MAC0460 / MAC5832 (2020)

EP2: linear regression, analytic solution

Goals:

- to implement and test the analytic solution for the linear regression task (see, for instance, [Slides of Lecture 03 (http://work.caltech.edu/slides/slides03.pdf)](http://work.caltech.edu/slides/slides03.pdf) and Lecture 03 of *Learning from Data*)
- to understand the core idea (*optimization of a loss or cost function*) for parameter adjustment in machine learning

This notebook makes use of additional auxiliary functions in util/

Linear regression

Given a dataset $\{(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(N)}, y^{(N)})\}$ with $\mathbf{x}^{(i)} \in \mathbb{R}^d$ and $y^{(i)} \in \mathbb{R}$, we would like to approximate the unknown function $f : \mathbb{R}^d \to \mathbb{R}$ (recall that $y^{(i)} = f(\mathbf{x}^{(i)})$) by means of a linear model h:

$$h(\mathbf{x}^{(i)}; \mathbf{w}, b) = \mathbf{w}^\top \mathbf{x}^{(i)} + b$$

Note that $h(\mathbf{x}^{(i)}; \mathbf{w}, b)$ is, in fact, an [affine transformation (https://en.wikipedia.org/wiki/Affine_transformation)](https://en.wikipedia.org/wiki/Affine_transformation) of $\mathbf{x}^{(i)}$. As commonly done, we will use the term "linear" to refer to an affine transformation.

The output of h is a linear transformation of $\mathbf{x}^{(i)}$. We use the notation $h(\mathbf{x}^{(i)}; \mathbf{w}, b)$ to make clear that h is a parametric model, i.e., the transformation h is defined by the parameters $\mathbf{w}$ and b. We can view vector $\mathbf{w}$ as a *weight* vector that controls the effect of each *feature* in the prediction.

By adding one component with value equal to 1 to the observations $\mathbf{x}^{(i)}$ -- artificial coordinate -- we can simplify the notation:

$$h(\mathbf{x}^{(i)}; \mathbf{w}) = \hat{y}^{(i)} = \mathbf{w}^\top \mathbf{x}^{(i)}$$

We would like to determine the optimal parameters $\mathbf{w}$ such that prediction $\hat{y}^{(i)}$ is as closest as possible to $y^{(i)}$ according to some error metric. Adopting the *mean square error* as such metric we have the following cost function:

$$J(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} \left(\hat{y}^{(i)} - y^{(i)}\right)^2$$

Thus, the task of determining a function h that is closest to f is reduced to the task of finding the values $\mathbf{w}$ that minimizes $J(\mathbf{w})$.

Now we will explore this model, starting with a simple dataset.

Import auxiliary functions

In [0]:

```
# all imports
import numpy as np
import time

# changed to work on colab
from util import get_housing_prices_data, r_squared
from plots import plot_points_regression

%matplotlib inline
```

The dataset

The first dataset we will use is a toy dataset. We will generate $N = 100$ observations with only one *feature* and a real value associated to each of them. We can view these observations as being pairs *(area of a real state in square meters, price of the real state)*. Our task is to construct a model that is able to predict the price of a real state, given its area.

In [111]:

