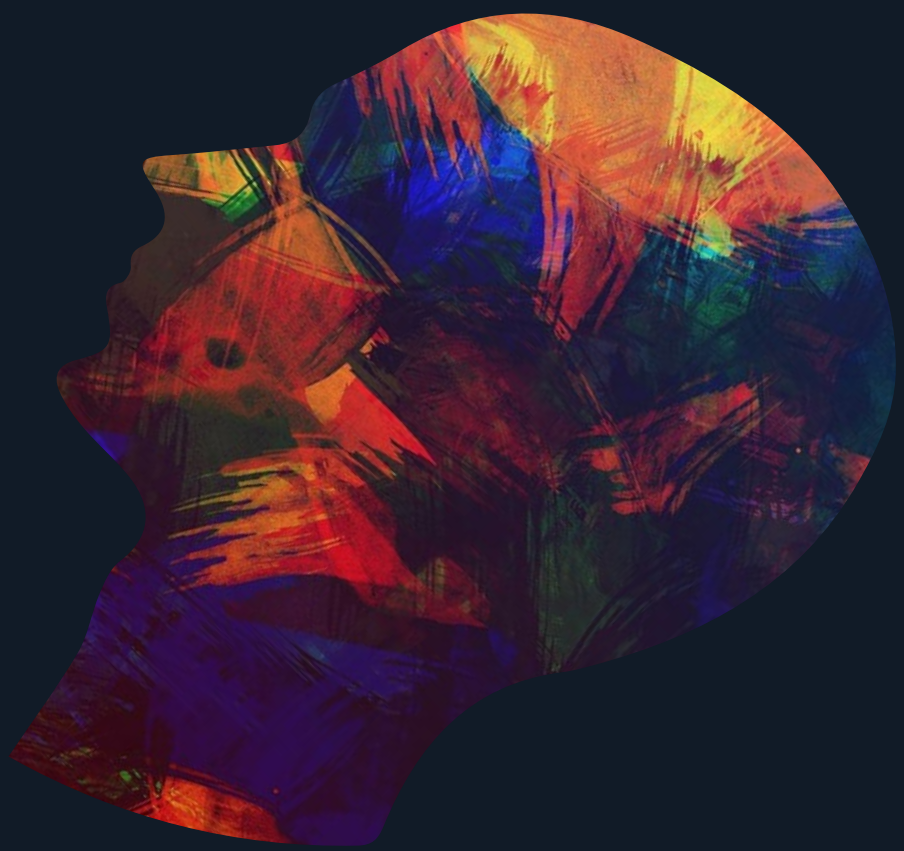
DEEP LEARNING INTERVIEWS

—REAL-WORLD DEEP LEARNING INTERVIEW PROBLEMS & SOLUTIONS—

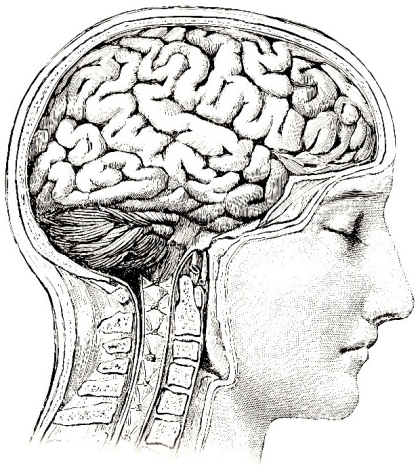
SECOND EDITION



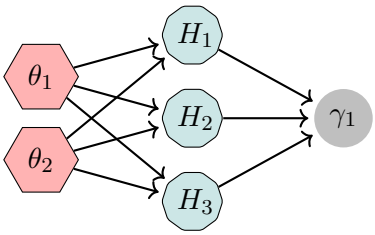
SHLOMO KASHANI

SHLOMO KASHANI

DEEP LEARNING INTERVIEWS



By Shlomo Kashani, M.Sc, QMUL, UK.



Published by Shlomo Kashani, Tel-Aviv, ISRAEL.
Visit: http://www.interviews.ai

Printing version: **VER. 26TH OCTOBER 2021**

Printed in the United States of America.
Library of Congress Cataloging-in-Publication Data
A catalog record for this book is available from the Library of Congress

COPYRIGHT.

the publisher nor author shall be liable for any loss of profit or any other commercial damages, including but not limited to special, incidental, consequential, or other damages.

Notices. Knowledge and best practice in this field are constantly changing. As new research and experience broaden our understanding, changes in research methods, professional practices, or medical treatment may become necessary. Practitioners and researchers must always rely on their own experience and knowledge in evaluating and using any information, methods, compounds, or experiments described herein. In using such information or methods they should be mindful of their own safety and the safety of others, including parties for whom they have a professional responsibility. To the fullest extent of the law, neither the Publisher nor the authors, contributors, or editors, assume any liability for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions, or ideas contained in the material herein.

FOREWORD.

We will build a machine that will fly.

— Joseph Michael Montgolfier, French Inventor/Aeronaut (1740-1810)

EEP learning interviews are technical, dense, and thanks to the fields competitiveness, often high-stakes. The prospect of preparing for one can be daunting, and the fear of failure can be paralyzing and many interviewees find their ideas slipping away alongside their confidence.

This book was written for you: an aspiring data scientist with a quantitative background, facing down the gauntlet of the interview process in an increasingly competitive field. For most of you, the interview process is the most significant hurdle between you and a dream job. Even though you have the ability, the background, and the motivation to excel in your target position, you might need some guidance on how to get your foot in the door.

Though this book is highly technical it is not too dense to work through quickly. It aims to be comprehensive, including many of the terms and topics involved in modern data science and deep learning. That thoroughness makes it unique; no other single work offers such breadth of learning targeted so specifically at the demands of the interview.

Most comparable information is available in a variety of formats, locations, structures, and resourcesblog posts, tech articles, and short books scattered across the internet. Those resources are simply not adequate to the demands of deep learning interview or exam preparation and were not assembled with this explicit purpose in mind. It is hoped that this book does not suffer the same shortcomings.

HIS books creation was guided by a few key principles: clarity and depth, thoroughness and precision, interest and accuracy. The volume was designed for use by job seekers in the fields of machine learning and deep learning whose abilities and background locate them firmly within STEM (science, technology, engineering, and mathematics). The book will still be of use to other readers, such as those still undergoing their initial education in a STEM field.

However, it is tailored most directly to the needs of **active job seekers and students attending M.Sc/Ph.D programmes in AI**. It is, in any case, a book for engineers, mathematicians, and computer scientists: nowhere does it include the kind of very basic background material that would allow it to be read by someone with no prior

knowledge of quantitative and mathematical processes.

The books contents are a large inventory of numerous topics relevant to deep learning job interviews and graduate level exams. Ideas that are interesting or pertinent have been excluded if they are not valuable in that context. That places this work at the forefront of the growing trend in education and in business to emphasize a core set of practical mathematical and computational skills. It is now widely understood that the training of every computer scientist must include a course dealing with the fundamental theorems of machine learning in a rigorous manner; Deep Learning appears in the curriculum of nearly every university; and this volume is designed as a convenient ongoing reference for graduates of such courses and programs.

The book is grounded in both academic expertise and on-the-job experience and thus has two goals. First, it compresses all of the necessary information into a coherent package. And second, it renders that information accessible and makes it easy to navigate. As a result, the book helps the reader develop a thorough understanding of the principles and concepts underlying practical data science. None of the textbooks I read met all of those needs, which are:

1. **Appropriate presentation level**. I wanted a friendly introductory text accessible to graduate students who have not had extensive applied experience as data scientists.

2. **A text that is rigorous** and builds a solid understanding of the subject without getting bogged down in too many technicalities.

3. **Logical and notational consistency among topics**. There are intimate connections between calculus, logistic regression, entropy, and deep learning theory, which I feel need to be emphasized and elucidated if the reader is to fully understand the field. Differences in notation and presentation style in existing sources make it very difficult for students to appreciate these kinds of connections.

4. **Manageable size**. It is very useful to have a text compact enough that all of the material in it can be covered in few weeks or months of intensive review. Most candidates will have only that much time to prepare for an interview, so a longer text is of no use to them.

   The text that follows is an attempt to meet all of the above challenges. It will inevitably prove more successful at handling some of them than others, but it has at least made a sincere and devoted effort.

A note about Bibliography

The book provides a carefully curated bibliography to guide further study, whether for interview preparation or simply as a matter of interest or job-relevant research. A comprehensive bibliography would be far too long to include here, and would be of little immediate use, so the selections have been made with deliberate attention to the value of each included text.

Only the most important books and articles on each topic have been included, and only those written in English that I personally consulted. Each is given a brief annotation to indicate its scope and applicability. Many of the works cited will be found to include very full bibliographies of the particular subject treated, and I recommend turning there if you wish to dive deeper into a specific topic, method, or process.

We have a web page for this book, where we list errata, examples, and any additional information. You can access this page at: http://www.interviews.ai. To comment or ask technical questions about this book, send email to: entropy@interviews.ai.

I would also like to solicit corrections, criticisms, and suggestions from students and other readers. Although I have tried to eliminate errors over the multi year process of writing and revising this text, a few undoubtedly remain. In particular, some typographical infelicities will no doubt find their way into the final version. I hope you will forgive them.

THE AUTHOR.

TEL AVIV ISRAEL, DECEMBER, 2020. FIRST PRINTING, DECEMBER 2020.

ACKNOWLEDGEMENTS.

The thanks and acknowledgements of the publisher are due to the following: My dear son, Amir Ivry, Matthew Isaac Harvey, Sandy Noymer, Steve foot and Velimir Gayevskiy.

Author's Biography.

When Shlomo typed his book in LaTeX, he wanted it to reflect some of his passions: AI, design, typography, and most notably coding. On a typical day, his two halves - the scientist and the artist - spend hours meticulously designing AI systems, from epilepsy prediction and pulmonary nodule detection, to training a computer-vision model on a cluster.

Shlomo spends whole days in a lab full of GPUs working on his many interesting research projects. Though research satisfies his itch for discovery, his most important scientific contribution, he says, is helping other researchers.

And the results are evident in his publications. But, although theoretical studies are important, practical experience has many great virtues. As the Head of AI at DeepOncology, he developed uses of Deep Learning for precise tumour detection, expanding and refining what human experts are capable of. The work, which relies on CNN's, marks the culmination of a career spent applying AI techniques to problems in medical AI. Shlomo holds an MSc in Digital Signal Processing (Distinction) from the University of London.

A personal note: In this first volume, I purposely present a coherent, cumulative, and content-specific **core curriculum** of the data science field, including topics such as information theory, Bayesian statistics, algorithmic differentiation, logistic regression, perceptrons, and convolutional neural networks.

I hope you will find this book stimulating. It is my belief that you **the postgraduate students and job-seekers** for whom the book is primarily meant will benefit from reading it; however, it is my hope that even the most experienced researchers will find it fascinating as well.

Shlomo Kashani,Tel-Aviv,ISRAEL.

About the Chief Editor.

Amir Ivry has been an applied research scientist in the fields of deep learning and speech signal processing since 2015. A direct PhD candidate in the Electrical and Computer Engineering Faculty in the Technion - Israel Institute of Technology, Amir is the author of over a dozen academic papers in leading IEEE journals and top-tier conferences. For his contribution to the field of hands-free speech communication using deep neural networks, Amir has received more than a dozen awards and honors, including back-to-back Jacobs citations for research excellence, and most recently the international speech communication association grant. Being only 28 years old, he has been cemented as a popular lecturer in the machine learning community, and delivered technological sessions for MIT, Google for startups, Alibaba, and more. Amir is currently holding a position as an applied research intern in Microsoft Advanced Technology Labs.

Contents

PART I
RUSTY NAIL

Chapter 1

How-to use this book

*The true logic of this world is in the **calculus** of probabilities.*

— James C. Maxwell

Contents

1.1 Introduction

First of all, welcome to world of Deep Learning Interviews.

1.1.1 What makes this book so valuable

ARGETED advertising. Deciphering dead languages. Detecting malignant tumours. Predicting natural disasters. Every year we see dozens of new uses for deep learning emerge from corporate R&R, academia, and plucky entrepreneurs. Increasingly, deep learning and artificial intelligence are ingrained in our cultural consciousness. Leading universities are dedicating programs to teaching them, and they make the headlines every few days.

That means jobs. It means intense demand and intense competition. It means a generation of data scientists and machine learning engineers making their way into

the workforce and using deep learning to change how things work. This book is for them, and for you. It is aimed at current or aspiring experts and students in the field possessed of a strong grounding in mathematics, an active imagination, engaged creativity, and an appreciation for data. It is hand-tailored to give you the best possible preparation for deep learning job interviews by guiding you through hundreds of fully solved questions.

That is what makes the volume so specifically valuable to students and job seekers: it provides them with the ability to speak confidently and quickly on any relevant topic, to answer technical questions clearly and correctly, and to fully understand the purpose and meaning of interview questions and answers.

Those are powerful, indispensable advantages to have when walking into the interview room.

The questions and problems the book poses are tough enough to cut your teeth on-and to dramatically improve your skills but theyre framed within thought provoking questions, powerful and engaging stories, and cutting edge scientific information. What are bosons and fermions? What is choriionic villus? Where did the Ebola virus first appear, and how does it spread? Why is binary options trading so dangerous?

Your curiosity will pull you through the book's problem sets, formulas, and instructions, and as you progress, you'll deepen your understanding of deep learning. There are intricate connections between calculus, logistic regression, entropy, and deep learning theory; work through the book, and those connections will feel intuitive.

1.1.2 What will I learn

Starting Your Career

Are you actively pursuing a career in deep learning and data science, or hoping to do so? If so, you're in luck everything from deep learning to artificial intelligence is in extremely high demand in the contemporary workforce. Deep learning professionals are highly sought after and also find themselves among the highest-paid employee groups in companies around the world.

So your career choice is spot on, and the financial and intellectual benefits of landing a solid job are tremendous. But those positions have a high barrier to entry: the deep learning interview. These interviews have become their own tiny industry, with HR employees having to specialize in the relevant topics so as to distinguish well-prepared job candidates from those who simply have a loose working knowledge of the material. Outside the interview itself, the difference doesn't always feel import-

ant. Deep learning libraries are so good that a machine learning pipeline can often be assembled with little high-skill input from the researcher themselves. But that level of ability won't cut it in the interview. You'll be asked practical questions, technical questions, and theoretical questions, and expected to answer them all confidently and fluently.

For unprepared candidates, that's the end of the road. Many give up after repeated post-interview rejections.

Advancing Your Career

Some of you will be more confident. Those of you with years on the job will be highly motivated, exceptionally numerate, and prepared to take an active, hands-on role in deep learning projects. You probably already have extensive knowledge in applied mathematics, computer science, statistics, and economics. Those are all formidable advantages.

But at the same time, it's unlikely that you will have prepared for the interview itself. Deep learning interviews especially those for the most interesting, autonomous, and challenging positions demand that you not only know how to do your job but that you display that knowledge clearly, eloquently, and without hesitation. Some questions will be straightforward and familiar, but others might be farther afield or draw on areas you haven't encountered since college.

There is simply no reason to leave that kind of thing to chance. Make sure you're prepared. Confirm that you are up-to-date on terms, concepts, and algorithms. Refresh your memory of fundamentals, and how they inform contemporary research practices. And when the interview comes, walk into the room knowing that you're ready for what's coming your way.

Diving Into Deep Learning

"Deep Learning Job Interviews" is organized into chapters that each consist of an Introduction to a topic, Problems illustrating core aspects of the topic, and complete Solutions. You can expect each question and problem in this volume to be clear, practical, and relevant to the subject. Problems fall into two groups, conceptual and application-based. Conceptual problems are aimed at testing and improving your knowledge of basic underlying concepts, while applications are targeted at practicing or applying what you've learned (most of these are relevant to Python and PyTorch). The chapters are followed by a reference list of relevant formulas and a selective bibliography for guide further reading.

1.1.3 How to Work Problems

In real life, like in exams, you will encounter problems of varying difficulty. A good skill to practice is recognizing the level of difficulty a problem poses. Job interviews will have some easy problems, some standard problems, and some much harder problems.

Each chapter of this book is usually organized into three sections: Introduction, Problems, and Solutions. As you are attempting to tackle problems, resist the temptation to prematurely peek at the solution; It is vital to allow yourself to struggle for a time with the material. Even professional data scientists do not always know right away how to resolve a problem. The art is in gathering your thoughts and figuring out a strategy to use what you know to find out what you don't.

PRB-1 CH.PRB- 1.1.

Problems outlined in grey make up the representative question set. *This set of problems is intended to cover the most essential ideas in each section. These problems are usually highly typical of what you'd see on an interview, although some of them are atypical but carry an important moral. If you find yourself unconfident with the idea behind one of these, it's probably a good idea to practice similar problems. This representative question set is our suggestion for a minimal selection of problems to work on. You are highly encouraged to work on more.*

SOL-1 CH.SOL- 1.1. *I am a solution.* ■

If you find yourself at a real stand-off, go ahead and look for a clue in one of the recommended theory books. Think about it for a while, and don't be afraid to read back in the notes to look for a key idea that will help you proceed. If you still can't solve the problem, well, we included the Solutions section for a reason! As you're reading the solutions, try hard to understand why we took the steps we did, instead of memorizing step-by-step how to solve that one particular problem.

If you struggled with a question quite a lot, it's probably a good idea to return to it in a few days. That might have been enough time for you to internalize the necessary ideas, and you might find it easily conquerable. If you're still having troubles, read over the solution again, with an emphasis on understanding why each step makes sense. One of the reasons so many job candidates are required to demonstrate their ability to resolves data science problems on the board, is that it hiring managers assume it reflects their true problem-solving skills.

In this volume, you will learn lots of concepts, and be asked to apply them in a variety of situations. Often, this will involve answering one really big problem by breaking it up into manageable chunks, solving those chunks, then putting the pieces back together. When you see a particularly long question, remain calm and look for a way to break it into pieces you can handle.

1.1.4 Types of Problems

Two main types of problems are presented in this book.

CONCEPTUAL: The first category is meant to test and improve your understanding of basic underlying concepts. These often involve many mathematical calculations. They range in difficulty from very basic reviews of definitions to problems that require you to be thoughtful about the concepts covered in the section.

An example in Information Theory follows.

PRB-2 CH.PRB- 1.2.

What is the distribution of maximum entropy, that is, the distribution which has the maximum entropy among all distributions on the bounded interval $[a, b]$,$(-\infty, +\infty)$

SOL-2 CH.SOL- 1.2.

The uniform distribution has the maximum entropy among all distributions on the bounded interval: $[a, b]$,$(-\infty, +\infty)$.
The variance of $U(a, b)$ *is* $\sigma^2 = 1/12(b - a)^2$.
Therefore the entropy is:

$$1/2 \log 12 + \log \sigma. \tag{1.1}$$

APPLICATION: Problems in this category are for practicing skills. It's not enough to understand the philosophical grounding of an idea: you have to be able to apply it in appropriate situations. This takes practice! mostly in Python or in one of the available Deep Learning Libraries such as PyTorch.

An example in PyTorch follows.

PRB-3 CH.PRB- 1.3.

Describe in your own words, what is the purpose of the following code in the context of training a Convolutional Neural Network.

```
    self.transforms = []
    if rotate:
      self.transforms.append(RandomRotate())
    if flip:
      self.transforms.append(RandomFlip())
```

SOL-3 CH.SOL- 1.3.

During the training of a Convolutional Neural Network, data augmentation, and to some extent dropout are used as core methods to decrease overfitting. Data augmentation is a regularization scheme that synthetically expands the data-set by utilizing label-preserving transformations to add more invariant examples of the same data samples. It is most commonly performed in real time on the CPU during the training phase whilst the actual training mode takes place on the GPU. This may consist for instance, random rotations, random flips, zooming, spatial translations etc. ■

PART II
KINDERGARTEN

CHAPTER 2

LOGISTIC REGRESSION

You should call it entropy for two reasons. In the first place, your uncertainty function has been used in statistical mechanics under that name. In the second place, and more importantly, no one knows what entropy really is, so in a debate you will always have the advantage.

— John von Neumann to Claude Shannon

Contents

2.1 Introduction

Multivariable methods are routinely utilized in statistical analyses across a wide range of domains. Logistic regression is the most frequently used method for modelling binary response data and binary classification.

When the response variable is binary, it characteristically takes the form of 1/0, with 1 normally indicating a success and 0 a failure. Multivariable methods usually assume a relationship between two or more independent, predictor variables, and one dependent, response variable. The predicted value of a response variable may be expressed as a sum of products, wherein each product is formed by multiplying the value of the variable and its coefficient. How the coefficients are computed? from a respective data set. Logistic regression is heavily used in supervised machine learning and has become the workhorse for both binary and multiclass classification problems. Many of the questions introduced in this chapter are crucial for truly understanding the inner-workings of artificial neural networks.

2.2 Problems

2.2.1 General Concepts

PRB-4 ❓ CH.PRB- 2.1.

True or False: *For a fixed number of observations in a data set, introducing more variables normally generates a model that has a better fit to the data. What may be the drawback of such a model fitting strategy?*

PRB-5 ❓ CH.PRB- 2.2.

Define the term ***"odds of success"*** *both qualitatively and formally. Give a numerical example that stresses the relation between probability and odds of an event occurring.*

PRB-6 ❓ CH.PRB- 2.3.

1. *Define what is meant by the term* ***"interaction"****, in the context of a logistic regression predictor variable.*

2. *What is the simplest form of an interaction? Write its formulae.*

3. *What statistical tests can be used to attest the significance of an interaction term?*

PRB-7 ❓ CH.PRB- 2.4.
True or False: *In machine learning terminology, unsupervised learning refers to the mapping of input covariates to a target response variable that is attempted at being predicted when the labels are known.*

PRB-8 ❓ CH.PRB- 2.5.
Complete the following sentence: *In the case of logistic regression, the response variable is the log of the odds of being classified in [...].*

PRB-9 ❓ CH.PRB- 2.6.
Describe how in a logistic regression model, a transformation to the response variable is applied to yield a probability distribution. Why is it considered a more informative representation of the response?

PRB-10 ❓ CH.PRB- 2.7.
Complete the following sentence: *Minimizing the negative log likelihood also means maximizing the [...] of selecting the [...] class.*

2.2.2 Odds, Log-odds

PRB-11 ❓ CH.PRB- 2.8.
Assume the probability of an event occurring is $p = 0.1$.

1. *What are the* ***odds*** *of the event occurring?.*

2. *What are the* ***log-odds*** *of the event occurring?.*

3. *Construct the* ***probability*** *of the event as a ratio that equals 0.1.*

PRB-12 ❓ CH.PRB- 2.9.

True or False: *If the odds of success in a binary response is* 4*, the corresponding probability of success is* 0.8*.*

PRB-13 ❓ CH.PRB- 2.10.

Draw a graph of ***odds to probabilities****, mapping the entire range of probabilities to their respective odds.*

PRB-14 ❓ CH.PRB- 2.11.

The logistic regression model is a subset of a broader range of machine learning models known as generalized linear models (GLMs), which also include analysis of variance (ANOVA), vanilla linear regression, etc. There are three components to a GLM; ***identify these three components for binary logistic regression.***

PRB-15 ❓ CH.PRB- 2.12.

Let us consider the logit transformation, i.e., log-odds. Assume a scenario in which the logit forms the linear decision boundary:

$$\log\left(\frac{\Pr(Y=1|X)}{\Pr(Y=0|X)}\right) = \theta_0 + \theta^T X, \tag{2.1}$$

for a given vector of systematic components X *and predictor variables* θ*. Write the mathematical expression for the hyperplane that describes the decision boundary.*

PRB-16 ❓ CH.PRB- 2.13.

True or False: *The logit function and the natural logistic (sigmoid) function are inverses of each other.*

2.2.3 The Sigmoid

The sigmoid (Fig. 2.1) also known as the logistic function, is widely used in binary classification and as a neuron activation function in artificial neural networks.

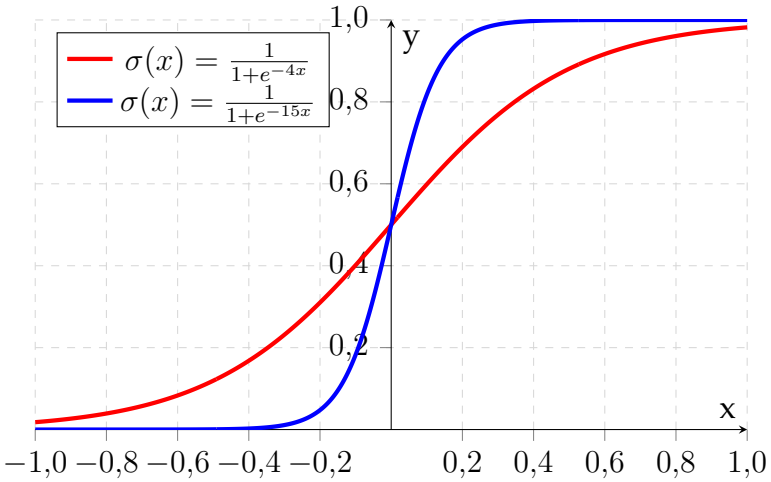


FIGURE 2.1: Examples of two sigmoid functions.

PRB-17 ❓ CH.PRB- 2.14.

Compute the derivative of the natural sigmoid function:

$$\sigma(x) = \frac{1}{1+e^{-x}} \in (0,1). \tag{2.2}$$

PRB-18 ❓ CH.PRB- 2.15.

Remember that in logistic regression, the hypothesis function for some parameter vector β and measurement vector x is defined as:

$$\begin{aligned} h_\beta(x) &= g(\beta^T x) = \frac{1}{1+e^{-\beta^T x}} \\ &= P(y=1|x;\beta), \end{aligned} \tag{2.3}$$

where y holds the hypothesis value.

Suppose the coefficients of a logistic regression model with independent variables are as follows: $\beta_0 = -1.5$, $\beta_1 = 3$, $\beta_2 = -0.5$.
Assume additionally, that we have an observation with the following values for the dependent variables: $x_1 = 1$, $x_2 = 5$. As a result, the logit equation becomes:

$$logit = \beta_0 + \beta_1 x_1 + \beta_2 x_2. \tag{2.4}$$

1. *What is the value of the **logit for this observation?***
2. *What is the value of the **odds for this observation?***
3. *What is the value of $P(y = 1)$ **for this observation?***

2.2.4 Truly Understanding Logistic Regression

PRB-19 ❓ CH.PRB- 2.16.

Proton therapy (PT) [2] is a widely adopted form of treatment for many types of cancer including breast and lung cancer (Fig. 2.2).

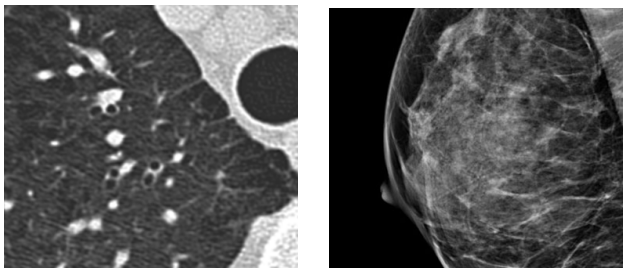


FIGURE 2.2: Pulmonary nodules (left) and breast cancer (right).

*A PT device which **was not properly calibrated** is used to simulate the treatment of cancer. As a result, the PT beam does not behave normally. A data scientist collects information relating to this simulation. The covariates presented in Table 2.1 are collected during*

*the experiment. The columns **Yes** and **No** indicate if the tumour was eradicated or not, respectively.*

	Tumour eradication	
Cancer Type	Yes	No
Breast	560	260
Lung	69	36

TABLE 2.1: Tumour eradication statistics.

Referring to Table 2.1:

1. *What is the explanatory variable and what is the response variable?*
2. *Explain the use of relative risk and odds ratio for measuring association.*
3. *Are the two variables positively or negatively associated?*
   Find the direction and strength of the association using both relative risk and odds ratio.
4. *Compute a 95% confidence interval (CI) for the measure of association.*
5. *Interpret the results and explain their significance.*

PRB-20 ❓ CH.PRB- 2.17.

Consider a system for radiation therapy planning (Fig. 2.3). Given a patient with a malignant tumour, the problem is to select the optimal radiation exposure time for that patient. A key element in this problem is estimating the probability that a given tumour will be eradicated given certain covariates. A data scientist collects information relating to this radiation therapy system.

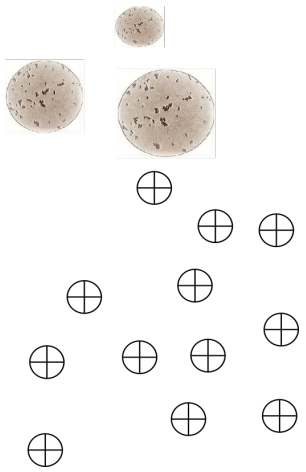


FIGURE 2.3: A multi-detector positron scanner used to locate tumours.

The following covariates are collected; X_1 *denotes time in milliseconds that a patient is irradiated with,* $X_2 =$ *holds the size of the tumour in centimeters, and* Y *notates a binary response variable indicating if the tumour was eradicated. Assume that each response' variable* Y_i *is a Bernoulli random variable with success parameter* p_i*, which holds:*

$$p_i = \frac{e^{\beta_0+\beta_1 x_1+\beta_2 x_2}}{1+e^{\beta_0+\beta_1 x_1+\beta_2 x_2}}. \tag{2.5}$$

The data scientist fits a logistic regression model to the dependent measurements and produces these estimated coefficients:

$$\begin{aligned} \hat{\beta}_0 &= -6, \\ \hat{\beta}_1 &= 0.05, \\ \hat{\beta}_2 &= 1. \end{aligned} \tag{2.6}$$

1. *Estimate the probability that, given a patient who undergoes the treatment for 40 milliseconds and who is presented with a tumour sized 3.5 centimetres, the system eradicates the tumour.*

2. *How many milliseconds the patient in part (a) would need to be radiated with to have exactly a 50% chance of eradicating the tumour?*

PRB-21 ❓ CH.PRB- 2.18.

Recent research [3] suggests that heating mercury containing dental amalgams may cause the release of toxic mercury fumes into the human airways. It is also presumed that drinking hot coffee, stimulates the release of mercury vapour from amalgam fillings (Fig. 2.4).

FIGURE 2.4: A dental amalgam.

To study factors that affect migraines, and in particular, patients who have at least four dental amalgams in their mouth, a data scientist collects data from 200K users with and without dental amalgams. The data scientist then fits a logistic regression model with an indicator of a second migraine within a time frame of one hour after the onset of the first migraine, as the binary response variable (e.g., migraine=1, no migraine=0). The data scientist believes that the frequency of migraines may be related to the release of toxic mercury fumes.

There are two independent variables:

1. X_1 = *1 if the patient has at least four amalgams; 0 otherwise.*

2. X_2 = *coffee consumption (0 to 100 hot cups per month).*

The output from training a logistic regression classifier is as follows:

```
Analysis of LR Parameter Estimates
Parameter    Estimate   Std.Err    Z-val   Pr>|Z|

Intercept    -6.36347   3.21362  -1.980   0.0477
$X_1$          -1.02411   1.17101   -0.875   0.3818
$X_2$           0.11904   0.05497    2.165   0.0304
```

1. *Using X_1 and X_2, express the **odds** of a patient having a migraine for a second time.*
2. *Calculate the **probability** of a second migraine for a patient that has at least four amalgams and drank 100 cups per month?*
3. *For users that have at least four amalgams, is **high** coffee intake associated with an **increased** probability of a second migraine?*
4. *Is there statistical evidence that having more than four amalgams is **directly** associated with a **reduction** in the probability of a second migraine?*

PRB-22 ❓ CH.PRB- 2.19.

To study factors that affect Alzheimer's disease using logistic regression, a researcher considers the link between gum (periodontal) disease and Alzheimer as a plausible risk factor [1]. The predictor variable is a count of gum bacteria (Fig. 2.5) in the mouth.

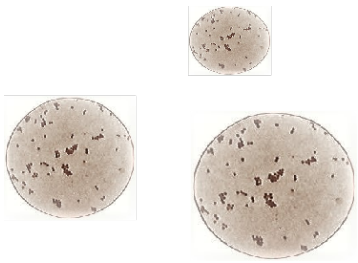


FIGURE 2.5: A chain of spherical bacteria.

The response variable, Y, measures whether the patient shows any remission (e.g. yes=1). The output from training a logistic regression classifier is as follows:

Parameter	DF	Estimate	Std
Intercept	1	-4.8792	1.2197
gum bacteria	1	0.0258	0.0194

1. *Estimate the probability of improvement when the count of gum bacteria of a patient is* 33.

2. *Find out the gum bacteria count at which the estimated probability of improvement is* 0.5.

3. *Find out the estimated odds ratio of improvement for an increase of* ***1*** *in the total gum bacteria count.*

4. *Obtain a* 99% *confidence interval for the true odds ratio of improvement increase of* ***1*** *in the total gum bacteria count. Remember that the most common confidence levels are* 90%, 95%, 99%, *and* 99.9%. *Table 9.1 lists the* z *values for these levels.*

Confidence Level	z
90%	1.645
95%	1.960
99%	**2.576**
99.9%	3.291

TABLE 2.2: Common confidence levels.

PRB-23 ❓ CH.PRB- 2.20.

Recent research [4] suggests that cannabis (Fig. 2.6) and cannabinoids administration in particular, may reduce the size of malignant tumours in rats.

FIGURE 2.6: Cannabis.

To study factors affecting tumour shrinkage, a deep learning researcher collects data from two groups; one group is administered with placebo (a substance that is not medicine) and the other with cannabinoids. His main research revolves around studying the relationship (Table 2.3) between the anticancer properties of cannabinoids and tumour shrinkage:

	Tumour Shrinkage In Rats		
Group	Yes	No	Sum
Cannabinoids	60	6833	6893
Placebo	130	6778	6909
Sum	190	13611	13801

TABLE 2.3: Tumour shrinkage in rats.

For the true odds ratio:

1. *Find the sample odds ratio.*
2. *Find the sample log-odds ratio.*
3. *Compute a 95% confidence interval ($z_{0.95} = 1.645$; $z_{0.975} = 1.96$) for the true log odds ratio and true odds ratio.*

2.2.5 The Logit Function and Entropy

PRB-24 ❓ CH.PRB- 2.21.

The entropy (see Chapter 4) of a single binary outcome with probability p to receive 1 is defined as:

$$H(p) \equiv -p \log p - (1-p) \log(1-p). \tag{2.7}$$

1. *At what p does $H(p)$ attain its maximum value?*
2. *What is the relationship between the entropy $H(p)$ and the logit function, given p?*

2.2.6 Python/PyTorch/CPP

PRB-25 ❓ CH.PRB- 2.22.

The following C++ code (Fig. 2.7) is part of a (very basic) logistic regression implementation module. For a theoretical discussion underlying this question, refer to problem 2.17.

```
1  #include ...
2  std::vector<double> theta {-6,0.05,1.0};
3  double sigmoid(double x) {
4   double tmp =1.0 / (1.0 + exp(-x));
5   std::cout << "prob=" << tmp<<std::endl;
6   return tmp;
7  }
8  double hypothesis(std::vector<double> x){
9   double z;
10  z=std::inner_product(std::begin(x), std::end(x),
     ↪  std::begin(theta), 0.0);
11  std::cout << "inner_product=" << z<<std::endl;
12  return sigmoid(z);
13 }
14 int classify(std::vector<double> x){
15  int hypo=hypothesis(x) > 0.5f;
16  std::cout << "hypo=" << hypo<<std::endl;
17  return hypo;
18 }
19 int main() {
20  std::vector<double> x1 {1,40,3.5};
21  classify(x1);
22 }
```

FIGURE 2.7: Logistic regression in CPP

1. *Explain the purpose of line* ***10****, i.e.,* ***inner_product****.*
2. *Explain the purpose of line* ***15****, i.e.,* ***hypo(x) > 0.5f****.*

3. *What does θ **(theta)** stand for in line 2?*

4. *Compile and run the code, you can use:*
   https://repl.it/languages/cpp11 to evaluate the code.
   What is the output?

PRB-26 ❓ CH.PRB- 2.23.

The following Python code (Fig. 2.8) runs a very simple linear model on a two-dimensional matrix.

```
1 import torch
2 import torch.nn as nn
3
4 lin = nn.Linear(5, 7)
5 data = (torch.randn(3, 5))
6
7 print(lin(data).shape)
8 >?
```

FIGURE 2.8: A linear model in PyTorch

Without actually running the code, determine what is the size of the matrix printed as a result of applying the linear model on the matrix.

PRB-27 ❓ CH.PRB- 2.24.

The following Python code snippet (Fig. 2.9) is part of a logistic regression implementation module in Python.

```python
from scipy.special import expit
import numpy as np
import math

def Func001(x):
 e_x = np.exp(x - np.max(x))
 return e_x / e_x.sum()

def Func002(x):
 return 1 / (1 + math.exp(-x))

def Func003(x):
 return x * (1-x)
```

FIGURE 2.9: Logistic regression methods in Python.

Analyse the methods Func001, Func002 *and* Func003 *presented in Fig. 2.9, find their purposes and* ***name them****.*

PRB-28 ❓ CH.PRB- 2.25.

The following Python code snippet (Fig. 2.10) is part of a machine learning module in Python.

```
^^I^^I
from scipy.special import expit
import numpy as np
import math
^^I^^I
def Func006(y_hat, y):
 if y == 1:
   return -np.log(y_hat)
 else:
   return -np.log(1 - y_hat)^^I
```

FIGURE 2.10: Logistic regression methods in Python.

Analyse the method Func006 presented in Fig. 2.10. What important concept in machine-learning does it implement?

PRB-29 ❓ CH.PRB- 2.26.

The following Python code snippet (Fig. 2.11) presents several different variations of the same function.

```
1  ^^I^^I
2  from scipy.special import expit
3  import numpy as np
4  import math
5
6  def Ver001(x):
7   return 1 / (1 + math.exp(-x))
8
9  def Ver002(x):
10  return 1 / (1 + (np.exp(-x)))
11
12 WHO_AM_I = 709
13
14 def Ver003(x):
15  return 1 / (1 + np.exp(-(np.clip(x, -WHO_AM_I, None))))
```

FIGURE 2.11: Logistic regression methods in Python.

1. *Which mathematical function do these methods implement?*
2. *What is significant about the number* 709 *in line 11?*
3. *Given a choice, which method would you use?*

2.3 Solutions

2.3.1 General Concepts

SOL-4 CH.SOL- 2.1.

True. *However, when an excessive and unnecessary number of variables is used in a logistic regression model, peculiarities (e.g., specific attributes) of the underlying data set disproportionately affect the coefficients in the model, a phenomena commonly referred to as "overfitting". Therefore, it is important that a logistic regression model does not start training with more variables than is justified for the given number of observations.* ■

SOL-5 CH.SOL- 2.2.

The odds of success are defined as the ratio between the probability of success $p \in [0, 1]$ *and the probability of failure* $1 - p$*. Formally:*

$$Odds(p) \equiv \left(\frac{p}{1-p} \right). \tag{2.8}$$

For instance, assuming the probability of success of an event is $p = 0.7$*. Then, in our example, the odds of success are* $7/3$*, or* 2.333 *to* 1*. Naturally, in the case of equal probabilities where* $p = 0.5$*, the odds of success is* 1 *to* 1*.*

■

SOL-6 CH.SOL- 2.3.

1. *An interaction is the product of two single predictor variables implying a* ***non-additive*** *effect.*

2. *The simplest interaction model includes a predictor variable formed by multiplying two ordinary predictors. Let us assume two variables* X *and* Z*. Then, the logistic regression model that employs the simplest form of interaction follows:*

$$\beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ, \tag{2.9}$$

   where the coefficient for the interaction term XZ *is represented by predictor* β_3*.*

3. *For testing the contribution of an interaction, two principal methods are commonly employed; the Wald chi-squared test or a likelihood ratio test between the model with and without the interaction term. Note: How does interaction relates to information theory? What added value does it employ to enhance model performance?*

■

SOL-7 CH.SOL- 2.4.

False. *This is exactly the definition of supervised learning; when labels are known then supervision guides the learning process.* ■

SOL-8 CH.SOL- 2.5.

In the case of logistic regression, the response variable is the log of the odds of being classified in a group of binary or multi-class responses. This definition essentially demonstrates that odds can take the form of a vector. ■

SOL-9 CH.SOL- 2.6.

When a transformation to the response variable is applied, it yields a probability distribution over the output classes, which is bounded between 0 and 1; this transformation can be employed in several ways, e.g., a softmax layer, the sigmoid function or classic normalization. This representation facilitates a soft-decision by the logistic regression model, which permits construction of probability-based processes over the predictions of the model. Note: What are the pros and cons of each of the three aforementioned transformations? ■

SOL-10 CH.SOL- 2.7.

*Minimizing the negative log likelihood also means maximizing the **likelihood** of selecting the **correct** class.* ■

2.3.2 Odds, Log-odds

SOL-11 CH.SOL- 2.8.

1. *The odds of the event occurring are, by definition:*

$$odds = (\frac{0.1}{0.9}) = 0.11. \tag{2.10}$$

2. *The log-odds of the event occurring are simply taken as the log of the odds:*

$$log\text{-}odds = \ln(0.1/0.9) = -2.19685. \tag{2.11}$$

3. *The probability may be constructed by the following representation:*

$$probability = \frac{odds}{odds + 1} = \frac{0.11}{1.11} = 0.1, \tag{2.12}$$

or, alternatively:

$$p = \frac{\exp(\ln odds)}{\exp(\ln odds) + 1} = \frac{0.11}{1.11} = 0.1. \tag{2.13}$$

Note: What is the intuition behind this representation?

SOL-12 CH.SOL- 2.9.

***True**. By definition of odds, it is easy to notice that $p = 0.8$ satisfies the following relation:*

$$odds = (\frac{0.8}{0.2}) = 4 \tag{2.14}$$

SOL-13 CH.SOL- 2.10.

The graph of odds to probabilities is depicted in Figure 2.12.

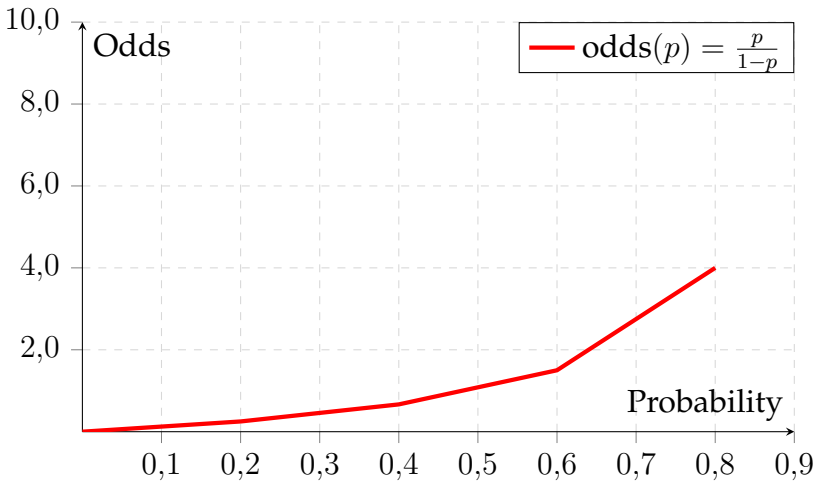


FIGURE 2.12: Odds vs. probability values.

SOL-14 CH.SOL- 2.11.

A binary logistic regression GLM consists of there components:

1. *Random component: refers to the probability distribution of the response variable* (Y)*, e.g., binomial distribution for* Y *in the binary logistic regression, which takes on the values* $Y = 0$ *or* $Y = 1$*.*

2. *Systematic component: describes the explanatory variables:* $(X_1, X_2, ...)$ *as a combination of linear predictors. The binary case does not constrain these variables to any degree.*

3. *Link function: specifies the link between random and systematic components. It says how the expected value of the response relates to the linear predictor of explanatory variables.*

   Note: Assume that Y *denotes whether a human voice activity was detected* $(Y = 1)$ *or not* $(Y = 0)$ *in a give time frame. Propose two systematic components and a link function adjusted for this task.*

■

SOL-15 CH.SOL- 2.12.

The hyperplane is simply defined by:

$$\theta_0 + \theta^T X = 0. \tag{2.15}$$

Note: Recall the use of the logit function and derive this decision boundary rigorously. ■

SOL-16 CH.SOL- 2.13.

True. *The logit function is defined as:*

$$z(p) = logit(p) = log\left(\frac{p}{1-p}\right), \tag{2.16}$$

for any $p \in [0, 1]$. A simple set of algebraic equations yields the inverse relation:

$$p(z) = \frac{\exp z}{1 + \exp z}, \tag{2.17}$$

which exactly describes the relation between the output and input of the logistic function, also known as the sigmoid. ■

2.3.3 The Sigmoid

SOL-17 CH.SOL- 2.14.

There are various approaches to solve this problem, here we provide two; direct derivation or derivation via the softmax function.

1. *Direct derivation:*
   $\frac{d}{dx}\sigma(x) = \frac{d}{dx}((1 + e^{-x})^{-1}) = -((1 + e^{-x})^{(-2)})\frac{d}{dx}(1 + e^{-x}) = \frac{e^{-x}}{(1+e^{-x})^2}$.

2. *Softmax derivation:*
   In a classification problem with mutually exclusive classes, where all of the values are positive and sum to one, a softmax activation function may be used. By definition, the softmax activation function consists of n terms, such that $\forall i \in [1, n]$:

$$f(\theta_i) = \frac{e^{\theta_i}}{\sum_k e^{v_k}} = \frac{1}{1 + e^{-\theta_i} \sum_{k \neq i} e^{\theta_k}}. \tag{2.18}$$

   *To compute the partial derivative of 2.18, we treat all θ_k where $k \neq i$ as **constants** and then differentiate θ_i using regular differentiation rules. For a given θ_i, let us define:*

$$\beta = \sum_{k \neq i} e^{\theta_k}, \tag{2.19}$$

   and

$$f(\theta_i) = \frac{1}{1 + \beta e^{-\theta_i}} = (1 + \beta e^{-\theta_i})^{-1}. \tag{2.20}$$

   It can now be shown that the derivative with respect to θ_i holds:

$$f'(\theta_i) = \left(1 + \beta e^{-\theta_i}\right)^{-2} \beta e^{-\theta_i}, \tag{2.21}$$

which can take on the informative form of:

$$f'(\theta_i) = f(\theta_i)(1 - f(\theta_i)). \tag{2.22}$$

It should be noted that 2.21 holds for any constant β, and for $\beta = 1$ it clearly reduces to the sigmoid activation function.

Note: Characterize the sigmoid function when its argument approaches $0, \infty$ and $-\infty$. What undesired properties of the sigmoid function do this values entail when considered as an activation function?

SOL-18 CH.SOL- 2.15.

1. *The logit value is simply obtained by substituting the values of the dependent variables and model coefficients into the linear logistic regression model, as follows:*

$$logit = \beta_0 + \beta_1 x_1 + \beta_2 x_2 = -1.5 + 3 \cdot 1 + -0.5 \cdot 5 = -1. \tag{2.23}$$

2. *According to the natural relation between the logit and the odds, the following holds:*

$$odds = e^{logit} = e^{\beta_0 + \beta_1 x_1 + \beta_2 x_2} = e^{-1} = 0.3678794. \tag{2.24}$$

3. *The **odds ratio** is, by definition:*

$$odds = \frac{P(y=1)}{P(y=0)}, \tag{2.25}$$

so the logistic response function is:

$$P(y=1) = \frac{1}{1 + e^{-logit}} = \frac{1}{1 + e^1} = 0.2689414. \tag{2.26}$$

2.3.4 Truly Understanding Logistic Regression

SOL-19 CH.SOL- 2.16.

1. *Tumour eradication (Y) is the response variable and cancer type (X) is the explanatory variable.*

2. *Relative risk (RR) is the ratio of risk of an event in one group (e.g., exposed group) versus the risk of the event in the other group (e.g., non-exposed group). The odds ratio (OR) is the ratio of odds of an event in one group versus the odds of the event in the other group.*

3. *If we calculate odds ratio as a measure of association:*

$$\hat{\theta} = \frac{560 \times 36}{69 \times 260} = 1.23745. \tag{2.27}$$

And the log-odds ratio is $(\log(1.23745)) = 0.213052$*:*

The odds ratio is ***larger*** *than one, indicating that the odds for a breast cancer is more than the odds for a lung cancer to be eradicated. Notice however, that this result is too close to one, which prevents conclusive decision regarding the odds relation.*

Additionally, if we calculate relative risk as a measure of association:

$$RR = \frac{\frac{560}{560+260}}{\frac{69}{69+36}} = 1.0392. \tag{2.28}$$

4. *The* 95% *confidence interval for the odds-ratio,* θ *is computed from the sample confidence interval for log odds ratio:*

$$\hat{\sigma}\left(\log(\hat{\theta})\right) = \sqrt{\frac{1}{560} + \frac{1}{260} + \frac{1}{69} + \frac{1}{36}} = 0.21886. \tag{2.29}$$

Therefore, the 95% CI for $\log(\theta)$ *is:*

$$0.213052 \pm 1.95 \times 0.21886 = (0.6398298, -0.2137241). \tag{2.30}$$

Therefore, the 95% CI for θ is:

$$(e^{-0.210}, e^{0.647}) = (0.810, 1.909). \tag{2.31}$$

5. *The CI $(0.810, 1.909)$ contains 1, which indicates that the true odds ratio is not significantly different from 1 and* ***there is not enough evidence*** *that tumour eradication is dependent on cancer type.*

■

SOL-20 CH.SOL- 2.17.

1. *By using the defined values for X_1 and X_2, and the known logistic regression model, substitution yields:*

$$\hat{p}(X) = \frac{e^{-6+0.05X_1+X_2}}{(1+e^{-6+0.05X_1+X_2})} = 0.3775. \tag{2.32}$$

2. *The equation for the predicted probability tells us that:*

$$\frac{e^{-6+0.05X_1+3.5}}{(1+e^{-6+0.05X_1+3.5})} = 0.5, \tag{2.33}$$

which is equivalent to constraining:

$$e^{-6+0.05X_1+3.5} = 1. \tag{2.34}$$

By taking the logarithm of both sides, we get that the number of milliseconds needed is:

$$X_1 = \frac{2.5}{0.05} = 50. \tag{2.35}$$

■

SOL-21 CH.SOL- 2.18.

For the purpose of this exercise, it is instructive to pre-define z as:

$$z\left(X_1, X_2\right) = -6.36 - 1.02 \times X_1 + 0.12 \times X_2. \tag{2.36}$$

1. *By employing the classic logistic regression model:*

$$\textit{odds} = \exp(z\left(X_1, X_2\right)). \tag{2.37}$$

2. *By substituting the given values of X_1, X_2 into $z\left(X_1, X_2\right)$, the probability holds:*

$$p = exp(z\left(1, 100\right))/(1 + exp(z\left(1, 100\right))) = 0.99. \tag{2.38}$$

3. *Yes. The coefficient for coffee consumption is positive (0.119) and the p-value is less than 0.05 (0.0304).*
   Note: Can you describe the relation between these numerical relations and the positive conclusion?

4. *No. The p-value for this predictor is $0.3818 > 0.05$.*
   Note: Can you explain why this inequality implicates a lack of statistical evidence?

■

SOL-22 CH.SOL- 2.19.

1. *The estimated probability of improvement is:*

$$\hat{\pi}(\textit{gum bacteria}) = \frac{\exp(-4.8792 + 0.0258 \times \textit{gum bacteria})}{1 + \exp(-4.8792 + 0.0258 \times \textit{gum bacteria})}.$$

   Hence, $\hat{\pi}(33) = 0.01748$.

2. *For* $\hat{\pi}(gum\ bacteria) = 0.5$ *we know that:*

$$\hat{\pi}(gum) = \frac{\exp(\hat{\alpha} + \hat{\beta}x)}{1 + \exp(\hat{\alpha} + \hat{\beta}x)} = 0.5 \tag{2.39}$$

$$gum\ bacteria = -\hat{\alpha}/\hat{\beta} = 4.8792/0.0258 = 189.116. \tag{2.40}$$

3. *The estimated odds ratio are given by:*

$$\exp(\hat{\beta}) = \exp(0.0258) = 1.0504. \tag{2.41}$$

4. *A* 99% *confidence interval for* β *is calculated as follows:*

$$\hat{\beta} \pm z_{0.005} \times ASE(\hat{\beta}) = \tag{2.42}$$
$$0.0258 \pm 2.576 \times 0.0194 \tag{2.43}$$
$$= (-0.00077, 0.9917). \tag{2.44}$$

Therefore, a 99% *confidence interval for the true odds ratio* $\exp(\beta)$ *is given by:*

$$(\exp(-0.00077), \exp(0.9917)) = (0.99923, 2.6958). \tag{2.45}$$

■

SOL-23 CH.SOL- 2.20.

1. *The sample odds ratio is:*

$$\hat{\theta} = \frac{130 \times 6833}{60 \times 6778} = 2.1842. \tag{2.46}$$

2. *The estimated standard error for* $\log\left(\hat{\theta}\right)$ *is:*

$$\hat{\sigma}\left(\log\hat{\theta}\right) = \sqrt{\frac{1}{60} + \frac{1}{6833} + \frac{1}{130} + \frac{1}{6778}} = 0.1570. \tag{2.47}$$

3. *According to previous sections, the* 95% *CI for the true log odds ratio is:*

$$0.7812 \pm 1.96 \times 0.1570 = (0.4734, 1.0889). \tag{2.48}$$

Correspondingly, the 95% *CI for the true odds ratio is:*

$$(e^{0.4734}, e^{1.0889}) = (1.6060, 2.9710). \tag{2.49}$$

■

2.3.5 The Logit Function and Entropy

SOL-24 CH.SOL- 2.21.

1. *The entropy (Fig. 2.13) has a maximum value of* $\log_2(2)$ *for probability* $p = 1/2$*, which is the most chaotic distribution. A lower entropy is a more predictable outcome, with zero providing full certainty.*

2. *The derivative of the entropy with respect to* p *yields* ***the negative of the logit*** *function:*

$$\frac{dH(p)}{dp} = -logit(p). \tag{2.50}$$

Note: The curious reader is encouraged to rigorously prove this claim.

■

2.3.6 Python, PyTorch, CPP

SOL-25 CH.SOL- 2.22.

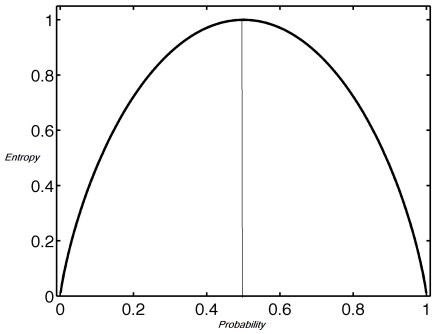


FIGURE 2.13: Binary entropy.

1. *During inference, the purpose of* ***inner_product*** *is to multiply the vector of logistic regression coefficients with the vector of the input which we like to evaluate, e.g., calculate the probability and binary class.*

2. *The line* ***hypo(x) > 0.5f*** *is commonly used for the evaluation of binary classification wherein probability values above 0.5 (i.e., a threshold) are regarded as TRUE whereas values below 0.5 are regarded as FALSE.*

3. *The term* θ ***(theta)*** *stands for the logistic regression coefficients which were evaluated during training.*

4. *The output is as follows:*

```
> inner_product=-0.5
> prob=0.377541
> hypo=0
```

FIGURE 2.14: Logistic regression in C++

SOL-26 CH.SOL- 2.23.

Because the second dimension of `lin` *is 7, and the first dimension of* `data` *is 3, the resulting matrix has a shape of* `torch.Size([3, 7])`.

■

SOL-27 CH.SOL- 2.24.

Ideally, you should be able to recognize these functions immediately upon a request from the interviewer.

1. *A softmax function.*
2. *A sigmoid function.*
3. *A derivative of a sigmoid function.*

■

SOL-28 CH.SOL- 2.25.

The function implemented in Fig. 2.10 is the `binary` *cross-entropy function.* ■

SOL-29 CH.SOL- 2.26.

1. *All the methods are variations of the sigmoid function.*
2. *In Python, approximately* $1.797e+308$ *holds the largest possible valve for a floating point variable. The logarithm of which is evaluated at* 709.78. *If you try to execute the following expression in Python, it will result in* `inf`: $np.log(1.8e+308)$.
3. *I would use* `Ver003` *because of its stability. Note: Can you entail why is this method more stable than the others?*

■

Chapter 3

PROBABILISTIC PROGRAMMING & BAYESIAN DL

Anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin.

— John von Neumann (1903-1957)

Contents

3.1 Introduction

HE Bayesian school of thought has permeated fields such as mechanical statistics, classical probability, and financial mathematics [13]. In tandem, the subject matter itself has gained attraction, particularly in the field of BML. It is not surprising then, that several new Python based probabilistic programming libraries such as PyMc3 and Stan [11] have emerged and have become widely adopted by the machine learning community.

This chapter aims to introduce the Bayesian paradigm and apply Bayesian inferences in a variety of problems. In particular, the reader will be introduced with real-life examples of conditional probability and also discover one of the most important results in Bayesian statistics: that the family of beta distributions is **conjugate to a binomial likelihood**. It should be stressed that Bayesian inference is a subject matter that students evidently find hard to grasp, since it heavily relies on rigorous probabilistic interpretations of data. Specifically, several obstacles hamper with the prospect of learning Bayesian statistics:

1. Students typically undergo merely basic introduction to classical probability and statistics. Nonetheless, what follows requires a very solid grounding in these fields.

2. Many courses and resources that address Bayesian learning do not cover essential concepts.

3. A strong comprehension of Bayesian methods involves numerical training and sophistication levels that go beyond first year calculus.

Conclusively, this chapter may be much harder to understand than other chapters. Thus, we strongly urge the readers to thoroughly solve the following questions and verify their grasp of the mathematical concepts in the basis of the solutions [8].

3.2 Problems

3.2.1 Expectation and Variance

PRB-30 ❓ CH.PRB- 3.1.
Define what is meant by a ***Bernoulli trial****.*

PRB-31 ❓ CH.PRB- 3.2.
The binomial distribution is often used to model the probability that k out of a group of n objects bare a specific characteristic. Define what is meant by a ***binomial random variable*** *X.*

PRB-32 ❓ CH.PRB- 3.3.
What does the following shorthand stand for?

$$X \sim \text{Binomial}(n,\, p) \tag{3.1}$$

PRB-33 ❓ CH.PRB- 3.4.
Find the probability mass function (PMF) of the following random variable:

$$X \sim \text{Binomial}(n,\, p) \tag{3.2}$$

PRB-34 ❓ CH.PRB- 3.5.
Answer the following questions:

1. *Define what is meant by (mathematical) expectation.*
2. *Define what is meant by variance.*
3. *Derive the expectation and variance of a the binomial random variable $X \sim \text{Binomial}(n,\, p)$ in terms of p and n.*

PRB-35 ❓ CH.PRB- 3.6.
Proton therapy (PT) is a widely adopted form of treatment for many types of cancer [6]. A PT device which ***was not properly calibrated*** *is used to treat a patient with pancreatic cancer (Fig. 3.1). As a result, a PT beam randomly shoots 200 particles independently and* ***correctly*** *hits cancerous cells with a probability of 0.1.*

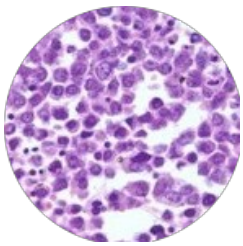


FIGURE 3.1: Histopathology for pancreatic cancer cells.

1. *Find the **statistical distribution** of the number of correct hits on cancerous cells in the described experiment. What are the expectation and variance of the corresponding random variable?*

2. *A radiologist using the device claims he was able to hit exactly 60 cancerous cells. How likely is it that he is **wrong**?*

3.2.2 Conditional Probability

PRB-36 ❓ CH.PRB- 3.7.
Given two events A and B in probability space H, which occur with probabilities $P(A)$ and $P(B)$, respectively:

1. *Define the conditional probability of A given B. Mind singular cases.*

2. *Annotate each part of the conditional probability formulae.*

3. *Draw an instance of Venn diagram, depicting the intersection of the events A and B. Assume that $A \bigcup B = H$.*

PRB-37 ❓ CH.PRB- 3.8.
*Bayesian inference amalgamates data information in the likelihood function with known **prior** information. This is done by conditioning the prior on the likelihood using the Bayes formulae. Assume two events A and B in probability space H, which occur with probabilities*

$P(A)$ and $P(B)$, respectively. Given that $A \bigcup B = H$, state the Bayes formulae for this case, interpret its components and annotate them.

