



# **Inteligencia Artificial & Machine Learning**

## **Aplicaciones en movilidad**

**Engineering** 

Founded by the Royal Academy of Engineering  
and Lloyd's Register Foundation

Dr. Iván S. Razo Zapata



# Aprendizaje Supervisado



## Tareas

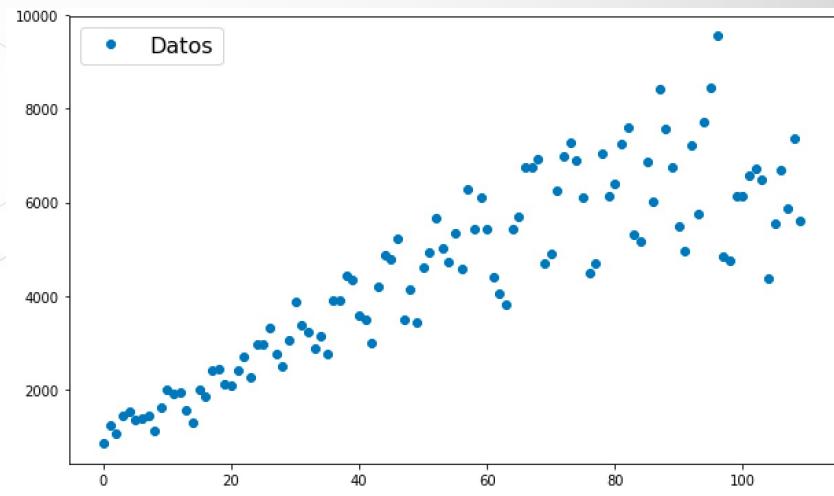
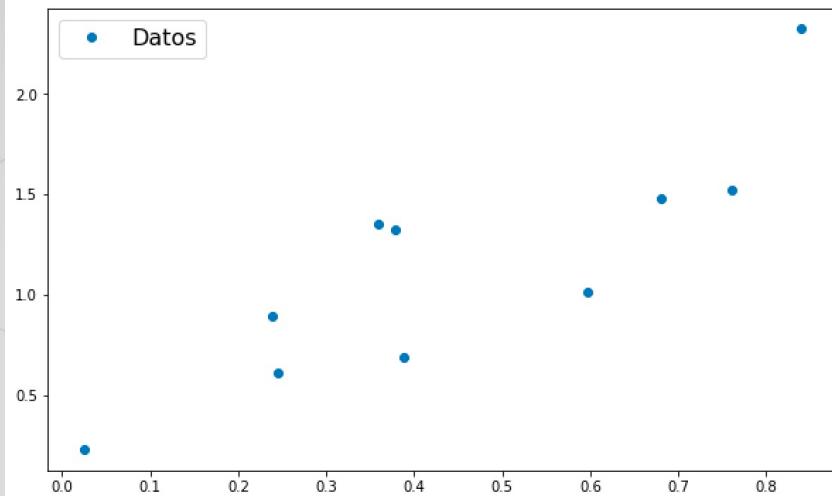
- Regresión
- Clasificación



# Regresión Lineal



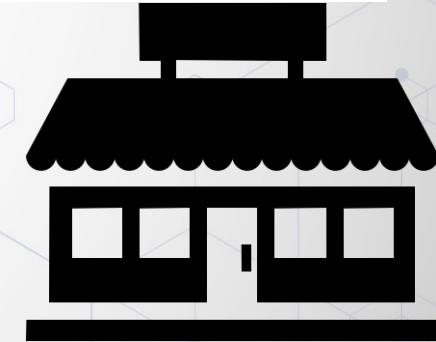
# Idea general – Predecir nuevos valores en base a datos del pasado



Peso del  
motor VS  
Consumo de  
combustible

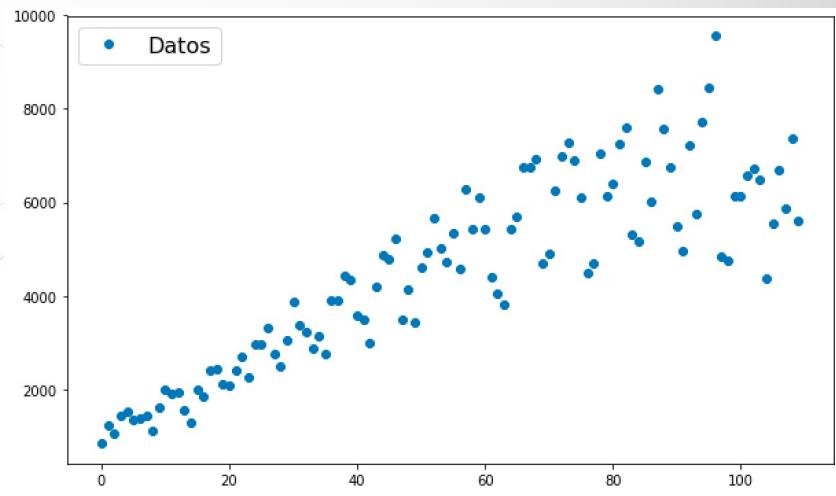
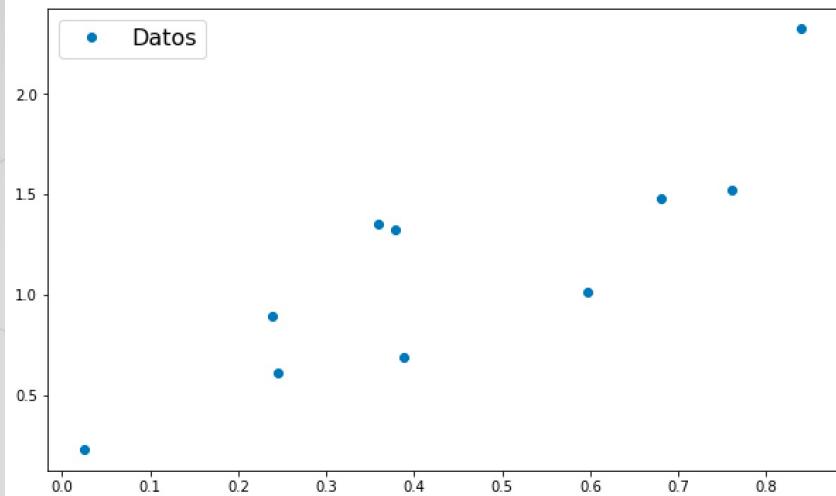


$m^2$  VS Valor(\$)



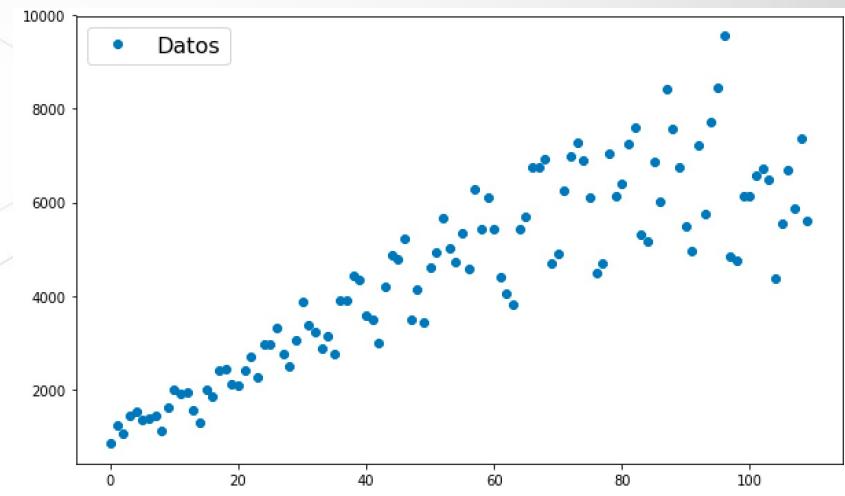
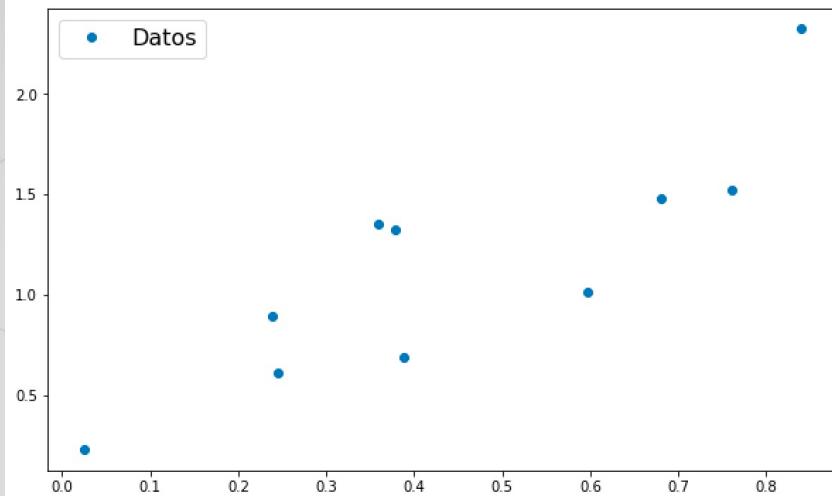
¿Qué otros procesos/fenómenos pueden dar origen a estos datos?

