Selected Exercises of Machine Learning: A Probabilistic Perspective

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1 Introduction

This is a collection of certain exercise solutions I did as I was reading through this book. As I am not a mathematician, the "proofs" listed here are rough and probably not rigorous. They only serve as a means to explain the concepts in a way that aids my own understanding.

2 Probability

Exercises

Exercise 2.1. **My neighbor has two children. Assuming that the gender of a child is like a coin flip, it is most likely, a priori, that my neighbor has one boy and one girl, with probability 1/2. The other possibilities, two boys or two girls, have probabilities 1/4 and 1/4.**

a. Suppose I ask him whether he has any boys, and he says yes. What is the probability that one child is a girl?

b. Suppose instead that I happen to see one of his children run by, and it is a boy. What is the probability that the other child is a girl?

a. Let G represent one girl, and B represent one boy. Since the neighbor has two children, we can state the entire sample space:

$$S = \{BB, BG, GB, GG\}$$

When the neighbor answers the question, this changes our beliefs about the other child. Using Bayes' theorem:

$$P(G = 1|B \geq 1) = \frac{P(B \geq 1|G = 1)P(G = 1)}{P(B \geq 1)} \tag{1}$$

$$= \frac{2/2 \times 1/2}{3/4} \tag{2}$$

$$= \frac{2}{3} \tag{3}$$

b. If we instead happen to see one of his children, this is a different way of looking at the problem. In this situation, learning the gender of one child tells us nothing about the gender of the other child. Therefore, the gender of the second child is a coin flip, 1/2.

Exercise 2.2. **Suppose a crime has been committed. Blood is found at the scene for which there is no innocent explanation. It is of a type which is present in 1% of the population.**

a. The prosecutor claims: "There is a 1% chance that the defendant would have the crime blood type if he were innocent. Thus there is a 99% chance that he is guilty". This is known as the prosecutor's fallacy. What is wrong with this argument?

b. The defender claims: "The crime occurred in a city of 800,000 people. The blood type would be found in approximately 8000 people. The evidence has provided a probability of just 1 in 8000 that

the defendant is guilty, and thus has no relevance". This is known as the defender's fallacy. What is wrong with this argument?

a. The defendant sharing the blood type does not mean that the defendant himself has a 99% probability of being guilty, just that he shares the same blood type as the guilty party, just like he shares the same blood type with 1% of the population. In a large enough city, there would be a large number of people fitting this description in a small geographical radius.

b. This statement assumes that the defendent is just as guilty (or just as non-guilty) as anyone else in that group of 8000 people. If there truly is no other evidence to tie this defendent to this crime, then that may be so, but if there were any other evidence (drives a similar car as the criminal, lives in the same area, or frequents the same locations), the probability that the defendant is guilty could be much higher.

Exercise 2.3. **Show that the variance of a sum is** $Var[X+Y] = Var[X] + Var[Y] + 2Cov[X,Y]$**, where** $Cov[X,Y]$ **is the covariance between** X **and** Y**.**

$$Var[X] + Var[Y] + 2Cov[X,Y] = E[(X-\mu_x)^2] + E[(Y-\mu_y)^2] + 2E[(X-\mu_x)(Y-\mu_y)] \tag{4}$$

$$= E[X^2 - 2X\mu_x + \mu_x^2] + E[Y^2 - 2Y\mu_y + \mu_y^2] + E[2XY - 2X\mu_y - 2Y\mu_x + 2\mu_x\mu_y] \tag{5}$$

$$= E[X^2 - 2X\mu_x + \mu_x^2 + Y^2 - 2Y\mu_y + \mu_y^2 + 2XY - 2X\mu_y - 2Y\mu_x + 2\mu_x\mu_y] \tag{6}$$

$$= E[X^2 + 2XY - 2X(\mu_x + \mu_y) + Y^2 - 2Y(\mu_x + \mu_y) + 2\mu_x\mu_y] \tag{7}$$

Note that $E(X+Y) = E(X) + E(Y) = \mu_x + \mu_y = \mu_{xy}$. Given this,

$$E[X^2 + 2XY - 2X(\mu_x + \mu_y) + Y^2 - 2Y(\mu_x + \mu_y) + 2\mu_x\mu_y] \tag{8}$$

$$= E[X^2 + 2XY - 2X\mu_{xy} + Y^2 - 2Y\mu_{xy} + 2\mu_x\mu_y] \tag{9}$$

$$= E[(X + Y - \mu_{xy})^2] \tag{10}$$

$$= Var[X+Y] \tag{11}$$

Exercise 2.4. **After your yearly checkup, the doctor has bad news and good news. The bad news is that you tested positive for a serious disease, and that the test is 99% accurate (i.e., the probability of testing positive given that you have the disease is 0.99, as is the probability of testing negative given that you don't have the disease). The good news is that this is a rare disease, striking only one in 10,000 people. What are the chances that you actually have the disease? (Show your calculations as well as giving the final result.)**

Since the test is 99% accurate, we know that $P(Y|D) = P(N|\ D) = 0.99$, where Y means a positive test result, N a negative test result, D means you

have the disease, and D means you do not have the disease. We also know the prior probability of having the disease: $P(D) = 0.0001$. Using Bayes' rule:

$$P(D|Y) = \frac{P(Y|D)P(D)}{P(Y)} \tag{12}$$

$$= \frac{0.99 \times 0.0001}{P(Y|D)P(D) + P(Y|\ D)P(\ D)} \tag{13}$$

$$= \frac{0.000099}{(0.99 \times 0.0001) + (0.01 \times 0.9999)} \tag{14}$$

$$= \frac{0.000099}{0.000099 + 0.009999} \tag{15}$$

$$= 0.0098 \tag{16}$$

So, there's about a 1% chance that you have the disease even though you tested positive for it.

Exercise 2.5. **Solve the Monty Hall problem.**

The key here is that the host will never open a door that has the car in it. So from that sense, the contestant does not disturb the original distribution, but it does give you additional information.

Let's say you originally pick the door with the car. Under these circumstances, which door the host will open is uniform (1/2). In this situation, it is worse for you to switch, and you'll only find yourself in this situation if you pick the door correctly the first time (1/3 chance).

Let's say you did not originally pick the door with the car. Under these circumstances, the door that the host will open is completely deterministic. Two doors will remain, one with the car, and the host will never choose that one. In this situation, it is better for you to switch, because you'll be gauranteed a car.

So, when you guess correctly the first time and switch, you're guaranteed to lose the car. If you guess incorrectly the first time and switch, you're guaranteed to win the car. The probability of guessing correctly the first time is 1/3, so switching will give you a winning probability of 2/3.

Exercise 2.6. **a. Let $H \in \{1, ..., K\}$ be a discrete random variable, and let e_1 and e_2 be the observed values of two other random variables E_1 and E_2. Suppose we wish to calculate the vector**

$$\vec{P}(H|e_1, e_2) = (P(H = 1|e_1, e_2), ..., P(H = K|e_1, e_2))$$

Which of the following sets of numbers are sufficient for the calculation?

i. $P(e_1, e_2), P(H), P(e_1|H), P(e_2|H)$

ii. $P(e_1, e_2), P(H), P(e_1, e_2|H)$

iii. $P(e_1|H), P(e_2|H), P(H)$

b. Now suppose we now assume $E_1 \perp E_2|H$ (i.e., E_1 and E_2 are conditionally independent given H). Which of the above 3 sets are sufficient now?

a. Let's use Bayes' Theorem to decompose this a bit:

$$P(H|e_1, e_2) = \frac{P(e_1, e_2, H)}{P(e_1, e_2)} \tag{17}$$

$$= \frac{P(e_1, e_2|H)P(H)}{P(e_1, e_2)} \tag{18}$$

$$= \frac{P(e_1|e_2, H)P(e_2)P(H)}{P(e_1, e_2)} \tag{19}$$

From this, we can see that **ii** is sufficient to solve this.

b. If we assume that they are now conditionally independent, then this allows **i** to be sufficient as well. Note that **iii** is still not sufficient, but if we know that E_1 and E_2 were unconditionally independent, this would be sufficient as well.

Exercise 2.7. **Show that pairwise independence between all pairs of variables does not necessarily imply mutual independence. It suffices to give a counterexample.**

Exercise 2.8. **In the text we said $X \perp Y|Z$ iff $p(x, y|z) = p(x|z)p(y|z)$ for all x, y, z such that $p(z) > 0$. Now prove the following alternative definition: $X \perp Y|Z$ iff there exist functions g and h such that $p(x, y|z) = g(x, z)h(y, z)$ for all x, y, z such that $p(z) > 0$.**

For this to be true, $g(x, z)h(y, z) = p(x|z)p(y|z)$ So by computing the marginal probabilities, we can see if they are equivalent.

$$p(x|z) = \sum_y p(x, y|z) \tag{20}$$

$$= \sum_y g(x, z)h(y, z) \tag{21}$$

$$= g(x, z) \sum_y h(y, z) \tag{22}$$

and therefore

$$\sum_y h(y, z) = \frac{p(x|z)}{g(x, z)}$$

Similarly we can find that

$$\sum_x g(x, z) = \frac{p(y|z)}{h(y, z)}$$

and we can note that

$$\sum_x \sum_y p(x, y|z) = \sum_x g(x, z) \sum_y h(y, z) = 1$$

so therefore

$$\sum_x \sum_y p(x, y|z) = \sum_x g(x, z) \sum_y h(y, z) \tag{23}$$

$$= \frac{p(y|z)}{h(y, z)} \frac{p(x|z)}{g(x, z)} \tag{24}$$

$$= 1 \tag{25}$$

which leads to

$$1 = \frac{p(y|z)}{h(y, z)} \frac{p(x|z)}{g(x, z)} \tag{26}$$

$$\frac{g(x, z)}{p(x|z)} = \frac{p(y|z)}{h(y, z)} \tag{27}$$

$$p(x|z)p(y|z) = g(x, z)h(y, z) \tag{28}$$

Exercise 2.9.
a. True or false? $(X \perp W|Z, Y) \wedge (X \perp Y|Z) \Rightarrow (X \perp Y, W|Z)$
b. True or false? $(X \perp Y|Z) \wedge (X \perp Y|W) \Rightarrow (X \perp Y|Z, W)$
a. Blowing out the component parts:

$$(X \perp W|Z, Y) \Leftrightarrow p(X, W|Z, Y) = p(X|Z, Y)p(W|Z, Y) \tag{29}$$

$$(X \perp Y|Z) \Leftrightarrow p(X, Y|Z) = p(X|Z)p(Y|Z) \tag{30}$$

$$(X \perp Y, W|Z) \Leftrightarrow p(X, Y, W|Z) = p(X|Z)p(Y|Z)p(W|Z) \tag{31}$$

so we can see if we can recreate the righthand side using what we know:
P(A,B) = P(A—B)P(B) P(A—B) = P(A,B)/P(B)
P(A,B—C,D) = P(A,B,D—C)/P(D)

$$p(X, Y, W|Z) = p(X, W|Z, Y)p(Y) \tag{32}$$

$$= p(X|Z, Y)p(W|Z, Y)p(Y) \tag{33}$$

$$= \frac{p(X, Y|Z)}{p(Y)} p(W|Z, Y)p(Y) \tag{34}$$

$$= p(X|Z)p(Y|Z)p(W|Z) \tag{35}$$

b. Blowing out the component parts:

$$(X \perp Y|Z) \Leftrightarrow p(X,Y|Z) = p(X|Z)p(Y|Z) \tag{36}$$
$$(X \perp Y|W) \Leftrightarrow p(X,Y|W) = p(X|W)p(Y|W) \tag{37}$$
$$(X \perp Y|Z,W) \Leftrightarrow p(X,Y|Z,W) = p(X|Z,W)p(Y|Z,W) \tag{38}$$

Note that W is in the conditioning set for the equation on the righthand side. There is no way to remove this from the conditioning set while also removing it from the lefthand side. Therefore this is false.

Exercise 2.10. **Given the Gamma density, show that the inverse Gamma is a Gamma with a change of variables to $Y = 1/X$.**

The Gamma is given by:

$$Ga(x|a,b) = \frac{b^a}{\tau(a)} x^{a-1} e^{-xb}$$

and the Inverse Gamma is given by:

$$IG(x|a,b) = \frac{b^a}{\tau(a)} x^{-(a+1)} e^{-b/x}$$

from these, it is easy to show that:

$$Ga(\frac{1}{x}|a,b) = \frac{b^a}{\tau(a)} (\frac{1}{x})^{a-1} e^{-b/x} \tag{39}$$
$$= \frac{b^a}{\tau(a)} x^{-1\times(a-1)} e^{-b/x} \tag{40}$$
$$= \frac{b^a}{\tau(a)} x^{-(a+1)} e^{-b/x} \tag{41}$$
$$= IG(x|a,b) \tag{42}$$

Exercise 2.11. **Show that the normalization constant for the Gaussian distribution is equal to $Z = \sigma\sqrt{2\pi}$.**

This is essentially just computing the integral

$$Z^2 = \int_0^{2\pi} \int_0^{\infty} r\, exp(-\frac{r^2}{2\sigma^2}) dr d\theta \tag{43}$$
$$= 2\pi \int_0^{\infty} r\, exp(-\frac{r^2}{2\sigma^2}) dr \tag{44}$$
$$= 2\pi\sigma^2 e^{-\frac{r^2}{2\sigma^2}} |_0^{\infty} \tag{45}$$
$$= 2\pi\sigma^2 \tag{46}$$

Therefore $Z = \sigma\sqrt{2\pi}$.

Exercise 2.12. **Show that**

$$I(X,Y) = H(X) - H(X|Y) = H(Y) - H(Y|X)$$

To show this, we must use the definitions of KL divergence, entropy, and conditional entropy. I will show the definitions here for clarity.

$$H(X) = -\sum_{k=1}^{K} p(X=k) log_2 p(X=k) \tag{47}$$

$$KL(X||Y) = -H(X) + H(X,Y) \tag{48}$$

$$H(Y|X) = \sum_x p(x) H(Y|X=x) \tag{49}$$

$$= H(X,Y) - H(X) \tag{50}$$

$$I(X,Y) = KL(p(X,Y)||p(X)p(Y)) \tag{51}$$

With these definitions, we can show that

$$I(X,Y) = KL(p(X,Y)||p(X)p(Y)) \tag{52}$$

$$= -H(p(X,Y)) + H(p(X,Y), p(X), pY()) \tag{53}$$

$$= \sum_{x\in X}\sum_{y\in Y} p(x,y) log\, p(x,y) - \sum_{x\in X}\sum_{y\in Y} p(x,y) log\, p(x)p(y) \tag{54}$$

$$= \sum_{x\in X}\sum_{y\in Y} p(x,y)(log\, p(y|x) + log\, p(x)) - \sum_{x\in X}\sum_{y\in Y} p(x,y)(log\, p(x) + log\, p(y)) \tag{55}$$

$$= -H(Y|X) + \sum_{x\in X}\sum_{y\in Y} p(x,y) log\, p(x) - \sum_{x\in X}\sum_{y\in Y} p(x,y)(log\, p(x) + log\, p(y)) \tag{56}$$

$$= -H(Y|X) + \sum_{x\in X} p(x) log\, p(x) - \sum_{x\in X} p(x) log\, p(x) + \sum_{y\in Y} p(y) log\, p(y) \tag{57}$$

$$= -H(Y|X) + \sum_{y\in Y} p(y) log\, p(y) \tag{58}$$

$$= -H(Y|X) + H(Y) \tag{59}$$

$$= H(Y) - H(Y|X) \tag{60}$$

Exercise 2.13. **Evaluate $I(X_1, X_2)$ where X has a bivariate normal distribution. Evaluate $I(X_1, X_2)$ at $\rho = -1$, $\rho = 0$, $\rho = 1$.**

The entropy for both multidimensional and single dimensional Gaussians is defined by:

$$h(\mathbf{X}) = \frac{1}{2} log_2[(2\pi e)^d \, det \, \Sigma] \tag{61}$$

$$h(X) = \frac{1}{2} log_2[2\pi e \sigma^2] \tag{62}$$

Using these, we can compute:

$$\begin{aligned}
I(X_1, X_2) &= H(X_1) - H(X_1|X_2) && (63)\\
&= H(X_1) - H(X_2, X_1) + H(X_2) && (64)\\
&= log_2[2\pi e \sigma^2] - H(X_2, X_1) && (65)\\
&= log_2[2\pi e] + log_2[\sigma^2] - H(X_2, X_1) && (66)\\
&= C + log_2[\sigma^2] - H(X_2, X_1) && (67)\\
&= C + 2log_2[\sigma] - \frac{1}{2} log_2[(2\pi e)^2 \, det \, \Sigma] && (68)\\
&= C + 2log_2[\sigma] - \frac{1}{2}[2C + log_2[det \, \Sigma]] && (69)\\
&= C + 2log_2[\sigma] - C - \frac{1}{2} log_2[\sigma^4(1-\rho^2)] && (70)\\
&= 2log_2[\sigma] - \frac{1}{2} log_2[\sigma^4(1-\rho^2)] && (71)
\end{aligned}$$

where $C = log_2[2\pi e]$. Now we can plug in various values for ρ. When $\rho = -1$,

$$\begin{aligned}
I(X_1, X_2) &= 2log_2[\sigma] - log_2[\sigma^4] && (72)\\
&= 2log_2[\sigma] - 4log_2[\sigma^4] && (73)\\
&= -2log_2[\sigma] && (74)
\end{aligned}$$

When $\rho = 0$,

$$\begin{aligned}
I(X_1, X_2) &= 2log_2[\sigma] - \frac{1}{2} log_2[\sigma^4] && (75)\\
&= 2log_2[\sigma] - 2log_2[\sigma] && (76)\\
&= 0 && (77)
\end{aligned}$$

When $\rho = 1$,

$$I(X_1, X_2) = 2log_2[\sigma]$$

Exercise 2.14. **Let X and Y be discrete random variables which are identically distributed (so $H(X) = H(Y)$) but not necessarily independent. Define**

$$r = 1 - \frac{H(Y|X)}{H(X)}$$

a. Show that $r = \frac{I(X,Y)}{H(X)}$

$$\frac{I(X,Y)}{H(X)} = \frac{H(Y) - H(Y|X)}{H(X)} \tag{78}$$

$$= \frac{H(X) - H(Y|X)}{H(X)} \tag{79}$$

$$= 1 - \frac{H(Y|X)}{H(X)} \tag{80}$$

b. Show that $0 \leq r \leq 1$

$$r = 1 - \frac{H(Y|X)}{H(X)} \tag{81}$$

$$= 1 - \frac{H(X,Y) - H(X)}{H(X)} \tag{82}$$

$$= 1 - H(X,Y) = 1 - H(X) \tag{83}$$

c. When is $r = 0$**?**

$r = 0$ when the entropy of X (or equivalently Y) $= 1$.

d. When is $r = 1$**?**

$r = 1$ when the entropy of X (or equivalently Y) $= 0$. This happens when X and Y is completely deterministic.

Exercise 2.15. **Let** $p(x)$ **be the empirical distribution and** $q(x|\theta)$ **be a model. Show that** $argmin_q \, KL(p||q)$ **is obtained by** $q(x) = q(x|\hat{\theta})$**, where** θ **is the MLE.**

Since

$$KL(p||q) = \sum_k p_k log \, p_k - \sum_k p_k log \, q_k$$

minimizing this is equivalent to maximizing

$$max_q \; -KL(p||q) = -\sum_k p_k log \, p_k + \sum_k p_k log \, q_k \qquad = \sum_k p_k log \, q_k \tag{84}$$

This is the maximum likelihood equation.

Exercise 2.16. **Derive the mean, mode, variance of** θ $Beta(a, b)$

The pdf of the beta distribution is given by

$$\frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha, \beta)}$$

Note that $B(\alpha, \beta)$ is a normalization constant, and in order to derive the moments of the distribution we will be using MLE, so for our purposes, we can ignore this constant.

The mode is defined as the peak of the distribution:

$$max\, x^{\alpha-1}(1-x)^{\beta-1} \equiv max\, log[x^{\alpha-1}(1-x)^{\beta-1}] \tag{85}$$
$$= max\, (\alpha-1)log(x) + (\beta-1)log(1-x) \tag{86}$$

by taking the derivative and setting it to 0, we get:

$$0 = \frac{\alpha-1}{x} + \frac{\beta-1}{1-x} \tag{87}$$
$$\frac{-\beta+1}{-1+x} = \frac{\alpha-1}{x} \tag{88}$$
$$x(-\beta+1) = (\alpha-1)(x-1) \tag{89}$$
$$-\beta x + x = -\alpha x - \alpha - x + 1 \tag{90}$$
$$\alpha x - \beta x + 2x = \alpha - 1 \tag{91}$$
$$x = \frac{\alpha-1}{\alpha+\beta-2} \tag{92}$$

The mean of the distribution is defined by:

$$E[x] = \int_0^1 xp(x)dx \tag{93}$$
$$= \int_0^1 x\frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha,\beta)}dx \tag{94}$$
$$= \frac{\alpha}{\alpha+\beta} \tag{95}$$

The variance of the distribution is defined by:

$$Var(X) = E[(X-\mu)^2] = E[X^2] - E[X]^2 \tag{96}$$
$$= E[X^2] - (\frac{\alpha}{\alpha+\beta})^2 \tag{97}$$
$$= \int_0^1 x^2 p(x)dx - (\frac{\alpha}{\alpha+\beta})^2 \tag{98}$$
$$= \int_0^1 x^2 \frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha,\beta)}dx - (\frac{\alpha}{\alpha+\beta})^2 \tag{99}$$
$$= \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)} \tag{100}$$

Exercise 2.17. **Suppose X, Y are two points sampled independently and uniformly at random from the interval $[0, 1]$. What is the expected location of the left most point?**

$$E[min(X,Y)] = \int_0^1 \int_0^1 min(X,Y)p(X,Y)dxdy \tag{101}$$

$$= \int_0^1 \int_0^1 min(X,Y)p(X)p(Y)dxdy \tag{102}$$

$$= \int_0^1 \int_0^1 min(X,Y)dxdy \tag{103}$$

$$= \frac{1}{2}\int_0^1 \int_0^1 X + Y - |X - Y|dxdy \tag{104}$$

$$= \frac{1}{3} \tag{105}$$

3 Generative Models for Discrete Data

Exercises

Exercise 3.1. **Derive Equation 3.22 by optimizing the log likelihood in Equation 3.11**

Equation 3.22 states $\hat{\theta}_{MLE} = \frac{N_1}{N}$.

