Today:

- Introduction
- The Language of Uncertainty
- Bayesian Probabilistic Modelling
- Bayesian Probabilistic Modelling of Functions
Introduction
With great power...

▶ Many engineering advances in ML

▶ Systems applied to toy data → deployed in real-life settings

▶ Control **handed-over** to automated systems; w many scenarios which can become **life-threatening** to humans
  ▶ Medical: automated decision making or recommendation systems
  ▶ Automotive: autonomous control of drones and self driving cars
  ▶ High frequency trading: ability to affect economic markets on global scale
  ▶ But all of these can be quite dangerous...
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Example: Medical Diagnostics

- **dAlbetes:** an exciting new startup (not really)
  - claims to automatically diagnose diabetic retinopathy
  - accuracy 99% on their 4 train/test patients
  - engineer trained **two** deep learning systems to predict probability $y$ given input fondus image $x$.

The engineer runs their system on your fondus image $x^*$ (RHS):

- Which model $f_1$, $f_2$ would you want the engineer to use for your diagnosis?
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The engineer runs their system on your fondus image $x^*$ (RHS):

- Which model $f_1, f_2$ would you want the engineer to use for your diagnosis? **None of these!** (‘I don’t know’)

![Eye image with graph](attachment:image.png)
Example: Autonomous Driving

Autonomous systems

▶ Range from simple robotic **vacuums** to **self-driving cars**

▶ Largely divided into systems which
  ▶ control behaviour w **rule-based** systems
  ▶ learn and **adapt to environment**

Both can use of ML tools

▶ ML for low-level feature extraction (**perception**)  
▶ reinforcement learning
Real-world example: assisted driving

▶ first fatality of assisted driving (June 2016)
▶ low-level system failed to distinguish white side of trailer from bright sky
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If system had identified its own uncertainty:

- alert user to take control over steering
- propagate uncertainty to decision making
In medical / robotics / science...

*can’t* use ML models giving a single point estimate (single value) in prediction

*must* use ML models giving an answer that says ‘10 but I’m uncertain’; or ‘10 ± 5’

Give me a *distribution* over possible outcomes!
In medical / robotics / science...

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▶ Give me a \textit{distribution} over possible outcomes!
**Example: Autonomous Driving (cnt)**

ML pipeline in **self-driving cars**

- **process raw sensory input** w perception models
  - eg image segmentation to find where other cars and pedestrians **are**
  - output fed into prediction model
    - eg where other car will **go**
  - output fed into ‘higher-level’ decision making procedures
    - eg **rule based system** (“cyclist to your left → do not steer left”)
- industry’s starting to use uncertainty for lots of components in the pipeline
  - eg **pedestrian prediction** models predict a distribution of pedestrian locations in X timesteps
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Efficient Computation of Collision Probabilities for Safe Motion Planning

Andrew Blake, Alejandro Bordallo, Majd Hawasly, Svetlin Penkov, Subramanian Ramamoorthy†, Alexandre Silva

Abstract—We address the problem of safe motion planning. As mobile robots and autonomous vehicles become increasingly more prevalent in human-centered environments, the need to ensure safety in the sense of guaranteed collision free behaviour has taken renewed urgency. Achieving this when perceptual modules provide only noisy estimates of objects in the environment requires new approaches. Working within a probabilistic framework for describing the environment, we present methods for efficiently calculating a probabilistic risk of collision for a candidate path. This may be used to stratify a set of candidate trajectories by levels of a safety threshold. Given such a stratification, based on user-defined thresholds, motion synthesis techniques could optimise for secondary criteria with the assurance that a primary safety criterion is already being satisfied. A key contribution of this paper is the use of a ‘convolution trick’ to factor the calculation of integrals providing bounds on collision risk, enabling an $O(1)$ computation even in cluttered and complex environments.

I. INTRODUCTION

[3]. Therefore, we can only treat such perception modules as being able to provide us with a probability distribution [4] over poses of the various objects in the scene. Achieving safe motion planning in such a setting will require the motion planning methods to turn these into probabilities of unsafe events (such as a collision of the robot with another agent), providing at least approximate assurance regarding the (non-)occurrence of these events.

Fig. 1: A visualisation of the motion planning problem that we strive to solve for a variety of motion synthesis methods. For instance, the Rapidly-exploring Random Tree (RRT) algorithm can utilise this probability within the search process. Likewise, a variational formulation of optimal control [5] could include this within the cost terms.

B. Related Work

The issue of safety in control and motion planning has been investigated from a number of different methodological
Uncertainty-Aware Driver Trajectory Prediction at Urban Intersections

Xin Huang\textsuperscript{1,2}, Stephen G. McGill\textsuperscript{1}, Brian C. Williams\textsuperscript{2}, Luke Fletcher\textsuperscript{1}, Guy Rosman\textsuperscript{1}

Abstract—Predicting the motion of a driver’s vehicle is crucial for advanced driving systems, enabling detection of potential risks towards shared control between the driver and automation systems. In this paper, we propose a variational neural network approach that predicts future driver trajectory distributions for the vehicle based on multiple sensors.

Our predictor generates both a conditional variational distribution of future trajectories, as well as a confidence estimate for different time horizons. Our approach allows us to handle inherently uncertain situations, and reason about information gain from each input, as well as combine our model with additional predictors, creating a mixture of experts.

