Introduction to Machine Learning-Exercise 1

Linear Algebra

1. (**15 pts**) A symmetric matrix A over $\mathbb{R}$ is called *positive semidefinite* (PSD) if for every vector $\mathbf{v}$, $\mathbf{v}^{\mathsf{T}} A\mathbf{v} \geq 0$.

   (a) Show that a symmetric matrix A is PSD if and only if it can be written as $A = XX^T$, if and only if all of its eigenvalues are non-negative.
   Hint: Recall that a real symmetric matrix A can be decomposed as $A = QDQ^T$, where Q is an orthogonal matrix whose columns are eigenvectors of A and D is a diagonal matrix with eigenvalues of A as its diagonal elements.

Proof: Fix a symmetric matrix A. The sequence of the proof will be like that:

A is a PSD → all its eigenvalues are non-negative → A can be written as $A = XX^T$ → A is a PSD.

Which gives us the wanted claim.

A is a PSD → all its eigenvalues are non-negative:

Lets assume that A is PSD. Let $\{v_1, v_2, \dots, v_n\}$ be the eigenvectors of A and $\{\alpha_1, \alpha_2, \dots, \alpha_n\}$ be its eigenvalues, by definition we know that:

$$\forall i: Av_i = \alpha_i v_i$$

And since A is a PSD so we conclude that:

$\forall i: v_i^T Av_i \geq 0 \rightarrow \forall i: v_i^T \alpha_i v_i \geq 0 \rightarrow \forall i: \alpha_i v_i^T v_i \geq 0$

And since $v_i^T v_i \geq 0$ for every vector so we conclude that $\forall i: \alpha_i \geq 0$ as wanted.

A’s eigenvalues are all non-negative → A can be written as $A = XX^T$:

Lets assume that all of A’s eigenvalues are non-negative. A can be decomposed as $A = QDQ^T$ as $D = diag(\alpha_1, \alpha_2, \dots, \alpha_n)$. Lets pay attention to the fact that if we define a matrix called D’ as $D' = diag(\sqrt{\alpha_1}, \sqrt{\alpha_2}, \dots, \sqrt{\alpha_n})$ then $D = D'D' \overset{since\ D'\ is\ symmetric}{=} D'D'^T$. And then we can write:

$A = \ QDQ^T = Q\,D'D'^T Q^T = \ QD'(QD')^T$ as wanted, cause we can take X=QD’.

A can be written as $A = XX^T$ → A is a PSD:

Lets assume A can be written as $A = XX^T$. Then for every vector v:

$$\forall v: v^T Av = v^T XX^T v = (X^T v)^T X^T v$$

And lets pay attention to that $(X^T v)^T X^T v$ is equal to the Euclidean norm of the matrix $X^T v$ powered by 2, and since the Euclidean norm is non-negative then its power by 2 is also non-negative.

So, we conclude that:

$$\forall v: v^T Av = (X^T v)^T X^T v \geq 0 \rightarrow A\ is\ PSD\ as\ wanted \qquad \blacksquare$$

   (b) Show that for all $\alpha, \beta \geq 0$ and PSD matrices $A, B \in \mathbb{R}^{n \times n}$, the matrix $\alpha A + \beta B$ is also PSD. Does this mean that the set of all $n \times n$ PSD matrices over $\mathbb{R}$ is a vector space over $\mathbb{R}$?

Proof:

Let $\alpha, \beta \geq 0$ and A,B PSD matrices. Then for every vector v:

$$v^T(\alpha A + \beta B)v = v^T \alpha A v + v^T \beta B v = \alpha v^T A v + \beta v^T B v$$

A is PSD so $v^T A v \geq 0$, and $\alpha \geq 0$ hence $\alpha v^T A v \geq 0$.

B is PSD so $v^T B v \geq 0$, and $\beta \geq 0$ hence $\beta v^T B v \geq 0$.

