IFT 6390 Fundamentals of Machine Learning
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Homework 1 - Theoretical part (Matteo Esposito)

1. **Probability warm-up: conditional probabilities and Bayes rule** [5 points]

   (a) Give the definition of the conditional probability of a discrete random variable X given a discrete random variable Y.

   (b) Consider a biased coin with probability 2/3 of landing on heads and 1/3 on tails. This coin is tossed three times. What is the probability that exactly two heads occur (out of the three tosses) given that the first outcome was a head?

   (c) Give two equivalent expressions of $P(X, Y)$:

   (i) as a function of $\mathbb{P}(X)$ and $\mathbb{P}(Y|X)$

   (ii) as a function of $\mathbb{P}(Y)$ and $\mathbb{P}(X|Y)$

   (d) Prove Bayes theorem:

   $$\mathbb{P}(X|Y) = \frac{\mathbb{P}(Y|X)\mathbb{P}(X)}{\mathbb{P}(Y)}.$$

   (e) A survey of certain Montreal students is done, where 55% of the surveyed students are affiliated with UdeM while the others are affiliated with McGill. A student is drawn randomly from this surveyed group.

   i. What is the probability that the student is affiliated with McGill?

   ii. Now let's say that this student is bilingual, and you know that 80% of UdeM students are bilingual while 50% of McGill students are. Given this information, what is the probability that this student is affiliated with McGill ?

(a)

$$P(X = x|Y = y) = \frac{P(X = x) \cap P(Y = y)}{P(Y = y)}$$

(b) Let T_n be the result of the nth toss.

$$\begin{aligned}
P((T_1 = H, T_2 = T) or (T_1 = T, T_2 = H)|T_0 = H) &= \frac{P(HHT) + P(HTH)}{P(H)} \\
&= \frac{2 * (1/3)^1 * (2/3)^2}{(2/3)} \\
&= \boxed{4/9}
\end{aligned}$$

(c) (i)

$$P(X, Y) = P(Y, X) = P(Y|X)P(X)$$

(ii)

$$P(X, Y) = P(X|Y)P(Y)$$

(d) Since $P(Y, X) = P(Y|X)P(X)$ and $P(X, Y) = P(X|Y)P(Y)$ and $P(X, Y) = P(Y, X)$ then,

$$\begin{aligned}
P(X|Y)P(Y) &= P(Y|X)P(X) \\
P(X|Y) &= \frac{P(Y|X)P(X)}{P(Y)} \qquad \square
\end{aligned}$$

(e) (i)

$$P(McGill) = 1 - P(UdeM) = \boxed{0.45}$$

(ii)

$$\begin{aligned}
P(McGill|bilingual) &= \frac{McGill \cap bilingual}{P(bilingual)} \\
&= \frac{P(McGill \cap bilingual)P(Mcgill)}{P(bilingual)} \\
&= \frac{P(McGill \cap bilingual)P(Mcgill)}{P(McGill \cap bilingual)P(Mcgill) + P(UdeM \cap bilingual)P(UdeM)} \\
&= \frac{(0.50)(0.45)}{(0.50)(0.45) + (0.80)(0.55)} \\
&= \boxed{45/133}
\end{aligned}$$

2. **Bag of words and single topic model** [12 points]

We consider a classification problem where we want to predict the topic of a document from a given corpus (collection of documents). The topic of each document can either be *sports* or *politics*. 2/3 of the documents in the corpus are about *sports* and 1/3 are about *politics*.

We will use a very simple model where we ignore the order of the words appearing in a document and we assume that words in a document are independent from one another given the topic of the document.

In addition, we will use very simple statistics of each document as features: the probabilities that a word chosen randomly in the document is either "goal", "kick", "congress", "vote", or any another word (denoted by *other*). We will call these five categories the vocabulary or dictionary for the documents: $V = \{"goal", "kick", "congress", "vote", other\}$.

Consider the following distributions over words in the vocabulary given a particular topic:

	$\mathbb{P}(\text{word} \mid \text{topic} = \textit{sports})$	$\mathbb{P}(\text{word} \mid \text{topic} = \textit{politics})$
word = "*goal*"	3/200	8/1000
word = "*kick*"	1/200	2/1000
word = "*congress*"	0	1/50
word = "*vote*"	5/1000	2/100
word = *other*	960/1000	950/1000

Table 1:

This table tells us for example that the probability that a word chosen at random in a document is "vote" is only 5/1000 if the topic of the document is *sport*, but it is 2/100 if the topic is *politics*.