We show how to augment the variational predictor with a physics-based predictor, and based on their confidence estimations, improve overall system performance. The resulting combined model is aware of the uncertainty associated with its predictions, which can help the vehicle autonomy to make decisions with more confidence. The model is validated on real-world urban driving data collected in multiple locations. This validation demonstrates that our approach improves the prediction error of a physics-based model by 25\% while successfully identifying the uncertain cases with 82\% accuracy.

1 Introduction

Probabilistic models, such as Gaussian Processes, have been used for deterministic results efficiently. However, these methods fail to capture the uncertain nature of human actions. Probabilistic predictions are very useful in many safety-critical tasks such as collision checking and risk-aware motion planning. They can express both the intrinsically uncertain

Fig. 1: Illustration of a motivating example where a vehicle is in front of an intersection. The sampled predicted trajectories using our approach are plotted in blue, where the groundtruth future trajectory is plotted in red. In parallel autonomy, the autonomous system can leverage the predicted driver trajectory to avert risk and improve the driving. This requires the system to be confident of its predicted trajectories.

urban driving prediction. Intersections, for instance, were responsible for 40\% of crashes happened in the United States in 2008 [9]. We therefore focus on predicting trajectories for vehicles driving in urban environments. This is more challenging than highway trajectory prediction due to more complicated environments with different road shapes and dynamic objects, as well as the variety of available driving actions for the driver. Additionally, in many cases it is crucial to be aware of the confidence of the prediction. In cases where those predictions cannot be accurately made, a later planning or parallel autonomy layer can take this into account, avoiding catastrophic outcomes due to mispredictions.
Sources of uncertainty

- Above are some examples of uncertainty

- Many other sources of uncertainty

- Test data is very dissimilar to training data
  - model trained on diabetes fondus photos of subpopulation A
  - never saw subpopulation B
    - “images are outside data distribution model was trained on”
  - desired behaviour
    - return a prediction (attempting to extrapolate)
    - +information that image lies outside data distribution
  - (model retrained w subpop. B labels \(\rightarrow\) low uncertainty on these)
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Sources of uncertainty (cnt)

- Uncertainty in model parameters that best explain data
  - large number of possible models can explain a dataset
  - uncertain which model parameters to choose to predict with
  - affects how we predict with new test points
Sources of uncertainty (cnt)

- Training labels are noisy
  - measurement imprecision
  - expert mistakes
  - crowd sourced labels

even infinity data $\rightarrow$ ambiguity inherent in data itself
Deep learning does not capture uncertainty:

- regression models output a single scalar/vector
- classification models output a probability vector (erroneously interpreted as model uncertainty)
Deep learning models are deterministic

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But when combined with *probability theory* can capture uncertainty in a principled way

→ known as **Bayesian Deep Learning**
Teaser: Uncertainty in Autonomous Driving
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Define model and train on data \( x_{\text{train}}, y_{\text{train}} \):

```python
from tensorflow.keras.layers import Input, Dense, Dropout

inputs = Input(shape=(1,))
x = Dense(512, activation="relu")(inputs)
x = Dropout(0.5)(x, training=True)
x = Dense(512, activation="relu")(x)
x = Dropout(0.5)(x, training=True)
outputs = Dense(1)(x)

model = tf.keras.Model(inputs, outputs)
model.compile(loss="mean_squared_error",
              optimizer="adam")
model.fit(x_train, y_train)
```
# do stochastic forward passes on x_test:
samples = [model.predict(x_test) for _ in range(100)]
m = np.mean(samples, axis=0)  # predictive mean
v = np.var(samples, axis=0)  # predictive variance

# plot mean and uncertainty
plt.plot(x_test, m)
plt.fill_between(x_test, m - 2*v**0.5, m + 2*v**0.5, alpha=0.1)  # plot two std (95% confidence)
Bayesian deep learning

All resources (including these slides): bdl101.ml

SLIDES
Slide decks from the talks.
- SLIDE DECK 1
- SLIDE DECK 2

DEMO
Demos mentioned in the slides
- UNCERTAINTY PLAYGROUND
- UNCERTAINTY VISUALISATION

RECAP
A quick recap of useful stuff.
- GAUSSIANS RECAP

NOTATION
Notation used in the slides:

MORE STUFF
OATML
Today and tomorrow we’ll understand why this code *makes sense*, and get a taste of

- the formal language of **uncertainty** (Bayesian probability theory)
- tools to use this language in **ML** (Bayesian prob. modelling)
- techniques to scale to real-world **deep learning** systems (modern variational inference)
- developing **big deep learning systems** which convey uncertainty
  - w **real-world** examples
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Basic concepts marked **green** (if you want to use as tools); Advanced topics marked **amber** (if you want to develop new stuff in BDL)
Bayesian Probability Theory: the Language of Uncertainty

Deriving the laws of *probability theory* from *rational degrees of belief*
import numpy as np

def toss():
    if np.random.rand() < 0.5:
        print('Heads')
    else:
        print('Tails')

unit wager: a ‘promise note’ where seller commits to pay note owner £1 if outcome of toss=‘heads’; a tradeable note; eg..
Betting game 1 (some philosophy for the soul)

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- **unit wager**: a ‘promise note’ where seller commits to pay note owner £1 if outcome of toss=‘heads’; a tradeable note; eg..