# Idea general – Predecir nuevos valores en base a datos del pasado



$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$

# Idea general – Predecir nuevos valores en base a datos del pasado

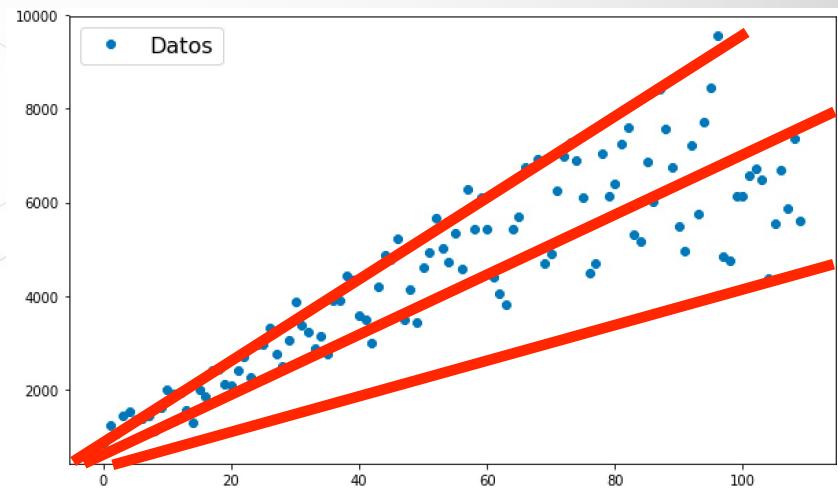
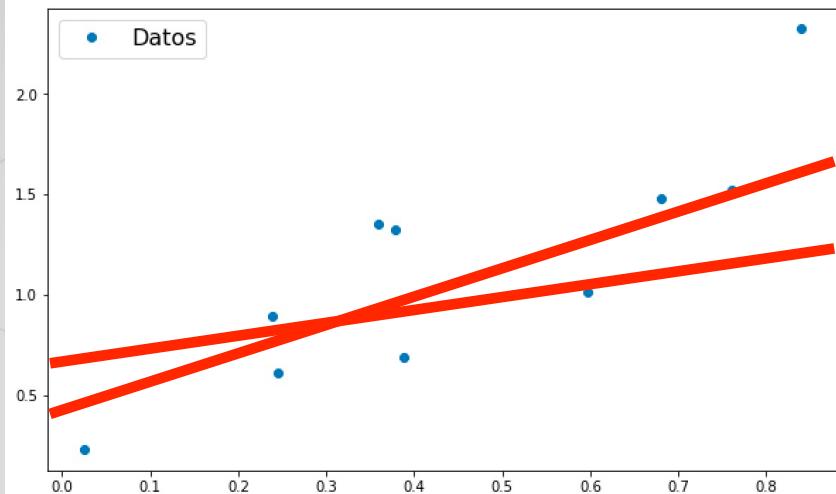


$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$

$$y_{new} = f(x_{new})$$



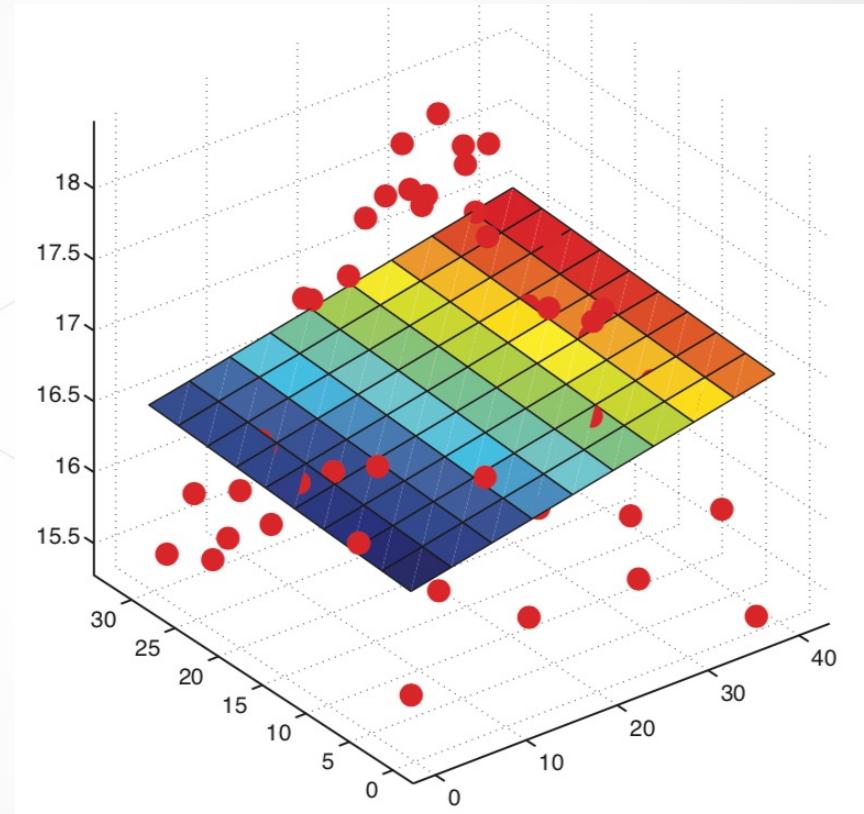
## Idea general



$$y_{new} = f(x_{new})$$



## Idea general



(Peso del motor, Km recorridos) VS Consumo de combustible

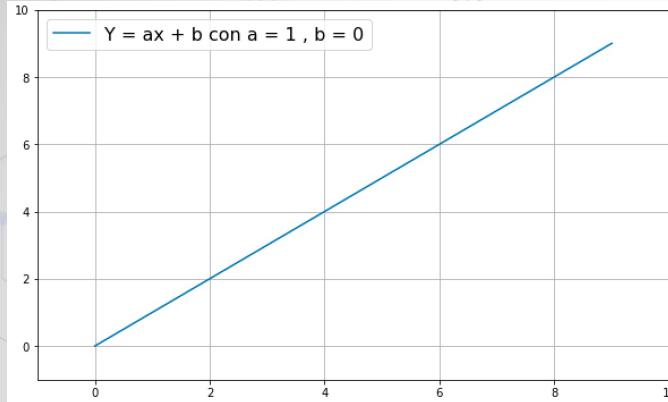
$$y = ax + b$$

# Primer modelo

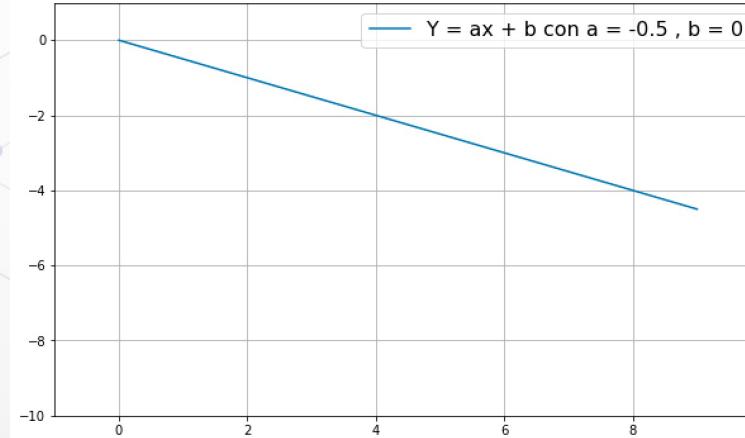
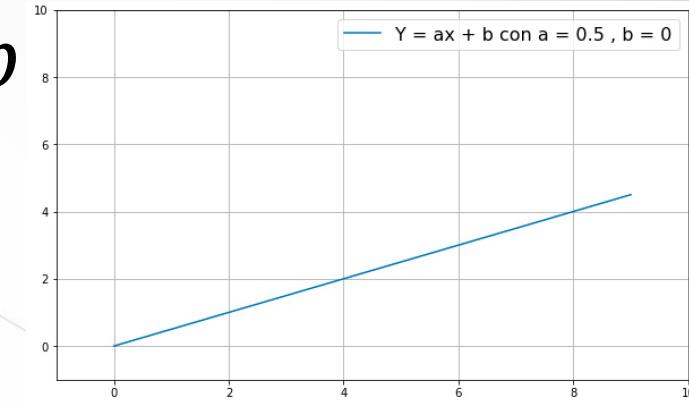
$$y = ax + b$$

Parámetros

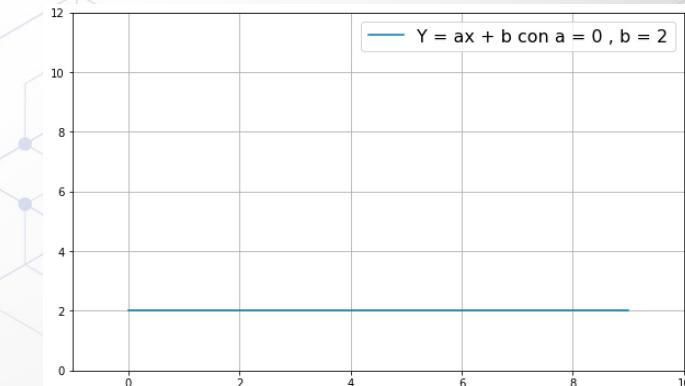
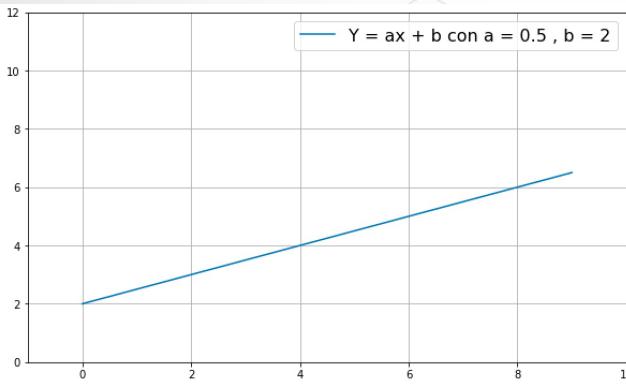
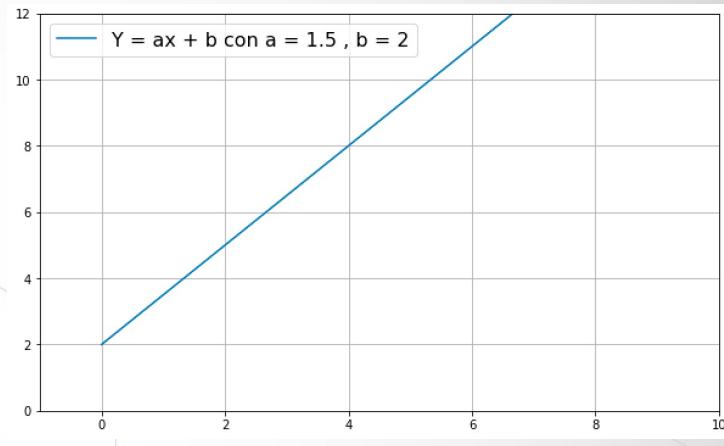
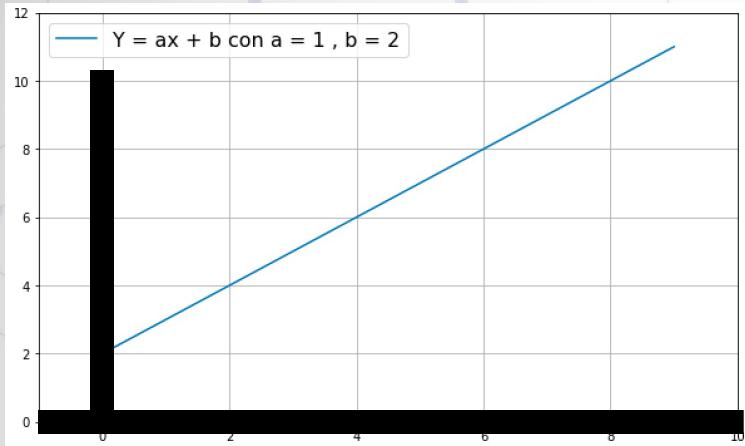
## Ideas básicas - parámetro a (pendiente)



