# 0_curve_fitting

October 22, 2020

## 1 Ajuste de curvas

[1]:
```
%pylab inline
import numpy as np
import matplotlib.pyplot as plt

from ipywidgets import interact, fixed, widgets
```

```
Populating the interactive namespace from numpy and matplotlib
```

El problema clásico de ajuste de curvas es dado un conjunto de puntos, encontrar la curva que **mejor** representa los datos. Donde **mejor** está sujeto a definición.

Para hacerlo más divertido, verémos el problema de ajuste de curvas como un problema de optimización y en particular como un método de aprendizaje de máquina *machine learning* supervisado.

Supongamos que tenemos un conjunto $m$ de datos de entrada $\mathbf{x}$ (en aprendizaje de máquina se les conoce como *features* ) y sus datos dependientes, $\mathbf{y}$ (*target* en aprendizaje de máquina). A este conjunto $(x^{(i)}, y^{(i)})$, le llamamos conjunto de entrenamiento. Queremos desarrollar un modelo $\hat{\mathbf{y}}$ que aproxime el valor de $\mathbf{y}$.

(Estamos asumiendo que y depende de x)

La primera aproximación es intentar una aproximación de forma lineal, conocida como *regresión lineal* , de la forma

$$\hat{\mathbf{y}} = \beta_0 + \beta_1 \mathbf{x}$$

(Es una recta)

Donde (si recuerdan Geometría Analítica) $\beta_0$ es el *interceptor* de la recta $\hat{\mathbf{y}}$ y $\beta_1$ es la *pendiente* de la recta. A $\hat{\mathbf{y}}$ se le conoce también como ***hipótesis*** y se le puede denotar con la variable $\mathbf{h}$. Si definimos que $x_0 \equiv 1$, podemos escribir la ***hipótesis*** de manera más compacta:

$$\hat{\mathbf{y}} = \sum_{j=0}^{n} \beta_j x_j = \beta^T \mathbf{x}$$

(Y es un plano en función de x.)

Con esta notación, podemos extender el formalismo a más dimensiones (en este caso $n$).

Vamos a tomar vectores verticales

Una posible definición de **mejor** es que el modelo (el cual está determinado por $\vec{\beta}$) minimice la suma de las diferencias entre el valor actual $\mathbf{y}$ y el predicho $\hat{\mathbf{y}}$ (a esta diferencia se le conoce como *error en la predicción* ), en otras palabras *minimizar* la suma del cuadrado de los *residuos*. La función a minimizar se conoce en aprendizaje de máquina como ***función de costo*** $\mathbf{J}$. Debido a que tenemos varios pares $(x_i, y_i)$, la función costo a minimizar es el *error cuadrático promedio*.

(Vamos a minimizar la suma de los errores al cuadrado)

$$\mathbf{J}(\beta_0, \beta_1) = \frac{1}{2n} \sum_{(x^{(i)}, y^{(i)}) \in X \times Y} (y^{(i)} - \hat{y}^{(i)}(x^{(i)}))^2 = \frac{1}{2n} \sum_{(x^{(i)}, y^{(i)}) \in X \times Y} (y^{(i)} - \beta_0 - \beta_1 x^{(i)})^2$$

El factor de 2 se agrega para simplificar cálculos posteriores. Visto así, el objetivo de un algoritmo supervisado de aprendizaje de máquina es encontrar $\beta_0$ y $\beta_1$ que minimiza la función de costo $\mathbf{J}(\beta_0, \beta_1)$. Esto se puede hacer mediante un algoritmo llamado ***gradient descent***.

## 1.1 Gradient descent

El gradiente de una función (hacia donde decrece la función, moverse en el sentido opuesto al gradiente) $g(x, y)$ es:

$$\nabla g(x, y) = \begin{bmatrix} \partial_x g \\ \partial_y g \end{bmatrix}$$

donde $\partial_x$, $\partial_y$ es la derivada parcial respecto a $x$ y $y$ respectivamente. el significado geométrico del gradiente de una función, es el vector que apunta en la dirección donde se maximiza el incremento de la función. Por lo tanto, si queremos minimizar la función, recorremos el vector en el sentido contrario.