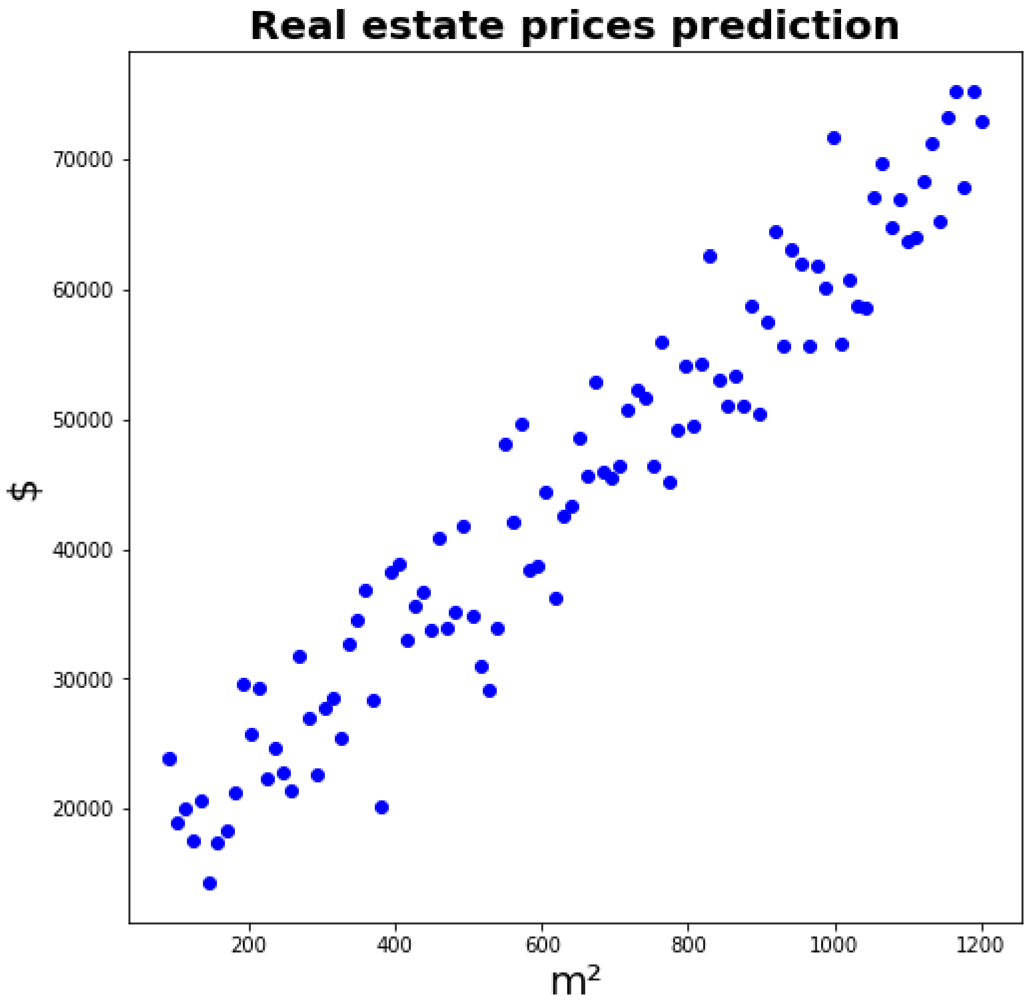
```
X, y = get_housing_prices_data(N=100)
```

```
X shape = (100, 1)

y shape = (100, 1)

X:
mean 645.0, sdt 323.65, max 1200.0, min 90.0

y:
mean 44699.359375, sdt 16302.68, max 75307.3671875, min 14315.726562
5
```

Ploting the data

In [112]:

```
plot_points_regression(X,
                       y,
                       title='Real estate prices prediction',
                       xlabel="m\u00b2",
                       ylabel='$')
```



The solution

Given $f : \mathbb{R}^{N\times d} \rightarrow \mathbb{R}$ and $\mathbf{A} \in \mathbb{R}^{N\times d}$, we define the gradient of f with respect to $\mathbf{A}$ as:

$$\nabla_{\mathbf{A}} f = \frac{\partial f}{\partial \mathbf{A}} = \begin{bmatrix} \frac{\partial f}{\partial \mathbf{A}_{1,1}} & \cdots & \frac{\partial f}{\partial \mathbf{A}_{1,m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial \mathbf{A}_{n,1}} & \cdots & \frac{\partial f}{\partial \mathbf{A}_{n,m}} \end{bmatrix}$$

Let $\mathbf{X} \in \mathbb{R}^{N\times d}$ be a matrix whose rows are the observations of the dataset (sometimes also called the *design matrix*) and let $\mathbf{y} \in \mathbb{R}^{N}$ be the vector consisting of all values of $y^{(i)}$ (i.e., $\mathbf{X}^{(i,:)} = \mathbf{x}^{(i)}$ and $\mathbf{y}^{(i)} = y^{(i)}$). It can be verified that:

$$J(\mathbf{w}) = \frac{1}{N}(\mathbf{X}\mathbf{w} - \mathbf{y})^T(\mathbf{X}\mathbf{w} - \mathbf{y})$$