And thus: $v^T(\alpha A + \beta B)v = \ \alpha v^T A v + \beta v^T B v \geq 0$, so the matrix $(\alpha A + \beta B)$ is PSD.

But this doesn't mean that the the set of all n x n PSD matrices over R is a vector space over R because the claim relies on that $\alpha\ and\ \beta$ are non-negative, meaning if we take a negative scalar then multiplying it by a PSD matrix A will not give us a PSD matrix, hence it is not closed under multiplication by a negative scalar.

Calculus and Probability

1. (**15 pts**) Let $X_1, ..., X_n$ be i.i.d $U([0, 1])$ (uniform) continuous random variables. Let $Y = \max(X_1, ..., X_n)$.

   (a) What is the PDF of Y? Write the mathematical formula and plot the PDF as well. Compute $\mathbb{E}[Y]$ and $\mathrm{Var}[Y]$ - how do they behave as a function of n as n grows large?

   (b) (**No need to submit**) Verify your answer empirically using Python.

Answer:

We know that the PDF of Y is the derivative of it's CDF, so we calculate the CDF first:

first, lets notice that for y between 0 and 1: $F_Y(y) = P(Y \leq y) = P(X_1 \leq Y)\ and\ P(X_2 \leq Y)\ and\ \dots\ P(X_n \leq Y) = \prod_{i=1}^{n} y = y^n$

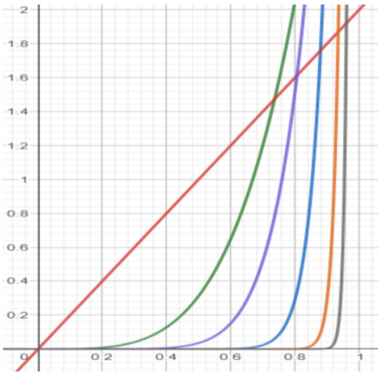
so, we conclude that:

$$F_Y(y) = \begin{cases} 0\ if\ y = 0 \\ y^n\ if\ 0 \leq y \leq 1 \\ 1\ if\ y > 1 \end{cases}$$

Thus:

$$f_Y(y) = \begin{cases} 0\ if\ y = 0 \\ n * y^{n-1}\ if\ 0 \leq y \leq 1 \\ 0\ if\ y > 1 \end{cases}$$

The plot of the CDF will look something like this:



Now, let’s compute E[Y]:

$$E[Y] = \int_{-\infty}^{\infty} y * f_Y(y)\, dy = \int_0^1 y * f_Y(y)\, dy = \int_0^1 y * n * y^{n-1}\, dy = \int_0^1 n * y^n\, dy = \frac{n * y^{n+1}}{n+1} /_0^1$$
$$= \frac{n}{n+1}$$

Notice that E[Y] as the n grows large it gets much closer to 1: $\lim_{n\to\infty} E[Y] = 1$

Now, let’s compute Var[Y]:

$$Var[Y] = E[Y^2] - (E[Y])^2 = \int_0^1 y^2 * n * y^{n-1} - (\frac{n}{n+1})^2 = \int_0^1 n * y^{n+1} - (\frac{n}{n+1})^2$$
$$= \frac{n * y^{n+2}}{n+2} /_0^1 - (\frac{n}{n+1})^2 = \frac{n}{n+2} - (\frac{n}{n+1})^2 = \cdots = \frac{n}{(n+2)(n+1)^2}$$

And notice that Var[Y] as the n grows it gets much closer to 0: $\lim_{n\to\infty} Var[Y] = 0$

Optimal Classifiers and Decision Rules

1. (**15 pts**)

(a) Let X and Y be random variables where Y can take values in $\mathcal{Y} = \{1, \ldots, L\}$. Let ℓ_{0-1} be the 0-1 loss function defined in class. Show that $h = \arg\min_{f:\mathcal{X}\to\mathcal{Y}} \mathbb{E}\left[\ell_{0-1}(Y, f(X))\right]$ is given by

$$h(x) = \arg\max_{i\in\mathcal{Y}} \mathbb{P}[Y = i | X = x]$$

(In class you proved this for binary classification, i.e. $\mathcal{Y} = \{0, 1\}$, here you are asked to generalize the result to L labels.)