(a) What is the probability that a random word in a document is "goal" given that the topic is *politics*?

(b) In expectation, how many times will the word "goal" appear in a document containing 200 words whose topic is *sports*?

(c) We draw randomly a document from the corpus. What is the probability that a random word of this document is "goal"?

(d) Suppose that we draw a random word from a document and this word is "kick". What is the probability that the topic of the document is *sports*?

(e) Suppose that we randomly draw two words from a document and the first one is "kick". What is the probability that the second word is "goal"?

(f) Going back to learning, suppose that you do not know the conditional probabilities given a topic or the probability of each topic (i.e. you don't have access to the information in table 1 or the topic distribution), but you have a dataset of N documents where each document is labeled with one of the topics *sports* and *politics*. How would you estimate the conditional probabilities (e.g., $\mathbb{P}(\text{word} = \text{"}goal\text{"} \mid \text{topic} = politics)$) and topic probabilities (e.g., $\mathbb{P}(\text{topic} = politics)$) from this dataset?

(a)

$$P(\text{"}goal\text{"}|politics) = \frac{8}{1000}$$

(b)

$$200 * P(\text{"}goal\text{"}|sports) = 200\left(\frac{3}{200}\right) = 3$$

(c)

$$\begin{aligned}
P(\text{"}goal\text{"}) &= P(\text{"}goal\text{"}|sports)P(sports) + P(\text{"}goal\text{"}|politics)P(politics) \\
&= \left(\frac{3}{200}\right)\left(\frac{2}{3}\right) + \left(\frac{8}{1000}\right)\left(\frac{1}{3}\right) \\
&= 0.0127
\end{aligned}$$

(d)

$$\begin{aligned}
P(sports|\text{"}kick\text{"}) &= \frac{P(\text{"}kick\text{"}|sports)P(sports)}{P(\text{"}kick\text{"}|sports)P(sports) + P(\text{"}kick\text{"}|politics)P(politics)} \\
&= \frac{\frac{1}{200} * \frac{2}{3}}{\frac{1}{200} * \frac{2}{3} + \frac{2}{1000} * \frac{1}{3}} \\
&= \frac{5}{6}
\end{aligned}$$

(e) Seeing as we calculated $P(sports|"kick")$ in the previous question, and knowing that the first word selected was "kick", we have that;

$$\begin{aligned} P("goal") &= \left(\frac{5}{6}\right)\left(\frac{3}{200}\right) + \left(\frac{1}{6}\right)\left(\frac{8}{1000}\right) \\ &= 0.0138 \end{aligned}$$

(f) For the conditional probabilities, we would take a count of all words in each of the 2 document classes then divide that by the total number of words found in all documents per document class. i.e.

$$P("goal"|politics) = \frac{\text{\# instances of "goal" in all politics documents}}{\text{\# words in all politics documents}}$$

For the topic probabilities, it would suffice to get a count of the number of documents classified as politics and sports and take the quotient of those totals and N (where N is total number of documents). i.e.

$$P("politics") = \frac{\text{\# labels = politics in dataset}}{N}$$

3. **Maximum likelihood estimation** [5 points]

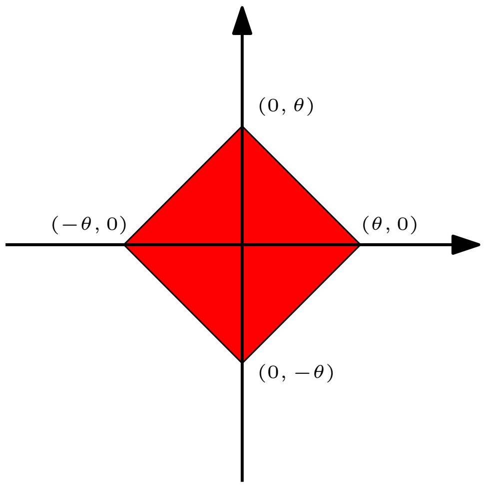
Let $\mathbf{x} \in \mathbb{R}^2$ be uniformly distributed over a diamond area with diagonals 2θ where θ is a parameter as shown in the figure. That is, the pdf of $\mathbf{x}$ is given by

$$f_\theta(\mathbf{x}) = \begin{cases} 1/2\theta^2 & \text{if } ||\mathbf{x}||_1 \leq \theta \\ 0 & \text{otherwise} \end{cases}$$

where $||\mathbf{x}||_1 = |x_1| + |x_2|$ is the L1 norm.