$$y = ax + b$$



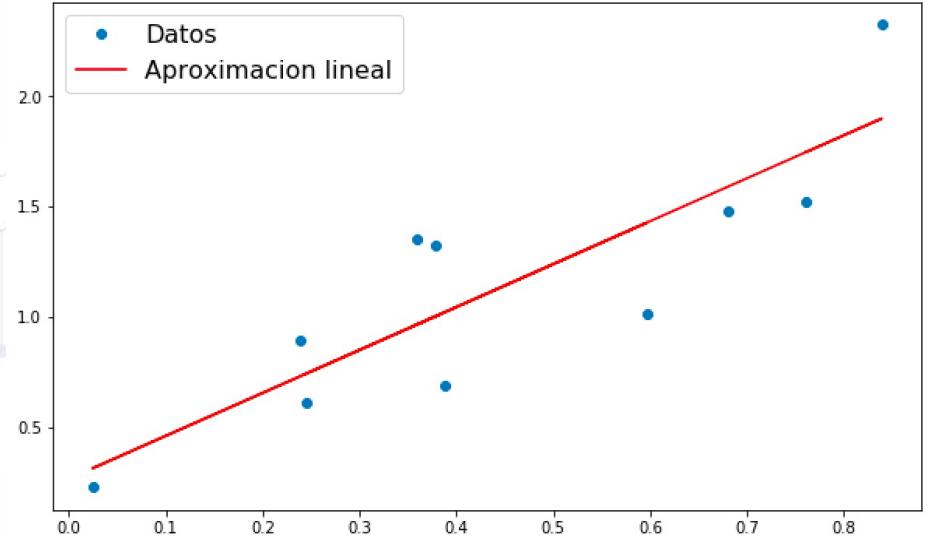
## Ideas básicas - parámetro b (intercepto - cruce con el eje y)



**a = 0**  
**b = 2**

## Ideas básicas

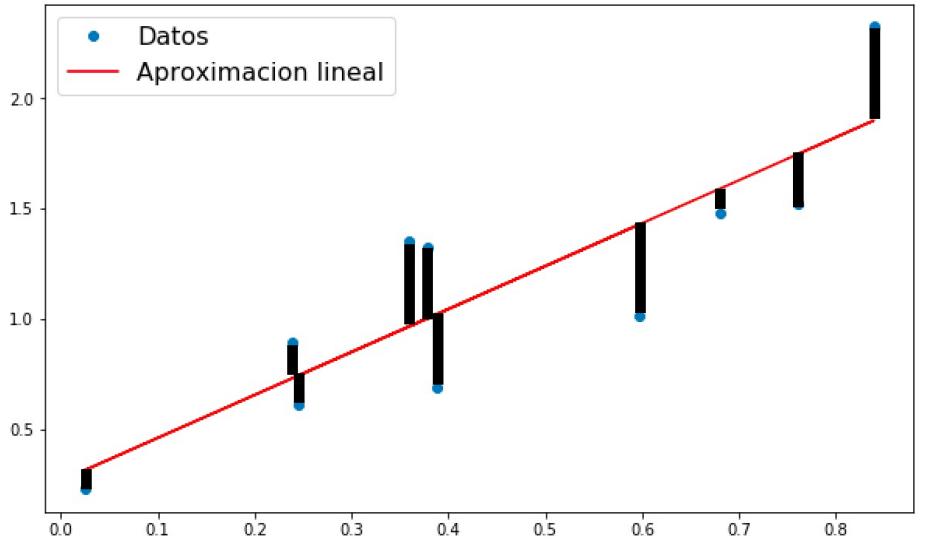
- **a**
  - Pendiente de la línea (slope)
- **b**
  - Intercepto
- ¿Cómo seleccionar los “mejores” valores de **a** y **b**?



$$y = ax + b$$

## Ideas básicas

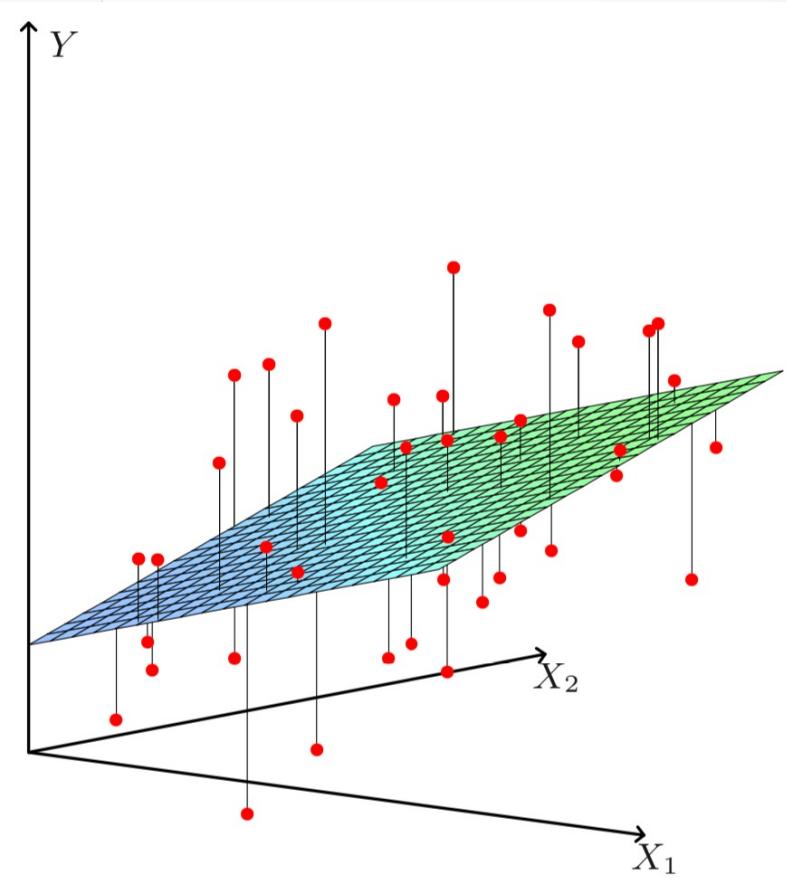
- **a**
- Pendiente de la línea (slope)
- **b**
- Intercepto
- ¿Cómo seleccionar los “mejores” valores de **a** y **b**?



Aprender en base a los datos observados

De los errores que se cometan durante la predicción

## Ideas básicas



## Ideas básicas

$$y = ax + b$$

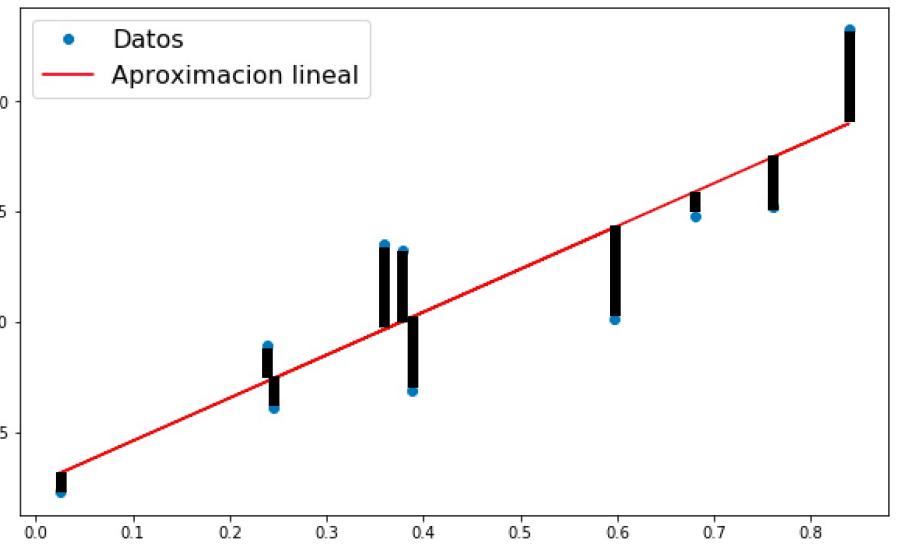
- Encontrar los valores para **a** y **b**
- Dos formas:
  - Solución iterativa con descenso de gradiente
    - El proceso comienza con valores aleatorios para a y b
  - Solución analítica

## Error

- Minimizar el **error cuadrático medio** entre nuestra estimación y los datos

$$\hat{y}_{a,b}(x^{(i)}) = ax^{(i)} + b$$

$$E(a, b) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

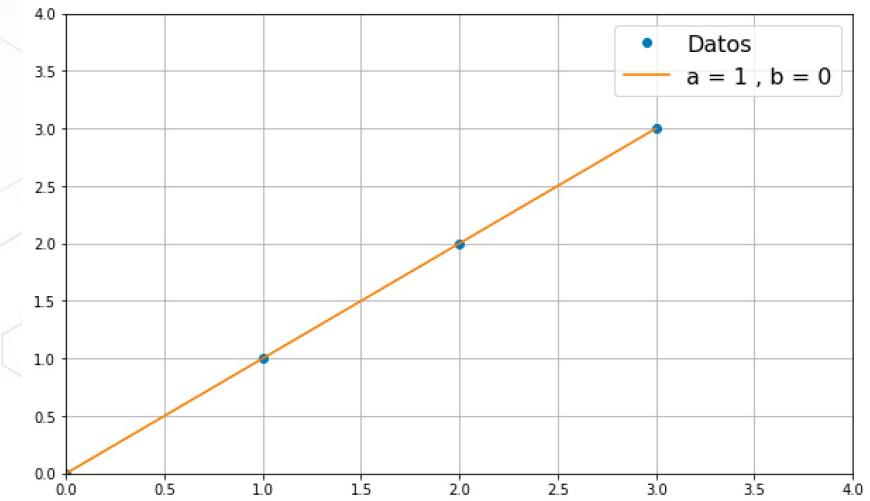


- Minimizar  $E(a,b)$  para **a** y **b**

## Ejemplo 1

- Caso “trivial”
- Datos =  $(1,1), (2,2), (3,3)$
- $a = 1, b = 0$

$$y = ax + b$$



$$E(a, b) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

$$E(a, b) = \frac{1}{2 \times 3} [((1 - 1)^2 + (2 - 2)^2 + (3 - 3)^2] = \frac{1}{6} [0^2 + 0^2 + 0^2] = 0$$