### 1.1.1 Algoritmo

1. Escoger un punto al azar, llama a este punto $\boldsymbol{B}_0$.
2. Calcular el gradiente de $\mathbf{J}$ en esa locación.
3. Actualiza la locación en el sentido opuesto a donde apunte el gradiente, específicamente resta a $\boldsymbol{B}_0$ el valor de $\alpha \nabla \mathbf{J}$, donde $\alpha$ es un número pequeño, conocido como ***learning rate***.
4. Repite los pasos 2 y 3 cuantas veces sea necesario.

Estamos buscando las betas

En pseudocódigo:

Repetir hasta que lograr convergencia {

$$\beta_{j+1} := \beta_j - \alpha \frac{\partial}{\partial \beta_j} \mathbf{J}(\beta)$$

}

Se deja como ejercicio de tarea, demostrar que

$$\frac{\partial}{\partial \beta_j}\mathbf{J}(\beta) = \frac{1}{m}\sum_{i=1}^{m}\left(\hat{y}(x^{(i)}) - y(x^{(i)})\right) \cdot x_j^{(i)}$$

Entonces:

Repetir hasta que lograr convergencia {

$$\beta_{j+1} := \beta_j - \alpha\frac{1}{m}\sum_{i=1}^{m}\left(\hat{y}(x^{(i)}) - y(x^{(i)})\right) \cdot x_j^{(i)}$$

}

[4]:
```
class RegresionLineal:
    def __init__(self, alpha=0.3, max_iters=100, tols=0.001):
        """
        Parámetros.
        ---------------
        alpha = Learning rate
        max_iters = Número máximo de iteraciones
        tols = definición de convergencia, que tanto nos estamos acercando
        """
        self.alpha = alpha
        self.max_iters = max_iters
        self.tols = tols
        self.breaking_iteration = None
        self.historia = {'costo':[], 'beta':[]}  # Con fines de graficación

    def gradientDescent(self, x, y):
        """
        Parámetros:
        ---------------
        x = vector de entrenamiento de features
        y = vector de entrenamiento de variable a predecir (target)
        """

        # ajustamos el vector de features
        unos = np.ones((x.shape[0], 1))
        Xt = x.reshape(x.shape[0], 1)
        Xt = np.concatenate((unos, Xt), axis=1)

        i = 0
        prep_J = 0
        m, n = Xt.shape
        self.beta = np.zeros(n)

        while i < self.max_iters:
            # Actualizamos beta (con la formula de betaj)
```

```
            self.beta = self.beta - self.alpha * self.gradiente(Xt, y)

            J = self.costo(Xt, y)

            #En el if estamos checando la convergencia
            if abs(J - prep_J) <= self.tols:
                print('La función convergió con beta: %s en la iteración %i' %␣
↪( str(self.beta), i ))
                self.breaking_iteration = i
                break
            else:
                prep_J = J

            self.historia['costo'].append(J)
            self.historia['beta'].append(self.beta)
            i += 1

    def hipotesis(self, x):
        #Producto punto
        return np.dot(x, self.beta)

    def costo(self, x, y):
        #La diferencia
        m = x.shape[0]
        error = self.hipotesis(x) - y
        return np.dot(error.T, error) / (2 * m)

    def gradiente(self, x, y):
        m = x.shape[0]
        error = self.hipotesis(x) - y
        return np.dot(x.T, error) / m
```

[7]:
```
r = RegresionLineal(alpha=0.03, max_iters=10000, tols=0)
r.gradientDescent(X, Y)
#X,Y se definen mas abajo
```

```
La función convergió con beta: [0.75016248 0.06388118] en la iteración 5247
```

