN (let's say we start with MSE).

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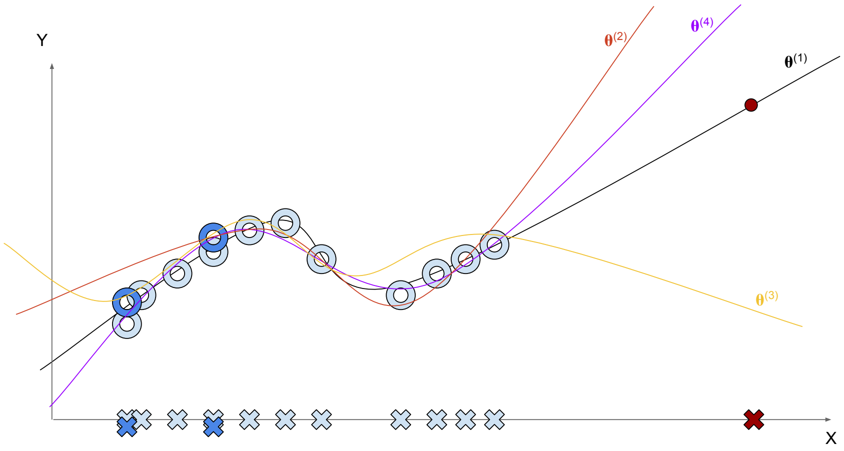

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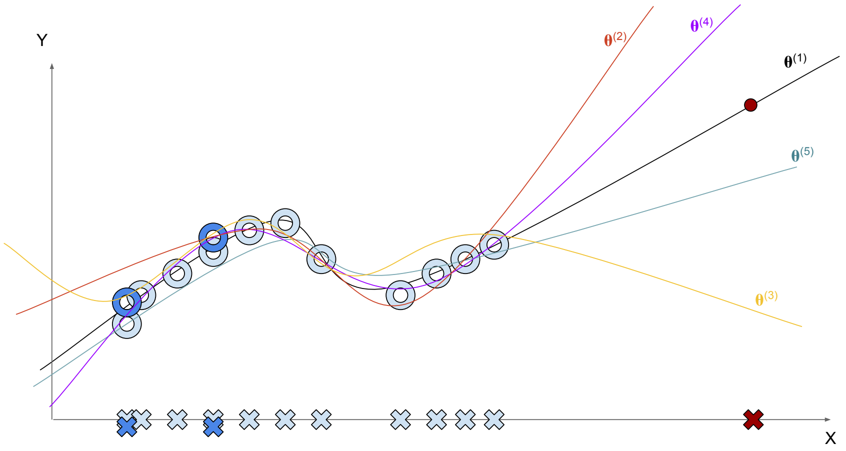

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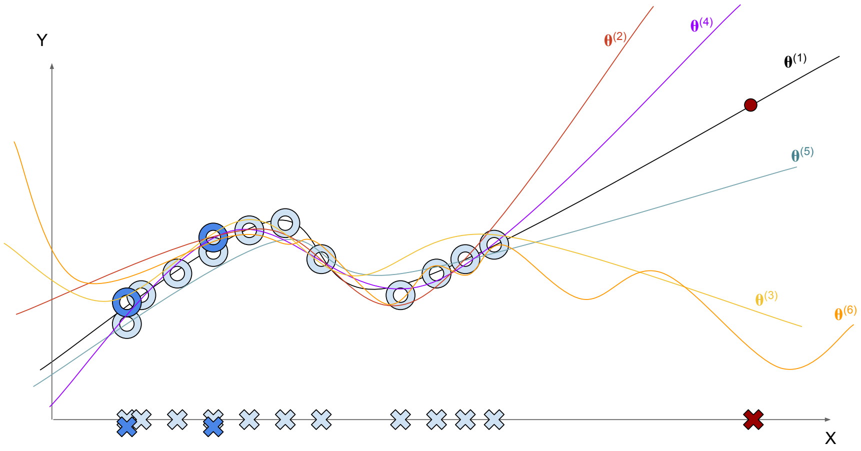

and $\mu(x; \theta^{(6)})$, with probability $p(\theta^{(6)}|\mathcal{D})$?