## Ejemplo 2

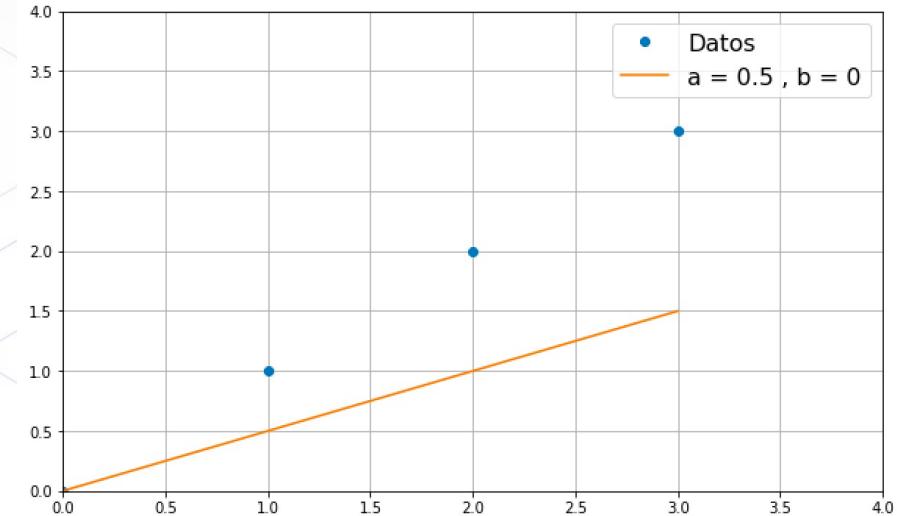
- Datos =  $(1,1), (2,2), (3,3)$
- $a = 0.5, b = 0$

$$E(a, b) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

$$E(a, b) = \frac{1}{2 \times 3} [((0.5 - 1)^2 + (1 - 2)^2 + (1.5 - 3)^2] = \frac{1}{6} [-0.5^2 + -1^2 + -1.5^2]$$

$$E(a, b) = \frac{1}{6} [0.25 + 1 + 2.25] = \frac{1}{6} [3.5] = \frac{3.5}{6} = 0.58$$

$$y = ax + b$$



## Ejemplo 3

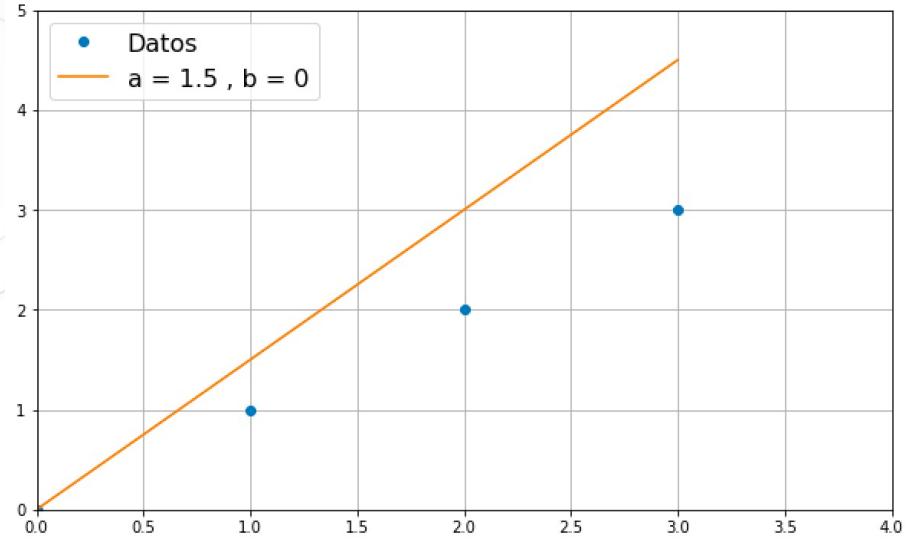
- Datos =  $(1,1), (2,2), (3,3)$
- $a = 1.5, b = 0$

$$E(a, b) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

$$E(a, b) = \frac{1}{2 \times 3} [((1.5 - 1)^2 + (3 - 2)^2 + (4.5 - 3)^2] = \frac{1}{6} [0.5^2 + 1^2 + 1.5^2]$$

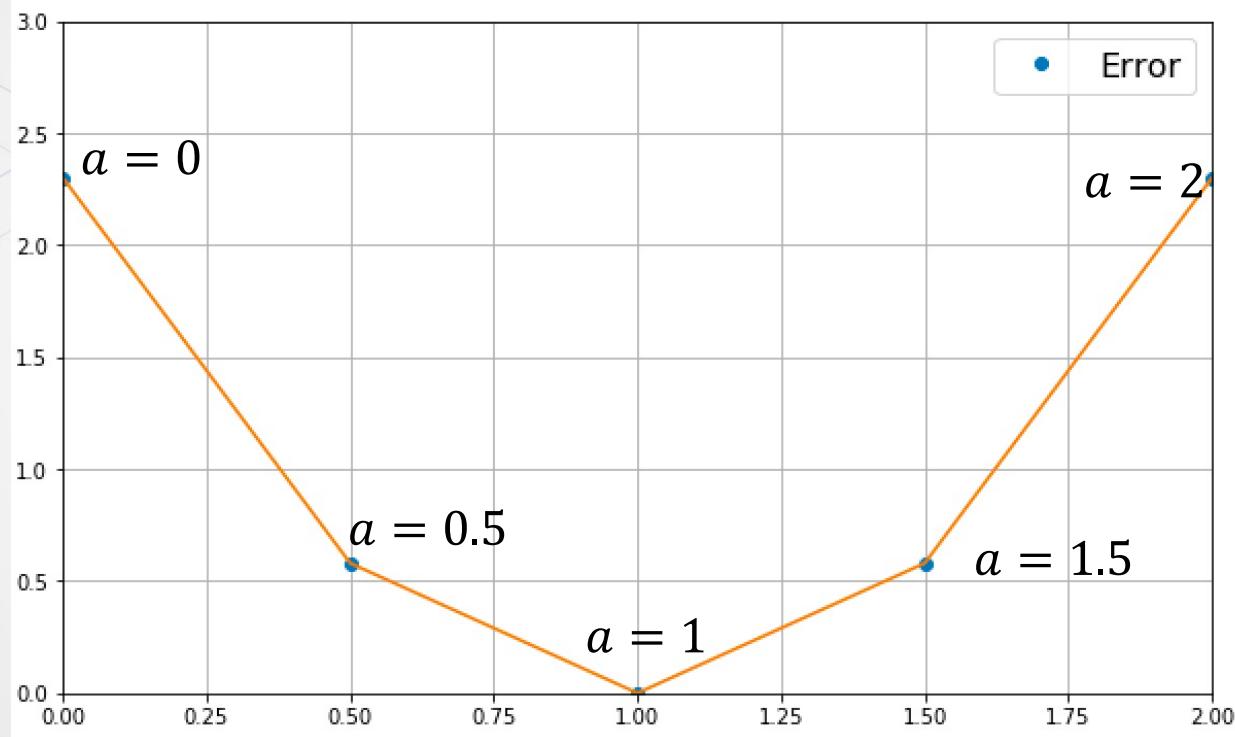
$$E(a, b) = \frac{1}{6} [0.25 + 1 + 2.25] = \frac{1}{6} [3.5] = \frac{3.5}{6} = 0.58$$