[8]:
```
objeto = RegresionLineal()
print(objeto.alpha)
print(objeto.max_iters)
print(objeto.tols)
```

```
0.3
100
0.001
```

### 1.1.2 Ejemplo

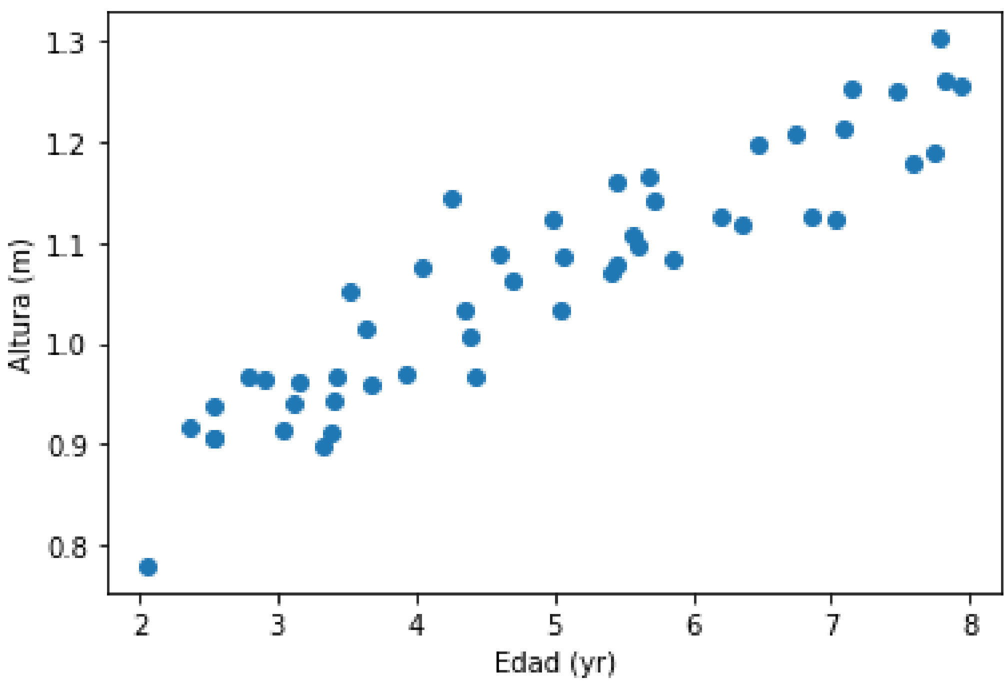
Los archivos **edad.dat** y **altura.dat** contienen las mediciones de las estaturas (en metros) de varios niños entre las edad de 2 y 8 años. Cada *tupla* de altura y edad, constituyen un ejemplo de entrenamiento $(x^{(i)}, y^{(i)})$ de nuestros datos. Hay $m = 50$ datos para entrenar que usaremos para realizar un modelo de regresión lineal.

[9]:
```
X = np.loadtxt('data/edad.dat')
Y = np.loadtxt('data/altura.dat')
```

Los datos se ven así:

[10]:
```
plt.scatter(X,Y, label="data")
plt.xlabel('Edad (yr)')
plt.ylabel('Altura (m)')
```

[10]:
```
Text(0, 0.5, 'Altura (m)')
```




**Ejercicio:** Usando el *widget* siguiente, trata de encontrar al "tanteo" cuál es la recta que mejor minimiza el error.

[11]:
```
def plotGuess(x, y, interceptor, pendiente):

    modelo = lambda x,b,m: b + m*x # función para graficar el modelo

    plt.scatter(X,Y, label="data")
```

```python
    plt.plot(X, modelo(X, interceptor, pendiente), label='Guess')
    plt.xlabel('Edad (yr)')
    plt.ylabel('Altura (m)')
    plt.legend(loc="best")
```

[12]:
```python
interact(plotGuess, x=fixed(X), y=fixed(Y), interceptor=(0,2,0.02),␣
↪pendiente=(0,2, 0.02));
```

```
interactive(children=(FloatSlider(value=1.0, description='interceptor', max=2.0, step=0.02), Fl
```