PRB-38 ❓ CH.PRB- 3.9.
*Define the terms **likelihood** and **log-likelihood** of a discrete random variable X given a fixed parameter of interest γ. Give a practical example of such scenario and derive its likelihood and log-likelihood.*

PRB-39 ❓ CH.PRB- 3.10.
*Define the term **prior distribution** of a likelihood parameter γ in the continuous case.*

PRB-40 ❓ CH.PRB- 3.11.
*Show the **relationship** between the prior, posterior and likelihood probabilities.*

PRB-41 ❓ CH.PRB- 3.12.
*In a Bayesian context, if a first experiment is conducted, and then another experiment is followed, what does the **posterior** become for the **next** experiment?*

PRB-42 ❓ CH.PRB- 3.13.
*What is the condition under which two events A and B are said to be **statistically independent**?*

3.2.3 Bayes Rule

PRB-43 ❓ CH.PRB- 3.14.
*In an experiment conducted in the field of particle physics (Fig. 3.2), a certain particle may be in two distinct **equally probable** quantum states: integer spin or half-integer spin. It is well-known that particles with integer spin are bosons, while particles with half-integer spin are fermions [4].*

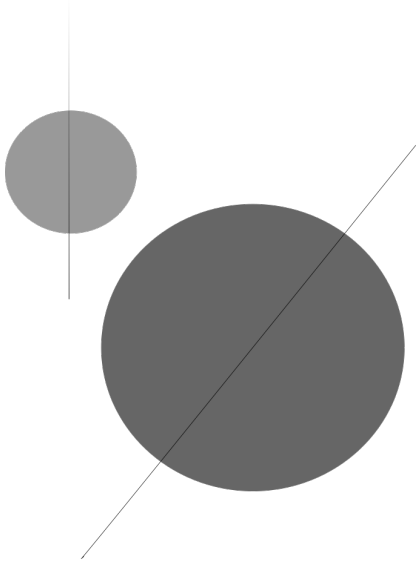


FIGURE 3.2: Bosons and fermions: particles with half-integer spin are fermions.

A physicist is observing two such particles, while at least one of which is in a half-integer state. What is the probability that ***both*** *particles are fermions?*

PRB-44 ❓ CH.PRB- 3.15.

During pregnancy, the Placenta Chorion Test [1] is commonly used for the diagnosis of hereditary diseases (Fig. 3.3). The test has a probability of 0.95 of being correct ***whether or not*** *a hereditary disease is present.*

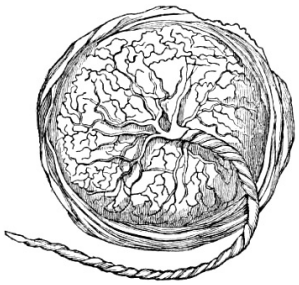


FIGURE 3.3: Foetal surface of the placenta

It is known that 1% of pregnancies result in hereditary diseases. Calculate the probability of a test indicating that a hereditary disease is present.

PRB-45 ❓ CH.PRB- 3.16.

The Dercum disease [3] is an extremely rare disorder of multiple painful tissue growths. In a population in which the ratio of females to males is equal, 5% of females and 0.25% of males have the Dercum disease (Fig. 3.4).

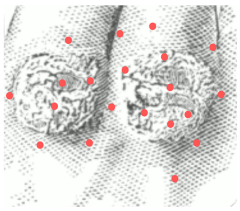


FIGURE 3.4: The Dercum disease

A person is chosen at random and that person has the Dercum disease. Calculate the probability that the person is female.

PRB-46 ❓ CH.PRB- 3.17.

There are numerous fraudulent binary options websites scattered around the Internet, and for every site that shuts down, new ones are sprouted like mushrooms. A ***fraudulent*** *AI*

based stock-market prediction algorithm utilized at the New York Stock Exchange, (Fig. 3.6) can correctly predict if a certain binary option [7] shifts states from 0 to 1 or the other way around, with 85% *certainty.*

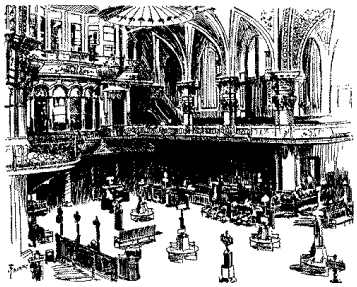


FIGURE 3.5: The New York Stock Exchange.

A financial engineer has created a portfolio consisting twice as many state-1 options then state-0 options. A stock option is selected at random and is determined by said algorithm to be in the state of 1. What is the probability that the prediction made by the AI is correct?

PRB-47 ❓ CH.PRB- 3.18.

In an experiment conducted by a hedge fund to determine if monkeys (Fig. 3.6) can outperform humans in selecting better stock market portfolios, 0.05 of humans and 1 out of 15 monkeys could correctly predict stock market trends correctly.

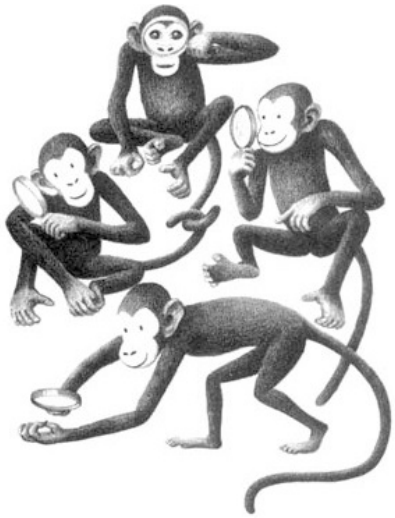


FIGURE 3.6: Hedge funds and monkeys.

From an equally probable pool of humans and monkeys an "expert" is chosen at random. When tested, that expert was correct in predicting the stock market shift. What is the probability that the expert is a ***human****?*

PRB-48 ❓ CH.PRB- 3.19.

During the cold war, the U.S.A developed a speech to text (STT) algorithm that could theoretically detect the hidden dialects of Russian sleeper agents. These agents (Fig. 3.7), were trained to speak English in Russia and subsequently sent to the US to gather intelligence. The FBI was able to apprehend ten such hidden Russian spies [9] and accused them of being "sleeper" agents.

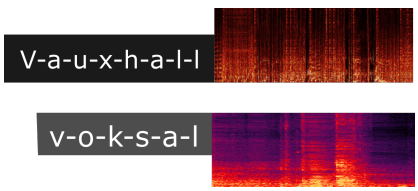


FIGURE 3.7: Dialect detection.

*The Algorithm relied on the acoustic properties of Russian pronunciation of the word (v-o-k-s-a-l) which was borrowed from English V-a-u-x-h-a-l-l. It was alleged that it is **impossible for Russians to completely hide** their accent and hence when a Russian would say V-a-u-x-h-a-l-l, the algorithm would yield the text "**v-o-k-s-a-l**". To test the algorithm at a diplomatic gathering where 20% of participants are Sleeper agents and the rest Americans, a data scientist randomly chooses a person and asks him to say V-a-u-x-h-a-l-l. A single letter is then chosen randomly from the word that was generated by the algorithm, which is observed to be an "l". What is the probability that the person is indeed a Russian sleeper agent?*

PRB-49 ❓ CH.PRB- 3.20.

During World War II, forces on both sides of the war relied on encrypted communications. The main encryption scheme used by the German military was an Enigma machine [5], which was employed extensively by Nazi Germany. Statistically, the Enigma machine sent the symbols X and Z Fig. (3.8) according to the following probabilities:

$$P(X) = \frac{2}{9} \tag{3.3}$$

$$P(Z) = \frac{7}{9} \tag{3.4}$$

A . —	N — .	& . ...
B — ...	O — — —	1 . — — —
C — . — .	P . — — .	2 .. — ..
D — ..	Q — — . —	3 ... — —
E .	R . — .	4 .... —
F .. — .	S ...	5 .....
G — — .	T —	6 — ....
H	U .. —	7 — — ..
I ..	V ... —	8 — — — ..
J . — — —	W . — —	9 — — — .
K — . —	X — .. —	0 — — — — —
L . — ..	Y — . — —	
M — —	Z — — ..	

FIGURE 3.8: The Morse telegraph code.

In one incident, the German military sent encoded messages while the British army used countermeasures to deliberately tamper with the transmission. Assume that as a result of the British countermeasures, an X is erroneously received as a Z (and mutatis mutandis) with a

probability $\frac{1}{7}$. If a recipient in the German military received a Z, what is the probability that a Z was actually transmitted by the sender?

3.2.4 Maximum Likelihood Estimation

PRB-50 ❓ CH.PRB- 3.21.
*What is **likelihood function** of the independent identically distributed (i.i.d) random variables:*
$X_1, \cdots, X_n$ *where* $X_i \sim \text{binomial}(n,\ p), \forall i \in [1, n]$,
and where p *is the parameter of interest?*

PRB-51 ❓ CH.PRB- 3.22.
*How can we derive the **maximum likelihood estimator (MLE)** of the i.i.d samples* $X_1, \cdots, X_n$ *introduced in Q. 3.21?*

PRB-52 ❓ CH.PRB- 3.23.
What is the relationship between the likelihood function and the log-likelihood function?

PRB-53 ❓ CH.PRB- 3.24.
Describe how to analytically find the MLE of a likelihood function?

PRB-54 ❓ CH.PRB- 3.25.
*What is the term used to describe **the first derivative** of the log-likelihood function?*

PRB-55 ❓ CH.PRB- 3.26.
*Define the term **Fisher information**.*

3.2.5 Fisher Information

PRB-56 ❓ CH.PRB- 3.27.

The 2014 west African Ebola (Fig. 9.10) epidemic has become the largest and fastest-spreading outbreak of the disease in modern history [2] with a death tool far exceeding all past outbreaks combined. Ebola (named after the Ebola River in Zaire) first emerged in 1976 in Sudan and Zaire and infected over 284 people with a mortality rate of 53%.

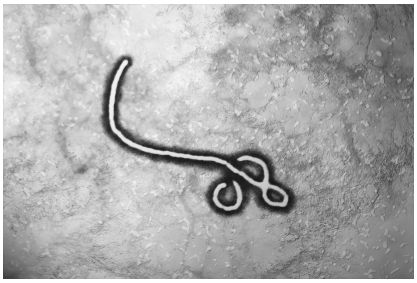


FIGURE 3.9: The Ebola virus.

This rare outbreak, underlined the challenge medical teams are facing in containing epidemics. A junior data scientist at the center for disease control (CDC) models the possible spread and containment of the Ebola virus using a numerical simulation. He knows that out of a population of k humans (the number of trials), x are carriers of the virus (success in statistical jargon). He believes the sample likelihood of the virus in the population, follows a Binomial distribution:

$$L(\gamma \mid y) = \left(\begin{array}{c} n \\ y \end{array} \right) \gamma^y (1-\gamma)^{n-y}, \qquad \gamma \in [0,1], \quad y = 1, 2, \ldots, n \tag{3.5}$$

As the senior researcher in the team, you guide him that his parameter of interest is γ, the proportion of infected humans in the entire population. The expectation and variance of the binomial distribution are:

$$E(y|\gamma, n) = n\gamma, \quad V(y|\gamma, n) = n\gamma(1-\gamma) \tag{3.6}$$

Answer the following; for the likelihood function of the form $L_x(\gamma)$:

1. *Find the log-likelihood function $l_x(\gamma) = \ln L_x(\gamma)$.*

2. *Find the gradient of $l_x(\gamma)$.*
3. *Find the Hessian matrix $H(\gamma)$.*
4. *Find the Fisher information $I(\gamma)$.*
5. *In a population spanning 10,000 individuals, 300 were infected by Ebola. Find the MLE for γ and the standard error associated with it.*

PRB-57 ❓ CH.PRB- 3.28.

In this question, you are going to derive the Fisher information function for several distributions. Given a probability density function (PDF) $f(X|\gamma)$, you are provided with the following definitions:

1. *The natural logarithm of the PDF $\ln f(X|\gamma) = \Phi(X|\gamma)$.*
2. *The first partial derivative $\Phi'(X|\gamma)$.*
3. *The second partial derivative $\Phi''(X|\gamma)$.*
4. *The Fisher Information for a continuous random variable:*

$$I(\gamma) = -\mathrm{E}_\gamma \left[\Phi'(X|\gamma)^2\right]. \tag{3.7}$$

Find the Fisher Information $I(\gamma)$ for the following distributions:

1. *The Bernoulli Distribution $X \sim B(1, \gamma)$.*
2. *The Poisson Distribution $X \sim Poiss(\theta)$.*

PRB-58 ❓ CH.PRB- 3.29.

1. ***True or False:*** *The Fisher Information is used to compute the Cramer-Rao bound on the variance of any unbiased maximum likelihood estimator.*
2. ***True or False:*** *The Fisher Information matrix is also the Hessian of the symmetrized KL divergence.*

3.2.6 Posterior & prior predictive distributions

PRB-59 ❓ CH.PRB- 3.30.
In chapter 3 we discussed the notion of a prior and a posterior distribution.

1. *Define the term* ***posterior distribution****.*
2. *Define the term* ***prior predictive distribution****.*

PRB-60 ❓ CH.PRB- 3.31.
Let y be the number of successes in 5 independent trials, where the probability of success is θ in each trial. Suppose your prior distribution for θ is as follows: $P(\theta = 1/2) = 0.25$, $P(\theta = 1/6) = 0.5$, and $P(\theta = 1/4) = 0.25$.

1. *Derive the* ***posterior distribution*** *$p(\theta|y)$* ***after*** *observing y.*
2. *Derive the* ***prior predictive distribution*** *for y.*

3.2.7 Conjugate priors

PRB-61 ❓ CH.PRB- 3.32.
In chapter 3 we discussed the notion of a prior and a posterior.

1. *Define the term* ***conjugate prior****.*
2. *Define the term* ***non-informative prior****.*

The Beta-Binomial distribution

PRB-62 ❓ CH.PRB- 3.33.
The Binomial distribution was discussed extensively in chapter 3. Here, we are going to show one of the most important results in Bayesian machine learning. Prove that the family of beta distributions is ***conjugate to a binomial likelihood****, so that if a prior is in that*

family then so is the posterior. That is, show that:

$$x \sim \text{Ber}(\gamma), \quad \gamma \sim \mathcal{B}(\alpha, \beta) \quad \Rightarrow \quad \gamma|x \sim \mathcal{B}(\alpha', \beta') \tag{3.8}$$

For instance, for h heads and t tails, the posterior is:

$$\mathcal{B}(h + \alpha, t + \beta) \tag{3.9}$$

3.2.8 Bayesian Deep Learning

PRB-63 ❓ CH.PRB- 3.34.

*A recently published paper presents a new layer for a new Bayesian neural network (BNN). The layer behaves as follows. During the feed-forward operation, each of the hidden neurons H_n , $n \in 1, 2$ in the neural network (Fig. 3.10) **may, or may not** fire independently of each other according to a known prior distribution.*

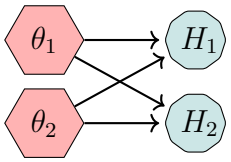


FIGURE 3.10: Likelihood in a BNN model.

The chance of firing, γ, is the same for each hidden neuron. Using the formal definition, calculate the likelihood function of each of the following cases:

1. *The hidden neuron is distributed according to $X \sim \text{binomial}(n, \gamma)$ random variable and fires with a probability of γ. There are 100 neurons and only 20 are **fired**.*
2. *The hidden neuron is distributed according to $X \sim Uniform(0, \gamma)$ random variable and fires with a probability of γ.*

PRB-64 ❓ CH.PRB- 3.35.

Your colleague, a veteran of the Deep Learning industry, comes up with an idea for for

*a BNN layer entitled **OnOffLayer**. He suggests that each neuron will stay **on** (the other state is off) following the distribution $f(x) = e^{-x}$ for $x > 0$ and $f(x) = 0$ otherwise (Fig. 3.11). X indicates the **time in** **seconds the neuron stays on**. In a BNN, 200 such neurons are activated independently in said OnOffLayer. The OnOffLayer is set to off (e.g. not active) **only if at least 150 of the neurons are shut down**. Find the probability that the OnOffLayer will be active for at least 20 seconds without being shut down.*

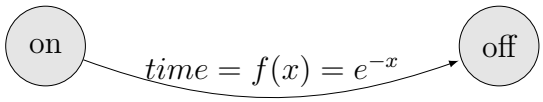


FIGURE 3.11: OnOffLayer in a BNN model.

PRB-65 ❓ CH.PRB- 3.36.

*A Dropout layer [12] (Fig. 3.12) is commonly used to regularize a neural network model by randomly equating several outputs (the crossed-out **hidden** node H) to 0.*

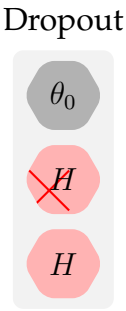


FIGURE 3.12: A Dropout layer (simplified form).

For instance, in PyTorch [10], a Dropout layer is declared as follows (3.1):

```
1 import torch
2 import torch.nn as nn
3 nn.Dropout(0.2)
```

CODE 3.1: Dropout in PyTorch

Where $nn.Dropout(0.2)$ *(Line #3 in 3.1) indicates that the probability of zeroing an element is* 0.2.

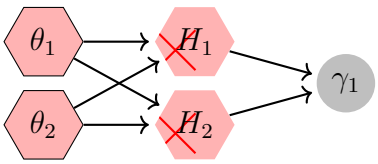


FIGURE 3.13: A Bayesian Neural Network Model

A new data scientist in your team suggests the following procedure for a Dropout layer which is based on Bayesian principles. Each of the neurons θ_n *in the neural network in (Fig. 8.33) may drop (or not) independently of each other exactly like a Bernoulli trial.*

During the training of a neural network, the Dropout layer randomly drops out outputs of the previous layer, as indicated in (Fig. 3.12). Here, for illustration purposes, all two neurons are dropped as depicted by the crossed-out ***hidden*** *nodes* H_n.

You are interested in the proportion θ *of dropped-out neurons. Assume that the chance of drop-out,* θ*, is* ***the same*** *for each neuron (e.g. a* ***uniform prior*** *for* θ*). Compute the* ***posterior*** *of* θ.

PRB-66 ❓ CH.PRB- 3.37.

A new data scientist in your team, who was formerly a Quantum Physicist, suggests the following procedure for a Dropout layer entitled ***QuantumDrop*** *which is based on Quantum principles and the* ***Maxwell Boltzmann distribution****. In the Maxwell-Boltzmann*

distribution, the likelihood of finding a particle with a particular velocity v is provided by:

$$n(v)dv = \frac{4\pi N}{V}\left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}} dv \tag{3.10}$$

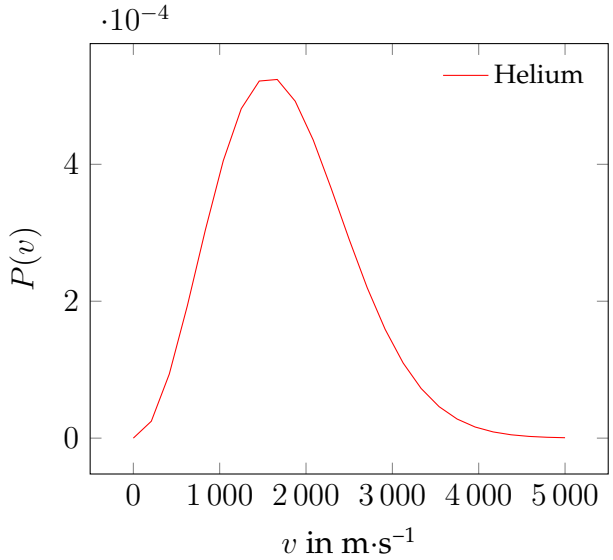


FIGURE 3.14: The Maxwell-Boltzmann distribution.

In the suggested QuantumDrop layer (3.15), each of the neurons behaves like a molecule and is distributed according to the Maxwell-Boltzmann distribution and ***fires only when the most probable speed is reached****. This speed is the velocity associated with the highest point in the Maxwell distribution (3.14). Using calculus, brain power and some mathematical manipulation, find the* ***most likely value (speed) at which the neuron will fire****.*

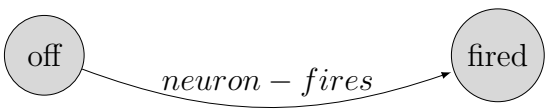


FIGURE 3.15: A QuantumDrop layer.

3.3 Solutions

3.3.1 Expectation and Variance

SOL-30 CH.SOL- 3.1.

The notion of a Bernoulli trial refers to an experiment with two dichotomous binary outcomes; success (x = 1), and failure (x = 0). ■

SOL-31 CH.SOL- 3.2.

A binomial random variable $X = k$ represents k successes in n mutually independent Bernoulli trials. ■

SOL-32 CH.SOL- 3.3.

The shorthand $X \sim \text{Binomial}(n, p)$ indicates that the random variable X has the binomial distribution (Fig. 3.16). The positive integer parameter n indicates the number of Bernoulli trials and the real parameter p, $0 < p < 1$ holds the probability of success in each of these trials.

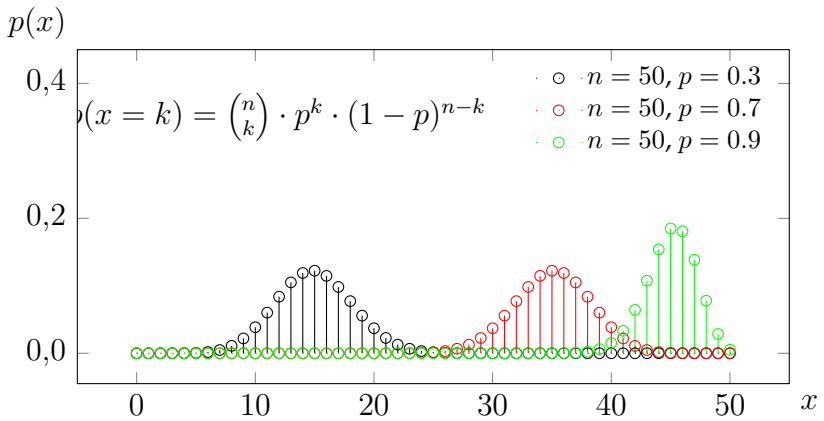


FIGURE 3.16: The binomial distribution.

■

SOL-33 CH.SOL- 3.4.

The random variable $X \sim \text{Binomial}(n,\, p)$ *has the following PMF:*

$$P(X = k) = \binom{n}{k} p^k \, (1-p)^{n-k} \,;\; k = 0,\, 1,\, 2,\, \ldots,\, n. \tag{3.11}$$

■

SOL-34 CH.SOL- 3.5.

The answers below regard a discrete random variable. The curious reader is encouraged to expend them to the continuous case.

1. *For a random variable* X *with probability mass function* $P(X = k)$ *and a set of outcomes* K*, the* expected value *of* X *is defined as:*

$$E[X] := \sum_{k \in K} kP(X = k). \tag{3.12}$$

Note: The expectation of X *may also be denoted by* μ_X*.*

2. *The* variance *of* X *is defined as:*

$$\text{Var}[X] := E\Big[(X - E[X])^2\Big]. \tag{3.13}$$

Note: The variance of X *may also be denoted by* σ_X^2*, while* σ_X *itself denotes the* **standard deviation** *of* X*.*

3. *The population mean and variance of a binomial random variable with parameters* n *and* p *are:*

$$E[X] = np \qquad\qquad V[X] = np(1-p) \tag{3.14}$$

Note: Why is this solution intuitive? What information theory-related phenomenon occurs when $p = 1/2$*?*

■

SOL-35 CH.SOL- 3.6.

1. *This scenario describes an experiment that is repeated 200 times independently with a success probability of* 0.1. *Thus, if the random variable* X *denotes the number of times success was obtained, then it is best characterized by the binomial distribution with parameters* $n = 200$ *and* $p = 0.1$. *Formally:*

$$X \sim \text{Binomial}(200,\ 0.1). \tag{3.15}$$

The expectation of X *is given by:*

$$x = E(x) = 200 \times 0.1 = 20, \tag{3.16}$$

and its respective variance is:

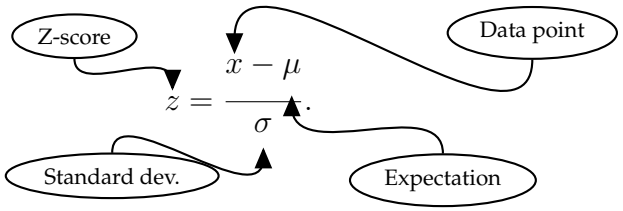
$$Var = 200 \times 0.10(1 - 0.10) = 18.0. \tag{3.17}$$

2. *Here we propose two distinguished methods to answer the question.*
Primarily, the straightforward solution is to employ the definition of the binomial distribution and substitute the value of X *in it. Namely:*

$$\begin{aligned} &P(X = 60; n = 200, p = 0.1) \\ &= \binom{200}{60} 0.1^{60} \left(1 - 0.1\right)^{200-60} \\ &\qquad =\approx 2.7 \times e^{-15}. \end{aligned} \tag{3.18}$$

This leads to an extremely high probability that the radiologist is mistaken.

The following approach is longer and more advanced, but grants the reader with insights and intuition regarding the results. To derive how wrong the radiologist is, we can employ an approximation by considering the standard normal distribution. In statistics, the ***Z-score*** *allows us to understand how far from the mean is a data point in units of standard deviation, thus revealing how likely it is to occur (Fig. 3.17).*



(3.19)

FIGURE 3.17: Z-score

Therefore, the probability of correctly hitting 60 cells is:

$$P(X \geq 60) = P(Z \geq \frac{60 - 20}{\sqrt{18.0}}) = P(Z \geq 9.428) \approx 0. \tag{3.20}$$

Again, the outcome shows the likelihood that the radiologist was wrong approaches 1. *Note: Why is the relation depicted in Fig. 3.17 deduces that Z is a standard Gaussian? Under what terms is this conclusion valid? Why does eq. (3.20) employs the cumulative distribution function and not the probability mass function?*

■

3.3.2 Conditional Probability

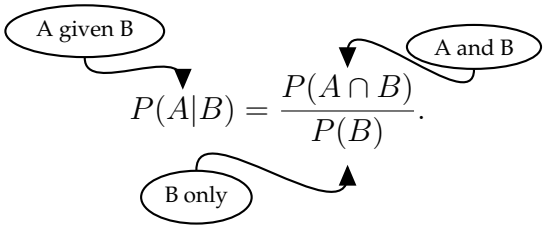
SOL-36 CH.SOL- 3.7.

1. *For two events A and B with $P(B) > 0$, the* conditional probability *of A given that B has occurred is defined as:*

$$P(A|B) = \frac{P(A \cap B)}{P(B)}. \tag{3.21}$$

It is easy to note that if $P(B) = 0$, this relation is not defined mathematically. In this case, $P(A|B) = P(A \cap B) = P(A)$.

2. *The annotated probabilities are displayed in Fig. 3.18:*



$$P(A|B) = \frac{P(A \cap B)}{P(B)}. \tag{3.22}$$

FIGURE 3.18: Conditional probability

3. *An example of a diagram depicting the intersected events A and B is displayed in Fig. 3.19:*

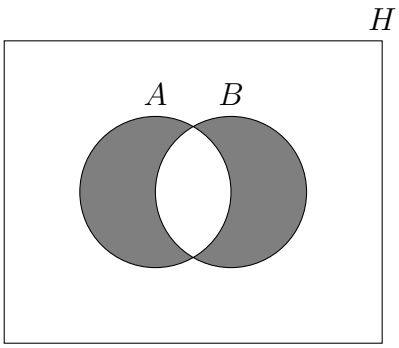


FIGURE 3.19: Venn diagram of the intersected events A and B in probability space H

■

SOL-37 CH.SOL- 3.8.

The Bayes formulae reads:

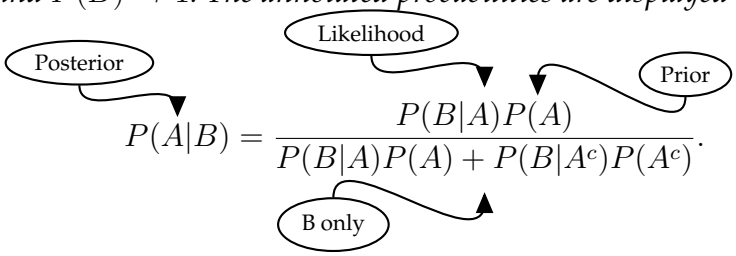
$$P(A|B) = \frac{P(B|A)P(A)}{P(B|A)P(A) + P(B|A^c)P(A^c)}, \tag{3.23}$$

where $P(A^c)$ is the complementary probability of $P(A)$. The interpretation of the elements in

Bayes formulae is as follows:

$$\textit{posterior probability} = \frac{\textit{likelihood of the data} \times \textit{prior probability}}{\textit{normalization constant}}. \tag{3.24}$$

Note: What is the important role of the normalization constant? Analyze the cases where $P(B) \to 0$ *and* $P(B) \to 1$. *The annotated probabilities are displayed in (Fig. 3.20):*



(3.25)

FIGURE 3.20: Annotated components of the Bayes formula (eq. 3.23)

SOL-38 CH.SOL- 3.9.

Given X *as a discrete randomly distributed variable and given* γ *as the parameter of interest, the likelihood and the log-likelihood of* X *given* γ *follows respectively:*

$$\mathcal{L}_\gamma(X = x) = p(X = x|\gamma) \tag{3.26}$$

$$\ell_\gamma(X = x) = \ln\left(p(X = x|\gamma)\right) \tag{3.27}$$

The term likelihood can be intuitively understood from this definition; it deduces how likely is to obtain a value x *when a prior information is given regarding its distribution, namely the parameter* γ. *For example, let us consider a biased coin toss with* $p_h = \gamma$. *Then:*

$$\mathcal{L}_\gamma(X = \text{“}h''\text{)} = p(X = \text{“}h''|\gamma) = \gamma. \tag{3.28}$$

$$\ell_\gamma(X = \text{“}h''\text{)} = \ln\left(p(X = \text{“}h''|\gamma)\right) = \ln\left(\gamma\right). \tag{3.29}$$

Note: The likelihood function may also follow continuous distributions such as the normal distribution. In the latter, it is recommended and often obligatory to employ the log-likelihood. Why? We encourage the reader to modify the above to the continuous case of normal distribution and derive the answer. ■

SOL-39 CH.SOL- 3.10.

