The kNN, or k-nearest neighbors algorithm, is a simple supervised learning algorithm, which works under the assumption that samples with similar features are more likely to share the same label. The algorithm is very straight-forward, although differing between trying to predict categoric and numeric labels: using a given distance metric (such as Euclidean, Manhattan, etc.), the algorithm finds the k closest samples to the sample we want to classify, and assigns the label that:

- 1. is most common (i.e. the mode) among the k neighbors, in the case of categoric labels;
- 2. is the average of the labels of the k neighbors, in the case of numeric labels.
  - 1. Considering the following data set:

|                       | У1 | У2 | <i>z</i> <sub>1</sub> | $z_2$ |
|-----------------------|----|----|-----------------------|-------|
| $x_1$                 | 1  | 1  | A                     | 1.4   |
| $x_2$                 | 2  | 1  | В                     | 0.5   |
| $x_3$                 | 2  | 3  | В                     | 2     |
| $x_4$                 | 3  | 3  | В                     | 2.2   |
| <i>x</i> <sub>5</sub> | 2  | 2  | Α                     | 0.7   |
| $x_6$                 | 1  | 2  | A                     | 1.2   |

Assuming kNN, with k = 3 applied within a leave-one-out schema:

- (a) Considering an  $z_1$  categoric output variable and the Euclidean distance, provide the prediction for  $x_1$ .
- (b) Considering an  $z_2$  numeric output variable and the cosine similarities, provide the mean regression estimate for  $x_1$ .
- (c) Considering a weighted-distance kNN, with Manhattan distance, identify both the **weighted-mode** estimate of  $x_1$  for a  $z_1$  outcome and the **weighted-mean** estimate of  $x_1$  for a  $z_2$  outcome.

Here, working with a leave-one-out schema means that, for each sample, we can pick its k neighbors from the pool of all the other samples, excluding itself (which, in theory, is always its closest neighbor, with null distance).

(a) The Euclidean distance is defined as the square root of the sum of the squared differences between the features of the two samples:

$$d(x_i, x_j) = \sqrt{\sum_{l=1}^{p} (x_i^{(l)} - x_j^{(l)})^2}$$

Since we're working with a leave-one-out schema, and trying to estimate the  $z_1$  label for  $x_1$ , we can pick the k neighbors from all samples except  $x_1$ . Below are illustrated the Euclidean distances between those samples and  $x_1$ , with the k closest neighbors highlighted in teal:

$$d(x_1, x_2) = \sqrt{(1-2)^2 + (1-1)^2} = 1$$

$$d(x_1, x_3) = \sqrt{5}$$
,  $d(x_1, x_4) = 2\sqrt{2}$ ,  $d(x_1, x_5) = \sqrt{2}$ ,  $d(x_1, x_6) = 1$ 

Knowing the k closest neighbors, we can now estimate the  $z_1$  label for  $x_1$ , by picking the most common label among them. In this case, the estimated label will be  $\mathbf{mode}(B, A, A) = A$ .

(b) Here, instead of the usual Euclidean/Manhattan distance, we're using the cosine similarities, which are defined as the cosine of the angle between the two vectors of features. As we know since high school, the cosine of the angle between two vectors is equal to the dot product of the two vectors divided by the product of their norms:

$$\cos(\vec{a}, \vec{b}) = \frac{\vec{a} \cdot \vec{b}}{\|\vec{a}\| \|\vec{b}\|}$$

Here, each sample is essentially a vector of features, hence the usage of this distance metric. The higher the cosine similarity, the closer the two vectors are, and vice versa: the cosine is equal to 1 when the two vectors are identical, and 0 when they are orthogonal.

Let's now compute the cosine similarities between  $x_1$  and the other samples, picking the k closest neighbors (once again, in teal):

$$\cos(x_1, x_2) = \frac{1 \cdot 2 + 1 \cdot 1}{\sqrt{2}\sqrt{5}} = \frac{3}{\sqrt{10}} = 0.94868, \quad \cos(x_1, x_3) = \frac{1 \cdot 2 + 1 \cdot 3}{\sqrt{2}\sqrt{13}} = \frac{5}{\sqrt{26}} = 0.98058$$

$$\cos(x_1, x_4) = \frac{1 \cdot 3 + 1 \cdot 3}{\sqrt{2}\sqrt{18}} = \frac{6}{\sqrt{36}} = 1, \quad \cos(x_1, x_5) = \frac{1 \cdot 2 + 1 \cdot 2}{\sqrt{2}\sqrt{8}} = \frac{4}{\sqrt{16}} = 1$$

$$\cos(x_1, x_6) = \frac{1 \cdot 1 + 1 \cdot 2}{\sqrt{2}\sqrt{5}} = \frac{3}{\sqrt{10}} = 0.94868$$