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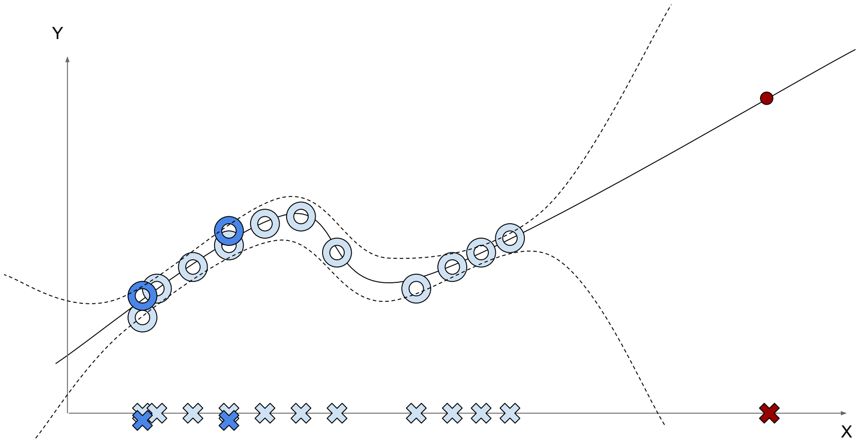

Suddenly, we are a lot less certain about predictions for x_*

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I want to say *yes*, because if we are going to talk about ‘ensembles’, then I feel like I owe a word such as ‘fancy’ to Bayes.

But honestly, I don’t feel like using the word ‘fancy’, because marginal and conditional probabilities are pretty basic.

Finally, I’m not sure it’s fair to explain something self-consistent (i.e., probability calculus) in terms of such a vaguely specified notion (i.e., ensembling).

But let’s build intuition, and expose differences!

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- Contrast this with stochasticity due to assessments of $\mu(x_*; \theta)$ for $\theta \sim \Theta|\mathcal{D}, \alpha$

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Committing to $\hat{\mu}(x_*)$ disregards the actual spread of predictions hiding uncertainty rather than exposing it.

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Bayesian Reasoning

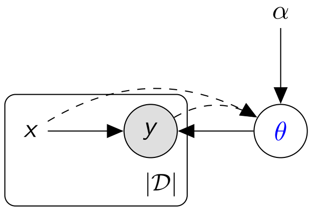
Reasoning with *parametric BNNs* involves averaging over parameters

- 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 $p(\mathcal{D}, \theta | \alpha, \mathcal{M})$ where $\mathcal{M}$ is the model assumptions — we omit $\mathcal{M}$ for brevity
- θ is only one *hypothesis* under this model
- the "worth" of each θ is quantified by $p(\theta | \mathcal{D}, \alpha)$
- uncertainty estimates are based on this posterior probability

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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Bayesian Inference

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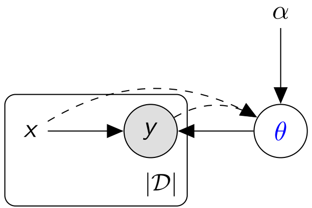

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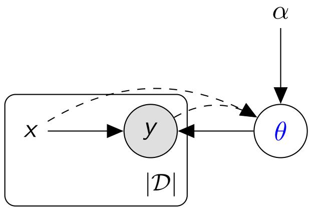

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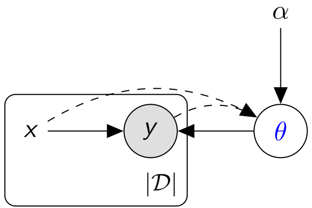

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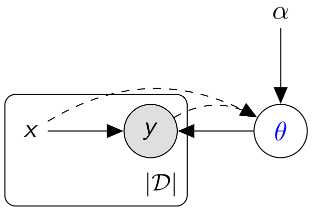

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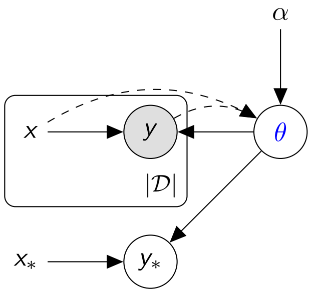
Posterior predictive distribution