*The continuous prior distribution, $f(\Gamma = \gamma)$ represents what is known about the probability of the value γ before the experiment has commenced. It is termed as being **subjective**, and therefore may vary considerably between researchers. By proceeding the previous example, $f(\Gamma = 0.8)$ holds the probability of randomly flipping a coin that yields "heads" with chance of 80% of times.* ■

SOL-40 CH.SOL- 3.11.

The essence of Bayesian analysis is to draw inference of unknown quantities or quantiles from the posterior distribution $p(\Gamma = \gamma|X = x)$, which is traditionally derived from prior beliefs and data information. Bayesian statistical conclusions about chances to obtain the parameter $\Gamma = \gamma$ or unobserved values of random variable $X = x$, are made in terms of probability *statements. These probability statements are conditional on the observed values of X, which is denoted as $p(\Gamma = \gamma|X = x)$, called posterior distributions of parameter γ. Bayesian analysis is a practical method for making inferences from data and prior beliefs using probability models for quantities we observe and for quantities which we wish to learn. Bayes rule provides a relationship of this form:*

$$\textit{posterior} \ \propto p(\mathbf{x}|\boldsymbol{\gamma})p(\boldsymbol{\gamma}) \propto \ \textit{data given prior} \times \ \textit{chance of prior} \ . \tag{3.30}$$

■

SOL-41 CH.SOL- 3.12.

*The posterior density summarizes what is known about the parameter of interest γ after the data **is observed**. In Bayesian statistics, the posterior density $p(\Gamma = \gamma|X = x)$ becomes the **prior** for this next experiment. This is part of the well-known Bayesian updating mechanism wherein we update our knowledge to reflect the actual distribution of data that we observed. To summarize, from the perspective of Bayes Theorem, we update the **prior distribution** to a **posterior distribution** after seeing the data.* ■

SOL-42 CH.SOL- 3.13.

Two events A and B are statistically independent if (and only if):

$$P(A \cap B) = P(A)P(B). \tag{3.31}$$

Note: Use conditional probability and rationalize this outcome. How does this property become extremely useful in practical researches that consider likelihood of normally distributed features? ■

3.3.3 Bayes Rule

SOL-43 CH.SOL- 3.14.

Let γ stand for the number of half-integer spin states, and given the prior knowledge that both states are equally probable:

$$P(\gamma = 2|\gamma \geq 1) \tag{3.32}$$

$$= \frac{P(\gamma = 2, \gamma \geq 1)}{P(\gamma \geq 1)} \tag{3.33}$$

$$= \frac{P(\gamma = 2)}{1 - P(\gamma = 0)} = \frac{1/4}{1 - 1/4} = \frac{1}{3} \tag{3.34}$$

Note: Under what statistical property do the above relations hold? ■

SOL-44 CH.SOL- 3.15.

Let event A indicate present hereditary-disease and let event B to hold a positive test result. The calculated probabilities are presented in Table 3.1. We were asked to find the probability of a test indicating that hereditary-disease is present, namely $P(B)$. According to the law of total probability:

$$\begin{aligned} P(B) &= P(B|A) * P(A) + P(B|\overline{A}) * P(\overline{A}) \\ &= [0.95 * 0.01] + [0.05 * 0.99] = 0.059 \end{aligned} \tag{3.35}$$

Note: In terms of performance evaluation, $P(B|A)$ is often referred to as the probability of

PROBABILITY	EXPLANATION
P(A)= 0.01	The probability of hereditary-disease.
P($\overline{A}$)=1-0.01=.99	The probability of no hereditary-disease.
P($\overline{B}$ | $\overline{A}$)=0.95	The probability that the test will yield a negative result [B̃] if hereditary-disease is NOT present [Ã].
P(B | $\overline{B}$)=1-0.95=.05	The probability that the test will yield a positive result [B] if hereditary-disease is NOT present [Ã] (probability of false alarm).
P(B | A)=0.95	The probability that the test will yield a positive result [B] if hereditary-disease is present [A] (probability of detection).
P($\overline{B}$ | A)=1-0.95=.05	The probability that the test will yield a negative result [B̃] if hereditary-disease is present [A].

TABLE 3.1: Probability values of hereditary-disease detection.

detection and $P(B|\overline{A})$ is considered the probability of false alarm. Notice that these measures do not, neither logically nor mathematically, combine to probability of 1. ■

SOL-45 CH.SOL- 3.16.

We first enumerate the probabilities one by one:

$$P(Dercum|female) = 0.05, \tag{3.36}$$

$$P(Dercum|male) = 0.0025, \tag{3.37}$$

$$P(male) = P(female) = 0.5. \tag{3.38}$$

We are asked to find $P(female|Dercum)$. Using Bayes Rule:

$$P(female|Dercum) = \frac{P(Dercum|female)P(female)}{P(Dercum)}. \tag{3.39}$$

However we are missing the term $P(Dercum)$. To find it, we apply the Law of Total Probability:

$$P(Dercum) = P(Dercum|female)P(female) + P(Dercum|male)P(male) = 0.05 \cdot 0.5 + 0.0025 \cdot 0.5 = 0.02625.$$

And finally, returning to eq. (3.39):

$$P(female|Dercum) = \frac{0.05 \cdot 0.5}{0.02625} \approx 0.9524 \tag{3.40}$$

Note: How could this result be reached with one mathematical equation? ■

SOL-46 CH.SOL- 3.17.
In order to solve this problem, we introduce the following events:

1. *AI: the AI predicts that the state of the stock option is 1.*
2. *$State1$: the state of the stock option is 1.*
3. *$State0$: the state of the stock option is 0.*

A direct application of Bayes formulae yields:

$$P(State1|AI) = \tag{3.41}$$
$$\frac{P(AI|State1)P(State1)}{P(AI|State1)P(State1)+P(AI|State0)P(State0)} \tag{3.42}$$
$$= \frac{0.85 \cdot 2/3}{0.85 \cdot 2/3 + 0.15 \cdot 1/3} \approx 0.9189.$$

■

SOL-47 CH.SOL- 3.18. *In order to solve this problem, we introduce the following events:*

1. *H: a human.*

2. *M: a monkey.*

3. *C: a correct prediction.*

By employing Bayes theorem and the Law of Total probability:

$$\begin{aligned} P(H|C) &= \frac{P(H \cap C)}{P(C)} \\ &= \frac{P(C|H)P(H)}{P(C|H)P(H) + P(C|M)P(M)} \\ &= \frac{\frac{1}{20} \cdot \frac{1}{2}}{\frac{1}{20} \cdot \frac{1}{2} + \frac{1}{15} \cdot \frac{1}{2}} \\ &\approx 0.42. \end{aligned} \tag{3.43}$$

Note: If something seems off in this outcome, do not worry - it is a positive sign for understanding of conditional probability. ■

SOL-48 CH.SOL- 3.19.

In order to solve this problem, we introduce the following events:

1. *RUS: a Russian sleeper agent is speaking.*

2. *AM: an American is speaking.*

3. *L: the TTS system generates an "l".*

We are asked to find the value of $P(RUS|L)$. Using Bayes Theorem we can write:

$$P(RUS|L) = \frac{P(L|RUS)P(RUS)}{P(L)}. \tag{3.44}$$

We were told that the Russians consist 1/5 of the attendees at the gathering, therefore:

$$P(RUS) = \frac{1}{5}. \tag{3.45}$$

Additionally, because "v-o-k-s-a-l" has a single l out of a total of six letters:

$$P(L|RUS) = \frac{1}{6}. \tag{3.46}$$

Additionally, because "V-a-u-x-h-a-l-l" has two l's out of a total of eight letters:

$$P(L|AM) = \frac{2}{8}. \tag{3.47}$$

An application of the Law of Total Probability yields:

$$\begin{aligned} P(L) &= P(AM)P(L|AM) + P(RUS)P(L|RUS) \\ &= \left(\frac{4}{5}\right)\left(\frac{2}{8}\right) + \left(\frac{1}{5}\right)\left(\frac{1}{6}\right) = \frac{7}{30}. \end{aligned} \tag{3.48}$$

Using Bayes Theorem we can write:

$$P(RUS|L) = \frac{\frac{1}{5}\left(\frac{1}{6}\right)}{\frac{7}{30}} = \frac{1}{7}. \tag{3.49}$$

Note: What is the letter by which the algorithm is most likely to discover a Russian sleeper agent? ■

SOL-49 CH.SOL- 3.20.

We are given that:
$P(X \text{ is erroneously received as a } Z) = 1/7$. *Using Bayes Theorem we can write:*

$$\begin{aligned} P(Z\ trans|Z\ received) &= \\ &= \frac{P(Z\ received|Z\ trans)P(Z\ trans)}{P(Z\ received)}. \end{aligned} \tag{3.50}$$

An application of the Law of Total Probability yields:

$$\begin{aligned} P(Z\ received) = \\ P(Z\ received|Z\ trans)P(Z\ trans) \\ +P(Z\ received|X\ trans)P(X\ trans) \\ = \frac{6}{7}\cdot\frac{7}{9}+\frac{1}{7}\cdot\frac{2}{9} \\ = \frac{44}{63}. \end{aligned}$$

So, using Bayes Rule, we have that

$$\begin{aligned} P(Z\ trans|Z\ received) \\ &= \frac{P(Z\ received|Z\ trans)P(Z\ trans)}{P(Z\ received)} \\ &= \frac{\frac{6}{7}\frac{7}{9}}{\frac{44}{63}} \\ &= \frac{44}{63} = 0.95. \end{aligned} \tag{3.51}$$

■

3.3.4 Maximum Likelihood Estimation

SOL-50 CH.SOL- 3.21.

For the set of i.i.d samples $X_1, \cdots, X_n$, the likelihood function *is the product of the probability functions:*

$$\begin{aligned} L(p) &= p(X_1 = x_1; p)p(X_2 = x_2; p)\cdots p(X_n = x_n; p) \\ &= \prod_{i=1}^{n}\binom{n}{x_i}p^{x_i}(1-p)^{n-x_i}. \end{aligned} \tag{3.52}$$

Note: What is the distribution of X^n when X is a Bernoulli distributed random variable?

■

SOL-51 CH.SOL- 3.22.

The maximum likelihood estimator (MLE) *of p is the value of all possible p values that maximizes $L(p)$. Namely, the p value that renders the set of measurements $X_1, \cdots, X_n$ as the* most likely. *Formally:*

$$\hat{p} = arg\, max_{0 \leq p \leq 1} L(p) \tag{3.53}$$

Note: The curious student is highly encouraged to derive $\hat{p}$ from $L(p)$. Notice that $L(p)$ can be extremely simplified. ■

SOL-52 CH.SOL- 3.23.

The log-likelihood *is the logarithm of the* likelihood *function. Intuitively, maximizing the likelihood function $L(\gamma)$ is equivalent to maximizing $\ln L(\gamma)$ in terms of finding the MLE $\hat{\gamma}$, since $\ln$ is a monotonically increasing function. Often, we maximize $\ln(f(\gamma))$ instead of the $f(\gamma)$. A common example is when $L(\gamma)$ is comprised of normally distribution random variables.*
Formally, if $X_1, \cdots, X_n$ are i.i.d, each with probability mass function (PMF) of $f_{X_i}(x_i \mid \gamma)$, then

$$f(\gamma) = \prod_{i=1}^{n} f_{X_i}(x_i \mid \gamma), \tag{3.54}$$

$$\ln(f(\gamma)) = \sum_{i=1}^{n} \ln f_{X_i}(x_i \mid \gamma). \tag{3.55}$$

■

SOL-53 CH.SOL- 3.24.

The general procedure for finding the MLE, given that the likelihood function is differentiable, is as follows:

1. *Start by differentiating the log-likelihood function $\ln(L(\gamma))$ with respect to a parameter of interest γ.*
2. *Equate the result to zero.*

3. *Solve the equation to find $\hat{\gamma}$ that holds:*

$$\frac{\partial \ln L(\hat{\gamma} \mid x_1, \cdots x_n)}{\partial \gamma} = 0 \tag{3.56}$$

4. *Compute the second derivative to verify that you indeed have a maximum rather than a minimum.*

■

SOL-54 CH.SOL- 3.25.

*The first derivative of the log-likelihood function is commonly known as the **Fisher score function**, and is defined as:*

$$\mathbf{u}(\gamma) = \frac{\partial \ln L(\gamma \mid x_1, \cdots x_n)}{\partial \gamma} \tag{3.57}$$

■

SOL-55 CH.SOL- 3.26.

***Fisher information**, is the term used to describe the expected value of the second derivatives (the curvature) of the log-likelihood function, and is defined by:*

$$\mathbf{I}(\gamma) = -E\left[\frac{\partial^2 \ln L(\gamma \mid x_1, \cdots x_n)}{\partial \gamma^2}\right] \tag{3.58}$$

■

3.3.5 Fisher Information

SOL-56 CH.SOL- 3.27.

1. *Given $L(\gamma)$:*

$$\ln L(\gamma) = \ln\left(\begin{array}{c} n \\ y \end{array} \right) + y * \ln(\gamma) + (n - y)\ln(1 - \gamma). \tag{3.59}$$

2. *To find the gradient, we differentiate once:*

$$g(\gamma) = y\gamma^{-1} - (n-y)(1-\gamma)^{-1} = \\ (\gamma(1-\gamma))^{-1}y - n(1-\gamma)^{-1}. \tag{3.60}$$

3. *The Hessian is generated by differentiating $g(\gamma)$:*

$$H(\gamma) = -y\gamma^{-2} - (n-y)(1-\gamma)^{-2} \tag{3.61}$$

4. *The Fisher information is calculated as follows:*

$$I(\gamma) = -E(H(\gamma)) = \frac{n}{\gamma(1-\gamma)}, \tag{3.62}$$

since:

$$E(y|\gamma, n) = n * \gamma \tag{3.63}$$

5. *Equating the gradient to zero and solving for our parameter γ, we get:*

$$\hat{\gamma} = \frac{y}{n} \tag{3.64}$$

In our case this equates to: $300/10000 = 0.03$. Regarding the error, there is a close relationship between the variance of γ and the Fisher information, as the former is the inverse of the latter:

$$\text{var}(\gamma) = [I(\gamma)]^{-1} \\ V(\gamma) = \frac{\gamma(1-\gamma)}{n} \tag{3.65}$$

Plugging the numbers from our question:

$$\hat{V}(\hat{\gamma}) = \frac{0.03(1-0.03)}{10000} = 2.9 \times 10^{-7}. \tag{3.66}$$

Statistically, the standard error that we are asked to find is the square root of eq. 3.66 which equals 5.3×10^{-4}. *Note: What desired property is revealed in this experiment? At was cost could we ensure a low standard error?*

■

SOL-57 CH.SOL- 3.28.

The Fisher Information for the distributions is as follows:

1. *Bernoulli:*

$$\Phi(x|\gamma) = x \log \gamma + (1 - x) \log(1 - \gamma), \tag{3.67}$$

$$\Phi'(x|\gamma) = \frac{x}{\gamma} - \frac{1 - x}{1 - \gamma}, \tag{3.68}$$

$$\Phi''(x|\gamma) = -\frac{x}{\gamma^2} - \frac{1 - x}{(1 - \gamma)^2}, \tag{3.69}$$

$$I(\gamma) = -\mathrm{E}_\gamma \left[\frac{X(1 - \gamma)^2 + (1 - X)\gamma^2}{\gamma^2(1 - \gamma)^2} \right] = \frac{1}{\gamma(1 - \gamma)}. \tag{3.70}$$

2. *Poisson:*

$$\begin{aligned} \lambda(x|\theta) &= x \log \theta - \log x! - \theta, \\ \lambda'(x|\theta) &= \frac{x - \theta}{\theta}, \\ \lambda''(x|\theta) &= -\frac{x}{\theta^2}, \\ I(\theta) &= -\mathrm{E}_\theta \left[\frac{(X - \theta)^2}{\theta^2} \right] = \frac{1}{\theta}. \end{aligned} \tag{3.71}$$

■

SOL-58 CH.SOL- 3.29.

1. *True.*
2. *True.*

■

3.3.6 Posterior & prior predictive distributions

SOL-59 CH.SOL- 3.30.

1. *Given a sample of the form* $\underline{x} = (x_1, \cdots, x_n)$ *drawn from a density* $p(\theta; \underline{x})$ *and* θ *is randomly generated according to a prior density of* $p(\theta)$*. Then the posterior density is defined by:*

$$p(\theta|\underline{x}) = \frac{p(\theta; \underline{x})p(\theta)}{p(\underline{x})}. \tag{3.72}$$

2. *The prior predictive density is:*

$$p(\underline{x}) = \int_{\theta \in \Theta} p(\theta; \underline{x})p(\theta)d\theta \tag{3.73}$$

■

SOL-60 CH.SOL- 3.31.

1. *The posterior* $p(\theta|y) \propto p(y|\theta)p(\theta)$ *is:*

$$\begin{cases} \binom{5}{y}(1/2)^y(1/2)^{5-y}0.25, & \theta = 1/2 \\ \binom{5}{y}(1/6)^y(5/6)^{5-y}0.5, & \theta = 1/6 \\ \binom{5}{y}(1/4)^y(3/4)^{5-y}0.25, & \theta = 1/4 \\ 0, & \textit{otherwise} \end{cases}$$

2. *The prior predictive distribution* $p(y)$*:*

$$\binom{5}{y}((1/2)^y(1/2)^{5-y}0.25 \tag{3.74}$$

$$+$$

$$(1/6)^y(5/6)^{5-y}0.5 + (1/4)^y(3/4)^{5-y}0.25). \tag{3.75}$$

■

3.3.7 Conjugate priors

SOL-61 CH.SOL- 3.32.

1. *A class $\mathcal{F}$ of prior distributions is said to form a conjugate family if the posterior density is in $\mathcal{F}$ for all each sample, whenever the prior density is in $\mathcal{F}$.*
2. *Often we would like a prior that favours no particular values of the parameter over others. Bayesian analysis requires prior information, however sometimes there is no particularly useful information before data is collected. In these situations, priors with "no information" are expected. Such priors are called* non-informative priors.

■

SOL-62 CH.SOL- 3.33.

If $x \sim \mathrm{B}(n, \gamma)$ *so*

$$p(x|\gamma) \propto \gamma^x(1-\gamma)^{n-x}$$

and the prior for γ *is* $\mathcal{B}(\alpha, \beta)$ *so*

$$p(\gamma) \propto \gamma^{\alpha-1}(1-\gamma)^{\beta-1}$$

then the posterior is

$$\gamma|x \sim \mathcal{B}(\alpha + x, \beta + n - x)$$

It is immediately clear the family of beta distributions is conjugate to a binomial likelihood.

■

3.3.8 Bayesian Deep Learning

SOL-63 CH.SOL- 3.34.

1. *The hidden neuron is distributed according to:*
   $X \sim \text{binomial}(n, \gamma)$ *random variable and fires with a probability of* γ*. There are 100 neurons and only 20 are* ***fired****.*

$$P(x = 20|\theta) = \begin{pmatrix} 100 \\ 20 \end{pmatrix} \theta^{20}(1-\theta)^{80} \tag{3.76}$$

2. *The hidden neuron is distributed according to:*
   $X\ uniform(0, \gamma)$ *random variable and fires with a probability of* γ*.*
   The uniform distribution is, of course, a very simple case:

$$f(x; a, b) = \frac{1}{b-a} \quad for \quad a \leq x \leq b \tag{3.77}$$

   Therefore:

$$f(x|\gamma) = \begin{cases} 0 & if\ \gamma < x\ or\ x < 0 \\ 1/\gamma & if\ 0 \leq x \leq \theta \end{cases} \tag{3.78}$$

■

SOL-64 CH.SOL- 3.35.

The provided distribution is from the exponential family. Therefore, a single neuron becomes inactive with a probability of:

$$p = P(X < 20) = \int_0^{20} e^{-x}\, dx = 1 - e^{-20}. \tag{3.79}$$

The OnOffLayer is off only if at least 150 out of 200 neurons are off. Therefore, this may be represented as a Binomial distribution and the probability for the layer to be off is:

$$V = \sum_{n \geq 150} \begin{pmatrix} 200 \\ n \end{pmatrix} \tilde{p}^n (1-\tilde{p})^{200-n} \tag{3.80}$$

Hence, the probability of the layer being active for at least 20 seconds is 1 minus this value:

$$[1 - V]. \tag{3.81}$$

■

SOL-65 CH.SOL- 3.36.

The observed data, e.g the dropped neurons are distributed according to:

$$(x_1, \ldots, x_n)|\theta \overset{iid}{\sim} \text{Bern}(\theta) \tag{3.82}$$

Denoting s and f as success and failure respectively, we know that the likelihood is:

$$p\left(x_1, \ldots, x_n|\theta\right) = \theta^s(1-\theta)^f \tag{3.83}$$

With the following parameters $\alpha = \beta = 1$ the beta distribution acts like Uniform prior:

$$\theta \sim \text{Beta}(\alpha, \beta), \text{ given } \alpha = \beta = 1 \tag{3.84}$$

*Hence, the **prior** density is:*

$$p(\theta) = \frac{1}{B(\alpha, \beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1} \tag{3.85}$$

*Therefore the **posterior** is:*

$$\begin{aligned} p\left(\theta|x_1, \ldots, x_n\right) &\propto p\left(x_1, \ldots, x_n|\theta\right) p(\theta) \\ &\propto \theta^S(1-\theta)^f\theta^{\alpha-1}(1-\theta)^{\beta-1} \\ &= \theta^{\alpha+s-1}(1-\theta)^{\beta+f-1} \end{aligned} \tag{3.86}$$

■

SOL-66 CH.SOL- 3.37.

Neurons are dropped whenever their value (or the equivalent quantum term- speed) reach

the most likely value:

$$n(v)dv = \frac{4\pi N}{V}\left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}} dv \tag{3.87}$$

From calculus, we know that in order to maximize a function, we have to equate its first derivative to zero:

$$\frac{d}{dv} n(v) = 0 \tag{3.88}$$

The constants can be taken out as follows:

$$\frac{d}{dv} v^2 e^{-\frac{mv^2}{2kT}} = 0 \tag{3.89}$$

Applying the chain rule from calculus:

$$2ve^{-\frac{mv^2}{2kT}} + v^2\left(-\frac{m}{2kT}2v\right)e^{-\frac{mv^2}{2kT}} = 0 \tag{3.90}$$

We notice that several terms cancel out:

$$v^2\frac{m}{2kT} = 1 \tag{3.91}$$

Now the quadratic equation can be solved yielding:

$$v_{most\_probable} = \sqrt{\frac{2kT}{m}} \tag{3.92}$$

Therefore, this is the most probable value at which the dropout layer will fire.

■

References

[1] M. Barati and P. 'Comparison of complications of chorionic villus sampling and amniocentesis'. In: 5.4 (2012), pp. 241–244 (cit. on p. 46).

[2] J. D. e. a. Bell BP Damon IK. 'Overview, Control Strategies, and Lessons Learned in the CDC Response to the 20142016 Ebola Epidemic.' In: *Morbidity and Mortality Weekly Report* 65.3 (2016), pp. 4–11 (cit. on p. 52).

[3] J. C. Cook and G. P. Gross. *Adiposis Dolorosa (Dercum, Anders Disease)*. StatPearls [Internet], 2019 (cit. on p. 47).

[4] G. Ecker. *Particles, Field, From Quantum Mechanics to the Standard Model of Particle Physics*. Springer., 2019 (cit. on p. 45).

[5] K. Gaj and A. Orlowski. 'Facts and Myths of Enigma: Breaking Stereotypes'. In: *International Conference on the Theory and Applications of Cryptographic Techniques*. 2003 (cit. on p. 50).

[6] B. Gottschalk. 'Techniques of Proton Radiotherapy: Transport Theory'. In: *arXiv* (2012) (cit. on p. 43).

[7] T. S. O. of Investor Education and Advocacy. *Binary options and Fraud* (cit. on p. 48).

[8] E. T. Jaynes. *Probability Theory as Logic*. Ed. by P. F. Fougère. Maximum-Entropy and Bayesian Methods. Kluwer, Dordrecht, 1990 (cit. on p. 42).

[9] D. o. J. National Security Division. *Conspiracy to Act as Unregistered Agents of a Foreign Government*. 2010 (cit. on p. 49).

[10] A. Paszke et al. 'Automatic differentiation in PyTorch'. In: *31st Conference on Neural Information Processing Systems*. 2017 (cit. on p. 56).

[11] J. Salvatier, T. V. Wiecki and C. Fonnesbeck. 'Probabilistic programming in Python using PyMC3'. In: *PeerJ Computer Science* 2 (Jan. 2016), e55 (cit. on p. 42).

[12] P. Sledzinski et al. 'The current state and future perspectives of cannabinoids in cancer biology'. In: *Cancer Medicine* 7.3 (2018), pp. 765–775 (cit. on p. 56).

[13] E. B. Starikov. 'Bayesian Statistical Mechanics: Entropy Enthalpy Compensation and Universal Equation of State at the Tip of Pen'. In: *Frontiers in Physics* 6 (2018), p. 2 (cit. on p. 42).

PART III
HIGH SCHOOL

CHAPTER 4

INFORMATION THEORY

A basic idea in information theory is that information can be treated very much like a physical quantity, such as mass or energy.

— Claude Shannon, 1985

Contents

4.1 Introduction

INDUCTIVE inference, is the problem of reasoning under conditions of incomplete information, or **uncertainty**. According to Shannon's theory [2], information and uncertainty are two sides of the same coin: the more uncertainty there is, the more information we gain by removing the uncertainty. Entropy plays central roles in many scientific realms ranging from physics and statistics to data science and economics. A basic problem in information theory is encoding large quantities of information [2].

Shannon's discovery of the fundamental laws of data compression and transmission marked the birth of information theory. In his fundamental paper of 1948, "*A Mathematical Theory of Communication*" [4], Shannon proposed a measure of the uncertainty associated with a random memory-less source, called *Entropy*.

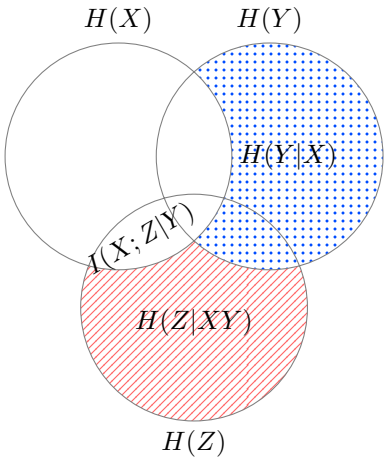
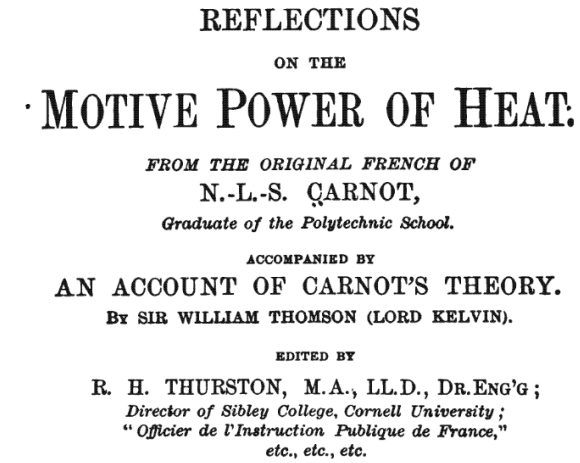


FIGURE 4.1: Mutual information

Entropy first emerged in thermodynamics in the 18^{th} century by Carnot, [1] in his pioneering work on steam entitled "*Reflection on the Motive Power of Fire*" (Fig. 4.2). Subsequently it appeared in statistical mechanics where it was viewed as a measure of *disorder*. However, it was Boltzmann (4.30) who found the connection between entropy and probability, and the notion of information as used by Shannon is a generalization of the notion of entropy. Shannon's entropy shares some instinct with Boltzmann's entropy, and likewise the mathematics developed in information theory is highly relevant in statistical mechanics.


REFLECTIONS

ON THE

MOTIVE POWER OF HEAT:

FROM THE ORIGINAL FRENCH OF

N.-L.-S. CARNOT,

Graduate of the Polytechnic School.

ACCOMPANIED BY

AN ACCOUNT OF CARNOT'S THEORY.

By SIR WILLIAM THOMSON (LORD KELVIN).

EDITED BY

R. H. THURSTON, M.A., LL.D., Dr. Eng'g;

Director of Sibley College, Cornell University;

"Officier de l'Instruction Publique de France,"

etc., etc., etc.

FIGURE 4.2: Reflection on the motive power of fire.

The **majority** of candidates I interview fail to come up with an answer to the following question: *what is the entropy of tossing a non-biased coin?* Surprisingly, even after I explicitly provide them with Shannon's formulae for calculating entropy (4.4), many are still unable to calculate simple logarithms. The purpose of this chapter is to present the aspiring data scientist with some of the most significant notions of entropy and to elucidate its relationship to probability. Therefore, it is primarily focused on basic quantities in information theory such as entropy, cross-entropy, conditional entropy, mutual information and Kullback-Leibler divergence, also known as relative entropy. It does not however, discuss more advanced topics such as the concept of 'active information' introduced by Bohm and Hiley [3].

4.2 Problems

4.2.1 Logarithms in Information Theory

It is important to note that all numerical calculations in this chapter use the binary logarithm $\log_2$. This specific logarithm produces units of bits, the commonly used units of information in the field on information theory.

PRB-67 ❓ CH.PRB- 4.1.