Note, as mentioned above, that the closest neighbors here are the ones with a higher cosine similarity:  $x_3$ ,  $x_4$ , and  $x_5$ . Since we're working with numeric labels for  $z_2$ , we can now estimate the mean regression estimate for  $x_1$  by averaging the values of  $z_2$  for those samples. In this case, the estimated value will be mean(2, 2.2, 0.7) = 1.6(3).

(c) Note that, here, we're working with a weighted-distance kNN, which means that we're assigning different weights to each sample based on its distance from the sample we're trying to estimate - a closer neighbor will have a bigger impact on the final estimate than a further neighbor. Note, also, that we're now working with the Manhattan distance, which is defined as the sum of the absolute differences between the features of the two samples:

$$d(x_i, x_j) = \sum_{l=1}^{p} |x_i^{(l)} - x_j^{(l)}|$$

Let's now compute the Manhattan distances between  $x_1$  and the other samples, picking the k closest neighbors (once again, in teal):

$$d(x_1, x_2) = |1 - 2| + |1 - 1| = 1$$

$$d(x_1, x_3) = 3$$
,  $d(x_1, x_4) = 4$ ,  $d(x_1, x_5) = 2$ ,  $d(x_1, x_6) = 1$ 

Now, the fun part begins: we have to correctly weigh each neighbor's label to estimate the label for  $x_1$ . We can do this by assigning a weight to each neighbor, based on its distance from  $x_1$ . The most common way to do this is by using the inverse of the distance. Regarding the weighted mode estimate of  $x_1$  for  $x_2$ :

$$\hat{z}_1 =$$
**weighted\_mode** $(1/1B, (1/1 + 1/2)A) = A$ 

The mean, of course, will take into account for the denominator the weights of each neighbor, instead of the amount of neighbors:

$$\hat{z}_2$$
 = weighted\_mean =  $\frac{1/1 \cdot 0.5 + 1/2 \cdot 0.7 + 1/1 \cdot 1.2}{1/1 + 1/2 + 1/1} = 0.82$ 

2. Consider the following training data set:

|                       | <i>y</i> <sub>1</sub> | <i>y</i> <sub>2</sub> | Z   |
|-----------------------|-----------------------|-----------------------|-----|
| $x_1$                 | 1                     | 1                     | 1.4 |
| $x_2$                 | 2                     | 1                     | 0.5 |
| $x_3$                 | 1                     | 3                     | 2   |
| <i>x</i> <sub>4</sub> | 3                     | 3                     | 2.5 |

- (a) Find the closed form solution for a linear regression, minimizing the sum of squared errors.
- (b) Predict the target value for the query vector  $x_{new} = \begin{bmatrix} 2 & 3 \end{bmatrix}^T$ .
- (c) Sketch the predicted three-dimensional hyperplane.
- (d) Compute both the MSE and MAE produced by the linear regression.
- (e) Are there biases on the residuals against any of the input variables?
- (f) Compute the closed form solution, considering Ridge regularization term with  $\lambda = 0.2$ .
- (g) Compare the hyperplanes obtained utilizing ordinary least squares and ridge regression.
- (h) Why is the Lasso regression usually preferred over Ridge regression for data spaces with a larger number of features?

In linear regression, we're trying to learn a linear function that maps the input features to the target variable. In other words, we're trying to find a function f such that:

$$f(x) = \sum_{i=1}^{p} w_i x_i + b$$

Here, the **bias**, b, is commonly written as  $w_0$ , and the **weights**,  $w_i$ , are the coefficients of the linear function - the bias is the intercept of the function, allowing us to effectively shift the function up or down.