To derive this, we must maximize the log likelihood. Formally, we have to find

$$argmax_\theta \, p(D|\theta) = \theta^{N_1}(1-\theta)^{N_0} \tag{106}$$
$$argmax_\theta \, log \, p(D|\theta) = N_1 log(\theta) + N_0 log(1-\theta) \tag{107}$$
$$argmin_\theta \; - log \, p(D|\theta) = -N_0 log(1-\theta) - N_1 log(\theta) \tag{108}$$

We will minimize this by taking the derivative equal to 0 and solving for θ:

$$0 = \frac{d}{d\theta} - N_0 log(1-\theta) - N_1 log(\theta) \tag{109}$$
$$= \frac{N_0}{1-\theta} - \frac{N_1}{\theta} \tag{110}$$
$$\frac{N_1}{\theta} = \frac{N_0}{1-\theta} \tag{111}$$
$$N_1(1-\theta) = N_0\theta \tag{112}$$
$$N_1 - N_1\theta = N_0\theta \tag{113}$$
$$N_1 = (N_0 + N_1)\theta \tag{114}$$
$$\frac{N_1}{N} = \theta \tag{115}$$

Exercise 3.2. **Derive the following:**

$$p(D) = \frac{[(\alpha_1)\cdots(\alpha_1 + N_1 - 1)][(\alpha_0)\cdots(\alpha_0 + N_0 - 1)]}{(\alpha)\cdots(\alpha + N - 1)} \tag{116}$$
$$= \frac{\Gamma(\alpha_1 + N_1)\Gamma(\alpha_0 + N_0)}{\Gamma(\alpha_1 + \alpha_0 + N)} \frac{\Gamma(\alpha_1 + \alpha_0)}{\Gamma(\alpha_1)\Gamma(\alpha_0)} \tag{117}$$

To derive this, we must use the identity $\Gamma(\alpha) = (\alpha - 1)!$. Also note that

$$\frac{\Gamma(\alpha + k)}{\Gamma(\alpha)} = (\alpha)\cdots(\alpha + k)$$

Using these, and the fact that $\alpha = \alpha_0 + \alpha_1$,

$$p(D) = \frac{[(\alpha_1)\cdots(\alpha_1+N_1-1)][(\alpha_0)\cdots(\alpha_0+N_0-1)]}{(\alpha)\cdots(\alpha+N-1)} \tag{118}$$

$$= \frac{(\Gamma(\alpha_1+N_1)/\Gamma(\alpha_1))(\Gamma(\alpha_0+N_0)/\Gamma(\alpha_0))}{\Gamma(\alpha+N)/\Gamma(\alpha)} \tag{119}$$

$$= \frac{\Gamma(\alpha_1+N_1)\Gamma(\alpha_0+N_0)/\Gamma(\alpha_1)\Gamma(\alpha_0)}{\Gamma(\alpha+N)/\Gamma(\alpha)} \tag{120}$$

$$= \frac{\Gamma(\alpha_1+N_1)\Gamma(\alpha_0+N_0)\Gamma(\alpha)}{\Gamma(\alpha+N)\Gamma(\alpha_1)\Gamma(\alpha_0)} \tag{121}$$

$$= \frac{\Gamma(\alpha_1+N_1)\Gamma(\alpha_0+N_0)}{\Gamma(\alpha+N)}\frac{\Gamma(\alpha)}{\Gamma(\alpha_1)\Gamma(\alpha_0)} \tag{122}$$

$$= \frac{\Gamma(\alpha_1+N_1)\Gamma(\alpha_0+N_0)}{\Gamma(\alpha_0+\alpha_1+N)}\frac{\Gamma(\alpha_0+\alpha_1)}{\Gamma(\alpha_1)\Gamma(\alpha_0)} \tag{123}$$

Exercise 3.3. **Show that**

$$p(x|n,D) = \binom{n}{x}\frac{B(x+\alpha_1', n-x+\alpha_0')}{B(\alpha_1',\alpha_0')}$$

reduces to $p(x=1|D) = \frac{\alpha_1'}{\alpha_0'+\alpha_1'}$ **when** $n=1$**.**

Let $n=1$, and $x \in \{0,1\}$. The Beta-Binomial model is given by:

$$Bb(x|a,b,n) = \binom{n}{x}\frac{B(x+a, n-x+b)}{B(a,b)}$$

Plugging what we know in,

$$Bb(1|\alpha_1',\alpha_0',1) = \binom{1}{1}\frac{B(1+\alpha_1', 1-1+\alpha_0')}{B(\alpha_1',\alpha_0')} \tag{124}$$

$$= \frac{\Gamma(1+\alpha_1')\Gamma(\alpha_0')/\Gamma(1+\alpha_1'+\alpha_0')}{\Gamma(\alpha_1')\Gamma(\alpha_0')/\Gamma(\alpha_1'+\alpha_0')} \tag{125}$$

$$= \frac{\Gamma(1+\alpha_1')\Gamma(\alpha_0')\Gamma(\alpha_1'+\alpha_0')}{\Gamma(1+\alpha_1'+\alpha_0')\Gamma(\alpha_0')\Gamma(\alpha_1')} \tag{126}$$

$$= \frac{\Gamma(1+\alpha_1')}{(\alpha_0'+\alpha_1'+1)\Gamma(\alpha_1')} \tag{127}$$

$$= \frac{(\alpha_1'+1)\Gamma(\alpha_1')}{(\alpha_0'+\alpha_1'+1)\Gamma(\alpha_1')} \tag{128}$$

$$= \frac{\alpha_1'+1}{\alpha_0'+\alpha_1'+1} \tag{129}$$

Exercise 3.4. **Suppose we toss a coin $n=5$ times. Let X be the number of heads. Let the prior probability of heads be $p(\theta) = Beta(\theta|1,1)$. Compute the posterior $p(\theta|X<3)$ up to normalization constant.**

The posterior can be given by $p(\theta|D) = p(D|\theta)p(\theta)$. By plugging in the likelihood (Binomial) and the prior (Beta), we get

$$p(\theta|D) = p(D|\theta)p(\theta) \tag{130}$$
$$\propto Beta(\theta|N_1 + \alpha, N_2 + \beta) \tag{131}$$

Since the number of heads is discrete and mutually exclusive,

$$p(\theta|X < 3) = p(\theta|X = 0) + p(\theta|X = 1) + p(\theta|X = 2) \tag{132}$$
$$\propto Beta(\theta|1, 5) + Beta(\theta|2, 4) + Beta(\theta|3, 3) \tag{133}$$
$$= \sum_{a=0}^{2} Beta(\theta|a + 1, 5 + 1 - a) \tag{134}$$

Exercise 3.5. **Let** $\phi = logit(\theta) = log\frac{\theta}{1-\theta}$**. Show that if** $p(\phi) \propto 1$**, then** $p(\theta) \propto Beta(\theta|0, 0)$**.**

Using the change of variables formula,

$$p(\phi) = p(logit(\theta)) \tag{135}$$
$$= \left|\frac{d\phi}{d\theta}\right| p(log\frac{\theta}{1-\theta}) \tag{136}$$
$$\propto \left|\frac{d}{d\theta}\left(\frac{\theta}{1-\theta}\right)\right| \tag{137}$$
$$= \theta^{-1}(1-\theta)^{-1} \tag{138}$$

Note that a $Beta(\theta|0, 0)$ distribution can be defined as

$$Beta(\theta|0, 0) = \frac{\theta^{0-1}(1-\theta)^{0-1}}{B(0, 0)} \tag{139}$$
$$\propto \theta^{-1}(1-\theta)^{-1} \tag{140}$$

This result is important, because it shows us that the uniform distribution transformed using the logit function is a $Beta(0, 0)$ distribution, which is an uninformative Beta distribution.

Exercise 3.6. **The Poisson pmf is defined as** $Poi(x|\lambda) = e^{-\lambda}\frac{\lambda^x}{x!}$**, for which** $x \in \{0, 1, 2, ...\}$ **where** $\lambda > 0$ **is the rate parameter. Derive the MLE.**

The MLE is defined as

$$argmax_\lambda p(x|\lambda) = e^{-\lambda}\frac{\lambda^x}{x!} \tag{141}$$
$$argmax_\lambda log\, p(x|\lambda) = -\lambda + xlog\lambda - logx! \tag{142}$$
$$argmin_\lambda - log\, p(x|\lambda) = \lambda - xlog\lambda + logx! \tag{143}$$

By taking the derivate and setting it to 0,

$$0 = \frac{d}{d\lambda} |\lambda - xlog\lambda + logx!| \tag{144}$$

$$= 1 - \frac{x}{\lambda} \tag{145}$$

$$\frac{x}{\lambda} = 1 \tag{146}$$

$$x = \lambda \tag{147}$$

Therefore, the MLE solution to the Poisson is $x = \lambda$.

Exercise 3.7. **a. Derive the posterior $p(\lambda|D)$ assuming a conjugate prior $p(\lambda) = Ga(\lambda|a, b) \propto \lambda^{a-1}e^{-\lambda b}$.**

The posterior is given by

$$p(\lambda|D) = p(D|\lambda)p(\lambda) \tag{148}$$

$$\propto e^{-\lambda}\frac{\lambda^x}{x!}\lambda^{a-1}e^{-\lambda b} \tag{149}$$

$$\propto \lambda^x\lambda^{a-1}e^{-\lambda}e^{-\lambda b} \tag{150}$$

$$= \lambda^{x+a-1}e^{-\lambda(b+1)} \tag{151}$$

$$= Ga(a + x, b + 1) \tag{152}$$

b. What does the posterior mean tend to as $a \to 0$ and $b \to 0$? (Recall that the mean of a $Ga(a, b)$ distribution is a/b.

The posterior mean tends to $Ga(0 + x, 0 + 1) = Ga(x, 1) \to x$ when $a \to 0$ and $b \to 0$.

Exercise 3.8. **Consider a uniform distribution centered on 0 with width $2a$. The density function is given by**

$$p(x) = \frac{1}{2a}I(x \in [-a, a])$$

a. Given a data set $x_1, ..., x_n$, what is the maximum likelihood estimate of a (call it $\hat{a}$)?

$$p(D|a) = \prod_{i=1}^{n} p(x_i|a) \tag{153}$$

$$= \prod_{i=1}^{n} \frac{1}{2a}I(x \in [-a, a]) \tag{154}$$

$$= \frac{1}{(2a)^n}\prod_{i=1}^{n} I(x \in [-a, a]) \tag{155}$$

Since, this is the quantity we want to maximize. Note that it is maximized as a is minimal (first term). The second term nullifies the first term for all x_i that is outside the interval $[-a, a]$. This means that the posterior is maximized for the smallest interval $[-a, a]$ that captures the full range of the data. Formally, the posterior is maximized when

$$\hat{a} = max(|x_i|)$$

b. What probability would the model assign a new data point x_{n+1} using $\hat{a}$?

Since $p(x_{n+1}) = \frac{1}{2\hat{a}} I(x_{n+1} \in [-\hat{a}, \hat{a}])$, it is obvious that x_{n+1} has probability $\frac{1}{2\hat{a}}$ if the point x_{n+1} is in the range $[-\hat{a}, \hat{a}]$, and 0 otherwise.

c. Do you see any problem with the above approach? Briefly suggest (in words) a better approach.

This approach suffers from the zero-count problem. In general, any probability specification that assigns zero probability to inputs that are possible is not ideal. A better solution would to use some Bayesian approach, or add Laplace smoothing.

Exercise 3.9. **Derive the posterior $p(\theta|D)$ of the uniform with a Pareto prior, and show that it can be expressed as a Pareto distribution.**

Note that the Pareto distribution is given by

$$Pareto(\theta|b, K) = bK^b\theta^{-(b+1)} I(\theta \geq K)$$

Using this,

$$\begin{aligned}
p(\theta|D) &= \frac{p(D, \theta)}{p(D)} && (156)\\
&= \frac{\frac{Kb^K}{\theta^{N+K+1}}}{\int_m^\infty \frac{Kb^K}{\theta^{N+K+1}} d\theta} I(\theta \geq max(D)) && (157)\\
&= \begin{cases} \frac{K\theta^{N+K-1}}{K(N+K)b^{N+K}} I(\theta \geq m) & if\, m \leq b \\ \frac{K\theta^{N+K-1}}{Kb^K(N+K)m^{N+K}} I(\theta \geq m) & if\, m > b \end{cases} && (158)\\
&= \frac{\theta^{N+K-1} I(\theta \geq m)}{N+K} \begin{cases} b^{-N-K} & if\, m \leq b \\ b^{-K} m^{-K-N} & if\, m > b \end{cases} && (159)\\
&\propto \theta^{N+K-1} b^{-K} m^{-K-N} I(\theta \geq m) && (160)\\
&= Pareto(\theta| - (K+N), m) && (161)
\end{aligned}$$

Exercise 3.10. **Let's say that taxicars are numbered uniformly like $p(x) = U(0, \theta)$.**

a. Suppose we see one taxi numbered 100, so $D = \{100\}$, $m = 100$, $N = 1$. Using a non-informative prior on θ of the form $p(\theta) = Pa(\theta|0, 0) \propto 1/\theta$, what is the posterior $p(\theta|D)$?

Recall from the previous exercise that the posterior is a Pareto of the form $Pa(\theta|N + K, max(m, b))$. The posterior is then given by

$$p(\theta|D) = p(D|\theta)p(\theta) \tag{162}$$
$$= U(0,\theta)Pa(\theta|0,0) \tag{163}$$
$$= Pa(\theta|N+0, max(100,0)) \tag{164}$$
$$= Pa(\theta|1,100) \tag{165}$$

b. Compute the posterior mean, mode and median number of taxis in the city, if such quantities exist.

We know the form of the posterior, so the posterior mean is the mean of the Pareto distribution, which is given by

$$\mu_{a,b} = \frac{ab}{a-1}$$

therefore, the mean of $Pa(\theta|1,100)$ is $\frac{100}{0}$, which is undefined.

The mode of a $Pa(\theta|a,b)$ is b, so the mode of the posterior is $m = 100$.

The median of a $Pa(\theta|a,b)$ is $2^{1/a}b$, so the mode of the posterior is $2^{1/1} \times 100 = 200$.

c. Compute the predictive density for the next taxicab number.

We can use the above equations to find the prior before witnessing the second taxicab. This prior will be the posterior after seeing the first taxicab number. This posterior is given by $Pa(\theta|1,m)$. Thus, using $b = m$ and $K = 1$, we can plug this into the equation above as

$$p(x|D,K,b) = \frac{K}{(N+K)b^N}I(x \leq m) + \frac{Kb^K}{(N+K)m^{N+K}}I(x > m) \tag{166}$$
$$= \frac{1}{(1+1)m^1}I(x \leq m) + \frac{m^1}{(1+1)x^{1+1}}I(x > m) \tag{167}$$
$$= \frac{1}{2m}I(x \leq m) + \frac{m}{2x^2}I(x > m) \tag{168}$$

d. Use the predictive density to compute the probability that the next taxi you will see (say, the next day) has number 100, 50, or 150, i.e. compute $p(x = 100|D,\alpha)$, etc.

$$p(x = 100|D,\alpha) = \frac{1}{2m}I(x \leq m) + \frac{m}{20000}I(x > m) \tag{169}$$
$$p(x = 50|d,\alpha) = \frac{1}{2m}I(x \leq m) + \frac{m}{5000}I(x > m) \tag{170}$$
$$p(x = 150|d,\alpha) = \frac{1}{2m}I(x \leq m) + \frac{m}{45000}I(x > m) \tag{171}$$

e. Briefly describe some ways we might make the model more accurate at prediction.

We are currently using an uninformative prior, which doesn't seem ideal. There are certain restrictions we could make on the distribution of taxi numbers.

Exercise 3.11. **The exponential distribution with parameter θ is given by $p(x|\theta) = \theta e^{-\theta x}$.**

a. Show that the MLE is given by $\hat{\theta} = 1/\bar{x}$, where $\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$.

The log likelihood is given by

$$log\, p(x|\theta) = \sum_{i=1}^{N} log(\theta e^{-\theta x_i}) \tag{172}$$

$$= \sum_{i=1}^{N} log(\theta) - \theta x_i \tag{173}$$

$$= Nlog(\theta) - \sum_{i=1}^{N} \theta x_i \tag{174}$$

$$= Nlog(\theta) - \theta \sum_{i=1}^{N} x_i \tag{175}$$

Setting the derivative to 0,

$$0 = \frac{d}{d\theta}\left| Nlog(\theta) - \theta \sum_{i=1}^{N} x_i \right| \tag{176}$$

$$= \frac{N}{\theta} - \sum_{i=1}^{N} x_i \tag{177}$$

$$\sum_{i=1}^{N} x_i = \frac{N}{\theta} \tag{178}$$

$$\theta = \frac{N}{\sum_{i=1}^{N} x_i} \tag{179}$$

$$= \frac{1}{\bar{x}} \tag{180}$$

b. Suppose we observe $X_1 = 5$, $X_2 = 6$, $X_3 = 4$. What is the MLE given this data?

The MLE is one over the arithmetic mean, which is $1/mean(5, 6, 4) = 1/5$.

c. Assume that an expert believe θ should have a prior distribution that is also exponential $p(\theta) = Expon(\theta|\lambda)$. Choose the prior parameter, call it $\hat{\lambda}$, such that $E[\theta] = 1/3$.

Note that the exponential distribution is just a special case of the Gamma distribution. In particular, $Expon(x|\theta) = Gamma(x|1, 1/\theta)$. Since we know that the mean of the Gamma distribution is a/b, then we can find the exponential with mean of $1/3$ through the Gamma:

$$Gamma(\theta|1, 3) = Expon(\theta|1/3)$$

d. What is the posterior $p(\theta|D, \hat{\lambda})$?

$$p(\theta|D, \hat{\lambda}) = p(D|\theta, \hat{\lambda})p(\hat{\lambda}) \tag{181}$$
$$= \prod_{i=1}^{N} \theta e^{-\theta x_i} \theta e^{-\theta\lambda} \tag{182}$$
$$= \prod_{i=1}^{N} \theta^2 e^{-\theta(x_i+\lambda)} \tag{183}$$
$$= \theta^{2N} \prod_{i=1}^{N} e^{-\theta\lambda - \theta x_i} \tag{184}$$
$$= \theta^{2N} e^{-\theta(\lambda + \sum_{i=1}^{N} x_i)} \tag{185}$$
$$= Gamma(\theta|2N, \lambda + \sum_{i=1}^{N} x_i) \tag{186}$$

e. Is the exponential prior conjugate to the exponential likelihood?

Yes, both the prior and the likelihood are of the Gamma distribution (remember the exponential distribution is a special case of the Gamma distribution).

f. What is the posterior mean, $E[\theta|D, \hat{\lambda}]$?

The posterior is a Gamma as shown above, which has a mean of a/b.

g. Explain why the MLE and posterior mean differ. Which is more reasonable in this example?

Since the posterior comes from an informative prior ($\hat{\lambda}$), the posterior and the MLE will be different, but equal as $N \to \infty$.

In this example, the posterior is more reasonable, since the prior is more informative.

Exercise 3.12. **The book discussed using a Beta prior for a Bernoulli rate parameter.**

a. Now consider the following prior, that believes the coin is fair, or is slightly biased towards tails:

$$p(\theta) = \begin{cases} 0.5 & if\, \theta = 0.5 \\ 0.5 & if\, \theta = 0.4 \\ 0 & otherwise \end{cases} \tag{187}$$
$$= 0.5I(\theta - 0.5 = 0) + 0.5I(\theta - 0.4 = 0) \tag{188}$$

Derive the MAP estimate under this prior as a function of N_1 and N.

The posterior is given by

$$
\begin{aligned}
p(\theta|D) &= p(D|\theta)p(\theta) && (189)\\
&= \theta^{N_1}(1-\theta)^{N_0}p(\theta) && (190)\\
&= \theta^{N_1}(1-\theta)^{N_0}(0.5I(\theta-0.5=0)+0.5I(\theta-0.4=0)) && (191)\\
&= 0.5^{N_1+N_0+1}I(\theta-0.5=0)+0.5(0.4^{N_1})(0.6^{N_0})I(\theta-0.4=0) && (192)
\end{aligned}
$$

Note that the prior is so restrictive that the likelihood is 0 for all θ except for 0.4 and 0.5. Thus, we can actually compute the likelihood for both of these values of θ and find which one maximizes the likelihood.

So, for each value of θ, the posterior is

$$
\begin{aligned}
p(0.4|D) &\propto (0.4^{N_1})(0.6^{N_0}) && (193)\\
p(0.5|D) &\propto 0.5^{N_1+N_0} && (194)
\end{aligned}
$$

These are functions of N_0 and N_1, and the value of θ that maximizes the posterior will depend of these. We can find these constraints by calling one the MAP and seeing the requirements needed for N_1 and N_0. Let's say that $\theta = 0.4$:

$$
\begin{aligned}
(0.4^{N_1})(0.6^{N_0}) &\geq 0.5^{N_1+N_0} && (195)\\
N_1 log(0.4) + N_0 log(0.6) &\geq (N_1+N_0)log(0.5) && (196)\\
N_1(log(0.4)-log(0.5)) &\geq N_0(log(0.5)-log(0.6)) && (197)\\
N_1 log(\frac{4}{5}) &\geq N_0 log(\frac{5}{6}) && (198)\\
N_1 &\geq \frac{log(5/6)}{log(4/5)}N_0 && (199)\\
&\approx 0.8171 N_0 && (200)
\end{aligned}
$$

Thus, when $N_1 \geq 0.8171N_0$, then $\theta_{MAP} = 0.4$, otherwise $\theta_{MAP} = 0.5$.

b. Suppose the true parameter is $\theta = 0.41$. Which prior leads to a better estimate when N is small? Which prior leads to a better estimate when N is large?

Note the "other" prior in this is when you use a $Beta(\theta|\alpha,\beta)$ prior, which leads to the MAP

$$\hat{\theta} = \frac{N_1+\alpha-1}{N_1+N_0+\alpha+\beta-2}$$

With small datasets, the prior can overwhelm the posterior. Thus, your choice of Beta could greatly influence the posterior in small datasets. For the handmade prior above, the worst that could happen is $\theta = 0.5$, which results in small error, whereas you could have worse error using a Beta prior.

For large datasets, note that the best you can do with the handmade prior is $\theta = 0.4$. When the true value is 0.41, this is not bad error, but note that

using a conjugate prior with large datasets tends to the MLE solution, which, with a large enough dataset can get arbitrarily precise.

Exercise 3.13. **Derive the posterior predictive distribution for a batch of data with the dirichlet-multinomial model.**

Note that the predictive distribution for a single data point is given by

$$p(X = j|D) = \frac{\alpha_j + N_j}{\alpha_0 + N}$$

Since the assumption is that all data points are i.i.d, we can use this as a jumping off point:

$$p(\tilde{D}|D, \alpha) = p(x_1|D, \alpha)p(x_2|D, \alpha, x_1) \cdots p(x_n|D, \alpha, x_1, x_2, \cdots, x_{n-1}) \tag{201}$$

$$= \frac{\prod_{j=1}^{K} \prod_{i=1}^{N_j^{new}-1} \alpha_j + N_j^{old} + i}{\prod_{i=1}^{N-1} \alpha + N^{old} + i} \tag{202}$$

$$= \frac{\prod_{j=1}^{K} (\alpha_j + N_j^{old} + N_j^{new} - 1)!/(\alpha_j + N_j^{old})!}{(\alpha + N^{old} + N - 1)!/(\alpha + N^{old})!} \tag{203}$$

$$= \frac{\prod_{j=1}^{K} \Gamma(\alpha_j + N_j)/\Gamma(\alpha_j + N_j^{old})}{\Gamma(\alpha + N)/\Gamma(\alpha + N^{old})} \tag{204}$$

$$= \frac{\Gamma(\alpha + N^{old})}{\Gamma(\alpha + N)} \prod_{j=1}^{K} \frac{\Gamma(\alpha_j + N_j)}{\Gamma(\alpha_j + N_j^{old})} \tag{205}$$

Exercise 3.14. **a. Suppose we compute the empirical distribution over letters of the Roman alphabet plus the space character (a distribution over 27 values) from 2000 samples. Suppose we see the letter "e" 260 times. What is $p(x_{2001} = e|D)$, if we assume $\theta \sim Dir(\alpha_1, ..., \alpha_{27})$, where $\alpha_k = 10$ for all k?**

Recall that the posterior predictive of the Dirichlet-multinomial model is

$$p(X = j|D) = \frac{\alpha_j + N_j}{\alpha_0 + N}$$

Given that $\alpha_k = 10$ for all k, this is simply

$$p(x_{2001} = e|D) = \frac{10 + 260}{\sum_{k=1}^{K} \alpha_k + 2000} \tag{206}$$

$$= \frac{270}{2270} \approx 0.119 \tag{207}$$

b. Suppose, in the 2000 samples, we saw "e" 260 times, "a" 100 times, and "p" 87 times. What is $p(x_{2001} = p, x_{2002} = a|D)$, if we assume $\theta \sim Dir(\alpha_1, ..., \alpha_{27})$, where $\alpha_k = 10$ for all k?

Note that

$$p(x_{2001} = p, x_{2002} = a|D) = p(x_{2001} = p|D)p(x_{2002} = a|D)$$

since they are conditionally independent events. Using the same framework as above, and letting $\alpha = \sum_{k=1}^{K} \alpha_k = 270$,

$$p(x_{2001} = p, x_{2002} = a|D) = \frac{\alpha_p + N_p}{\alpha + N} \frac{\alpha_a + N_a}{\alpha + N} \tag{208}$$

$$= \frac{97 \times 110}{(270 + 2000)^2} \tag{209}$$

$$\approx 0.0021 \tag{210}$$

Exercise 3.15. **Suppose $\theta \sim \beta(\alpha_1, \alpha_2)$, and we believe that $E[\theta] = m$ and $var[\theta] = v$. Using Equation 2.62, solve for α_1 and α_2 in terms of m and v. What values do you get if $m = 0.7$ and $v = 0.22$?**

Equation 2.62 states that

$$mean = \frac{a}{a+b}, mode = \frac{a-1}{a+b-2}, var = \frac{ab}{(a+b)^2(a+b+1)}$$

for a Beta distribution. Using these, we get a system of equations

$$m = \frac{a}{a+b} \tag{211}$$

$$m(a+b) = a \tag{212}$$

$$mb = a(1-m) \tag{213}$$

$$b = \frac{a(1-m)}{m} \tag{214}$$

By plugging this into the variance function above, it can be shown that

$$a = m\left(\frac{m(1-m)}{v} - 1\right)$$

which you can then plug back into the equation for b above to get

$$b = (1-m)\left(\frac{m(1-m}{v} - 1\right)$$

If $m = 0.7$ and $v = 0.2^2 = 0.04$, then

$$a = 0.7\left(\frac{0.7(1-0.7)}{0.04} - 1\right) = 2.975$$

and

$$b = (1-0.7)\left(\frac{0.7(1-0.7)}{0.04} - 1\right) = 1.275$$

Exercise 3.16. **Suppose $\theta \sim \beta(\alpha_1, \alpha_2)$ and we believe that $E[\theta] = m$ and $p(l < \theta < u) = 0.95$. Write a program that can solve for α_1 and α_2 in terms of m, and u.**

We know the mean, so we can write

$$m = \frac{\alpha_1}{\alpha_1 + \alpha_2} \tag{215}$$

$$m(\alpha_1 + \alpha_2) = \alpha_1 \tag{216}$$

$$m\alpha_2 = \alpha_1 - m\alpha_1 \tag{217}$$

$$\alpha_2 = \frac{\alpha_1}{m} - \alpha_1 \tag{218}$$

We are given the quantiles, which we can express as

$$\int_l^u \frac{1}{B(\alpha_1, \alpha_2)} \theta^{\alpha_1 - 1}(1-\theta)^{\alpha_2 - 1} d\theta = I_u(\alpha_1, \alpha_2) - I_l(\alpha_1, \alpha_2) \tag{219}$$

where $I_x(\alpha_1, \alpha_2) = \int_0^x Beta(\alpha_1, \alpha_2)$ is the regularized incomplete beta function. We can minimize the squared discrepancy between this and 0.95:

$$0 = \frac{d}{d\theta}[(I_u(\alpha_1, \alpha_2)d\theta - I_l(\alpha_1, \alpha_2)d\theta - 0.95)^2] \tag{220}$$

$$0 = I_u(\alpha_1, \alpha_2) - I_l(\alpha_1, \alpha_2) - 0.95 \tag{221}$$

Since this exercise involves writing a program, the code for this program is found in an IPython notebook in this same directory.

Exercise 3.17. **Suppose we toss a coin N times and observe N_1 heads. Let $N_1 \sim Bin(N, \theta)$ and $\theta \sim Beta(1, 1)$. Show that the marginal likelihood is $p(N_1|N) = 1/(N+1)$.**

The key here is that N_1 and N are sufficient statistics. Remember that the posterior of the Beta-Binomial model is given by

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} \tag{222}$$

$$= Beta(\theta|N_1 + a, N_0 + b) \tag{223}$$

$$p(D) = \frac{p(D|\theta)p(\theta)}{Beta(\theta|N_1 + a, N_0 + b)} \tag{224}$$

The marginal likelihood is given by

$$p(N_1|N) = \int_\theta \frac{p(N_1|\theta, N)p(\theta|N)}{p(N_1, N)} d\theta \tag{225}$$

$$= \int_\theta \frac{Bin(N_1|\theta, N)Beta(\theta|1, 1)}{Beta(\theta|N_1 + 1, N_0 + 1)} d\theta \tag{226}$$

Since we are marginalizing over θ, we can rewrite these using Beta functions, like

$$p(N_1|N) = \binom{N}{N_1} \frac{B(N_1+1, N-N_1+1)}{B(N_1+1, N-N_1+1)/B(N_1, N-N_1)} \tag{227}$$

$$= \binom{N}{N_1} \frac{B(N_1+1, N-N_1+1)}{B(1,1)} \tag{228}$$

$$= \binom{N}{N_1} \frac{\Gamma(N_1+1)\Gamma(N-N_1+1)}{\Gamma(N+2)} \tag{229}$$

$$= \frac{N!}{N_1!(N-N_1)!} \frac{\Gamma(N_1+1)\Gamma(N-N_1+1)}{\Gamma(N+2)} \tag{230}$$

$$= \frac{N!N_1!(N-N_1)!}{N_1!(N-N_1)!(N+1)!} \tag{231}$$

$$= \frac{N!}{(N+1)N!} \tag{232}$$

$$= \frac{1}{N+1} \tag{233}$$

Exercise 3.18. **Suppose we toss a coin $N = 10$ times and observe $N_1 = 9$ heads. Let the null hypothesis be that the coin is fair, and the alternative be that the coin can have any bias, so $p(\theta) = Unif(0,1)$. Derive the Bayes factor $BF_{1,0}$ in favor of the biased coin hypothesis. What if $N = 100$ and $N_1 = 90$?**

The Bayes factor is defined as

$$BF_{1,0} = \frac{p(D|alt)}{p(D|null)}$$

Let's look into the null hypothesis first. The null hypothesis says that the coin is not biased, meaning $\theta = 0.5$. Thus, the likelihood is

$$p(N_1|\theta = 0.5) = \binom{N}{N_1} 0.5^{N_1} 0.5^{N-N_1} = \binom{N}{N_1} 0.5^N$$

Note that the alternative hypothesis marginalizes across all θ, and as we saw in the last exercise, this is $\frac{1}{N+1}$.

So, the Bayes Factor is

$$BF_{1,0} = \frac{1}{\binom{N}{N_1}(N+1)0.5^N} \tag{234}$$

$$= \frac{2^N}{\binom{N}{N_1}(N+1)} \tag{235}$$

Thus, is $N = 10$ and $N_1 = 9$, then the Bayes Factor is 9.31. This is moderately strong evidence to accept the alternative.

If $N = 100$ and $N_1 = 90$, then the Bayes Factor is 7.251×10^{14}. This is very strong evidence to accept the alternative.

Exercise 3.19. **This question sets up Naive Bayes as a linear classifier. a. Write down an expression for the log posterior odds ratio, in terms of the features and the parameters.**

The log posterior odds ratio is

$$log\frac{p(c=1|x_i)}{p(c=2|x_i)} = log\frac{p(x_i|c=1,\theta)p(c=1)}{p(x_i|c=2,\theta)p(c=2)} \tag{236}$$

$$= log\frac{p(x_i|c=1,\theta)}{p(x_i|c=2,\theta)} \tag{237}$$

$$= logp(x_i|c=1,\theta) - logp(x_i|c=2,\theta) \tag{238}$$

$$= \phi(x_i)^T\beta_1 - \phi(x_i)^T\beta_2 \tag{239}$$

$$= \phi(x_i)^T(\beta_1 - \beta_2) \tag{240}$$

b. Intuitively, words that occur in both classes are not very "discriminative", and therefore should not affect our beliefs about the class label. Consider a particular word w. State the conditions on $\theta_{1,w}$ and $\theta_{2,w}$ (or equivalently the conditions on $\beta_{1,w}$, $\beta_{2,w}$) under which the presence or absence of w in a test document will have no effect on the class posterior (such a word will be ignored by the classifier). Hint: using your previous result, figure out when the posterior odds ratio is $0.5/0.5$**.**

For a word w to have no effect on the posterior, the log posterior odds should equal 1. Since the model is linear, we can narrow this down to one word. We also note that we are considering words that exist in both classes, so $\phi(x_{i,w}) = 1$. So,

$$1 = \phi(x_i)^T(\beta_1 - \beta_2) \tag{241}$$

$$\beta_1 = \beta_2 \tag{242}$$

$$log\frac{\theta_{1,w}}{1-\theta_{1,w}} = log\frac{\theta_{2,w}}{1-\theta_{2,w}} \tag{243}$$

$$\frac{\theta_{1,w}}{1-\theta_{1,w}} = \frac{\theta_{2,w}}{1-\theta_{2,w}} \tag{244}$$

$$\theta_{1,w}(1-\theta_{2,w}) = \theta_{2,w}(1-\theta_{1,w}) \tag{245}$$

$$\theta_{1,w} - \theta_{1,2}\theta_{2,w} = \theta_{2,w} - \theta_{1,w}\theta_{2,w} \tag{246}$$

$$\theta_{1,w} = \theta_{2,w} \tag{247}$$

c. Let there be n_1 documents of class 1 and n_2 be the number of documents in class 2, where $n_1 = n_2$ (since e.g., we get much more non-spam than spam; this is an example of class imbalance). If we use

the above estimate for $\theta_{c,w}$, will word w be ignored by our classifier? Explain why or why not.

Since the word is in all documents, then the given estimates $\hat{\theta}_{cw}$ are

$$\hat{\theta}_{1w} = \frac{1+n_1}{2+n_1} \tag{248}$$

$$\hat{\theta}_{2w} = \frac{1+n_2}{2+n_2} \tag{249}$$

Since $n_1 \neq n_2$, these quantities are not equal. We saw in part (b) that the necessary requirement for the model to ignore a word is for $\theta_{1w} = \theta_{2w}$, so we can be sure that the model will not ignore this word.

d. What other ways can you think of which encourage "irrelevant" words to be ignored?

Weighting each word by frequency using TF-IDF for example.

Exercise 3.20. **a. How would you specify a "full" model that doesn't use Naive Bayes assumption? How many parameters would it have?**

The Naive Bayes assumption allows for significant simplification in the model specification. Without it, the best you could do is to use the chain-rule of probability:

$$p(x_{1:D}|y=c) = p(x_1|y=c)p(x_2|x_1, y=c)\cdots p(x_D|x_1, ..., x_{D-1}, y=c)$$

The Naive Bayes assumption allows us to trim down the contingency table to a workable amount. Since the features are binary, the number of parameters in the full model is 2^D.

b. Assume the number of features D is fixed. Let there be N training cases. If the sample size N is very small, which model (naive Bayes or full) is likely to give lower test set error, and why?

The number of parameters in the naive Bayes model is DC vs. 2^D for the full model. So, if N is very small while D remains fixed, it is very likely that the full model will be over-parameterized and overfit on the training set. Therefore, in this case, the naive Bayes model will perform better on the test set, since it avoids the curse of dimensionality.

c. What if the sample size N was very large?

In this case, the conditional independence assumption that the naive Bayes model uses may be too restrictive to capture the patterns in the data, and therefore the full model will likely perform better.

d. What is the computational complexity of fitting the full and naive Bayes model as a function of N and D?

Both of the models are $O(ND)$ worst case, since we can assume that it takes $O(D)$ time to convert a bit array to an array index.

e. What is the computational complexity at test time for the full and naive Bayes model?

The complexity for naive Bayes at test time is $O(CD)$. For the full model, we loop through the classes and lookup the joint probability to use as the prediction. So, the complexity is $O(CD)$. Note that in the full model, D is a much larger number than in naive Bayes.

f. Suppose the test case has missing data. Let x_v be the visible features of size v, and x_h be the hidden (missing) features of size h, where $v+h=D$. What is the computational complexity of computing $p(y|x_v,\hat{\theta})$ for the full and naive Bayes models, as a function of v and h?

The naive Bayes model could just skip over the missing features, so therefore the complexity would still be $O(CD)$. The full model, however, would have to create entries for all possible combinations of missing and non-missing features, which would be $O(2^h D)$.

Exercise 3.21. **Derive equation 3.76**

$$I(X,Y) = \sum_{x_j}\sum_{y} p(x_j,y) log \frac{p(x_j,y)}{p(x_j)p(y)} \tag{250}$$

$$= \sum_{x_j}\sum_{y} p(x_j|y)p(y) log \frac{p(x_j|y)p(y)}{p(x_j)p(y)} \tag{251}$$

$$= \sum_{x_j}\sum_{y} p(x_j|y)p(y) log \frac{p(x_j|y)}{p(x_j)} \tag{252}$$

Since it is given that the features are binary, we can expand the summation:

$$I(X,Y) = \sum_{x_j}\sum_{y} p(x_j|y)p(y) log \frac{p(x_j|y)}{p(x_j)} \tag{253}$$

$$= \sum_{y} p(x_j|y)p(y) log \frac{p(x_j|y)}{p(x_j)} + (1-p(x_j|y)p(y) log \frac{1-p(x_j|y)}{1-p(x_j)} \tag{254}$$

$$= \sum_{y} \theta_{jy}\pi_y log \frac{\theta_{jy}}{\theta_j} + (1-\theta_{jy})\pi_y log \frac{1-\theta_{jy}}{1-\theta_j} \tag{255}$$

4 Gaussian Models

Exercises

Exercise 4.1. **Let $X \sim U(1,1)$ and $Y = X^2$. Clearly Y is dependent on X (in fact, Y is uniquely determined by X). However, show that $\rho(X,Y) = 0$. Hint: if $X \sim U(a,b)$ then $E[X] = (a+b)/2$ and $var[X] = (ba)^2/12$.**

Let's plug things into the definition of correlation:

$$\rho(X,Y) = \frac{cov(X,Y)}{\sigma_X \sigma_Y} \tag{256}$$

$$= \frac{E[XY] - E[X]E[Y]}{\sigma_X \sigma_Y} \tag{257}$$

$$= \frac{E[X^3] - E[X]E[X^2]}{\sigma_X \sigma_{X^2}} \tag{258}$$

Note that to show this equals 0, we just have to show that the numerator is equal to 0. To do this, we will compute each term:

$$E[X^3] = \frac{1}{2}\int_{-1}^{1} u^3 p(u) du = 0$$

$$E[X^2] = \frac{1}{2}\int_{-1}^{1} u^2 p(u) du = \frac{1}{3}$$

$$E[X] = \frac{-1+1}{2} = 0$$

So we have

$$\rho(X,Y) = \frac{E[X^3] - E[X]E[X^2]}{\sigma_X \sigma_{X^2}} \tag{259}$$

$$= \frac{0 - 0 \times \frac{1}{3}}{\sigma_X \sigma_{X^2}} \tag{260}$$

$$= 0 \tag{261}$$

Exercise 4.2. **Let $X \sim N(0,1)$ and $Y = WX$, where $p(W = 1) = p(W = 1) = 0.5$. It is clear that X and Y are not independent, since Y is a function of X.**

a. Show that $Y \sim N(0,1)$.

So, W randomly changes the sign half the time on X. Thus,

$$Y \sim \frac{1}{2}N(0,1) - \frac{1}{2}N(0,1)$$

Let's write the distribution out for this:

$$p(Y|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(WX-\mu)^2}{2\sigma^2}} \tag{262}$$

$$= \frac{1}{2\sqrt{2\pi\sigma^2}} e^{-\frac{(-X-\mu)^2}{2\sigma^2}} + \frac{1}{2\sqrt{2\pi\sigma^2}} e^{-\frac{(X-\mu)^2}{2\sigma^2}} \tag{263}$$

$$= \frac{1}{2\sqrt{2\pi}} e^{-\frac{(-X)^2}{2}} + \frac{1}{2\sqrt{2\pi}} e^{-\frac{X^2}{2}} \tag{264}$$

$$= \frac{1}{2\sqrt{2\pi}} \left(e^{-\frac{X^2}{2}} + e^{-\frac{X^2}{2}} \right) \tag{265}$$

$$= \frac{1}{2\sqrt{2\pi}} \left(2e^{-\frac{X^2}{2}} \right) \tag{266}$$

$$= \frac{1}{\sqrt{2\pi}} e^{-\frac{X^2}{2}} \tag{267}$$

$$= N(0,1) \tag{268}$$

b. Show that $cov[X,Y] = 0$**.**

$$cov[X,Y] = E[XY] - E[X]E[Y] \tag{269}$$

$$= E[E[XY|W]] - E[X]E[WX] \tag{270}$$

$$= \frac{1}{2}E[X^2] + \frac{1}{2}E[-X^2] - E[X]E[WX] \tag{271}$$

$$= \frac{1}{2}E[X^2] + \frac{1}{2}E[X^2] - E[X]E[WX] \tag{272}$$

$$= E[X^2] - E[X](\frac{1}{2}E[^2] + \frac{1}{2}E[-X^2]) \tag{273}$$

$$= E[X^2] - E[X^2] \tag{274}$$

$$= 0 \tag{275}$$

Exercise 4.3. **Prove that** $-1 \leq \rho(X,Y) \leq 1$

$$\rho(X,Y) = \frac{cov(X,Y)}{\sigma_X \sigma_Y}$$

This is trivial to prove with the Cauchy-Swartz inequality which states that

$$|cov(X,Y)| \leq \sqrt{\sigma_X^2 \sigma_Y^2}$$

because for $\rho(X,Y)$ to be > 1 or < -1, then $|cov(X,Y)| > \sqrt{\sigma_X^2 \sigma_Y^2}$, which is false.

Exercise 4.4. **Show that, if** $Y = aX + b$ **for some parameters** $a > 0$ **and** b**, then** $\rho(X,Y) = 1$**. Similarly show that if** $a < 0$**, then** $\rho(X,Y) = -1$**.**

$$\rho(X,Y) = \frac{cov(X,Y)}{\sigma_X \sigma_Y} \tag{276}$$

$$= \frac{E[(X - E[X])(Y - E[Y])]}{\sqrt{E[(X - E[X])^2]E[(Y - E[Y])^2]}} \tag{277}$$

$$\tag{278}$$

Note that the quantity $(Y - E[Y])$ can be written as

$$Y - E[Y] = aX + b - E[aX + b] \tag{279}$$

$$= aX + b - b - aE[X] \tag{280}$$

$$= a(X - E[X]) \tag{281}$$

Plugging this, we get

$$\rho(X,Y) = \frac{aE[(X - E[X])(X - E[X])]}{|a|\sqrt{E[(X - E[X])^2]E[(X - E[X])^2]}} \tag{282}$$

$$= \frac{E[(X - E[X])(X - E[X])]}{E[(X - E[X])^2]} \tag{283}$$

$$= \frac{E[(X - E[X])^2]}{E[(X - E[X])^2]} \tag{284}$$

$$= 1 \tag{285}$$

If $a < 0$, then this changes to

$$\rho(X,Y) = \frac{aE[(X - E[X])^2]}{|a|\sqrt{E[(X - E[X])^2]E[(X - E[X])^2]}} \tag{286}$$

$$= -\frac{E[(X - E[X])^2]}{E[(X - E[X])^2]} \tag{287}$$

$$= -1 \tag{288}$$

Exercise 4.5. **Derive the normalization constant for multivariate Gaussian.**

We are trying to show that

$$(2\pi)^{D/2}|\Sigma|^{1/2} = \int exp(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu))dx$$

Using eigenvalue decomposition on $\Sigma = U\Lambda U^T$, we can write this as

$$(2\pi)^{D/2}|\Sigma|^{1/2} = \int exp(-\frac{1}{2}(x-\mu)^T U\Lambda^{-1}U^T(x-\mu))dx \tag{289}$$

$$= \int exp(-\frac{1}{2}u^T\Lambda^{-1}u)du \tag{290}$$

$$= \int exp(-\frac{1}{2}\sum_d \frac{u_d^2}{\lambda_d})du \tag{291}$$

$$= \prod_{i=1}^{D} \int exp(-\frac{u_i^2}{2\lambda_i})du \tag{292}$$

Note that this is the product of single dimensional Gaussians. We know that $\int exp(-\frac{u^2}{2\sigma^2}) = \sqrt{2\pi\sigma^2}$, and so we can rewrite this expression as

$$\prod_{i=1}^{D} \int exp(-\frac{u_i^2}{2\lambda_i})du = \prod_{i=1}^{D} \sqrt{2\pi\lambda_i} \tag{293}$$

$$= (2\pi)^{D/2} \prod_{i=1}^{D} \lambda_i^{1/2} \tag{294}$$

$$= (2\pi)^{D/2}|\Sigma|^{1/2} \tag{295}$$

Exercise 4.6. **Derive the pdf of the bivariate Guassian with Σ given.**
Note that

$$\Sigma^{-1} = \frac{1}{\sigma_1^2\sigma_2^2 - \rho^2\sigma_1^2\sigma_2^2}\begin{bmatrix} \sigma_2^2 & -\rho\sigma_1\sigma_2 \\ -\rho\sigma_1\sigma_2 & \sigma_1^2 \end{bmatrix} \tag{296}$$

and

$$(x-\mu)^T\Sigma^{-1}(x-\mu) = \frac{1}{\sigma_1^2\sigma_2^2-\rho^2\sigma_1^2\sigma_2^2}\begin{bmatrix}x_1-\mu_1 & x_2-\mu_2\end{bmatrix}\begin{bmatrix}\sigma_2^2 & -\rho\sigma_1\sigma_2\\ -\rho\sigma_1\sigma_2 & \sigma_1^2\end{bmatrix}\begin{bmatrix}x_1-\mu_1\\ x_2-\mu_2\end{bmatrix} \tag{297}$$

$$= \frac{1}{\sigma_1^2\sigma_2^2-\rho^2\sigma_1^2\sigma_2^2}\begin{bmatrix}\sigma_1^2(x_1-\mu_1)+\rho\sigma_1\sigma_2(x_2-\mu_n) & \rho\sigma_1\sigma_2(x_1-\mu_1)+\sigma_2^2(x_2-\mu_n)\end{bmatrix}\begin{bmatrix}x_1-\mu_1\\ x_2-\mu_2\end{bmatrix} \tag{298}$$

$$= \frac{1}{\sigma_1^2\sigma_2^2-\rho^2\sigma_1^2\sigma_2^2}(x_1-\mu_1)(\sigma_1^2(x_1-\mu_1)+\rho\sigma_1\sigma_2(x_2-\mu_2))+(x_2-\mu_2)(\rho\sigma_1\sigma_2(x_1-\mu_1)+\sigma_2^2(x_2-\mu_2)) \tag{299}$$

$$= \frac{1}{\sigma_1^2\sigma_2^2-\rho^2\sigma_1^2\sigma_2^2}\sigma_1^2(x_1-\mu_1)^2+2\rho\sigma_1\sigma_2(x_1-\mu_1)(x_2-\mu_2)+\sigma_2^2(x_2-\mu_2)^2 \tag{300}$$

$$= \frac{1}{1-\rho^2}\frac{\sigma_1^2(x_1-\mu_1)^2}{\sigma_1^2\sigma_2^2}+\frac{2\rho\sigma_1\sigma_2(x_1-\mu_1)(x_2-\mu_2)}{\sigma_1^2\sigma_2^2}+\frac{\sigma_2^2(x_2-\mu_2)^2}{\sigma_1^2\sigma_2^2} \tag{301}$$

$$= \frac{1}{1-\rho^2}\left(\frac{(x_1-\mu_1)^2}{\sigma_1^2}+\frac{(x_2-\mu_2)^2}{\sigma_2^2}+2\rho\frac{(x_1-\mu_1)}{\sigma_1}\frac{(x_2-\mu_2)}{\sigma_2}\right) \tag{302}$$

We see that this is the quantity requested of us in the exercise.