$$y = ax + b$$



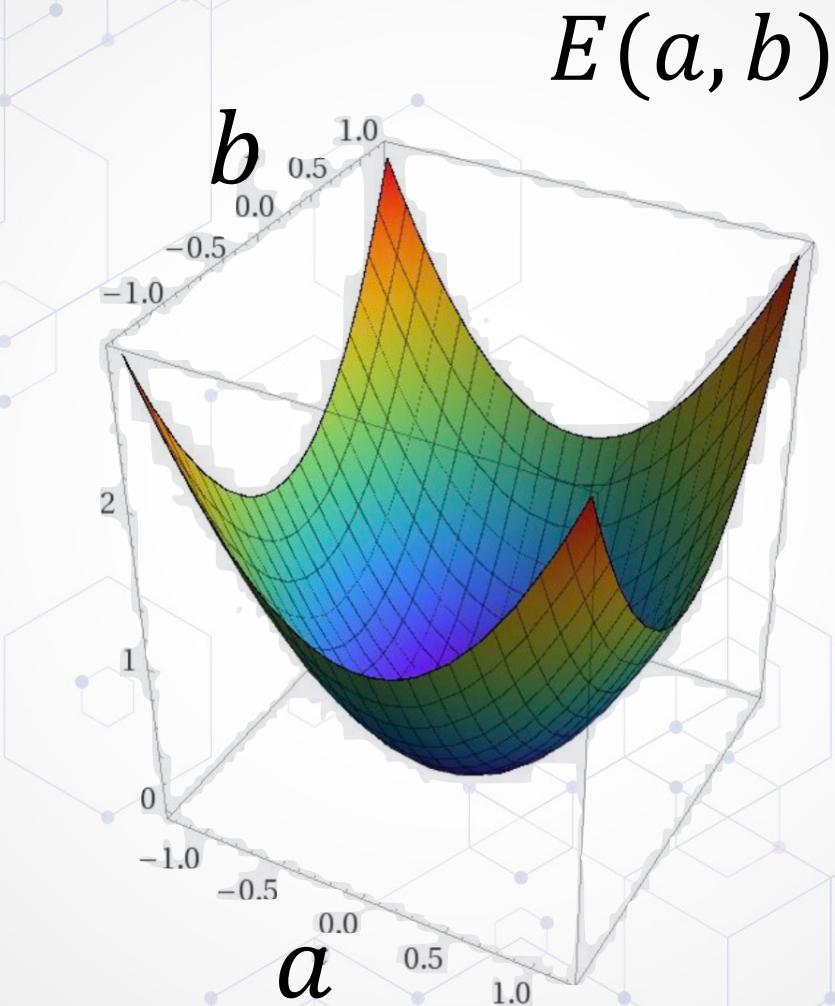
## Curva de error – b fija

$$E(a, b = 0)$$

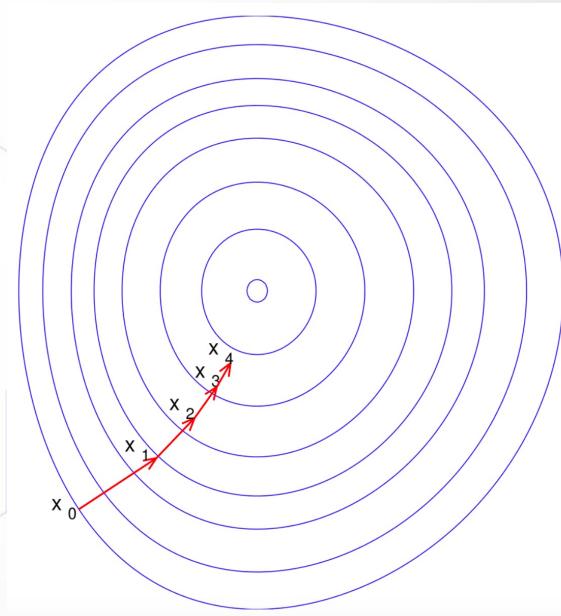
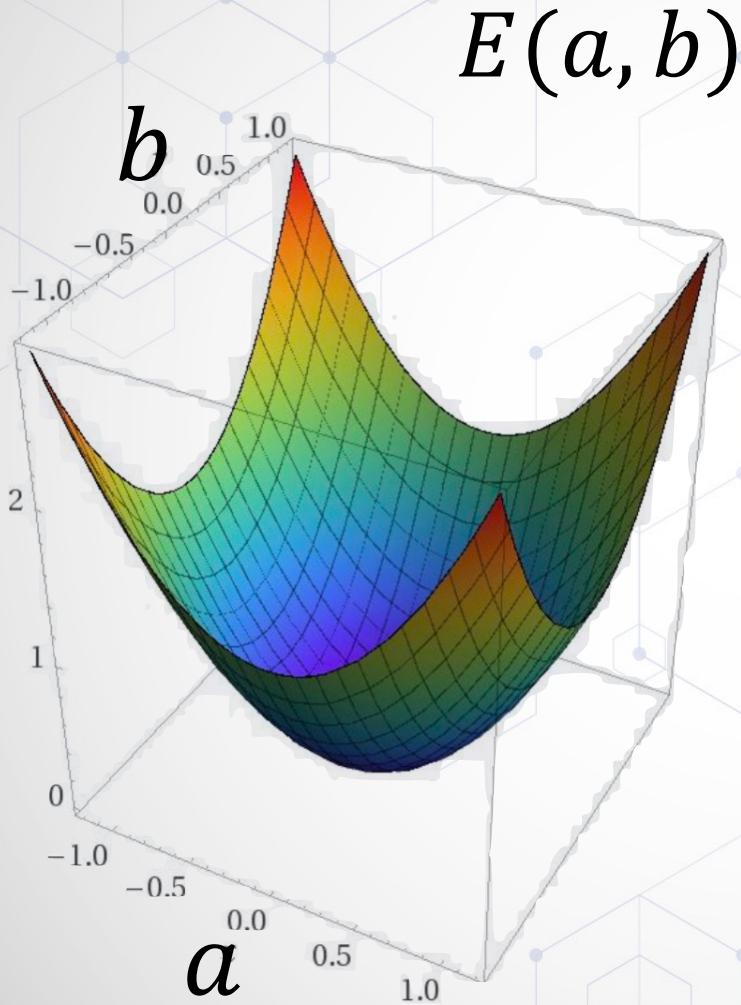


Al alejarnos del valor óptimo el error se incrementa

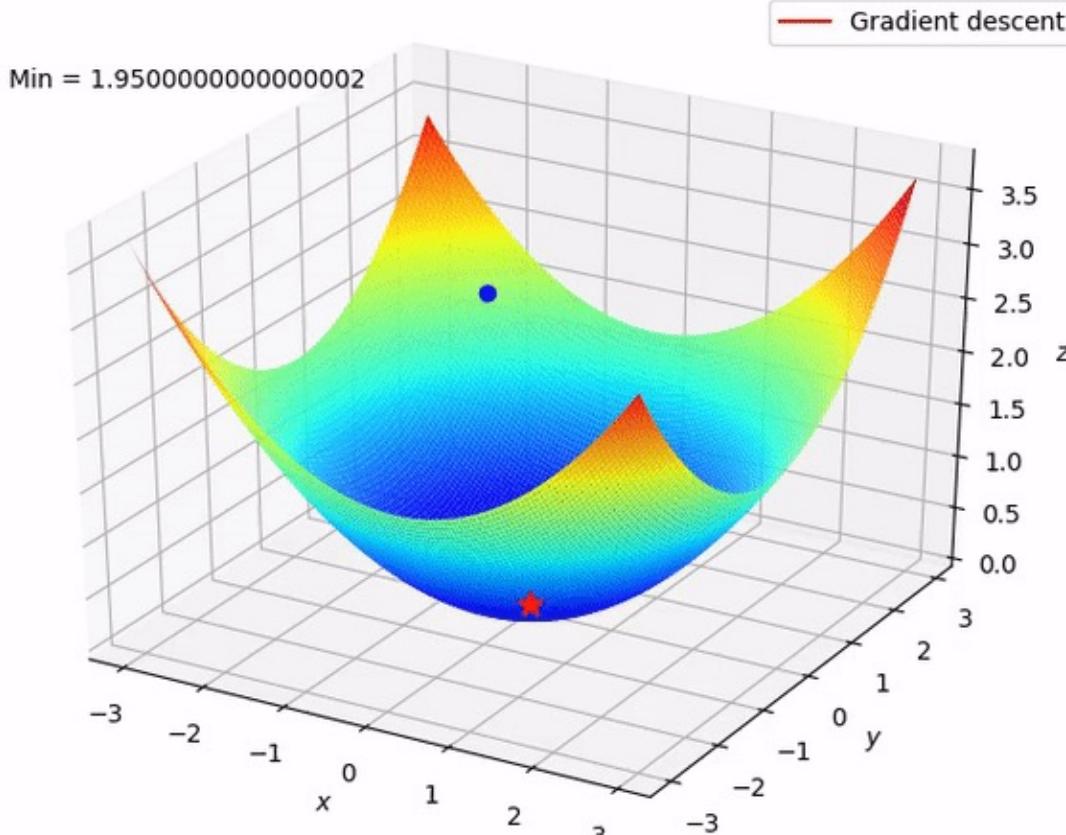
## Superficie de error



## Solución iterativa con descenso de gradiente



# Solución iterativa con descenso de gradiente



# ¿Cómo?

## Solución iterativa con descenso de gradiente

- Iniciando con valores aleatorios **a** y **b**
- Actualizar el valor de **a** y **b** de manera iterativa hasta llegar al punto mínimo

$$E(a, b) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

$$\nabla E(a, b)$$

$$a \leftarrow a - \alpha \frac{\partial E(a, b)}{\partial a}$$

$$b \leftarrow b - \alpha \frac{\partial E(a, b)}{\partial b}$$

## Solución iterativa con descenso de gradiente

- Iniciando con valores aleatorios **a** y **b**
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 $\alpha$ 

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Tasa de aprendizaje (learning rate): Hyperparámetro

## Solución iterativa con descenso de gradiente

$$\hat{y}_{a,b}(x^{(i)}) = ax^{(i)} + b$$

$$E(a, b) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

$$a \leftarrow a - \alpha \frac{\partial}{\partial a} E(a, b)$$

$$a \leftarrow a - \alpha \frac{\partial}{\partial a} \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

$$a \leftarrow a - \alpha \frac{2}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)}) \frac{\partial}{\partial a} (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})$$

$$a \leftarrow a - \alpha \frac{2}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)}) \frac{\partial}{\partial a} (ax^{(i)} + b - y^{(i)})$$

$$a \leftarrow a - \alpha \frac{1}{m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)}) x^{(i)}$$

## Solución iterativa con descenso de gradiente

$$\hat{y}_{a,b}(x^{(i)}) = ax^{(i)} + b$$

$$E(a, b) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

$$b \leftarrow b - \alpha \frac{\partial}{\partial b} E(a, b)$$

$$b \leftarrow b - \alpha \frac{\partial}{\partial b} \frac{1}{2m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})^2$$

$$b \leftarrow b - \alpha \frac{1}{m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)}) \frac{\partial}{\partial b} (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})$$

$$b \leftarrow b - \alpha \frac{1}{m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)}) \frac{\partial}{\partial b} (ax^{(i)} + b - y^{(i)})$$

$$b \leftarrow b - \alpha \frac{1}{m} \sum_{i=1}^m (\hat{y}_{a,b}(x^{(i)}) - y^{(i)})$$

## Solución iterativa con descenso de gradiente

$a \leftarrow$  valor aleatorio, p.ej.  $\in [0,1]$   
 $b \leftarrow$  valor aleatorio, p.ej.  $\in [0,1]$