- would you pay p=£0.01 for a unit wager on ‘heads’?
  - pay a penny to buy a note where I commit to paying £1 if ‘heads’

- p=£0.99?
  - pay 99 pence for a note where I commit to paying £1 if ‘heads’

- up to £0.05?, £0.95 or above?, ...
Betting game 1 (some philosophy for the soul)

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- **Unit wager:** note seller commits to paying £1 if outcome='heads'

- would you **sell** a unit wager at £p for ‘heads’?
  - you get £p for the note, and have to pay £1 if heads

- up to £0.05?, £0.95 or above?, ...
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▶ Unit wager: note seller commits to paying £1 if outcome=‘heads’

▶ what if you have to set price £p, and commit to either sell unit wager at £p for ‘heads’, or buy one?
    ▶ I decide whether to sell to you, or buy from you
    ▶ I sell: you pay £p to buy note where I commit to paying £1 if heads
    ▶ I buy: you get £p for note, and have to pay me £1 if heads

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Beliefs as willingness to wager

- A person with degree of belief $p$ in event $A$ is assumed to be willing to pay $\leq \pounds p$ for a unit wager on $A$
- and is willing to sell such a wager for any price $\geq \pounds p$
- This $p$ captures our degree of belief about the event $A$ taking place (aka uncertainty, confidence)
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Rational beliefs

- Two notes (unit wagers):
  - Note 1: ‘outcome=heads’
  - Note 2: ‘outcome=tails’

  you decide $p$ for note 1 and $q$ for note 2; I decide whether to buy from you or sell you each note at the price you determined

- if $p + q < 1$ then I will buy from you note 1 for £$p$ and also note 2 for £$q$

- whatever outcome you give me £$1$; but because I gave you $p + q < 1$, you lost £$1 - p - q$

- **Dutch book**: a set of unit wager notes where you decide the odds (wager price) and I decide whether to buy or sell each note ... and you are guaranteed to always lose money.
Rational beliefs

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Set of beliefs is called **rational** if no Dutch book exists.
Setup

- Def sample space $X$ of simple events (possible outcomes)
  - e.g. experiment flipping two coins $X = \{HH, HT, TH, TT\}$
- Let $A$ be an event (a subset of $X$). $A$ holding true $=$ at least one of the outcomes in $A$ happened
  - e.g. “at least one heads” $\leftrightarrow A = \{HH, HT, TH\}$
- Write $p_A$ for belief of event $A$ (your wager on $A$ happening, assuming all wagers are unit wagers)
Formalism (rational beliefs $\equiv$ prob theory)

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Can show that $\{p_A\}_{A \subseteq X}$ are rational beliefs iff $\{p_A\}_{A \subseteq X}$ satisfies laws of probability theory

- Already showed that $p_A + p_{A^c} = 1$
- Try to devise other betting games at home (bdl101.ml/betting)
Formalism (rational beliefs = prob theory)

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Can derive the laws of prob theory from rational beliefs!
- $\rightarrow$ if you want to be rational, must follow laws of probability (otherwise someone can take advantage of your model)
Probability as belief vs frequency

Above known as **Bayesian prob theory**

- forms an **interpretation of the laws of probability**, and formalises our notion of uncertainty in events

- vs ‘Frequency as probability’
  - only applicable to repeatable events (eg, try to answer ‘will Trump win 2020’)
  - also other issues; eg p-hacking
  - Psychology journal banning p values

(although there are problems w Bayesian arguments as well)
‘Real-world’ example

DID THE SUN JUST EXPLODE? (IT’S NIGHT, SO WE’RE NOT SURE)

THIS NEUTRINO DETECTOR MEASURES WHETHER THE SUN HAS GONE NOVA.

THEN, IT ROLLS TWO DICE. IF THEY BOTH COME UP SIX, IT TELLS US. OTHERWISE, IT TELLS THE TRUTH.

LET’S TRY.

DETECTOR! HAS THE SUN GONE NOVA?

(ROLL)

YES.

FREQUENTIST STATISTICIAN:

THE PROBABILITY OF THIS RESULT HAPPENING BY CHANCE IS \[
\frac{1}{36} = 0.027.
\]

SINCE \( p < 0.05 \), I CONCLUDE THAT THE SUN HAS EXPLODED.

BAYESIAN STATISTICIAN:

BET YOU $50 IT HASN’T.

[https://xkcd.com/1132/]
Bayesian Probabilistic Modelling (an Introduction)

Simple idea: “If you’re doing something which doesn’t follow from the laws of probability, then you’re doing it wrong”
can’t do ML without **assumptions**

- **must** make some assumptions about how data was generated
- there always exists some **underlying process** that generated obs
- in Bayesian probabilistic modelling we make our assumptions about underlying process **explicit**
- want to **infer** underlying process (find dist that generated data)
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eg – astrophysics: gravitational lensing

- there exists a physics process magnifying far away galaxies

- Nature chose lensing coeff → gravitational lensing mechanism → transform galaxy

- We **observe** transformed galaxies, want to **infer** lensing coeff
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**eg – cats vs dogs classification**

- there exist some underlying rules we don’t know
  - **eg** “if has pointy ears then cat”
  - We **observe** pairs (image, “cat” / “no cat”), and want to **infer** underlying mapping from images to labels
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**eg** – Gaussian density estimation

- I tell you the process I used to generate data and give 5 data points

\[ x_n \sim \mathcal{N}(x_n; \mu, \sigma^2), \quad \sigma = 1 \]