Exercise 4.7. **Compute the conditional probability distribution of the given bivariate Gaussian.**

Note that the conditional probability of two Gaussians is a Gaussian. Also the conditional probability distribution is given by

$$p(x_1|x_2) = N(x_1|\mu_{1|2},\Sigma_{1|2}) \tag{303}$$

$$\mu_{1|2} = \mu_1+\Sigma_{12}\Sigma_{22}^{-1}(x_2-\mu_2) \tag{304}$$

$$\Sigma_{1|2} = \Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} \tag{305}$$

It simplifies things greatly that we are considering a bivariate Gaussian, since Σ_{jk} becomes a scalar. Thus, after plugging in to the equations given in the problem,

$$p(x_2|x_1) = N(x_2|\mu_{2|1},\Sigma_{2|1}) \tag{306}$$

$$\mu_{2|1} = \mu_2+\sigma_1\sigma_2(\rho\frac{\sigma_2}{\sigma_1}(x_1-\mu_1)) \tag{307}$$

$$= \mu_2+\rho\sigma_2^2(x_1-\mu_1) \tag{308}$$

$$\Sigma_{2|1} = \sigma_1\sigma_2\frac{\sigma_2}{\sigma_1}-\sigma_1\sigma_2\rho^2\frac{\sigma_2}{\sigma_1} \tag{309}$$

$$= \sigma_2^2+\rho^2\sigma_2^2 \tag{310}$$

$$p(x_2|x_1) = N(x_2|\mu_2+\rho\sigma_2^2(x_1-\mu_1),\rho^2\sigma_2^2) \tag{311}$$

If $\sigma_2 = \sigma_1 = 1$, then

$$p(x_2|x_1) = N(x_2|\mu_2 + \rho(x_1 - \mu_1), \rho^2)$$

Exercise 4.8. **This exercise is shown in the R notebook "ch4-8.ipynb"**

Exercise 4.9. **Suppose you have two sensors with known (and different) variances ν_1 and ν_2, but unknown and same mean μ. What is the posterior $p(\mu|D)$, assuming a non-informative prior for μ?**

In section 4.4.2.1 we saw that the posterior of some observed data from some noisy measurements of this is given by

$$p(\mu|y_1, y_2, ..., y_n) = 0p(\mu|D, \Sigma) \qquad = N(\mu|m_N, V_N) \tag{312}$$

$$V_N^{-1} = V_0^{-1} + N\Sigma^{-1} \tag{313}$$

$$m_N = V_N(\Sigma^{-1}(N\bar{x}) + V_0^{-1}m_0) \tag{314}$$

$$\tag{315}$$

By assuming an uninformative prior, we are saying that $V_0 = \infty I$, which simplifies these to

$$p(\mu|D, \Sigma) = N(\mu|\bar{x}, \frac{1}{N}\Sigma) \tag{316}$$

$$\tag{317}$$

TODO

Exercise 4.10. **Derive the information form results of Section 4.3.1.**

The information form the Gaussian distribution is given by

$$N(x|\xi, \Lambda) = (2\pi)^{D/2}|\Lambda|^{1/2}exp\left[-\frac{1}{2}(x^T\Lambda x + \xi^T\Lambda^{-1}\xi - 2x^T\xi)\right] \tag{318}$$

$$\propto exp\left[-\frac{1}{2}(x^T\Lambda x + \xi^T\Lambda^{-1}\xi - 2x^T\xi)\right] \tag{319}$$

$$= exp\left[-\frac{1}{2}\begin{pmatrix}x_1\\x_2\end{pmatrix}^T\begin{pmatrix}\Lambda_{11} & \Lambda_{12}\\\Lambda_{21} & \Lambda_{22}\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix} + \begin{pmatrix}\xi_1\\\xi_2\end{pmatrix}^T\begin{pmatrix}\Lambda_{11} & \Lambda_{12}\\\Lambda_{21} & \Lambda_{22}\end{pmatrix}^{-1}\begin{pmatrix}\xi_1\\\xi_2\end{pmatrix} - 2\begin{pmatrix}x_1\\x_2\end{pmatrix}^T\begin{pmatrix}\xi_1\\\xi_2\end{pmatrix}\right] \tag{320}$$

$$= exp[-\frac{1}{2}x_2(x_1\Lambda_{12} + x_2\Lambda_{22}) + x_1(x_1\Lambda_{11} + x_2\Lambda_{21}) + \tag{321}$$

$$\begin{pmatrix}\xi_1\\\xi_2\end{pmatrix}^T\begin{pmatrix}I & 0\\-\Lambda_{22}^{-1}\Lambda_{21} & I\end{pmatrix}\begin{pmatrix}(\Lambda_{11} - \Lambda_{12}\Lambda_{22}^{-1}\Lambda_{21})^{-1} & 0\\0 & \Lambda_{22}^{-1}\end{pmatrix}\begin{pmatrix}I & -\Lambda_{12}\Lambda_{22}^{-1}\\0 & I\end{pmatrix}\begin{pmatrix}\xi_1\\\xi_2\end{pmatrix} - 2x_1\xi_1 - 2x_2\xi_2] \tag{322}$$

$$N(x|\xi, \Lambda) = N(x|\Sigma^{-1}\mu, \Sigma^{-1})$$

The statements we are trying to prove is

$$p(x_1) = N(x_1|\mu_1, \Sigma_{11}) \tag{323}$$
$$p(x_2) = N(x_2|\mu_2, \Sigma_{22}) \tag{324}$$
$$p(x_1|x_2) = N(x_1|\mu_{1|2}, \Sigma_{1|2}) \tag{325}$$
$$\mu_{1|2} = \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \tag{326}$$
$$\Sigma_{1|2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} = \Lambda_{11}^{-1} \tag{327}$$

Exercise 4.11. **Derive equation 4.209**

The posterior is given by

$$p(\mu, \Sigma|D) = \frac{p(D|\mu, \Sigma)p(\mu, \Sigma)}{p(D)} \tag{328}$$
$$\propto p(D|\mu, \Sigma)NIW(\mu, \Sigma|m_0, \kappa_0, \upsilon_0, S_0) \tag{329}$$
$$= (2\pi)^{ND/2}|\Sigma|^{-\frac{N}{2}} exp(-\frac{N}{2}(\mu - \bar{x})^T\Sigma^{-1}(\mu - \bar{x}) - \frac{1}{2}tr(\Sigma^{-1}S_{\bar{x}})) \tag{330}$$
$$\times NIW(\mu, \Sigma|m_0, \kappa_0, \upsilon_0, S_0) \tag{331}$$
$$\propto |\Sigma|^{-\frac{N}{2}} exp(-\frac{N}{2}(\mu - \bar{x})^T\Sigma^{-1}(\mu - \bar{x}) - \frac{1}{2}tr(\Sigma^{-1}S_{\bar{x}})) \tag{332}$$
$$\times |\Sigma|^{-\frac{\upsilon_0+D+2}{2}} exp(-\frac{\kappa_0}{2}(\mu - m_0)^T\Sigma^{-1}(\mu - m_0) - \frac{1}{2}tr(\Sigma^{-1}S_0)) \tag{333}$$
$$= |\Sigma|^{-\frac{\upsilon_0+D+2+N}{2}} exp(-\frac{N}{2}(\mu - \bar{x})^T\Sigma^{-1}(\mu - \bar{x}) - \frac{\kappa_0}{2}(\mu - m_0)^T\Sigma^{-1}(\mu - m_0) \tag{334}$$
$$- \frac{1}{2}tr(\Sigma^{-1}S_0) - \frac{1}{2}tr(\Sigma^{-1}S_{\bar{x}})) \tag{335}$$
$$= |\Sigma|^{-\frac{\upsilon_N+D+2}{2}} exp(-\frac{\kappa_N}{2}(\mu - m_N)^T\Sigma^{-1}(\mu - m_N) - \frac{1}{2}tr(\Sigma^{-1}S_N)) \tag{336}$$
$$= NIW(\mu, \Sigma|m_N, \kappa_N, \upsilon_N, S_N) \tag{337}$$

Exercise 4.12. **a. Derive the BIC score for a Gaussian with dimension D will full covariance matrix.**

The BIC is given by

$$BIC = log\, p(D|\hat{\mu}, \hat{\Sigma}) - \frac{d}{2} log(N) \tag{338}$$
$$= -\frac{N}{2} tr(\hat{\Sigma}^{-1}\hat{S}) - \frac{N}{2} log(|\hat{\Sigma}|) - \frac{d}{2} log(N) \tag{339}$$
$$= -\frac{N}{2} tr(\hat{\Sigma}^{-1}\hat{\Sigma}) - \frac{N}{2} log(|\hat{\Sigma}|) - \frac{d}{2} log(N) \tag{340}$$
$$= -\frac{Nd}{2} - \frac{N}{2} log(|\hat{\Sigma}|) - \frac{d}{2} log(N) \tag{341}$$
$$= -\frac{1}{2}(Nd + dlog(N) + Nlog(|\hat{\Sigma}|)) \tag{342}$$

b. Derive the BIC for a Gaussian with diagonal covariance matrix.

Note that for diagonal matrices, the determinant is just the product of the diagonals. Thus, we can reduce the above equation to

$$BIC = log\, p(D|\hat{\mu}, \hat{\Sigma}) - \frac{d}{2} log(N) \tag{343}$$
$$= -\frac{1}{2}(Nd + dlog(N) + Nlog(|\hat{\Sigma}|)) \tag{344}$$
$$= -\frac{1}{2}(Nd + dlog(N) + Nlog(\prod_{i=1}^{d} \sigma_i)) \tag{345}$$
$$= -\frac{1}{2}(Nd + dlog(N) + N\sum_{i=1}^{d} log(\sigma_i)) \tag{346}$$

Exercise 4.13. **Compute the sample size needed to compute the given Bayesian credible interval.**

From the text, we see that the posterior of the mean is given by

$$p(\mu|D, \Sigma) = N(\mu|m_N, V_N) \tag{347}$$
$$V_N^{-1} = V_0^{-1} + N\Sigma^{-1} \tag{348}$$
$$m_N = V_N(\Sigma^{-1}(N\bar{x}) + V_0^{-1} m_0) \tag{349}$$

Plugging these into what's given in the problem we get

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2} \tag{350}$$
$$\frac{N}{\sigma^2} = \frac{1}{\sigma_N^2} - \frac{1}{\sigma_0^2} \tag{351}$$
$$N = \frac{\sigma^2}{\sigma_N^2} - \frac{\sigma^2}{\sigma_0^2} \tag{352}$$
$$= \sigma^2 \left(\frac{1}{\sigma_N^2} - \frac{1}{\sigma_0^2} \right) \tag{353}$$

Plugging in the known values, we see that

$$N = \sigma^2 \left(\frac{1}{\sigma_N^2} - \frac{1}{\sigma_0^2} \right) \tag{354}$$

$$= 4 \left(\frac{1}{\sigma_N^2} - \frac{1}{9} \right) \tag{355}$$

$$\tag{356}$$

Now all we need to know is σ_N^2 to compute this. For this, we know that the interval must be of width 1. We can use this to show that

$$u - l = 1 = (\mu_N + 1.96\sigma_N) - (\mu_N - 1.96\sigma_N) \tag{357}$$

$$1 + \mu_N - 1.96\sigma_N = \mu_N + 1.96\sigma_N \tag{358}$$

$$1 = 3.92\sigma_N \tag{359}$$

$$\sigma_N = \frac{1}{3.92} \tag{360}$$

$$\sigma_N^2 = \frac{1}{3.92^2} \tag{361}$$

Now we can plug everything in to get

$$N = 4 \left(\frac{1}{\sigma_N^2} - \frac{1}{9} \right) \tag{362}$$

$$= 4 \left(3.92^2 - \frac{1}{9} \right) \tag{363}$$

$$\approx 61.02 \tag{364}$$

For sample sizes we always round up, so the sample size is $N = 62$.

Exercise 4.14. **a. Calculate the MAP estimate of μ for a 1-d Gaussian.**
The posterior is given by

$$p(\mu|D) \propto p(D|\mu)p(\mu) \tag{365}$$

$$= N(\mu, m_N, V_N) \tag{366}$$

$$V_N^{-1} = V_0^{-1} + N\Sigma^{-1} \tag{367}$$

$$m_N = V_N(\Sigma^{-1}(N\bar{x}) + V_0^{-1}m_0) \tag{368}$$

Because the mode is the mean of a Gaussian, we can compute the posterior mean of the distribution and this will be the MAP estimate.

$$p(\mu|D) = N(\mu, m_N, V_N) \tag{369}$$
$$m_N = V_N(\Sigma^{-1}(N\bar{x}) + V_0^{-1}m_0) \tag{370}$$
$$= V_N(\frac{N\bar{x}}{\sigma^2} + \frac{m}{s^2}) \tag{371}$$
$$V_N = \left(\frac{1}{s^2} + \frac{N}{\sigma^2}\right)^{-1} = \frac{s^2\sigma^2}{\sigma^2 + Ns^2} \tag{372}$$
$$m_N = \frac{s^2\sigma^2}{\sigma^2 + Ns^2}\left(\frac{N\bar{x}}{\sigma^2} + \frac{m}{s^2}\right) \tag{373}$$
$$= \frac{N\bar{x}s^2\sigma^2}{\sigma^2(\sigma^2 + Ns^2)} + \frac{s^2\sigma^2 m}{s^2(\sigma^2 + Ns^2)} \tag{374}$$
$$= \frac{N\bar{x}s^2}{\sigma^2 + Ns^2} + \frac{\sigma^2 m}{\sigma^2 + Ns^2} \tag{375}$$
$$= \frac{N\bar{x}s^2 + \sigma^2 m}{\sigma^2 + Ns^2} \tag{376}$$

This is the MAP estimate of the mean.

b. Show that as the number of samples n, the MAP estimate converges to the MLE.

$$\hat{\mu}_{MAP} = \frac{N\bar{x}s^2 + \sigma^2 m}{\sigma^2 + Ns^2} \tag{377}$$
$$\hat{\mu}_{MLE} = \bar{x} \tag{378}$$

So, we need to show that as n tends to infinity, the MAP solution converges to $\bar{x}$. Thus

$$\lim_{n\to\infty} \frac{N\bar{x}s^2 + \sigma^2 m}{\sigma^2 + Ns^2} = \frac{N\bar{x}s^2}{Ns^2} = \frac{Ns^2}{Ns^2}\bar{x} = \bar{x} \tag{379}$$

c. Suppose n is small and fixed. What does the MAP estimate converge to if we increase the prior variance s^2?

This is similar to the previous section, but now we are taking the limit of s^2 to ∞.

$$\lim_{s\to\infty} \frac{N\bar{x}s^2 + \sigma^2 m}{\sigma^2 + Ns^2} = \frac{Ns^2\bar{x}}{Ns^2} = \frac{Ns^2}{Ns^2}\bar{x} = \bar{x} \tag{380}$$

So, increasing the prior variance to ∞ yields the MLE. This makes sense, since the prior with infinite variance is an uninformative prior.

c. Suppose n is small and fixed. What does the MAP estimate converge to if we decrease the prior variance s^2?

This is similar to the previous section, but now we are taking the limit of s^2 to 0.

$$\lim_{s\to 0} \frac{N\bar{x}s^2 + \sigma^2 m}{\sigma^2 + Ns^2} = \frac{\sigma^2 m}{\sigma^2} = \frac{\sigma^2}{\sigma^2} m = m \tag{381}$$

So, as the prior variance tends to 0, the MAP converges to the prior mean m. This makes sense, because a prior with a variance of 0 encodes the belief that we are absolutely certain of the prior mean.

Exercise 4.15. **a. Show how to sequentially update the covariance estimate.**

The sample covariance is given by

$$\hat{\Sigma} = C_n = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - m_n)(x_i - m_n)^T$$

Note that we can update the cumulative mean as

$$m_{n+1} = \frac{x_{n+1} + nm_n}{n+1}$$

What we are trying to show is that

$$C_{n+1} = \frac{n-1}{n} C_n + \frac{1}{n+1} (x_{n+1} - m_n)(x_{n+1} - m_n)^T \tag{382}$$

$$nC_{n+1} = (n-1)C_n + \frac{n}{n+1} (x_{n+1} - m_n)(x_{n+1} - m_n)^T \tag{383}$$

$$nC_{n+1} - (n-1)C_n = \frac{n}{n+1} (x_{n+1} - m_n)(x_{n+1} - m_n)^T \tag{384}$$

This form is a little easier to work with. Using this definition and the following definitions:

$$C_n = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - m_n)(x_i - m_n)^T \tag{385}$$

$$C_{n+1} = \frac{1}{n} \sum_{i=1}^{n+1} (x_i - m_{n+1})(x_i - m_{n+1})^T \tag{386}$$

We can show that

$$nC_{n+1} - (n-1)C_n = \sum_{i=1}^{n+1}(x_i - m_{n+1})(x_i - m_{n+1})^T - \sum_{i=1}^{n}(x_i - m_n)(x_i - m_n)^T \tag{387}$$

$$= \sum_{i=1}^{n+1} x_i x_i^T - m_{n+1}m_{n+1}^T - \sum_{i=1}^{n} x_i x_i^T - m_n m_n^T \tag{388}$$

$$= x_{n+1}x_{n+1}^T - (n+1)m_{n+1}m_{n+1}^T - nm_n m_n^T \tag{389}$$

$$= x_{n+1}x_{n+1}^T - nm_n m_n^T - (n+1)\left(\frac{x_{n+1} + nm_n}{n+1}\right)\left(\frac{x_{n+1} + nm_n}{n+1}\right)^T \tag{390}$$

$$= x_{n+1}x_{n+1}^T - nm_n m_n^T - \frac{1}{n+1}(x_{n+1} + nm_n)(x_{n+1} + nm_n)^T \tag{391}$$

$$= x_{n+1}x_{n+1}^T - nm_n m_n^T - \frac{1}{n+1}(x_{n+1}x_{n+1}^T + nx_{n+1}m_n + nm_n x_{n+1} + n^2 m_n m_n^T) \tag{392}$$

$$= \frac{n}{n+1}x_{n+1}x_{n+1}^T - nm_n m_n^T - \frac{n^2}{n+1}m_n m_n^T - \frac{n}{n+1}x_{n+1}m_n - \frac{n}{n+1}m_n x_{n+1} \tag{393}$$

$$= \frac{n}{n+1}x_{n+1}x_{n+1}^T - \frac{n(n+1)}{n+1}m_n m_n^T - \frac{n^2}{n+1}m_n m_n^T \tag{394}$$

$$= \frac{n}{n+1}x_{n+1}x_{n+1}^T - \frac{n}{n+1}m_n m_n^T \tag{395}$$

$$= \frac{n}{n+1}(x_{n+1} - m_n)(x_{n+1} - m_n)^T \tag{396}$$

which is what we intended to show.

b. What is the big-O run time of this sequential update?

This procedure is $O(d^2)$, because we only have to compute one inner product at a time.

c. Show how to incrementally update the precision matrix.

Let $u = (x_{n+1} - m_n)$. Then

$$C_{n+1}^{-1} = \left(\frac{n-1}{n}C_n + \frac{1}{n+1}uu^T\right)^{-1} \tag{397}$$

and we are trying to show that

$$C_{n+1}^{-1} = \frac{n}{n-1}\left[C_n^{-1} - \frac{C_n^{-1}uu^T C_n^{-1}}{\frac{n^2-1}{n} + u^T C_n^{-1}u}\right] \tag{398}$$

Using the matrix inversion lemma provides us with

$$C_{n+1}^{-1} = \left(\frac{n-1}{n}C_n + \frac{1}{n+1}uu^T\right)^{-1} \tag{399}$$

$$= \frac{n}{n-1}C_n^{-1} - \frac{\frac{n}{n-1}C_n^{-1}\frac{1}{n+1}uu^T\frac{n}{n-1}C_n^{-1}}{1+\frac{1}{n+1}u^T\frac{n}{n-1}C_n^{-1}u} \tag{400}$$

$$= \frac{n}{n-1}C_n^{-1} - \frac{\frac{n^2}{(n-1)^2(n+1)}C_n^{-1}uu^TC_n^{-1}}{1+\frac{n}{(n-1)(n+1)}u^TC_n^{-1}u} \tag{401}$$

$$\tag{402}$$

Note that

$$\frac{n^2}{(n-1)^2(n+1)} = \frac{n}{n-1}\frac{n}{(n-1)(n+1)}$$

and

$$(n-1)(n+1)(1+\frac{n}{(n-1)(n+1)}B) = (n-1)(n+1)+nB = n^2-1+nB$$

Using these we see that

$$C_{n+1}^{-1} = \frac{n}{n-1}C_n^{-1} - \frac{\frac{n^2}{(n-1)^2(n+1)}C_n^{-1}uu^TC_n^{-1}}{1+\frac{n}{(n-1)(n+1)}u^TC_n^{-1}u} \tag{403}$$

$$= \frac{n}{n-1}\left[C_n^{-1} - \frac{nC_n^{-1}uu^TC_n^{-1}}{n^2-1+nu^TC_n^{-1}u}\right] \tag{404}$$

$$= \frac{n}{n-1}\left[C_n^{-1} - \frac{C_n^{-1}uu^TC_n^{-1}}{\frac{n^2-1}{n}u^TC_n^{-1}u}\right] \tag{405}$$

d. What's the big-O complexity of this procedure?
This procedure is also $O(d^2)$.