Run the following Python code (4.3) in a Python interpreter. What are the results?

```
import math
import numpy
print (math.log(1.0/0.98)) # Natural log (ln)
print (numpy.log(1.0/0.02)) # Natural log (ln)

print (math.log10(1.0/0.98)) # Common log (base 10)
print (numpy.log10(1.0/0.02)) # Common log (base 10)

print (math.log2(1.0/0.98)) # Binary log (base 2)
print (numpy.log2(1.0/0.02)) # Binary log (base 2)
```

FIGURE 4.3: Natural (ln), binary ($\log_2$) and common ($\log_{10}$) logarithms.

PRB-68 ❓ CH.PRB- 4.2.

The three basic laws of logarithms:

1. ***First law***

$$\log A + \log B = \log AB. \tag{4.1}$$

Compute the following expression:

$$\log_{10} 3 + \log_{10} 4.$$

2. ***Second law***

$$\log A^n = n \log A. \tag{4.2}$$

Compute the following expression:

$$\log_2 4^6.$$

3. ***Third law***

$$\log A - \log B = \log \frac{A}{B}. \tag{4.3}$$

Therefore, subtracting $\log B$ *from* $\log A$ *results in* $\log \frac{A}{B}$.

Compute the following expression:

$$\log_e 15 - \log_e 3.$$

4.2.2 Shannon's Entropy

PRB-69 ❓ CH.PRB- 4.3.
Write Shannon's famous general formulae for ***uncertainty***.

PRB-70 ❓ CH.PRB- 4.4.
Choose exactly ***one, and only one*** *answer.*

1. *For an event which is* ***certain to happen****, what is the entropy?*
   - *(a)* 1.0
   - *(b)* 0.0
   - *(c) The entropy is undefined*
   - *(d)* -1
   - *(e)* 0.5
   - *(f)* $\log_2(N)$, *N being the number of possible events*

2. *For N* ***equiprobable events****, what is the entropy?*

   (a) 1.0

   (b) 0.0

   (c) The entropy is undefined

   (d) -1

   (e) 0.5

   (f) $\log_2(N)$

PRB-71 ❓ CH.PRB- 4.5.

Shannon found that entropy was the only function satisfying ***three natural properties****. Enumerate these properties.*

PRB-72 ❓ CH.PRB- 4.6.

In information theory, minus the logarithm of the probability of a symbol (essentially the number of bits required to represent it efficiently in a binary code) is defined to be the ***information*** *conveyed by transmitting that symbol. In this context, the entropy can be interpreted as the expected information conveyed by transmitting a single symbol from an alphabet in which the symbols occur with the probabilities π_k.*
Mark the correct answer*: Information is a/an* ***[decrease/increase]*** *in uncertainty.*

PRB-73 ❓ CH.PRB- 4.7.

Claud Shannon's paper "A mathematical theory of communication" [4], marked the birth of information theory. Published in 1948, it has become since the Magna Carta of the information age. Describe in your own words what is meant by the term ***Shannon bit****.*

PRB-74 ❓ CH.PRB- 4.8.

With respect to the notion of ***surprise*** *in the context of information theory:*

1. *Define what it actually meant by being* ***surprised****.*

2. *Describe how it is related to the likelihood of an event happening.*

3. ***True or False:*** *The less likely the occurrence of an event, the smaller information it conveys.*

PRB-75 ❓ CH.PRB- 4.9.

*Assume a source of signals that transmits a given message a with probability P_a. Assume further that the message is encoded into an ordered series of ones and zeros (a bit string) and that a receiver has a decoder that converts the bit string back into its respective message. Shannon devised a formulae that describes the **size** that the mean length of the bit string can be **compressed to**. Write the formulae.*

PRB-76 ❓ CH.PRB- 4.10.

Answer the following questions:

1. *Assume a source that provides a constant stream of N **equally likely** symbols $\{x_1, x_2, \ldots, x_N\}$. What does Shannon's formulae (4.4) reduce to in this particular case?*

2. *Assume that each equiprobable pixel in a monochrome image that is fed to a DL classification pipeline, can have values ranging from 0 to 255. Find the entropy in **bits**.*

PRB-77 ❓ CH.PRB- 4.11.

Given Shannon's famous general formulae for uncertainty (4.4):

$$H = -\sum_{a=1}^{N} P_a \log_2 P_a \qquad \textit{(bits per symbol).} \tag{4.4}$$

1. *Plot a graph of the curve of probability vs. uncertainty.*

2. ***Complete the sentence:*** *The curve is **[symmetrical/asymmetrical]**.*

3. ***Complete the sentence:*** *The curve rises to a* ***[minimum/maximum]*** *when the two symbols are equally likely (P_a = 0.5).*

PRB-78 ❓ CH.PRB- 4.12.

Assume we are provided with biased coin for which the event 'heads' is assigned probability p, and 'tails' - a probability of $1-p$. Using (4.4), the respective entropy is:

$$H(p) = -p \log p - (1-p) \log (1-p) . \tag{4.5}$$

Therefore, $H \geq 0$ and the maximum possible uncertainty is attained when $p = 1/2$, is $H_{\max} = \log_2 2$.
Given the above formulation, describe a helpful property of the entropy that ***follows from the concavity of the logarithmic function.***

PRB-79 ❓ CH.PRB- 4.13.

True or False: *Given random variables X, Y and Z where $Y = X + Z$ then:*

$$H(X,Y) = H(X,Z). \tag{4.6}$$

PRB-80 ❓ CH.PRB- 4.14.

What is the entropy of a ***biased coin****? Suppose a coin is biased such that the probability of 'heads' is $p(x_h) = 0.98$.*

1. ***Complete the sentence:*** *We can predict 'heads' for each flip with an accuracy of [___]%.*

2. ***Complete the sentence:*** *If the result of the coin toss is 'heads', the amount of Shannon information gained is [___] bits.*

3. ***Complete the sentence:*** *If the result of the coin toss is 'tails', the amount of Shannon information gained is [___] bits.*

4. ***Complete the sentence:*** *It is always true that the more information is associated with an outcome, the* ***[more/less]*** *surprising it is.*

5. *Provided that the ratio of tosses resulting in 'heads' is $p(x_h)$, and the ratio of tosses resulting in 'tails' is $p(x_t)$, and also provided that $p(x_h)+p(x_t) = 1$, what is formulae for the **average surprise**?*

6. *What is the value of the **average surprise** in bits?*

4.2.3 Kullback-Leibler Divergence (KLD)

PRB-81 ❓ CH.PRB- 4.15.
Write the formulae for the Kullback-Leibler divergence between two discrete probability density functions P and Q.

PRB-82 ❓ CH.PRB- 4.16.
Describe one intuitive interpretation of the KL-divergence with respect to bits.

PRB-83 ❓ CH.PRB- 4.17.

1. ***True or False:** The KL-divergence is not a symmetric measure of similarity, i.e.:*

$$\mathrm{D}_{KL}(P\|Q) \neq \mathrm{D}_{KL}(Q\|P).$$

2. ***True or False:** The KL-divergence satisfies the triangle inequality.*

3. ***True or False:** The KL-divergence is not a distance metric.*

4. ***True or False:** In information theory, KLD is regarded as a measure of the information gained when probability distribution Q is used to approximate a true probability distribution P.*

5. ***True or False:** The units of KL-divergence are units of information.*

6. ***True or False:** The KLD is always non-negative, namely:*

$$\mathrm{D}_{KL}(P\|Q) \geq 0.$$

.

7. ***True or False:*** *In a decision tree,* ***high*** *information gain indicates that adding a split to the decision tree results in a* ***less*** *accurate model.*

PRB-84 ❓ CH.PRB- 4.18.
Given two distributions f_1 and f_2 and their respective joint distribution f, write the formulae for the mutual information *of f_1 and f_2.*

PRB-85 ❓ CH.PRB- 4.19.
The question was commented out but remained here for the consistency of the numbering system.

4.2.4 Classification and Information Gain

PRB-86 ❓ CH.PRB- 4.20.
There are several measures by which one can determine how to optimally split attributes in a decision tree. List the three most commonly used measures and write their formulae.

PRB-87 ❓ CH.PRB- 4.21.
Complete the sentence: *In a decision tree, the attribute by which we choose to split is the one with* ***[minimum/maximum]*** *information gain.*

PRB-88 ❓ CH.PRB- 4.22.
To study factors affecting the decision of a frog to jump (or not), a deep learning researcher from a Brazilian rain-forest, collects data pertaining to several independent binary co-variates.

FIGURE 4.4: A Frog in its natural habitat. Photo taken by my son.

*The binary response variable **Jump** indicates whether a jump was observed. Referring to Table (4.1), each row indicates the observed values, columns denote features and rows denote labelled instances while class label (**Jump**) denotes whether the frog had jumped.*

Observation	Green	Rain	Jump
$x1$	1	0	+
$x2$	1	1	+
$x3$	1	0	+
$x4$	1	1	+
$x5$	1	0	+
$x6$	0	1	+
$x7$	0	0	−
$x8$	0	1	−

TABLE 4.1: Decision trees and frogs.

Without explicitly determining the information gain values for each of the three attributes, which attribute should be chosen as the attribute by which the decision tree should be first partitioned? e.g which attribute has the highest predictive power regarding the decision of the frog (Fig. 4.4) to jump.

PRB-89 ❓ CH.PRB- 4.23.

This question discusses the link between binary classification, information gain and decision trees. Recent research [5] suggests that Cannabis (Fig. 4.5), and Cannabinoids administration in particular may reduce the size of malignant tumours in rodents. The data (Table 9.2) comprises a training set of feature vectors with corresponding class labels which a researcher intents classifying using a decision tree.

FIGURE 4.5: Cannabis

To study factors affecting tumour shrinkage, the deep learning researcher collects data regrading two independent binary variables; θ_1 (T/F) indicating whether the rodent is a female, and θ_2 (T/F) indicating whether the rodent was administrated with Cannabinoids. The binary response variable, γ, indicates whether tumour shrinkage was observed (e.g. shrinkage=+, no shrinkage=-). Referring to Table (9.2), each row indicates the observed values, columns (θ_i) denote features and class label (γ) denotes whether shrinkage was observed.

γ	θ_1	θ_2
+	T	T
-	T	F
+	T	F
+	T	T
-	F	T

TABLE 4.2: Decision trees and Cannabinoids administration

1. *Describe what is meant by **information gain**.*
2. *Describe in your own words how does a decision tree work.*
3. *Using log_2, and the provided dataset, calculate the sample entropy $H(\gamma)$.*
4. *What is the information gain $IG(X_1) \equiv H(\gamma) - H(|\theta_1)$ for the provided training corpus?*

PRB-90 ❓ CH.PRB- 4.24.

To study factors affecting the expansion of stars, a physicist is provided with data regrading two independent variables; θ_1 (T/F) indicating whether a star is dense, and θ_2 (T/F) indicating whether a star is adjacent to a black-hole. He is told that the binary response variable, γ, indicates whether expansion was observed.

e.g.:
expansion=+, no expansion=-. Referring to table (4.3), each row indicates the observed values, columns (θ_i) denote features and class label (γ) denotes whether expansion was observed.

γ (expansion)	θ_1 (dense)	θ_2 (black-hole)
+	F	T
+	T	T
+	T	T
-	F	T
+	T	F
-	F	F
-	F	F

TABLE 4.3: Decision trees and star expansion.

1. *Using log_2 and the provided dataset, calculate the sample entropy $H(\gamma)$ (expansion) before splitting.*
2. *Using log_2 and the provided dataset, calculate the **information gain** of $H(\gamma|\theta_1)$.*

3. *Using log_2 and the provided dataset, calculate the* ***information gain*** *of $H(\gamma|\theta_2)$.*

PRB-91 ❓ CH.PRB- 4.25.

To study factors affecting tumour shrinkage in humans, a deep learning researcher is provided with data regrading two independent variables; θ_1 (S/M/L) indicating whether the tumour is small(S), medium(M) or large(L), and θ_2 (T/F) indicating whether the tumour has undergone radiation therapy. He is told that the binary response variable, γ, indicates whether tumour shrinkage was observed (e.g. shrinkage=+, no shrinkage=-).

Referring to table (4.4), each row indicates the observed values, columns (θ_i) denote features and class label (γ) denotes whether shrinkage was observed.

γ (shrinkage)	θ_1	θ_2
-	S	F
+	S	T
-	M	F
+	M	T
+	H	F
+	H	T

TABLE 4.4: Decision trees and radiation therapy.

1. *Using log_2 and the provided dataset, calculate the sample entropy $H(\gamma)$ (shrinkage).*
2. *Using log_2 and the provided dataset, calculate the entropy of $H(\gamma|\theta_1)$.*
3. *Using log_2 and the provided dataset, calculate the entropy of $H(\gamma|\theta_2)$.*
4. ***True or false:** We should split on a specific variable that minimizes the information gain, therefore we should split on θ_2 (radiation therapy).*

4.2.5 Mutual Information

PRB-92 ❓ CH.PRB- 4.26.

Shannon described a communications system consisting five elements (4.6), two of which are the source S and the destination D.

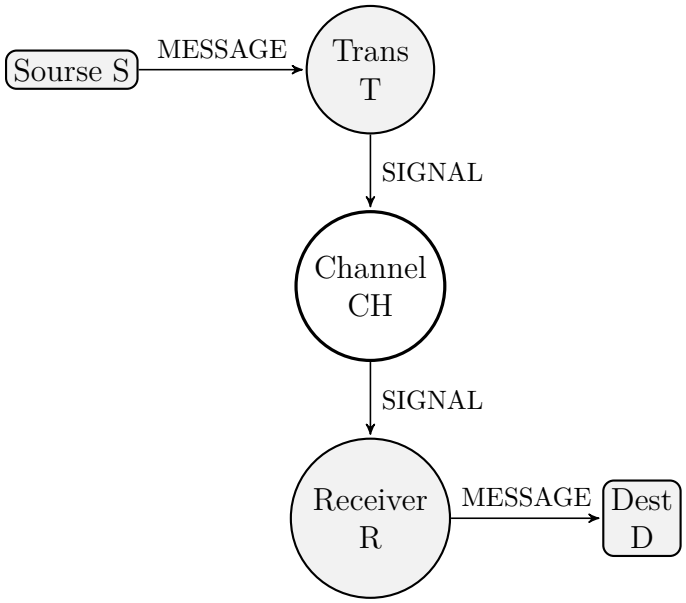


FIGURE 4.6: Shannon's five element communications system.

1. *Draw a Venn diagram depicting the relationship between the entropies of the source $H(S)$ and of the destination $H(D)$.*
2. *Annotate the part termed **equivocation**.*
3. *Annotate the part termed **noise**.*
4. *Annotate the part termed **mutual information**.*
5. *Write the formulae for **mutual information**.*

PRB-93 ❓ CH.PRB- 4.27.
Complete the sentence: *The relative entropy $D(p||q)$ is the measure of (a) [___] between*

two distributions. It can also be expressed as a measure of the (b)[___] of assuming that the distribution is q when the (c)[___] distribution is p.

PRB-94 ❓ CH.PRB- 4.28.

Complete the sentence: *Mutual information is a Shannon entropy-based measure of dependence between random variables. The mutual information between X and Z can be understood as the (a) [___] of the (b) [___] in X given Z:*

$$I(X;Z) := H(X) - H(X \mid Z), \tag{4.7}$$

where H is the Shannon entropy, and $H(X \mid Z)$ is the conditional entropy of Z given X.

4.2.6 Mechanical Statistics

Some books have a tendency of sweeping "unseen" problems under the rug. We will not do that here. This subsection may look intimidating and for a good reason; it involves equations that, unless you are a physicists, you have probably never encountered before. Nevertheless, the ability to cope with new concepts lies at the heart of every job interview.

For some of the questions, you may need these constants:

PHYSICAL CONSTANTS

k	Boltzmanns constant	1.381×10^{-23} J K^{-1}
c	Speed of light in vacum	2.998×10^{8}m s^{-1}
h	Planck's constant	6.626×10^{-34} J s

PRB-95 ❓ CH.PRB- 4.29.

What is the expression for the Boltzmann probability distribution?

PRB-96 ❓ CH.PRB- 4.30.

Information theory, quantum physics and thermodynamics are closely interconnected. There are several equivalent formulations for the second law of thermodynamics. One approach to describing uncertainty stems from Boltzmanns fundamental work on entropy *in*

statistical mechanics. Describe what is meant by ***Boltzmanns entropy.***

PRB-97 ❓ CH.PRB- 4.31.
From Boltzmanns perspective, what is the entropy of an octahedral dice (4.7)?

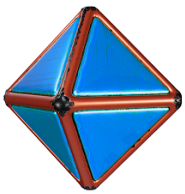


FIGURE 4.7: An octahedral dice.

4.2.7 Jensen's inequality

PRB-98 ❓ CH.PRB- 4.32.

1. *Define the term concave function.*
2. *Define the term convex function.*
3. *State Jensen's inequality and its implications.*

PRB-99 ❓ CH.PRB- 4.33.
True or False: *Using Jensen's inequality, it is possible to show that the KL divergence is always greater or equal to zero.*

4.3 Solutions

4.3.1 Logarithms in Information Theory

SOL-67 CH.SOL- 4.1.

Numerical results (4.8) are provided using Python interpreter version 3.6.

```
import math
import numpy
print (math.log(1.0/0.98)) # Natural log (ln)
> 0.02020270731751947
print (numpy.log(1.0/0.02)) # Natural log (ln)
> 3.912023005428146
print (math.log10(1.0/0.98)) # Common log (base 10)
> 0.008773924307505152
print (numpy.log10(1.0/0.02)) # Common log (base 10)
> 1.6989700043360187
print (math.log2(1.0/0.98)) # Binary log (base 2)
> 0.02914634565951651
print (numpy.log2(1.0/0.02)) # Binary log (base 2)
> 5.643856189774724
```

FIGURE 4.8: Logarithms in information theory.

SOL-68 CH.SOL- 4.2.

The logarithm base is explicitly written in each solution.

1. $$\log_{10} 3 + \log_{10} 4 = \log_{10}(3 \times 4) = \log_{10} 12.$$

2. $$\log_2 4^6 = 6 \log_2 4.$$

3. $$\log_e 15 - \log_e 3 = \log_e \tfrac{15}{3} = \log_e 5.$$

4.3.2 Shannon's Entropy

SOL-69 CH.SOL- 4.3.

Shannons famous general formulae for uncertainty is:

$$\boxed{H = -\sum_{a=1}^{N} P_a \log_2 P_a \quad \textit{(bits per symbol).}} \tag{4.8}$$

SOL-70 CH.SOL- 4.4.

1. *No information is conveyed by an event which is a-priori known to occur for certain (P_a = 1), therefore the entropy is* 0.
2. *Equiprobable events mean that* $P_i = 1/N \ \forall i \in [1, N]$. *Therefore for* N *equally-likely events, the entropy is* $\log_2(N)$.

SOL-71 CH.SOL- 4.5.

The three properties are as follows:

1. $H(X)$ *is always non-negative, since information cannot be lost.*
2. *The uniform distribution maximizes* $H(X)$, *since it also maximizes uncertainty.*
3. *The additivity property which relates the sum of entropies of two independent events. For instance, in thermodynamics, the total entropy of two isolated systems which co-exist in equilibrium is the sum of the entropies of each system in isolation.*

SOL-72 CH.SOL- 4.6.

*Information is an **[increase]** in uncertainty.* ■

SOL-73 CH.SOL- 4.7.

*The Shannon bit has two distinctive states; it is either 0 or 1, but never both at the same time. Shannon devised an experiment in which there is a question whose only two possible answers were **equally likely to happen**.*
*He then defined **one bit** as the amount of information gained (or alternatively, the amount of entropy removed) once an answer to the question has been learned. He then continued to state that when the a-priori probability of any one possible answer is higher than the other, the answer would have conveyed less than one bit of information.* ■

SOL-74 CH.SOL- 4.8.

The notion of surprise is directly related to the likelihood of an event happening. Mathematically is it inversely proportional to the probability of that event.
*Accordingly, learning that a high-probability event has taken place, for instance the sun rising, is **much less of a surprise** and gives less information than learning that a low-probability event, for instance, rain in a hot summer day, has taken place. Therefore, the less likely the occurrence of an event, the greater information it conveys.*
*In the case where an event is a-priori known to occur for certain ($P_a = 1$), then no information is conveyed by it. On the other hand, an extremely intermittent event conveys a lot of information as it **surprises** us and informs us that a very improbable state exists. Therefore, the statement in part 3 is false.*

■

SOL-75 CH.SOL- 4.9.

*This quantity I_{Sh}, represented in the formulae is called the **Shannon information of the source**:*

$$I_{Sh} = -\sum_a p_a \log_2 p_a. \tag{4.9}$$

It refers to the mean length in bits, per message, into which the messages can be compressed

to. It is then possible for a communications channel to transmit I_{Sh} bits per message with a capacity of I_{Sh}. ■

SOL-76 CH.SOL- 4.10.

1. *For N equiprobable events it holds that $P_i = 1/N, \forall i \in [1, N]$. Therefore if we substitute this into Shannon's equation we get:*

$$H_{equiprobable} = -\sum_{i=1}^{N} \frac{1}{N} \log_2 \frac{1}{N}. \tag{4.10}$$

Since N does not depend on i, we can pull it out of the sum:

$$\begin{aligned} H_{equiprobable} &= -(\frac{1}{N} \log_2 \frac{1}{N}) \sum_{i=1}^{N} 1 && (4.11) \\ &= -\left(\frac{1}{N} \log_2 \frac{1}{N}\right) N \\ &= -\log_2 \frac{1}{N} && (4.12) \\ &= \log_2 N. \end{aligned}$$

It can be shown that for a given number of symbols (i.e., N is fixed) the uncertainty H has its largest value only when the symbols are equally probable.

2. *The probability for each pixel to be assigned a value in the given range is:*

$$p_i = 1/256. \tag{4.13}$$

Therefore the entropy is:

$$H = -(256)(1/256)(-8) = 8 \text{ [bits/symbol]}. \tag{4.14}$$

■

SOL-77 CH.SOL- 4.11.

Refer to Fig. 4.9 for the corresponding illustration of the graph, where information is shown as a function of p. It is equal to 0 for $p = 0$ and for $p = 1$. This is reasonable because for such values of p the outcome is certain, so no information is gained by learning the outcome. The entropy in maximal uncertainty equals to 1 bit for $p = 0.5$. Thus, the information gain is maximal when the probabilities of two possible events are equal. Furthermore, for the entire range of probabilities between $p = 0.4$ and $p = 0.6$ the information is close to 1 bit. ■

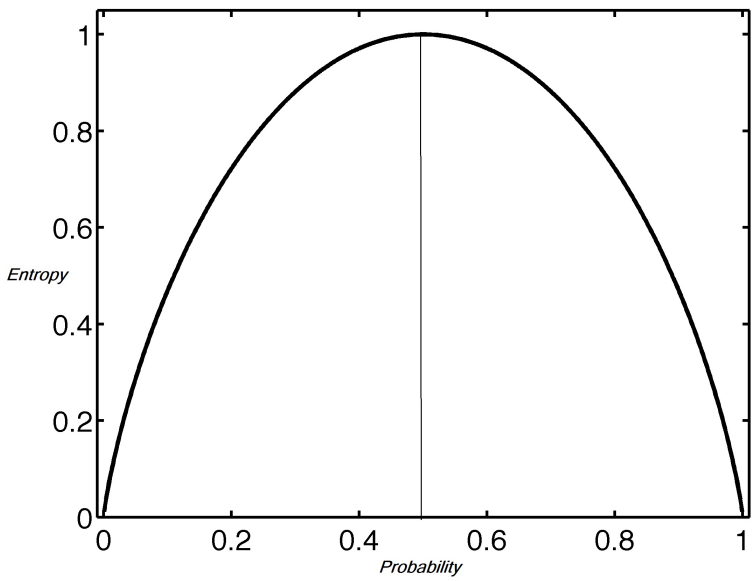


FIGURE 4.9: H vs. Probability

SOL-78 CH.SOL- 4.12.

An important set of properties of the entropy follows from the concavity of the entropy, which follows from the concavity of the logarithm. Suppose that in an experiment, we cannot decide whether the actual probability of 'heads' is p_1 or p_2. We may decide to assign probability q to the first alternative and probability $1 - q$ to the second. The actual probability of 'heads' then is the mixture $qp_1 + (1 - q)p_2$. The corresponding entropies satisfy the inequality:

$$S\left(qp_1 + (1-q)p_2\right) \geq qS\left(p_1\right) + (1-q)\,S\left(p_2\right), \tag{4.15}$$

These probabilities, are equal in the extreme cases where $p_1 = p_2$, or $q = 0$, or $q = 1$. ■

SOL-79 CH.SOL- 4.13.

Given (X, Y), we can determine X and $Z = Y - X$. Conversely, given (X, Z), we can determine X and $Y = X + Z$. Hence, $H(X, Y) = H(X, Z)$ due to the existence of this bijection. ■

SOL-80 CH.SOL- 4.14.

The solution and numerical calculations are provided using $\log_2$.

1. *We can predict 'heads' for each flip with an accuracy of $p(x_h) = 98\%$.*
2. *According to Fig. (4.10), if the result of the coin toss is 'heads', the amount of Shannon information gained is $\log_2(1/0.98)$ [bits] .*

```
import math
import numpy
print (math.log2(1.0/0.98)) # Binary log (base 2)
> 0.02914634565951651
print (numpy.log2(1.0/0.02)) # Binary log (base 2)
> 5.643856189774724
```

FIGURE 4.10: Shannon information gain for a biased coin toss.

3. *Likewise, if the result of the coin toss is 'tails', the amount of Shannon information gained is $\log_2(1/0.02)$ [bits] .*
4. *It is always true that the **more** information is associated with an outcome, the **more** surprising it is.*
5. *The formulae for the **average surprise** is:*

$$H(x) = p(x_h) \log \frac{1}{p(x_h)} + p(x_t) \log \frac{1}{p(x_t)}. \tag{4.16}$$

6. *The value of the* ***average surprise*** *in bits is (4.11):*

$$H(x) = [0.98 \times 0.0291] + [0.02 \times 5.643] \\ = 0.1414 \textit{ [bits]}. \tag{4.17}$$

```
import autograd.numpy as np
def binaryEntropy (p):
 return -p*np.log2(p) -(1-p)*np.log2(1-p)
 print ("binaryEntropy(p) is:{}
  ↪  bits".format(binaryEntropy(0.98)))
> binaryEntropy(p) is:0.1414 bits
```

FIGURE 4.11: Average surprise

4.3.3 Kullback-Leibler Divergence

SOL-81 CH.SOL- 4.15.

For discrete probability distributions P and Q, the Kullback-Leibler divergence ***from*** *P* ***to*** *Q, the KLD is defined as:*

$$\begin{aligned} D(P \parallel Q) &= \sum_x P(x) \log \frac{P(x)}{Q(x)} \\ &= \mathrm{E}_P \left[\log \frac{1}{Q(x)} - \log \frac{1}{P(x)} \right] \\ &= \underbrace{H_P(Q)}_{\textit{Cross Entropy}} - \underbrace{H(P)}_{\textit{Entropy}}. \end{aligned} \tag{4.18}$$

SOL-82 CH.SOL- 4.16.

One interpretation is the following: the KL-divergence indicates the average number of ***additional bits*** *required for transmission of values $x \in X$ which are distributed according to $P(x)$, but we erroneously encoded them according to distribution $Q(x)$. This makes sense since you have to "pay" for additional bits to compensate for not knowing the true distribution, thus using a code that was optimized according to other distribution. This is one of the reason that the KL-divergence is also known as relative entropy. Formally, the cross entropy has an information interpretation quantifying how many bits are wasted by using the wrong code:*

$$H_P(Q) = \sum_x \underbrace{P(x)}_{\text{Sending } P} \overbrace{\log \frac{1}{Q(x)}}^{\text{code for } Q}. \tag{4.19}$$

SOL-83 CH.SOL- 4.17.

1. ***True*** *KLD is a non-symmetric measure, i.e. $D(P \parallel Q) \neq D(Q \parallel P)$.*
2. ***False*** *KLD does not satisfy the triangle inequality.*
3. ***True*** *KLD is not a distance metric.*
4. ***True*** *KLD is regarded as a measure of the information* ***gain****. Notice that, however, KLD is the* ***amount*** *of information* ***lost****.*
5. ***True*** *The units of KL divergence are units of information (bits, nats, etc.).*
6. ***True*** *KLD is a non-negative measure.*
7. ***True*** *Performing splitting based on highly informative event usually leads to low model generalization and a less accurate one as well.*

SOL-84 CH.SOL- 4.18.

Formally, mutual information attempts to measure how correlated two variables are with each other:

$$\begin{aligned} I(X;Y) &= \sum_{x,y} P(x,y) \log \frac{P(x,y)}{P(x)P(y)} \\ &= \mathrm{E}\left[\log \frac{1}{P(x)} + \log \frac{1}{P(y)} - \log \frac{1}{P(x,y)}\right] \\ &= H(X) + H(Y) - H(X,Y). \end{aligned} \tag{4.20}$$

Regarding the question at hand, given two distributions f_1 and f_2 and their joint distribution f, the mutual information *of f_1 and f_2 is defined as $I(f_1, f_2) = H(f, f_1 f_2)$. If the two distributions are independent, i.e. $f = f_1 \cdot f_2$, the mutual information will vanish. This concept has been widely used as a similarity measure in image analysis.* ■

SOL-85 CH.SOL- 4.19.

The question was commented out but remained here for the consistency of the numbering system. ■

4.3.4 Classification and Information Gain

SOL-86 CH.SOL- 4.20.

The three most widely used methods are:

1.

$$\textit{Entropy}\ (t) = -\sum_{i=0}^{c-1} p(i) \log_2 p(i). \tag{4.21}$$

2.

$$1 - \sum_{i=0}^{c-1} [p(i)]^2 \tag{4.22}$$

3.

$$\textit{Classification error } (t) = 1 - \max_i [p(i)]. \tag{4.23}$$

■

SOL-87 CH.SOL- 4.21.

In a decision tree, the attribute by which we choose to split is the one with ***[maximum]*** *information gain.* ■

SOL-88 CH.SOL- 4.22.

It is clear that the entropy will be ***decreased more*** *by first splitting on Green rather than on Rain.*

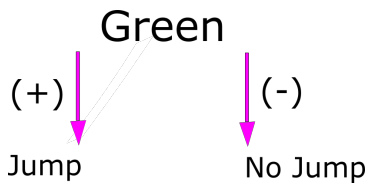


FIGURE 4.12: First split.