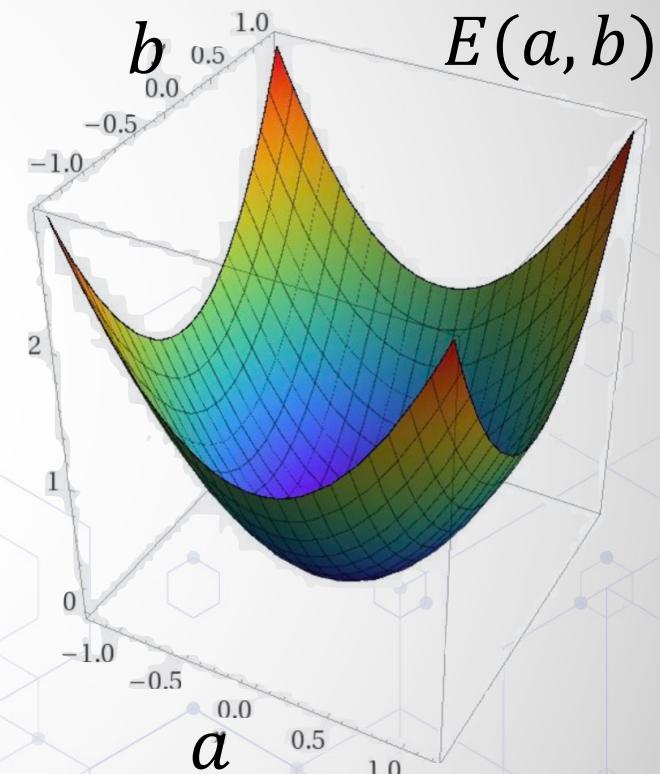
Repetir {

$$a \leftarrow a - \alpha \frac{1}{m} \sum_{i=1}^m (ax^{(i)} + b - y^{(i)})x^{(i)}$$

$$b \leftarrow b - \alpha \frac{1}{m} \sum_{i=1}^m (ax^{(i)} + b - y^{(i)})$$

}

$$\hat{y}_{a,b}(x^{(i)}) = ax^{(i)} + b$$



## Solución iterativa con descenso de gradiente

$a \leftarrow$  valor aleatorio, p.ej.  $\in [0,1]$   
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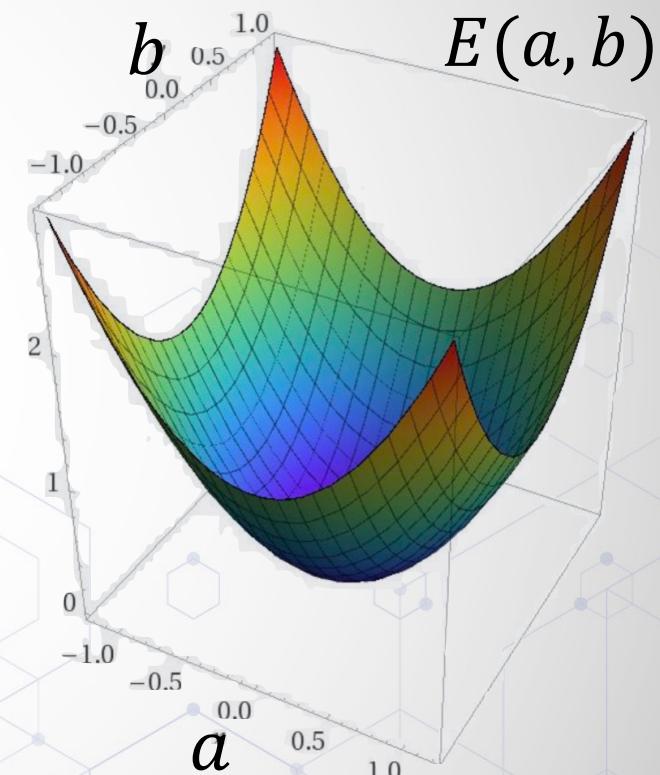
Repetir {

$$a \leftarrow a - \alpha \frac{1}{m} \sum_{i=1}^m (\hat{y} - y^{(i)}) x^{(i)}$$

$$b \leftarrow b - \alpha \frac{1}{m} \sum_{i=1}^m (\hat{y} - y^{(i)})$$

}

$$\hat{y}_{a,b}(x^{(i)}) = ax^{(i)} + b$$



## Solución iterativa con descenso de gradiente

$a \leftarrow$  valor aleatorio, p.ej.  $\in [0,1]$   
 $b \leftarrow$  valor aleatorio, p.ej.  $\in [0,1]$

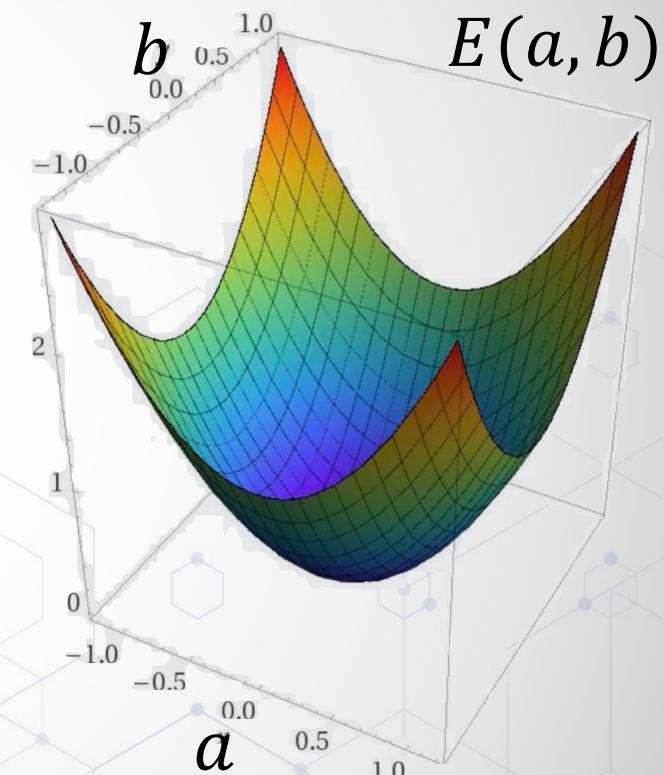
Repetir {

$$a \leftarrow a - \alpha \frac{1}{m} \sum_{i=1}^m (\text{Error}) x^{(i)}$$

$$b \leftarrow b - \alpha \frac{1}{m} \sum_{i=1}^m (\text{Error})$$

}

$$\hat{y}_{a,b}(x^{(i)}) = ax^{(i)} + b$$





# Regresión Lineal

Implementación en Python



## Solución iterativa con descenso de gradiente

$a \leftarrow$  valor aleatorio, p.ej.  $\in [0,1]$   
 $b \leftarrow$  valor aleatorio, p.ej.  $\in [0,1]$

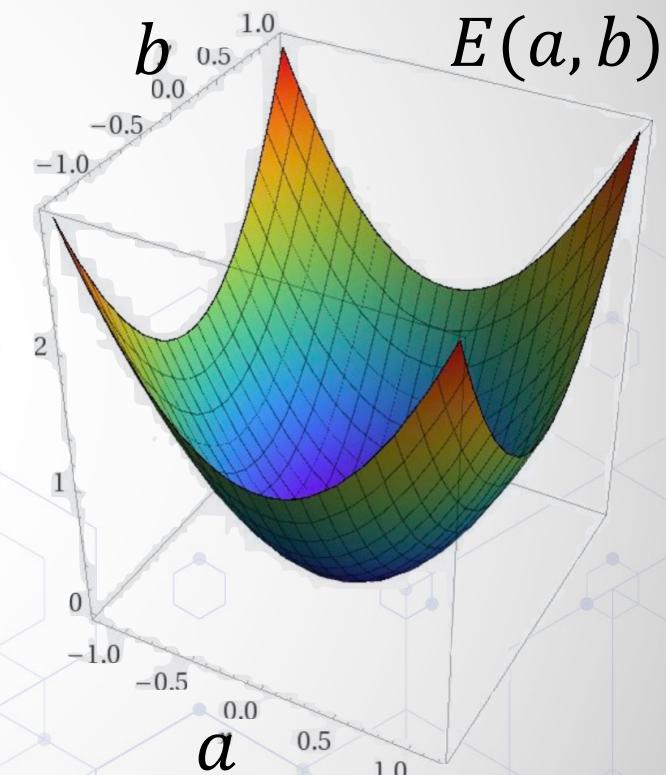
Repetir {

$$a \leftarrow a - \alpha \frac{1}{m} \sum_{i=1}^m (\text{Error}) x^{(i)}$$

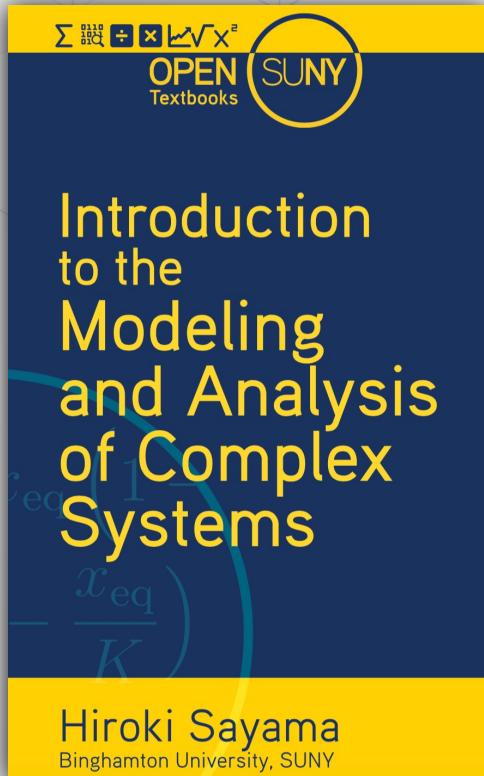
$$b \leftarrow b - \alpha \frac{1}{m} \sum_{i=1}^m (\text{Error})$$

}

$$\hat{y}_{a,b}(x^{(i)}) = ax^{(i)} + b$$



# Idea general



## Three essential components of computer simulation

**Initialize.** You will need to set up the initial values for all the state variables of the system.

**Observe.** You will need to define how you are going to monitor the state of the system. This could be done by just printing out some variables, collecting measurements in a list structure, or visualizing the state of the system.

**Update.** You will need to define how you are going to update the values of those state variables in every time step. This part will be defined as a function, and it will be executed repeatedly.