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

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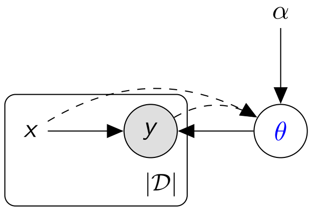
Bayesian Inference

Posterior inference



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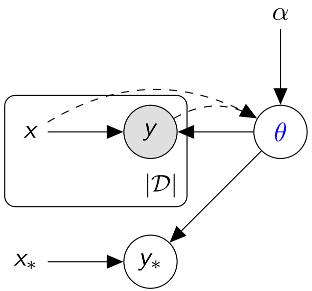

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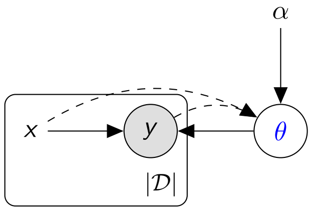

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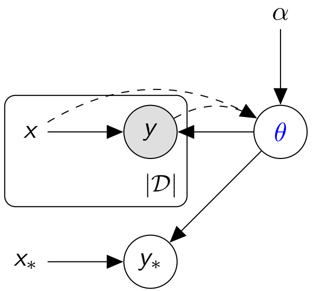

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Conditional independence
$Y_* \perp \mathcal{D} \mid \theta$

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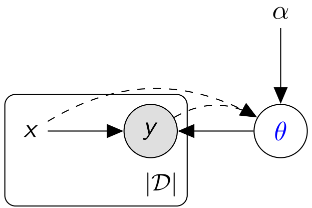

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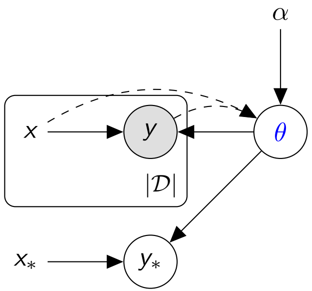

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Terminology

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, it usually has to do with assessing a decision rule.

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

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

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

MLE

$$\pi = {}^1/_K \mathbf{1}_K$$
$$\theta = \langle \theta^{(1)}, \ldots, \theta^{(K)} \rangle$$

Bayes

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

$\mathbf{1}_K$ is a K-dimensional vector where every element is 1.

MLE

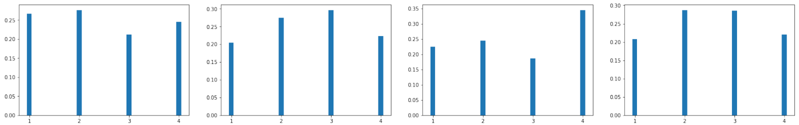
- parameters are **given**
- where do they come from?

Bayes

- parameters are rvs (there's no search for parameters, they come from the prior, stochastically)
- but it's worth asking, what does it mean to impose a Dirichlet prior on mixing coefficients π?
- what does it mean to impose a Dirichlet prior on the parameters of each likelihood component $\theta^{(z)}$?

What makes good mixing coefficients?

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



The question you have to think about is: Can we make any assumptions before observing data?

For example, let's see what happens as we vary our choice of prior for mixing coefficients

- Here you see 4 models that are likely under this prior. Each of these models gives every component of the mixture roughly the same opportunity to generate data points.

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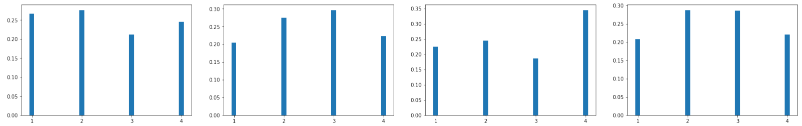
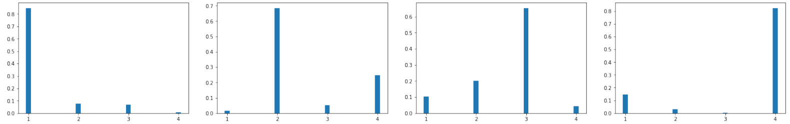


$\pi \sim \mathrm{Dir}(1 \times \mathbf{1}_K)$



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- This prior is different, each model prefers few components. Clearly, there's no reason to prefer component 1 systematically over the others, so this prior supports coefficients that reveal different winners each time.