- you **observe** the points \( \{x_1, ..., x_5\} \), and want to **infer** my \( \mu \)
- Reminder: Gaussian density with mean \( \mu \) and variance \( \sigma^2 \)

\[
p(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}\]
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X Which $\mu$ generated my data?
V What’s the probability that $\mu = 10$ generated my data? (want to infer distribution over $\mu$!)
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eg – Gaussian density estimation

These are the hypotheses we’ll play with

I chose a Gaussian (one of those) from which I generated data
Generative story / model

In Bayesian probabilistic modelling

- want to represent our beliefs / assumptions about how data was generated explicitly

- eg via *generative story* [‘My assumptions are...’]:
  - Someone (me / Nature / etc) selected parameters $\mu^*, \sigma^*$
  - Generated $N$ data points $x_n \sim \mathcal{N}(\mu^*, \sigma^*^2)$
  - Gave us $D = \{x_1, ..., x_N\}$
  - → how would you formalise this process?

- Bayesian probabilistic model:
  - prior [what I believe params might look like]
    $$\mu \sim \mathcal{N}(0, 10), \quad \sigma = 1$$
  - likelihood [how I believe data was generated given params]
    $$x_n \mid \mu, \sigma \sim \mathcal{N}(\mu, \sigma^2)$$

- will update prior belief on $\mu$ conditioned on data you give me (infer distribution over $\mu$): $\mu \mid \{x_1, ..., x_N\}$
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    \[ \mu \mid \{x_1, ..., x_N\} \]
Can you find my Gaussian?

How can you infer $\mu$? (find distribution)

Everything follows the laws of prob..

- **Sum rule**

  $$p(X = x) = \sum_y p(X = x, Y = y) = \int p(X = x, Y) \, dY$$

- **Product rule**

  $$p(X = x, Y = y) = p(X = x | Y = y) p(Y = y)$$

- **Bayes rule**

  $$p(X = x | Y = y, H) = \frac{p(Y = y | X = x, H) p(X = x | H)}{p(Y = y | H)}$$

Note: $H$ is often omitted in conditional for brevity
Can you find my Gaussian?

Remember: products, ratios, marginals, and conditionals of Gaussians are Gaussian!

Properties of Gaussian distributions:
If $x_1, x_2$ follow a joint Gaussian distribution:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12}^T & \Sigma_{22} \end{bmatrix}\right),$$

then each marginal is Gaussian:

$$x_1 \sim \mathcal{N}(\mu_1, \Sigma_{11}),$$

each conditional is Gaussian:

$$x_1|x_2 \sim \mathcal{N}(\mu_1 + \Sigma_{12} \Sigma_{22}^{-1}(x_2 - \mu_2), \Sigma_{11} - \Sigma_{12} \Sigma_{22} \Sigma_{22}^T),$$

any linear combination is Gaussian:

$$Ax_1 + Bx_2 + C \sim \mathcal{N}(A\mu_1 + B\mu_2 + C, A\Sigma_{11} A^T + B\Sigma_{22} B^T)$$

and the product of the marginal densities is an (unnormalised) Gaussian:

$$\mathcal{N}(x; \mu_1, \Sigma_{11})\mathcal{N}(x; \mu_2, \Sigma_{22}) = C \cdot \mathcal{N}\left(x; (\Sigma_{11}^{-1} + \Sigma_{22}^{-1})^{-1}(\Sigma_{11}^{-1}\mu_1 + \Sigma_{22}^{-1}\mu_2), (\Sigma_{11}^{-1} + \Sigma_{22}^{-1})^{-1}\right)$$

with $C = \mathcal{N}(\mu_1; \mu_2, \Sigma_{11} + \Sigma_{22})$.

More here.

Visualising Gaussian likelihoods:

Summary (and playground) here: bdl101.ml/gauss
Inference

Bayes rule:

\[ p(X = x | Y = y, \mathcal{H}) = \frac{p(Y = y | X = x, \mathcal{H})p(X = x | \mathcal{H})}{p(Y = y | \mathcal{H})}, \]

and in probabilistic modelling:

\[
\begin{align*}
\text{Posterior} & \quad \text{Likelihood} \quad \text{Prior} \\
p(\mu | \mathcal{D}, \sigma, \mathcal{H}) & = \frac{p(\mathcal{D} | \mu, \sigma, \mathcal{H})p(\mu | \sigma, \mathcal{H})}{p(\mathcal{D} | \sigma, \mathcal{H})}
\end{align*}
\]

with model evidence \( p(\mathcal{D} | \sigma, \mathcal{H}) = \int p(\mathcal{D} | \mu, \sigma, \mathcal{H})p(\mu | \sigma, \mathcal{H})d\mu \) (sum rule).

**Likelihood**

- we explicitly assumed data comes iid from a Gaussian
- compute \( p(\mathcal{D} | \mu, \sigma) = \text{multiply all } p(x_n | \mu, \sigma) \) (product rule)
- prob of observing data points for given params
The Likelihood in more detail

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Reducing dataset from 5 points to 1:

- What does the likelihood look like?
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Likelihood as a function of parameters

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![Graph showing likelihood as a function of parameters with a peak at x=0 and labeled parameters m=1, s=1 and pdf=0.241970724519]
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and with smaller $\sigma$..

- Trying to max lik will get “absolutely certain that $\sigma = 0$ & $\mu = 0$”
- Does this make sense? (I told you $x_n \sim \mathcal{N}$!)
- MLE failure
Reducing dataset from 5 points to 1:

- What does the likelihood look like?