Using basic matrix derivative concepts we can compute the gradient of $J(\mathbf{w})$ with respect to $\mathbf{w}$:

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \frac{2}{N}(\mathbf{X}^T\mathbf{X}\mathbf{w} - \mathbf{X}^T\mathbf{y})$$

Thus, when $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$ we have

$$\mathbf{X}^T\mathbf{X}\mathbf{w} = \mathbf{X}^T\mathbf{y}$$

Hence,

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Note that this solution has a high computational cost. As the number of variables (*features*) increases, the cost for matrix inversion becomes prohibitive. See [this text (http://cs229.stanford.edu/notes/cs229-notes1.pdf)](http://cs229.stanford.edu/notes/cs229-notes1.pdf) for more details.

Exercise 1

Using only **NumPy** (a quick introduction to this library can be found [here (http://cs231n.github.io/python-numpy-tutorial/)](http://cs231n.github.io/python-numpy-tutorial/)), complete the two functions below. Recall that $\mathbf{X} \in \mathbb{R}^{N\times d}$; thus you will need to add a component of value 1 to each of the observations in $\mathbf{X}$ before performing the computation described above.

NOTE: Although the dataset above has data of dimension $d = 1$, your code must be generic (it should work for $d \geq 1$)

In [0]:

```
def normal_equation_weights(X, y):
    """
    Calculates the weights of a linear function using the normal equation metho
d.
    You should add into X a new column with 1s.

    :param X: design matrix
    :type X: np.ndarray(shape=(N, d))
    :param y: regression targets
    :type y: np.ndarray(shape=(N, 1))
    :return: weight vector
    :rtype: np.ndarray(shape=(d+1, 1))
    """

    # START OF YOUR CODE:

    # X matrix with ones in the beggining of each observation
    X_add = np.hstack((np.ones((X.shape[0],1)), X))

    # Mutiplication of X and its transpose
    X_m = np.dot(X_add.T, X_add)

    # Inverse of multiplication
    X_mi = np.linalg.inv(X_m)

    # Result
    w = np.dot(np.dot(X_mi, X_add.T), y)

    # END YOUR CODE

    return w
```

In [114]:

```
# test of function normal_equation_weights()

w = 0  # this is not necessary
w = normal_equation_weights(X, y)
print("Estimated w = ", w)
```

```
Estimated w =  [[13346.65989702]
 [   48.60883972]]
```

In [0]:

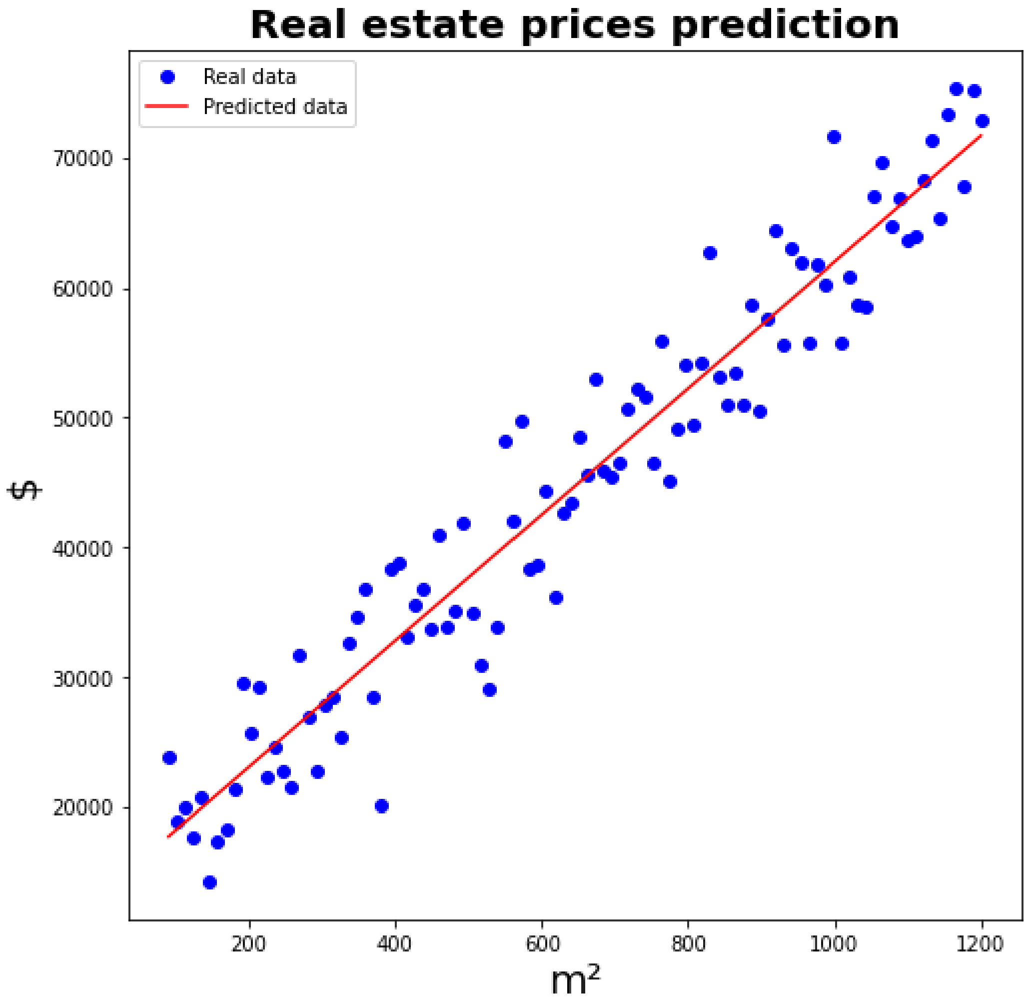
```
def normal_equation_prediction(X, w):
    """
    Calculates the prediction over a set of observations X using the linear func
tion
    characterized by the weight vector w.
    You should add into X a new column with 1s.

    :param X: design matrix
    :type X: np.ndarray(shape=(N, d))
    :param w: weight vector
    :type w: np.ndarray(shape=(d+1, 1))
    :param y: regression prediction
    :type y: np.ndarray(shape=(N, 1))
    """

    # START OF YOUR CODE:

    # X matrix with ones in the beggining of each observation
    X_add = np.hstack((np.ones((X.shape[0],1)), X))

    # Results with generated weights
    prediction = np.dot(X_add, w)

    # END YOUR CODE

    return prediction
```

You can use the R^2 (https://pt.wikipedia.org/wiki/R%C2%B2) metric to evaluate how well the linear model fits the data.

It is expected that R^2 is a value close to 0.5.

In [116]:

```
# test of function normal_equation_prediction()
prediction = normal_equation_prediction(X, w)
r_2 = r_squared(y, prediction)
plot_points_regression(X,
                       y,
                       title='Real estate prices prediction',
                       xlabel="m\u00b2",
                       ylabel='$',
                       prediction=prediction,
                       legend=True,
                       r_squared=r_2)
```



$R^2 = 0.5178$

Additional tests

Let us compute a prediction for $x = 650$

In [117]:

```
# Let us use the prediction function
x = np.asarray([650]).reshape(1,1)
prediction = normal_equation_prediction(x, w)
print("Area = %.2f  Predicted price = %.4f" %(x[0], prediction))

# another way of computing the same
y = np.dot(np.asarray((1,x)), w)
print("Area = %.2f  Predicted price = %.4f" %(x, y))
```

```
Area = 650.00  Predicted price = 44942.4057
Area = 650.00  Predicted price = 44942.4057
```

Exercise 2: Effect of the number of samples

Change the number of samples N and observe how processing time varies.

In [118]:

```
# Testing different values for N
X, y = get_housing_prices_data(N=1000000)
init = time.time()
w = normal_equation_weights(X, y)
prediction = normal_equation_prediction(X,w)
init = time.time() - init

print("Execution time = {:.8f}(s)".format(init))
```

```
X shape = (1000000, 1)

y shape = (1000000, 1)

X:
mean 645.0000610351562, sdt 320.43, max 1200.0, min 90.0

y:
mean 44249.4765625, sdt 16511.39, max 88606.1875, min 517.9199829101
562
Execution time = 0.03417253(s)
```

Executei este notebook na ferramenta Colab, da Google. Os tempos obtidos foram os seguintes:

- N = 100 -> Execution time = 0.00313520(s)
- N = 1000 -> Execution time = 0.00441623(s)
- N = 10000 -> Execution time = 0.00300860(s)
- N = 100000 -> Execution time = 0.00449181(s)
- N = 1000000 -> Execution time = 0.02990961(s)

Para N = 10000000 não consegui executar o algoritmo.