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Say we have $K = 4$ components, I show a few samples for

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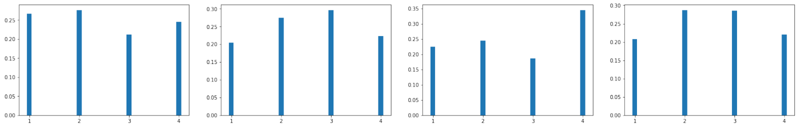
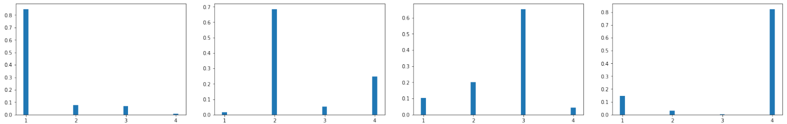
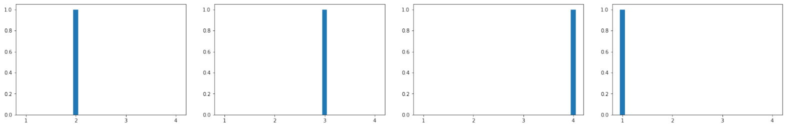


$\pi \sim \mathrm{Dir}(1 \times \mathbf{1}_K)$



$\pi \sim \mathrm{Dir}(0.1 \times \mathbf{1}_K)$



The question you have to think about is: Can we make any assumptions before observing data?

For example, let's see what happens as we vary our choice of prior for mixing coefficients

- Here you see 4 models that are likely under this prior. Each of these models gives every component of the mixture roughly the same opportunity to generate data points.
- This prior is different, each model prefers few components. Clearly, there's no reason to prefer component 1 systematically over the others, so this prior supports coefficients that reveal different winners each time.
- This prior likes very sparse mixing coefficients. Again, there's no reason to prefer any one component over any other. But it seems like a good idea to prefer sparse mixtures. The Dirichlet prior allows us to express a preference: every model is possible (literally, every way to mix for components), but some models are preferred (for example, the sparse ones).

What makes good mixing coefficients?

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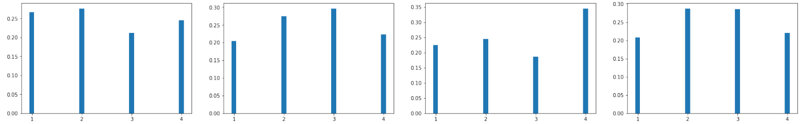

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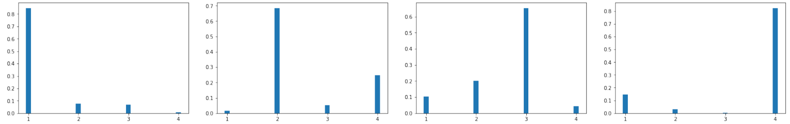

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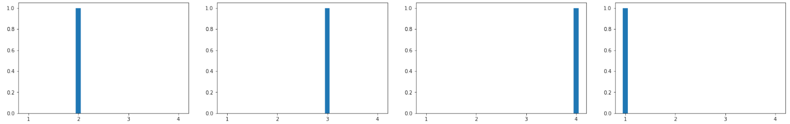