And with all data:
Reducing dataset from 5 points to 1:

▷ What does the likelihood look like?

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Likelihood function shows how well every value of $\mu$, $\sigma$ predicted what would happen.
The Posterior in more detail

\[ p(\mu|D, \sigma, \mathcal{H}) = \frac{p(D|\mu, \sigma, \mathcal{H})p(\mu|\sigma, \mathcal{H})}{p(D|\sigma, \mathcal{H})} \]

with model evidence \( p(D|\sigma, \mathcal{H}) = \int p(D|\mu, \sigma, \mathcal{H})p(\mu|\sigma, \mathcal{H})d\mu \) (sum rule). In contrast to the likelihood, posterior would say

‘with the data you gave me, this is what I currently think \( \mu \) could be, and I might become more certain if you give me more data’

- normaliser = marginal likelihood = evidence = sum of likelihood * prior
  - (but often difficult to calculate... more in the next lecture)
Eg, inference w prior = ‘we believe data is equally likely to have come from one of the 5 Gaussians w σ = 1’

\[ p(\mu = \mu_i | \sigma, \mathcal{H}) = \frac{1}{5} \text{ and } p(\mu \neq \mu_i \text{ for all } i | \sigma, \mathcal{H}) = 0 \]

then marginal likelihood is

\[ p(\mathcal{D} | \sigma, \mathcal{H}) = \sum_i p(\mathcal{D} | \mu = \mu_i, \sigma, \mathcal{H}) p(\mu = \mu_i | \sigma, \mathcal{H}) \]

\[ = \sum_i p(\mathcal{D} | \mu = \mu_i, \sigma, \mathcal{H}) \frac{1}{5} \]

and posterior is

\[ p(\mu = \mu_i | \sigma, \mathcal{D}, \mathcal{H}) = \frac{1/5 p(\mathcal{D} | \mu = \mu_i, \sigma, \mathcal{H})}{\sum_i 1/5 p(\mathcal{D} | \mu = \mu_i, \sigma, \mathcal{H})} \]
where \( p(\mathcal{D}|\mu = \mu_i, \sigma = 1, \mathcal{H}) \) is given by

- marginal likelihood of \( \sigma = 1 \) = \( p(\mathcal{D}|\sigma = 1, \mathcal{H}) \) = ‘prob that data came from single Gaussian with param \( \sigma = 1 \)’

- similarly, marginal likelihood of hypothesis = \( p(\mathcal{D}|\mathcal{H}) \) = ‘prob that data came from single Gaussian (with some \( \mu, \sigma \)’
Bayesian Probabilistic Modelling of Functions
Why uncertainty over functions

- Example going beyond beliefs over statements (‘heads happened’) / scalars (µ)

- Would want to know uncertainty (ie belief) of system in prediction

- Want to know distribution over outputs for each input \( x = \text{dist} \) over functions

- First, some preliminaries.. (history, and notation)
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Linear regression [Gauss, 1809]

Given a set of $N$ input-output pairs $\{(x_1, y_1), ..., (x_N, y_N)\}$

- eg average number of accidents for different driving speeds

- assumes exists linear func mapping vectors $x_i \in \mathbb{R}^Q$ to $y_i \in \mathbb{R}^D$ (with $y_i$ potentially corrupted with observation noise)

- model is linear trans. of inputs: $f(x) = Wx + b$, $W$ some $D$ by $Q$ matrix over reals, $b$ real vector with $D$ elements

- Different params $W, b$ define different linear trans
  - aim: find params that (eg) minimise $1/N \sum_i ||y_i - (Wx_i + b)||^2$

- but relation between $x$ and $y$ need not be linear
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- Assumes there exists a linear function mapping vectors $x_i \in \mathbb{R}^Q$ to $y_i \in \mathbb{R}^D$ (with $y_i$ potentially corrupted with observation noise)

- Model is linear transformation of inputs: $f(x) = Wx + b$, where $W$ is some $D$ by $Q$ matrix over reals, $b$ is a real vector with $D$ elements

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Linear basis function regression [Gergonne, 1815; Smith, 1918]

- input \( x \) fed through \( K \) fixed scalar-valued non-linear trans. \( \phi_k(x) \)

- collect into a feature vector \( \phi(x) = [\phi_1(x), \ldots, \phi_K(x)] \)

- do linear regression with \( \phi(x) \) vector instead of \( x \) itself

- with scalar input \( x \), trans. can be
  - wavelets parametrised by \( k \): \( \cos(k\pi x)e^{-x^2/2} \)
  - polynomials of degrees \( k \): \( x^k \)
  - sinusoidals with various frequencies: \( \sin(kx) \)

- When \( \phi_k(x) := x_k \) and \( K = Q \), basis function regr. = linear regr.

- basis functions often assumed fixed and orthogonal to each other (optimal combination is sought)

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Parametrised basis functions

**Parametrised** basis functions [Bishop, 2006; many others]

- eg basis functions $\phi_{w_k, b_k}$ where scalar-valued function $\phi_k$ is applied to inner-product $w_k^T x + b_k$
  - $\phi_k$ often def’d to be identical for all $k$ (only params change)
  - eg $\phi_k(\cdot) = \tanh(\cdot)$, giving $\phi_{w_k, b_k}(x) = \tanh(w_k^T x + b_k)$

- feature vector = basis functions’ outputs = input to linear trans.

