Sai Nikhil (02/27/2021) thirandas.s@northeastern.edu

Problem 1. *Naive Bayes classifier. Consider a binary classification problem where there are eight data points in the training set. That is,*

$$\mathcal{D} = \{(-1,-1,-1,-),(-1,-1,1,+),(-1,1,-1,+),(-1,1,1,-),\\ (1,-1,-1,+),(1,-1,1,-),(1,1,-1,-),(1,1,1,+)\}$$

where each tuple (x_1, x_2, x_3, y) represents a training example with input vector (x_1, x_2, x_3) and class label y
a) (10 points) Construct a naive Bayes classifier for this problem and evaluate its accuracy on the training set. Measure accuracy as the fraction of correctly classified examples.
b) (10 points) Transform the input space into a higher-dimensional space

$$\left(x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2x_3, x_1^2, x_2^2, x_3^2, x_1^2x_2, x_1x_2^2, x_1x_3^2, x_2^2x_3, x_2x_3^2\right)$$

and repeat the previous step.
Carry out all steps manually and show all your calculations. Discuss your main observations.

Solution.

a)

Let us re-order and write the training set as follows,

x_1	x_2	x_3	y
-1	-1	-1	$-$
-1	1	1	$-$
1	-1	1	$-$
1	1	-1	$-$
-1	-1	1	$+$
-1	1	-1	$+$
1	-1	-1	$+$
1	1	1	$+$

The input vector and class label are both discrete in this case. We have, $\mathcal{X}_j = \{-1, 1\}$ and $\mathcal{Y} = \{-, +\}$. The posterior for a class is given by,

$$p(y \mid \boldsymbol{x}) \propto p(\boldsymbol{x} \mid y)p(y)$$

After applying Naive Bayes assumption, we have,

$$p\left(x_1, x_2, \ldots, x_d \mid y\right) = \prod_{j=1}^{d} p\left(x_j \mid y\right)$$

We know that class conditional is given by,

$$P(X_j = l|Y = k) = \frac{\#\text{ times } X_j = l \wedge Y = k}{\#\text{ times } Y = k} = \frac{m_{j,l,k}}{n_k}$$

In order to avoid $\frac{0}{0}$ issues, we can evaluate class conditional using smoothing, where the smoothing parameter $\ell = 1$. The new form of class conditional thus becomes,

$$P(X_j = l|Y = k) = \frac{m_{j,l,k} + \ell}{n_k + \ell|\mathcal{X}_j|} = \frac{m_{j,l,k} + 1}{n_k + 2}$$

From the training data, the class conditionals are as follows:

$$\begin{aligned}
P(X_1 = -1|Y = -) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_1 = 1|Y = -) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_1 = -1|Y = +) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_1 = 1|Y = +) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_2 = -1|Y = -) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_2 = 1|Y = -) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_2 = -1|Y = +) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_2 = 1|Y = +) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_3 = -1|Y = -) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_3 = 1|Y = -) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_3 = -1|Y = +) &= \frac{2+1}{4+2} = \frac{1}{2} \\
P(X_3 = 1|Y = +) &= \frac{2+1}{4+2} = \frac{1}{2}
\end{aligned}$$

The class probability after applying smoothing is of the form,

$$P(Y = k) = \alpha_k = \frac{n_k + \ell}{n + \ell|\mathcal{Y}|} = \frac{n_k + 1}{n + 2}$$

The class probabilities are,

$$P(Y = -) = \frac{4+1}{8+2} = \frac{1}{2} \quad \text{and} \quad P(Y = +) = \frac{4+1}{8+2} = \frac{1}{2}$$

Therefore,

$$\begin{aligned}
P(\boldsymbol{x} = (-1, -1, -1)|Y = -) &= \prod_{j=1}^{3} P(X_j = -1|Y = -) \\
&= P(X_1 = -1|Y = -) \times P(X_2 = -1|Y = -) \times P(X_3 = -1|Y = -) \\
&= \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} = \frac{1}{8}
\end{aligned}$$

Similarly,

$$\begin{aligned}
P(\boldsymbol{x} = (-1, 1, 1)|Y = -) &= \frac{1}{8} \\
P(\boldsymbol{x} = (1, -1, 1)|Y = -) &= \frac{1}{8} \\
P(\boldsymbol{x} = (1, 1, -1)|Y = -) &= \frac{1}{8} \\
P(\boldsymbol{x} = (-1, -1, 1)|Y = +) &= \frac{1}{8} \\
P(\boldsymbol{x} = (-1, 1, -1)|Y = +) &= \frac{1}{8} \\
P(\boldsymbol{x} = (1, -1, -1)|Y = +) &= \frac{1}{8} \\
P(\boldsymbol{x} = (1, 1, 1)|Y = +) &= \frac{1}{8}
\end{aligned}$$

Let, $P(\boldsymbol{x}) = k$. Hence the posteriors are,

$$\begin{aligned}
P(Y = -|\boldsymbol{x} = (-1, -1, -1)) &= \frac{P(\boldsymbol{x} = (-1, -1, -1)|Y = -) \times P(Y = -)}{P(\boldsymbol{x})} \\
&= \frac{\frac{1}{8} \times \frac{1}{2}}{k} \\
&= \frac{1}{16k}
\end{aligned}$$

Similarly,

$$\begin{aligned}
P(Y = -|\boldsymbol{x} = (-1, 1, 1)) &= \frac{1}{16k} \\
P(Y = -|\boldsymbol{x} = (1, -1, 1)) &= \frac{1}{16k} \\
P(Y = -|\boldsymbol{x} = (1, 1, -1)) &= \frac{1}{16k} \\
P(Y = +|\boldsymbol{x} = (-1, -1, 1)) &= \frac{1}{16k} \\
P(Y = +|\boldsymbol{x} = (-1, 1, -1)) &= \frac{1}{16k} \\
P(Y = +|\boldsymbol{x} = (1, -1, -1)) &= \frac{1}{16k} \\
P(Y = +|\boldsymbol{x} = (1, 1, 1)) &= \frac{1}{16k}
\end{aligned}$$

and the complementary posterior probabilities are,

$$
\begin{aligned}
P(Y=+|\boldsymbol{x}=(-1,-1,-1)) &= \frac{1}{16k}\\
P(Y=+|\boldsymbol{x}=(-1,1,1)) &= \frac{1}{16k}\\
P(Y=+|\boldsymbol{x}=(1,-1,1)) &= \frac{1}{16k}\\
P(Y=+|\boldsymbol{x}=(1,1,-1)) &= \frac{1}{16k}\\
P(Y=-|\boldsymbol{x}=(-1,-1,1)) &= \frac{1}{16k}\\
P(Y=-|\boldsymbol{x}=(-1,1,-1)) &= \frac{1}{16k}\\
P(Y=-|\boldsymbol{x}=(1,-1,-1)) &= \frac{1}{16k}\\
P(Y=-|\boldsymbol{x}=(1,1,1)) &= \frac{1}{16k}
\end{aligned}
$$

We classify a dataset $\boldsymbol{x}$ as $+$ if, $P(Y=+|\boldsymbol{x}) > P(Y=-|\boldsymbol{x})$, else we classify it with $-$.

With that logic, the first 4 training examples in the re-ordered set in the above table are classified correctly with a $-$. Rest all are incorrectly classified.

Hence, the accuracy $= \frac{4}{8} \times 100\% = 50\%$.

b)

The training data is,

x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	y
-1	-1	-1	1	1	1	-1	1	1	1	-1	-1	-1	-1	-1	$-$
-1	1	1	-1	-1	1	-1	1	1	1	1	-1	-1	1	1	$-$
1	-1	1	-1	1	-1	-1	1	1	1	-1	1	1	1	-1	$-$
1	1	-1	1	-1	-1	-1	1	1	1	1	1	1	-1	1	$-$
-1	-1	1	1	-1	-1	1	1	1	1	-1	-1	-1	1	-1	$+$
-1	1	-1	-1	1	-1	1	1	1	1	1	-1	-1	-1	1	$+$
1	-1	-1	-1	-1	1	1	1	1	1	-1	1	1	-1	-1	$+$
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	$+$

In the above table,

$$
x_4 = x_1x_2, x_5 = x_1x_3, x_6 = x_2x_3, x_7 = x_1x_2x_3, x_8 = x_1^2, x_9 = x_2^2,
$$
$$
x_{10} = x_3^2, x_{11} = x_1^2x_2, x_{12} = x_1x_2^2, x_{13} = x_1x_3^2, x_{14} = x_2^2x_3, x_{15} = x_2x_3^2
$$

Let,

$$
P(X_j = l|Y = k) = \alpha_{j,l,k}
$$

Therefore,

	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9	α_{10}	α_{12}	α_{12}	α_{13}	α_{14}	α_{15}
$X_j = -1, Y = -$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{5}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$X_j = -1, Y = +$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$X_j = 1, Y = -$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{6}$	$\frac{5}{6}$	$\frac{5}{6}$	$\frac{5}{6}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$X_j = 1, Y = +$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{5}{6}$	$\frac{5}{6}$	$\frac{5}{6}$	$\frac{5}{6}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$

The class probabilities are,

$$
P(Y=-) = \frac{4+1}{8+2} = \frac{1}{2} \quad \text{and} \quad P(Y=+) = \frac{4+1}{8+2} = \frac{1}{2}
$$

Let $P(\boldsymbol{x}) = k \ \forall \boldsymbol{x}$.
Therefore,

$$\begin{aligned} P(Y=-|\boldsymbol{x}=(-1,-1,-1,1,1,1,-1,1,1,1,-1,-1,-1,-1,-1)) &= \frac{P(\boldsymbol{x}|Y=-)\times P(Y=-)}{P(\boldsymbol{x})} \\ &= \frac{\frac{1}{2^{11}}\times\frac{5^4}{6^4}\times\frac{1}{2}}{k} \\ &= \frac{5^4}{2^{12}\times 6^4 k} \end{aligned}$$

and

$$\begin{aligned} P(Y=+|\boldsymbol{x}=(-1,-1,-1,1,1,1,-1,1,1,1,-1,-1,-1,-1,-1)) &= \frac{\frac{1}{2^{11}}\times\frac{5^3}{6^4}\times\frac{1}{2}}{k} \\ &= \frac{5^3}{2^{12}\times 6^4 k} \end{aligned}$$

Therefore from above two equations for first vector, $P(Y=+|\boldsymbol{x}) \leq P(Y=-|\boldsymbol{x})$.
$\implies$ The vector should be classified as $-$, which is as given.
For second vector,

$$\begin{aligned} P(Y=-|\boldsymbol{x}) &= \frac{\frac{1}{2^{11}}\times\frac{5^4}{6^4}\times\frac{1}{2}}{k} \\ &= \frac{5^4}{2^{12}\times 6^4 k} \\ P(Y=+|\boldsymbol{x}) &= \frac{\frac{1}{2^{11}}\times\frac{5^3}{6^4}\times\frac{1}{2}}{k} \\ &= \frac{5^3}{2^{12}\times 6^4 k} \end{aligned}$$

Here also, $P(Y=+|\boldsymbol{x}) \leq P(Y=-|\boldsymbol{x}) \implies$ The vector should be classified as $-$, which is as given.
For third and fourth vectors,

$$\begin{aligned} P(Y=-|\boldsymbol{x}) &= \frac{\frac{1}{2^{11}}\times\frac{5^4}{6^4}\times\frac{1}{2}}{k} \\ &= \frac{5^4}{2^{12}\times 6^4 k} \\ P(Y=+|\boldsymbol{x}) &= \frac{\frac{1}{2^{11}}\times\frac{5^3}{6^4}\times\frac{1}{2}}{k} \\ &= \frac{5^3}{2^{12}\times 6^4 k} \end{aligned}$$

Here also, $P(Y=+|\boldsymbol{x}) \leq P(Y=-|\boldsymbol{x}) \implies$ The vector should be classified as $-$, which is as given.

For fifth, sixth, seventh and eighth vectors,

$$\begin{aligned} P(Y=+|\boldsymbol{x}) &= \frac{\frac{1}{2^{11}}\times\frac{5^4}{6^4}\times\frac{1}{2}}{k} \\ &= \frac{5^4}{2^{12}\times 6^4 k} \end{aligned}$$

$$
\begin{aligned}
P(Y=-|\boldsymbol{x}) &= \frac{\frac{1}{2^{11}} \times \frac{5^3}{6^4} \times \frac{1}{2}}{k} \\
&= \frac{5^3}{2^{12} \times 6^4 k}
\end{aligned}
$$

Here, $P(Y=+|\boldsymbol{x}) > P(Y=-|\boldsymbol{x}) \implies$ The vector should be classified as +, which is as given.
Hence, the accuracy $= \frac{8}{8} \times 100\% = 100\%$.

Observations:

1. Clearly the feature $x_7 = x_1x_2x_3$ is alone enough to classify input vectors correctly with 100% accuracy in case b).
2. Features x_2^2 and x_3^2 are redundant as they as produce the same output as x_1^2. Similarly, $x_1^2x_2$ is same as x_2, $x_1x_2^2$ and $x_1x_3^2$ are same as x_1, $x_2^2x_3$ is same as x_3, $x_2x_3^2$ is same as x_2. Such redundant features should be removed while performing Naive Bayes classification. However, in this special case, their presence doesn't effect the classification.

□

Problem 2. *Consider a binary classification problem in which we want to determine the optimal decision surface. A point* x *is on the decision surface if* $P(Y=1 \mid \mathrm{x}) = P(Y=0 \mid \mathrm{x})$.

a) (10 points) Find the optimal decision surface assuming that each class-conditional distribution is defined as a two-dimensional Gaussian distribution:

$$
p(\mathbf{x} \mid Y=i) = \frac{1}{(2\pi)^{d/2} \left|\boldsymbol{\Sigma}_i\right|^{1/2}} \cdot e^{-\frac{1}{2}(\mathbf{x}-\mathbf{m}_i)^T \boldsymbol{\Sigma}_i^{-1}(\mathbf{x}-\mathbf{m}_i)}
$$

where $i \in \{0,1\}, \mathbf{m}_0 = (1,2), \mathbf{m}_1 = (6,3), \boldsymbol{\Sigma}_0 = \boldsymbol{\Sigma}_1 = \mathbf{I}_2, P(Y=0) = P(Y=1) = \frac{1}{2}, \mathbf{I}_d$ *is the d-dimensional identity matrix, and* $|\boldsymbol{\Sigma}_i|$ *is the determinant of* $\boldsymbol{\Sigma}_i$.

b) (5 points) Generalize the solution from part (a) using $\mathbf{m}_0 = (m_{01}, m_{02}), \mathbf{m}_1 = (m_{11}, m_{12}), \boldsymbol{\Sigma}_0 = \boldsymbol{\Sigma}_1 = \sigma^2\mathbf{I}_2$ *and* $P(Y=0) \neq P(Y=1)$.

c) (10 points) Generalize the solution from part (b) to arbitrary covariance matrices $\boldsymbol{\Sigma}_0$ *and* $\boldsymbol{\Sigma}_1$*. Discuss the shape of the optimal decision surface.*

Solution.

a)

For optimal decision surface, we have, $P(Y=0 \mid \mathbf{x}) = P(Y=1 \mid \mathbf{x})$.

$$
\text{Let, } \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}
$$

Therefore,

$$
\begin{gathered}
P(\mathbf{x} \mid Y=0) \cdot P(Y=0) = P(\mathbf{x} \mid Y=1) \cdot P(Y=1) \\
\implies \frac{1}{(2\pi)^{d/2} \left|\boldsymbol{\Sigma}_0\right|^{1/2}} \cdot e^{-\frac{1}{2}(\mathbf{x}-\mathbf{m}_0)^T \boldsymbol{\Sigma}_0^{-1}(\mathbf{x}-\mathbf{m}_0)} \cdot \frac{1}{2} = \frac{1}{(2\pi)^{d/2} \left|\boldsymbol{\Sigma}_1\right|^{1/2}} \cdot e^{-\frac{1}{2}(\mathbf{x}-\mathbf{m}_1)^T \boldsymbol{\Sigma}_1^{-1}(\mathbf{x}-\mathbf{m}_1)} \cdot \frac{1}{2} \\
\implies (x_1-1)^2 + (x_2-2)^2 = (x_1-6)^2 + (x_2-3)^2
\end{gathered}
$$

$$\boxed{5x_1 + x_2 = 20}$$

b)

Let, $P(Y=0) = \alpha$ and $P(Y=1) = 1-\alpha$

Therefore,

$$P(\mathbf{x} \mid Y=0) \cdot P(Y=0) = P(\mathbf{x} \mid Y=1) \cdot P(Y=1)$$

$$\frac{1}{(2\pi)^{d/2} \left|\boldsymbol{\Sigma}_0\right|^{1/2}} \cdot e^{-\frac{1}{2}(\mathbf{x}-\mathbf{m}_0)^T \boldsymbol{\Sigma}_0^{-1}(\mathbf{x}-\mathbf{m}_0)} \cdot \alpha = \frac{1}{(2\pi)^{d/2} \left|\boldsymbol{\Sigma}_1\right|^{1/2}} \cdot e^{-\frac{1}{2}(\mathbf{x}-\mathbf{m}_1)^T \boldsymbol{\Sigma}_1^{-1}(\mathbf{x}-\mathbf{m}_1)} \cdot (1-\alpha)$$

$$\implies (x_1 - m_{01})^2 + (x_2 - m_{02})^2 - (x_1 - m_{11})^2 - (x_1 - m_{12})^2 = 2\sigma^2 \ln\left(\frac{\alpha}{1-\alpha}\right)$$

$$\boxed{(m_{11} - m_{01})x_1 + (m_{12} - m_{02})x_2 + \frac{(m_{01}^2 + m_{02}^2 - m_{11}^2 - m_{12}^2)}{2} - \sigma^2 \ln\left(\frac{\alpha}{1-\alpha}\right) = 0}$$

c)

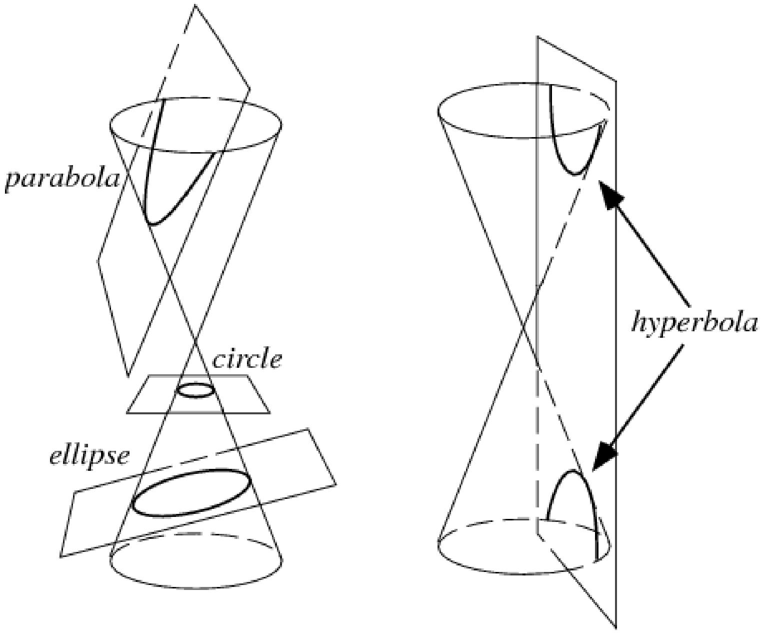
Generalizing the above equation, we get,

$$e^{\frac{(\mathbf{x}-\mathbf{m}_0)^T \boldsymbol{\Sigma}_0^{-1}(\mathbf{x}-\mathbf{m}_0) - (\mathbf{x}-\mathbf{m}_1)^T \boldsymbol{\Sigma}_1^{-1}(\mathbf{x}-\mathbf{m}_1)}{2}} = \frac{\alpha}{1-\alpha}\sqrt{\frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_0|}}$$

$$(\mathbf{x}-\mathbf{m}_0)^T \boldsymbol{\Sigma}_0^{-1} (\mathbf{x}-\mathbf{m}_0) - (\mathbf{x}-\mathbf{m}_1)^T \boldsymbol{\Sigma}_1^{-1} (\mathbf{x}-\mathbf{m}_1) - 2\ln\left(\frac{\alpha}{1-\alpha}\sqrt{\frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_0|}}\right) = 0$$

Upon substituting constants, this will be simplified to the form,

$$\boxed{Ax_1^2 + Bx_2^2 + Cx_1x_2 + Dx_1 + Ex_2 + F = 0}$$



This is the generic equation of a conic section in a 2-D plane as shown above. The shape of the conic will depend on following values:

$$\Delta = \begin{vmatrix} A & \frac{1}{2}C & \frac{1}{2}D \\ \frac{1}{2}C & B & \frac{1}{2}E \\ \frac{1}{2}D & \frac{1}{2}E & F \end{vmatrix}, \quad J = \begin{vmatrix} A & \frac{1}{2}C \\ \frac{1}{2}C & B \end{vmatrix}, \quad I = A + B,$$

$$K = \begin{vmatrix} A & \frac{1}{2}D \\ \frac{1}{2}D & F \end{vmatrix} + \begin{vmatrix} B & \frac{1}{2}E \\ \frac{1}{2}E & F \end{vmatrix}$$

The appropriate cases for different conics are given below:

Δ	J	$\Delta/1$	K	Type of conic
$\neq 0$	< 0			hyperbola
$\neq 0$	0			parabola
$\neq 0$	> 0	< 0		ellipse
$\neq 0$	> 0	> 0		(imaginary ellipse)
0	< 0			intersecting lines
0	> 0			point
0	0		< 0	distinct parallel lines
0	0		> 0	(imaginary parallel lines)
0	0		0	coincident lines

□

Problem 3. *Problem 3. (55 points) Consider a multivariate linear regression problem of mapping $\mathbb{R}^d$ to $\mathbb{R}$, with two different objective functions. The first objective function is the sum of squared errors, as presented in class; i.e., $\sum_{i=1}^{n} e_i^2$, where $e_i = w_0 + \sum_{j=1}^{d} w_j x_{ij} - y_i$. The second objective function is the sum of square Euclidean distances to the hyperplane; i.e., $\sum_{i=1}^{n} r_i^2$, where r_i is the Euclidean distance between point (x_i, y_i) to the hyperplane $f(x) = w_0 + \sum_{j=1}^{d} w_j x_j$.*

a) (10 points) Derive a gradient descent algorithm to find the parameters of the model that minimizes the sum of squared errors.

b) (20 points) Derive a gradient descent algorithm to find the parameters of the model that minimizes the sum of squared distances.

c) (20 points) Implement both algorithms and test them on 3 datasets. Datasets can be randomly generated, as in class, or obtained from resources such as UCI Machine Learning Repository. Compare the solutions to the closed-form (maximum likelihood) solution derived in class and find the R^2 in all cases on the same dataset used to fit the parameters; i.e., do not implement cross-validation. Briefly describe the data you use and discuss your results.

d) (5 points) Normalize every feature and target using a linear transform such that the minimum value for each feature and the target is 0 and the maximum value is 1. The new value for feature j of data point i can be found as

$$x_{ij}^{new} = \frac{x_{ij} - \min_{k \in \{1,2,\ldots,n\}} x_{kj}}{\max_{k \in \{1,2,\ldots,n\}} x_{kj} - \min_{k \in \{1,2,\ldots,n\}} x_{kj}}$$

where n is the dataset size. The new value for the target i can be found as

$$y_i^{new} = \frac{y_i - \min_{k \in \{1,2,\ldots,n\}} y_k}{\max_{k \in \{1,2,\ldots,n\}} y_k - \min_{k \in \{1,2,\ldots,n\}} y_k}$$

Measure the number of steps towards convergence and compare with the results from part (c). Briefly discuss your results.

Solution.

a)

Given: A set of observations

$$D = \{(x_i, y_i)\}_{i=1}^{n}, (x_{i,}y_i) \in \mathbb{R}^d \times \mathbb{R}$$

Objective: Find best linear approximator

$$f(x) = \omega_0 + \sum_{j=1}^{d} \omega_j x_j$$

Minimize sum of squares $= \sum_{i=1}^{n} \left(f\left(x_i\right) - y_i\right)^2$

Rewrite: Minimize,

$$SSE = \sum_{i=1}^{n} \left(w_0 + \sum_{j=1}^{d} w_j x_{ij} - y_i \right)^2$$

Suppose, $\boxed{x_{i0} = 1}$,

$$SSE\left(w_0, w_1, \cdots w_d\right) = \sum_{i=1}^{n} \left(\sum_{j=0}^{d} w_j x_{ij} - y_i \right)^2$$

Writing in vector form, we get,

$$\boxed{SSE(\mathbf{w}) = (\mathbf{xw} - \mathbf{y})^T (\mathbf{xw} - \mathbf{y})}$$

Hence,

$$\boxed{\nabla SSE(\mathbf{w}) = 2\mathbf{x}^T (\mathbf{xw} - \mathbf{y})}$$

For gradient descent, $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \cdot \nabla SSE\left(\mathbf{w}^{(t)}\right)$, where $\eta \in (0, 1]$

$$\boxed{\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - 2\eta \mathbf{x}^T \left(\mathbf{xw}^{(t)} - \mathbf{y}\right)}$$

b)

Given: A set of observations

$$D = \{(x_i, y_i)\}_{i=1}^{n}, (x_{i,}y_i) \in \mathbb{R}^d \times \mathbb{R}$$

Objective: Find best linear approximator

$$f(x) = \omega_0 + \sum_{j=1}^{d} \omega_j x_j$$

Minimize sum of squared euclidian distances,

$$\begin{aligned} SSED &= \sum_{i=1}^{n} \frac{\left(f\left(x_i\right) - y_i\right)^2}{\|\mathbf{w}\|^2 + 1} \\ &= \sum_{i=1}^{n} \frac{\left(w_0 + \sum_{j=1}^{d} w_j x_i - y_i\right)^2}{\|\mathbf{w}\|^2 + 1} \end{aligned}$$

Suppose, $\boxed{x_{i0} = 1}$,

$$
\begin{aligned}
SSED(w_0, w_1, \cdots w_d) &= \sum_{i=1}^{n} \frac{\left(\sum_{j=0}^{d} w_j x_{ij} - y_i\right)^2}{\|w\|^2 + 1} \\
&= \frac{\sum_{i=1}^{n} \left(\sum_{j=0}^{d} w_j x_{ij} - y_i\right)^2}{\sum_{k=1}^{d} w_k^2 + 1} \\
&= \frac{SSE\left(w_0, w_1, \ldots w_d\right)}{\sum_{k=1}^{d} w_k^2}
\end{aligned}
$$

$$
\implies \boxed{SSED(\mathbf{w}) = \frac{SSE(\mathbf{w})}{\|\mathbf{w}\|^2 + 1}}
$$

Hence,

$$
\frac{\partial(SSED)}{\partial w_0} = \frac{\left(\sum_{k=1}^{d} w_k^2 + 1\right) \times \frac{\partial}{\partial w_0}(SSE) - SSE \times 0}{\left(\sum_{k=1}^{d} w_k^2 + 1\right)^2}
$$

and, when $1 \leq p \leq d$,

$$
\frac{\partial(SSED)}{\partial w_p} = \frac{\left(\sum_{k=1}^{d} w_k^2 + 1\right) \times \frac{\partial(SSE)}{\partial w_P} - SSE \times (2w_p)}{\left(\sum_{k=1}^{d} w_k^2 + 1\right)^2}
$$

We modify $\mathbf{w}$ vector by putting, $w_0 = 0$ to get $\mathbf{w}_2$,
Hence,

$$
\boxed{\nabla SSED(\mathbf{w}, \mathbf{w}_2) = \frac{\left(\|\mathbf{w}_2\|^2 + 1\right) \times \nabla SSE(\mathbf{w}) - 2 \times SSE(\mathbf{w}) \times \mathbf{w}_2}{\left(\|\mathbf{w}_2\|^2 + 1\right)^2}}
$$

Let for $\mathbf{t}^{th}$ step, the modified $\mathbf{w}^{(t)}$ be $\mathbf{w}_2{}^{(t)}$.
So, for gradient descent, $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \cdot \nabla SSED\left(\mathbf{w}^{(t)}, \mathbf{w}_2{}^{(t)}\right)$, where $\eta \in (0, 1]$

$$
\boxed{\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \left(\frac{\left(\|\mathbf{w}_2{}^{(t)}\|^2 + 1\right) \times \nabla SSE(\mathbf{w}^{(t)}) - 2 \times SSE(\mathbf{w}^{(t)}) \times \mathbf{w}_2{}^{(t)}}{\left(\|\mathbf{w}_2{}^{(t)}\|^2 + 1\right)^2} \right)}
$$

c) & d)

For code, please look into **GradientDescent.ipynb**.

Output:

1)
Actual weights = [1 2]
WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Raw dataset results:
Weights from Maximum Likelihood = [1.25499004 1.98981147]
Weights from Sum of Squared Error = [1.25888602 1.98237399] Number of iterations taken = 336
Weights from Sum of Squared Euclidean Distance Error = [1.79207960e-03 4.21289384e+00] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9423719488680293
R^2 for Sum of Squared Error = 0.9423585914916401

R^2 for Sum of Squared Euclidean Distance Error = -0.3125292809590352

WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Normalized dataset results:
Weights from Maximum Likelihood = [0.08428984 0.82866939]
Weights from Sum of Squared Error = [0.080403 0.83608681] Number of iterations taken = 232
Weights from Sum of Squared Euclidean Distance Error = [0.00183914 0.9647496] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9405070723861864
R^2 for Sum of Squared Error = 0.9404306160582103
R^2 for Sum of Squared Euclidean Distance Error = 0.9110184877290902

2)
Actual weights = [1 2 3]
WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Raw dataset results:
Weights from Maximum Likelihood = [1.23021267 2.02393632 3.01567512]
Weights from Sum of Squared Error = [1.23897042 2.01566028 3.00716707] Number of iterations taken = 411
Weights from Sum of Squared Euclidean Distance Error = [9.11827650e-04 3.10726850e+00 4.17204299e+00] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9810229751608907
R^2 for Sum of Squared Error = 0.981012314928364
R^2 for Sum of Squared Euclidean Distance Error = 0.7807863494298954

WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Normalized dataset results:
Weights from Maximum Likelihood = [0.02130786 0.40205078 0.5999009]
Weights from Sum of Squared Error = [0.01296103 0.41063084 0.60728349] Number of iterations taken = 326
Weights from Sum of Squared Euclidean Distance Error = [3.44419144e-04 4.20719822e-01 6.19044100e-01] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9815491309587564
R^2 for Sum of Squared Error = 0.9813044292617724
R^2 for Sum of Squared Euclidean Distance Error = 0.9800893873012639

3)
Actual weights = [1 2 3 4]
WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Raw dataset results:
Weights from Maximum Likelihood = [1.23175493 2.00920529 3.02320381 4.00696197]
Weights from Sum of Squared Error = [1.24252118 2.00268153 3.01665139 3.99957899] Number of iterations taken = 544
Weights from Sum of Squared Euclidean Distance Error = [4.19130419e-04 2.71024299e+00 3.76068168e+00 4.83138405e+00] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9915521623406103
R^2 for Sum of Squared Error = 0.9915472787565527
R^2 for Sum of Squared Euclidean Distance Error = 0.9292159669387261

WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Normalized dataset results:
Weights from Maximum Likelihood = [-0.09614229 0.25250589 0.37625801 0.50156219]
Weights from Sum of Squared Error = [-0.1068754 0.25926529 0.38285911 0.5086211] Number of iterations taken = 410

Weights from Sum of Squared Euclidean Distance Error = [-0.00150743 0.19394194 0.32020437 0.44452522]
Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9915165897073519
R^2 for Sum of Squared Error = 0.9912062933639023
R^2 for Sum of Squared Euclidean Distance Error = 0.9681003338416297

4)
+++++++++++++START WITH N = 300 and D = 15+++++++++++++
Actual weights = [1 2 4 4 2 4 4 1 4 2 4 5 1 1 2 3]
WARNING: Convergence not obtained for ¡function SSE at 0x7fd54d030700¿
WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Raw dataset results:
Weights from Maximum Likelihood = [1.11379202 2.00029796 3.99977594 4.00013072 2.00049968 4.00002218 3.99985206 1.0002666 4.00036985 1.9999127 3.99993452 5.00038289 1.00011637 1.00009822 2.00048834 3.00036932]
Weights from Sum of Squared Error = [6.55525175e+303 inf inf inf inf inf inf inf inf inf inf inf inf inf inf inf]
Number of iterations taken = 91
Weights from Sum of Squared Euclidean Distance Error = [-9.01336498e-06 -1.37630440e+02 4.59005871e+02 -8.54542452e+01 1.48951236e+03 3.87126499e+02 7.20603366e+02 9.57736517e+02 -4.30511843e+02 2.89074535e+02 -1.68475555e+03 -3.16648651e+02 -4.24806071e+02 -6.64258165e+02 -1.77869449e+02 8.49412333e+01] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9999998167501309
R^2 for Sum of Squared Error = nan
R^2 for Sum of Squared Euclidean Distance Error = -60694.73590778983

WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Normalized dataset results:
Weights from Maximum Likelihood = [-0.34941459 0.08970206 0.18447254 0.18363183 0.09199215 0.18160336 0.18226469 0.04420227 0.18116071 0.09201079 0.18117562 0.22684705 0.0449425 0.0456999 0.09390231 0.13825206]
Weights from Sum of Squared Error = [-0.44835348 0.09889455 0.19320891 0.19519339 0.11112236 0.19363335 0.19811723 0.06018336 0.19083287 0.10666284 0.1936614 0.24515874 0.05618911 0.05946077 0.10792598 0.14598463]
Number of iterations taken = 2354
Weights from Sum of Squared Euclidean Distance Error = [-0.00040218 0.05428484 0.1527442 0.14297237 0.02808748 0.14070359 0.13078585 -0.01279373 0.14730324 0.04002846 0.13681534 0.16844793 0.00216292 -0.0042922 0.04477235 0.1073495] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9983488145823171
R^2 for Sum of Squared Error = 0.9901491922153589
R^2 for Sum of Squared Euclidean Distance Error = 0.8965566890039539

++++++++++++++++++++END++++++++++++++++++++

5)
+++++++++++++START WITH N = 300 and D = 25+++++++++++++
Actual weights = [1 3 2 5 2 5 4 1 3 1 3 1 4 4 4 3 1 3 5 3 5 5 3 5 3 3]
WARNING: Convergence not obtained for ¡function SSE at 0x7fd54d030700¿
WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Raw dataset results:
Weights from Maximum Likelihood = [1.22925544 2.99969538 2.00006519 5.00030685 1.99979471 5.00023927 4.00007528 1.00006182 3.00008527 0.99998621 2.99981107 0.99994666 3.99955583 4.00009405 4.00028369 2.99966477 0.99996969 2.99997628 4.9998824 3.00034224 5.00004925 5.00005719 3.00025455 5.00035179 3.00024262 2.99992421]
Weights from Sum of Squared Error = [-inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf -inf] Number of iterations taken = 86
Weights from Sum of Squared Euclidean Distance Error = [2.51767061e-06 -9.88697125e+02 9.00873261e+01 -1.92963409e+03 -2.35525810e+02 -6.63291427e+00 3.39117084e+02 1.23302792e+03 -5.27756261e+02 -5.23797684e+01

7.74342188e+02 -2.31359030e+03 7.23699252e+02 1.13881796e+03 -6.94846143e+02 6.90815058e+02 -7.71019832e+02 2.95505655e+01 -5.05390598e+02 -1.16050678e+02 7.23553196e+02 5.31881742e+02 -8.56822317e+02 2.41791437e+03 -1.83191668e+02 1.18182893e+03] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9999999206838287
R^2 for Sum of Squared Error = nan
R^2 for Sum of Squared Euclidean Distance Error = -74297.25730943335

WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Normalized dataset results:
Weights from Maximum Likelihood = [-0.73555493 0.09176588 0.0614537 0.14867511 0.06219864 0.1512127 0.11995057 0.02880507 0.08949756 0.03048697 0.09011332 0.02959466 0.1202821 0.11760331 0.11932968 0.08863317 0.02941539 0.09008425 0.14911477 0.08947689 0.14974749 0.1513679 0.08862665 0.1500807 0.09039517 0.08904543]
Weights from Sum of Squared Error = [-0.88373584 0.10526709 0.06790168 0.16733445 0.0713776 0.16155003 0.1281091 0.0360564 0.09922515 0.04951841 0.09450599 0.04241477 0.13061328 0.13824017 0.13591043 0.09478696 0.04239259 0.09853011 0.16628535 0.09452441 0.1664138 0.16376364 0.09904652 0.15497507 0.104135 0.10571228]
Number of iterations taken = 2637
Weights from Sum of Squared Euclidean Distance Error = [-0.00055953 0.02456858 0.02461456 0.06228102 0.01216935 0.10581652 0.08061827 -0.01311681 0.03975548 -0.06745841 0.06509645 -0.04019028 0.06899602 0.0218671 0.04168255 0.05616815 -0.04176067 0.04496383 0.07029958 0.06111526 0.07544612 0.09448006 0.03683481 0.12744838 0.02232875 0.00885513] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9992785843911158
R^2 for Sum of Squared Error = 0.9873395915423594
R^2 for Sum of Squared Euclidean Distance Error = 0.7054469437702278

++++++++++++++++++++END++++++++++++++++++++

6)
+++++++++++++START WITH N = 500 and D = 15+++++++++++++
Actual weights = [4 4 1 4 5 5 4 2 1 2 2 1 2 3 2 4]
WARNING: Convergence not obtained for ¡function SSE at 0x7fd54d030700¿
WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Raw dataset results:
Weights from Maximum Likelihood = [4.19197647 4.00005829 1.00003433 4.00027826 4.99966552 5.00011521 4.00037878 1.99982901 1.00012679 2.00001082 2.00009117 0.99995515 2.00054615 3.00000614 2.00020594 3.99984357]
Weights from Sum of Squared Error = [1.08520046e+303 inf inf inf inf inf inf inf inf inf inf inf inf inf inf inf]
Number of iterations taken = 85
Weights from Sum of Squared Euclidean Distance Error = [-2.45393323e-06 1.35503230e+03 -1.09638282e+03 -9.69297195e+02 1.46620462e+03 -1.24861283e+03 1.46405201e+03 -1.34609076e+03 5.40068547e+02 7.58014339e+01 3.30850235e+02 5.37074487e+02 -2.33809938e+03 2.15320324e+02 -1.00568218e+02 1.53771598e+03] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9999998259936541
R^2 for Sum of Squared Error = nan
R^2 for Sum of Squared Euclidean Distance Error = -134470.54599720868

WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Normalized dataset results:
Weights from Maximum Likelihood = [-0.51998462 0.18128726 0.04334654 0.18172096 0.22789152 0.22804701 0.18111454 0.09002892 0.04452301 0.09141063 0.09048435 0.04540351 0.08991154 0.13577932 0.0896705 0.1810057
]
Weights from Sum of Squared Error = [-0.58397535 0.19031205 0.05168271 0.18973635 0.23574162 0.2327261 0.1899888 0.09780599 0.056224 0.09949582 0.0978154 0.05392619 0.09997114 0.14498114 0.09949853 0.18661719]
Number of iterations taken = 1724
Weights from Sum of Squared Euclidean Distance Error = [-0.00094496 0.11321581 -0.03037624 0.11940295

0.17014407 0.19162951 0.11360697 0.02330995 -0.05022218 0.02387642 0.02854233 -0.0268557 0.00724938 0.06304645 0.00974125 0.13576683] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9984722644103742
R^2 for Sum of Squared Error = 0.995347449159415
R^2 for Sum of Squared Euclidean Distance Error = 0.7925571678154589

++++++++++++++++++++END+++++++++++++++++++++

7)
+++++++++++++START WITH N = 500 and D = 25+++++++++++++
Actual weights = [3 1 4 1 3 5 5 4 5 4 1 2 3 4 5 2 5 1 2 1 3 2 1 1 2 3]
WARNING: Convergence not obtained for ¡function SSE at 0x7fd54d030700¿
WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Raw dataset results:
Weights from Maximum Likelihood = [3.24497527 1.00028751 3.99993721 1.0000767 2.99997367 5.00030765 5.00010002 4.000008 5.00028374 4.00049966 0.9997872 1.99978382 3.00006563 4.00001772 5.00016734 1.99997228 5.00055664 0.99983617 1.99990638 1.00008227 3.00002484 1.99976782 0.99994172 0.99967888 1.9996288 2.9995631
]
Weights from Sum of Squared Error = [9.45550614e+298 4.95770499e+300 4.96664283e+300 4.81437234e+300 4.83837582e+300 4.87131164e+300 4.77213033e+300 4.72443157e+300 4.82788492e+300 4.90858866e+300 4.86871021e+300 4.66732369e+300 4.97032502e+300 4.67548743e+300 4.64735652e+300 4.74008072e+300 4.75269017e+300 4.72077171e+300 4.73918214e+300 4.70027626e+300 4.83761292e+300 4.73605989e+300 4.76102506e+300 4.83220060e+300 4.95664850e+300 4.76815571e+300] Number of iterations taken = 79
Weights from Sum of Squared Euclidean Distance Error = [-3.44913351e-06 -2.30382376e+03 -1.68883000e+03 -5.33322120e+02 -2.63620894e+02 -4.55335563e+02 7.13082385e+02 1.14981595e+03 2.81436092e+02 -9.93246841e+02 -1.03359936e+03 1.53598228e+03 -1.93038709e+03 1.93220568e+03 2.21970667e+03 7.16513300e+02 1.12826392e+03 5.84547956e+02 5.95279613e+02 6.99372538e+02 -5.16760648e+02 5.17075312e+02 3.22830092e+02 -7.14757806e+02 -1.94186255e+03 6.22466736e+02] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9999999104829829
R^2 for Sum of Squared Error = -inf
R^2 for Sum of Squared Euclidean Distance Error = -138630.36464914665

WARNING: Convergence not obtained for ¡function SSED at 0x7fd54d030b80¿
Normalized dataset results:
Weights from Maximum Likelihood = [-0.76601335 0.03380109 0.13802622 0.03389831 0.10405455 0.17179754 0.1722516 0.13703769 0.17363995 0.13801589 0.0339626 0.06854687 0.10352891 0.13759839 0.17226761 0.06840241 0.1726181 0.03344793 0.06869985 0.03553007 0.10343633 0.06902528 0.03491455 0.0357838 0.06932436 0.10229722]
Weights from Sum of Squared Error = [-0.84572459 0.04146822 0.14695777 0.03918924 0.11303719 0.17697531 0.17865866 0.14287515 0.18181098 0.14472318 0.0367957 0.07431063 0.11100301 0.14555811 0.18153574 0.07446155 0.1804489 0.0382179 0.07687837 0.04168635 0.10744186 0.07285991 0.03951204 0.0428857 0.07259151 0.10572461]
Number of iterations taken = 1883
Weights from Sum of Squared Euclidean Distance Error = [-0.00106577 -0.04368339 0.06024521 -0.02618336 0.01729601 0.13130755 0.12086351 0.08685847 0.10540002 0.07899458 -0.00605082 0.00964694 0.03522075 0.0657044 0.09481498 0.00551846 0.10701359 -0.02024717 -0.01123888 -0.02950712 0.06863788 0.02846556 -0.0215508 -0.03754629 0.03267755 0.06693289] Number of iterations taken = 100000
R^2 for Maximum Likelihood = 0.9990941254620707
R^2 for Sum of Squared Error = 0.9955182734431118
R^2 for Sum of Squared Euclidean Distance Error = 0.6682149738210033

++++++++++++++++++++END+++++++++++++++++++++

Datasets 1, 2 & 3 are picked from a normal distribution in (0, 1) and have size=100. Datasets 4, 5, 6 & 7 are picked from a integer uniform distribution from [0, 100] and have size and dimension combinations coming from {300, 500} and {15, 25}.

Observations (without normalization):

1. When input values are small (chosen from a normal distribution in $(0, 1)$), the sum of squared errors does converge but the sum of squared euclidean distances does not converge. The R^2 value for SSE is better than R^2 value for $SSED$ mostly because of over-engineering involved when modeling using $SSED$ i.e., there is no single local optimum in case of $SSED$.

2. As we increase the number of features (1 to 2 to 3), the R^2 tends to get closer to 1 thus yielding a solution close to $\mathbf{w_{ML}}$.

Observations (with normalization):

1. For smaller input values (chosen from a normal distribution in $(0, 1)$), the sum of squared errors does converge but the sum of squared euclidean distances does not converge. The R^2 value for SSE is better than R^2 value for $SSED$ for the above mentioned reason. However, the improvement because of normalization is relatively high when the number of features are less.

2. This time I tested with larger input values (chosen integers from uniform distribution in $[1, 100]$), the sum of squared errors does not converge. This is mostly due to overflow issues. The sum of squared euclidean distances does not converge but after running 100,000 iterations we get a decent solution. The R^2 value for SSE is undefined and R^2 value for $SSED$ is much less than zero which implies that the model is performing poorly.

3. Normalizing the larger input value data we get pretty good results. This time the sum of squared errors and the sum of squared euclidean distances both converge. The R^2 value for SSE is better than R^2 value for $SSED$ because of no single definite local optimum.

4. As we increase the number of features (15 to 25), for both SSE/SSED , the R^2 tends to get away from 1, although in both cases it is much close to 1. This is contrary to the observation stated above. This can be explained by the curse of dimensionality.

□