Entrenamos la regresión lineal con un *learning rate* de $\alpha = 0.03$

[13]:
```python
r = RegresionLineal(alpha=0.03, max_iters=10000, tols=0.0000001)
r.gradientDescent(X, Y)
```

```
La función convergió con beta: [0.73300235 0.06700325] en la iteración 1190
```

[14]:
```python
r.historia
```

[14]:
```
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array([0.71826232, 0.06968501]),
array([0.71836206, 0.06966687]),
array([0.71846148, 0.06964878]),
array([0.7185606 , 0.06963075]),
array([0.7186594 , 0.06961277]),
array([0.7187579 , 0.06959485]),
array([0.71885608, 0.06957699]),
array([0.71895396, 0.06955918]),
…]}

**Ejercicio:** Agrega un *widget* de interacción en el cual puedas modificar $\alpha$. ¿Qué observas?

[15]:
```
def plotModelo(x,y,rl,iteracion):
    modelo = lambda x,b,m: b + m*x # función para graficar el modelo

    _beta = rl.historia['beta'][iteracion]

    fig, ax = plt.subplots(1,2, figsize=(10,6))
    ax[0].scatter(x,y, label="datos")
    ax[0].plot(x, modelo(x, _beta[0], _beta[1]), label="int: %1.2f, pen: %1.2f"␣
↪% (_beta[0], _beta[1]))
    ax[0].set_xlabel('Edad (yr)')
    ax[0].set_ylabel('Altura (m)')
    ax[0].legend(loc="best")
    #ax[0].set_xlim(0, max(x))
    #ax[0].set_ylim(0, max(y))

    costo  = rl.historia['costo']

    iteraciones = [i for i in range(0, len(costo))]
    ax[1].plot(iteraciones, costo, 'g', label="costo")
    ax[1].plot(iteracion, costo[iteracion], 'or', label="iteracion")
    ax[1].set_xlabel('Iteraciones')
    ax[1].set_ylabel('Costo')
    ax[1].legend(loc="best")
```

[16]:
```
plotModelo(X,Y, r, 5246)
#El ultimo numero es la ultima iteracion
```

```
       ␣
↪---------------------------------------------------------------------------

       IndexError                                Traceback (most recent call␣
↪last)

       <ipython-input-16-39f5651b10b2> in <module>
   ----> 1 plotModelo(X,Y, r, 5246)
         2 #El ultimo numero es la ultima iteracion


       <ipython-input-15-6cee49b1aa08> in plotModelo(x, y, rl, iteracion)
         2     modelo = lambda x,b,m: b + m*x # función para graficar el modelo
         3
   ----> 4     _beta = rl.historia['beta'][iteracion]
         5
         6     fig, ax = plt.subplots(1,2, figsize=(10,6))
```

```
IndexError: list index out of range
```

[17]:
```
ultima_iteracion = (r.breaking_iteration - 1) if r.breaking_iteration else (r.
 ↪max_iters - 1)

interact(plotModelo, x=fixed(X), y=fixed(Y), rl=fixed(r),␣
 ↪iteracion=(0,ultima_iteracion,10)); #El 10 es el cambio en el interact
```

```
interactive(children=(IntSlider(value=590, description='iteracion', max=1189, step=10), Output
```

**Ejercicio**: Modifica el *widget* que creaste, para que dibujes la última iteración ¿Tienes una mejor intuición de $\alpha$?

## 1.2 Una cosa más...

A pesar de que la regresión lineal (obtenida con el *gradient descent* ) parece un algoritmo muy simple, los conceptos son los mismos que para algoritmos de aprendizaje de máquina más avanzados, i.e. minimizar una función de costo. Estos algoritmos simplemente reemplazan el modelo linear con un modelo más complejo (y con una función de costo más compleja). De cierta manera, los algoritmos de aprendizaje de máquina son problemas de optimización.