Answer:

Denote $g = \arg min_{f:X\to Y} E\left[l_{0-1}\left(Y, f(x)\right)\right], h(x) = \arg max_{i\in Y} P[Y = i|X = x]$. We need to prove g=h.

It holds that:

$$E\left[l_{0-1}\left(Y, f(x)\right)\right] = \sum_{x\in X} \sum_{i=1}^{L} P[X = x, Y = i] * l\left(i, f(x)\right)$$
$$= \sum_{x\in X} \left(P[X = x] \sum_{i=1}^{L} P(Y = i|X = x) * l\left(i, f(x)\right) \right)$$

That is because when Y=f(x) then l(I,f(x)=0 and thus its Pr it’s not calculated in the sum operator.

$$\Big\downarrow$$
$$= \sum_{x\in X} \left(P[X = x] * \left[1 - P[Y = f(x)|X = x]\right] \right)$$
$$\geq_{by\ the\ choice\ of\ h} \sum_{x\in X} \left(P[X = x] * \left[1 - P[Y = h(x)|X = x]\right] \right) = E\left[l_{0-1}\left(Y, h(x)\right)\right]$$

And thus, we conclude that h satisfies that $E\left[l_{0-1}\left(Y, h(x)\right)\right]$ is minimal the same as g, so g=h as wanted.

Notice that intuitively the second line in the equation(which is above the black arrow) is minimized when the maximum $P(Y = i|X = x)$ is not calculated in the sum operator, which happens when the loss function outputs 0 on these probabilities, which means when we choose f to be h(h by definition gives the maximum among those probabilities).

(b) Let X and Y be random variables where Y can take values in $\mathcal{Y} = \{0, 1\}$. Let Δ be the following asymmetric loss function:

$$\Delta(y, \hat{y}) = \begin{cases} 0 & y = \hat{y} \\ a & y = 0, \hat{y} = 1 \\ b & y = 1, \hat{y} = 0, \end{cases}$$

where $a, b \in (0, 1]$ (note that this loss function generalizes the 0-1 loss defined in class). Compute the optimal decision rule h for the loss function Δ, i.e. the decision rule which satisfies:

$$h = \arg \min_{f:\mathcal{X} \to \mathcal{Y}} \mathbb{E}\left[\Delta(Y, f(X))\right]$$

Answer:

For any $f: X \to Y$ it holds that:

$$E\big[\Delta\big(Y, f(x)\big)\big] = \sum_{x \in X} \sum_{y \in Y = \{0,1\}} P[X = x, Y = y] * \Delta\big(y, f(x)\big)$$

$$= \sum_{x \in X} \left(P[X = x] \sum_{y \in Y = \{0,1\}} P[Y = y|X = x] * \Delta\big(y, f(x)\big) \right)$$

$$= P[X = x] * \big[P[Y = 0|X = x] * \Delta\big(0, f(x)\big) + P[Y = 1|X = x] * \Delta\big(1, f(x)\big)\big]$$

We can see from the equation above, which we want to minimize its result, that if we predict that f(x)=0 then we "pay" $P[X = x] * P[Y = 1|X = x] * \Delta\big(1, f(x)\big) = P[X = x] * P[Y = 1|X = x] * b$, as $\Delta\big(0, f(x)\big) = 0$, and if we predict that f(x)=1 then we "pay" $P[X = x] * P[Y = 0|X = x] * \Delta\big(0, f(x)\big) = P[X = x] * P[Y = 0|X = x] * a$.

Thus, we conclude that the optimal decision rule h which satisfies the expected loss is minimal will predict that h(x)=0 when $b * P[Y = 1|X = x] < a * P[Y = 0|X = x]$, else it should predict that h(x)=1, more formally:

$$h(x) = \begin{cases} 0 \; if \; b * P[Y = 1|X = x] < a * P[Y = 0|X = x] \\ 1 \; else: b * P[Y = 1|X = x] \geq a * P[Y = 0|X = x] \end{cases} = \begin{cases} 0 \; if \; \dfrac{P[Y = 1|X = x]}{P[Y = 0|X = x]} < \dfrac{a}{b} \\ 1 \qquad\qquad otherwise \end{cases}$$

2. (**15 pts**) Let X and Y be random variables where X can take values in some set $\mathcal{X}$ and Y can take values in $\mathcal{Y} = \{0, 1\}$ (i.e. binary label space). Assume we wish to find a predictor $h : \mathcal{X} \to [0, 1]$ (note that the hypothesis can output any number between 0 and 1) which minimizes $\mathbb{E}[\Delta_{log}(Y, h(X))]$, where Δ_{log} is the following loss function known as the *log-loss*:

$$\Delta_{log}(y, \hat{y}) = -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y}).$$

Find the predictor $h : \mathcal{X} \to [0, 1]$ which minimizes $\mathbb{E}[\Delta_{log}(Y, h(X))]$ (the final answer should be very intuitive).

Note: This loss function may seem odd at first, but it is very important and we'll discuss it further in the future.

Answer:

Note: we were told in the recitation, as I remember, to consider log as ln, so I solved the question with this consideration.

For any $f: X \to Y$ it holds that:

$$E\left[\Delta\left(Y, f(x)\right)\right] = \sum_{x \in X} \sum_{y \in Y = \{0,1\}} P[X = x, Y = y] * \Delta_{log}\left(y, f(x)\right)$$

$$= \sum_{x \in X} \left(P[X = x] \sum_{y \in Y = \{0,1\}} P[Y = y | X = x] * \Delta_{log}\left(y, f(x)\right) \right)$$

This transition is simply by compensating in Δ_{log} y=0, and then y=1…

$$= P[X = x] * \left[P[Y = 0 | X = x] * \Delta_{log}\left(0, f(x)\right) + P[Y = 1 | X = x] * \Delta_{log}\left(1, f(x)\right)\right]$$

$$= P[X = x] * \left[P[Y = 0 | X = x] * -\log\left(1 - f(x)\right) + P[Y = 1 | X = x] * -\log\left(f(x)\right)\right]$$

Denote $g(z) = -P[Y = 0 | X = x] * \log(1 - z) - P[Y = 1 | X = x] * \log(z)$ as z=f(x) which is our prediction for some x, and we want to find the minimum of this function g, meaning which z=f(x) should we predict so it gives us the minimum value.

notice that our variable is z=f(x) and that $P[Y = 0 | X = x], P[Y = 1 | X = x]$ are parameters.

To calculate the minimum, we first find the derivative of g:

$$g'(z) = -P[Y = 0 | X = x] * \frac{-1}{1 - z} - P[Y = 1 | X = x] * \frac{1}{z} = \frac{P[Y = 0 | X = x]}{1 - z} - \frac{P[Y = 1 | X = x]}{z}$$

$$= \frac{z * P[Y = 0 | X = x] - P[Y = 1 | X = x] + z * P[Y = 1 | X = x]}{(1 - z)z}$$

$$= \frac{z(P[Y = 0 | X = x] + P[Y = 1 | X = x]) - P[Y = 1 | X = x]}{z(1 - z)}$$

P[Y=0|X=x] +P[Y=1|X=x] =1

$$= \frac{z - P[Y = 1 | X = x]}{z(1 - z)}$$

And thus, we get the minimum when:

$$z - P[Y = 1 | X = x] = 0 \to z = P[Y = 1 | X = x]$$

Thus, we conclude that the wanted predictor h is given by:

$$h(x) = P[Y = 1 | X = x]$$

intuitively, when we predict h(x) to be $P[Y = 1 | X = x]$ then if this probability is “high“(closer to 1) then our prediction is indeed closer to 1 which is more likely the real value of x and if this probability is “small” then our prediction is indeed closer to 0 which is more likely the real value of of x, and thus we minimize the error.

3. (**10 pts**)

Let X and Y be random variables taking values in $\mathcal{X} = \mathbb{R}$ and $\mathcal{Y} = \{0, 1\}$ respectively, and assume that given $Y = 0$, X is distributed normally with mean μ and variance σ_0^2, i.e. $X \sim \mathcal{N}(\mu, \sigma_0^2)$, and similarly, given $Y = 1$, $X \sim \mathcal{N}(\mu, \sigma_1^2)$, where $\sigma_0 \neq \sigma_1$. Also assume $\Pr[Y = 1] = p_1$.

Find the optimal decision rule for this distribution and the zero-one loss, i.e. find $h : \mathbb{R} \to \{0, 1\}$ which minimizes $\mathbb{E}[\ell_{0-1}(Y, h(X))]$ where ℓ_{0-1} is the zero-one loss defined in class (write the decision rule only in terms of $x, \mu, \sigma_0, \sigma_1$ and p_1).

Answer:

In class we saw that the decision rule h that minimizes the expected 0-1 loss in the binary case is given by:

$$h(x) = \begin{cases} 1 \; if \; P(Y=1|X=x) > P(Y=0|X=x) \\ 0 \qquad\qquad\qquad else \end{cases}$$

now we want to find the values of x that hold:

$$P(Y=1|X=x) > P(Y=0|X=x)$$

Using Bayes theorem for continuous variables we get that the upper statement is equivalent to:

$$\frac{f_x(x|Y=1) * P(Y=1)}{f_x(x)} > \frac{f_x(x|Y=0) * P(Y=0)}{f_x(x)}$$

$$\frac{f_x(x|Y=1) * p_1}{f_x(x)} > \frac{f_x(x|Y=0) * (1-p_1)}{f_x(x)}$$

The equation above holds when:

$$f_x(x|Y=1) * p_1 > f_x(x|Y=0) * (1-p_1)$$

$$\frac{p_1}{\sqrt{2\pi{\sigma_1}^2}} * e^{-\frac{(x-\mu)^2}{2{\sigma_1}^2}} > \frac{(1-p_1)}{\sqrt{2\pi{\sigma_2}^2}} * e^{-\frac{(x-\mu)^2}{2{\sigma_2}^2}}$$

$$e^{-\frac{(x-\mu)^2}{2{\sigma_1}^2}+\frac{(x-\mu)^2}{2{\sigma_2}^2}} > \frac{(1-p_1) * \sqrt{2\pi{\sigma_1}^2}}{p_1 * \sqrt{2\pi{\sigma_2}^2}}$$

$$-\frac{(x-\mu)^2}{2{\sigma_1}^2} + \frac{(x-\mu)^2}{2{\sigma_2}^2} > \ln\left(\frac{(1-p_1) * \sigma_1}{p_1 * \sigma_2}\right)$$

$$(x-\mu)^2({\sigma_1}^2 - {\sigma_2}^2) > 2{\sigma_1}^2{\sigma_2}^2 * \ln\left(\frac{(1-p_1) * \sigma_1}{p_1 * \sigma_2}\right)$$

$$(x-\mu)^2 > \frac{2{\sigma_1}^2{\sigma_2}^2 * \ln\left(\frac{(1-p_1) * \sigma_1}{p_1 * \sigma_2}\right)}{({\sigma_1}^2 - {\sigma_2}^2)}$$

$$x-\mu > \sqrt{\frac{2{\sigma_1}^2{\sigma_2}^2 * \ln\left(\frac{(1-p_1)*\sigma_1}{p_1*\sigma_2}\right)}{({\sigma_1}^2-{\sigma_2}^2)}} \ \boldsymbol{or}\ x-\mu < -\sqrt{\frac{2{\sigma_1}^2{\sigma_2}^2 * \ln\left(\frac{(1-p_1)*\sigma_1}{p_1*\sigma_2}\right)}{({\sigma_1}^2-{\sigma_2}^2)}}$$

$$x > \mu + \sqrt{\frac{2{\sigma_1}^2{\sigma_2}^2 * \ln\left(\frac{(1-p_1)*\sigma_1}{p_1*\sigma_2}\right)}{({\sigma_1}^2-{\sigma_2}^2)}} \ \boldsymbol{or}\ x < \mu - \sqrt{\frac{2{\sigma_1}^2{\sigma_2}^2 * \ln\left(\frac{(1-p_1)*\sigma_1}{p_1*\sigma_2}\right)}{({\sigma_1}^2-{\sigma_2}^2)}}$$

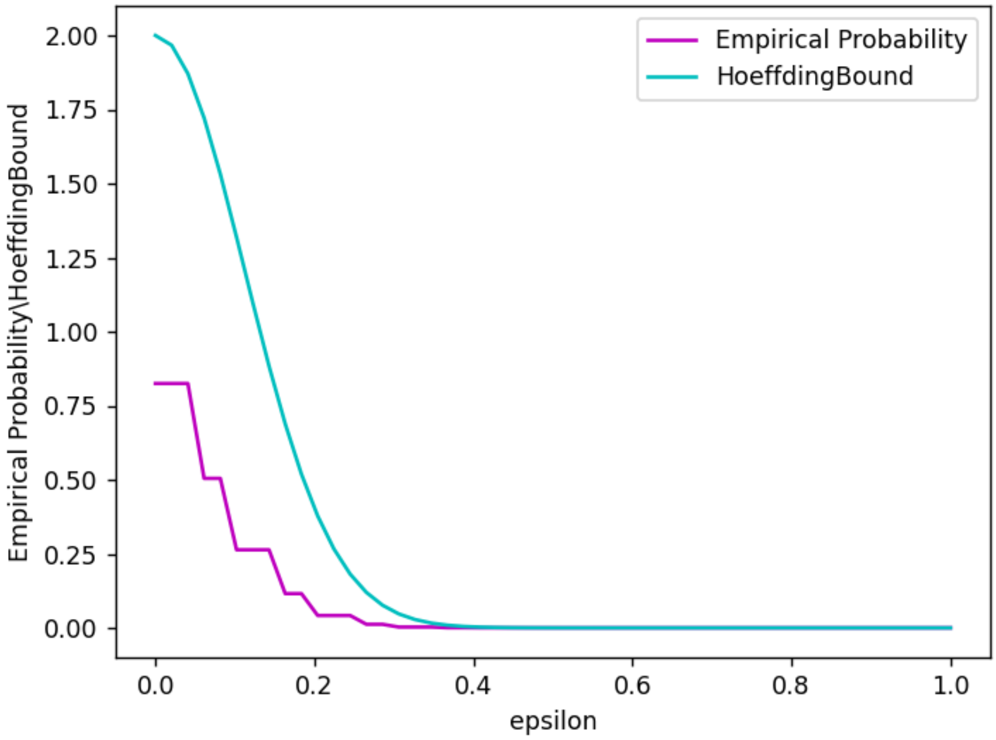
In these cases we predict that h(x)=1, otherwise [meaning that x is between these values] we predict that h(x)=0.

So, to sum up, our optimal decision rule h is:

$$h(x) = \begin{cases} 0\ if\ \mu - \sqrt{\frac{2{\sigma_1}^2{\sigma_2}^2 * \ln\left(\frac{(1-p_1)*\sigma_1}{p_1*\sigma_2}\right)}{({\sigma_1}^2-{\sigma_2}^2)}} < x < \mu + \sqrt{\frac{2{\sigma_1}^2{\sigma_2}^2 * \ln\left(\frac{(1-p_1)*\sigma_1}{p_1*\sigma_2}\right)}{({\sigma_1}^2-{\sigma_2}^2)}} \\ 1 \qquad\qquad\qquad\qquad otherwise \end{cases}$$

Programming Assignment

Question 1:



Question 2:

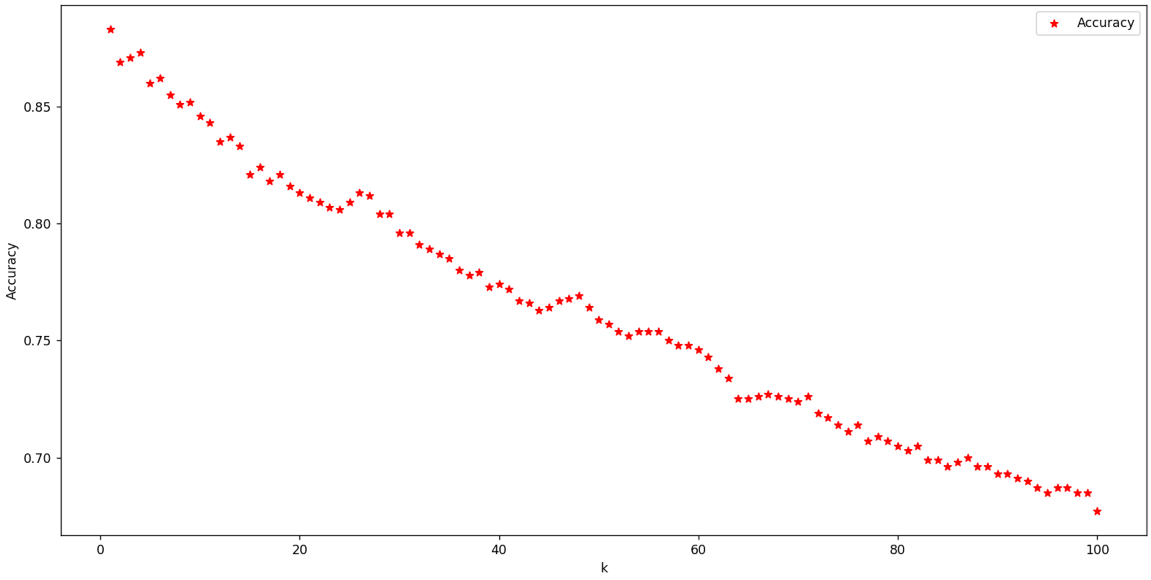
2b:

The accuracy of the prediction is: 0.846(84.6%).

In a completely random predictor, I would have expected to get an accuracy of 0.1(10%), since there are ten possibilities for the label: {0,1, 2, … ,9}, assuming that in the test set contains equal images of each label.

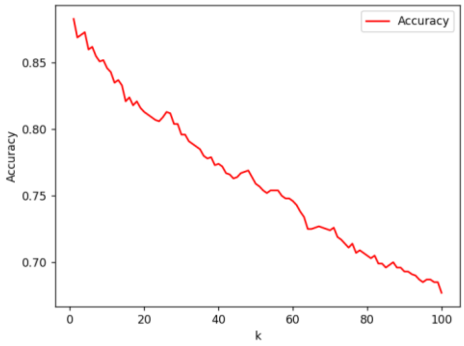
Note: if the test set is not uniformly distributed as said above, then the accuracy the prediction would change depending on the distribution.

2c:



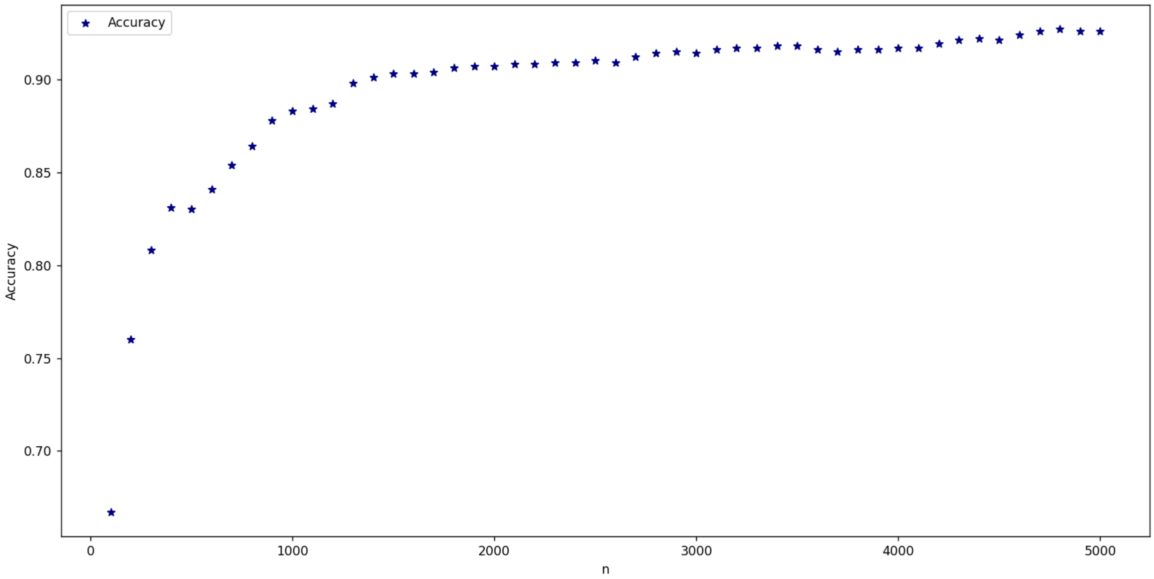
We can see from the plot above that k=1 is the best k, because it gives the highest accuracy.

Also, we can see that when k=2 the accuracy is worse than k=1 but then it rises up again when k=3 and then rises up again when k=4(still worse than k=1), meaning that k=4 is the second best k. this thing, meaning that the accuracy goes down and then rises up again, happens also for higher k values but I think that it happens less, meaning that after k=4 in general we can say that there is decline in the accuracy. Maybe the explanation of this might be that when k is big enough then in the k nearest images there are more images with different labels of the query image, and such there is more mistakes and less accuracy.



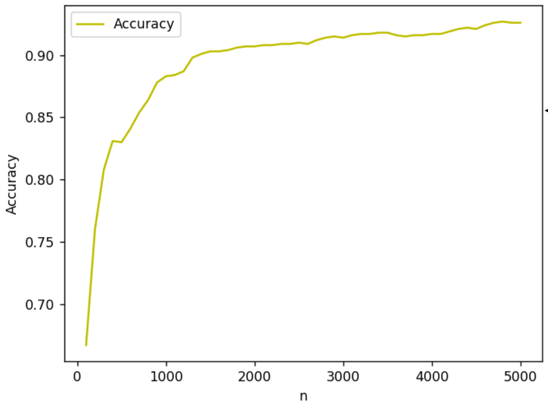
This is the same graph but not scattered, I think the one above is better cause we can see more obvious the points.

2d:



As we can see from the plot above, when k=1(which is the best k according to the previous question) as n increases the accuracy of our prediction gets better. And that makes sense cause intuitively when we train the machine on a large amount of images, training set, mistakes are made less meaning that accuracy gets better.

Note: the difference in the accuracies is more noticeable among the smallest values of n, meaning that when n is small as long as we increase it the accuracy gets better significantly, but after certain value of n, say n~2000, the accuracy gets better but not that much. That makes sense also because it must be a kind of a maximum accuracy which we can get to, mistakes will be made. I also think about this positively, cause this means that after a certain number of training data the usefulness of more and more data is negligible, and thus no need to get more training data…



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