Exercise 2: Effect of the data dimension

Test your code for data with $d > 1$. You can create your own dataset (if you do so, you can share the code by posting it to the moodle's Forum -- only the code for the dataset generation!). If you have no idea on how to generate such dataset, you can use existing datasets such as the one in scikit-learn [https://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_boston.html#sklearn.datasets.load_boston (https://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_boston.html#sklearn.datasets.load_boston)](https://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_boston.html#sklearn.datasets.load_boston)

If you used an existing dataset or one generated by a colleague, please acknowledge the fact clearly. Thanks!

Dataset 1: boston house-prices

Para o meu primeiro teste com o caso multidimensional, usarei o dataset [aqui disponivel (https://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_boston.html#sklearn.datasets.load_boston)](https://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_boston.html#sklearn.datasets.load_boston). Tal D possui 13 dimensões e 506 observações.

In [119]:

```
# Testing with boston house-prices dataset
# The 1's in variables names are here due to scope reasons

from sklearn.datasets import load_boston
X1, y1 = load_boston(return_X_y=True)

# Weights vector
w1 = normal_equation_weights(X1, y1)
# Predictions
p1 = normal_equation_prediction(X1, w1)

# Calculating the mean square error
J1 = ((p1 - y1)**2).mean()

print("Mean square error: " + str(J1))

# Printing some samples
print("\nComparing some values")
for i in [0, 5, 54, 76, 96, 213, 278, 376, 399, 412, 490]:
    print("Actual | predicted y = {:.2f} | {:.2f}".format(y1[i], p1[i]))
```

```
Mean square error: 21.894831181729206

Comparing some values
Actual | predicted y = 24.00 | 30.00
Actual | predicted y = 28.70 | 25.26
Actual | predicted y = 18.90 | 15.36
Actual | predicted y = 20.00 | 22.95
Actual | predicted y = 21.40 | 24.73
Actual | predicted y = 28.10 | 25.22
Actual | predicted y = 29.10 | 30.35
Actual | predicted y = 13.90 | 17.74
Actual | predicted y = 6.30 | 10.89
Actual | predicted y = 17.90 | 1.72
Actual | predicted y = 8.10 | 3.66
```

Dataset 2: Diabetes

Esse segundo dataset possui 10 dimensões e 442 exemplos. Tal dados mostram a quantificação da evolução da doença 1 ano a partir das medições. A referencia pode ser consultada [aqui (https://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_diabetes.html#sklearn.datasets.load_diabetes)](https://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_diabetes.html#sklearn.datasets.load_diabetes).

In [120]:

```
# Testing with diabetes dataset
# The 2's in variables names are here due to scope reasons

from sklearn.datasets import load_diabetes
X2, y2 = load_diabetes(return_X_y=True)

# Weights vector
w2 = normal_equation_weights(X2, y2)
# Predictions
p2 = normal_equation_prediction(X2, w2)

# Calculating the mean square error
J2 = ((p2 - y2)**2).mean()

print("Mean square error: " + str(J2))

# Printing some samples
print("\nComparing some values")
for i in [0, 5, 54, 76, 96, 213, 278, 376, 399, 412, 440]:
    print("Actual | predicted y = {:.2f} | {:.2f}".format(y2[i], p2[i]))
```

```
Mean square error: 2859.6903987680657

Comparing some values
Actual | predicted y = 151.00 | 206.12
Actual | predicted y = 97.00 | 106.35
Actual | predicted y = 182.00 | 139.11
Actual | predicted y = 170.00 | 191.17
Actual | predicted y = 150.00 | 207.72
Actual | predicted y = 49.00 | 98.58
Actual | predicted y = 102.00 | 111.45
Actual | predicted y = 121.00 | 211.26
Actual | predicted y = 232.00 | 189.19
Actual | predicted y = 261.00 | 232.98
Actual | predicted y = 220.00 | 211.86
```

In [0]: