Bootcamp Machine Learning



Module07 Multivariate Linear Regression

Module07 - Multivariate Linear Regression

Building on what you did on the previous modules you will extend the linear regression to handle more than one features. Then you will see how to build polynomial models and how to detect overfitting.

Notions of the module

Multivariate linear hypothesis, multivariate linear gradient descent, polynomial models. Training and test sets, overfitting.

Useful Ressources

You are strongly advise to use the following resource: Machine Learning MOOC - Stanford Here are the sections of the MOOC that are relevant for today's exercises:

Week 2:

Multivariate Linear Regression:

- Multiple Features (Video + Reading)
- Gradient Descent for Multiple Variables (Video + Reading)
- Gradient Descent in Practice I- Feature Scaling (Video + Reading)
- Gradient Descent in Practice II- Learning Rate (Video + Reading)
- Features and Polynomial Regression (Video + Reading)
- Review (Reading + Quiz)

General rules

- The Python version to use is 3.7, you can check with the following command: python -V
- The norm: during this bootcamp you will follow the Pep8 standards
- The function eval is never allowed.
- The exercises are ordered from the easiest to the hardest.
- Your exercises are going to be evaluated by someone else, so make sure that your variable names and function names are appropriate and civil.
- Your manual is the internet.
- You can also ask questions in the #bootcamps channel in 42AI's Slack workspace.
- If you find any issues or mistakes in this document, please create an issue on our dedicated Github repository.

Helper

Ensure that you have the right Python version.

```
> which python
/goinfre/miniconda/bin/python
> python -V
Python 3.7.*
> which pip
/goinfre/miniconda/bin/pip
```

Exercise 00 - Linear Regression with Class

Exercise 01 - Ai Key Notions

Interlude - To the Multivariate Universe and Beyond!

Exercise 02 - Multivariate Hypothesis - Iterative Version

Interlude - Even More Linear Algebra Tricks!

Exercise 03 - Multivariate hypothesis - vectorized version

Interlude - Evaluate

Exercise 04 - Vectorized Cost Function

Interlude - Improve with the Gradient

Exercise 05 - Multivariate Linear Gradient

Interlude - Gradient Descent

Exercise 06 - Multivariate Gradient Descent

Exercise 07 - Multivariate Linear Regression with Class

Exercise 08 - Practicing Multivariate Linear Regression

Exercise 9 - Question Time!

Interlude - Introducing Polynomial Models

Exercise 10 - Polynomial models

Exercise 11 - Let's Train Polynomial Models!

Interlude - Plotting Curves With Matplotlib

Exercise 12 - Let's PLOT some Polynomial Models!

Interlude - Lost in Overfitting

Exercise 13 - DataSpliter

Exercise 14 - Machine Learning for Grown-ups: Training and Test Sets

Exercise 15 - Question Time!

Exercise 00 - Linear Regression with Class

Turn-in directory: ex00

Files to turn in: mylinearregression.py

Authorized modules: numpy, staticmethod decorator

Forbidden modules: sklearn

AI Classics:

These exercises are key assignments from the previous module. If you haven't completed them yet, you should finish them first before you continue with today's exercises.

Objective:

Write a class that contains all methods necessary to perform Linear Regression.

Instructions:

In this exercise, you will not learn anything new but don't worry, it's for your own good! You are expected to write your own MyLinearRegression class which looks similar to the sklearn.linear_model.LinearRegression class:

```
class MyLinearRegression():
    """
    Description:
        My personnal linear regression class to fit like a boss.
    """
    def __init__(self, thetas, alpha=0.001, max_iter=1000):
        self.alpha = alpha
        self.max_iter = max_iter
        self.thetas = thetas

#... other methods ...
```

You will add the following methods:

- fit_(self, x, y)
- predict_(self, x)
- cost_elem_(y, y_hat)
- cost_(y, y_hat).

You have already implemented these functions, you just need a few adjustments so that they all work well within your MyLinearRegression class.

```
import numpy as np
from mylinearregression import MyLinearRegression as MyLR
x = np.array([[12.4956442], [21.5007972], [31.5527382], [48.9145838], [57.5088733]])
y = np.array([[37.4013816], [36.1473236], [45.7655287], [46.6793434], [59.5585554]])
lr1 = MyLR([2, 0.7])
# Example 0.0:
```

```
lr1.predict(x)
array([[10.74695094],
         [17.05055804],
[24.08691674],
         [36.24020866],
[42.25621131]])
MyLR.cost_elem_(y, lr1.predict(x))
array([[710.45867381],
         [364.68645485],
[469.96221651],
[108.97553412],
         [299.37111101]])
MyLR.cost_(y, lr1.predict(x))
195.34539903032385
lr2 = MyLR([0, 0], alpha=5e-8, n_cycle = 1500000)
lr2.fit(x, y)
lr2.theta
array([[1.40709365],
         [1.1150909]])
lr2.predict(x)
array([[15.3408728],
         [25.38243697],
[36.59126492],
         [55.95130097],
[65.53471499]])
MyLR.cost_elem_(y, lr2.predict(x))
array([[486.66604863],
         [115.88278416],
[84.16711596],
[85.96919719],
         [ 35.71448348]])
MyLR.cost_(y, lr2.predict(x))
 80.83996294128525
```

Exercise 01 - AI Key Notions:

These questions highlight key notions from the previous modules. Making sure you can formulate a clear answer to each of them is necessary before you keep going. Discuss them with a fellow student if you can.

Are you able to clearly and simply explain:

- 1 What is a *hypothesis* and what is its goal? (It's a second chance for you to say something intelligible, no need to thank us!)
- 2 What is a cost function and what does it represent?
- 3 What is linear gradient descent and what does it do? (hint: you have to talk about J, its gradient, and θ)
- 4 What happens if you choose a *learning rate* that is too large?
- 5 What happens if you choose a very small learning rate, but still a sufficient number of cycles?
- 6 Can you explain MSE and what it measures?

Interlude - To the Multivariate Universe and Beyond!

Until now we've used a very simple hypothesis: $h_{\theta}(x) = \theta_0 + \theta_1 x$ With this very simple hypothesis we found a way to evaluate and improve our predictions.

That's all very neat, but we live in a world full of complex phenomena that a model using this hypothesis would fail miserably at predicting. If we take weather forecasting for example, how easy do you think it would be to predict tomorrow's temperature with just one variable (say, the current atmospheric pressure)? A model based on just one variable is too simple to account for the complexity of this phenomenon.

Now what if, on top of the atmospheric pressure, we could take into account the current temperature, humidity, wind, sunlight, and any useful information we can get our hands on?

We'd need a model where more than one variable (or even thousands of variables) are involved. That's what we call a **multivariate model**. And that's today's topic!

Predict

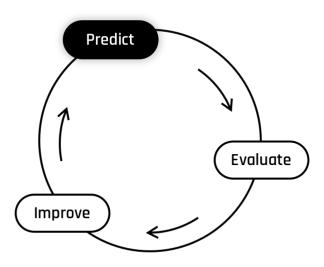


Figure 1: The Learning Cycle - Predict

Representing the examples as an $(m \times n)$ matrix

First we need to reconsider how we represent the training examples. Now that we want to characterize each training example with not just one, but many variables, we need more than a vector. We need a **matrix**!

So instead of an x vector of dimension $m \times 1$, we now have a matrix of dimension $m \times n$, where n is the number of **features** (or variables) that characterize each training example. We call it the **design matrix**, denoted by a capital X.

$$X = \begin{bmatrix} x_1^{(1)} & \dots & x_n^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(m)} & \dots & x_n^{(m)} \end{bmatrix}$$

Where:

- $x^{(i)}$ is the feature vector of the i^{th} training example, $(i^{th}$ row of the X matrix),
- x_i is the j^{th} column of the X matrix,
- $x_j^{(i)}$ is the j^{th} feature of the i^{th} training example (at the intersection of the i^{th} ,row and the j^{th} column of the X matrix). It's a real number.

The multivariate hypothesis

Then, we must update our hypothesis to take more than one feature into account.

$$\hat{y}^{(i)} = \theta_0 + \theta_1 x_1^{(i)} + \dots + \theta_n x_n^{(i)}$$
 for $i = 1, ..., m$

Where:

- $\hat{y}^{(i)}$ is the model's prediction for the i^{th} example,
- $x_1^{(i)}$ is the first feature of the i^{th} example,
- $x_n^{(i)}$ is the n^{th} feature of the i^{th} example,
- θ is a vector of dimension (n+1), the parameter vector.

You will notice that we end up with two indices: i and j. They should not be confused:

- i refers to one of the m examples in the dataset (line number in the X matrix),
- j refers to one of the n features that describe each example (column number in the X matrix).

Exercise 02 - Multivariate Hypothesis - Iterative Version

Turn-in directory: ex02/

Files to turn in: prediction.py

Forbidden functions: None

Remarks: n/a

Objective:

Manipulate the hypothesis to make prediction. You must implement the following formula as a function:

$$\hat{y}^{(i)} = \theta_0 + \theta_1 x_1^{(i)} + \dots + \theta_n x_n^{(i)}$$
 for $i = 1, ..., m$

Where:

- \hat{y} is a vector of dimension m: the vector of predicted values,
- $\hat{y}^{(i)}$ is the i^{th} component of the \hat{y} vector: the predicted value for the i^{th} example,
- θ is a vector of dimension (n+1): the parameter vector,
- θ_i is the j^{th} component of the parameter vector,
- X is a matrix of dimensions $m \times n$: the design matrix,
- $x^{(i)}$ is the i^{th} row of the X matrix: the feature vector of the i^{th} example,
- x_i is the j^{th} column of the X matrix,
- $x_j^{(i)}$ is the element at the intersection of the i^{th} row and the j^{th} column of the X matrix: the j^{th} feature of the i^{th} example.

Instructions:

In the prediction.py file, create the following function as per the instructions given below:

```
def simple_predict(x, theta):
    """Computes the prediction vector y_hat from two non-empty numpy.ndarray.
    Args:
        x: has to be an numpy.ndarray, a matrix of dimension m * n.
        theta: has to be an numpy.ndarray, a vector of dimension (n + 1) * 1.
    Returns:
        y_hat as a numpy.ndarray, a vector of dimension m * 1.
        None if x or theta are empty numpy.ndarray.
        None if x or theta dimensions are not matching.
        None if x or theta are not of the expected type objects.
    Raises:
        This function should not raise any Exception.
    """
        ... Your code ...
```

```
import numpy as np
x = np.arange(1,13).reshape((4,-1))
```

```
# Example 1:
theta1 = np.array([5, 0, 0, 0])
simple_predict(x, theta1)
# Ouput:
array([5., 5., 5., 5.])
# Do you understand why y_hat contains only 5's here?

# Example 2:
theta2 = np.array([0, 1, 0, 0])
simple_predict(x, theta2)
# Output:
array([1, 4., 7., 10.])
# Do you understand why y_hat == x[:,0] here?

# Example 3:
theta3 = np.array([-1.5, 0.6, 2.3, 1.98])
simple_predict(X, theta3)
# Output:
array([ 9.64, 24.28, 38.92, 53.56])

# Example 4:
theta4 = np.array([-3, 1, 2, 3.5])
simple_predict(x, theta4)
# Output:
array([12.5, 32., 51.5, 71.])
```

Interlude - Even More Linear Algebra Tricks!

As you already did before with the univariate hypothesis, the multivariate hypothesis can be vectorized as well.

If you add a column of 1's as the first column of the X matrix, you get what we'll call the X' matrix. Then, you can calculate \hat{y} by multiplying X' and θ .

$$X' \cdot \theta = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_n^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(m)} & \dots & x_n^{(m)} \end{bmatrix} \cdot \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} = \begin{bmatrix} \theta_0 + \theta_1 x_1^{(1)} + \dots + \theta_n x_n^{(1)} \\ \vdots \\ \theta_0 + \theta_1 x_1^{(m)} + \dots + \theta_n x_n^{(m)} \end{bmatrix} = \begin{bmatrix} \hat{y}^{(1)} \\ \vdots \\ \hat{y}^{(m)} \end{bmatrix} = \hat{y}$$

Another way of understanding this algebra trick is to pretend that each training example has an artificial x_0 feature that is always equal to 1. This simplifies the equations because now, each x_j feature has its corresponding θ_j parameter in the multiplication.

$$\theta_0 x_0^{(i)} + \theta_1 x_1^{(i)} + \dots + \theta_n x_n^{(i)} = \theta \cdot x'^{(i)}$$

Exercise 03 - Multivariate hypothesis - vectorized version

Turn-in directory: ex03/

Files to turn in: prediction.py

Forbidden functions: None

Remarks: n/a

Objective:

You must implement the following formula as a function:

$$\hat{y} = X' \cdot \theta = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_n^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(m)} & \dots & x_n^{(m)} \end{bmatrix} \cdot \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} = \begin{bmatrix} \theta_0 + \theta_1 x_1^{(1)} + \dots + \theta_n x_n^{(1)} \\ \vdots \\ \theta_0 + \theta_1 x_1^{(m)} + \dots + \theta_n x_n^{(m)} \end{bmatrix}$$

Where:

- \hat{y} is a vector of dimension m: the vector of predicted values,
- X is a matrix of dimensions $m \times n$: the design matrix,
- X' is a matrix of dimensions $m \times (n+1)$: the design matrix onto which a column of 1's was added as a first column,
- θ is a vector of dimension (n+1),: the parameter vector,
- $x^{(i)}$ is the i^{th} row of the X matrix,
- x_j is the j^{th} column of the X matrix,
- $x_j^{(i)}$ is the intersection of the i^{th} row and the j^{th} column of the X matrix: the j^{th} feature of the i^{th} training example.