■

SOL-89 CH.SOL- 4.23.

1. *Information gain is the expected reduction in entropy caused by partitioning values in a dataset according to a given attribute.*
2. *A decision tree learning algorithm chooses the next attribute to partition the currently selected node, by first computing the information gain from the entropy, for instance, as a splitting criterion.*
3. *There are 3 positive examples corresponding to Shrinkage=+, and 2 negative examples*

corresponding to Shrinkage=-. Using the formulae:

$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i) \tag{4.24}$$

and the probabilities:

$$P(\gamma = +) = \frac{3}{5}, \tag{4.25}$$

$$P(\gamma = -) = \frac{2}{5}, \tag{4.26}$$

the overall entropy before splitting is (4.13):

$$\begin{aligned} E_{orig} &= -(3/5)\log(3/5) - (2/5)\log(2/5) \\ &= H(\gamma) \approx 0.97095[bits/symbol]. \end{aligned} \tag{4.27}$$

```
import autograd.numpy as np
 def binaryEntropy (p):
  return -p*np.log2(p) -(1-p)*np.log2(1-p)

print ("binaryEntropy(p) is:{} bits".format(binaryEntropy(4/7)))
> binaryEntropy(p) is: 0.97095 bits
```

FIGURE 4.13: Entropy before splitting.

4. *If we split on θ_1, (4.5) the relative shrinkage frequency is:*

Total	$\theta_1 = T$	$\theta_1 = F$
⊕	3	0
⊖	1	1

TABLE 4.5: Splitting on θ_1.

To compute the information gain (IG) based on feature θ_1, we must first compute the entropy of γ after a split based on θ_1, $H(\gamma|\theta_1)$:

$$H(\gamma|\theta_1) = -\sum_{j=1}^{v}\left[\sum_{i=1}^{k} P(\gamma=\gamma_i|\theta_1=\theta_j)\log_2 P(\gamma=\gamma_i|\theta_1=\theta_j)\right] P(\theta_1=\theta_j).$$

Therefore, using the data for the the relative shrinkage frequency (4.5), the information gain after splitting on θ_1 is:

$$\begin{aligned} E_{\theta_1=T} &= -\frac{3}{4}\log\frac{3}{4} - \frac{1}{4}\log\frac{1}{4} = 0.8112, \\ E_{\theta_1=F} &= -\frac{0}{1}\log\frac{0}{1} - \frac{1}{1}\log\frac{1}{1} = 0.0. \end{aligned} \tag{4.28}$$

Now we know that $P(\theta_1 = T) = \boxed{4/5}$ and $P(\theta_1 = F) = \boxed{1/5}$, therefore:

$$\begin{aligned} \Delta &= E_{orig} - \boxed{(4/5)}E_{\theta_1=T} - \boxed{(1/5)}E_{\theta_1=F} \\ &= 0.97095 - (4/5) * 0.8112 - (1/5) * (0.0) \\ &=\approx 0.32198 \textit{ [bits/symbol].} \end{aligned} \tag{4.29}$$

■

SOL-90 CH.SOL- 4.24.

There are 4 positive examples corresponding to Expansion=+, and 3 negative examples

corresponding to Expansion=-.

1. *The overall entropy before splitting is (4.14):*

$$\begin{aligned} E_{orig} &= -(4/7)\log(4/7) - (3/7)\log(3/7) \\ &= 0.9852281 \textit{ [bits/symbol].} \end{aligned} \tag{4.30}$$

```
import autograd.numpy as np
 def binaryEntropy (p):
  return -p*np.log2(p) -(1-p)*np.log2(1-p)

print ("binaryEntropy(p) is:{} bits".format(binaryEntropy(4/7)))
> binaryEntropy(p) is:0.9852281 bits
```

FIGURE 4.14: Entropy before splitting.

2. *If we split on θ_1, (4.6) the relative star expansion frequency is:*

Total	$\theta_1 = T$	$\theta_1 = F$
⊕	3	1
⊖	0	3

TABLE 4.6: Splitting on θ_1.

Therefore, the information gain after splitting on A is:

$$\begin{aligned} E_{\theta_1=T} &= -\frac{3}{3}\log\frac{3}{3} - \frac{0}{3}\log\frac{0}{3} = 0.0, \\ E_{\theta_1=F} &= -\frac{3}{4}\log\frac{3}{4} - \frac{1}{4}\log\frac{1}{4} = 0.81127. \end{aligned} \tag{4.31}$$

Now we know that $P(\theta_1 = T) = \boxed{3/7}$ *and* $P(\theta_1 = F) = \boxed{4/7}$*, therefore:*

$$\begin{aligned}\Delta &= E_{orig} - \boxed{(3/7)}E_{\theta_1=T} - \boxed{(4/7)}E_{\theta_1=F} \\ &= 0.98522 - (3/7) * 0.0 - (4/7) * (0.81127) \\ &= 0.52163 \textit{ [bits/symbol].}\end{aligned} \tag{4.32}$$

3. *If we split on* θ_2*, (4.7) the relative star expansion frequency is:*

Total	$\theta_2 = T$	$\theta_2 = F$
+	3	1
-	1	2

TABLE 4.7: Splitting on θ_2.

The information gain after splitting on B is:

$$\begin{aligned}E_{\theta_2=T} &= -\frac{3}{4}\log\frac{3}{4} - \frac{1}{4}\log\frac{1}{4} = 0.0.8112, \\ E_{\theta_2=F} &= -\frac{1}{3}\log\frac{1}{3} - \frac{2}{3}\log\frac{2}{3} = 0.9182.\end{aligned} \tag{4.33}$$

Now we know that $P(\theta_2 = T) = \boxed{4/7}$ *and* $P(\theta_2 = F) = \boxed{3/7}$*, therefore:*

$$\begin{aligned}\Delta &= E_{orig} - \boxed{(4/7)}E_{\theta_2=T} - \boxed{(3/7)}E_{\theta_2=F} \\ &= 0.98522 - (4/7) * 0.8122 - (3/7) * (0.9182) \\ &0.1275 \textit{ [bits/symbol].}\end{aligned}$$

$$\begin{aligned}\Delta &= 0.98522 - (4/7) * 0.8122 - (3/7) * (0.9182) \\ &0.1275 \textit{ [bits/symbol].}\end{aligned} \tag{4.34}$$

■

SOL-91 CH.SOL- 4.25.

1.

$$\begin{aligned} H(\gamma) &= -\left(\frac{2}{6}\log_2\frac{2}{6} + \frac{4}{6}\log_2\frac{4}{6}\right) \\ H(\gamma) &= -\left(\frac{1}{3}\log_2\frac{1}{3} + \frac{2}{3}\log_2\frac{2}{3}\right) \\ &\approx 0.92 \textit{ [bits/symbol].} \end{aligned} \tag{4.35}$$

2.

$$\begin{aligned} H(\gamma|\theta_1) = -\frac{1}{3}\left(\frac{1}{2}\log_2\frac{1}{2} + \frac{1}{2}\log_2\frac{1}{2}\right) - \\ \frac{1}{3}\left(\frac{1}{2}\log_2\frac{1}{2} + \frac{1}{2}\log_2\frac{1}{2}\right) - \frac{1}{3}\left(1\log_2 1\right). \\ H(\gamma|\theta_1) = \frac{1}{3}(1) + \frac{1}{3}(1) + \frac{1}{3}(0). \\ H(\gamma|\theta_1) = \frac{2}{3} \approx 0.66\textit{[bits/symbol].} \end{aligned} \tag{4.36}$$

3.

$$\begin{aligned} H(\gamma|\theta_2) &= -\frac{1}{2}\left(\frac{1}{3}\log_2\frac{1}{3} + \frac{2}{3}\log_2\frac{2}{3}\right) - \frac{1}{2}\left(1\log_2 1\right). \\ H(\gamma|\theta_2) &= \frac{1}{2}\left(\log_2 3 - \frac{2}{3}\right). \\ H(\gamma|\theta_2) &= \frac{1}{2}\log_2 3 - \frac{1}{3} \approx 0.46 \textit{ [bits/symbol].} \end{aligned} \tag{4.37}$$

4. ***False.***

4.3.5 Mutual Information

SOL-92 CH.SOL- 4.26.

1. The diagram is depicted in Fig. 4.15.

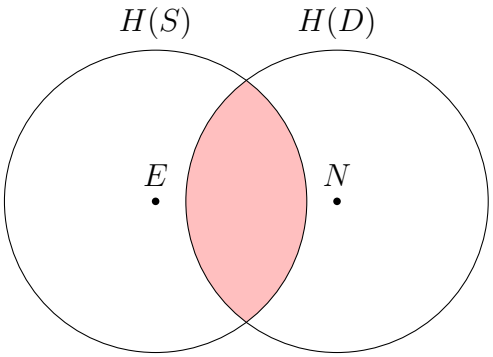


FIGURE 4.15: Mutual Information between $H(S)$ & $H(D)$.

2. ***Equivocation*** *is annotated by* E.
3. ***Noise*** *is annotated by* N.
4. *The intersection (shaded area) in (4.15) corresponds to mutual information of the source* $H(S)$ *and of the destination* $H(D)$.
5. *The formulae for mutual information is:*

$$H(S;D) = H(S) - E = H(D) - N. \tag{4.38}$$

■

SOL-93 CH.SOL- 4.27.

The relative entropy $D(p||q)$ *is the measure of* ***difference*** *between two distributions. It can also be expressed like a measure of the* ***inefficiency*** *of assuming that the distribution is* q *when the* ***true*** *distribution is* p. ■

SOL-94 CH.SOL- 4.28.

Mutual information is a Shannon entropy-based measure of dependence between random variables. The mutual information between X *and* Z *can be understood as the* ***reduction*** *of*

*the **uncertainty** in X given Z:*

$$I(X;Z) := H(X) - H(X \mid Z), \tag{4.39}$$

where H is the Shannon entropy, and $H(X \mid Z)$ is the conditional entropy of Z given X. ■

4.3.6 Mechanical Statistics

SOL-95 CH.SOL- 4.29.
Is this question valuable? ■

SOL-96 CH.SOL- 4.30.
Boltzmann related the degree of disorder of the state of a physical system to the logarithm of its probability. If, for example, the system has n non-interacting and identical particles, each capable of existing in each of K equally likely states, the leading term in the logarithm of the probability of finding the system in a configuration with n_1 particles in state 1, n_2 in state 2, etc, is given by the Boltzmann entropy $\mathcal{H}_\pi = -\sum_1^K \pi_i \log(\pi_i)$, *where $\pi_i = n_i/n$.* ■

SOL-97 CH.SOL- 4.31.
There are 8 equiprobable events in each roll of the dice, therefore:

$$H = -\sum_{i=1}^{8} \frac{1}{8} \log_2 \frac{1}{8} = 3 \text{ [bits]} . \tag{4.40}$$

■

4.3.7 Jensen's inequality

SOL-98 CH.SOL- 4.32.

1. *A function f is concave in the range $[a, b]$ if $f\phi 2$ is negative in the range $[a, b]$.*
2. *A function f is convex in the range $[a, b]$ if $f\phi 2$ is positive in the range $[a, b]$.*

3. *The following inequality was published by J.L. Jensen in 1906:*

   (Jensen's Inequality) *Let f be a function convex up on (a, b). Then for any $n \geq 2$ numbers $x_i \in (a, b)$:*

$$f\left(\frac{\sum_{i=1}^{n} x_i}{n}\right) \leq \frac{\sum_{i=1}^{n} f(x_i)}{n},$$

   and that the equality is attained if and only if f is linear or all x_i are equal.

   For a convex down function, the sign of the inequality changes to $\geq$.

   Jensen's inequality states that if f is convex in the range $[a, b]$, then:

$$\frac{f(a) + f(b)}{2} \geq f\left(\frac{a+b}{2}\right).$$

   Equality holds if and only if $a = b$. Jensen's inequality states that if f is concave in the range $[a, b]$, then:

$$\frac{f(a) + f(b)}{2} \leq f\left(\frac{a+b}{2}\right).$$

   Equality holds if and only if $a = b$.

■

SOL-99 CH.SOL- 4.33.

True *The non-negativity of KLD can be proved using Jensen's inequality.* ■

References

[1] S. Carnot. *Reflections on the Motive Power of Fire: And Other Papers on the Second Law of Thermodynamics*. Dover books on physics. Dover Publications, 2012 (cit. on p. 86).

[2] T. M. Cover and J. A. Thomas. *Elements of Information Theory*. John Wiley and Sons, Inc., 2006 (cit. on p. 86).

[3] B. J. Hiley. 'From the Heisenberg Picture to Bohm: a New Perspective on Active Information and its relation to Shannon Information'. In: *Proc. Conf. Quantum Theory: reconsideration of foundations* (2002), pp. 141–162 (cit. on p. 87).

[4] C. Shannon. 'A mathematical theory of communication'. In: *Bell System Technical Journal* 27 (1948), pp. 379–423 (cit. on pp. 86, 90).

[5] P. Sledzinski et al. 'The current state and future perspectives of cannabinoids in cancer biology'. In: *Cancer Medicine* 7.3 (2018), pp. 765–775 (cit. on p. 96).

CHAPTER 5

DEEP LEARNING: CALCULUS, ALGORITHMIC DIFFERENTIATION

*The true logic of this world is in the **calculus** of probabilities.*

— James C. Maxwell

Contents

5.1 Introduction

ALCULUS is the mathematics of change; the differentiation of a function is key to almost every domain in the scientific and engineering realms and calculus is also very much *central* to DL. A standard curriculum of *first year calculus* includes topics such as limits, differentiation, the derivative, Taylor series, integration, and the integral. Many aspiring data scientists who lack a relevant mathematical background and are shifting careers, hope to easily enter the field but frequently encounter a mental barricade.

$f(x)$	$f'(x)$
$\sin(x)$	$\cos(x)$
$\cos(x)$	$-\sin(x)$
$\log(x)$	$\frac{1}{x}$
e^x	e^x

Thanks to the rapid advances in processing power and the proliferation of GPUs, it is possible to lend the burden of computation to a computer with high efficiency and precision. For instance, extremely fast implementations of backpropagation, the gradient descent algorithm, and *automatic differentiation* (AD) [5] brought artificial intelligence from a mere concept to reality.

Calculus is frequently taught in a way that is very burdensome to the student, therefore I tried incorporating the writing of Python code snippets into the learning process and the usage of:
DAGs (**D**irected **A**cyclic **G**raphs). Gradient descent is the essence of optimization in deep learning, which requires efficient access to first and second order derivatives that AD frameworks provide. While older AD frameworks were written in C++ ([4]), the newer ones are Python-based such as Autograd ([10]) and JAX ([3], [1]).

Derivatives are also crucial in graphics applications. For example, in a rendering technique entitled *global illumination*, photons bounce in a synthetically generated scene while their direction and colour has to be determined using derivatives based on the specific material each photon hits. In ray tracing algorithms, the colour of the pixels is determined by tracing the trajectory the photons travel from the eye of the observer through a synthetic 3D scene.

A function is usually represented by a **DAG**. For instance, one commonly used form is to represent intermediate values as nodes and operations as arcs (5.2). One other commonly used form is to represent not only the values but also the operations as nodes (5.11).

The first representation of a function by a DAG goes back to [7].

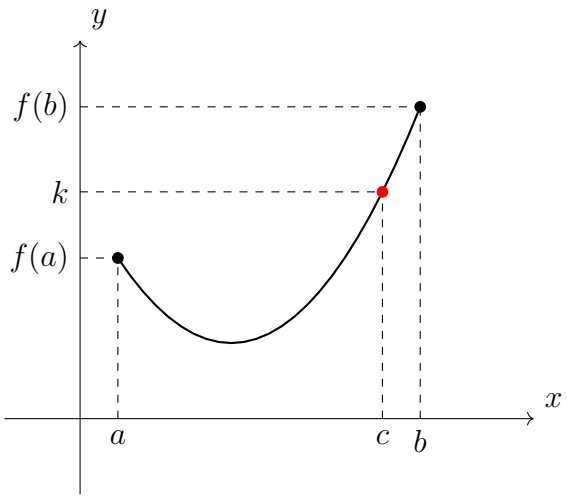


FIGURE 5.1: Intermediate value theorem

Manual differentiation is tedious and error-prone and practically unusable for real-time graphics applications wherein numerous successive derivatives have to be repeatedly calculated. Symbolic differentiation on the other hand, is a computer based method that uses a collection of differentiation rules to analytically calculate an exact derivative of a function resulting in a purely symbolic derivatives. Many symbolic differentiation libraries utilize what is known as *operator-overloading* ([9]) for both the forward and reverse forms of differentiation, albeit they are not quite as fast as AD.

5.2 Problems

5.2.1 AD, Gradient descent & Backpropagation

AD [5] is the application of the chain rule to functions by computers in order to automatically compute derivatives. AD plays a significant role in training deep learning algorithms and in order to understand AD you need a solid grounding in Calculus. As opposed to numerical differentiation, AD is a procedure for establishing **exact** derivatives without any truncation errors. AD breaks a computer program into a series of fundamental mathematical operations, and the gradient or Hessian of the computer program is found by successive application of the chain rule (5.1) to it's elementary constituents.

For instance, in the C++ programming language, two techniques ([4]) are commonly utilized in transforming a program that calculates numerical values of a function into a program which calculates numerical values for derivatives of that function; (1) an operator overloading approach and (2) systematic source code transformation.

$$\frac{\partial}{\partial t} f(g(t))\bigg|_{t=t_0} = \left(\frac{\partial}{\partial s} f(s)\bigg|_{s=g(t_0)}\right)\left(\frac{\partial}{\partial t} g(t)\bigg|_{t=t_0}\right) \tag{5.1}$$

One notable feature of AD is that the values of the derivatives produced by applying AD, as opposed to numerical differentiation (finite difference formulas), are **exact and accurate**. Two variants of AD are widely adopted by the scientific community: the forward mode or the reverse mode where the underlying distinction between them is the order in which the chain rule is being utilized. The forward mode, also entitled tangent mode, propagates derivatives from the dependent towards the independent variables, whereas the reverse or adjoint mode does exactly the opposite. AD makes heavy use of a concept known as dual numbers (DN) first introduced by Clifford ([2]).

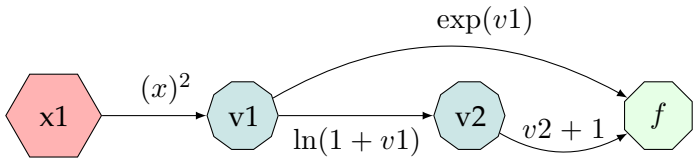


FIGURE 5.2: A Computation graph with intermediate values as nodes and operations as arcs.

5.2.2 Numerical differentiation

PRB-100 ❓ CH.PRB- 5.1.

1. *Write the formulae for the **finite difference rule** used in numerical differentiation.*
2. *What is the main problem with this formulae?*

3. *Indicate one problem with software tools which utilize numerical differentiation and successive operations on floating point numbers.*

PRB-101 ❓ CH.PRB- 5.2.

1. *Given a function $f(x)$ and a point a, define the **instantaneous rate of change** of $f(x)$ at a.*
2. *What other commonly used alternative name does the instantaneous rate of change have?*
3. *Given a function $f(x)$ and a point a, define the **tangent line** of $f(x)$ at a.*

5.2.3 Directed Acyclic Graphs

There are two possible ways to traverse a **DAG** (**D**irected **A**cyclic **G**raph). One method is simple. Start at the bottom and go through all nodes to the top of the computational tree. That is nothing else than passing the corresponding computation sequence top down. Based on this method, the so called forward mode or of AD was developed [8]. In contrast to this forward mode the reverse mode was first used by Speelpenning [13] who passed the underlying graph top down and propagated the gradient backwards.

PRB-102 ❓ CH.PRB- 5.3.

1. *State the definition of the derivative $f(c)$ of a function $f(x)$ at $x = c$.*
2. *With respect to the* **DAG** *depicted in 5.3:*

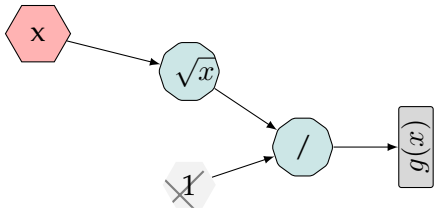


FIGURE 5.3: An expression graph for $g(x)$. Constants are shown in gray, crossed-out since derivatives should not be propagated to constant operands.

(a) Traverse the graph 5.3 and find the function $g(x)$ it represents.

(b) Using the definition of the derivative, find $g'(9)$.

PRB-103 ❓ CH.PRB- 5.4.

1. *With respect to the expression graph depicted in 5.4, traverse the graph and find the function $g(x)$ it represents.*

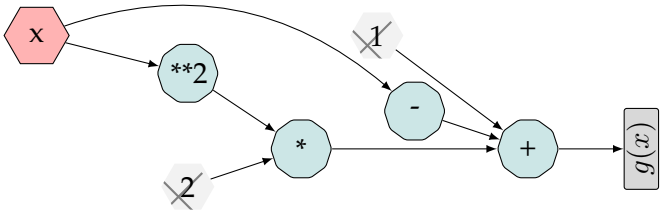


FIGURE 5.4: An expression graph for $g(x)$. Constants are shown in gray, crossed-out since derivatives should not be propagated to constant operands.

2. *Using the definition of the derivative find the derivative of $g(x)$.*

5.2.4 The chain rule

PRB-104 ❓ CH.PRB- 5.5.

1. *The **chain rule** is key concept in differentiation. Define it.*

2. *Elaborate how the chain rule is utilized in the context of neural networks.*

5.2.5 Taylor series expansion

The idea behind a Taylor series is that if you know a function and all its derivatives at one point $x = a$, you can approximate the function at other points near a. As an example, take $f(x) = \sqrt{x}$. You can use Taylor series to approximate $\sqrt{10}$ by knowing $f(9)$ and all the derivatives $f'(9)$, $f''(9)$.

The MacLaurin series (5.2) is a special case of Taylor series when $f(0)$, $f'(0)$ are known:

$$f(x) = f(0) + xf'(0) + \frac{x^2}{2!}f''(0) + \frac{x^3}{3!}f'''(0) + \cdots = \sum_{p=0}^{\infty} \frac{x^p}{p!} f^{(p)}(0) \tag{5.2}$$

For instance, the Maclaurin expansion of $cos(x)$ is:

$$\begin{aligned} f(x) &= \cos x, \quad f'(x) = -\sin x, \\ f''(x) &= -\cos x, \quad f'''(x) = \sin x \end{aligned} \tag{5.3}$$

When evaluated at 0 results in:

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \tag{5.4}$$

PRB-105 ❓ CH.PRB- 5.6.

Find the Taylor series expansion for:

1.

$$\frac{1}{1-x} \tag{5.5}$$

2.

$$e^x \tag{5.6}$$

3.

$$\sin(x) \tag{5.7}$$

4.

$$\cos(x) \tag{5.8}$$

PRB-106 ❓ CH.PRB- 5.7.
Find the Taylor series expansion for:

$$\log(x) \tag{5.9}$$

PRB-107 ❓ CH.PRB- 5.8.
Find the Taylor series expansion centered at $x = -3$ for:

$$f(x) = 5x^2 - 11x + 1 \tag{5.10}$$

PRB-108 ❓ CH.PRB- 5.9.
Find the 101th degree Taylor polynomial centered at $x = 0$ for:

$$f(x) = \cos(x) \tag{5.11}$$

PRB-109 ❓ CH.PRB- 5.10.
At $x = 1$, compute the first 7 terms of the Taylor series expansion of:

$$f(x) = \ln 3x. \tag{5.12}$$

5.2.6 Limits and continuity

Theorem 1 (L'Hopital's rule)**.**

$$[\lim_{x\to a}\frac{f(x)}{g(x)} = \lim_{x\to a}\frac{f'(x)}{g'(x)}]. \tag{5.13}$$

PRB-110 ❓ CH.PRB- 5.11.
Find the following limits:

1. $\lim_{x\to 3}\dfrac{e^{x^3}-e^{27}}{3x-9}$
2. $\lim_{x\to 0}\dfrac{e^{x^2}-x-1}{3\cos x - x - 3}$
3. $\lim_{x\to\infty}\dfrac{x-\ln x}{\sqrt[100]{x}+4}$

5.2.7 Partial derivatives

PRB-111 ❓ CH.PRB- 5.12.

1. ***True or false**: When applying a partial derivative, there are two variables considered constants - the dependent and independent variable.*
2. *Given $g(x,y)$, find its partial derivative with respect to x:*

$$g(x,y) = x^2y + yx + 8y. \tag{5.14}$$

PRB-112 ❓ CH.PRB- 5.13.

The gradient of a two-dimensional function is given by

$$\nabla f(x,y) = \frac{\partial f}{\partial x} i + \frac{\partial f}{\partial y} j \tag{5.15}$$

1. *Find the gradient of the function:*

$$f(x,y) = xy^2 - y^2 + x^3 \tag{5.16}$$

2. *Given the function:*

$$g(x,y) = x^2 y = xy^2 - y - 1, \tag{5.17}$$

evaluate it at $(-1,0)$*, directed at* $(1,1)$*.*

PRB-113 ❓ CH.PRB- 5.14.
Find the partial derivatives of:

$$f(x,y) = 3\sin^2(x-y) \tag{5.18}$$

PRB-114 ❓ CH.PRB- 5.15.
Find the partial derivatives of:

$$z = 2\sin(x)\sin(y) \tag{5.19}$$

5.2.8 Optimization

PRB-115 ❓ CH.PRB- 5.16.
Consider $f(x) = \dfrac{x^2+1}{(x+2)^2}$.

1. *Where is* $f(x)$ *well defined?*

2. *Where is $f(x)$ increasing and decreasing?*

3. *Where is $f(x)$ reaching minimum and maximum values.*

PRB-116 ❓ CH.PRB- 5.17.
Consider $f(x) = 2x^3 - x$.

1. *Derive $f(x)$ and conclude on its behavior.*

2. *Derive once again and discuss the concavity of the function $f(x)$.*

PRB-117 ❓ CH.PRB- 5.18.

Consider the function

$$f(x, y) = 2x^2 - xy + y^2,$$

and find maximum, minimum, and saddle points.

5.2.9 The Gradient descent algorithm

PRB-118 ❓ CH.PRB- 5.19.

The gradient descent algorithm can be utilized for the minimization of convex functions. Stationary points are required in order to minimize a convex function. A very simple approach for finding stationary points is to start at an arbitrary point, and move along the gradient at that point towards the next point, and repeat until converging to a stationary point.

1. *What is the term used to describe the vector of all partial derivatives for a function $f(x)$?*

2. *Complete the sentence: when searching for a minima, if the derivative is positive, the function is **increasing/decreasing**.*

3. *The function x^2 as depicted in 5.5, has a derivative of $f'(x) = 2x$. Evaluated at $x = -1$, the derivative equals $f'(x = -1) = -2$. At $x = -1$, the function is **decreasing** as x gets larger. We will happen if we wish to find a **minima** using gradient descent, and increase (decrease) x by **the size of the gradient**, and then again repeatedly keep jumping?*

4. *How this phenomena can be alleviated?*

5. ***True or False:** The gradient descent algorithm is guaranteed to find a local minimum if the learning rate is correctly decreased and a finite local minimum exists.*

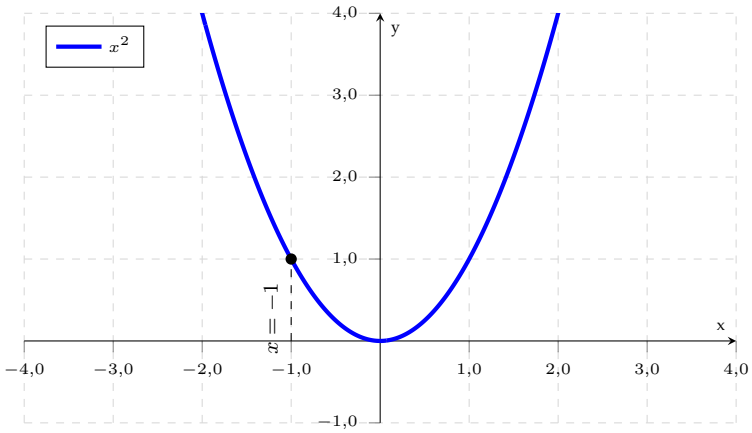


FIGURE 5.5: x^2 Function

PRB-119 ❓ CH.PRB- 5.20.

1. *Is the data linearly separable?*

X_1	X_2	Y
1	1	+
12	12	−
4	5	−
12	12	+

(5.20)

2. *What is loss function for linear regression?*

3. *What is the gradient descent algorithm to minimize a function $f(x)$?*

5.2.10 The Backpropagation algorithm

The most important, expensive and hard to implement part of any hardware realization of ANNs is the non-linear activation function of a neuron. Commonly applied activation functions are the sigmoid and the hyperbolic tangent. In the most used learning algorithm in present day applications, back-propagation, the derivatives of the sigmoid function are needed when back propagating the errors.

The backpropagation algorithm looks for the minimum of the error function in weight space using the method of gradient descent.

PRB-120 ❓ CH.PRB- 5.21.

1. *During the training of an ANN, a sigmoid layer applies the sigmoid function to every element in the forward pass, while in the backward pass the chain rule is being utilized as part of the backpropagation algorithm. With respect to the backpropagation algorithm, given a sigmoid $\sigma(x) = \frac{e^x}{1+e^x}$ activation function, and a J as the cost function, annotate each part of equation (5.21):*

$$dZ = \frac{dJ}{d\sigma(x)}\frac{d\sigma(x)}{dx} = dA \cdot \sigma(x) \cdot \Big(1 - \sigma(x)\Big) \tag{5.21}$$

2. *Code snippet 5.6 provides a pure Python-based (e.g. not using Autograd) implementation of the forward pass for the sigmoid function. Complete the backward pass that directly computes the analytical gradients.*

```
class Sigmoid:
 def forward(self,x):
   self.x = x
   return 1/(1+np.exp(-x))
 def backward(self, grad):
   grad_input = [???]
   return grad_input
```

FIGURE 5.6: Forward pass for the sigmoid function.

PRB-121 ❓ CH.PRB- 5.22.

This question deals with the effect of customized transfer functions. Consider a neural network with hidden units that use x^3 and output units that use $\sin(2x)$ as transfer functions. Using the chain rule, starting from $\partial E/\partial y_k$, derive the formulas for the weight updates Δw_{jk} and Δw_{ij}. Notice - do not include partial derivatives in your final answer.

5.2.11 Feed forward neural networks

Understanding the inner-workings of Feed Forward Neural Networks (FFNN) is crucial to the understanding of other, more advanced Neural Networks such as CNN's.

> A Neural Network (NN) is an interconnected assembly of simple processing elements, *units* or *nodes*, whose functionality is loosely based on the animal neuron. The processing ability of the network is stored in the inter-unit connection strengths, or *weights*, obtained by a process of adaptation to, or *learning* from, a set of training patterns. [6]

The *Backpropagation Algorithm* is the most widely used learning algorithm for FFNN. Backpropagation is a training method that uses the *Generalized Delta Rule*. Its basic idea is to perform a gradient descent on the total squared error of the network output, considered as a function of the weights. It was first described by *Werbos* and made popular by *Rumelhart*'s, *Hinton*'s and *Williams*' paper [12].

5.2.12 Activation functions, Autograd/JAX

Activation functions, and most commonly the sigmoid activation function, are heavily used for the construction of NNs. We utilize Autograd ([10]) and the recently published JAX ([1]) library to learn about the relationship between activation functions and the Backpropagation algorithm.

Using a logistic, or sigmoid, activation function has some benefits in being able to easily take derivatives and then interpret them using a logistic regression model. Autograd is a core module in PyTorch ([11]) and adds inherit support for automatic differentiation for all operations on tensors and functions. Moreover, one can implement his own custom Autograd function by sub classing the autograd *Function* and implementing the forward and backward passes which operate on PyTorch tensors. PyTorch provides a simple syntax (5.7) which is transparent to both CPU/GPU support.

```
import torch
from torch.autograd import Function
class DLFunction(Function):
 @staticmethod
 def forward(ctx, input):
  ...

 @staticmethod
 def backward(ctx, grad_output):
 ...
```

FIGURE 5.7: PyTorch syntax for autograd.

PRB-122 ❓ CH.PRB- 5.23.

1. ***True or false:*** *In Autograd, if any input tensor of an operation has requires_grad=True, the computation will be tracked. After computing the backward pass, a gradient w.r.t. this tensor is accumulated into .grad attribute*

2. ***True or false:*** *In Autograd, multiple calls to backward will sum up previously computed gradients if they are not zeroed.*

PRB-123 ❓ CH.PRB- 5.24.

Your friend, a veteran of the DL community wants to use logistic regression and implement custom activation functions using Autograd. Logistic regression is used when the variable y that we want to predict can only take on discrete values (i.e. classification). Considering a binary classification problem (y = 0 or y = 1) (5.8), the hypothesis function could be defined so that it is bounded between $[0, 1]$ *in which we use some form of logistic function, such as the* ***sigmoid function****. Other, more efficient functions exist such as the* ***ReLU*** *(Rectified Linear Unit) which we discussed later. Note: The weights in (5.8) are only meant for illustration purposes and are not part of the solution.*

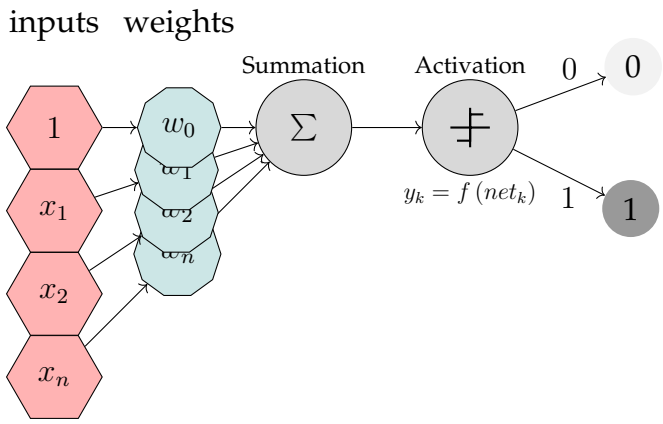


FIGURE 5.8: A typical binary classification problem.

1. *Given the sigmoid function:* $g(x) = \frac{1}{1+e^{-z}}$ *what is the expression for the corresponding hypothesis in logistic regression?*
2. *What is the decision boundary?*
3. *What does* $h_\Theta(x) = 0.8$ *mean?*
4. *Using an Autograd based Python program, implement both the forward and backward pass for the sigmoid activation function and evaluate it's derivative at* $x = 1$

5. *Using an Autograd based Python program, implement both the forward and backward pass for the ReLU activation function and evaluate it's derivative at* $x = 1$

PRB-124 ❓ CH.PRB- 5.25.

For real values, $-1 < x < 1$ *the hyperbolic tangent function is defined as:*

$$\tanh^{-1} x = \frac{1}{2}[\ln(1+x) - \ln(1-x)] \tag{5.22}$$

On the other hand, the artanh function, which returns the ***inverse*** *hyperbolic tangent of its argument x, is implemented in numpy as arctanh().*

Its derivative is given by:

$$(arctanh(x))' = \frac{1}{1-x^2} \tag{5.23}$$

Your friend, a veteran of the DL community wants to implement a custom activation function for the arctanh function using Autograd. Help him in realize the method.

1. *Use this numpy array as an input* $[[0.37, 0.192, 0.571]]$ *and evaluate the result using pure Python.*

2. *Use the PyTorch based* $torch.autograd.Function$ *class to implement a custom Function that implements the forward pass for the arctanh function in Python.*

3. *Use the PyTorch based* $torch.autograd.Function$ *class to implement a custom Function that implements the backward pass for the arctanh function in Python.*

4. *Name the class ArtanhFunction, and using the gradcheck method from torch.autograd, verify that your numerical values equate the analytical values calculated by gradcheck. Remember you must implement a method entitled* $.apply(x)$ *so that the function can be invoked by Autograd.*

5.2.13 Dual numbers in AD

Dual numbers (DN) are analogous to complex numbers and augment real numbers

with a dual element by adjoining an infinitesimal element $\mathbf{d}$, for which $\mathbf{d}^2 = 0$.

PRB-125 ❓ CH.PRB- 5.26.

1. *Explain how AD uses floating point numerical rather than symbolic expressions.*
2. *Explain the notion of DN as introduced by ([2]).*
3. *What arithmetic operations are possible on DN?.*
4. *Explain the relationship between a Taylor series and DN.*

PRB-126 ❓ CH.PRB- 5.27.

1. *Expand the following function using DN:*

$$\sin(x + \dot{x}\mathbf{d}) \tag{5.24}$$

2. *With respect to the expression graph depicted in 5.9:*

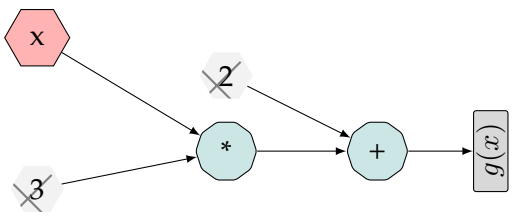


FIGURE 5.9: An expression graph for $g(x)$. Constants are shown in gray, crossed-out since derivatives should not be propagated to constant operands.

   (a) *Traverse the graph 5.9 and find the function $g(x)$ it represents.*
   (b) *Expand the function $g(x)$ using DN.*

3. *Show that the general identity:*

$$g(x + \dot{x}\mathbf{d}) = g(x) + g'(x)\dot{x}\mathbf{d} \tag{5.25}$$

holds in this particular case too.

4. *Using the derived DN, evaluate the function $g(x)$ at $x = 2$.*
5. *Using an Autograd based Python program implement the function and evaluate it's derivative at $x = 2$.*

PRB-127 ❓ CH.PRB- 5.28.

With respect to the expression graph depicted in 5.10:

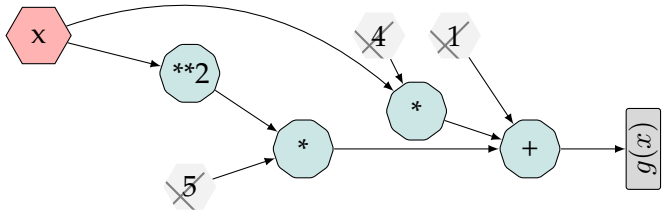


FIGURE 5.10: An expression graph for $g(x)$. Constants are shown in gray, crossed-out since derivatives should not be propagated to constant operands.

1. *Traverse the graph 5.10 and find the function $g(x)$ it represents.*
2. *Expand the function $g(x)$ using DN.*
3. *Using the derived DN, evaluate the function $g(x)$ at $x = 5$.*
4. *Using an AutoGrad based Python program implement the function and evaluate it's derivative at $x = 5$.*

5.2.14 Forward mode AD

PRB-128 ❓ CH.PRB- 5.29.

When differentiating a function using forward-mode AD, the computation of such an expression can be computed from its corresponding directed a-cyclical graph by propagating the numerical values.

1. *Find the function, $g(A, B, C)$ represented by the expression graph in 5.11.*

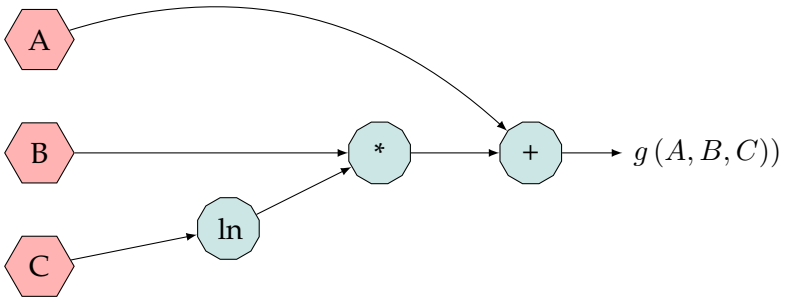


FIGURE 5.11: A computation graph for $g(x)$

2. *Find the partial derivatives for the function $g(x)$.*

PRB-129 ❓ CH.PRB- 5.30.

Answer the following given that a computational graph of a function has N inputs and M outputs.

1. ***True or False**?:*
   (a) *Forward and reverse mode AD always yield the same result.*
   (b) *In reverse mode AD there are fewer operations (time) and less space for intermediates (memory).*
   (c) *The cost for forward mode grows with N.*
   (d) *The cost for reverse mode grows with M.*

PRB-130 ❓ CH.PRB- 5.31.

1. *Transform the source code in code snippet 5.1 into a function $g(x_1, x_2)$.*

CODE 5.1: A function, $g(x_1, x_2)$ in the C programming language.

```
float g( float x1 , float x2) {
 float v1, v2, v3 , v4 , v5;
 v1=x1;
 v2=x2;
 v3 = v1 * v2;
 v4 = ln (v1 );
 v5 = v3 + v4;
 return v5;
}
```

2. *Transform the function $g(x_1, x_2)$ into an expression graph.*
3. *Find the partial derivatives for the function $g(x_1, x_2)$.*

5.2.15 Forward mode AD table construction

PRB-131 ❓ CH.PRB- 5.32.

1. *Given the function:*

$$f(x_1, x_2) = x_1 x_2 + ln(x_1) \tag{5.26}$$

and the graph 5.1, annotate each vertex (edge) of the graph with the partial derivatives that would be propagated in forward mode AD.

2. *Transform the graph into a **table** that computes the **function**: $g(x_1, x_2)$ evaluated at $(x1; x2) = (e^2; \pi)$ using forward-mode AD.*
3. *Write and run a Python code snippet to prove your results are correct.*
4. *Describe the role of **seed values** in forward-mode AD.*

5. *Transform the graph into a **table** that computes the **derivative** of $g(x_1, x_2)$ evaluated at $(x1; x2) = (e^2; \pi)$ using forward-mode AD for x_1 as the chosen independent variable.*

6. *Write and run a Python code snippet to prove your results are correct.*

5.2.16 Symbolic differentiation

In this section, we introduce the basic functionality of the SymPy (SYMbolic Python) library commonly used for symbolic mathematics as a means to deepen your understanding in both Python and calculus. If you are using Sympy in a Jupyter notebook in Google Colab (e.g. https://colab.research.google.com/) then rendering sympy equations requires MathJax to be available within each cell output. The following is a hook function that will make this possible:

CODE 5.2: Sympy in Google Colab

```
from IPython.display import Math, HTML
def enable_sympy_in_cell():
display(HTML("<script
 ↪  src='https://cdnjs.cloudflare.com/ajax/libs/"
"mathjax/2.7.3/latest.js?config=default'>
</script>"))
get_ipython().events.register('pre_run_cell',
 ↪  enable_sympy_in_cell)
```

After successfully registering this hook, SymPy rendering (5.3) will work correctly:

CODE 5.3: Rendering Sympy in Google Colab

```
import sympy
from sympy import *
init_printing()
x, y, z = symbols('x y z')
Integral(sqrt(1/x), (x, 0, oo))
```

It is also recommended to use the latest version of Sympy:

CODE 5.4: Updating Sympy

```
> pip install --upgrade sympy
```

5.2.17 Simple differentiation

PRB-132 ❓ CH.PRB- 5.33.
Answer the following questions:

1. *Which differentiation method is inherently prone to rounding errors?*
2. *Define the term symbolic differentiation.*

PRB-133 ❓ CH.PRB- 5.34.
Answer the following questions:

1. *Implement the sigmoid function* $\sigma(x) = \frac{1}{1+e^{-x}}$ *symbolically using a Python based SymPy program.*
2. *Differentiate the sigmoid function using SymPy and compare it with the analytical derivation* $\sigma'(x) = \sigma(x)(1 - \sigma(x))$.
3. *Using SymPy, evaluate the gradient of the sigmoid function at* $x = 0$.
4. *Using SymPy, plot the resulting gradient of the sigmoid function.*

5.2.18 The Beta-Binomial model

PRB-134 ❓ CH.PRB- 5.35.

You will most likely not be given such a long programming task during a face-to-face interview. Nevertheless, an extensive home programming assignment is typically given at many of the start-ups I am familiar with. You should allocate around approximately four to six hours to completely answer all questions in this problem.

We discussed the Beta-Binomial model extensively in chapter 3. Recall that the Beta-Binomial distribution is frequently used in Bayesian statistics to model the number of successes in n trials. We now employ SymPy to do the same; demonstrate computationally how a prior distribution is updated to develop into a posterior distribution after observing the data via the relationship of the Beta-Binomial distribution.

Provided the probability of success, the number of successes after n trials follows a binomial distribution. Note that the beta distribution is a conjugate prior for the parameter of the binomial distribution. In this case, the likelihood function is binomial, and a beta prior distribution yields a beta posterior distribution.

Recall that for the Beta-Binomial distribution the following relationships exist:

Prior of θ	*Beta(a,b)*
Likelihood	*binomial (n, θ)*
Posterior of θ	*Beta $(a + x, b + n - x)$*
Posterior Mean	$(a + x)/(a + b + n - x)$

(5.27)

1. *Likelihood: The starting point for our inference problem is the Likelihood, the probability of the **observed** data. Find the Likelihood function symbolically using sympy. Convert the SymPy representation to a purely Numpy based callable function with a Lambda expression. Evaluate the Likelihood function at $\theta = 0.5$ with 50 successful trials out of 100.*

2. *Prior: The Beta Distribution. Define the Beta distribution which will act as our **prior** distribution symbolically using sympy. Convert the SymPy representation to a purely Numpy based callable function. Evaluate the Beta Distribution at $\theta : 0.5, a : 2, b : 7$*

3. *Plot the Beta distribution, using the Numpy based function.*

4. *Posterior: Find the **posterior** distribution by multiplying our Beta prior by the Binomial Likelihood symbolically using sympy. Convert the SymPy representation to*

a purely Numpy based callable function. Evaluate the Posterior Distribution at $\theta : 0.5, a : 2, b : 7$

5. *Plot the posterior distribution, using the Numpy based function.*

6. *Show that the posterior distribution has the same functional dependence on* θ *as the prior, and it is just* ***another Beta distribution****.*

7. *Given:*
   Prior : $\text{Beta}(\theta|a = 2, b = 7) = 56\theta\,(-\theta + 1)^6$ *and:*
   Likelihood : $\text{Bin}(r = 3|n = 6, \theta) = 19600\theta^3\,(-\theta + 1)^{47}$ *find the resulting posterior distribution and plot it.*

5.3 Solutions

5.3.1 Algorithmic differentiation, Gradient descent

5.3.2 Numerical differentiation

SOL-100 CH.SOL- 5.1.

1. *The formulae is:*

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}. \tag{5.28}$$

2. *The main problem with this formulae is that it suffers from numerical instability for small values of* h*.*

3. *In some numerical software systems, the number* $\sqrt{2}$ *may be represented as the a floating point number* ≈ 1.414213562*. Therefore, the result of:*
   $float\left(\sqrt{(2)}\right) * float\left(\sqrt{(2)}\right)$ *may equal* ≈ 2.000000446*.*

■

SOL-101 CH.SOL- 5.2.

1. *The instantaneous rate of change equals:*

$$\lim_{h \to 0} \frac{f(a+h) - f(a)}{a+h-a}. \tag{5.29}$$

2. *The instantaneous rate of change of $f(x)$ at a is also commonly known as the tangent line of $f(x)$ at a.*

3. *Given a function $f(x)$ and a point a, the tangent (Fig. 5.12) line of $f(x)$ at a is a line that touches $f(a)$ but does not cross $f(x)$ (sufficiently close to a).*

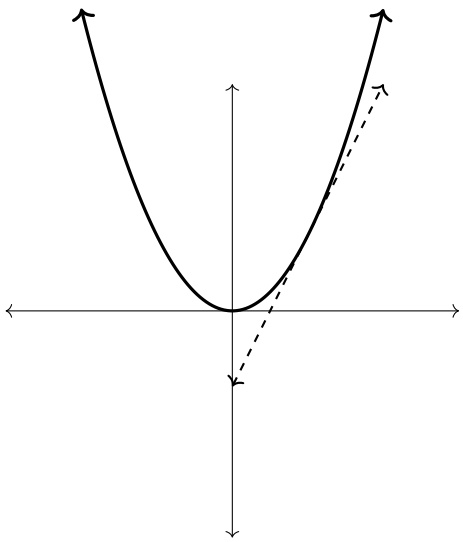


FIGURE 5.12: A Tangent line

5.3.3 Directed Acyclic Graphs

SOL-102 CH.SOL- 5.3.

1. *The definition is:*

$$f'(c) = \lim_{h \to 0} \frac{f(c+h) - f(c)}{h}.$$

2. *If we traverse the graph 5.3 from left to right we derive the following function:*

$$g(x) = \frac{1}{\sqrt{x}}. \tag{5.30}$$

$$\begin{aligned}
f'(9) &= \lim_{h \to 0} \frac{1/\sqrt{9+h} - 1/\sqrt{9}}{h} \\
&= \lim_{h \to 0} \frac{\sqrt{9} - \sqrt{9+h}}{\sqrt{9} \cdot \sqrt{9+h} \cdot h} \\
&= \lim_{h \to 0} \frac{(3 - \sqrt{9+h})(3 + \sqrt{9+h})}{3\sqrt{9+h} \cdot (3 + \sqrt{9+h}) \cdot h} \\
&= \lim_{h \to 0} \frac{9 - (9+h)}{9\sqrt{9+h} \cdot h + 3 \cdot (9+h) \cdot h} \\
&= -\frac{1}{9 \cdot 3 + 3 \cdot 9} \\
&= -\frac{1}{54}
\end{aligned}$$

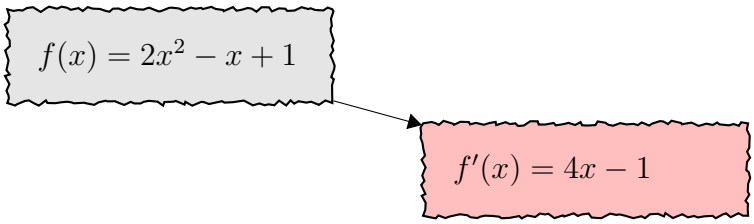
■

SOL-103 CH.SOL- 5.4.

1. *The function $g(x) = 2x^2 - x + 1$ represents the expression graph depicted in 5.4.*

2. *By the definition:*

$$\begin{aligned} f'(x) &= \lim_{h\to 0} \frac{f(x+h)-f(x)}{x+h-x} \\ &= \lim_{h\to 0} \frac{2(x+h)^2-(x+h)+1-2x^2+x-1}{h} \\ &= \lim_{h\to 0} \frac{2(x^2+2xh+h^2)-x-h+1-2x^2+x-1}{h} \\ &= \lim_{h\to 0} \frac{2x^2+4xh+2h^2-x-h+1-2x^2+x-1}{h} \\ &= \lim_{h\to 0} \frac{4xh+2h^2-h}{h} \\ &= \lim_{h\to 0} 4x+2h-1 \\ &= 4x-1. \end{aligned} \tag{5.31}$$



5.3.4 The chain rule

SOL-104 CH.SOL- 5.5.

1. *The chain rule states that the partial derivative of $E = E(x, y)$ with respect to x can be calculated via another variable $y = y(x)$, as follows:*

$$\frac{\partial E}{\partial x} = \frac{\partial E}{\partial y} \cdot \frac{\partial y}{\partial x} \tag{5.32}$$

2. *For instance, the chain rule [8] is applied in neural networks to calculate the change in*

its weights resulting from tuning the cost function. This derivative is calculated via a chain of partial derivatives (e.g. of the activation functions).

■

5.3.5 Taylor series expansion

SOL-105 CH.SOL- 5.6.

1.

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n = 1 + x + x^2 + x^3 \quad (\textit{when } -1 < x < 1) \tag{5.33}$$

2.

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \tag{5.34}$$

3.

$$\sin x = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots \tag{5.35}$$

4.

$$\cos x = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n} = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots \tag{5.36}$$

■

SOL-106 CH.SOL- 5.7.

$$\log x = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}\,(x-1)^n}{n} = (x-1) - \frac{(x-1)^2}{2} + \frac{(x-1)^3}{3} - \frac{(x-1)^4}{4} + \cdots \tag{5.37}$$

■

SOL-107 CH.SOL- 5.8.

In this case, all derivatives can be computed:

$$\begin{aligned} f^0(x) &= 5x^2 - 11x + 1, \\ f^0(-3) &= 79, \\ f^1(x) &= 10x - 11, \\ f^1(-3) &= -41, \\ f^2(x) &= 10, \\ f^2(-3) &= 10, \\ f^n(x) &= 0,\ \forall n \geq 3. \end{aligned} \tag{5.38}$$

■

SOL-108 CH.SOL- 5.9.

The immediate answer is 1. Refer to eq. 5.36 to verify this logical consequence. ■

SOL-109 CH.SOL- 5.10.

By employing eq. 5.37, one can substitute x by $3 - x$ and generate the first 7 terms of the x-dependable outcome before assigning the point $x = 1$.

■

5.3.6 Limits and continuity

SOL-110 CH.SOL- 5.11.

1. *With an indeterminate form* $0/0$*, L'Hopital's rule holds. We look at*

$$\lim_{x\to 3} \frac{3x^2 e^{x^3}}{3} = 9e^{27},$$

which equals to the original limit.

2. *Again, we yield* $0/0$ *at interim, so we look at the first order derivative*

$$\lim_{x\to 0} \frac{2xe^x - 1}{-3\sin x - 1} = 1.$$

The original limit is also equal to 1*.*

3. *This time, the intermediate form is of* ∞/∞ *and L'Hopital applies as well. The quotient of the derivatives is*

$$\frac{1 - \frac{1}{x}}{0.01x^{-99/100}} = 100(x-1)x^{1/99}$$

As $x \to \infty$*, this goes to* ∞*, so the original limit is equal to* ∞ *also.*

■

5.3.7 Partial derivatives

SOL-111 CH.SOL- 5.12.

1. *True.*

2. *By treating* y *as constant, one can derive that*

$$\frac{\partial g}{\partial x} = 2xy + y. \tag{5.39}$$

■

SOL-112 CH.SOL- 5.13.

1.

$$\begin{aligned}\boldsymbol{\nabla} f(x,y) &= \frac{\partial f}{\partial x}\boldsymbol{i} + \frac{\partial f}{\partial y}\boldsymbol{j} \\ &= \left(y^2 + 3x^2\right)\boldsymbol{i} + (2xy - 2y)\,\boldsymbol{j}\end{aligned} \tag{5.40}$$

2. *It can be shown that* $\nabla g(x,y) = (2xy + y^2)\,\boldsymbol{i} + (x^2 + 2xy - 1)\,\boldsymbol{j}$ *at* $(-1,0)$ *equals* $(0,0)$. *According to the definition of directional derivative:*

$$\frac{(0,0)\cdot(1,1)}{|(1,1)|} = 0 \tag{5.41}$$

■

SOL-113 CH.SOL- 5.14.

$$\begin{aligned}\frac{\partial f}{\partial x} &= 6\sin(x-y)\cos(x-y) \\ \frac{\partial f}{\partial y} &= -6\sin(x-y)\cos(x-y)\end{aligned} \tag{5.42}$$

■

SOL-114 CH.SOL- 5.15.

$$\begin{aligned}\frac{\partial z}{\partial x} &= 2\cos x \sin y \\ \frac{\partial z}{\partial y} &= 2\sin x \cos y\end{aligned} \tag{5.43}$$

■

5.3.8 Optimization

SOL-115 CH.SOL- 5.16.

1. *The function is only defined where* $x \neq -2$, *in the domain of:* $(-\infty, -2) \cup (-2, +\infty)$.

2. *By a simple quotient-based derivation:*

$$f'(x) = \frac{2(x+2)(2x-1)}{(x+2)^4}. \tag{5.44}$$

   Namely, expect for the ill-defined $x = -2$, *the critical point of* $x = 0.5$ *should be considered. For* $x > 0.5$, *the derivative is positive and the function increases, in contrast to* $x < 0.5$.

3. *The requested coordinate is* $(0.5, 0.2)$.

■

SOL-116 CH.SOL- 5.17.

1. $f'(x) = 6x^2 - 1$, *which entails the behavior of the function changes around the points* $x = \pm\frac{1}{\sqrt{6}}$. *The derivative is negative between* $x = -\frac{1}{\sqrt{6}}$ *and* $x = \frac{1}{\sqrt{6}}$, *i.e., it decreases in the domain, and increases otherwise.*

2. *The second derivative is* $f''(x) = 12x$, *which means the function is concave for negative* x *values and convex otherwise.*

■

SOL-117 CH.SOL- 5.18.

The function should be derived according to each variable separately and be equated to 0, as follows:

$$f_x(x, y) = 4x - y = 0\,, \quad f_y(x, y) = -y + 2y = 0\,.$$

So, the solution to these equations yield the coordinate $(0, 0)$, *and* $f(0, 0) = 0$.

Let us derive the second order derivative, as follows:

$$\frac{\partial^2 f}{\partial x^2}(x, y) = 4\,, \ \frac{\partial^2 f}{\partial y^2}(x, y) = 2\,, \ \frac{\partial^2 f}{\partial x \partial y}(x, y) = -1\,,$$

Also, the following relation exists:

$$D(x,y) = \frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2 = 7\,,$$

Thus, the critical point $(0,0)$ *is a minimum.* ■

5.3.9 The Gradient descent algorithm

SOL-118 CH.SOL- 5.19.

1. *It is the gradient of a function which is mathematically represented by:*

$$\nabla f(x,y) = \begin{pmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} \end{pmatrix} \tag{5.45}$$

2. *Increasing.*
3. *We will keep jumping between the same two points without ever reaching a minima.*
4. *This phenomena can be alleviated by using a* ***learning rate or step size****. For instance,* $x+ = 2 * \eta$ *where* η *is a learning rate with small value such as* $\eta = 0.25$*.*
5. *True.*

■

SOL-119 CH.SOL- 5.20.

1. *The point (12,12) has two classes, so the classes cannot be separated by any line.*
2.

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2 \tag{5.46}$$

3. *Simple but fundamental algorithm for minimizing f. Just repeatedly move in the direction of the negative gradient*
   (a) *Start with initial guess $\theta^{(0)}$, step size η*
   (b) *For $k = 1, 2, 3, \ldots$:*
      i. *Compute the gradient $\nabla f(\theta^{(k-1)})$*
      ii. *Check if gradient is close to zero; is so stop, otherwise continue*
      iii. *Update $\theta^{(k)} = \theta^{(k-1)} - \eta \nabla f(\theta^{(k-1)})$*
   (c) *Return final $\theta^{(k)}$ as approximate solution θ^**

5.3.10 The Backpropagation algorithm

SOL-120 CH.SOL- 5.21.

1. *The annotated parts of equation (5.21) appear in (5.47):*

$$\begin{aligned} \sigma(x) = \frac{e^x}{1+e^x} &= \textit{The Sigmoid activation function} \\ &\sigma(x) \cdot \Big(1 - \sigma(x)\Big) \\ \textit{The deriviative of the Sigmoid activation function} &= \\ 1Z &= \textit{The input} \\ dZ &= \textit{The error introduced by input } Z. \\ A &= \textit{The output} \\ dA &= \textit{The error introduced by output } A. \end{aligned} \tag{5.47}$$

2. *Code snippet 5.13 provides an implementation of both the forward and backward passes for the sigmoid function.*

```python
class Sigmoid:
 def forward(self,x):
  self.x = x
  return 1/(1+np.exp(-x))

 def backward(self, grad):
  grad_input = self.x*(1-self.x) * grad
  return grad_input
```

FIGURE 5.13: Forward and backward passes for the sigmoid activation function in pure Python.

SOL-121 CH.SOL- 5.22.

The key concept in this question is merely understanding that the transfer function and ***its derivatives*** *are changing compared to traditional activation functions, namely:*

$$\frac{\partial E}{\partial y_k} = (y_k - d_k) \tag{5.48}$$

$$\frac{\partial E}{\partial net_k} = \frac{\partial E}{\partial y_k} \cdot \frac{\partial y_k}{\partial net_k} = (y_k - d_k) \cdot 2\cos(2net_k) \tag{5.49}$$

$$\Delta w_{jk} = -\eta \frac{\partial E}{\partial w_{jk}} = -\eta \frac{\partial E}{\partial net_k} \cdot \frac{\partial net_k}{\partial w_{jk}} = -\eta \cdot (y_k - d_k) \cdot 2\cos(2net_k) \cdot y_j \tag{5.50}$$

$$\frac{\partial E}{\partial y_j} = \sum_k \left(\frac{\partial E}{\partial net_k} \cdot \frac{\partial net_k}{\partial y_j} \right) = \sum_k \left(\frac{\partial E}{\partial net_k} w_{jk} \right) \tag{5.51}$$

$$\frac{\partial E}{\partial net_j} = \frac{\partial E}{\partial y_j} \cdot \frac{\partial y_j}{\partial net_j} = \frac{\partial E}{\partial y_j} \cdot 3net_j^2 \tag{5.52}$$

$$\begin{aligned} \Delta w_{ij} &= -\eta \frac{\partial E}{\partial w_{ij}} \\ &= -\eta \frac{\partial E}{\partial net_j} \cdot \frac{\partial net_j}{\partial w_{ij}} \\ &= -\eta \cdot (\textstyle\sum_k [(y_k - d_k) \cdot 2\cos(2net_k) \cdot w_{jk}]) \cdot 3net_j^2 \cdot y_i \end{aligned} \tag{5.53}$$

■

5.3.11 Feed forward neural networks

5.3.12 Activation functions, Autograd/JAX

SOL-122 CH.SOL- 5.23.

1. *True.*
2. *True.*

■

SOL-123 CH.SOL- 5.24.

The answers are as follows:

1. $h_\Theta(x) = g(\Theta^T x) = \frac{1}{1+e^{-\Theta^T x}}$.
2. *The decision boundary for the logistic sigmoid function is where* $h_\Theta(x) = 0.5$ *(values less than 0.5 mean false, values equal to or more than 0.5 mean true).*
3. *That there is a 80% chance that the instance is of the corresponding class, therefore:*
   - $h_\Theta(x) = g(\Theta_0 + \Theta_1 x_1 + \Theta_2 x_2)$. *We can predict* $y = 1$ *if* $x_0 + x_1 + x_2 \geq 0$.
4. *The code snippet in 5.14 implements the function using Autograd.*

```python
from torch.autograd import Function
class Sigmoid(Function):
 @staticmethod
 def forward(ctx, x):
  output = 1 / (1 + torch.exp(-x))
  ctx.save_for_backward(output)
  return output

 @staticmethod
 def backward(ctx, grad_output):
  output,  = ctx.saved_tensors
  grad_x = output * (1 - output) * grad_output
  return grad_x
```

FIGURE 5.14: Forward and backward for the sigmoid function in Autograd.

5. *The code snippet in 5.15 implements the function using Autograd.*

```python
from torch.autograd import Function
class ReLU(torch.autograd.Function):
 @staticmethod
 def forward(ctx, input):
  ctx.save_for_backward(input)
  return input.clamp(min=0)

 @staticmethod
 def backward(ctx, grad_output):
  input, = ctx.saved_tensors
  grad_input = grad_output.clone()
  grad_input[input < 0] = 0
  return grad_input
```

FIGURE 5.15: Forward and backward for the ReLU function in Autograd.

SOL-124 CH.SOL- 5.25. *The answers are as follows:*

1. *Code snippet 5.16 implements the forward pass using pure Python.*

```
import numpy as np
xT = torch.abs(torch.tensor([[0.37,0.192,0.571]],
requires_grad=True)).type(torch.DoubleTensor)
xT_np=xT.detach().cpu().numpy()
print ("Input: \n",xT_np)
arctanh_values = np.arctanh(xT_np)
print ("Numpy:", arctanh_values)
> Numpy: [[0.38842311 0.1944129  0.64900533]]
```

FIGURE 5.16: Forward pass for equation (5.23) using pure Python.

2. *Code snippet 5.17 implements the forward pass using Autograd.*

```
import torch
from torch.autograd import Function
class ArtanhFunction(Function):
 @staticmethod
 def forward(ctx, x):
  ctx.save_for_backward(x)
  r = (torch.log_(1 + x).sub_(torch.log_(1 - x))).mul_(0.5)
  return r
```

FIGURE 5.17: Forward pass for equation (5.23).

3. *Code snippet 5.18 implements the backward pass using Autograd.*

```
from torch.autograd import Function
class ArtanhFunction(Function):
@staticmethod
 input, = ctx.saved_tensors
 out= grad_output / (1 - input ** 2)
 print ("backward:{}".format(out))
 return out
```

FIGURE 5.18: Backward pass for equation (5.23).

4. *Code snippet 5.19 verifies the correctness of the implementation using gradcheck.*

```
import numpy as np

xT =
 ↪  torch.abs(torch.tensor([[0.11,0.19,0.57]],requires_grad=True))
.type(torch.DoubleTensor)
arctanh_values_torch = arctanhPyTorch(xT)
print ("Torch:", arctanh_values_torch)
from torch.autograd import gradcheck, Variable
f = ArtanhFunction.apply
test=gradcheck(lambda t: f(t), xT)
print(test)

> PyTorch version: 1.7.0
> Torch: tensor([[0.3884, 0.1944, 0.6490]], dtype=torch.float64,
>    grad_fn=<ArtanhFunctionBackward>)
> backward:tensor([[1.1586, 1.0383,1.4838]], dtype=torch.float64,
       grad_fn=<CopyBackwards>)
```

FIGURE 5.19: Invoking arctanh using gradcheck

5.3.13 Dual numbers in AD

SOL-125 CH.SOL- 5.26.

The answers are as follows:

1. *The procedure of AD is to use verbatim text of a computer program which calculates a numerical value and to transform it into the text of a computer program called the transformed program which calculates the desired derivative values. The transformed computer program carries out these derivative calculations by repeated use of the chain rule however applied to* ***actual floating point values*** *rather than to a symbolic representation.*

2. *Dual numbers extend all numbers by adding a second component* $x \mapsto x + \dot{x}\mathbf{d}$ *where* $x + \dot{x}$ *is the* ***dual part****.*

3. *The following arithmetic operations are possible on DN:*

   (a) $\mathbf{d}^2 = 0$

   (b) $(x + \dot{x}\mathbf{d}) + (y + \dot{y}\mathbf{d}) = x + y + (\dot{x} + \dot{y})\mathbf{d}$

   (c) $-(x + \dot{x}\mathbf{d}) = -x - \dot{x}\mathbf{d}$

   (d) $\frac{1}{x+\dot{x}d} = \frac{1}{x} - \frac{\dot{x}}{x^2}d$

4. *For* $f(x + \dot{x}\mathbf{d})$ *the Taylor series expansion is:*

$$f(x + \dot{x}\mathbf{d}) = f(x) + \frac{f'(x)}{1!}\dot{x}\mathbf{d} + \ldots 0 \tag{5.54}$$

The immediate and important result is that all higher-order terms $(n >= 2)$ ***disappear*** *which provides closed-form mathematical expression that represents a function and its derivative.*

SOL-126 CH.SOL- 5.27.

The answers are as follows:

1.

$$\sin(x + \dot{x}\mathbf{d}) = \sin(x) + \cos(x)\dot{x}\mathbf{d} \tag{5.55}$$

2. *If we traverse the graph 5.9 from left to right we drive the following simple function:*

$$g(x) = 3 * x + 2 \tag{5.56}$$

3. *We know that:*

$$g(x) = 3 * x + 2 \tag{5.57}$$

$$g'(x) = 3 \tag{5.58}$$

Now if we expand the function using DN:

$$g(x + \dot{x}\mathbf{d}) = 3 * (x + \dot{x}\mathbf{d}) + 2 = \tag{5.59}$$
$$3 * x + 3 * (\dot{x}\mathbf{d}) + 2 \tag{5.60}$$

Rearranging:

$$3 * x + 2 + 3 * (\dot{x}\mathbf{d}) \tag{5.61}$$

But since $g(x) = 3 * x + 2$ then:

$$g(x + \dot{x}\mathbf{d}) = g(x) + g'(x)\dot{x}\mathbf{d} \tag{5.62}$$

4. *Evaluating the function $g(x)$ at $x = 2$ using DN we get:*

$$g(x = 2) = (3 * 2 + 2) + (3)\dot{x}\mathbf{d} = \tag{5.63}$$
$$8 + (3)\dot{x}\mathbf{d} \tag{5.64}$$

5. *The code snippet in 5.20 implements the function using Autograd.*

```python
import autograd.numpy as np
from autograd import grad
x = np.array([2.0], dtype=float)
def f1(x):
 return 3*x + 2
grad_f1 = grad(f1)
print(f1(x)) # > 8.0
print(grad_f1(x)) # > 3.0
```

FIGURE 5.20: Autograd

SOL-127 CH.SOL- 5.28. *The answers are as follows:*

1. *If we traverse the graph 5.9 from left to right we drive the following function:*

$$g(x) = 5 * x^2 + 4 * x + 1 \tag{5.65}$$

2. *We know that:*

$$g(x_1) = 5 * x^2 + 4 * x + 1 \tag{5.66}$$

$$g'(x_1) = 10 * x_1 + 4 \tag{5.67}$$

Now if we expand the function using DN we get:

$$g(x + \dot{x}\mathbf{d}) = 5 * (x + \dot{x}\mathbf{d})^2 + 4 * (x + \dot{x}\mathbf{d}) + 1 = \tag{5.68}$$

$$5 * (x^2 + 2 * x + \dot{x}\mathbf{d} + (\dot{x}\mathbf{d})^2) + 4 * x + 4 * (\dot{x}\mathbf{d}) + 1 \tag{5.69}$$

However by definition $(\mathbf{d}^2) = 0$ *and therefore that term vanishes. Rearranging the terms:*

$$(5 * x^2 + 4 * x + 1) + (10 * x + 4)\dot{x}\mathbf{d} \tag{5.70}$$

But since $g(x) = (5 * x^2 + 4 * x + 1)$ *then:*

$$g(x + \dot{x}\mathbf{d}) = g(x) + g'(x)\dot{x}\mathbf{d} \tag{5.71}$$

3. *Evaluating the function* $g(x)$ *at* $x = 5$ *using DN we get:*

$$g(x = 4) = (5 * 5^2 + 4 * 5 + 1) + (10 * 5 + 4)\dot{x}\mathbf{d} = 146 + (54)\dot{x}\mathbf{d} \tag{5.72}$$

4. *The code snippet in 5.21 implements the function using Autograd.*

```
import autograd.numpy as np
from autograd import grad
x = np.array([5.0], dtype=float)
def f1(x):
 return 5*x**2 + 4*x +1
grad_f1 = grad(f1)
print(f1(x)) # > 146.0
print(grad_f1(x)) # > 54.0
```

FIGURE 5.21: Autograd

■

5.3.14 Forward mode AD

SOL-128 CH.SOL- 5.29.
The answers are as follows:

1. *The function $g(x)$ represented by the expression graph in 5.11 is:*

$$g(x) = A + B * ln(C) \tag{5.73}$$

2. *For a logarithmic function:*

$$\frac{d}{dx}\ln(x) = \frac{1}{x} \tag{5.74}$$

Therefore, the partial derivatives for the function $g(x)$ are:

$$\begin{aligned} \frac{\partial f}{\partial A} &= 1 \\ \frac{\partial f}{\partial B} &= ln(C) \\ \frac{\partial f}{\partial C} &= B * \frac{1}{C} \end{aligned} \tag{5.75}$$

SOL-129 CH.SOL- 5.30. *The answers are as follows:*

1. *True. Both directions yield the exact same results.*
2. *True. Reverse mode is more efficient than forward mode AD (why?).*
3. *True.*
4. *True.*

SOL-130 CH.SOL- 5.31.
The answers are as follows:

1. *The function is*

$$f(x_1, x_2) = x_1 x_2 + ln(x_1) \tag{5.76}$$

2. *The graph associated with the forward mode AD is as follows:*

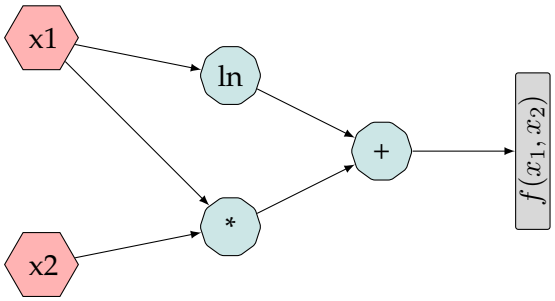


FIGURE 5.22: A Computation graph for $g(x_1, x_2)$ in 5.1

3. *The partial derivatives are:*

$$\begin{aligned} \frac{\partial f}{\partial x_1} &= x_2 - \frac{1}{(x_1)} \\ \frac{\partial f}{\partial x_2} &= x_1 \end{aligned} \tag{5.77}$$

■

5.3.15 Forward mode AD table construction

SOL-131 CH.SOL- 5.32.

The answers are as follows:

1. *The graph with the intermediate values is depicted in (5.23)*

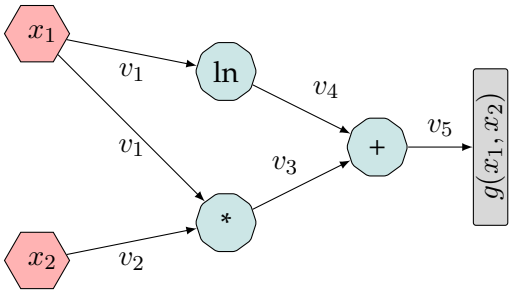


FIGURE 5.23: A derivative graph for $g(x_1, x_2)$ in 5.1

2. *Forward mode AD for* $g(x_1, x_2) = \ln(x_1) + x_1 x_2$ *evaluated at* $(x_1, x_2) = (e^2, \pi)$.

Forward-mode function evaluation		
$v_{-1} = x_1$		$= e^2$
$v_0 = x_2$		$= \pi$
v_1	$= \ln v_{-1}$	$= \ln(e^2) = 2$
v_2	$= v_{-1} \times v_0$	$= e^2 \times \pi = 23.2134$
v_3	$= v_1 + v_2$	$2 + 23.2134 = 25.2134$
f	$= v_3$	$=\approx 25.2134$

TABLE 5.1: Forward-mode AD table for $y = g(x_1, x_2) = \ln(x_1) + x_1 x_2$ evaluated at $(x_1, x_2) = (e^2; \pi)$ and setting $\dot{x}_1 = 1$ to compute $\frac{\partial y}{\partial x_1}$.

3. *The following Python code (5.24) proves that the numerical results are correct:*

```
import math
print (math.log(math.e*math.e) + math.e*math.e*math.pi)
> 25.2134^^I
```

FIGURE 5.24: Python code- AD of the function $g(x_1, x_2)$

4. *Seed values indicate the values by which the dependent and independent variables are initialized to before being propagated in a computation graph. For instance:*

$$\dot{v}_1 = \frac{\partial x_1}{\partial x_1} = 1$$
$$\dot{v}_2 = \frac{\partial x_2}{\partial x_1} = 0$$

Therefore we set $\dot{x}_1 = 1$ *to compute* $\frac{\partial y}{\partial x_1}$.

5. *Here we construct a table for the forward-mode AD for the derivative of* $f(x_1, x_2) = \ln(x_1) + x_1 x_2$ *evaluated at* $(x_1, x_2) = (e^2, \pi)$ *while setting* $\dot{x}_1 = 1$ *to compute* $\frac{\partial y}{\partial x_1}$*.. In forward-mode AD a derivative is called a* ***tangent****.*

In the derivation that follows, note that mathematically using manual differentiation:

$$\begin{aligned} &\tfrac{\mathrm{d}}{\mathrm{d}x_1}\left[\ln(x) + x_2 x\right] \\ &= \tfrac{\mathrm{d}}{\mathrm{d}x_1}[\ln(x_1)] + x_2 \cdot \tfrac{\mathrm{d}}{\mathrm{d}x_1}[x_1] \\ &= \tfrac{1}{x_1} + x_2 \cdot 1 \\ &= \tfrac{1}{x_1} + x_2 \end{aligned}$$

and also since $\frac{d}{dx}\ln(x) = \frac{1}{x}$ *then* $\dot{v}_1 = \frac{1}{v_{-1}} * \dot{v}_{-1} = \dot{v}_{-1}/v_{-1} = \frac{1}{e^2} * 1 = 1/e^2$.

Forward-mode AD derivative evaluation
$v_{-1} = x_1 = e^2$
$v_0 = x_2 = \pi$
$\dot{v}_{-1} = \dot{x}_1 = 1$
$\dot{v}_0 = \dot{x}_2 = 0$
$\dot{v}_1 = \dot{v}_{-1}/v_{-1} = 1/e^2$
$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1} = 1 \times \pi + 0 \times e^2 = \pi$
$\dot{v}_4 = \dot{v}_1 + \dot{v}_2 = 1/e^2 + \pi$
$\boldsymbol{\dot{f} = \dot{v}_4 = 1/e^2 + \pi = \approx 3.2769}$

TABLE 5.3: Forward-mode AD table for $y = g(x_1, x_2) = \ln(x_1) + x_1 x_2$ evaluated at $(x_1, x_2) = (e^2; \pi)$ and setting $\dot{x}_1 = 1$ (seed values are mentioned here: 3) to compute $\frac{\partial y}{\partial x_1}$.

6. *The following Python code (5.25) proves that the numerical results are correct:*

```python
import autograd.numpy as np
from autograd import grad
import math

x1 = math.e* math.e
x2 = math.pi

def f1(x1,x2):
return (np.log(x1) + x1*x2)

grad_f1 = grad(f1)

print(f1(x1,x2)) # > 25.2134
print(grad_f1(x1,x2)) # > 3.2769
```

FIGURE 5.25: Python code- AD of the function $g(x_1, x_2)$

5.3.16 Symbolic differentiation

5.3.17 Simple differentiation

SOL-132 CH.SOL- 5.33.

The answers are as follows:

1. *Approximate methods such as numerical differentiation suffer from numerical instability and truncation errors.*

2. *In symbolic differentiation, a symbolic expression for the derivative of a function is calculated. This approach is quite slow and requires symbols parsing and manipulation. For example, the number $\sqrt{2}$ is represented in SymPy as the object Pow(2,1/2). Since SymPy employees exact representations Pow(2,1/2)*Pow(2,1/2) will always equal 2.*

SOL-133 CH.SOL- 5.34.

1. *First:*

```
import sympy
sympy.init_printing()
from sympy import Symbol
from sympy import diff, exp, sin, sqrt
y = Symbol('y')
y = sympy.Symbol("y")
sigmoid = 1/(1+sympy.exp(-y))^^I
```

FIGURE 5.26: Sigmoid in SymPy

2. *Second:*

```
sig_der=sym.diff(sigmoid, y)
```

FIGURE 5.27: Sigmoid gradient in SymPy

3. *Third:*

```
sig_der.evalf(subs={y:0})
> 0.25
```

FIGURE 5.28: Sigmoid gradient in SymPy

4. *The plot is depicted in 5.29.*

```
1 p = sym.plot(sig_der);
```

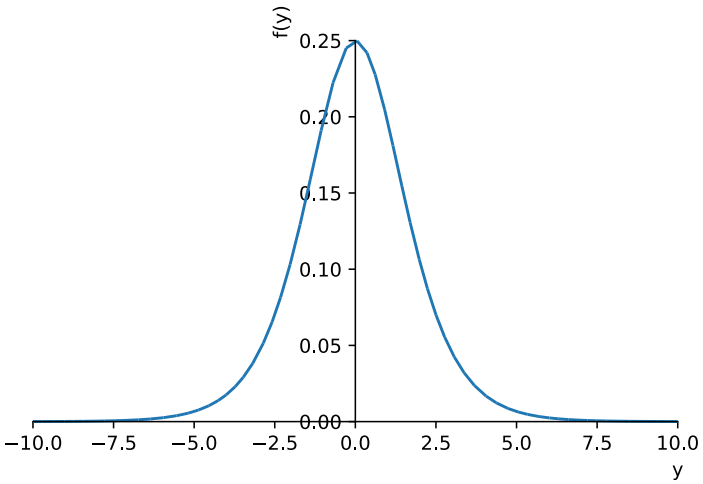


FIGURE 5.29: SymPy gradient of the Sigmoid() function

5.3.18 The Beta-Binomial model

SOL-134 CH.SOL- 5.35.

To correctly render the generated LaTeX in this problem, we import and configure several libraries as depicted in 5.30.

```
import numpy as np
import scipy.stats as st
import matplotlib.pyplot as plt
import sympy as sp
sp.interactive.printing.
init_printing(use_latex=True)
from IPython.display import display, Math, Latex
maths = lambda s: display(Math(s))
latex = lambda s: display(Latex(s))^^I
```

FIGURE 5.30: SymPy imports

1. *The Likelihood function can be created as follows. Note the specific details of generating the Factorial function in SymPy.*

```
n = sp.Symbol('n', integer=True, positive=True)
r = sp.Symbol('r', integer=True, positive=True)
theta = sp.Symbol('theta')
# Create the function symbolically
from sympy import factorial
cNkSym=  (factorial(n))/ (factorial(r) *factorial(n-r))
cNkSym.evalf()
binomSym= cNkSym*((theta **r)*(1-theta)**(n-r))
binomSym.evalf()
#Convert it to a Numpy-callable function
binomLambda = sp.Lambda((theta,r,n), binomSym)
maths(r"\operatorname{Bin}(r|n,\theta) = ")
display (binomLambda.expr)
#Evaluating the SymPy version results in:
> binomSym.subs({theta:0.5,r:50,n:100})
#Evaluating the pure Numpy version results in:
> binomLambda(0.5,50,100)= 0.07958923
```

FIGURE 5.31: Likelihood function using SymPy

The Symbolic representation results in the following LaTeX:

$$\mathrm{Bin}(r|n,\theta) = \frac{\theta^r \left(-\theta+1\right)^{n-r} n!}{r!\,(n-r)!} \tag{5.78}$$

2. *The Beta distribution can be created as follows.*

```
a = sp.Symbol('a', integer=False, positive=True)
b = sp.Symbol('b', integer=False, positive=True)
#mu = sp.Symbol('mu', integer=False, positive=True)
# Create the function symbolically
G = sp.gamma
# The normalisation factor
BetaNormSym = G(a + b)/(G(a)*G(b))
# The functional form
BetaFSym = theta**(a-1) * (1-theta)**(b-1)
BetaSym=BetaNormSym * BetaFSym
BetaSym.evalf() # this works
# Turn Beta into a function
BetaLambda = sp.Lambda((theta,a,b), BetaNormSym * BetaFSym)
maths(r"\operatorname{Beta}(\theta|a,b) = ")
display(BetaSym)
#Evaluating the SymPy version results in:
> BetaLambda(0.5,2,7)=0.4375
#Evaluating the pure Numpy version results in:
> BetaSym.subs({theta:0.5,a:2,b:7})=0.4375
```

FIGURE 5.32: Beta distribution using SymPy

The result is:

$$\text{Beta}(\theta|a,b) = \frac{\theta^{a-1}\Gamma(a+b)}{\Gamma(a)\Gamma(b)}(-\theta+1)^{b-1} \tag{5.79}$$

3. *The plot is depicted in 5.33.*

```
%pylab inline
mus = arange(0,1,.01)
# Plot for various values of a and b
for ab in [(.1,.1),(.5,.5),(2,20),(2,3), (1,1)]:
plot(mus, vectorize(BetaLambda)(mus,*ab), label="a=%s b=%s" % ab)
legend(loc=0)
xlabel(r"$\theta$", size=22)
```

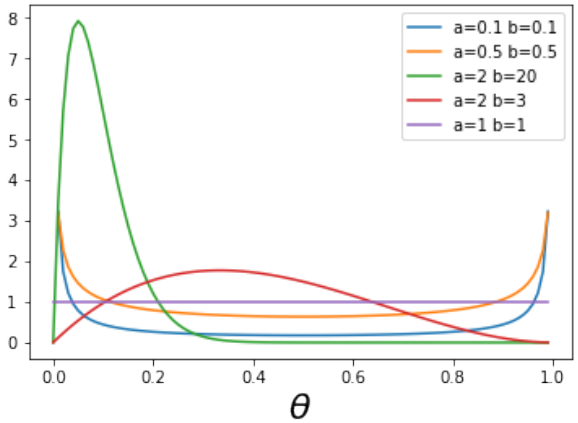


FIGURE 5.33: A plot of the Beta distribution

4. *We can find the posterior distribution by multiplying our Beta prior by the Binomial Likelihood.*

```
a = sp.Symbol('a', integer=False, positive=True)
b = sp.Symbol('b', integer=False, positive=True)
BetaBinSym=BetaSym * binomSym
# Turn Beta-bin into a function
BetaBinLambda = sp.Lambda((theta,a,b,n,r), BetaBinSym)
BetaBinSym=BetaBinSym.powsimp()
display(BetaBinSym)
maths(r"\operatorname{Beta}(\theta|a,b) \times
 ↪  \operatorname{Bin}(r|n,\theta) \propto %s" %
 ↪  sp.latex(BetaBinSym))
> BetaBinSym.subs({theta:0.5,a:2,b:7,n:10,r:3})= 0.051269
> BetaBinLambda (0.5,2,7, 10,3)= 0.051269
```

FIGURE 5.34: A plot of the Beta distribution

The result is:

$$\text{Beta}(\theta|a,b) \times \text{Bin}(r|n,\theta) \propto \frac{\theta^{a+r-1}\left(-\theta+1\right)^{b+n-r-1} n!}{r!\,(n-r)!\Gamma(a)\Gamma(b)}\Gamma(a+b)$$

So the posterior distribution has the same functional dependence on θ as the prior, it is just another Beta distribution.

5. *Mathematically, the relationship is as follows:*

$$
\begin{aligned}
&\textbf{Prior}: \\
&\text{Beta}(\theta|a=2,b=7) \\
&= 56\theta\left(-\theta+1\right)^{6} \\
&\textbf{Likelihood}: \\
&\text{Bin}(r=3|n=6,\theta) = 19600\theta^{3}\left(-\theta+1\right)^{47} \\
&\textbf{Posterior}(\textbf{normalised}): \\
&\text{Beta}(\theta|2,7)\times\text{Bin}(3|50,\theta) = 1097600\theta^{4}\left(-\theta+1\right)^{53}
\end{aligned}
\tag{5.80}
$$

```
prior = BetaLambda(theta,2,7)
maths("\mathbf{Prior}:\operatorname{Beta}(\theta|a=2,b=7) = %s" %
 ↪  sp.latex(prior))
likelihood = binomLambda(theta,3,50) # = binomLambda(0.5,3,10)
maths("\mathbf{Likelihood}: \operatorname{Bin}(r=3|n=6,\theta) =
 ↪  %s" % sp.latex(likelihood))
posterior = prior * likelihood
posterior=posterior.powsimp()
maths(r"\mathbf{Posterior
 ↪  (normalised)}:\operatorname{Beta}(\theta|2,7) \times
 ↪  \operatorname{Bin}(3|50,\theta)=%s"
posterior.subs({theta:0.5})
plt.plot(mus, (sp.lambdify(theta,posterior))(mus), 'r')
xlabel("$\\theta$", size=22)
```

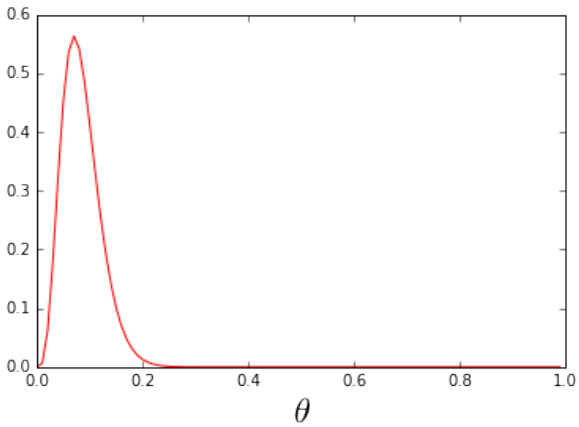


FIGURE 5.35: A plot of the Posterior with the provided data samples.

References

[1] J. Bradbury et al. *JAX: composable transformations of NumPy programs*. 2018 (cit. on pp. 123, 136).

[2] W. K. Clifford. 'Preliminary Sketch of Bi-quaternions'. In: *Proceedings of the London Mathematical Society 4* (1873), pp. 381–95 (cit. on pp. 125, 139).

[3] R. Frostig et al. *JAX: Autograd and XLA*. 2018 (cit. on p. 123).

[4] A. Griewank, D. Juedes and J. Utke. 'Algorithm 755; ADOL-C: a package for the automatic differentiation of algorithms written in C/C++'. In: *ACM Transactions on Mathematical Software* 22.2 (June 1996), pp. 131–167 (cit. on pp. 123, 125).

[5] A. Griewank and A. Walther. *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*. Second. USA: Society for Industrial and Applied Mathematics, 2008 (cit. on pp. 123, 124).

[6] K. Gurney. *An Introduction to Neural Networks*. 1 Gunpowder Square, London EC4A 3DE, UK: UCL Press, 1998 (cit. on p. 135).

[7] L. V. Kantorovich. 'On a mathematical symbolism convenient for performing machine calculations'. In: *Dokl. Akad. Nauk SSSR*. Vol. 113. 4. 1957, pp. 738–741 (cit. on p. 123).

[8] G. Kedem. 'Automatic differentiation of computer programs'. In: *ACM Transactions on Mathematical Software (TOMS)* 6.2 (1980), pp. 150–165 (cit. on pp. 126, 149).

[9] S. Laue. *On the Equivalence of Forward Mode Automatic Differentiation and Symbolic Differentiation*. 2019. arXiv: 1904.02990 [cs.SC] (cit. on p. 124).

[10] D. Maclaurin, D. Duvenaud and R. P. Adams. 'Autograd: Effortless gradients in numpy'. In: *ICML 2015 AutoML Workshop*. Vol. 238. 2015 (cit. on pp. 123, 136).

[11] A. Paszke et al. 'Automatic differentiation in PyTorch'. In: (2017) (cit. on p. 136).

[12] D. Rumelhart, G. Hinton and R. Williams. 'Learning representations by back propagating errors'. In: *Nature 323* (1986), pp. 533–536 (cit. on p. 135).

[13] B. Speelpenning. *Compiling fast partial derivatives of functions given by algorithms*. Tech. rep. Illinois Univ Urbana Dept of Computer Science, 1980 (cit. on p. 126).