Note that we always want to make the best predictions possible, of course: for that purpose, we'll want our function f to be as close as possible to the actual target values. In other words, we want to minimize the error between the predicted values and the actual values. The most common way to do this is by minimizing the sum of squared errors (SSE) - that, as we have noted in other sheets, essentially encapsulates the MLE method - which is defined as:

$$SSE = (XW - Z)^{T}(XW - Z) = (\hat{Z} - Z)^{T}(\hat{Z} - Z)$$

Considering that we're trying to minimize the error, we can take the derivative of the SSE with respect to the weights and set it to zero:

$$\frac{\partial SSE}{\partial w_i} = 0 \leftrightarrow \frac{\partial}{\partial w_i} (\hat{Z} - Z)^T (\hat{Z} - Z) = 0$$

After performing some maniacal algebra, we can find the closed form solution for the weights:

$$W = (X^T X)^{-1} X^T Z$$

(a) We've derived the closed form solution for the weights, above, so most of our work is done here. Considering the training data set, we can say that X and Z are the following matrices (note that X's first column is all ones, letting the neutral element for the bias,  $w_0$ , shift the function up or down):

$$X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 3 \\ 1 & 3 & 3 \end{bmatrix}, \quad Z = \begin{bmatrix} 1.4 \\ 0.5 \\ 2 \\ 2.5 \end{bmatrix}$$

After plugging these matrices into the closed form solution, we gather the following weight vector (numpy calculations in the notebook):

$$W = \begin{bmatrix} 0.275 \\ 0.02 \\ 0.645 \end{bmatrix}$$

(b) As we have mentioned in the motivation for this exercise, the predictions,  $f(x) = \hat{z}$ , are given by the following equation:

$$\hat{z} = \sum_{i=1}^{p} w_i x_i + w_0$$

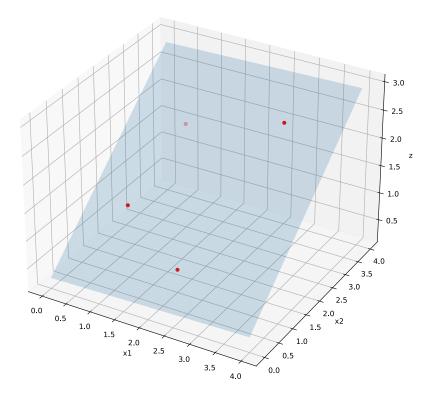
Plugging our values onto the afore-mentioned equation (note how  $x_0 = 1$  in order to allow for matrix multiplication), we get the following:

$$\hat{z} = W^T \cdot x_{new} = \begin{bmatrix} 0.275 \\ 0.02 \\ 0.645 \end{bmatrix}^T \cdot \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = 2.25$$

(c) The three-dimensional hyperplane for the linear regression in question is the one defined by the following equation:

$$\hat{z} = \begin{bmatrix} 0.275 \\ 0.02 \\ 0.645 \end{bmatrix}^T \cdot x = 0.275 + 0.02x_1 + 0.645x_2$$

With the aid of Python's matplotlib library, we can plot the hyperplane in three dimensions, as shown in the figure below:



(d) We're asked to compute both the MSE (Mean Squared Error) and the MAE (Mean Absolute Error) produced by the linear regression in hands. They're defined as follows:

MSE = 
$$\frac{1}{n} \sum_{i=1}^{n} (\hat{z}_i - z_i)^2$$

MAE = 
$$\frac{1}{n} \sum_{i=1}^{n} |\hat{z}_i - z_i|$$

We'll need, of course, to compute the estimates,  $\hat{z}$ , for each of the training set's original samples. We can do this by plugging the training set's input vectors into the linear regression's equation:

$$\hat{z} = \begin{bmatrix} 0.275 \\ 0.02 \\ 0.645 \end{bmatrix}^T \cdot x$$

The obtained estimates are the following:

$$\hat{z} = \begin{bmatrix} 0.94 \\ 0.96 \\ 2.23 \\ 2.27 \end{bmatrix}$$

With these estimates, we can compute the MSE and MAE:

$$\mathbf{MSE} = \frac{1}{4} \sum_{i=1}^{4} (\hat{z}_i - z_i)^2 = \frac{1}{4} \left( (0.94 - 1.4)^2 + \dots + (2.27 - 2.5)^2 \right) = 0.13225$$

$$\mathbf{MAE} = \frac{1}{4} \sum_{i=1}^{4} |\hat{z}_i - z_i| = \frac{1}{4} (|0.94 - 1.4| + \dots + |2.27 - 2.5|) = 0.345$$

(e) The residues are defined as the difference between the actual target values and the predicted values,  $\hat{z}$ . For our linear regression, considering the given training data, we have the following residues:

$$r_1 = 1.4 - 0.94 = 0.46$$
,  $r_2 = 0.5 - 0.96 = -0.46$ ,  $r_3 = 2 - 2.23 = -0.23$ ,  $r_4 = 2.5 - 2.27 = 0.23$ 

Plotting the residues against each feature doesn't show a particular skew in the data against any particular feature, hence we can't say that any of the features is more important than the others (and, as such, we can't say that there's any underlying bias).

(f) The Ridge regularization technique aims to **tune** a linear regression model, by adding a penalty term to the SSE. This penalty, usually denoted by  $\lambda$ , changes the closed form solution for the weights, W, to the following:

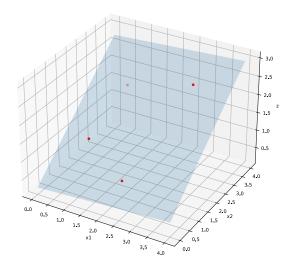
$$W = (X^T X + \lambda I)^{-1} X^T Z$$

where I is the identity matrix. The regularization term,  $\lambda$ , is a hyperparameter that controls the amount of regularization applied to the model, in order to avoid overfitting. The larger the value of  $\lambda$ , the more the regression will shift from its original solution.

With  $\lambda = 0.2$ , as given by the question's statement, we can compute the new weights, W, as follows:

$$W = (X^T X + 0.2I)^{-1} X^T Z = \begin{bmatrix} 0.238123 \\ 0.0522205 \\ 0.629293 \end{bmatrix}$$

(g) The Ridge regression's hyperplane is the one shown in the figure below:



The norm of the vector describing the model's hyperplane is, as expected, smaller than the one obtained in the previous question. This is due to the regularization term, which aims precisely to reduce the model's weights' magnitude.

- (h) LASSO, or Least Absolute Shrinkage and Selection Operator, is another regularization technique that aims to tune a linear regression model. It differs from Ridge regression in that it adds a penalty term to the SSE, but this term is the sum of the absolute values of the weights, instead of the sum of their squares. With LASSO, the coefficients are shrunk towards zero, which means that some of them will be reduced to zero, effectively removing them from the model this is a so-called **feature selection**, since it'll happen to the least relevant features of the model. Ridge regression, on the other hand, will only reduce the weights' magnitude, but will never set them to zero. This way, LASSO is more likely to produce a sparse (and better) model, with fewer features, than Ridge regression, regarding data sets with a large number of features.
  - 3. Considering the following training data, with z as an ordinal variable:

|                  | <i>y</i> <sub>1</sub> | y <sub>2</sub> | z |
|------------------|-----------------------|----------------|---|
| $\overline{x_1}$ | 1                     | 1              | 1 |
| $x_2$            | 2                     | 1              | 1 |
| $x_3$            | 1                     | 3              | 0 |
| $x_4$            | 3                     | 3              | 0 |

- (a) Find a linear regression using the closed form solution.
- (b) Assuming an output threshold  $\theta = 0.5$ , provide the predicted class for  $x_{new} = \begin{bmatrix} 2 & 2.5 \end{bmatrix}^T$ .
- (a) We already know that the closed form solution of a linear regression is given by:

$$W = (X^T X)^{-1} X^T Z$$

Looking at the data set, we can already write both *X* and *Z*:

$$X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 3 \\ 1 & 3 & 3 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

Plugging them into the closed form solution, we obtain:

$$W = (X^T X)^{-1} X^T Z = \begin{bmatrix} 1.5 \\ -2.22045e - 16 \\ -0.5 \end{bmatrix}$$

(b) Output thresholds are used to convert the output of a linear regression model into a class label - considering binary labels, the threshold  $\theta$  is used to determine whether the output is 0 or 1 (considering whether or not  $\hat{z}$  is greater than  $\theta$ ). In this case, we can compute the output of the model for the new sample,  $x_{new}$ , as follows:

$$\hat{z} = W^T \cdot x_{new} = \begin{bmatrix} 1.5 \\ -2.22045e - 16 \\ -0.5 \end{bmatrix}^T \cdot \begin{bmatrix} 1 \\ 2 \\ 2.5 \end{bmatrix} = 0.25$$

Since this estimation does not surpass the defined threshold,  $\theta = 0.5$ , the predicted class for  $x_{new}$  is 0.

4. Considering the data below to learn the following model, compare:

$$z = w_1 y_1 + w_2 y_2 + \epsilon, \epsilon \sim \mathcal{N}(0, 0.1)$$

$$\begin{array}{c|cccc} & y_1 & y_2 & z \\ \hline x_1 & 3 & -1 & 2 \\ x_2 & 4 & 2 & 1 \\ x_3 & 2 & 2 & 1 \end{array}$$

- (a)  $w = \begin{bmatrix} w_1 & w_2 \end{bmatrix}^T$ , using an MLE approach.
- (b) w using the Bayesian approach, assuming  $p(w) = N(w \mid \mu = [0, 0], \Sigma = \begin{bmatrix} 0.2 & 0 \\ 0 & 0.2 \end{bmatrix})$ .

As has been noted in the motivation for Linear Regression in this solution sheet, the default approach to learn a linear regression model is to use the Maximum Likelihood Estimation (MLE) approach. However, we might want to regularize the model, in order to avoid overfitting. This can be done by using a Bayesian approach, which will add a prior distribution to the model's weights, in order to penalize them (note that this is where the  $\lambda$  parameter in both Ridge and LASSO comes from). In this case, we'll use a Gaussian prior distribution, with mean  $\mu = [0,0]$  and covariance matrix  $\Sigma = \begin{bmatrix} 0.2 & 0 \\ 0 & 0.2 \end{bmatrix}$ .

As we know, in a Bayesian approach (and considering a MAP estimation), the posterior distribution is given by:

8

$$\begin{aligned} \operatorname{argmax}_{w} p(w \mid X, Z) &= \operatorname{argmax}_{w} p(X, Z \mid w) p(w) \\ &= \operatorname{argmax}_{w} \prod_{i=1}^{N} p(z_{i} \mid x_{i}, w) p(w) \\ &= \operatorname{argmax}_{w} \log p(w) + \sum_{i=1}^{N} \log p(z_{i} \mid x_{i}, w) * \\ &= \operatorname{argmax}_{w} \log \left( \frac{1}{(2\pi)^{D/2} \sqrt{\det \Sigma}} \right) \cdot \left( -\frac{1}{2} (w - \mu)^{T} \Sigma^{-1} (w - \mu) \right) + \sum_{i=1}^{N} \log p(z_{i} \mid x_{i}, w) \\ &= \cdots \\ &= \operatorname{argmin}_{w} (w - \mu)^{T} \Sigma^{-1} (w - \mu) + \sum_{i=1}^{N} \frac{1}{\tau^{2}} \cdot (z_{i} - w^{T} x_{i})^{2} * * \\ &= \operatorname{argmax}_{w} w^{T} \Sigma^{-1} w + \frac{1}{\tau^{2}} \cdot (Z - Xw)^{T} (Z - Xw) \end{aligned}$$

\* Note that the logarithm of a product is the sum of the logarithms of the factors.

\*\* We use  $\tau$  to denote the standard deviation of the noise,  $\epsilon$ .

After some more magical algebra, we'll be able to obtain the closed form solution for the weights, w, as follows:

$$w = (X^{T}X + \tau^{2}\Sigma^{-1})^{-1}X^{T}Z$$

 $\lambda$  is the parameter that controls the regularization strength:

$$\lambda = \frac{\tau^2}{\sigma^2}$$

(a) This is the standard MLE approach, where we don't consider any prior distribution for the weights and the usual closed form solution  $(W = (X^T X)^{-1} X^T Z)$ . We're given both X and Z, so we can compute the weights as follows:

$$X = \begin{bmatrix} 1 & 3 & -1 \\ 1 & 4 & 2 \\ 1 & 2 & 2 \end{bmatrix}, \quad Z = \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}, \quad W = (X^T X)^{-1} X^T Z = \begin{bmatrix} 1.66667 \\ 0 \\ -0.333333 \end{bmatrix}$$

(b) In this case, we have to solve the problem as stated in the (rather long) motivation above - utilizing  $W = (X^TX + \tau^2\Sigma^{-1})^{-1}X^TZ$ . Here, of course,  $\tau = 0.1$  and  $\Sigma = \begin{bmatrix} 0.2 & 0 \\ 0 & 0.2 \end{bmatrix}$ . We can compute the weights as follows:

$$X = \begin{bmatrix} 1 & 3 & -1 \\ 1 & 4 & 2 \\ 1 & 2 & 2 \end{bmatrix}, \quad Z = \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}, \quad W = (X^T X + \tau^2 \Sigma^{-1})^{-1} X^T Z = (X^T X + \frac{\tau^2}{\sigma^2})^{-1} X^T Z = \begin{bmatrix} 0.77865 \\ 0.25955 \\ -0.288854 \end{bmatrix}$$

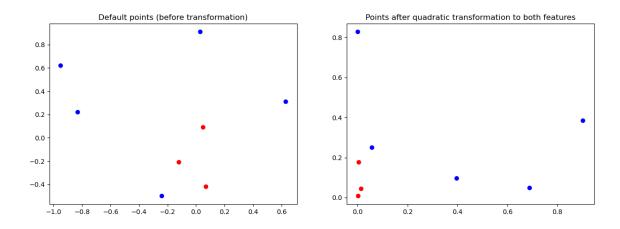
\*\*\* Note how  $\Sigma = 0.2^2 I$ , and as such  $\sigma = 0.2$ .

5. Identify a transformation to aid linearly modelling the data set below.

|                       | y <sub>1</sub> | y <sub>2</sub> | Z |
|-----------------------|----------------|----------------|---|
| $x_1$                 | -0.95          | 0.62           | 0 |
| $x_2$                 | 0.63           | 0.31           | 0 |
| $x_3$                 | -0.12          | -0.21          | 1 |
| $x_4$                 | -0.24          | -0.5           | 0 |
| <i>x</i> <sub>5</sub> | 0.07           | -0.42          | 1 |
| $x_6$                 | 0.03           | 0.91           | 0 |
| <i>x</i> <sub>7</sub> | 0.05           | 0.09           | 1 |
| $x_8$                 | -0.83          | 0.22           | 0 |

Sketch the predicted surface.

A good way to try to understand good transformations to apply to a data set is to plot the samples and try to find a pattern in the data. In this case, we can see that the labels seem to shift from 1 to 0 with the increase of the point's distance from the origin. This is a good indication that we should apply a quadratic transformation to the data, since it'll make the data more linearly separable.

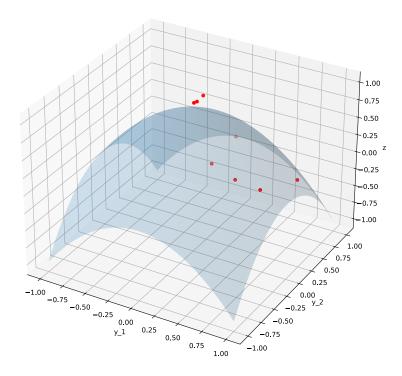


In order to sketch the predicted surface, we'll need to find the weight matrix associated with the regression; for that, instead of considering the inputs matrix, X, we're going to consider the transformed inputs matrix,  $\Phi$ :

$$\Phi(x) = \begin{bmatrix} 1 & x_1^{(1)} & x_1^{(2)} \\ \vdots & \vdots & \vdots \\ 1 & x_n^{(1)} & x_n^{(2)} \end{bmatrix}$$

$$\Phi = \begin{bmatrix} 1 & 0.9025 & 0.3844 \\ 1 & 0.3969 & 0.0961 \\ 1 & 0.0144 & 0.0441 \\ 1 & 0.0576 & 0.25 \\ 1 & 0.0049 & 0.1764 \\ 1 & 0.0009 & 0.8281 \\ 1 & 0.0025 & 0.0081 \\ 1 & 0.6889 & 0.0484 \end{bmatrix}, \quad W = (\Phi^T \Phi)^{-1} \Phi^T Z = \begin{bmatrix} 0.816775 \\ -0.864807 \\ -0.950784 \end{bmatrix}$$

As such, the regression's equation is given by  $0.816775 - 0.864807x_1^2 - 0.950784x_2^2$  - can't forget that the quadratic transformation to the data is not only felt in the weight parameters, but also in the input parameters!.



6. Consider both logarithmic and quadratic transformations for the data set below:

|                       | <i>y</i> <sub>1</sub> | Z    |
|-----------------------|-----------------------|------|
| $\overline{x_1}$      | 3                     | 1.5  |
| $x_2$                 | 4                     | 9.3  |
| <i>x</i> <sub>3</sub> | 6                     | 23.4 |
| $x_4$                 | 10                    | 45.8 |
| <i>x</i> <sub>5</sub> | 12                    | 60.1 |

7.

$$\phi_1(x_1) = \log(x_1), \quad \phi_2(x_2) = x_2^2$$

- (a) Plot both of the closed form regressions.
- (b) Which transformation minimizes the sum of squared errors on the original data?