Be careful:

- The x argument your function will receive as an input corresponds to X, the $m \times n$ matrix. Not X'.
- theta is an (n+1) dimension vector.
- You have to transform x to fit theta's dimension!

Instructions:

In the prediction.py file, write the predict_ function as per the instructions given below:

```
def predict_(x, theta):
    """Computes the prediction vector y_hat from two non-empty numpy.ndarray.
    Args:
        x: has to be an numpy.ndarray, a vector of dimension m * n.
        theta: has to be an numpy.ndarray, a vector of dimension (n + 1) * 1.
    Returns:
        y_hat as a numpy.ndarray, a vector of dimension m * 1.
        None if x or theta are empty numpy.ndarray.
        None if x or theta dimensions are not matching.
        None if x or theta are not of the expected type objects.
        Raises:
        This function should not raise any Exception.
```

```
... Your code ...
```

```
import numpy as np
x = np.arange(1,13).reshape((4,-1))

# Example 1:
theta1 = np.array([5, 0, 0, 0])
predict_(x, theta1)
# Ouput:
array([5., 5., 5., 5.])
# Do you understand why y_hat contains only 5's here?

# Example 2:
theta2 = np.array([0, 1, 0, 0])
predict_(x, theta2)
# Output:
array([ 1.,  4.,  7., 10.])
# Do you understand why y_hat == x[:,0] here?

# Example 3:
theta3 = np.array([-1.5, 0.6, 2.3, 1.98])
predict_(X, theta3)
# Output:
array([ 9.64, 24.28, 38.92, 53.56])

# Example 4:
theta4 = np.array([-3, 1, 2, 3.5])
predict_(x, theta4)
# Output:
array([ 12.5, 32., 51.5, 71. ])
```

Interlude - Evaluate

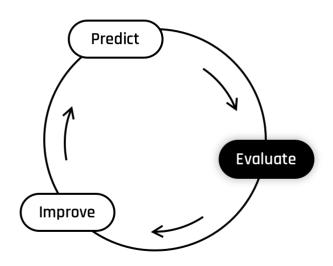


Figure 2: The Learning Cycle - Evaluate

Back to the Cost Function

How is our model doing?

To evaluate our model, remember before we used a **metric** called the **cost function** (also known as **loss function**). The cost function is basically just a measure of how wrong the model is, in all of its predictions.

Two modules ago, we defined the cost function as the average of the squared distances between each prediction and its expected value (distances represented by the dotted lines in the figure below) :

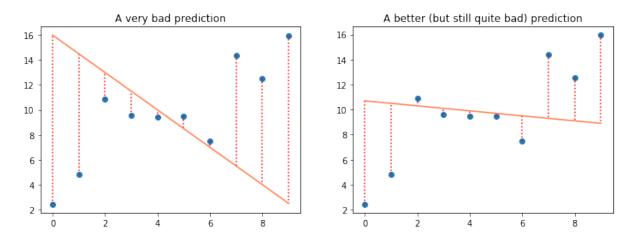


Figure 3: Distances between predicted and expected values

The formula was the following:

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (\hat{y}^{(i)} - y^{(i)})^2$$

And its vectorized form:

$$J(\theta) = \frac{1}{2m}(\hat{y} - y) \cdot (\hat{y} - y)$$

So, now that we moved to multivariate linear regression, what needs to change? You may have noticed that variables such as x_j and θ_j don't intervened in the equation. Indeed, the cost function only uses the predictions (\hat{y}) and the expected values (y), so the inner workings of the model don't matter to its evaluation metric.

This means we can use the exact same cost function as we did before!

Exercise 04 - Vectorized Cost Function

Turn-in directory: ex04/ Files to turn in: cost.py Forbidden functions: None Remarks: n/a

Objective:

Understand and manipulate cost function for multivariate linear regression. You must implement the following formula as a function:

$$J(\theta) = \frac{1}{2m}(\hat{y} - y) \cdot (\hat{y} - y)$$

Where:

- \hat{y} is a vector of dimension m, the vector of predicted values,
- y is a vector of dimension m, the vector of expected values.

Instructions:

In the cost.py file, create the following function as per the instructions given below:

```
def cost_(y, y_hat):
    """Computes the mean squared error of two non-empty numpy.ndarray, without any for loop.
    The two arrays must have the same dimensions.
Args:
    y: has to be an numpy.ndarray, a vector.
    y_hat: has to be an numpy.ndarray, a vector.
Returns:
    The mean squared error of the two vectors as a float.
    None if y or y_hat are empty numpy.ndarray.
    None if y and y_hat does not share the same dimensions.
    None if y or y_hat are not of the expected type objects.
Raises:
    This function should not raise any Exceptions.
"""
... Your code ...
```

```
import numpy as np
X = np.array([0, 15, -9, 7, 12, 3, -21])
Y = np.array([2, 14, -13, 5, 12, 4, -19])

# Example 1:
cost_(X, Y)
# Output:
2.142857142857143

# Example 2:
cost_(X, X)
# Output:
0.0
```

Interlude - Improve with the Gradient

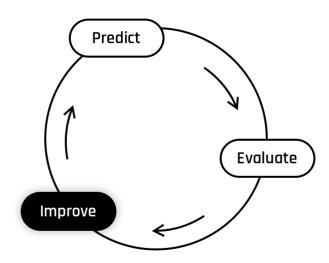


Figure 4: The Learning Cycle: Improve

Multivariate Gradient

From our multivariate linear hypothesis we can derive our multivariate gradient. It looks a lot like the one we saw yesterday, but instead of having just two components, the gradient now has as many as there are parameters. This means that now we need to calculate $\nabla(J)_0, \nabla(J)_1, \dots, \nabla(J)_n$

If we take the univariate equations we used yesterday and replace the formula for $\nabla(J)_1$ by a more general $\nabla(J)_j$, we get the following:

$$\nabla(J)_0 = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})$$

$$\nabla(J)_j = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} \quad \text{for j = 1, ..., n}$$

Where:

- $\nabla(J)$ is a vector of dimension (n+1), the gradient vector,
- $\nabla(J)_j$ is the j^{th} component of $\nabla(J)$, the partial derivative of J with respect to θ_j ,
- y is a vector of dimension m, the vector of expected values,
- $y^{(i)}$ is a scalar, the i^{th} component of vector y,
- $x^{(i)}$ is the feature vector of the i^{th} example,
- $x_i^{(i)}$ is a scalar, the j^{th} feature value of the i^{th} example,
- $h_{\theta}(x^{(i)})$ is a scalar, the model's estimation of $y^{(i)}$. (It can also be denoted $\hat{y}^{(i)}$).