# Idea general

## Regresión lineal (descenso por gradiente)

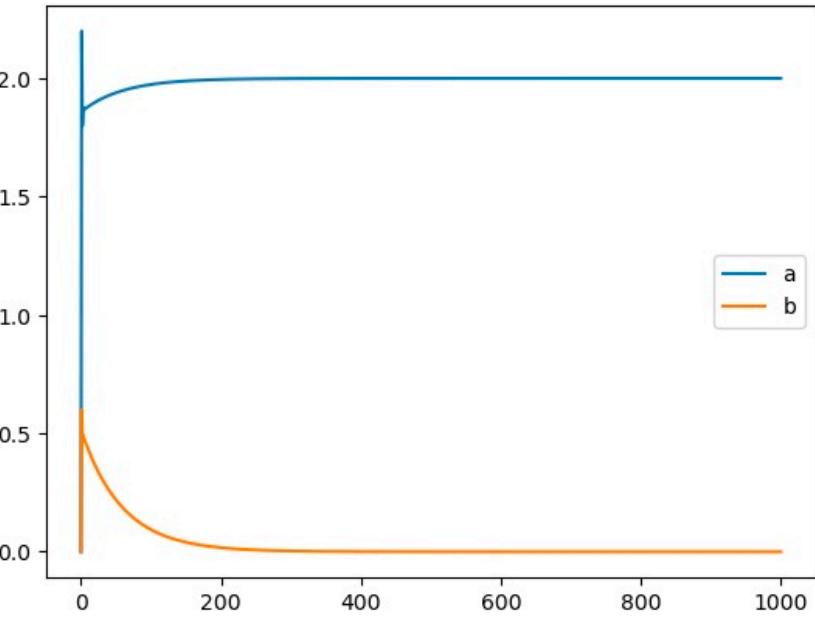
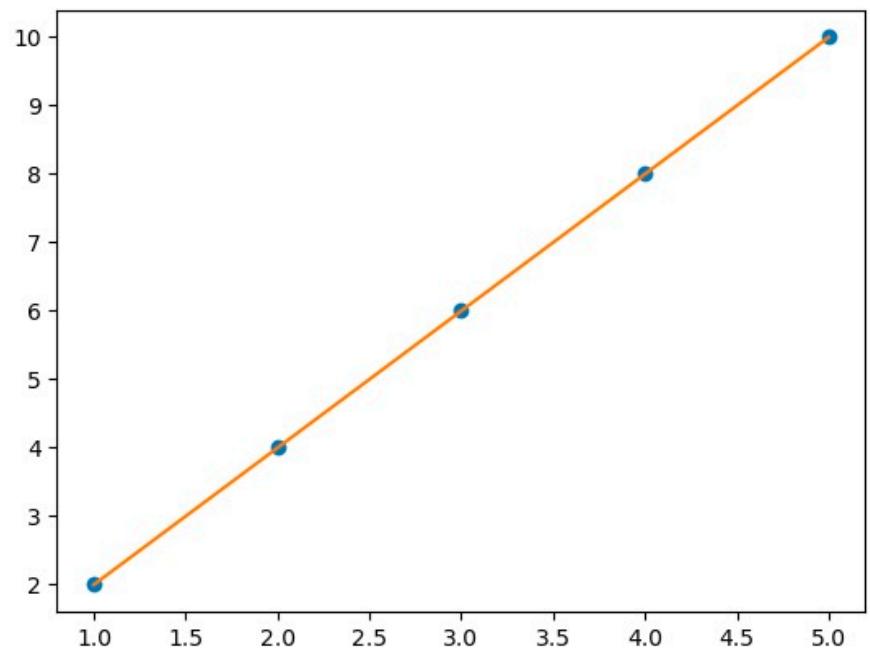
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## Idea general





## Polinomios

$$y = ax + b$$

$$y = \theta_0 + \theta_1 x$$

## Polinomios

$$y = ax + b$$

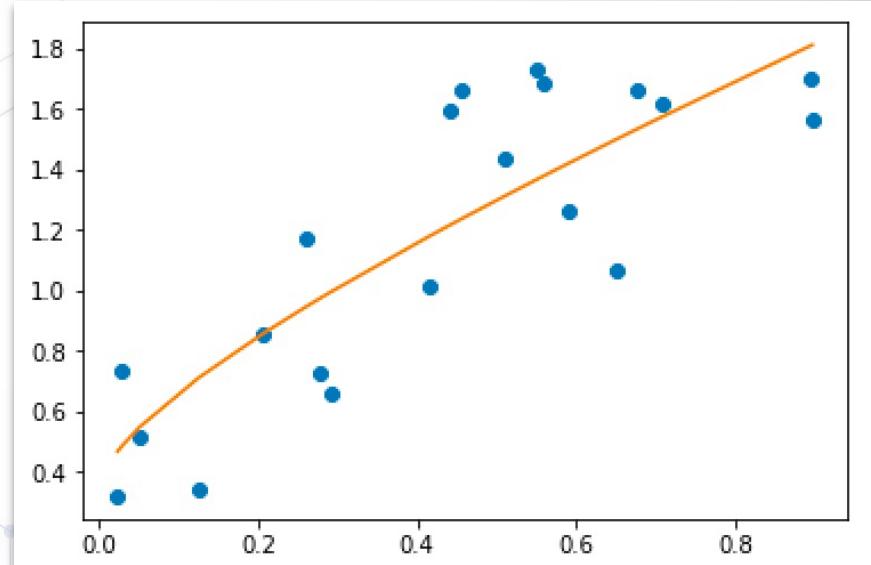
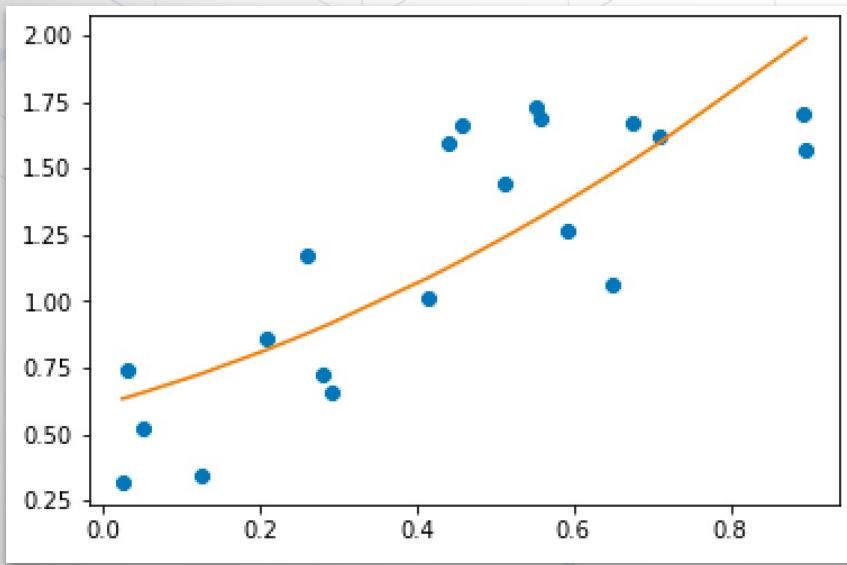
$$y = \theta_0 + \theta_1 x$$

$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

## Polinomios

$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

$$y = \theta_0 + \theta_1 x + \theta_2 \sqrt{x}$$



## Polinomios

$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

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

$$\theta_0 = \theta_0 - \alpha \frac{\partial E(\theta)}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial E(\theta)}{\partial \theta_1}$$

$$\theta_2 = \theta_2 - \alpha \frac{\partial E(\theta)}{\partial \theta_2}$$

## Polinomios

$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

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

$$\frac{\partial E(\theta)}{\partial \theta_0} = \frac{\partial}{\partial \theta_0} \frac{1}{2m} \sum_{i=1}^m (\hat{y}_\theta(x) - y)^2$$

$$= \frac{\partial}{\partial \theta_0} \frac{1}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y)^2$$

$$= \frac{2}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y) \frac{\partial}{\partial \theta_0} (\theta_0 + \theta_1 x + \theta_2 x^2 - y)$$

$$= \frac{1}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y) 1$$

$$\theta_0 = \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y)$$

## Polinomios

$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

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

$$\frac{\partial E(\theta)}{\partial \theta_1} = \frac{\partial}{\partial \theta_1} \frac{1}{2m} \sum_{i=1}^m (\hat{y}_\theta(x) - y)^2$$

$$= \frac{\partial}{\partial \theta_1} \frac{1}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y)^2$$

$$= \frac{2}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y) \frac{\partial}{\partial \theta_1} (\theta_0 + \theta_1 x + \theta_2 x^2 - y)$$

$$= \frac{1}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y) x$$

$$\theta_1 = \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y) x$$

## Polinomios

$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

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

$$\frac{\partial E(\theta)}{\partial \theta_2} = \frac{\partial}{\partial \theta_2} \frac{1}{2m} \sum_{i=1}^m (\hat{y}_\theta(x) - y)^2$$

$$= \frac{\partial}{\partial \theta_2} \frac{1}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y)^2$$

$$= \frac{2}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y) \frac{\partial}{\partial \theta_2} (\theta_0 + \theta_1 x + \theta_2 x^2 - y)$$

$$= \frac{1}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y) x^2$$

$$\theta_2 = \theta_2 - \alpha \frac{1}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x + \theta_2 x^2 - y) x^2$$

## Polinomios

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_n x^n$$

$\theta \leftarrow$  valores aleatorios, p.ej.  $\in [0,1]$

Repetir {

$$\theta_j \leftarrow \theta_j - \alpha \times \sum_{i=1}^m (\theta x^i - y^i) x^j$$

}



## Generalización a múltiples dimensiones

- Solución iterativa con descenso de gradiente

$$y = ax + b$$

$$y = bx_0 + ax_1 \quad x_0 = 1$$

$$y = \theta_0x_0 + \theta_1x_1$$

$$y = \theta_0x_0 + \theta_1x_1 + \theta_2x_2 + \dots + \theta_nx_n$$

## Generalización a múltiples dimensiones

$\theta \leftarrow \text{valores aleatorios, p.ej. } \in [0,1]$

Repetir {

$$\theta_j \leftarrow \theta_j - \alpha \times \sum_{i=1}^m (\theta x^i - y^i) x_j^i$$