- in vector form:
  - $W_1$ a matrix of dimensions $Q$ by $K$
  - $b_1$ a vector with $K$ elements
  - $\phi_{w_1, b_1}(x) = \phi(w_1 x + b_1)$
  - $W_2$ a matrix of dimensions $K$ by $D$
  - $b_2$ a vector with $D$ elements
  - model output: $f_{W_1, b_1, W_2, b_2}(x) = \phi_{w_1, b_1}(x)W_2 + b_2$

- want to find $W_1, b_1, W_2, b_2$ that minimise $1/N \sum_i \|y_i - f_{W_1, b_1, W_2, b_2}(x_i)\|^2$
Parametrised basis functions

**Parametrised** basis functions [Bishop, 2006; many others]

- eg basis functions $\phi_{w_k, b_k}$ where scalar-valued function $\phi_k$ is applied to inner-product $w_k^T x + b_k$
  - $\phi_k$ often def’d to be identical for all $k$ (only params change)
  - eg $\phi_k(\cdot) = \tanh(\cdot)$, giving $\phi_{w_k, b_k}(x) = \tanh(w_k^T x + b_k)$

- feature vector = basis functions’ outputs = input to linear trans.

- in vector form:
  - $W_1$ a matrix of dimensions $Q$ by $K$
  - $b_1$ a vector with $K$ elements
  - $\phi_{W_1, b_1}(x) = \phi(W_1 x + b_1)$
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Hierachy of parametrised basis functions [Rumelhart et al., 1985]
- called “NNs” for historical reasons

- **layers**
  - ‘feature vectors’ in hierarchy
  - linear trans. = ‘inner product’ layer = ‘fully connected’ layer
  - ‘input layer’, ‘output layer’, ‘hidden layers’
  - trans. matrix = weight matrix = \( W \);
    
    intercept = bias = \( b \)

- **units**
  - elements in a layer

- **feature vector** (overloaded term)
  - often refers to the penultimate layer (at top of model just before softmax / last linear trans.)
  - denote feature vector

\[
\phi(x) = [\phi_1(x), \ldots, \phi_K(x)] \text{ with } K \text{ units (a } K \text{ by } 1 \text{ vector)}
\]

\[
\Phi(X) = [\phi(x_1)^T, \ldots, \phi(x_N)^T], \text{ N by } K \text{ matrix}
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  - denote feature vector
    \( \phi(x) = [\phi_1(x), \ldots, \phi_K(x)] \) with \( K \) units (a \( K \) by 1 vector)
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**Hierarchy of parametrised basis functions**

- **regression**
  - compose multiple basis function layers into a regression model
  - result of last trans. also called “model output”; often no non-linearity here

- **classification**
  - further compose a **softmax** function at the end; also called “logistic” for 2 classes
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- “building blocks”
  - layers are simple
  - modularity in layer composition → versatility of deep models
  - many engineers work in field → lots of tools that scale well
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Assumptions for the moment

- we’ll use deep nets, and denote $W$ to be the weight matrix of the last layer and $b$ the bias of last layer

- (for the moment) look only at last layer $W$, everything else fixed – ie weights other than $W$ do not change
  - later we’ll worry about other layers

- assume that $y$ is scalar
  - so $W$ is $K$ by 1
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  - both will simplify derivations here (but pose no difficulty otherwise)

- then $f^W(x) = \sum w_k \phi_k(x) = W^T \phi(x)$ with $\phi(x)$ a ‘frozen’ feature vec for some NN

- some notation you’ll need to remember...
  $X, x, N, x_n, Q, D, K, D = \{(x_1, y_1), .., (x_N, y_N)\} = X, Y$
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Generative story

Want to put dist over functions..

- difficult to put belief over funcs., but easy to put over NN params

- assumptions for the moment: our data was generated from the fixed $\phi$ (NN) using some $W$ (which we want to infer)
Generative story

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**Generative story** [what we assume about the data]

- Nature chose \( W \) which def’s a func: \( f^W(x) := W^T \phi(x) \)
- generated **func. values** with inputs \( x_1, \ldots, x_N \): \( f_n := f^W(x_n) \)
- corrupted func. values with noise [also called ”obs noise”]
  \[ y_n := f_n + \epsilon_n, \quad \epsilon_n \sim \mathcal{N}(0, \sigma^2) \]
  [additive Gaussian noise w param \( \sigma \)]
- we’re given **observations** \( \{(x_1, y_1), \ldots, (x_N, y_N)\} \) and \( \sigma = 1 \)
Model

- **qs**
  - how can we find function value \( f^* \) for a new \( x^* \)?
  - how can we find our confidence in this prediction?
  - → ‘everything follows from the laws of probability theory’

- we build a **model**:
  - put prior dist over params \( W \)
    \[
    p(W) = \mathcal{N}(W; 0_K, s^2 I_K)
    \]
  - likelihood [conditioned on \( W \) generate obs by adding gaussian noise]
    \[
    p(y|W, x) = \mathcal{N}(y; W^T \phi(x), \sigma^2)
    \]
  - prior belief “\( w_k \) is more likely to be in interval \([-1, 1]\) than in \([100, 200]\)” means that the **func. values** are likely to be more smooth than erratic (we’ll see later why)
  - we want to infer \( W \) (find dist over \( W \) given \( D \))
qs