Vectorized Form

As usual, we can use some linear algebra magic to get a more compact (and computationally efficient) formula.

First we can use our convention that each training example has an extra $x_0 = 1$ feature, and replace the gradient formulas above by one single equation that is valid for all j components:

$$\nabla(J)_j = \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$
 for $j = 0, ..., n$

And this generic equation can then be rewritten in a vectorized form:

$$\nabla(J) = \frac{1}{m} X^{\prime T} (X^{\prime} \theta - y)$$

Where:

- $\nabla(J)$ is the gradient vector of dimension (n+1),
- X' is a matrix of dimensions $m \times (n+1)$, the design matrix onto which a column of 1's was added as the first column,
- X'^T means the matrix has been transposed,
- θ is a vector of dimension (n+1), the parameter vector,
- y is a vector of dimension m, the vector of expected values.

The vectorized equation can output the entire gradient vector all at once, in one calculation! So if you understand the linear algebra operations, you can forget about the equations we presented at the top of the page and simply use the vectorized one.

Exercise 05 - Multivariate Linear Gradient

 $\begin{array}{ccc} \text{Turn-in directory}: & \text{ex}05/\\ \text{Files to turn in}: & \text{gradient.py} \\ \text{Forbidden functions}: & \text{None} \\ & \text{Remarks}: & \text{n/a} \\ \end{array}$

Objective:

Understand and manipulate the concept of gradient in the case of multivariate formulation. You must implement the following formula as a function:

$$\nabla(J) = \frac{1}{m} X'^{T} (X'\theta - y)$$

Where:

- $\nabla(J)$ is a vector of dimension (n+1), the gradient vector,
- X is a matrix of dimensions $m \times n$, the design matrix,
- X' is a matrix of dimensions $m \times (n+1)$, the design matrix onto which a column of 1's was added as a first column,
- θ is a vector of dimension (n+1), the parameter vector,
- y is a vector of dimension m, the vector of expected values.

Instructions:

In the gradient.py file, create the following function as per the instructions given below:

```
def gradient(x, y, theta):
    """Computes a gradient vector from three non-empty numpy.ndarray, without any for-loop.
    The three arrays must have the compatible dimensions.
Args:
    x: has to be an numpy.ndarray, a matrix of dimension m * n.
    y: has to be an numpy.ndarray, a vector of dimension m * 1.
    theta: has to be an numpy.ndarray, a vector (n + 1) * 1.
Returns:
    The gradient as a numpy.ndarray, a vector of dimensions n * 1, containg the result of
    the formula for all j.
    None if x, y, or theta are empty numpy.ndarray.
    None if x, y and theta do not have compatible dimensions.
    None if x or y or theta are not of the expected type objects.
Raises:
    This function should not raise any Exception.
"""
    ... Your code ...
```

```
[ 13, -2, 14],
        [ -7, 14, -1],
        [ -8, -4, 6],
        [ -5, -9, 6],
        [ 1, -5, 11],
        [ 9, -11, 8]])
y = np.array([2, 14, -13, 5, 12, 4, -19])
theta1 = np.array([3,0.5,-6])

# Example :
gradient(x, y, theta1)
# Output:
array([ -33.71428571, -37.35714286, 183.14285714, -393.])

# Example :
theta2 = np.array([0,0,0])
gradient(x, y, theta2)
# Output:
array([ -0.71428571,  0.85714286, 23.28571429, -26.42857143])
```

Interlude - Gradient Descent

Now comes the fun part: gradient descent!

The algorithm is not that different from the one used in univariate linear regression. As you might have guessed, what will change is that the j indice needs to run from 0 to n instead of 0 to 1. So all you need is a more generic algorithm, which can be expressed in pseudocode as the following:

repeat until convergence { compute $\nabla(J)$ $\theta_j \leftarrow \theta_j - \alpha \nabla(J)_j$

If you started to like vectorized forms, you might have noticed that that the θ_j notation is actually redundant here, since all components of θ need to be updated simultaneously. θ is a vector, $\nabla(J)$ also, they both have dimension (n+1). So all we need to do is this:

si

repeat until convergence {**compute** $\nabla(J)\theta \leftarrow \theta - \alpha\nabla(J)$ }

Where:

- θ is the entire parameter vector,
- α (alpha) is the learning rate (a small number, usually between 0 and 1),
- $\nabla(J)$ is the entire gradient vector.

Note: Do you still wonder why there is a subtraction in the equation?

By definition, the gradient indicates the direction towards which we should adjust the θ parameters if we wanted to *increase* the cost. But since our optimization objective is to *minimize* the cost, we move θ in the opposite direction of the gradient (hence the name *gradient descent*).

Exercise 06 - Multivariate Gradient Descent

Turn-in directory: ex06/ Files to turn in: fit.py Authorized modules: numpy

Forbidden functions : any function that performs derivatives for you

Objective:

Understand and manipulate the concept of gradient descent in the case of multivariatelinear regression. Implement a function to perform linear gradient descent (LGD) for multivariate linear regression.

Instructions:

In this exercise, you will implement linear gradient descent to fit your multivariate model to the dataset. The pseudocode of the algorithm is the following:

```
repeat until convergence {compute \nabla(J)\theta \leftarrow \theta - \alpha\nabla(J)}
```

Where:

- $\nabla(J)$ is the entire gradient vector,
- θ is the entire parameter vector,
- α (alpha) is the learning rate (a small number, usually between 0 and 1).