Exercise 4.16. **Derive an expression for the log likelihood ratio with an arbitrary covariance matrix.**

$$log\frac{p(y=1|x)}{p(y=0|x)} = log\frac{p(x|y=1)}{p(x|y=0)} + log\frac{p(y=1)}{p(y=0)} \tag{406}$$

$$= log\frac{N(x|\mu_1,\Sigma_1)}{N(x|\mu_2,\Sigma_2)} + log\frac{p(y=1)}{p(y=0)} \tag{407}$$

$$= log\frac{(2\pi)^{D/2}|\Sigma_1|^{1/2}exp(-\frac{1}{2}(x-\mu_1)^T\Sigma_1^{-1}(x-\mu_1)}{(2\pi)^{D/2}|\Sigma_0|^{1/2}exp(-\frac{1}{2}(x-\mu_0)^T\Sigma_0^{-1}(x-\mu_0)} + log\frac{p(y=1)}{p(y=0)} \tag{408}$$

$$= log\frac{|\Sigma_1|^{1/2}}{|\Sigma_0|^{1/2}}exp(-\frac{1}{2}(x-\mu_1)^T\Sigma_1^{-1}(x-\mu_1) - \frac{1}{2}(x-\mu_0)^T\Sigma_0^{-1}(x-\mu_0)) + log\frac{p(y=1)}{p(y=0)} \tag{409}$$

$$= log\frac{|\Sigma_1|^{1/2}}{|\Sigma_0|^{1/2}} - \frac{1}{2}(x-\mu_1)^T\Sigma_1^{-1}(x-\mu_1) - \frac{1}{2}(x-\mu_0)^T\Sigma_0^{-1}(x-\mu_0) + log\frac{p(y=1)}{p(y=0)} \tag{410}$$

We can simplify this further if we make assumptions about the problem. For example, if the covariance matrix is shared ($\Sigma_j = \Sigma$), then

$$log\frac{p(y=1|x)}{p(y=0|x)} = log\frac{|\Sigma|^{1/2}}{|\Sigma|^{1/2}} - \frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1) - \frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0) + log\frac{p(y=1)}{p(y=0)} \tag{411}$$

$$= 1 + log\frac{p(y=1)}{p(y=0)} - \frac{1}{2}\left[tr((x-\mu_1)^T\Sigma^{-1}(x-\mu_1)) + tr((x-\mu_0)^T\Sigma^{-1}(x-\mu_0))\right] \tag{412}$$

$$= 1 + log\frac{p(y=1)}{p(y=0)} - \frac{1}{2}\left[tr((x-\mu_1)^T\Sigma^{-1}(x-\mu_1) + (x-\mu_0)^T\Sigma^{-1}(x-\mu_0))\right] \tag{413}$$

$$\tag{414}$$

Further, if the covariance matrix is shared and diagonal, then

$$log\frac{p(y=1|x)}{p(y=0|x)} = 1 + log\frac{p(y=1)}{p(y=0)} - \frac{1}{2}\left[tr((x-\mu_1)^T\Sigma^{-1}(x-\mu_1) + (x-\mu_0)^T\Sigma^{-1}(x-\mu_0))\right] \tag{415}$$

$$= 1 + log\frac{p(y=1)}{p(y=0)} - \frac{1}{2}\left[\sum_{i=1}^{N}\frac{(x_i-\mu_1)^2}{\sigma_i} + \frac{(x_i-\mu_0)^2}{\sigma_i}\right] \tag{416}$$

Finally, if the covariance is shared and spherical ($\Sigma = \sigma^2 I$), then

$$log\frac{p(y=1|x)}{p(y=0|x)} = 1 + log\frac{p(y=1)}{p(y=0)} - \frac{1}{2}\left[\sum_{i=1}^{N}\frac{(x_i-\mu_1)^2}{\sigma} + \frac{(x_i-\mu_0)^2}{\sigma}\right] \quad (417)$$

$$= 1 + log\frac{p(y=1)}{p(y=0)} - \frac{N}{2\sigma}\sum_{i=1}^{N}(x_i-\mu_1)^2 + (x_i-\mu_0)^2 \quad (418)$$

Exercise 4.17. **Compute the misclassification rate of LDA and QDA on the height/weight dataset.**

The code for this can be found in ch4-17.ipynb.

Exercise 4.18. **Consider a 3 class naive Bayes classifier with one binary feature and one Gaussian feature.**

a. Compute $p(y|x_1 = 0, x_2 = 0)$.

The naive Bayes classifier can be written as

$$p(y|x_1=0,x_2=0) = p(y)p(x_1=0|y)p(x_2=0|y) \quad (419)$$

$$= Mu(y|\pi,1)Ber(x_1=0|\theta)N(x_2=0|\mu,\sigma^2) \quad (420)$$

$$= Mu(y,\begin{bmatrix}0.5\\0.25\\0.25\end{bmatrix},1)Ber(x_1=0|\begin{bmatrix}0.5\\0.5\\0.5\end{bmatrix})N(x_2=0|\begin{bmatrix}-1\\0\\1\end{bmatrix},\begin{bmatrix}1\\1\\1\end{bmatrix}) \quad (421)$$

$$\propto \begin{bmatrix}0.5\\0.25\\0.25\end{bmatrix} \oplus \begin{bmatrix}0.5\\0.5\\0.5\end{bmatrix} \oplus \begin{bmatrix}0.2419707\\0.3989423\\0.2419707\end{bmatrix} \quad (422)$$

$$= \begin{bmatrix}0.060492675\\0.0498677875\\0.0302463375\end{bmatrix} \quad (423)$$

$$= \begin{bmatrix}0.4302258233\\0.3546612864\\0.2151129116\end{bmatrix} \quad (424)$$

b. Compute $p(y|x_1 = 0)$.

We can compute this by noting that

$$p(y|x_1=0) = \sum_{i=1}^{3} p(y=i)p(x_1=0|y=i) \quad (425)$$

$$= \sum_{i=1}^{3} \pi_i Ber(x_1=0|\theta_i) \quad (426)$$

$$= 0.5\sum_{i=1}^{3}\pi_i = 0.5 \quad (427)$$

c. Compute $p(y|x_2 = 0)$.
We can compute this in a similar fashion:

$$p(y|x_2 = 0) = \sum_{i=1}^{3} \pi_i p(x_2 = 0|y = i) \tag{428}$$

$$= \sum_{i=1}^{3} \pi_i N(\mu_i, \sigma_i^2) \tag{429}$$

$$= 0.5 \times 0.2419707 + 0.25 \times 0.3989423 + 0.25 \times 0.2419707 \tag{430}$$

$$= 0.341706275 \tag{431}$$

Exercise 4.19. **Derive the QDA decision boundary for a binary classification problem where $\Sigma_1 = k\Sigma_0$.**

The QDA formulation is given by

$$p(y = c|x, \theta) = \frac{\pi_c |2\pi\Sigma_c|^{1/2} exp(-\frac{1}{2}(x - \mu_c)^T \Sigma_c^{-1}(x - \mu_c))}{\sum_c \pi_c |2\pi\Sigma_c|^{1/2} exp(-\frac{1}{2}(x - \mu_c)^T \Sigma_c^{-1}(x - \mu_c))} \tag{432}$$

Assume that Σ is of dimensionality D. Formulating this as a binary problem and plugging in the fact that $\Sigma_1 = k\Sigma_0$, we get

$$p(y = 1|x, \theta) = \frac{\pi_1 |2\pi k\Sigma_0|^{1/2} exp(-\frac{1}{2}(x - \mu_1)^T k\Sigma_0^{-1}(x - \mu_1))}{\pi_0 |2\pi\Sigma_0|^{1/2} exp(-\frac{1}{2}(x - \mu_0)^T \Sigma_0^{-1}(x - \mu_0)) + \pi_1 |2\pi k\Sigma_0|^{1/2} exp(-\frac{1}{2}(x - \mu_1)^T k\Sigma_0^{-1}(x - \mu_1))} \tag{433}$$

$$= \frac{\pi_1 k^D exp(-\frac{1}{2}(x - \mu_1)^T k\Sigma_0^{-1}(x - \mu_1))}{\pi_0 exp(-\frac{1}{2}(x - \mu_0)^T \Sigma_0^{-1}(x - \mu_0)) + \pi_1 k^D exp(-\frac{1}{2}(x - \mu_1)^T k\Sigma_0^{-1}(x - \mu_1))} \tag{434}$$

$$= \frac{\pi_1 k^D exp(-\frac{k}{2} tr(\Sigma_0^{-1}(x - \mu_1)(x - \mu_1)^T)}{\pi_0 exp(-\frac{1}{2} tr(\Sigma_0^{-1}(x - \mu_0)(x - \mu_0)^T) + \pi_1 k^D exp(-\frac{k}{2} tr(\Sigma_0^{-1}(x - \mu_1)(x - \mu_1)^T)} \tag{435}$$

$$= \frac{\pi_1 k^D exp(-\frac{k}{2} tr(\Sigma_0^{-1} xx^T) - \frac{k}{2} tr(\Sigma_0^{-1} \mu_1 \mu_1^T))}{\pi_0 exp(-\frac{1}{2} tr(\Sigma_0^{-1} xx^T) - \frac{1}{2} tr(\Sigma_0^{-1} \mu_0 \mu_0^T)) + \pi_1 k^D exp(-\frac{k}{2} tr(\Sigma_0^{-1} xx^T) - \frac{k}{2} tr(\Sigma_0^{-1} \mu_1 \mu_1^T))} \tag{436}$$

Let $a = tr(\Sigma_0^{-1} xx^T)$ and $b_c = tr(\Sigma_0^{-1} \mu_c \mu_c^T)$. Then

$$p(y=1|x,\theta) = \frac{\pi_1 k^D \frac{exp(-\frac{k}{2}a)}{exp(-\frac{k}{2}b_1)}}{\pi_0 \frac{exp(-\frac{1}{2}a)}{exp(-\frac{1}{2}b_0)} + \pi_1 k^D \frac{exp(-\frac{k}{2}a)}{exp(-\frac{k}{2}b_1)}} \tag{437}$$

$$= \frac{\pi_1 k^D exp(-\frac{k}{2}a)}{\pi_0 exp(-\frac{1}{2}a - \frac{k}{2}b_1 + \frac{1}{2}b_0) + \pi_1 k^D exp(-\frac{k}{2}a)} \tag{438}$$

$$= \frac{1}{\pi_0 \pi_1^{-1} k^{-D} exp(\frac{k}{2}a - \frac{1}{2}a - \frac{k}{2}b_1 + \frac{1}{2}b_0) + 1} \tag{439}$$

$$= \frac{1}{\pi_0 \pi_1^{-1} k^{-D} exp(\frac{1}{2}((k-1)a - kb_1 + b_0)) + 1} \tag{440}$$

$$= \pi_0^{-1} \pi_1 k^D Sigm(\nu) \tag{441}$$

where

$$\nu = -\frac{1}{2}((k-1)a + kb_1 + b_0) \tag{442}$$

$$= -\frac{1}{2}((k-1)tr(\Sigma_0^{-1} x x^T) + ktr(\Sigma_0^{-1}\mu_1\mu_1^T) + tr(\Sigma_0^{-1}\mu_0\mu_0^T)) \tag{443}$$

$$= -\frac{1}{2}((k-1)tr(\Sigma_0^{-1} x x^T) + (k-1)tr(\Sigma_0^{-1}\mu_1\mu_1^T) + tr(\Sigma_0^{-1}\mu_1\mu_1^T) + tr(\Sigma_0^{-1}\mu_0\mu_0^T)) \tag{444}$$

$$= -\frac{1}{2}((k-1)(x-\mu_1)^T\Sigma_0^{-1}(x-\mu_1) + tr(\Sigma_0^{-1}\mu_1\mu_1^T) + tr(\Sigma_0^{-1}\mu_0\mu_0^T)) \tag{445}$$

$$= -\frac{1}{2}((k-1)(x-\mu_1)^T\Sigma_0^{-1}(x-\mu_1) + (\mu_1-\mu_0)^T\Sigma_0^{-1}(\mu_1-\mu_0)) \tag{446}$$

$$= -\frac{k-1}{2}(x-\mu_1)^T\Sigma_0^{-1}(x-\mu_1) - \frac{1}{2}(\mu_1-\mu_0)^T\Sigma_0^{-1}(\mu_1-\mu_0) \tag{447}$$

Thus, since class 1 is a scaled version of class 2, the decision boundary scales this class as well.

Exercise 4.20. **See the textbook for the full problem description.**

a. GaussI, LinLog.

Note that we are only considering performance on the training set, and only considering a loss function that is a function of the conditional likelihood, not the joint likelihood.

Logistic regression maximizes the conditional likelihood, whereas LDA and QDA maximize the joint likelihood. Since we are only considering training set performance, maximizing the conditional likelihood will be sufficient in minimizing the given loss function. Thus

$L(GaussI) \geq L(LinLog)$.

b. GaussX, QuadLog.

Again, on the surface they seem equivalent, however the logistic model maximizes the conditional likelihood. So similarly

$L(GaussX) \geq L(QuadLog)$.

c. LinLog, QuadLog.

The QuadLog model has more parameters and is therefore more flexible. It might not perform as well on the test set, but on the training set it will likely perform better. Thus

$L(LinLog) \geq L(QuadLog)$.

d. GaussI, QuadLog.

The GaussI model is likely too restrictive, thus

$L(GaussI) \geq L(QuadLog)$.

e. In general is it true that the negative log likelihood loss function behaves similarly to the misclassification rate ($L(M) > L(M')$ implies $R(M) < R(M')$)?

This is not true because of the discretized nature of the misclassification rate. For example, one model could lower the log likelihood loss but still not be better "enough" to improve the misclassification rate.

Exercise 4.21. **TODO**

Exercise 4.22. **Class the points using the QDA model described in the text.**

a. $x = [-0.5, 0.5]$**.**

Note that the normalization constants for the problem described is given by

$$Z_c = \pi_c |2\pi\Sigma_c|^{-1/2} \tag{448}$$

$$Z_1 = \frac{1}{3}|2\pi 0.7I|^{-1/2} = 0.2273643491 \tag{449}$$

$$Z_2 = Z_3 = \frac{1}{3}|2\pi \begin{bmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{bmatrix}|^{-1/2} = 0.2054679336 \tag{450}$$

Another quantity that is useful to compute up front is

$$M_c = (x - \mu_c)^T \Sigma_c^{-1} (x - \mu_c) \tag{451}$$

$$M_1 = \begin{bmatrix} -0.5 \\ 0.5 \end{bmatrix}^T \begin{bmatrix} 0.7 & 0 \\ 0 & 0.7 \end{bmatrix}^{-1} \begin{bmatrix} -0.5 \\ 0.5 \end{bmatrix} = 0.714286 \tag{452}$$

$$M_2 = \begin{bmatrix} -1.5 \\ -0.5 \end{bmatrix}^T \begin{bmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{bmatrix}^{-1} \begin{bmatrix} -1.5 \\ -0.5 \end{bmatrix} = 2.83333 \tag{453}$$

$$M_3 = \begin{bmatrix} 0.5 \\ -0.5 \end{bmatrix}^T \begin{bmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{bmatrix}^{-1} \begin{bmatrix} 0.5 \\ -0.5 \end{bmatrix} = 0.833333 \tag{454}$$

A final quantity that will use is

$$P_c = Z_c exp(-\frac{1}{2}M_c) \tag{455}$$

$$P_1 = Z_1 exp(-\frac{1}{2}M_1) = 0.1590805683 \tag{456}$$

$$P_2 = Z_2 exp(-\frac{1}{2}M_2) = 0.0498303871 \tag{457}$$

$$P_3 = Z_3 exp(-\frac{1}{2}M_3) = 0.1354530358 \tag{458}$$

We can then plug these into the equation for QDA to get

$$p(y = 1|x, \theta) = \frac{P_1}{P_1 + P_2 + P_3} = 0.4619547118 \tag{459}$$

$$p(y = 2|x, \theta) = \frac{P_2}{P_1 + P_2 + P_3} = 0.1447026645 \tag{460}$$

$$p(y = 3|x, \theta) = \frac{P_3}{P_1 + P_2 + P_3} = 0.3933426237 \tag{461}$$

Thus, we would classify this point to class 1.
b. Classify $x = [0.5, 0.5]$**.**
We can utilize the same machinery for this.

$$M_c = (x - \mu_c)^T \Sigma_c^{-1} (x - \mu_c) \tag{462}$$

$$M_1 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}^T \begin{bmatrix} 0.7 & 0 \\ 0 & 0.7 \end{bmatrix}^{-1} \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} = 0.714286 \tag{463}$$

$$M_2 = \begin{bmatrix} -0.5 \\ -0.5 \end{bmatrix}^T \begin{bmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{bmatrix}^{-1} \begin{bmatrix} -0.5 \\ -0.5 \end{bmatrix} = 0.5 \tag{464}$$

$$M_3 = \begin{bmatrix} -0.5 \\ 1.5 \end{bmatrix}^T \begin{bmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{bmatrix}^{-1} \begin{bmatrix} -0.5 \\ 1.5 \end{bmatrix} = 3.83333 \tag{465}$$

And

$$P_c = Z_c exp(-\frac{1}{2}M_c) \tag{466}$$

$$P_1 = Z_1 exp(-\frac{1}{2}M_1) = 0.1590805683 \tag{467}$$

$$P_2 = Z_2 exp(-\frac{1}{2}M_2) = 0.1600185876 \tag{468}$$

$$P_3 = Z_3 exp(-\frac{1}{2}M_3) = 0.03022365758 \tag{469}$$

We can then plug these into the equation for QDA to get

$$p(y=1|x,\theta) = \frac{P_1}{P_1+P_2+P_3} = 0.4553970201 \tag{470}$$

$$p(y=2|x,\theta) = \frac{P_2}{P_1+P_2+P_3} = 0.4580822707 \tag{471}$$

$$p(y=3|x,\theta) = \frac{P_3}{P_1+P_2+P_3} = 0.08652070925 \tag{472}$$

Thus we would classify this point to class 2.

5 Bayesian Statistics

Exercises

Exercise 5.1. **Prove that a mixture of conjugate priors is indeed conjugate.**

We are trying to show that

$$p(\theta|D) = \sum_k p(z=k|D)p(\theta|D, z=k)$$

with a prior of the form

$$p(\theta) = \sum_k p(z=k)p(\theta|z=k)$$

We know that the posterior can be given by

$$\begin{aligned}
p(\theta|D) &= \frac{p(D|\theta)p(\theta)}{p(D)} && (473)\\
&= \frac{p(D|\theta)\sum_k p(\theta|z=k)p(z=k)}{p(D)} && (474)\\
&= p(D|\theta)\frac{\sum_k p(\theta|z=k)}{p(D)} && (475)\\
&= \frac{\sum_k p(D|\theta, z=k)p(\theta|z=k)}{p(D)} && (476)\\
&= \frac{\sum_k p(\theta, z=k|D)p(D)p(\theta|z=k)}{p(D)\sum_k p(\theta, z=k)} && (477)\\
&= \frac{\sum_k p(\theta, z=k|D)p(\theta|z=k)}{\sum_k p(\theta|z=k)p(z=k)} && (478)\\
&= \frac{\sum_k p(\theta, z=k|D)}{\sum_k p(z=k)} && (479)\\
&= \sum_k p(\theta, z=k|D) && (480)\\
&= \sum_k p(z=k|D)p(\theta|D, z=k) && (481)
\end{aligned}$$

Exercise 5.2. **Optimal threshold on classification probability.**

a. What is θ as a function of λ_{01} and λ_{10}?

The model can be expressed as

$$p(y|x) = 1 - p(y=0|x) = p(y=1|x) = p_1 = \hat{y}$$

The loss function can be expressed as

$$L(y, \hat{y}) = y(1-\hat{y})\lambda_{01} + \hat{y}(1-y)\lambda_{10} \tag{482}$$
$$L(0, \hat{y}) = \hat{y}\lambda_{10} \tag{483}$$
$$L(1, \hat{y}) = (1-\hat{y})\lambda_{01} \tag{484}$$

The quantity we are trying to minimize is the expected loss function. This is given by

$$E[L(y, \hat{y})] = p_0 L(0, \hat{y}) + p_1 L(1, \hat{y}) \tag{485}$$
$$= p_0 \hat{y}\lambda_{10} + p_1 \lambda_{01}(1-\hat{y}) \tag{486}$$

We can take the derivate with respect to $\hat{y}$ and set this to zero, which give us

$$0 = \frac{d}{d\hat{y}}(p_0\lambda_{10}\hat{y} + p_1\lambda_{01} - \hat{y}p_1\lambda_{01}) \tag{487}$$
$$= p_0\lambda_{10} - p_1\lambda_{01} \tag{488}$$
$$p_1\lambda_{01} = p_0\lambda_{10} \tag{489}$$
$$p_1\lambda_{01} = (1-p_1)\lambda_{10} \tag{490}$$
$$p_1\lambda_{01} + p_1\lambda_{10} = \lambda_{10} \tag{491}$$
$$p_1(\lambda_{01} + \lambda_{10}) = \lambda_{10} \tag{492}$$
$$p_1 = \frac{\lambda_{10}}{\lambda_{01} + \lambda_{10}} \tag{493}$$

Thus we see that the decision boundary occurs when $p_1 = \frac{\lambda_{10}}{\lambda_{01}+\lambda_{10}}$. If p_1 is greater than this quantity, we will classify this with class 1, and 0 otherwise.

b. Show a loss matrix where the threshold is 0.1**.**

This is accomplished by plugging in to the quantity derived above:

$$0.1 = \frac{\lambda_{10}}{\lambda_{01} + \lambda_{10}} \tag{494}$$
$$0.1\lambda_{01} + 0.1\lambda_{10} = \lambda_{10} \tag{495}$$
$$0.1\lambda_{01} = 0.9\lambda_{10} \tag{496}$$
$$\lambda_{01} = 9\lambda_{10} \tag{497}$$

Thus, a loss function of the following form will be sufficient:

$$\begin{bmatrix} 0 & 9\lambda_{10} \\ \lambda_{10} & 0 \end{bmatrix}$$

Exercise 5.3. **Reject option in classifiers.**

a. Show that the minimum risk is obtained if decide $Y = j$ **if** $p(Y = j|x) \geq p(Y = k|x)$ **for all** k **and** $p(Y = j|x) \geq 1 - \frac{\lambda_r}{\lambda_s}$**.**

Note that the first part of this has been shown above, namely that the most likely class will be chosen. The second part, the reject option, will be shown in this exercise.

The expected posterior loss in this case is given by

$$\rho(\hat{y}|x) = \sum_{k=1}^{C} p(y = k|x)L(y = k, \hat{y})$$

Let's say that the correct class is j. Then, the posterior loss is

$$\rho(\hat{y}|x) = \sum_{k=1}^{C} p(y = k|x)L(y = k, \hat{y}) \tag{498}$$

$$= \sum_{k \neq j} p(y = k|x)\lambda_s \tag{499}$$

$$= (1 - p(y = j|x))\lambda_s \tag{500}$$

We need to see when this quantity is better than the reject option. If the reject option is chosen, then the posterior loss is given by

$$\rho(\hat{y}|x) = \sum_{k=1}^{C} p(y = k|x)\lambda_r = \lambda_r$$

Thus for us not to choose the reject option,

$$(1 - p(y = j|x))\lambda_s \geq \lambda_r \tag{501}$$

$$1 - p(y = j|x) \geq \frac{\lambda_r}{\lambda_s} \tag{502}$$

$$1 - \frac{\lambda_r}{\lambda_s} = p(y = j|x) \tag{503}$$

b. Qualitatively describe what happens as λ_r/λ_s increases from 0 to 1.