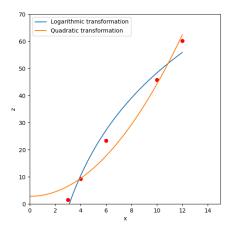
(a) As it was seen above, using  $\Phi$  transformations, we effectively go from utilizing the input matrix, X, directly, to using the transformed input matrix,  $\Phi$ . For starters, let's compute the transformed input matrices, for each transformation:

$$X = \begin{bmatrix} 3 \\ 4 \\ 6 \\ 10 \\ 12 \end{bmatrix}, \quad \Phi_1 = \begin{bmatrix} 1 & 1.09861 \\ 1 & 1.38629 \\ 1 & 1.79176 \\ 1 & 2.30259 \\ 1 & 2.48491 \end{bmatrix}, \quad \Phi_2 = \begin{bmatrix} 1 & 9 \\ 1 & 16 \\ 1 & 36 \\ 1 & 100 \\ 1 & 144 \end{bmatrix}$$

We'll have, then, two weight matrices,  $W_1$  and  $W_2$ , associated with each transformation (and, as such, two different linear regressions):

$$W_1 = (\Phi_1^T \Phi_1)^{-1} \Phi_1^T Z = \begin{bmatrix} -47.0212 \\ 41.3945 \end{bmatrix}, \quad W_2 = (\Phi_2^T \Phi_2)^{-1} \Phi_2^T Z = \begin{bmatrix} 2.78947 \\ 0.413615 \end{bmatrix}$$

$$\hat{z}_1 = -47.0212 + 41.3945 \log(x)$$
  $\hat{z}_2 = 2.78947 - 0.413615x^2$ 



(b) The sum of squared errors for each transformation is rather easy to compute:

$$\hat{z}_1 = -47.0212 + 41.3945 \log(x) = \begin{bmatrix} -1.54473 \\ 10.3637 \\ 27.1477 \\ 48.2931 \\ 55.8402 \end{bmatrix}, \quad \hat{z}_2 = 2.78947 - 0.413615x^2 = \begin{bmatrix} 6.51201 \\ 9.40731 \\ 17.6796 \\ 44.151 \\ 62.3501 \end{bmatrix}$$

$$SSE_1 = \sum_{i=1}^{n} (z_i - \hat{z}_1)^2 = (1.5 + 1.54473)^2 + \dots = 48.8088$$

$$SSE_2 = \sum_{i=1}^{n} (z_i - \hat{z}_2)^2 = (1.5 - 6.51201)^2 + \dots = 65.6365$$

We choose the model that minimizes the sum of squared errors, which is the first one, applying the logarithmic transformation.

- 8. Select the criteria promoting a smoother regression model:
- (a) Applying Ridge and Lasso regularizations to linear regression models.
- (b) Increasing the depth of a decision tree regressor.
- (c) Increasing the k parameter of a kNN regressor.
- (d) Parametrizing a kNN regressor with uniform weights, instead of the default distance-based weights.

In order to answer this question, we need to understand what *smoothing a regression model* means. In the context of linear regression, we can say that a model is smoother when the weights are smaller - it'll be easier to generalize the model to unseen data, avoiding overfitting to training data, and to discard noise. In that sense, both LASSO and Ridge regularizations are good candidates to smooth a linear regression model.

Regarding decision trees, smoother models are those with smaller depths - very deep trees tend to overfit the data, creating a model whose regression is very close to the training data (the regression will shift up and down according to the samples it sees in its path). As such, increasing the depth of a decision tree regressor will make the model less smooth.

As for kNN regressors, it's intuitive that, for both categoric and numeric variables, a larger k will make the model smoother - with more samples, the mean/mode picked will stabilize, making the model less sensitive to noise (and, in the limit case, picking always the same label, regardless of the input). As such, we have a smoother model with increasing levels of k.

Finally, regarding the weights of a kNN regressor, we can say that the default distance-based weights are smoother than the uniform weights. The distance-based weights are a function of the distance between the input and the samples in the training set, and, as such, they'll be smaller for samples that are farther away from the input. As such, the model will be smoother, as it'll be less sensitive to noise.