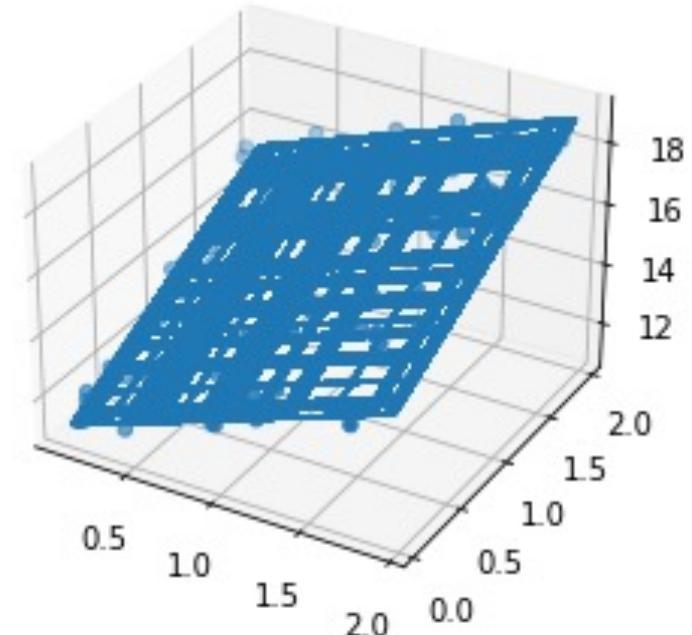
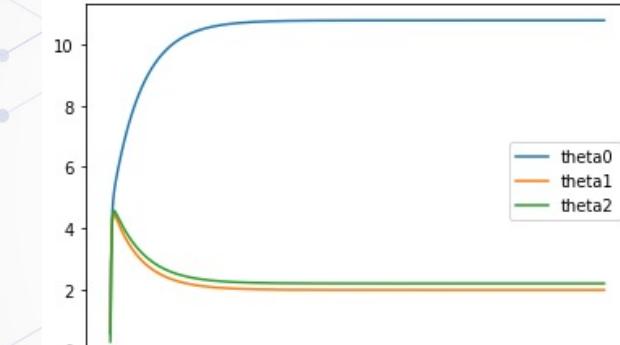
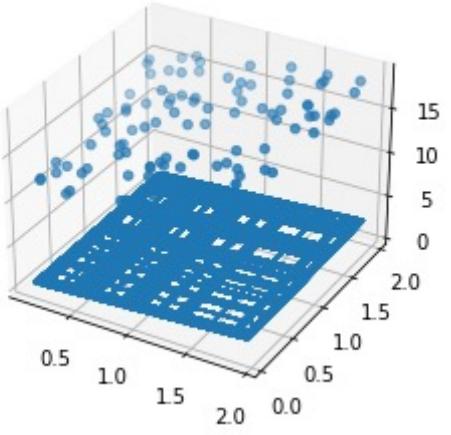
}

Para cada j (característica)

i dato/muestra

## Múltiples dimensiones

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$





## Datos reales

### sklearn.datasets.load\_diabetes

```
sklearn.datasets.load_diabetes(*, return_X_y=False, as_frame=False)
```

[\[source\]](#)

Load and return the diabetes dataset (regression).

Samples total 442

Dimensionality 10

Features real,  $-.2 < x < .2$

Targets integer 25 - 346

**Note:** The meaning of each feature (i.e. `feature_names`) might be unclear (especially for `lbg`) as the documentation of the original dataset is not explicit. We provide information that seems correct in regard with the scientific literature in this field of research.

Read more in the [User Guide](#).

## Datos reales

# Datos

```
from sklearn import datasets
```

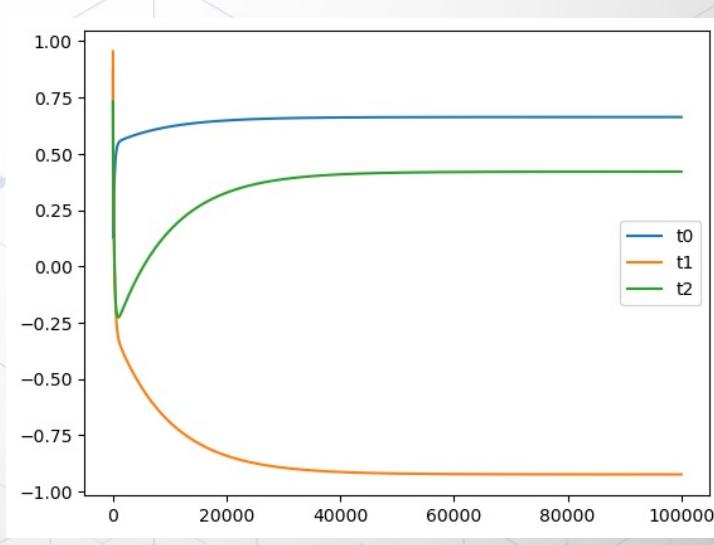
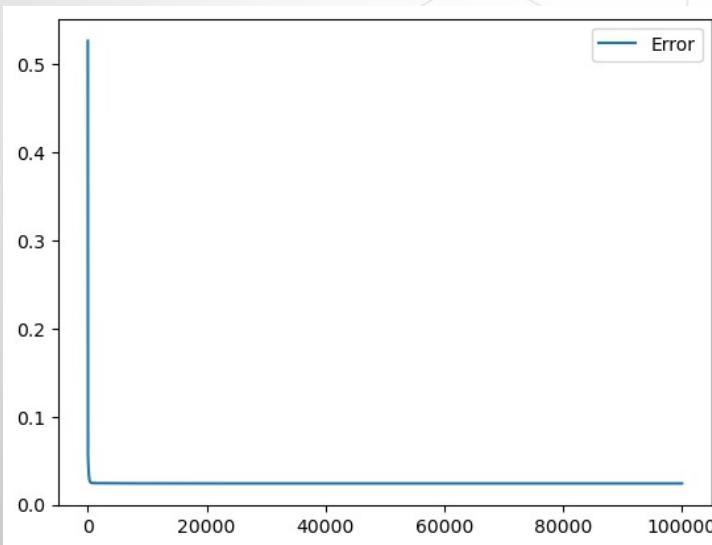
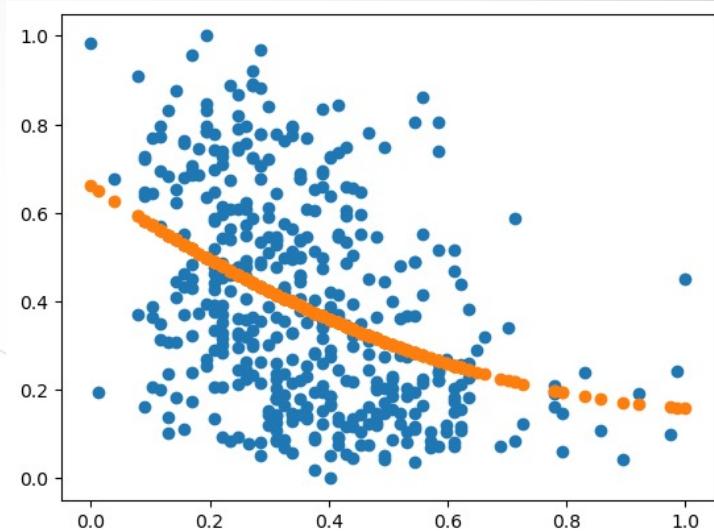
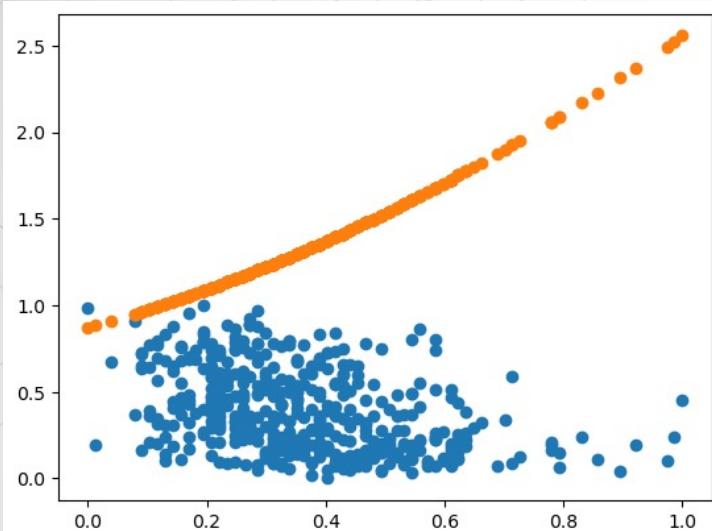
```
xT, y = datasets.load_diabetes(return_X_y=True)
```

```
x = xT[:,6]
```

```
m = x.size
```

```
plt.plot(x,y,'o')
```

## Datos reales





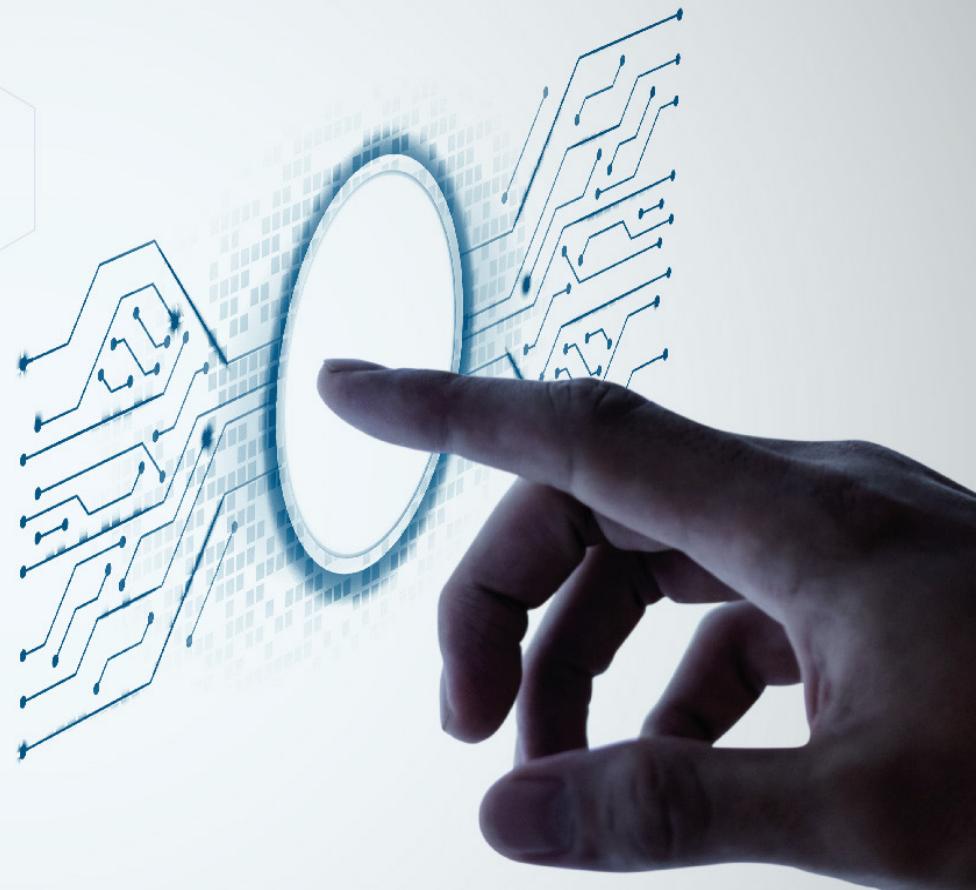
## Tarea moral

- Condiciones de paro
- Descenso estocástico
- Batch learning

# Engineering X

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## GRACIAS



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