Note that we will choose class j if it is the most likely class and if

$$p(y = j|x) \geq 1 - \frac{\lambda_r}{\lambda_s}$$

When the quantity λ_r/λ_s is 0, this means that $\lambda_r = 0$. Note that λ_r is the risk of rejection, and when this is 0, we will choose to reject often. In fact, we will only choose not to reject when $p(y = j|x) = 1$.

When the quantity is 1, that means that the risk of rejection is infinitely high. Thus, this is equivalent to a classifier with no reject option.

Exercise 5.4. **Suppose it costs** \$10 **to misclassify and** \$3 **for a human to manually classify.**

a. Suppose $p(y = 1|x) = 0.2$**. Which decision minimizes expected loss?**

The expected loss function is given by

$$\rho(\hat{y}|x) = p_1 L(1, \hat{y}) + (1 - p_1)L(0, \hat{y})$$

We can use this to plug in each decision

$$\rho(0|x) = (1 - 0.2) \times 10 = 8 \tag{504}$$
$$\rho(1|x) = 0.2 \times 10 = 2 \tag{505}$$
$$\rho(r|x) = 3 \tag{506}$$

Thus, we would class this to class 0.

b. Now suppose $p(y = 1|x) = 0.4$**.**

Similarly we will plug the numbers in

$$\rho(0|x) = (1 - 0.4) \times 10 = 6 \tag{507}$$
$$\rho(1|x) = 0.4 \times 10 = 4 \tag{508}$$
$$\rho(r|x) = 3 \tag{509}$$

Thus in this case, we will choose the reject option.

c. Show that there are thresholds θ_0 **and** θ_1 **such that if** $p_1 \leq \theta_0$**, we will classify to** 0**,** $\theta_0 \leq p_1 \leq \theta_1$ **we will classify as reject, and** $p_1 \geq \theta_1$ **we will classify as** 1**.**

Let's run through each decision

$$\rho(0|x) = (1 - p_1) \times 10 = 10 - 10p_1 = \rho_0 \tag{510}$$
$$\rho(1|x) = p_1 \times 10 = 10p_1 = \rho_1 \tag{511}$$
$$\rho(r|x) = 3 = \rho_r \tag{512}$$

Let's say the correct choice is class 0. Then

$$10 - 10p_1 \geq 10p_1 \rightarrow 1 - p_1 \geq p_1 \rightarrow p_1 \leq 0.5 \tag{513}$$
$$10p_1 \leq 3 \rightarrow p_1 \leq 0.3 \tag{514}$$

Now if the correct class is 1, then

$$10p_1 \geq 10 - 10p_1 \rightarrow p_1 \geq 1 - p_1 \rightarrow p_1 \geq 0.5 \tag{515}$$
$$10 - 10p_1 \leq 3 \rightarrow 1 - p_1 \leq 0.3 \rightarrow p_1 \geq 0.7 \tag{516}$$

Thus, the thetas are $\theta_0 = 0.3$ and $\theta_1 = 0.7$.

Exercise 5.5. **Newsvendor problem**

$$E_\pi(Q) = \int_Q^\infty (P-C)Qf(D)dD + \int_0^Q (P-C)Df(D) - \int_0^Q C(Q-D)f(D)dD \tag{517}$$

$$= (P-C)Q\int_Q^\infty f(D)dD + (P-C)\int_0^Q Df(D)dD - CQ\int_0^Q f(D)dD + C\int_0^Q Df(D)dD \tag{518}$$

$$= (P-C)Q(1-F(Q)) + P\int_0^Q Df(D)dD - CQ\int_0^Q f(D)dD \tag{519}$$

$$= (P-C)Q(1-F(Q)) + P\int_0^Q Df(D)dD - CQF(Q) \tag{520}$$

$$= (P-C)Q - (P-C)QF(Q) + P\int_0^Q Df(D)dD - CQF(Q) \tag{521}$$

$$= (P-C)Q - PQF(Q) + CQF(Q) + P\int_0^Q Df(D) - CQF(Q) \tag{522}$$

$$= (P-C)Q - PQF(Q) + P\int_0^Q Df(D) \tag{523}$$

$$= (P-C)Q - PQF(Q) + PQF(Q) - P\int_0^Q F(D)dD \tag{524}$$

$$= (P-C)Q - P\int_0^Q F(D)dD \tag{525}$$

Now we will take the derivate wrt Q. We then see that

$$\frac{d}{dQ}(P-C)Q - P\int_0^Q F(D)dD = (P-C) - PF(Q)$$

By setting this quantity to 0, we see that

$$0 = (P-C) - PF(Q) \tag{526}$$

$$PF(Q) = (P-C) \tag{527}$$

$$F(Q) = \frac{P-C}{P} \tag{528}$$

Exercise 5.6. **Let $B = p(D|H_1)/p(D|H_0)$ be the Bayes factor of model 1. Suppose we plot two ROC curves, one computed by thresholding B, and the other computed by thresholding $p(H_1|D)$. Will they be the same or different?**

If we threshold on B, we are saying that the decision rule is given by

$$I(f(x) > B) = I(f(x) > \frac{p(D|H_1)}{p(D|H_0)})$$

Compare this if we threshold with $p(H_1|D)$:

$$I(f(x) > p(H_1|D))$$

The domains are different for the two, but are they still monotonically related? We note that as B increases to ∞, we favor H_1 more heavily. Thus it makes sense that as B increases, so should $p(H_1|D)$.

Similarly, as B decreases towards 0, so should $p(H_0|D)$ decrease as well. Thus, the ROC curves should be the same.

Exercise 5.7. **Bayes model averaging improves predictive accuracy.**

For this exercise, note the following properties of KL-divergence:

$$KL(q||p) = -\sum_x p(x) log\, q(x) + p(x) log\, p(x) \tag{529}$$

$$= -\sum_x p(x)(log\, q(x) + log\, p(x)) \tag{530}$$

$$= -\sum_x p(x) log\, q(x) p(x) \tag{531}$$

The expectation of the loss function of the plugin approximation is given by

$$E[L(\Delta, p^m)] = E[-log(p^m(\Delta))] \tag{532}$$

$$= E[-log(p(\Delta|m, D))] \tag{533}$$

$$= -\sum_{m \in M} p(\Delta|m, D) p(m|D) log(p(\Delta|m, D)) \tag{534}$$

The loss function of the Bayes model averaging estimate is given by

$$E[L(\Delta, p^{BMA})] = E[-log(p^{BMA}(\Delta))] \tag{535}$$

$$= -E[log(\sum_{m \in M} p(\Delta|m, D) p(m|D))] \tag{536}$$

$$= -\sum_{m \in M} p(\Delta|m, D) p(m|D) log(\sum_{m \in M} p(\Delta|m, D) p(m|D)) \tag{537}$$

One way to show that the Bayes model averaging is superior is to show that the difference between the two is ≥ 0. So, if we take the difference,

$$E[L(\Delta, p^m)] - E[L(\Delta, p^{BMA})] = -\sum_{m\in M} p(\Delta|m,D)p(m|D)log(p(\Delta|m,D)) \tag{538}$$

$$+ \sum_{m\in M} p(\Delta|m,D)p(m|D)log(\sum_{m\in M} p(\Delta|m,D)p(m|D)) \tag{539}$$

$$= -\sum_{m\in M} p(\Delta|m,D)p(m|D)(log\, p(\Delta|m,D) + log \sum_{m\in M} p(\Delta|m,D)p(m|D)) \tag{540}$$

$$= -\sum_{m\in M} p(m|D) \sum_{m\in M} p(\Delta|m,D)log\, p(\Delta|m,D) \sum_{m\in M} p(\Delta|m,D)p(m|D) \tag{541}$$

$$= -\sum_{m\in M} p(\Delta|m,D)log\, p(\Delta|m,D) \sum_{m\in M} p(\Delta|m,D)p(m|D) \tag{542}$$

$$= KL(p(\Delta|m,D), \sum_{m\in M} p(\Delta|m,D)p(m|D)) \tag{543}$$

$$\geq 0 \tag{544}$$

Exercise 5.8. **MLE and model selection for a 2d discrete distribution.**
a. Write down the joint probability distribution $p(x, y|\theta)$ as a 2×2 table, in terms of $\theta = (\theta_1, \theta_2)$

The likelihood can be factorized as

$$p(x, y|\theta) = p(y|x, \theta_2)p(x|\theta_1) = p(y|x, \theta_2)\theta_1$$

Using the definition of $p(y|x, \theta_2)$ shown in the problem, this can be shown to be

	y=0	y=1
x=0	$\theta_1\theta_2$	$\theta_1 - (1 - \theta_2)$
x=1	$\theta_1(1 - \theta_2)$	$\theta_1\theta_2$

b. With the given dataset, what is the MLE of θ_1 and θ_2?

The MLE of θ_1 is the proportion of xs that are 1. This means that $\theta_1^{MLE} = \frac{4}{7}$.

The MLE of θ_2 is the proportion of times that x and y agree. This means that $\theta_2^{MLE} = \frac{2}{7}$.

To compute the likelihood ($p(D|\hat{\theta}, M_2)$), we can use the 2×2 table to compute them. This gives us

$$p(D|\hat{\theta}, M_2) = \prod_{i=1}^{N} p(x_i, y_i|\hat{\theta}) \tag{545}$$

Plugging in the data given, this is

$$p(D|\hat{\theta}, M_2) = \theta_1^7 \theta_2^4 (1-\theta_2)^3 \tag{546}$$

$$= \frac{4}{7}^7 \frac{2}{7}^4 (1-\frac{2}{7})^3 \tag{547}$$

c. Now consider a model with 4 parameters, representing $p(x, y|\theta) = \theta_{x,y}$. What is the MLE of θ? What is $p(D|\hat{\theta}, M_4)$ where M_4 denotes this 4-parameter model?

This situation is similar. Each $\theta_{x,y}$ is essentially one of the cells in the 2×2 table. Thus the MLE of θ is given by

$$\hat{\theta} = \begin{bmatrix} \frac{1-\sum x}{N} \frac{1-\sum y}{N}(1-p(x)) \\ \frac{1-\sum x}{N} \frac{\sum y}{N}(1-p(x)) \\ \frac{\sum x}{N} \frac{1-\sum y}{N}(1-p(x)) \\ \frac{\sum xy}{N}(1-p(x)) \end{bmatrix} \tag{548}$$

$$= \begin{bmatrix} (3/7)(4/7)(1/2) \\ (3/7)(3/7)(1/2) \\ (4/7)(4/7)(1/2) \\ (2/7)(1/2) \end{bmatrix} \tag{549}$$

$$= \begin{bmatrix} 12/98 \\ 9/98 \\ 16/98 \\ 4/98 \end{bmatrix} \tag{550}$$

$$\tag{551}$$

This needs to be normalized, and when it is it becomes

$$\hat{\theta} = \begin{bmatrix} 0.2926829268 \\ 0.2195121951 \\ 0.3902439024 \\ 0.09756097561 \end{bmatrix} \tag{552}$$

$$\tag{553}$$

To compute the likelihood, we take the data, figure out which $\theta_{x,y}$ is relevant, and take the product. Thus

$$p(D|\hat{\theta}, M_4) = \theta_{0,0}^2 \theta_{0,1} \theta_{1,0}^2 \theta_{1,1}^2 \tag{554}$$

$$= 0.2926829268^2 \times 0.2195121951 \times 0.3902439024 \times 0.09756097561^2 \tag{555}$$

d. Which model would be picked using leave-one-out CV?

This would be extremely tedious to calcualte for both models by hand, but we note that the second model has more parameters and thus would likely fit better (or at least as well). Thus, it is likely that the second model will be chosen for CV.

e. Compute the BIC for both models? Which model does it prefer?

The BIC is given by

$$BIC(M, D) = p(D|\hat{\theta}) - \frac{dof(M)}{2} logN$$

Let's look at the model complexity penalization term. For the two parameter model, this is given by

$$\frac{2}{2} logN = log7 \approx 0.845$$

For the four parameter model, this is

$$\frac{4}{2} logN = 2log7 \approx 1.690$$

Thus, for the four parameter model to be preferred, it would have to have a higher likelihood of $\geq log7$. This is very unlikely (and is in fact not the case), so the BIC would prefer the simpler model.

Exercise 5.9. **Prove that the posterior median is the optimal estimate under L1 loss.**

The median is given by

$$p(y < a|x) = \int_{-\infty}^{a} p(y|x) = \int_{a}^{\infty} p(y|x) = p(y \geq a|x) = 0.5 \tag{556}$$

The posterior expected loss under L1 loss is given by

$$\rho(a|x) = E[abs(y - a)|x]$$

By taking the derivative wrt a, we see that

$$\begin{aligned}
\frac{d}{da}\rho(a|x) &= \frac{d}{da} E[abs(y - a)|x] && (557)\\
&= E[\frac{d}{da} abs(y - a)|x] && (558)\\
&= E[\frac{a - y}{|a - y|}|x] && (559)\\
&= \int \frac{a - y}{|a - y|} p(\frac{a - y}{|a - y|}|x) dx && (560)\\
&= \int sgn(a - y) p(sgn(a - y)|x) dx && (561)
\end{aligned}$$

So, the quantity we are minimizing is the sign of the quantity $a - y$. Note that $\forall a < y, sgn(a - y) = -1$ and $\forall a > y, sgn(a - y) = 1$. Thus the as above y "cancel out" the as below y. Thus, we want to maximize the number of $a - y$ that cancel each other out. This will occur at the median.

Exercise 5.10. **If $L_{FN} = cL_{FP}$, show that we should pick $\hat{y} = 1$ iff $p(y = 1|x)/p(y = 0|x) > \tau$, where $\tau = \frac{c}{1+c}$.**

The text here is misprinted. In the example they give, $c = 2$, meaning that false negatives are twice as bad as false positives. They then say that this would cause the model to have a decision threshold of $2/3$, meaning that it would err on the side of saying negative. Since false negatives are more costly, this doesn't make sense.

$$\rho(\hat{y} = 0|x) = cL_{FP}p(y = 1|x) \tag{562}$$
$$\rho(\hat{y} = 1|x) = L_{FP}p(y = 0|x) \tag{563}$$
$$\tag{564}$$

We should pick class 1 iff

$$\rho(\hat{y} = 0|x) > \rho(\hat{y} = 1|x) \tag{565}$$
$$cL_{FP}p(y = 1|x) > L_{FP}p(y = 0|x) \tag{566}$$
$$cp(y = 1|x) > p(y = 0|x) \tag{567}$$
$$\frac{p(y = 1|x)}{p(y = 0|x)} > \frac{1}{c} \tag{568}$$

The above equation makes more sense. Let $c = 2$. This means that classifying something wrongly as negative is twice as bad as classifying something wrongly as positive. So, we should err on the side of classifying things as positive.

In this case, we just have to show that the ratio is $> \frac{1}{2}$ before we classify as positive. This is in line with intuition.

6 Frequentist Statistics

Exercises

Exercise 6.1. **Suppose we have a completely random dataset with N_1 examples of class 1, and N_2 examples of class 2, where $N_1 = N_2$. What is the best misclassification rate any method can achieve? What is the estimated misclassification rate of the same method using LOOCV?**

The misclassification rate is given by

$$\frac{1}{N}\sum_{i=1}^{N} I(\hat{y}_i \neq y_i) = \frac{1}{N_1 + N_2}\sum_{i=1}^{N} y(1-\hat{y}) \tag{569}$$

Since the input x tells us nothing about the output y, the best classification rate we could possibly do is $\frac{1}{K}$, where K is the number of classes. Thus, in this case, the best we could do is $\frac{1}{2}$. For LOOCV, we see that this is given by

$$R(m, D, N) = \frac{1}{N}\sum_{i=1}^{N} L(y_i, f_m^{-i}(x_i))$$

Since the dataset is random, $f_m^{-i}(x_i) = f_m(x_i)$. This is identical to the equation above, which means that we would get the same answer from LOOCV as we did the simple misclassification rate in this case.

Exercise 6.2. **James Stein estimator for Gaussian means.**
a. Find the ML-II estimate of m_0 and τ_0^2.

The two stage model is given by

$$Y_i|\theta_i \sim N(\theta_i, 500), \theta_i|\mu \sim N(m_0, \tau_0^2)$$

The quantity we must optimize is given by

$$p(D|\theta_i, \mu) = \prod_{n=1}^{N} N(\theta_i, 500)N(m_0|\tau_0^2) \tag{570}$$

$$log\, p(D|\theta_i, \mu) = \sum_{n=1}^{N} log\, N(\theta_i, 500) + \sum_{n=1}^{N} log\, N(m_0|tau_0^2) \tag{571}$$

$$\propto -\sum_{n=1}^{N}(y_i - \theta_i)^2 - \sum_{n=1}^{N} log\sqrt{2\pi\tau_0^2} - \frac{(y_i - m_0)^2}{2\tau_0^2} \tag{572}$$

To find the ML-II estimate, we maximize this quantity with respect to m_0:

$$\frac{d}{dm_0} log\, p(D|\theta_i, \mu) = \frac{d}{dm_0}(-\sum_{n=1}^{N} \frac{(y_i - m_0)^2}{2\tau_0^2}) \tag{573}$$

$$= \frac{d}{dm_0}(-\sum_{n=1}^{N} \frac{1}{2\tau_0^2}(y_i^2 - 2m_0 y_i + m_0^2)) \tag{574}$$

$$= \frac{d}{dm_0}(\sum_{n=1}^{N} \frac{1}{2\tau_0^2}(2m_0 y_i - m_0^2)) \tag{575}$$

$$= \frac{d}{dm_0}(\sum_{n=1}^{N} \frac{1}{\tau_0^2} m_0 y_i) - \frac{N^2}{\tau_0^2} m_0 \tag{576}$$

$$= \frac{d}{dm_0}(\frac{N}{\tau_0^2} \sum_{n=1}^{N} m_0 y_i) - \frac{N^2}{\tau_0^2} m_0 \tag{577}$$

$$= -\frac{N^2}{\tau_0^2} m_0 + \frac{N}{\tau_0^2} \sum_{n=1}^{N} y_i \tag{578}$$

Setting this equal to 0, we get

$$0 = -\frac{N^2}{\tau_0^2} m_0 + \frac{N}{\tau_0^2} \sum_{n=1}^{N} y_i \tag{579}$$

$$\frac{N^2}{\tau_0^2} m_0 = \frac{N}{\tau_0^2} \sum_{n=1}^{N} y_i \tag{580}$$

$$N m_0 = \sum_{n=1}^{N} y_i \tag{581}$$

$$m_0 = \frac{1}{N} \sum_{n=1}^{N} y_i \tag{582}$$

Thus we see that the ML-II of m_0 is just the arithmetic mean of the dataset. We can similarly do this analysis for τ_0^2:

$$\frac{d}{d\tau_0^2} log\, p(D|\theta_i, \mu) \propto \frac{d}{d\tau_0^2}(-\sum_{n=1}^{N}(y_i - \theta_i)^2 - \sum_{n=1}^{N} log\sqrt{2\pi\tau_0^2} - \frac{(y_i - m_0)^2}{2\tau_0^2}) \tag{583}$$

$$= \frac{d}{d\tau_0^2}(-Nlog\sqrt{2\pi\tau_0^2} - \frac{N}{2\tau_0^2}\sum_{n=1}^{N}(y_i - m_0)^2) \tag{584}$$

$$= \frac{d}{d\tau_0^2}(-Nlog\sqrt{2\pi\tau_0^2}) - \frac{N\sum_{n=1}^{N}(y_i - m_0)^2}{4\tau_0^4} \tag{585}$$

$$= -\frac{N}{2\tau_0^2} - \frac{N\sum_{n=1}^{N}(y_i - m_0)^2}{4\tau_0^4} \tag{586}$$

Again, setting this to 0 gives us

$$0 = -\frac{N}{2\tau_0^2} - \frac{N\sum_{n=1}^{N}(y_i - m_0)^2}{4\tau_0^4} \tag{587}$$

$$\frac{N}{2\tau_0^2} = \frac{N\sum_{n=1}^{N}(y_i - m_0)^2}{4\tau_0^4} \tag{588}$$

$$\frac{2\tau_0^2}{4\tau_0^4} = \frac{N}{N\sum_{n=1}^{N}(y_i - m_0)^2} \tag{589}$$

$$\frac{1}{2\tau_0^2} = \frac{1}{\sum_{n=1}^{N}(y_i - m_0)^2} \tag{590}$$

$$\tau_0^2 = \frac{1}{2}\sum_{n=1}^{N}(y_i - m_0)^2 \tag{591}$$

b. Find the posterior estimates of $E[\theta_i|y_i, m_0, \tau_0]$ and $var[\theta_i|y_i, m_0, \tau_0]$ for $i = 1$.

Note that as the data tends to ∞, the ML estimate coverges to the expected value of the actual parameter. So, the posterior estimate of $E[\theta_1|y_1, m_0, \tau_0]$ is given by

$$E[\theta_1|y_1, m_0, \tau_0] = N(\frac{y_1}{N}, \frac{1}{2}(y_1 - \frac{y_1}{N})^2) \tag{592}$$

$$= N(\frac{y_1}{N}, \frac{1}{2}(\frac{N-1}{N}y_1)^2) \tag{593}$$

$$= N(\frac{y_1}{N}, \frac{(N-1)^2}{2N^2}y_1^2) \tag{594}$$

Plugging in the data, this gives us

$$E[\theta_1|y_1, m_0, \tau_0] = N(\frac{y_1}{N}, \frac{(N-1)^2}{2N^2}y_1^2) \tag{595}$$

$$= N(\frac{1505}{6}, \frac{25}{72}1505^2) \tag{596}$$

c. Give a 95% credible interval for $p(\theta_i|y_i, m_0, \tau_0)$ for $i = 1$. Do you trust this interval?

The 95% confidence interval is given by $m_0 \pm 1.96\frac{\sigma^2}{\sqrt{N}}$. Plugging the numbers in, we get

$$m_0 \pm 1.96\frac{\sigma^2}{\sqrt{N}} = \frac{1505}{6} \pm 1.96\frac{\frac{25}{72}1505^2}{\sqrt{6}} \tag{597}$$

This interval is very wide.

d. What do you expect would happen to your estimates if σ^2 were much smaller (say $\sigma^2 = 1$)? You do not need to compute the numerical answer; just briefly explain what would happen qualitatively, and why.

If the σ^2 were much smaller, this would not affect the variance of θ_i, which is affected only by m_0 and τ_0^2. Thus, this would have no effect on the interval width.

Exercise 6.3. **Show that $\hat{\sigma}^2 = \frac{1}{N}\sum_{n=1}^{N}(x_n - \hat{\mu})^2$ is a biased estimator of σ_2.**

To show this, we note that

$$E[\hat{\sigma^2}] = E[\frac{1}{N}\sum_{n=1}^{N}(x_n - \hat{\mu})^2] \tag{598}$$

$$= \frac{1}{N}E[\sum_{n=1}^{N}x_n^2 - 2\sum_{n=1}^{N}x_n\hat{\mu} + \sum_{n=1}^{N}\hat{\mu}^2] \tag{599}$$

$$= \frac{1}{N}E[\sum_{n=1}^{N}x_n^2 - 2N\hat{\mu}^2 + \sum_{n=1}^{N}\hat{\mu}^2] \tag{600}$$

$$= E[\frac{1}{N}\sum_{n=1}^{N}x_n^2] - 2E[\hat{\mu}^2] + E[\frac{1}{N}\sum_{n=1}^{N}\hat{\mu}^2] \tag{601}$$

$$= E[x^2] - 2E[\hat{\mu}^2] + E[\hat{\mu}^2] \tag{602}$$

$$= E[x^2] - E[\hat{\mu}^2] \tag{603}$$

Note that the definition of variance says that

$$\sigma^2 = E[x^2] - E[x]^2$$

So, if we define $\sigma_x^2 = E[x^2] - E[x]^2$ and $\sigma_{\hat{\mu}}^2 = E[\hat{\mu}^2] - E[\hat{\mu}]^2$, then

$$\begin{aligned}
\sigma_x^2 - \sigma_{\hat{\mu}}^2 &= (E[x^2] - E[x]^2) - (E[\hat{\mu}^2] - E[\hat{\mu}]^2) && (604)\\
&= E[x^2] - E[\hat{\mu}]^2 - E[x]^2 + E[\hat{\mu}]^2 && (605)\\
&= E[x^2] - E[\hat{\mu}]^2 && (606)\\
&= E[\hat{\sigma^2}] && (607)
\end{aligned}$$

The last two lines is valid because $E[x]^2 = E[\hat{\mu}]^2$, since $\hat{\mu}$ is an unbiased estimator.