You are expected to write a function named fit_ as per the instructions bellow:

```
def fit_(x, y, theta, alpha, max_iter):
    """
    Description:
        Fits the model to the training dataset contained in x and y.
    Args:
            x: has to be a numpy.ndarray, a matrix of dimension m * n: (number of training
    examples, number of features).
        y: has to be a numpy.ndarray, a vector of dimension m * 1: (number of training
    examples, 1).
        theta: has to be a numpy.ndarray, a vector of dimension (n + 1) * 1: (number of
    features + 1, 1).
        alpha: has to be a float, the learning rate
        max_iter: has to be an int, the number of iterations done during the gradient
    descent
    Returns:
        new_theta: numpy.ndarray, a vector of dimension (number of features + 1, 1).
        None if there is a matching dimension problem.
        None if any of the parameter is not of the expected type object.
Raises:
        This function should not raise any Exception.
"""
        ... your code here ...
```

Hopefully, you have already implemented a function to calculate the multivariate gradient.

Examples:

```
import numpy as np
x = np.array([[0.2, 2., 20.], [0.4, 4., 40.], [0.6, 6., 60.], [0.8, 8., 80.]])
y = np.array([[19.6], [-2.8], [-25.2], [-47.6]])
theta = np.array([[42.], [1.], [1.]])

# Example 0:
theta2 = fit_(x, y, theta, alpha = 0.0005, max_iter=42000)
theta2
# Output:
array([[41.99..],[0.97..], [0.77..], [-1.20..]])

# Example 1:
predict_(x, theta2)
# Output:
array([[19.5992..], [-2.8003..], [-25.1999..], [-47.5996..]])
```

Remarks:

- You can create more training data by generating an x array with random values and computing the corresponding y vector as a linear expression of x. You can then fit a model on this artificial data and find out if it comes out with the same θ coefficients that first you used.
- It is possible that θ_0 and θ_1 become "[nan]". In that case, it means you probably used a learning rate that is too large.

Exercise 07 - Multivariate Linear Regression with Class

Turn-in directory: ex07/

Files to turn in: mylinearregression.py

Authorized modules: Numpy Forbidden modules: sklearn

Objective:

Upgrade your Linear Regression class so it can handle multivariate hypotheses.

Instructions:

You are expected to upgrade your own MyLinearRegression class from Module06. You will upgrade the following methods to support multivariate linear regression:

- predict_(self, x)
- fit_(self, x, y)

Depending on how you implement your methods, you might need to update other methods. ## Examples:

```
import numpy as np
from mylinearregression import MyLinearRegression as MyLR
X = np.array([[1., 1., 2., 3.], [5., 8., 13., 21.], [34., 55., 89., 144.]])
Y = np.array([[23.], [48.], [218.]])
mylr = MyLR([[1.], [1.], [1.], [1.], [1]])
mylr.predict_(X)
array([[8.], [48.], [323.]])
mylr.cost_elem_(X,Y)
array([[225], [0.], [11025]])
mylr.cost_(X,Y)
mylr.alpha = 1.6e-4
mylr.max_iter = 2000000
mylr.fit_(X, Y)
mylr.theta
array([[18.188..], [2.767..], [-0.374..], [1.392..], [0.017..]])
mylr.predict_(X)
array([[23.417..], [47.489..], [218.065...]])
```

```
# Example 5:
mylr.cost_elem_(X,Y)
# Output:
array([[0.174..], [0.260..], [0.004..]])

# Example 6:
mylr.cost_(X,Y)
# Output:
0.0732..
```

Exercise 08 - Practicing Multivariate Linear Regression

Turn-in directory: ex08/

Files to turn in: multivariate_linear_model.py

Authorized modules: numpy, matplotlib

Forbidden modules: sklearn

Remarks: Read the doc

Objective:

Fit a linear regression model to a dataset with multiple features. Plot the model's predictions and interpret the graphs.

Instructions:

Yesterday you performed a univariate linear regression on a dataset to make predictions based on ONE feature (well done!). Now, it's time to dream bigger. Lucky you are, we give you a new dataset with multiple features that you will find in the resources attached. The dataset is called <code>spacecraft_data.csv</code> and it describes a set of spacecrafts with their price, as well as a few other features. A description of the dataset is provided in the file named <code>spacecraft_data_description.txt</code>.

Part One: Univariate Linear Regression

To start, we'll build on yesterday's work and see how a univariate model can predict spaceship prices. As you know, univariate models can only process ONE feature at a time. So to train each model, you need to select a feature and ignore the other ones.

Instructions:

In the first part of the exercise, you will train three different univariate models to predict spaceship prices. Each model will use a different feature of the spaceships. For each feature, your program has to perform a gradient descent from a new set of thetas, plot or generate a graph, print the final value of the thetas and the MSE of the corresponding model.

Age

Select the Age feature as your x vector, and Sell_price as your y vector. Train a first model, myLR_age, and generate price predictions (\hat{y}) .

Produce a scatter plot with both sets of data points on the same graph, as follows:

- The actual prices, given by $(x_{age}^{(i)}, y^{(i)})$ for i = 0....m
- The predicted prices, represented by $(x_{age}^{(i)}, \hat{y}^{(i)})$ for i = 0...m (see example below),

Thrust

Select the Thrust_power feature as your x vector, and Sell_price as your y vector. Train a second model, myLR_thrust, and generate price predictions (\hat{y}) .

Produce a scatter plot with both sets of data points on the same graph, as follows:

- The actual prices, given by $(x_{thrust}^{(i)}, y^{(i)})$ for i = 0...m
- The predicted prices, represented by $(x_{thrust}^{(i)}, \hat{y}^{(i)})$ for i=0...m (see example below),

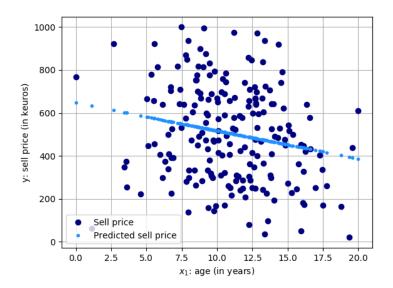


Figure 5: Plot of the selling prices of spacecrafts with respect to their age, as well as our first model's price predictions.

Total distance

Select the Terameters feature as your x vector, and Sell_price as your y vector. Train a third model, myLR_distance, and make price predictions (\hat{y}) .