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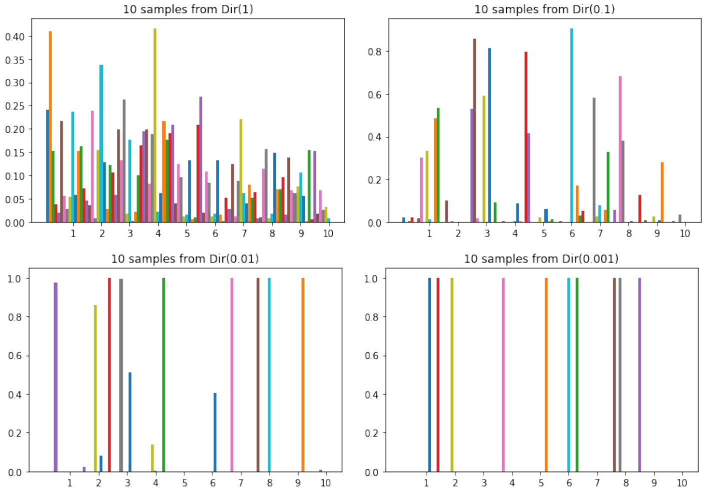
What makes a good conditional?

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



How about the components themselves? Similar story.

Do we want components that each can generate everything? That is, no specialisation whatsoever.

Or do we prefer components that generate only a selected subset of the support?

Clearly, why should component 1 prefer any particular subset of the support? It should not, thus it's prior does not express a preference for one particular subset, it express a preference for any distribution that focuses on only a small subset. Distributions that meet this 'requirement' are not preferred over one another.

The idea of allowing components to change like that may be scary. But think of it this way, we are not committing to any one such distribution. We are averaging **all** of them out to get to quantities such as the evidence and the posterior predictive distribution. There's no risk in that. The risk is precisely in arbitrarily picking any one configuration when so many alternatives exist.

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 identity of clusters
  uniform marginals

All of that is essentially very clear a priori

- that is, before we collect observations
- by simply considering the nature of problem

Yes, there's an elephant in the room.

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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?

Yes, there's an elephant in the room.

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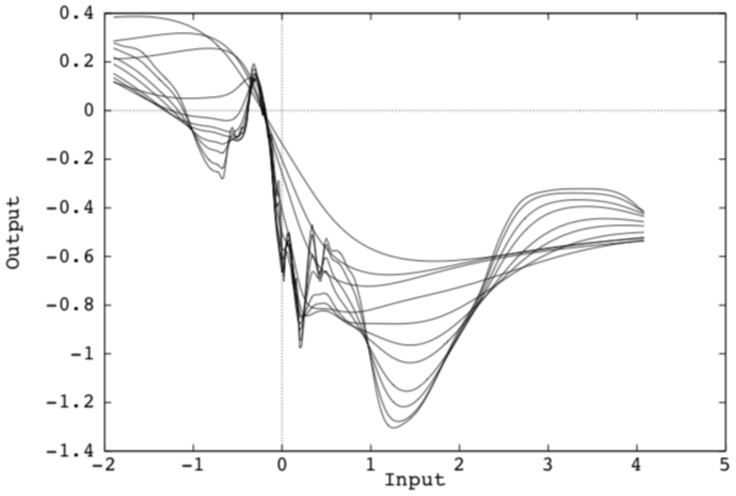
Sampling from these priors and performing forward passes with the network will expose a range of functions

- 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 $x^{(1)}, \dots, x^{(N)}$ the density $p(f(x^{(1)}), \dots, f(x^{(N)}))$ 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. $x_i \stackrel{\text{def}}{=} x^{(i)}$.

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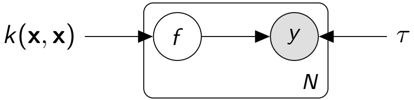
GP prior

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



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

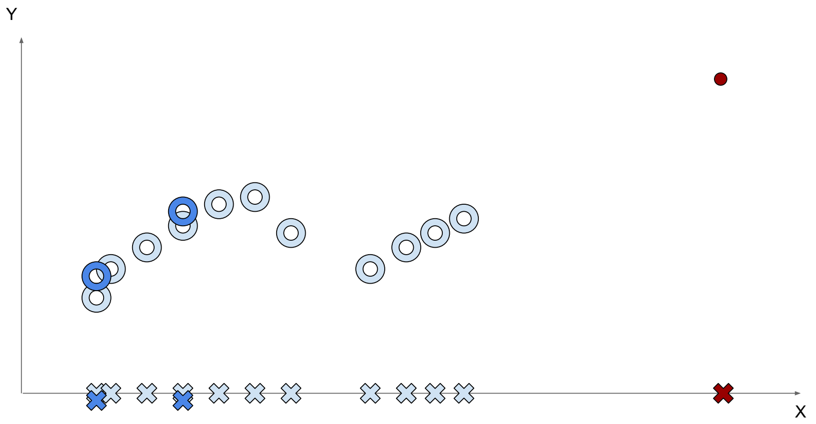
Posterior

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

Posterior predictive distribution:

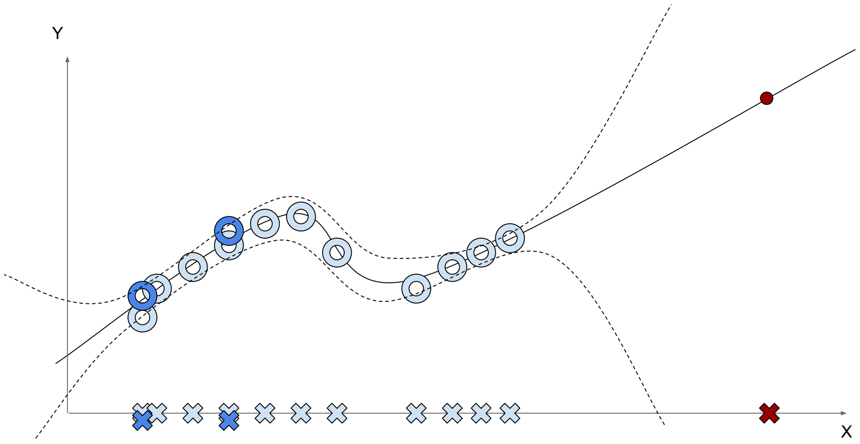
$$Y_*|x_*,\mathbf{x},\mathbf{y} \sim \mathcal{N}\big(k(x_*,\mathbf{x})(\mathbf{K} + \tau^{-1}\mathbf{I}_N)^{-1}\mathbf{y},\; k(x_*,x_*) + \tau^{-1} - k(x_*,\mathbf{x})(\mathbf{K} + \tau^{-1}\mathbf{I}_N)^{-1}k(x_*,\mathbf{x})^\top\big)$$

Uncertainty illustrated (revisited)



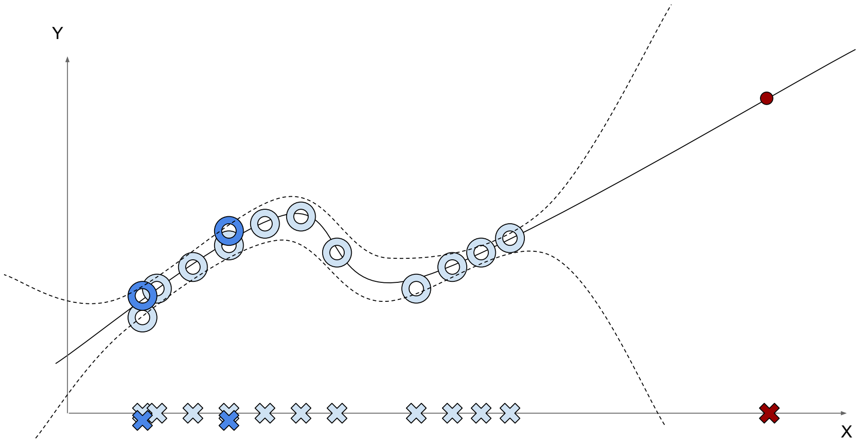
Let's get back to this

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: $k : \mathcal{X} \times X \to \mathbb{R}$ 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

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

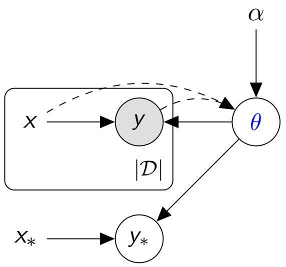
- kernels for text are fewer, less convenient, and less well-understood
- x can be very high-dimensional (and perhaps we have less intuitions to choose a kernel)