Let's investigate the quantity $\sigma_{\hat{\mu}}^2$:

$$\begin{aligned}
\sigma_{\hat{\mu}}^2 &= Var[\hat{\mu}] && (608)\\
&= \frac{1}{N^2} Var[\sum_{n=1}^{N} x_n] && (609)\\
&= \frac{1}{N^2} \sum_{n=1}^{N} Var[x] && (610)\\
&= \frac{N}{N^2} Var[x] && (611)\\
&= \frac{1}{N} Var[x] && (612)\\
&= \frac{1}{N} \sigma_x^2 && (613)
\end{aligned}$$

Therefore,

$$\begin{aligned}
E[\hat{\sigma}^2] &= \sigma_x^2 - \frac{1}{N}\sigma_x^2 && (614)\\
&= \frac{N-1}{N}\sigma_x^2 && (615)
\end{aligned}$$

Exercise 6.4. **Estimate σ^2 when μ is known.**

We saw before that $E[\hat{\sigma^2}] = \sigma_x^2 - \sigma_{\hat{\mu}}^2$. If μ is known, then $\sigma_{\hat{\mu}}^2 = 0$. Thus,

$$E[\hat{\sigma^2}] = \sigma_x^2$$

which means the estimate is unbiased.

7 Linear Regression

Exercises

Exercise 7.1. **Behavior of training set error with increasing sample size.**

There are two sources of errors to be seen. One is measurement error, this is the irreducible error given in the noise of the problem. The other is approximation error, which is the error in finding the coefficients.

When the sample size is small, the training set error will be overly optimistic of the measurement error. That is, the model may overfit and thus understate this error source. As training size increases, either the model must become much more complex (so as to continue overfitting), or the overfitting will stop and the measurement error will converge to the measurement error of the problem.

As the model gets more complex, for a given sample size the approximation error will increase, since there are more parameters to estimate.

Let's combine the two intuitions. For a complex model with small sample size, the measurement error will be understated and the approximation error will be higher. As the sample size increases, the measurement error will tend towards the problem definition and the approximation error will decrease. This will cause the training set error to increase to a plateau as sample size increases.

Exercise 7.2. **Compute the MLE for W in the given data.**

The weight matrix W is given by

$$W = (X^T X)^{-1} X^T Y$$

We are given a single x vector that we expand using basis functions into

$$X = \begin{bmatrix} \phi(0) \\ \phi(0) \\ \phi(0) \\ \phi(1) \\ \phi(1) \\ \phi(1) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

In order to compute the MLE, we need to compute the quantity $(X^T X)^{-1}$. This is given by

$$(X^T X)^{-1} = \left(\begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}^T \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \right)^{-1} = \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{3} \end{bmatrix} \tag{616}$$

We use this quantity to compute the weight matrix:

$$W = (X^T X)^{-1} X^T Y \tag{617}$$

$$= \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{3} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}^T \begin{bmatrix} -1 & -1 \\ -1 & -2 \\ -2 & -1 \\ 1 & 1 \\ 1 & 2 \\ 2 & 1 \end{bmatrix} \tag{618}$$

$$= \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{3} \end{bmatrix} \begin{bmatrix} -4 & -4 \\ 4 & 4 \end{bmatrix} \qquad = \begin{bmatrix} -\frac{4}{3} & -\frac{4}{3} \\ \frac{4}{3} & \frac{4}{3} \end{bmatrix} \tag{619}$$

Exercise 7.3. **Derive the MLE for ridge regression if the input is mean centered.**

The formula for the model is given by

$$J(w, w_0) = (y - Xw - w_0 1)^T (y - Xw - w_0 1) + \lambda w^T w$$

We must optimize this for both w and w_0. The key to this is to understand that the mean of a matrix can be given by

$$\bar{X} = (1^T 1)^{-1} 1^T X$$

since $(1^T 1) = N$, which means $(1^T 1)^{-1} = 1/N$, and $1^T X = \sum_i X$. So, if X is mean centered, then this quantity is 0.

Let's optimize for w_0 first:

$$\frac{d}{w_0} J(w, w_0) = \frac{d}{w_0}(y^T y - y^T X w - y^T w_0 1 - w^T X^T y + \tag{620}$$

$$w^T X^T X w + w^T X^T w_0 1 - 1^T w_0^T y + 1^T w_0^T X w + 1^T w_0^T w_0 1 + \lambda w^T w) \tag{621}$$

$$= \frac{d}{w_0}(-y^T w_0 1 + w^T X^T w_0 1 - 1^T w_0^T y + 1^T w_0^T X w + 1^T w_0^T w_0 1) \tag{622}$$

$$= -1^T y + w^T X^T - 1^T y + w^T X^T + 2 w_0 1^T 1 \tag{623}$$

$$= -2^T y + 2 w^T X^T + 2 w_0 1^T 1 \tag{624}$$

Setting this equal to 0 we get

$$0 = -2^T y + 1^T w^T X^T + 2w_0 1^T 1 \tag{625}$$
$$= -1^T y + 1^T w^T X^T + w_0 1^T 1 \tag{626}$$
$$w_0 1^T 1 = 1^T y + w^T X^T \tag{627}$$
$$w_0 = (1^T 1)^{-1} 1^T y + (1^T 1)^{-1} 1^T w^T X^T \tag{628}$$
$$= (1^T 1)^{-1} 1^T y \tag{629}$$
$$= \bar{y} \tag{630}$$

Now let's look at w. Optimizing for this we get

$$\frac{d}{w} J(w, w_0) = \frac{d}{w}(y^T y - y^T X w - y^T w_0 1 - w^T X^T y + \tag{631}$$
$$w^T X^T X w + w^T X^T w_0 1 - 1^T w_0^T y + 1^T w_0^T X w + 1^T w_0^T w_0 1 + \lambda w^T w) \tag{632}$$
$$= \frac{d}{w}(-y^T X w - w^T X^T y + w^T X^T X w + w^T X^T w_0 1 + 1^T w_0^T X w + \lambda w^T w) \tag{633}$$
$$= -y^T X - y^T X + 2X^T X w + 1^T w_0^T X + 1^T w_0^T X + 2\lambda w \tag{634}$$
$$= -2y^T X + 2^T w_0^T X + 2\lambda w + 2X^T X w \tag{635}$$
$$= -y^T X + 1^T w_0^T X + \lambda w + X^T X w \tag{636}$$
$$= (X^T X + \lambda I) w - y^T X + 1^T \bar{y}^T X \tag{637}$$
$$= (X^T X + \lambda I) w - (y^T + 1^T \bar{y}^T) X \tag{638}$$
$$= (X^T X + \lambda I) w - (y^T + ||y||) X \tag{639}$$

Setting this equal to 0 we get

$$0 = (X^T X + \lambda I) w - (X^T y + X^T w_0)^T \tag{640}$$
$$(X^T X + \lambda I) w = (X^T y + X^T (y^T - w^T X))^T \tag{641}$$
$$(X^T X + \lambda I) w = (X^T y + X^T y^T - X^T w^T X)^T \tag{642}$$
$$(X^T X + \lambda I) w = (X^T (y + y^T - w^T X))^T \tag{643}$$

Exercise 7.4. **Show that the MLE for the error variance in linear regression is given by the empircal variance of the residual errors.**

Each residual is i.i.d and normal. Therefore, the likelihood is given by

$$L(y, \hat{y}) = \prod_{i=1}^{N} N(y - w^T x, \sigma^2) \tag{644}$$

$$log\, L(y, \hat{y}) = \sum_{i=1}^{N} log\, N(y - w^T x, \sigma^2) \tag{645}$$

$$= -\sum_{i=1}^{N} log(\sqrt{2\pi\sigma^2}) + \frac{(y_i - w^T x_i)^2}{2\sigma^2} \tag{646}$$

$$= -Nlog(\sqrt{2\pi\sigma^2}) + \sum_{i=1}^{N} \frac{(y_i - w^T x_i)^2}{2\sigma^2} \tag{647}$$

Taking the derivative of this wrt σ^2, we get

$$\frac{d}{d\sigma^2}(-Nlog(\sqrt{2\pi\sigma^2}) + \sum_{i=1}^{N} \frac{(y_i - w^T x_i)^2}{2\sigma^2}) = -\frac{N}{2\sigma^2} + \frac{(y_i - w^T x_i)^2}{2\sigma^4} \tag{648}$$

$$\tag{649}$$

Setting this to zero, get get

$$0 = -\frac{N}{2\sigma^2} + \frac{(y_i - w^T x_i)^2}{2\sigma^4} \tag{650}$$

$$\frac{N}{2\sigma^2} = \frac{(y_i - w^T x_i)^2}{2\sigma^4} \tag{651}$$

$$2N\sigma^4 = 2\sigma^2 (y_i - w^T x_i)^2 \tag{652}$$

$$N\sigma^2 = (y_i - w^T x_i)^2 \tag{653}$$

$$\sigma^2 = \frac{1}{N} \sum_{i=1}^{N} (y_i - w^T x_i)^2 \tag{654}$$

Exercise 7.5. **Derive the MLE for the offset term in linear regression.**
The loss function with the offset term separated is given by

$$L(y, \hat{y}) = \frac{1}{N} \sum_{i=1}^{N} (y - w^T x_i - w_0)^T (y - w^T x_i - w_0)$$

Taking the derivative of this with respect to w_0 we get

$$\frac{d}{dw_0} L(y, \hat{y}) = \frac{1}{N} \sum_{i=1} y - w^T x_i - w_0 \tag{655}$$

Setting this to 0 we see that

$$0 = \frac{1}{N}\sum_{i=1}^{N} y - w^T x_i - w_0 \tag{656}$$

$$w_0 = \frac{1}{N}\sum_{i=1}^{N} y - w^T x_i \tag{657}$$

$$= \bar{y} - \bar{x}^T w \tag{658}$$

If we similarly solve for w, then

$$\frac{d}{dw}L(y,\hat{y}) = \frac{d}{dw}((y - w^T X - w_0)^T(y - w^T X - w_0)) \tag{659}$$

$$= 2(y - w^T X - w_0)X^T \tag{660}$$

$$= (2y - 2w^T X - 2w_0)X^T \tag{661}$$

$$= 2X^T y - 2w^T X^T X - 2w_0 X^T \tag{662}$$

Setting this equal to 0 we get

$$0 = 2X^T y - 2w^T X^T X - 2w_0 X^T \tag{663}$$

$$wX^T X = X^T y - w_0 X^T \tag{664}$$

$$w = (X^T X)^{-1}X^T y - (X^T X)^{-1} w_0 X^T \tag{665}$$

$$= (X^T X)^{-1}X^T y - (X^T X)^{-1}(\bar{y} - \bar{X}^T w)X^T \tag{666}$$

$$= (X^T X)^{-1}X^T y - (X^T X)^{-1}X^T \bar{y} + (X^T X)^{-1}\bar{X}^T w X^T \tag{667}$$

$$= (X^T X)^{-1}X^T (y - \bar{y}) + (X^T X)^{-1}\bar{X}^T w X^T \tag{668}$$

$$w - (X^T X)^{-1}\bar{X}X^T w = (X^T X)^{-1}X^T y_c \tag{669}$$

$$w(1 - (X^T X)^{-1}\bar{X}X^T) = (X^T X)^{-1}X^T y_c \tag{670}$$

$$w = (1 - (X^T X)^{-1}\bar{X}X^T)^{-1}(X^T X)^{-1}X^T y_c \tag{671}$$

$$= (X^T X)^{-1}X^T y_c - (\bar{X}X^T)^{-1}(X^T X)(X^T X)^{-1}X^T y_c \tag{672}$$

$$= (X^T X)^{-1}X^T y_c - (\bar{X}X^T)X^T y_c \tag{673}$$

$$= ((X - \bar{X})^T(X - \bar{X}))^{-1}((X - \bar{X})^T)y_c \tag{674}$$

$$= (X_c^T X_c)^{-1}X_c y_c \tag{675}$$

Exercise 7.6. **Derive the MLE for simple linear regression.**

Simple linear regression is just linear regression in the 1d case. The loss function is given by

$$L(y, \hat{y}) = \frac{1}{2} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)^2 \tag{676}$$

where we use $\frac{1}{2}$ instead of $\frac{1}{N}$ because this will be easier to take the derivative of. Taking the derivative wrt w_0, we get

$$\frac{d}{dw_1} L(y, \hat{y}) = \frac{d}{dw_1} \frac{1}{2} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)^2 \tag{677}$$

$$= \sum_{i=1}^{N} y_i - w_1 x_i - w_0 \tag{678}$$

Setting this equal to 0, we get

$$0 = \sum_{i=1}^{N} y_i - w_1 x_i - w_0 \tag{679}$$

$$N w_0 = \sum_{i=1}^{N} y_i - w_1 x_i \tag{680}$$

$$w_0 = \frac{1}{N} \sum_{i=1}^{N} y_i - \frac{1}{N} w_1 \sum_{i=1}^{N} x_i \tag{681}$$

$$= \bar{y} - w_1 \bar{x} \tag{682}$$

Taking the derivative of the loss function wrt w_1, we get

$$\frac{d}{dw_1} L(y, \hat{y}) = \frac{d}{dw_1} \frac{1}{2} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)^2 \tag{683}$$

$$= \sum_{i=1}^{N} (y_i - w_1 x_i - w_0) x_i \tag{684}$$

Setting this equal to 0, we get

$$0 = \sum_{i=1}^{N}(y_i - w_1 x_i - w_0)x_i \tag{685}$$

$$= \sum_{i=1}^{N} y_i x_i - w_1 x_i^2 - w_0 x_i \tag{686}$$

$$w_1 \sum_{i=1}^{N} x_i^2 = \sum_{i=1}^{N} x_i y_i - (\bar{y} - w_1 \bar{x})x_i \tag{687}$$

$$w_1 \sum_{i=1}^{N} x_i^2 = \sum_{i=1}^{N} x_i y_i - \bar{y}\sum_{i=1}^{N} x_i + w_1 \bar{x}\sum_{i=1}^{N} x_i \tag{688}$$

$$w_1 \sum_{i=1}^{N} x_i^2 = \sum_{i=1}^{N} x_i y_i - N\bar{x}\bar{y} + N w_1 \bar{x}^2 \tag{689}$$

$$+N w_1 \bar{x}^2 \tag{690}$$

$$w_1 \sum_{i=1}^{N} x_i^2 - N w_1 \bar{x}^2 = \sum_{i=1}^{N} x_i y_i - N\bar{x}\bar{y} \tag{691}$$

$$w_1 (\sum_{i=1}^{N} x_i^2 - N\bar{x}^2) = \sum_{i=1}^{N} x_i y_i - N\bar{x}\bar{y} \tag{692}$$

$$w_1 = \frac{\sum_{i=1}^{N} x_i y_i - N\bar{x}\bar{y}}{\sum_{i=1}^{N} x_i^2 - N\bar{x}^2} \tag{693}$$

Exercise 7.7. **Sufficient statistics for online linear regression.**
a. What are the minimal set of statistics that we need to estimate w_1?

Using the definitions defined in the problem text, we see that

$$w_1 = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2} = \frac{N C_{xy}^{(n)}}{N C_{xx}^{(n)}} = \frac{C_{xy}^{(n)}}{C_{xx}^{(n)}} \tag{694}$$

b. What are the minimal set of statistics that we need to estimate w_0?

We can see that

$$w_0 = \bar{y} - w_1 \bar{x} = \bar{y}^{(n)} - \frac{C_{xy}^{(n)}}{C_{xx}^{(n)}} \bar{x}^{(n)} \tag{695}$$

c. Derive equation for online updating $\bar{y}$.

We see that

$$\bar{y}^{(n+1)} = \frac{1}{n+1}\sum_{i=1}^{n+1} y_i \tag{696}$$

$$= \frac{1}{n+1}(n\bar{y} + y_{n+1}) \tag{697}$$

$$= \frac{n}{n+1}\bar{y} + \frac{1}{n+1}y_{n+1} \tag{698}$$

$$= \bar{y} - \frac{1}{n+1}\bar{y} + \frac{1}{n+1}y_{n+1} \tag{699}$$

$$= \bar{y} - \frac{1}{n+1}(\bar{y} + y_{n+1}) \tag{700}$$

d. Derive the update equation for C_{xy}

$$C_{xy}^{(n+1)} = \frac{1}{n+1}\sum_{i=1}^{n+1}(x_i - \bar{x}^{(n+1)})(y_i - \bar{y}^{(n+1)}) \tag{701}$$

$$= \frac{1}{n+1}(x_{n+1} - \bar{x}^{(n+1)})(y_{n+1} - \bar{y}^{(n+1)}) + \frac{1}{n+1}\sum_{i=1}^{n}(x_i - \bar{x}^{(n+1)})(y_i - \bar{y}^{(n+1)}) \tag{702}$$

$$= \frac{1}{n+1}(x_{n+1}y_{n+1} - x_{n+1}\bar{y}^{(n+1)} - y_{n+1}\bar{x}^{(n+1)} + \bar{x}^{(n+1)}\bar{y}^{(n+1)}) \tag{703}$$

$$+ \frac{1}{n+1}\sum_{i=1}^{n}(x_i y_i - x_i\bar{y}^{(n+1)} - y_i\bar{x}^{(n+1)} - \bar{x}^{(n+1)}\bar{y}^{(n+1)}) \tag{704}$$

By plugging in the equation we derived in part c., we can see that

$$C_{xy}^{(n+1)} = \frac{1}{n+1}\left[x_{n+1}y_{n+1} + nC_{xy}^{(n)} + n\bar{x}^{(n)}\bar{y}^{(n)} - (n+1)\bar{x}^{(n+1)}\bar{y}^{(n+1)}\right] \tag{705}$$

Parts e. and f. can be found in the IPython notebook ch7-7.ipynb

Exercise 7.8. **Bayesian linear regression in 1d with known σ^2**

a. Compute unbiased estimate of $\hat{\sigma}^2$, using w as the MLE.

This is implemented in code in the IPython notebook ch7-8.ipynb.

b. Assume $p(w) = p(w_0)p(w_1)$, and $p(w_0)$ is uniform and $p(w_1)$ is $N(0,1)$. What is $p(w)$?

An uniformative uniform prior can be expressed as a normal with infinite variance (or zero precision). Thus

$$p(w) = N(0,\infty)N(0,1) \tag{706}$$

$$= N(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}\infty & 0\\0 & 1\end{bmatrix}) \tag{707}$$

c. Compute the marginal posterior of the slope $p(w_1|D, \sigma^2)$. What is $E[w_1|D, \sigma^2]$ and $var[w_1|D, \sigma^2]$?

Using the results from 7.6.1, we see that the posterior is given by

$$p(w|x, y, \sigma^2) = N(w|w_N, V_N) \tag{708}$$

$$w_N = \frac{1}{\sigma^2} V_N \sum_{i=1}^{N} x_i y_i \tag{709}$$

$$V_N = \frac{\sigma^2}{\sigma^2 + \sum_{i=1}^{N} x_i^2} \tag{710}$$

By plugging in the data provided, we get

$$p(w|x, y, \sigma^2) = N(w|0.012567, 0.000407)$$

These two parameters to the distribution are the expected value and the variance, respectively,

d. What is a 95% credible interval for w_1?

Since the posterior is Gaussian, we note that the 95% credible interval is given by $\mu \pm 1.96\sigma^2$. From the numbers given, this is

$$0.012567 \pm 1.96 \times 0.000407 = [0.01176928, 0.01336472]$$

8 Logistic Regression

Exercises

Exercise 8.1. **Spam classification using logistic regression.**
This exercise is written in the IPython notebook ch8-1-2.ipynb.

Exercise 8.2. **Spam classification using Naive Bayes.**
This exercise is written in the IPython notebook ch8-1-2.ipynb.

Exercise 8.3. **Gradient and Hessian of log-likelihood for multinomial logistic regression.**

a. Derive the derivative of the sigmoid function.

The sigmoid function is given by

$$\sigma(a) = \frac{1}{1+e^{-a}}$$

Taking the derivative of this, we get

$$\frac{d}{da}\sigma(a) = \frac{d}{da}\frac{1}{1+e^{-a}} \tag{711}$$

$$= -\frac{1}{(1+e^{-a})^2}\frac{d}{da}(1+e^{-a}) \tag{712}$$

$$= -\frac{1}{(1+e^{-a})^2)} \times -e^{-a} \tag{713}$$

$$= \frac{e^{-a}}{(1+e^{-a})^2} \tag{714}$$

$$= e^{-a}\sigma(a)^2 \tag{715}$$

$$= (\frac{1}{\sigma(a)} - 1)\sigma(a)^2 \tag{716}$$

$$= \sigma(a)(1-\sigma(a)) \tag{717}$$

b. Using the previous result and chain rule of calculus, derive an expression for the gradient of the log likelihood.

The NLL is given by

$$NLL(w) = \sum_{i=1}^{N} log(1 + exp(-\tilde{y}_i w^T x_i))$$

The gradient of this is the derivative of this wrt w, which is

$$\frac{d}{dw}NLL(w) = \frac{d}{dw}\sum_{i=1}^{N} log(1 + exp(-\tilde{y}_i w^T x_i)) \tag{718}$$

$$= \sum_{i=1}^{N} \sigma(\tilde{y}_i w^T x_i) x_i \tilde{y}_i \tag{719}$$

We note that $\tilde{y} \in [-1, 1]$. Therefore, when $\tilde{y} = 1$ we get

$$\frac{d}{dw} NLL(w) = \sum_{i=1}^{N} \sigma(w^T x_i) x_i = \sum_{i=1}^{N} \mu_i x_i$$

and when $\tilde{y} = -1$ we get

$$\frac{d}{dw} NLL(w) = -\sum_{i=1}^{N} \sigma(-w^T x_i) x_i = -\sum_{i=1}^{N} (1 - \sigma(w^T x_i)) x_i = -\sum_{i=1}^{N} (1 - \mu_i) x_i$$

Therefore, using the fact that $y \in [0, 1]$, we can rewrite this as

$$\frac{d}{dw} NLL(w) = \sum_{i=1}^{N} (\mu_i - y_i) x_i$$

c. Prove that the Hessian is positive definite.
The Hessian is given by

$$H = X^T S X$$

where $S = diag(\mu_1(1 - \mu_1), ..., \mu_n(1 - \mu_n))$. Since we know that $0 \geq \mu_i \leq 1$, we know that S is positive. Therefore

$$\begin{aligned} H &= X^T S X && (720) \\ &= tr(X^T S X) && (721) \\ &= \sum_i \sum_j X_{ij} S_{ij} X_{ij} && (722) \\ &= \sum_i \sum_j X_{ij}^2 S_{ij} && (723) \end{aligned}$$

Since $X_{ij}^2 \geq 0 \, \forall X_{ij}$, then H must be positive definite.