Produce a scatter plot with both sets of data points on the same graph, as follows:

- The actual prices, given by $(x_{distance}^{(i)}, y^{(i)})$ for i = 0...m
- The predicted prices, represented by $(x_{distance}^{(i)}, \hat{y}^{(i)})$ for i = 0...m (see example below),

Reminder:

- After executing the fit_ method, you may obtain $\theta = \text{array}([[\mathtt{nan}, \mathtt{nan}]])$. If it happens, try reducing your learning rate.
- Be aware that you also need to set the appropriate number of cycles used in the fit_ function. If it's too low, you might not allowed enough cycles for the gradient descent to reach the optimal thetas values. Try to find a value that gets you the best score, but that doesn't make the training last forever.

Hint:

First, try plotting the data points (x_j, y) . Then you can guess initial theta values that are not too far off. This will help your algorithm converge more easily.

```
import pandas as pd
import numpy as np
form mylinearregression import MyLinearRegression as MyLR

data = pd.read_csv("spacecraft_data.csv")
X = np.array(data[['Age']])
Y = np.array(data[['Sell_price']])
myLR_age = MyLR([[1000.0], [-1.0]], alpha = 2.5e-5, max_iter = 100000)
myLR_age.fit_(X[:,0].reshape(-1,1), Y)

RMSE_age = myLR_age.mse_(X[:,0].reshape(-1,1),Y)
print(RMSE_age)
57636.77729...
```

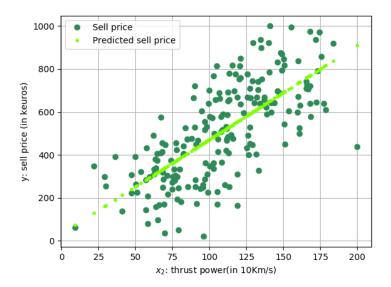


Figure 6: Plot of the selling prices of spacecrafts with respect to the thrust power of their engines, as well as our second model's price predictions.

How accurate is your model when you only take one feature into account?

Part Two: Multivariate Linear Regression (A New Hope)

Now, it's time for your first multivariate linear regression!

Instructions:

Here, you will train a single model that will take all features into account. Your program is expected to perform steps similar to the ones in the part one (fitting, displaying or generating 3 graphs, printing the thetas and the MSE).

Training the model

- Train a single multivariate linear regression model on all three features.
- Display and interpret the resulting theta parameters. What can you say about the role that each feature plays in the price prediction?
- Evaluate the model with the Mean Squared Error. How good is your model doing, compared to the other three that you trained in Part One of this exercise?

```
import pandas as pd
import numpy as np
from mylinearregression import MyLinearRegression as MyLR

data = pd.read_csv("spacecraft_data.csv")
X = np.array(data[['Age','Thrust_power','Terameters']])
Y = np.array(data[['Sell_price']])
my_lreg = MyLR([1.0, 1.0, 1.0, 1.0], alpha = 1e-4, max_iter = 600000)

my_lreg.mse_(X,Y)
# Output:
144044.877...
```

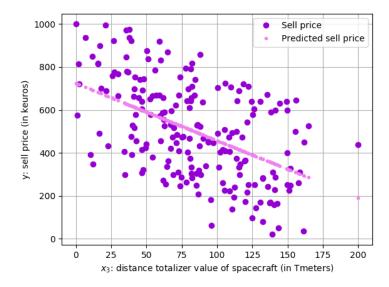


Figure 7: Plot of the selling prices of spacecrafts with respect to the terameters driven, as well as our third model's price predictions.

```
my_lreg.fit_(X,Y)
my_lreg.theta
# Output:
array([[334.994...],[-22.535...],[5.857...],[-2.586...]])

my_lreg.mse_(X,Y)
# Output:
586.896999...
```

Examples:

Plotting the predictions

Here we'll plot the model's predictions just like we did in Part One. We'll make three graphs, each one displaying the predictions and the actual prices as a function of ONE of the features.

- On the same graph, plot the actual and predicted prices on the y axis , and the Age feature on the x axis. (see figure below)
- On the same graph, plot the actual and predicted prices on the y axis, and the Thrust power feature on the x axis. (see figure below)
- On the same graph, plot the actual and predicted prices on the y axis, and the distance feature on the x axis. (see figure below)

Can you see any improvement on these three graphs, compared to the three that you obtained in Part One? Can you relate your observations to the MSE value that you just calculated?

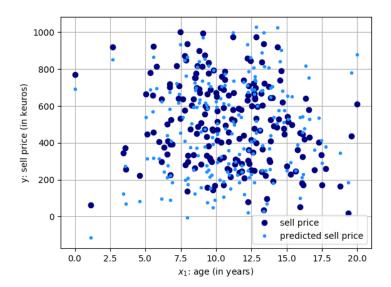


Figure 8: Spacecraft sell prices of and predicted sell prices with the multivariate hypothesis, with respect to the age feature

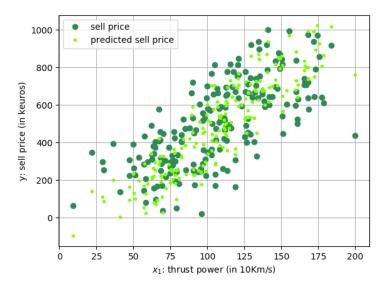


Figure 9: Spacecraft sell prices predicted sell prices with the multivariate hypothesis, with respect to the thrust power of the engines

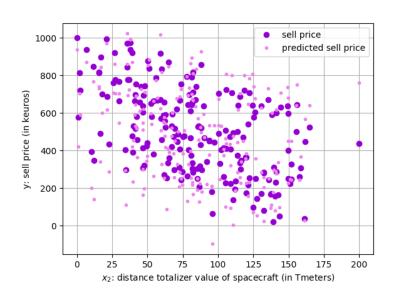


Figure 10: Spacecraft sell prices and predicted sell prices with the multivariage hypothesis, with respect to the driven distance (in terameters)

Exercise 9 - Question Time!

Are you able to clearly and simply explain:

- 1 What is the main difference between univariate and multivariate linear regression, in terms of variables?
- 2 Is there a minimum number of variables needed to perform a multivariate linear regression? If yes, which one?
- 3 Is there a maximum number of variables needed to perform a multivariate linear regression? If yes, which one?
- 4 Is there a difference between univariate and multivariate linear regression in terms of performance evaluation?
- 5 What does it mean geometrically to perform a multivariate gradient descent with two variables?

Interlude - Introducing Polynomial Models

You probably noticed that the method we use is called *linear regression* for a reason: the model generates all of its predictions on a straight line. However, we often encounter features that don't have a linear relationship with the predicted variable, like in the figure below:

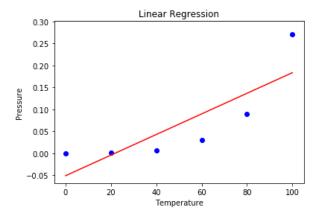


Figure 11: Non-linear relationship

In that case, we are stuck with a straight line that can't fit the data points properly. In this example, what if we could express y not as a function of x, but also of x^2 , and maybe even x^3 and x^4 ? We could make a hypothesis that draws a nice **curve** that would better fit the data. That's where polynomial features can help!