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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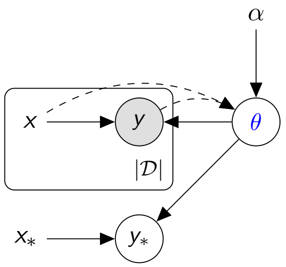

That is,

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

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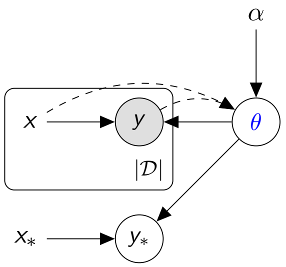

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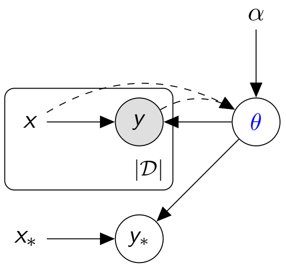

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Let's learn a proxy $q(\theta|\lambda)$!

Variational Bayes

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.

Variational Bayes is the variational inference you know and love, where as good Bayesians we only optimise our choice of $q(\theta)$, not our choice of $p(\mathcal{D}, \theta)$.

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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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&= \arg\min_{q(\theta)} \ -\mathbb{E}_{q(\theta)}\left[\log \frac{p(\theta,\mathcal{D})}{q(\theta|\lambda)}\right] && \text{property of log} \\
&= \arg\max_{q(\theta)} \ \mathbb{E}_{q(\theta)}\left[\log p(\theta,\mathcal{D})\right] + \mathbb{H}(q(\theta)) && \text{ELBO}
\end{aligned}
$$

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

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

ELBO continued

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\end{aligned}$$

Recall

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

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

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If we have the same exponential family for $p(\theta)$ and $q(\theta|\lambda)$, then

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

is known in closed form.

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

Choosing λ

How should we choose λ?

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How can we approach the following problem?

$$\arg\max_{\lambda} \ \mathbb{E}_{q(\theta|\lambda)}\left[\log p(\mathcal{D}|\theta)\right] - \underbrace{\mathrm{KL}(q(\theta|\lambda)||p(\theta))}_{\text{closed form}}$$

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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

Remember the *law of the unconscious statistician*?

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

We used it for VAEs, and we are going to use it now for BNNs.

Reparameterised Gradients

Assume we pick $q(\theta|\lambda)$ from a reparameterisable family
e.g. location-scale distributions

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

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where $\epsilon^{(k)}\sim\phi(\epsilon)$, $\theta^{(k)}=t(\epsilon^{(k)},\lambda)$, and $I\sim\mathcal{U}(1/N)$

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where $\epsilon^{(k)} \sim \phi(\epsilon)$, $\theta^{(k)} = t(\epsilon^{(k)},\lambda)$, and $I \sim \mathcal{U}(1/N)$

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

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Training now gives you a point estimate for λ
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- $q(\theta|\mathcal{D})$ approximates the true posterior $p(\theta|\mathcal{D})$
- it should prefer models that are likely after observing data $\mathcal{D}$ in light of whatever prior assumptions we made
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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

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

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

Outline

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

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

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

GP based on $\hat{k}$

We can immediately define a GP using this new kernel

$$
\begin{aligned}
b_s &\sim \mathcal{N}(0, l_0^{-2}) \\
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\end{aligned}
\qquad
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\mathbf{Y}|\mathbf{f} &\sim \mathcal{N}(\mathbf{f}, \tau^{-1}\mathbf{I}_N)
\end{aligned}
$$

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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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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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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- $\mathbf{w}_r = z(\mathbf{m}_r + \boldsymbol{\sigma} \odot \epsilon) + (1-z)\boldsymbol{\sigma} \odot \epsilon$
  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

$$
\begin{aligned}
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
\end{aligned}
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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.

Inferences

Marginal likelihood: get estimates via importance sampling to compare different hyperparameters

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- do not disable dropout at test time

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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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- all we need is to sample the mask once per data point
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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)

CNN and RNN variants Gal and Ghahramani (2016a,c)

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