Suppose that n samples $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ are drawn independently according to $f_\theta(\mathbf{x})$.

(a) Let $f_\theta(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$ denote the joint pdf of n independent and identically distributed (i.i.d.) samples drawn according to $f_\theta(\mathbf{x})$. Express $f_\theta(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$ as a function of $f_\theta(\mathbf{x}_1), f_\theta(\mathbf{x}_2), \ldots, f_\theta(\mathbf{x}_n)$



(b) We define the maximum likelihood estimate by the value of θ which maximizes the likelihood of having generated the dataset D from the distribution $f_\theta(\mathbf{x})$. Formally,

$$\theta_{MLE} = \arg\max_{\theta \in \mathbb{R}^+} f_\theta(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n),$$

Find the maximum likelihood estimate of θ.

(a)

$$\begin{aligned} L(\theta) &= f_\theta(x_1, x_2, \ldots, x_n) \\ &= \prod_{i=1}^{n} f_\theta(x_i) \\ &= \left(\frac{1}{2\theta^2}\right)\left(\frac{1}{2\theta^2}\right)\cdots\left(\frac{1}{2\theta^2}\right) \end{aligned}$$

$$L(\theta) = \begin{cases} \frac{1}{(2\theta^2)^n} & ||x_i||_1 \leq \theta \quad i = (1, \ldots, n) \\ 0 & \text{Otherwise} \end{cases}$$

(b) We can see that the value of θ that will maximize $L(\theta)$ will have to be the smallest value of θ such that $\theta \geq ||x_i||_1$. Therefore,

$$\hat{\theta} = max(||x_1||_1, ||x_2||_1, \ldots, ||x_n||_1)$$

4. **Maximum likelihood meets histograms** [10 points]

Let $X_1, X_2, \cdots, X_n$ be n i.i.d data points drawn from a piece-wise constant probability density function over N equal size bins between 0 and 1 $(B_1, B_2, \cdots, B_N)$, where the constants are $\theta_1, \theta_2, \cdots, \theta_N$.

$$p(x; \theta_1, \cdots, \theta_N) = \begin{cases} \theta_j & \frac{j-1}{N} \leq x < \frac{j}{N} \text{ for } j \in \{1, 2, \cdots, N\} \\ 0 & \text{otherwise} \end{cases}$$

We define μ_j for $j \in \{1, 2, \cdots, N\}$ as $\mu_j \coloneqq \sum_{i=1}^{n} \mathbb{1}(X_i \in B_j)$.

(a) Using the fact that the total area underneath a probability density function is 1, express θ_N in terms of the other constants.

(b) Write down the log-likelihood of the data in terms of $\theta_1, \theta_2, \cdots, \theta_{N-1}$ and $\mu_1, \mu_2, \cdots, \mu_{N-1}$.

(c) Find the maximum likelihood estimate of θ_j for $j \in \{1, 2, \cdots, N\}$.

(a)

$$\sum_{j=1}^{N} \frac{\theta_j}{N} = 1$$

$$\sum_{j=1}^{N-1} \frac{\theta_j}{N} + \frac{\theta_N}{N} = 1$$

$$\theta_N = N - \sum_{j=1}^{N-1} \theta_j$$

(b)

$$\mathcal{L}(\theta) = log(L(\theta)) = log\left(\prod_{j=1}^{N}\left(\frac{\theta_j}{N}\right)^{\mu_j}\right) = log\left(\left(\frac{\theta_N}{N}\right)^{\mu_j}\prod_{j=1}^{N-1}\left(\frac{\theta_j}{N}\right)^{\mu_j}\right)$$

$$= log\left(\left(1 - \sum_{j=1}^{N-1}\frac{\theta_j}{N}\right)^{n-\sum_{j=1}^{N-1}\mu_j}\prod_{j=1}^{N-1}\left(\frac{\theta_j}{N}\right)^{\mu_j}\right)$$

$$= \left(n - \sum_{j=1}^{N-1}\mu_j\right) log\left(1 - \sum_{j=1}^{N-1}\frac{\theta_j}{N}\right) + \left(\sum_{j=1}^{N-1}\mu_j log\left(\frac{\theta_j}{N}\right)\right)$$

Staying aligned with the problem statement, the above expression should be our final answer. We can however simplify it some more.

$$\mathcal{L}(\theta) = \mu_N log\left(\frac{\theta_N}{N}\right) + \sum_{j=1}^{N-1}\mu_j log\left(\frac{\theta_j}{N}\right)$$

(c) Assume $k \in \{1, \dots, N\}$, then

$$\frac{\partial}{\partial \theta_k}(\mathcal{L}(\theta_k)) = -\frac{\mu_N}{1 - \sum_{j=1}^{N-1} \theta_j} + \frac{\mu_k}{\theta_k} = 0 \iff \frac{\mu_N}{1 - \sum_{j=1}^{N-1} \theta_j} = \frac{\mu_k}{\theta_k}$$

Rerranging our terms, we have that,

$$\theta_k = \frac{\mu_k \theta_N}{\mu_N}$$

To maximize this we assume $\mu_N = n$ and $\theta_N = N$, in the case where all points fall into one bin and therefore,

$$\hat{\theta_k} = \frac{\mu_k N}{n} \quad \forall\, k \in \{1, \dots, N\}$$

5. **Histogram methods** [10 points]

Consider a dataset $\{x_j\}_{j=1}^n$ where each point $x \in [0, 1]^d$. Let $f(x)$ be the true unknown data distribution. You decide to use a histogram method to estimate the density $f(x)$ and divide each dimension into m bins.

(a) Show that for a measurable set S, $\mathbb{E}_{x \sim f}[\mathbb{1}_{\{x \in S\}}] = \mathbb{P}_{x \sim f}(x \in S)$, where $\mathbb{1}_{\{x \in S\}} = 1$ if $x \in S$ and 0 otherwise.

(b) Combining the result of the previous question with the Law of Large Numbers, show that the estimated probability of falling in bin i, as given by the histogram method, tends to $\mathbb{P}_{x \sim f}(x \in V_i) = \int_{V_i} f(x)dx$, the true probability of falling in bin i, as $n \to \infty$. V_i denotes the volume occupied by bin i.

(c) Consider the MNIST dataset with 784 dimensions (i.e. $x \in [0, 1]^{784}$). We divide each dimension into 2 bins. How many digits (base 10) does the total number of bins have?

(d) Assuming a uniform distribution over all bins, how many data points would you need to get k points per bin on average?

(e) Assuming a uniform distribution over all bins, what is the probability that a particular bin is empty, as a function of d, m and n?

(a) We use the definition of expectation of a continuous rv and the fact that all points $\notin S$ will not contribute to the expectation to yield the following:

$$\mathbb{E}_{x \sim f}[\mathbb{1}_{\{x \in S\}}] = \int_{x \sim f} f(x)\mathbb{1}_{\{x \in S\}} dx = \int_S f(x)dx = \mathbb{P}_{x \sim f}(x \in S)$$

(b) Given a region V_i, we can leverage the LLN and the previous expression to assert that,

$$\mathbb{P}_{x\sim f}(x \in V_i) = \int_{V_i} f(x)dx = \mathbb{E}_{x\sim f}[\mathbb{1}_{\{x\in S\}}]$$

(c)

$$\# \text{ bins} = 2^{784} = 10^{784*log_{10}2} = 10^{\sim 236}$$

Therefore, 237 digits.

(d) If we assume a uniform distribution, to be able to get k points per bin on average, we would need to satidfy the following expression:

$$k = \frac{\# \text{ points}}{\# \text{ bins}} = \frac{n}{m}$$

Therefore, given our previous result, we would need

$$\frac{n}{2^{784}} = k \iff n = k * 2^{784} \text{ points}$$

(e) The probability of a point falling into a bin is given by $\frac{1}{m^d}$ therefore, the probability of not falling into a bin is $1 - \frac{1}{m^d}$. If we extend this to the case where a bin will never receive a point we have that,

$$P(\text{Empty bin}) = \left(1 - \frac{1}{m^d}\right)^n$$

6. **Gaussian Mixture** [10 points]

Let $\mu_0, \mu_1 \in \mathbb{R}^d$, and let Σ_0, Σ_1 be two $d \times d$ positive definite matrices (i.e. symmetric with positive eigenvalues).
We now introduce the two following pdf over $\mathbb{R}^d$:

$$f_{\mu_0,\Sigma_0}(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{det(\Sigma_0)}} e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma_0^{-1}(\mathbf{x}-\mu_0)}$$

$$f_{\mu_1,\Sigma_1}(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{det(\Sigma_1)}} e^{-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma_1^{-1}(\mathbf{x}-\mu_1)}$$

These pdf correspond to the multivariate Gaussian distribution of mean μ_0 and covariance Σ_0, denoted $\mathcal{N}_d(\mu_0, \Sigma_0)$, and the multivariate Gaussian distribution of mean μ_1 and covariance Σ_1, denoted $\mathcal{N}_d(\mu_1, \Sigma_1)$.

We now toss a balanced coin Y, and draw a random variable X in $\mathbb{R}^d$, following this process : if the coin lands on tails ($Y = 0$) we draw X from $\mathcal{N}_d(\mu_0, \Sigma_0)$, and if the coin lands on heads ($Y = 1$) we draw X from $\mathcal{N}_d(\mu_1, \Sigma_1)$.

(a) Calculate $\mathbb{P}(Y = 0|X = \mathbf{x})$, the probability that the coin landed on tails given $X = \mathbf{x} \in \mathbb{R}^d$, as a function of μ_0, μ_1, Σ_0, Σ_1, and $\mathbf{x}$. Show all the steps of the derivation.

(b) Recall that the Bayes optimal classifier is $h_{Bayes}(\mathbf{x}) = \underset{y\in\{0,1\}}{\operatorname{argmax}} \mathbb{P}(Y = y|X = \mathbf{x})$. Show that in this setting if $\Sigma_0 = \Sigma_1$ the Bayes optimal classifier is linear in $\mathbf{x}$.

(a) We can use Bayes Rule here,

$$\mathbb{P}(Y = 0|X = \mathbf{x}) = \frac{P(X = \mathbf{x}|Y = 0)P(Y = 0)}{P(X = \mathbf{x})}$$
$$= \frac{P(X = \mathbf{x}|Y = 0)P(Y = 0)}{P(X = \mathbf{x}|Y = 0)P(Y = 0) + P(X = \mathbf{x}|Y = 1)P(Y = 1)}$$

and from the information above we know that Y represents a fair coin toss with probability 0.5 of 1 and of 0. Therefore, we can exclude it from the calculation since it appears in both the numerator and denominator.

$$\mathbb{P}(Y = 0|X = \mathbf{x}) = \frac{f_{\mu_0,\Sigma_0}(\mathbf{x}) * \frac{1}{2}}{f_{\mu_0,\Sigma_0}(\mathbf{x}) * \frac{1}{2} + f_{\mu_1,\Sigma_1}(\mathbf{x}) * \frac{1}{2}}$$
$$= \frac{f_{\mu_0,\Sigma_0}(\mathbf{x})}{f_{\mu_0,\Sigma_0}(\mathbf{x}) + f_{\mu_1,\Sigma_1}(\mathbf{x})}$$
$$= \frac{\frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{det(\Sigma_0)}}e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma_0^{-1}(\mathbf{x}-\mu_0)}}{\frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{det(\Sigma_0)}}e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma_0^{-1}(\mathbf{x}-\mu_0)} + \frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{det(\Sigma_1)}}e^{-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma_1^{-1}(\mathbf{x}-\mu_1)}}$$
$$= \frac{\sqrt{det(\Sigma_1)}e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma_0^{-1}(\mathbf{x}-\mu_0)}}{\sqrt{det(\Sigma_1)}e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma_0^{-1}(\mathbf{x}-\mu_0)} + \sqrt{det(\Sigma_0)}e^{-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma_1^{-1}(\mathbf{x}-\mu_1)}}$$

(b) If we let $\Sigma_0 = \Sigma_1 = \Sigma$, we have that,

$$\mathbb{P}(Y = 0|X = \mathbf{x}) = \frac{e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0)}}{e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0)} + e^{-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1)}}$$

and to determine the decision boundary and show that the classifier is linear in x, we set $\mathbb{P}(Y = 0|X = \mathbf{x}) = \mathbb{P}(Y = 1|X = \mathbf{x})$, yielding the following:

$$\begin{aligned}
\mathbb{P}(Y = 0|X = \mathbf{x}) &= \mathbb{P}(Y = 1|X = \mathbf{x}) \\
\frac{e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0)}}{e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0)} + e^{-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1)}} &= \frac{e^{-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1)}}{e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0)} + e^{-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1)}} \\
e^{-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0)} &= e^{-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1)} \\
\frac{1}{2}(\mathbf{x} - \mu_0)^T\Sigma^{-1}(\mathbf{x} - \mu_0) &= \frac{1}{2}(\mathbf{x} - \mu_1)^T\Sigma^{-1}(\mathbf{x} - \mu_1) \\
||x - \mu_0|| &= ||x - \mu_1|| \quad \square
\end{aligned}$$