Polynomial features

First we get to do some feature engineering. We create new features by raising our initial x feature to the power of 2, and then 3, 4... as far as we want to go. For each new feature we need to create a new column in the dataset.

Polynomial Hypothesis

Now that we created our new features, we can combine them in a linear hypothesis that looks just the same as what we're used to:

$$\hat{y} = \theta_0 + \theta_1 x + \theta_2 x^2 + \dots + \theta_n x^n$$

It's a little strange because we are building a linear combination, not with different features but with different powers of the same feature. This is a first way of introducing non-linearity in a regression model!

Exercise 10 - Polynomial models

Turn-in directory: ex10/

Files to turn in: polynomial_model.py

Authorized modules : numpy Forbidden modules : sklearn

Objective:

Broaden the comprehension of the notion of hypothesis. Create a function that takes a vector x of dimension m and an integer n as input, and returns a matrix of dimensions $m \times n$.

Each column of the matrix contains x raised to the power of j, for j = 1, 2, ..., n:

$$x \mid x^2 \mid x^3 \mid \dots \mid x^n$$

Instructions:

In the polynomial_model.py file, create the following function as per the instructions given below:

```
def add_polynomial_features(x, power):
    """Add polynomial features to vector x by raising its values up to the power given in
        argument.
    Args:
        x: has to be an numpy.ndarray, a vector of shape m * 1.
        power: has to be an int, the power up to which the components of vector x are going to
        be raised.
        Returns:
            The matrix of polynomial features as a numpy.ndarray, of shape m * n, containg he
        polynomial feature values for all training examples.
            None if x is an empty numpy.ndarray.
        Raises:
            This function should not raise any Exception.
        """
            ... Your code ...
```

```
4,
5,
          16,
25,
                     64,
125,
                                 256, 1024, 4096],
625, 3125, 15625]])
```

Exercise 11 - Let's Train Polynomial Models!

Turn-in directory: ex11/

Files to turn in: polynomial_train.py

Authorized modules : numpy Forbidden modules : sklearn

Objective:

Manipulation of polynomial hypothesis.

It's training time! Let's train some polynomial models, and see if those with higher polynomial degree perform better!

Instructions:

Write a program which:

- Reads and loads are_blue_pills_magic.csv,
- Trains **six** separate linear regression models with polynomials hypothesis where their degree are ranging from 1 to 6,
- Evaluates and prints the evaluation score (MSE) of each of the six models,
- Plots a barplot showing the MSE score of the models in functions of the polynomial degree of the hypothesis,
- Plots the 6 models and the data points on the same figure. Used lineplot style for the models and scaterplot for the data points. Add more prediction points to have smooth curves for the models.

You will used Micrograms as feature and Score as target. The implementation of the method fit_based on the simple gradient descent lakes of efficiency and sturdiness, which will lead to the impossibility of converging for polynomial models with high degree or with features having several orders of magnitude of difference. See the starting values for some thetas below to help you to get acceptable parameters values for the models.

According to your evaluation scores only, what is the best hypothesis (or model) between the trained models? According to the last plot, why is is not true? Which phenomenom do you observed here?

Starting points:

You will not be able to get acceptable parameters for models 4, 5 and 6. Thus you can start the fit process for those models with:

```
theta4 = np.array([-20, 160, -80, 10, -1]).reshape(-1,1)
theta5 = np.array([1140, -1850, 1110, -305, 40, -2]).reshape(-1,1)
theta6 = np.array([9110, -18015, 13400, -4935, 966, -96.4, 3.86]).reshape(-1,1)
```

Teminology Note:

The **degree** of a polynomial expression is its highest exponent. E.g.: The polynomial degree of $5x^3 - x^6 + 2x^2$ is 6.

Here in this equation, you don't see any terms with x, x^4 and x^5 , but we can still say they exist. It's just that their coefficient is 0. This means that a polynomial linear regression model can lower the impact of any term by bringing its corresponding θ_i closer to 0.

Interlude - Plotting Curves With Matplotlib

You have been asked to plot straight lines in the module 05. Now you are working with polynomial models, the hypothesis functions are not straight lines, but curves.

Plotting curves is a bit more tricky, because if you do not have enough data point, you will get an ugly broken line instead of a smooth curve.

Here's a way to do it.

Let's begin with a simple dataset:

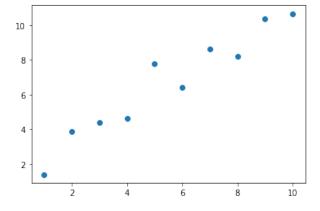


Figure 12: Scatter plot of a dataset

Now, we build a polynomial model of degree 3 and plot its hypothesis function $h(\theta)$.

```
from polynomial_model import add_polynomial_features
from mylinearregression import MyLinearRegression as MyLR

# Build the model:
x_ = add_polynomial_features(x, 3)
my_lr = MyLR(np.ones(4).reshape(-1,1)).fit_(x_, y)

# Plot:
## To get a smooth curve, we need a lot of data points
continuous_x = np.arange(1,10.01, 0.01).reshape(-1,1)
x_ = add_polynomial_features(continuous_x, 3)
y_hat = my_lr.predict_(continuous_x)
```

```
plt.scatter(x,y)
plt.plot(continuous_x, y_hat, color='orange')
plt.show()
```

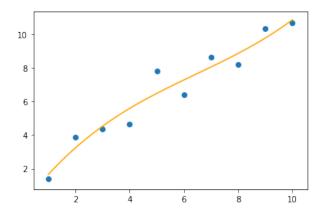


Figure 13: Scatter plot of a dataset, and on top, a plot of the polynomial hypothesis function

Exercise 12 - Let's Think about Polynomial Models!

 $\begin{array}{ccc} \text{Turn-in directory}: & \text{ex}12/\\ & \text{Files to turn in}: & \text{answer.txt} \\ \text{Authorized modules}: & \text{your brain} \\ & \text{Forbidden modules}: & \text{n/a} \\ \end{array}$

Objective:

It's reflection time!