Exercise 8.4. **Gradient and Hessian of log-likelihood for multinomial logistic regression.**
a. Derive the Jacobian of the softmax.
The softmax function is given by

$$S(\eta_i)_k = \frac{e^{\eta_{ik}}}{\sum_{j=1}^{J} e^{\eta_{ij}}}$$

Let's look at the derivative in the case where $\eta_{ij} = \eta_{ik}$. In this case, the derivative is

$$\frac{\partial \mu_{ik}}{\partial \eta_{ij}} = \frac{\partial \mu_{ij}}{\partial \eta_{ij}} = \frac{\partial}{\partial \eta_{ij}} \frac{e^{\eta_{ij}}}{\sum_{j=1}^{J} e_{ij}^{\eta}} \tag{724}$$

$$= \frac{e^{\eta_{ij}}}{\sum_{j=1}^{J} e^{\eta_{ij}}} - \frac{e^{2\eta_{ij}}}{(\sum_{j=1}^{J} e^{\eta_{ij}})^2} \tag{725}$$

Now let's look at the case when $\eta_{ij} \neq \eta_{ik}$. In this case, the derivative is

$$\frac{\partial \mu_{ik}}{\partial \eta_{ij}} = -\frac{e^{\eta_{ik}+\eta_{ij}}}{(\sum_{j=1}^{J} e^{\eta_{ij}})^2} \tag{726}$$

We can combine these into one equation using $\delta_{jk} = I(j = k)$ as follows:

$$\frac{\partial \mu_{ik}}{\partial \eta_{ij}} = \delta_{jk} \left(\frac{e^{\eta_{ij}}}{\sum_{j=1}^{J} e^{\eta_{ij}}} - \frac{e^{\eta_{ij}+\eta_{ik}}}{(\sum_{j=1}^{J} e^{\eta_{ij}})^2} \right) - (1 - \delta_{jk}) \frac{e^{\eta_{ik}+\eta_{ij}}}{(\sum_{j=1}^{J} e^{\eta_{ij}})^2} \tag{727}$$

$$= \delta_{jk}(\mu_{ij} - \mu_{ij}\mu_{ik}) - (1 - \delta_{jk})\mu_{ij}\mu_{ik} \tag{728}$$

$$= \delta_{jk}\mu_{ij} - \delta_{jk}\mu_{ij}\mu_{ik} - \mu_{ij}\mu_{ik} + \delta_{jk}\mu_{ij}\mu_{ik} \tag{729}$$

$$= \delta_{jk}\mu_{ij} - \mu_{ij}\mu_{ik} \tag{730}$$

$$= \mu_{ij}(\delta_{jk} - \mu_{ik}) \tag{731}$$

b. Show that $\bigtriangledown_{w_c} l = \sum_i (y_{ic} - \mu_{ic}) x_i$.
The log likelihood is given by

$$l(W) = \sum_{i=1}^{N} \left[\left(\sum_{c=1}^{C} y_{ic} w_c^T x_i \right) - log \left(\sum_{c'=1}^{C} exp(w_{c'}^T x_i) \right) \right] \tag{732}$$

$$= \sum_{i=1}^{N} \sum_{c=1}^{C} y_{ic} w_c^T x_i - \sum_{i=1}^{N} log \sum_{c'=1}^{C} exp(w_{c'}^T x_i) \tag{733}$$

The likelihood for a particular class c is given by

$$l(w_c) = \sum_{i=1}^{N} y_{ic} w_c^T x_i - \sum_{i=1}^{N} log \sum_{c'=1}^{C} exp(w_{c'}^T x_i) \tag{734}$$

$$= w_c \sum_{i=1}^{N} y_{ic} x_i - \sum_{i=1}^{N} log \sum_{c'=1}^{C} exp(w_{c'}^T x_i) \tag{735}$$

$$\tag{736}$$

Taking the derivative of this wrt w_c, we get

$$\nabla_{w_c} l = \sum_{i=1}^{N} y_{ic} x_i - \sum_{i=1}^{N} x_i \frac{e^{w_c^T x_i}}{\sum_{c'=1}^{C} e^{w_{c'}^T x_i}} \tag{737}$$

$$= \sum_{i=1}^{N} y_{ic} x_i - \mu_{ic} x_i \tag{738}$$

$$= \sum_{i=1}^{N} (y_{ic} - \mu_{ic}) x_i \tag{739}$$

c. Derive the block submatrix of the Hessian for the classes c and c'.

We must take the derivative of the equation derived above.

$$\nabla^2_{w_c} l = \nabla_{w_c} \nabla_{w_c} l = \nabla_{w_c} \sum_{i=1}^{N} (y_{ic} - \mu_{ic}) x_i \tag{740}$$

$$= -\sum_{i=1}^{N} \mu_{ic} (\delta_{cc'} - \mu_{ic'}) x_i \tag{741}$$

Exercise 8.5. **Symmetric version of l_2 regularized multinomial logistic regression.**

In this problem, we are asked to optimize a regularized multinomial model, where the problem is overspecified (there are C parameters and only $C - 1$ degrees of freedom). In particular we are asked to optimize

$$\sum_{i=1}^{N} log\, p(y_i|x_i, W) - \lambda \sum_{c=1}^{C} w_c^T w_c = \sum_{i=1}^{N} w_{c0} + w_c^T x_i - log(\sum_{c=1}^{C} e^{w_{c0} + w_c^T x_i}) - \lambda \sum_{c=1}^{C} w_c^T w_c \tag{742}$$

Using the definition of the gradient defined in previous problems, we can derive the derivative of this optimizer wrt w as

$$\frac{d}{w_c} \sum_{i=1}^{N} log\, p(y_i|x_i, W) - \lambda \sum_{c=1}^{C} w_c^T w_c = \sum_{i=1}^{N} (y_{ic} - \mu_{ic}) x_i - 2\lambda w_c \tag{743}$$

Note that at the optimum, the gradient is necessarily 0. Thus we have

$$0 = -2\lambda w_c \tag{744}$$

$$w_c = \sum_{j=1}^{J} w_{cj} = 0 \tag{745}$$

Exercise 8.6. **Elementary properties of l_2 regularized logistic regression.**
a. The cost function has multiple locally optimal solutions.

This is False. For this to be false, the cost function would have to be convex. That occurs when the Hessian is strictly positive. The likelihood is convex, as is shown in the text, so the Hessian of the regularization term need be strictly positive. The Hessian of this term is λ.

b. Let $\hat{w}$ be global optimum. $\hat{w}$ is sparse?

False. Regularization penalizes the weight vectors, but does not induce sparsity. Regularization pushes the weight vectors towards zero, but quadratically. Another way to think about this is that the curvature is positive, and therefore will only tend to zero at the limits.

c. If the training data is linearly separable, then some weights w_j might become infinite if $\lambda = 0$.

This is true. If the data is linearly separable and there is no regularization, then the weights can go to infinity, since they control the steepness of the sigmoid curve. Regularization would prevent this, obvoiusly.

d. The likelihood on the training set always increases as we increase λ.

False. As we increase λ, we restrict degrees of freedom. Thus we incur bias on the training set for a reduction in variance.

d. The likelihood on the test set always increases as we increase λ.

False. As we increase λ, we do in fact perform better on the test set, but only to a point. At some point, the regularization term overwhelms, and the model becomes too rigid to be useful even on the test set.

9 Generalized linear models and the exponential family

Exercises

Exercise 9.1. **Conjugate prior for univariate Gaussian in exponential family form.**

Let's start backwards. We are told that the conjugate prior is given by

$$N(\mu|\gamma, \lambda(2\alpha-1))Ga(\lambda|\alpha,\beta) \propto exp(-\frac{\lambda(2\alpha-1)}{2}(\mu-\gamma)^2)\lambda^{\alpha-1}exp(-\lambda\beta) \tag{746}$$

$$= exp(-\frac{\lambda(2\alpha-1)}{2}(\mu-\gamma)^2 - \lambda\beta)\lambda^{\alpha-1} \tag{747}$$

$$= exp(-\frac{\lambda}{2}\left[(2\alpha-1)(\mu-\gamma)^2 - 2\beta\right])\lambda^{\alpha-1} \tag{748}$$

In the problem, we are asked to parameterize this distribution using μ and $\lambda = 1/\sigma^2$. Thus, the likelihood is given by

$$p(D|\mu,\lambda) = \prod_{i=1}^{N} \frac{\lambda}{\sqrt{2\pi}} exp(-\frac{\lambda}{2}(x_i-\mu)^2) \tag{749}$$

$$= \lambda^N (2\pi)^{-N/2} \prod_{i=1}^{N} exp(-\frac{\lambda}{2}(x_i-\mu)^2) \tag{750}$$

$$= \lambda^N (2\pi)^{-N/2} exp(-\frac{\lambda}{2}\sum_{i=1}^{N}(x_i-\mu)^2) \tag{751}$$

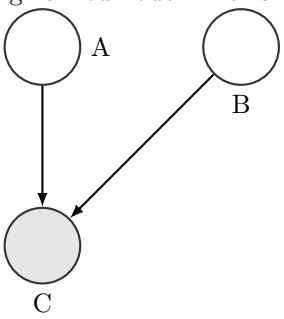
10 Directed graphical models (Bayes nets)

Exercises

Exercise 10.1. **Consider the DAG in Figure 10.14(a). Construct a new DAG where you marginalize out X.**

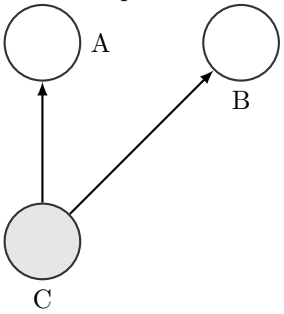
The important thing to note here is that while conditioning a variable acts like a "blocker" node, marginalizing a node does the opposite. It removes the node from the DAG, and adjusts all nodes accordingly.

To illustrate some properties of marginalization, let a shaded node mean a marginalized node. In this case

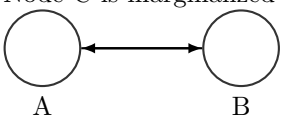


Node C is marginalized and this DAG reduces to

In other words, since A and B are parents of C, marginalizing on C will make A and B independent of each other. Another situation is



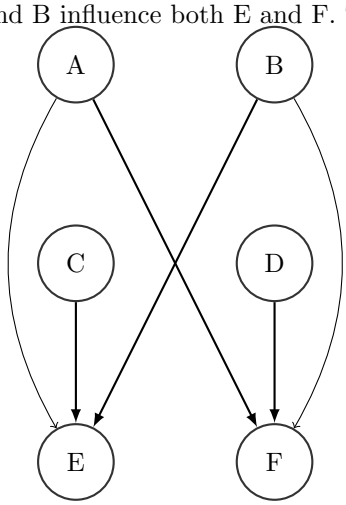
Node C is marginalized and this DAG reduces to



In this situation, C is a parent of A and B. Marginalizing out C causes and A and B to be dependent to each other.

Applying these rules to the DAG in the problem text, we note that node X is both a child and a parent node. By marginalizing X, it removes the dependence

on A and B, but adds dependencies to A and B through the children of X. In other words, by removing X, now A and B influence E and F. Particularly, both A and B influence both E and F. The DAG then looks like



As you can see, both nodes A and B now affect E and F.

Exercise 10.2. **Bayes ball.**

a. Consider the DAG in Figure 10.14(b). List all variables that independent of A given evidence on B.

"Given evidence on B" is another way of saying "conditional on B". To find all of the variables that are independent of A, we look at all the paths that each variable can arrive at A through, and examine them with the knowledge of B.

Let's go through the nodes then.

Node C: this node is a parent of A, and thus is not independent of A, even knowing B.

Node D: from node D, we can reach A through $\{D, B, A\}$, $\{D, G, E, C, A\}$, and $\{D, G, I, H, C, A\}$. Conditioning on B blocks $\{D, B, A\}$, but not the others. Therefore, D is not independent of A, conditioned on B.

Node E: we can reach node A using $\{E, C, A\}$, which is unblocked. Therefore node E is not independent of node A.

Node F: we can reach node A using $\{F, C, A\}$, which is unblocked. Therefore node F is not independent of node A.

Node G: we can reach node A using $\{G, E, C, A\}$, $\{G, D, B, A\}$, or $\{G, I, H, F, C, A\}$. The path $\{G, D, B, A\}$ is blocked, but the others are not, and therefore node G is reachable from node A.

Node H: we can reach node A using $\{H, F, C, A\}$, $\{H, I, G, E, C, A\}$, or $\{H, I, G, D, B, A\}$. The path $\{H, I, G, D, B, A\}$ is blocked, but the others are not, and therefore node H is reachable from node A.

Node I: we can reach node A using $\{I, H, F, C, A\}$, $\{I, G, D, B, A\}$, or $\{I, G, E, C, A\}$. The path $\{I, G, D, B, A\}$ is blocked, but the others are not, and therefore node I is reachable from node A.

Thus, the only node that is independent to A conditioning on B is B.

b. Consider the DAG in Figure 10.14(c). List all variables that are independent of A given evidence on J.

Note that since G is the sole parent of J and J has no children, conditioning on J is equivalent to conditioning on G.

Next, let's identify the hidden nodes. These are $\{H, I\}$. This means that nodes C, F are blocked from the rest of the DAG and are independent of A.

For the remaining nodes, note that conditioning on G opens up paths to A, since all paths to A from other nodes that go through G will go through a v-structure node. Thus, nodes $\{B, D, E\}$ are all not independent of A.

Thus, nodes $\{G, J, H, I, C, F\}$ are all independent of A after conditiong on J.

Exercise 10.3. **Markov blanked for a DGM.**

We want to prove that the conditional for a node is given by the conditional of the node with its parents times the conditional of its children with itself. The conditional is given by

$$p(X_i|X_{-i}) = \frac{p(X_{-i}|X_i)p(X_i)}{p(X_{-i})} \tag{752}$$

$$= \frac{p(X_i)\prod_{t\neq i}^{T} p(X_t|pa(X_t), X_i)}{\prod_{t\neq i}^{T} p(X_t|pa(X_t))} \tag{753}$$

Note that for the children X_c of X_i, $pa(X_c) = X_i$. Thus, the numerator becomes

$$p(X_i|X_{-i}) = \frac{p(X_i)\prod_{Y_j\in ch(X_i)} p(Y_j|pa(Y_j))\prod_{t\neq i}^{T} p(X_t|pa(X_t), X_i)}{\prod_{t\neq i}^{T} p(X_t|pa(X_t))} \tag{754}$$

Note that Equation 10.7 comes in handy here. it says that $p(X_{1:V}) = \prod_{t=1}^{V} p(x_t|pa(x_t))$. What follows from this is that nodes are not affected by nodes that aren't its parents. Thus, we can write this quantity as

$$p(X_i|X_{-i}) = \frac{p(X_i|pa(X_i))\prod_{Y_j\in ch(X_i)} p(Y_j|pa(Y_j))\prod_{t\neq i}^{T} p(X_t|pa(X_t))}{\prod_{t\neq i}^{T} p(X_t|pa(X_t))} \tag{755}$$

$$= p(X_i|pa(X_i)) \prod_{Y_j\in ch(X_i)} p(Y_j|pa(Y_j)) \tag{756}$$

Exercise 10.4. **Hidden variables in DGMs.**

a. Assuming all nodes (including H) are binary and all CPDs are tabular, prove that the model on the left has 17 free parameters.

In general, a variable with K states have $K-1$ free parameters. So, binary variables will have 1 free parameter. Thus $p(X_i)$ has 1 free parameter.

We can write $P(X_n|X_{n-1},...,X_1)$ as $P(X_n = n|X_{n-1} = m,...,X_1 = a) = T_{nm...a}$. Since we are dealing with binary variables, we note that $T_{nm...a}$ is indexed with a binary string of length n. The number of states in a binary string of length n is 2^{n-1}. Thus, $P(X_n|X_{n-1},...,X_1)$ has 2^{n-1} free parameters.

The joint distribution of this particular DGM is given by

$$p(X_{1:6}) = p(X_1)p(X_2)p(X_3)\sum_h p(H = h|X_{1:3})p(X_4|H = h)p(X_5|H = h)p(X_6|H = h) \tag{757}$$

Going left to right from each term in the joint, the number of free parameters are given by

$$1 + 1 + 1 + 2^3 + 2 + 2 + 2 = 17$$

b. Assuming all nodes are binary and all CPDs are tabular, prove that the model on the right has 59 free parameters.

The joint is given by

$$p(X_{1:6}) = p(X_1)p(X_2)p(X_3)p(X_4|X_{1:3})p(X_5|X_{1:4})p(X_6|X_{1:5})$$

Following the similar process above, we see that the number of free parameters are given by

$$1 + 1 + 1 + 2^3 + 2^4 + 2^5 = 59$$

c. Suppose we have a data set $D = X_{1:6}^n$ for $n = 1 : N$, where we observe the Xs but not H, and we want to estimate the parameters of the CPDs using maximum likelihood. For which model is this easier?

Computing the MLE for DGM models means counting the proportion that fall onto the entry of the CPD. Thus, with less free parameters, this is easier to estimate.

For very large N, the more complex model is preferred, because it models more interaction that may be useful. But for anything less than a very large N, the simpler model is easier to estimate the CPDs using maximum likelihood.

Exercise 10.5. **Bayes net for a rainy day.** The joint distribution is given by

$$P(V, R, G, S) = P(V)P(G)P(R|V, G)P(S|G) \tag{758}$$

a. Write down an expression for $P(S = 1|V = 1)$ in terms of α, β, γ, and δ.

We note that $p(x_i) = p(x_i|pa(x_i))$. Thus,

$$P(S = 1|V = 1) = P(S = 1|V = 1, G) = \sum_{g\in G} P(S = 1|G = g)P(G = g) \tag{759}$$

$$= \alpha(1 - \gamma) + (1 - \alpha)(1 - \beta) \tag{760}$$

b. Write down an expression for $P(S = 1|V = 0)$. Is this the same or different?

Since V is not a predecessor of S, this expression would be the same as $P(S = 1|V = 1)$.

c. Find ML estimates of α, β, and γ using the given dataset.

ML estimates of a CPT is just the proportion of counts that fall into the given cell of the table.

Since $\alpha = P(G = 0)$, then $\alpha = \frac{1}{3}$. Since $\beta = P(G = 1|S = 0)$, then $\beta = 0$. Since $\gamma = P(G = 0|S = 0)$, then $\gamma = 1$.

Note that these ML estimate for β falls into the zero-count problem.

Exercise 10.6. **Fishing nets.**

a. Classify the fish as salmon or sea bass.

We first note that

$$p(X_2|X_1, X_4) = p(X_1)p(X_2|X_1)p(X_4|X_2) \tag{761}$$

This much is true from exercise 10.3. Because we know the fish is thin, we "select" this column from the $p(X_4|X_2)$ matrix, and then can formulate this as a series of matrix multiplications:

$$p(X_2|X_1, X_4) = \begin{bmatrix}0.5 & 0 & 0 & 0.5\end{bmatrix} \begin{bmatrix}0.9 & 0.1\\ 0.3 & 0.7\\ 0.4 & 0.6\\ 0.8 & 0.2\end{bmatrix} \begin{bmatrix}0.6\\ 0.05\end{bmatrix} \tag{762}$$

$$= 0.38 \tag{763}$$

Thus, there is a 38% chance that the fish is a sea bass, and 62% chance that the fish is a salmon. So, we'd classify this as a salmon.

Suppose all we know is that the fish is thin and medium lightness. What season is it now, most likely?

Now we are interested in predicting $p(X_1|X_3, X_4)$. This probability is given by

$$p(X_1|X_3, X_4) \propto p(X_3|X_2)p(X_4|X_2)p(X_2|X_1)p(X_1) \tag{764}$$

$$= (\begin{bmatrix}0.33 & 0.1\end{bmatrix} \otimes \begin{bmatrix}0.6 & 0.05\end{bmatrix}) \begin{bmatrix}0.9 & 0.1\\ 0.3 & 0.7\\ 0.4 & 0.6\\ 0.8 & 0.2\end{bmatrix}^T \begin{bmatrix}0.25 & 0.25 & 0.25 & 0.25\end{bmatrix} \tag{765}$$

$$= \begin{bmatrix}0.044675 & 0.015725 & 0.02055 & 0.03985\end{bmatrix} \tag{766}$$

We can normalize this vector by dividing by its norm to get

$$p(X_1|X_3, X_4) = \begin{bmatrix} 0.3698262 & 0.1301738 & 0.1701159 & 0.3298841 \end{bmatrix}$$

Thus, it is more likely that it is either fall or winter, with winter being slightly more likely.

Exercise 10.7. **Removing leaves in BN20 networks.**

a. Show that we can safely remove all the hidden leaf nodes without affecting the posterior over the disease nodes.

This is a more informal proof. Note that this graph is directed, and thus $z_{1:3}$ affects $x_{1:4}$, but not the other way around. Therefore, nodes x_3 and x_5 will have no affect on the posterior $p(z_{1:3}|x_1, x_2, x_4)$, and therefore this posterior can be modeled using either graphs.

b. Show that we can analytically remove the leaves that are in the "off state", by absorbing their effect into the prior of the parents.

The posterior is given by

$$p(z_{1:d}|x_{i\in on}, x_{j\in off}) = p(z_{1:d}) \prod_{i\in on} p(x_i|pa(x_i)) \prod_{j\in off} p(x_j|pa(x_j)) \tag{767}$$

$$= p(z_{1:d}) \prod_{i\in on} p(x_i|pa(x_i)) \prod_{j\in off} p(x_j|pa(x_j)) \tag{768}$$

$$= p^*(z_{1:d}) \prod_{i\in on} p(x_i|pa(x_i)) \tag{769}$$

where $p^*(z_{1:d}) = p(z_{1:d}) \prod_{j\in off} p(x_j|pa(x_j))$.

Exercise 10.8. **Handling negative findings in the QMR network.**

Piggybacking off of the last exercise, we know that the absorption of the negative findings is given by

$$p(z_{1:d}) \prod_{j\in f^-} p(x_j|pa(x_j)) = \prod_{d=1}^{D} p(z_d) \prod_{j\in f^-} p(x_j|pa(x_j)) \tag{770}$$

We can see that there are $|D| \times |f^-|$ terms in this, and so therefore this operation will take $O(|D||f^-|)$ time.

Exercise 10.9. **Moralization does not introduce new independence statements.**

While moralization is not described in the text up to this point, the problem text describes it. Consider a node C with two parents, A and B. Now consider that we moralize A and B by adding an undirected edge connecting them. This makes the joint distribution

$$p(A, B, C) = p(C|A, B)p(A, B)$$

as opposed to without moralization, which says the joint is given by

$$p(A, B, C) = p(C|A, B)p(A)p(B)$$

Essentially, moralization removes the assumption of independence between the two parents. Thus, if they aren't independent, then moralization would reduce the CI assumptions in the model. If the parents are in fact independent, then $p(A, B) = p(A)p(B)$, and moralization has no effect.