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\[ p(w | x, y) \propto p(y) p(w | x) / p(y | x) \]
\[ p(w|x,y) = p(y|x, w) p(w|x) / p(y|x) \]

only terms top \[ \propto p(y|x, w) p(w) \]
\[
\rho(w|x,y) = \frac{\rho(w)}{\rho(y|x) \rho(w|x)} \\
= \rho(y|x,w) \rho(w) \\
= \prod_n \mathcal{N}(y_n | w^T \phi(x_n), \sigma^2) \mathcal{N}(w|0, \mathbf{I} s^2)
\]
\[ p(w|x, y) \]
\[ = \frac{p(y|x, w) p(w|x)}{p(y|x)} \]
\[ \propto p(y|x, w) p(w) \]
\[ = \prod_n \mathcal{N}(y_n; w^T \phi(x), \sigma^{-2}) \mathcal{N}(w; 0, s^2 I) \]
\[ = \prod_n e^{-\frac{1}{2} \sigma^{-2} (y_n - w^T \phi(x))^2} \cdot e^{-\frac{1}{2} s^{-2} w^T w} \]
Analytic inference w functions [new technique!]

\[ p(w | x, y) \]

\[ = p(y | x, w) \frac{p(w)}{p(y | x)} \]

only term

\[ \propto p(y | x, w) p(w) \]

\[ = \left[ \prod_n N(y_n; w^T \phi(x_n), \sigma^{-2}) \right] N(w; 0, s^2 I) \]

\[ = \left[ \prod_n e^{-\frac{1}{2\sigma^{-2}} (y_n - w^T \phi(x_n))^2} \right] e^{-\frac{1}{2} s^{-2} w^T w} \]

\[ \propto e^{\frac{n}{2} \sum_{n \sigma^{-2}} (y_n - w^T \phi(x_n))^2 + s^{-2} w^T w} \]
\[ \rho(w|x,y) = \frac{\rho(w)}{\rho(y|x)} \]
\[ = \frac{\rho(y|x,w)\rho(w)}{\rho(y|x)} \]

\[ \propto \rho(y|x,w) \rho(w) \]

\[ = \left[ \prod_n \mathcal{N}(y_n; \mathbf{w}^T \phi(x_n), \sigma^2) \right] \mathcal{N}(\mathbf{w}; \mathbf{0}, s^2 I) \]

\[ = \prod_n e^{\frac{1}{2\sigma^2} (y_n - \mathbf{w}^T \phi(x_n))^2} \cdot e^{-\frac{1}{2} s^{-2} \mathbf{w}^T \mathbf{w}} \]

\[ \propto \mathcal{E} \left\{ -\frac{1}{2} \sum_n \sigma^{-2} (y_n - \mathbf{w}^T \phi(x_n))^2 + s^{-2} \mathbf{w}^T \mathbf{w} \right\} \]

"\(w\) terms:

\[ \frac{1}{n} \sum_n \sigma^{-2} (\cdot 2 y_n \mathbf{w}^T \phi(x_n) + \left( \mathbf{w}^T \phi(x_n) \right)^T (\mathbf{w}^T \phi(x_n)) \]

\[ + s^{-2} \mathbf{w}^T \mathbf{w} \]

\[ = \phi^T(x_n) \mathbf{w} = \mathbf{w}^T \phi(x_n) \]
\[ \sigma^{-2} \sum_n \left( \gamma_n \phi_t \right) \] 
\[ + \sigma^{-2} \sum_n \phi_t \phi_t^\top \gamma_n \] 
\[ + \sum_n \gamma_n \gamma_n^\top \]
Analytic inference w functions [new technique!]

\[
\begin{align*}
\mathbf{w} & = \mathbf{\Sigma}^{-2} \sum_{n} (-2 y_n \mathbf{w}^T \phi (x_n)) \\
& \quad + \mathbf{\Sigma}^{-2} \sum_{n} \mathbf{w}^T \phi (x_n) \phi (x_n)^T \mathbf{w} \\
& \quad + S^{-2} \mathbf{w}^T \mathbf{w} \\
& = \mathbf{w}^T \left[ \mathbf{\Sigma}^{-2} \sum_{n} \phi (x_n) \phi (x_n)^T + S^{-2} \mathbf{I}_k \right] \mathbf{w} \\
& \quad - 2 \mathbf{w}^T \mathbf{\Sigma}^{-2} \sum_{n} y_n \phi (x_n)
\end{align*}
\]
Analytic inference w functions [new technique!]

\[ \begin{align*}
\mathbf{w}^\top \Sigma^{-1} \sum_n \left( -2 \gamma_n \mathbf{w}^\top \phi(t_n) \right) \\
+ \sigma^{-2} \sum_n \mathbf{w}^\top \phi(t_n) \phi(t_n)^\top \mathbf{w} \\
+ \sigma^{-2} \sum_n \mathbf{w}^\top \phi(t_n) \phi(t_n)^\top \mathbf{w} \\
+ \sigma^{-2} \sum_n \mathbf{w}^\top \phi(t_n) \phi(t_n)^\top \mathbf{w} \\
= \mathbf{w}^\top \left[ \sigma^{-2} \sum_n \phi(t_n) \phi(t_n)^\top + \sigma^{-2} \mathbf{1}_k \right] \mathbf{w} \\
- 2 \mathbf{w}^\top \sigma^{-2} \sum_n \gamma_n \phi(t_n) \\
\text{Known} \quad \rho(\mathbf{w}|y) \sim \mathcal{N}(\mu^*, \Sigma^*) \\
(\mathbf{w} - \mu^*) \Sigma^{-1} (\mathbf{w} - \mu^*) = \mathbf{w}^\top \Sigma^{-1} \mathbf{w} - 2 \mathbf{w}^\top \Sigma^{-1} \mu^* + \mu^* \Sigma^{-1} \mu^*.
\end{align*} \]
Analytic inference w functions [new technique!]

\[
\begin{align*}
\Sigma' &= (\sigma^{-2} \sum_n \phi(x_n)\phi(x_n)^T + s^{-2} I_K)^{-1} \\
\mu' &= \Sigma'\sigma^{-2} \sum_n (y_n\phi(x_n))
\end{align*}
\]

and in vector form:

\[
\begin{align*}
\Sigma'\sigma^{-2} \Phi(X)^T Y
\end{align*}
\]
Analytic predictions with functions

How do we predict function values $y^*$ for new $x^*$?

- use prob theory to perform preds!

$$p(y^*|x^*, X, Y)$$

$$= \int p(y^*, W|x^*, X, Y) dW \quad \text{sum rule}$$

$$= \int p(y^*|x^*, W, X, Y) p(W|X, Y) dW \quad \text{product rule}$$

$$= \int p(y^*|x^*, W) p(W|X, Y) dW \quad \text{model assumptions}$$

- how to eval? [a new technique!]
  - likelihood $p(y^*|x^*, W)$ is Gaussian
  - posterior $p(W|X, Y)$ is Gaussian (from above)
  - so predictive $p(y^*|x^*, X, Y)$ is Gaussian..
Analytic predictions with functions

\[ p(y^* | x^*, \mathcal{D}) = \mathcal{N}(\mu^* | \Sigma^*) \]

\[ \mu^* = E_{\rho(y^* | x^*, \mathcal{D})} \Sigma^* \]
Analytic predictions with functions

\[ p(y^* | x^*, D) = \mathcal{N}(\mu^*, \Sigma^*) \]

\[ \mu^* = E_{p(y^* | x^*, D)} \bar{Y}^* \]

\[ = \int p(y^* | x^*, D) \cdot y^* \, dy^* \]
Analytic predictions with functions

\[ p(y^*|x^*, 0) = N(\mu^*, \Sigma^*) \]

\[ \mu^* = E_{p(y^*|x^*, 0)}[y^*] \]

\[ = \int p(y^*|x^*, 0) \cdot y^* \, dy^* \]

\[ = \int y^* \left( \int p(y^*|x^*, w) p(w|0) \, dw \right) \, dy^* \]
$p(y^* | x^*, D) = \mathcal{N}(\mu^*, \Sigma^*)$

$\mu^* = E_{p(y^* | x^*, D)}[y^*]$

$= \int p(y^* | x^*, D) \cdot y^* \, dy^*$

$= \int y^* \left( \int p(y^* | x^*, w) p(w | D) \, dw \right) \, dy^*$

$= \int \left( \int y^* p(y^* | x^*, w) \, dy^* \right) p(w | D) \, dw$

$E_{\mu^*} (y^*) = \omega \phi(x^*)$
Analytic predictions with functions

\[ p(y^*|x^*, \mathbf{D}) = \mathcal{N}(\mu^*, \Sigma^*) \]

\[ \mu^* = \mathbb{E}_{p(y^*|x^*, \mathbf{D})}[y^*] \]

\[ = \int p(y^*|x^*, \mathbf{D}) \cdot y^* \, dy^* \]

\[ = \int \int p(y^*|x^*, \mathbf{w}) p(w|D) \, dw \, dy^* \]

\[ = \int \left( \int p(y^*|x^*, \mathbf{w}) \, dy^* \right) p(w|D) \, dw \]

\[ \mathbb{E}_{\text{Post}}(y^*) = \mathbf{w}^T \phi(x^*) \]

\[ = \left\{ \mathbf{w}^T p(w|D) \, dw \right\} \phi(x^*) = \mu^T \phi(x^*) \]

\[ \mathbb{E}_{\text{Post}}[w]^T = \mu^T \]
Analytic predictions with functions

\[ \mu^* = E_{\pi(x^*)} \sum \gamma^* \]

\[ = \int \gamma^* \left( \int p(y^* | x^*, w) \right) p(w | \theta) d w \] d \gamma^*

\[ = \int \left( \int \gamma^* p(y^* | x^*, w) d y^* \right) p(w | \theta) d w \]

\[ = w^T \phi(x^*) = \mu^T \phi(x^*) \]

\[ E_{\text{post}} [w]^T = \mu^T \]

- Homework: Predictive variance
What you should be able to do now

- perform density estimation with scalars
- know when MLE fails (and why)
- use Bayes law to make more informed decisions in your life
- win against your friends in a series of bets
- argue with frequentists about how to interpret the laws of probability
- argue with philosophers about the nature of subjective beliefs
- use Bayesian probability in ML correctly
- perform predictions in Bayesian probabilistic modelling correctly
What we will cover next

In the next lecture we’ll

▶ decompose uncertainty into epistemic and aleatoric components

▶ use uncertainty in regression **correctly**

▶ develop tools to scale the ideas above to large deep models

▶ develop **big deep learning systems** which convey uncertainty
  ▶ w **real-world** examples