Instructions:

Based on the plots you made in the previous exercise for each model you built, answer the following questions (in answers.txt):

- 1. From a purely intuitive point of view, which hypothesis (i.e. which polynomial degree) seems to **better** represent the relationship between y and x?
- 2. Go back to your answer for the previous exercise. What polynomial degree had you identified as the most accurate on the dataset? Is it the same one as the curve you just picked as the most representative of the relationship between y and x?
- 3. Find the plot that illustrates that same hypothesis you had found was the most accurate in the previous exercise. Take a closer look at the curve. What do you think? Does it seem to properly represent the relationship between y and x?

Interlude - Lost in Overfitting

The two previous exercises lead you, dear reader, to a very dangerous territory: the realm of **overfitting**. You did not see it coming but now, you are in a bad situation...

By increasing the polynomial degree of your model, you increased its complexity.

Is it wrong?

Not always.

Some models are indeed very complex because the relationships they represent are very complex as well.

But, if you look at the plots for the previous exercise's best model, you should feel that something is wrong.

Something is rotten in the state of our model...

Take a look at the following plot.

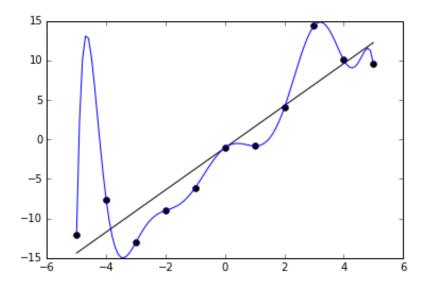


Figure 14: Overfitting hypothesis

You can see that the prediction line fits each data point perfectly, but completely misses out on capturing the relationship between x and y properly.

And now, if we add some brand new data points to the dataset, we see that the predictions on those new examples are way off.

This situation is called overfitting, because the model is doing an excessively good job at fitting the data. It is literally bending over backward to account for the data's minute details. But most the data's irregularities are just noise, and they should in fact be ignored. So because the model overfit, it can't generalize to new data.

The training set, the test set, and the happy data scientist

To be able to detect overfitting, you should always evaluate your model on new data.

New data means, data that your model hasn't seen during training. It's the only way to make sure your model isn't *cheating*. To do so, now and forever, you must always divide your dataset in (at least) two parts: one for the training, and one for the evaluation of your model.

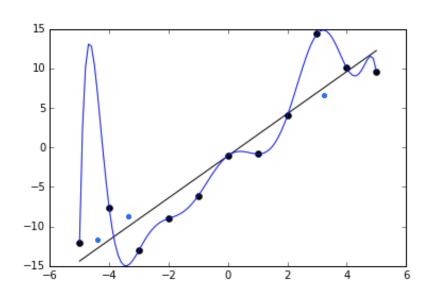


Figure 15: Generalization errors resulting from overfitting

Exercise 13 - DataSpliter

Turn-in directory: ex13/

Files to turn in: data_spliter.py

Authorized modules : Numpy Forbidden modules : sklearn

Objective:

Learn how to split a dataset into a **training set** and a **test set**.

Instructions:

You must implement a function that **shuffles** and **splits** a dataset it in two parts: a **training set** and a **test set**.

- Your function will shuffle and split the X matrix while keeping a certain **proportion** of the examples for training, and the rest for testing.
- Your function will also shuffle and split the y vector while making sure that the order of the rows in the output match the order of the rows in the split X output.

In the data_spliter.py file, you have to code the following function as per the instructions given below:

Be careful!

- The dataset has to be randomly shuffled *before* it is split into training and test sets.
- Unless you use the same seed in your randomization algorithm, you won't get the same results twice.

Examples:

The following examples are just an indication of possible outputs. As long as you have shuffled datasets with their corresponding y values, your function is working correctly.

```
import numpy as np
x1 = np.array([1, 42, 300, 10, 59])
y = np.array([0, 1, 0, 1, 0])

# Example 1:
data_spliter(x1, y, 0.8)
# Output:
```

```
(array([ 1, 59, 42, 300]), array([10]), array([0, 0, 1, 0]), array([1]))
data_spliter(x1, y, 0.5)
(array([59, 10]), array([ 1, 300, 42]), array([0, 1]), array([0, 0, 1]))
x2 = np.array([[ 1, 42],
                 [ 10, 42]])
y = np.array([0, 1, 0, 1, 0])
data_spliter(x2, y, 0.8)
(array([[ 10, 42],
 [500, 50],

[59, 1],

[300, 10]]),

array([[1, 42]]),

array([0, 1, 0, 1]),
 array([0]))
data_spliter(x2, y, 0.5)
(array([[59, 1],
         [10, 42]]),
 array([[300, 10],
         [ 1, 42]]),
 array([0, 0]),
 array([1, 1, 0]))
```

Exercise 14 - Machine Learning for Grown-ups: Trantor guacamole business

Turn-in directory: ex14/

Files to turn in: space_avocado.py benchmark_train.py models.csv

Ressources: space_avocado.csv

Authorized modules : numpy Forbidden modules : sklearn

Objective:

Let's do Machine Learning for "real"!

Introduction:

The dataset is constitued of 5 columns:

- index: not relevant.
- weight: the avocado weight order (in ton).
- prod_distance: distance from where the avocado ordered is produced (in Mkm).
- time_delivery: time between the order and the receipt (in days).
- target: price of the order (in space money). It contains the data of all the avocado purchase made by Trantor administration (guacamole is a serious business there).

Instructions:

You have to explore different models and select the best you find. To do this:

- Split your space_avocado.csv dataset into a training and a test set.
- Use your polynomial_features method on your training set.
- Consider several Linear Regression models with polynomial hypotheses with a maximum degree of 4.
- Evaluate your models on the test set.

According to your model evaluations, what is the best hypothesis you can get?

- Plot the evaluation curve which help you to select the best model (evaluation metrics vs models).
- Plot the true price and the predicted price obtain via your best model (3D representation or 3 scatterplots).

The training of all your models can take a long time. Thus you need to train only the best one. But, you should return in benchmark_train.py the program which perform the training of all the models and save the parameters of the different models into a CSV file. In models.csv one must find the parameters of all the models you have explored and trained. In space_avocado.py train the model based on the best hypothesis you find and load the other models from models.csv. Then evaluate and plot the different graphics as asked before.

Exercise 15 - Question Time!

Are you able to clearly and simply explain:

- 1 What is overfitting?
- 2 What do you think underfitting might be?
- 3 Why is it important to split the data set in a training and a test set?
- 4 If a model overfits, what will happen when you compare its performance on the training set and the test set?
- 5 If a model underfits, what do you think will happen when you compare its performance on the training set and the test set?