Aproximación por mínimos cuadrados

Motivación. Ajuste discreto lineal. Ajuste polinómico. Ajustes potencial y exponencial. Ejemplos con Python

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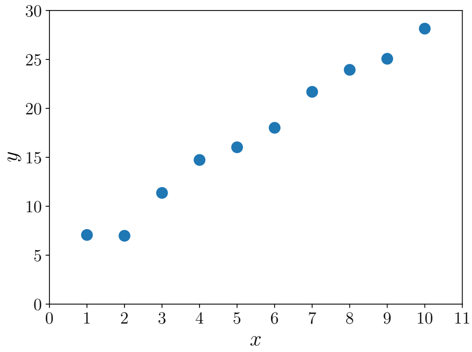
Cálculo Avanzado • 2023

Datos:

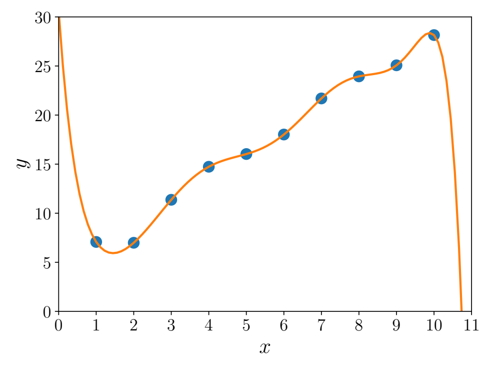
x_i	y_i	x_i	y_i
1	7.07	6	18.02
2	6.99	7	21.69
3	11.37	8	23.94
4	14.73	9	25.07
5	16.03	10	28.15

Figura:



Ajuste exacto: polinomio de grado 9

$$
\begin{aligned}
P_9(x) = {} & 30.63 - 55.47x + 53.23x^2 \\
& - 30.82x^3 12.24x^4 - 3.21x^5 \\
& + 0.53x^6 - 0.053x^7 + 0.0029x^8 \\
& - 6.4 \times 10^{-5} x^9
\end{aligned}
$$



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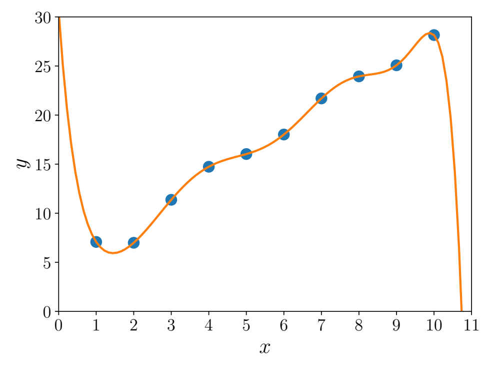

Aproximación lineal:

$$y = a_1\, x + a_0$$

- Problema **minimax**:

$$E_\infty(a_0, a_1) = \max_{1 \le i \le 10} \{|y_i - (a_1 x_i + a_0)|\}$$

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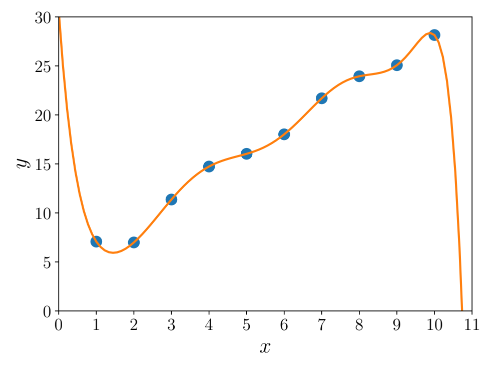

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$$E_1(a_0, a_1) = \sum_{i=1}^{10} |y_i - (a_1 x_i + a_0)|$$

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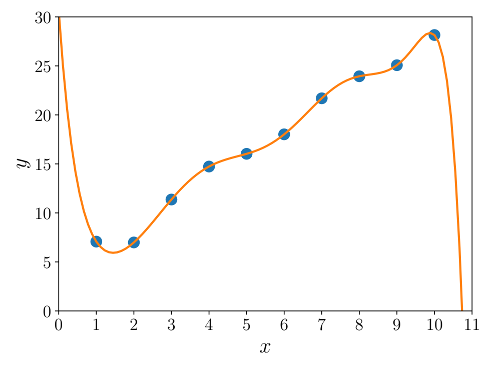

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$$y = a_1\, x + a_0$$

- Problema **minimax**:

$$E_\infty(a_0, a_1) = \max_{1 \leq i \leq 10} \{|y_i - (a_1 x_i + a_0)|\}$$

- Desviación absoluta:

$$E_1(a_0, a_1) = \sum_{i=1}^{10} |y_i - (a_1 x_i + a_0)|$$

- **Mínimos cuadrados:**

$$E_2(a_0, a_1) = \sum_{i=1}^{10} [y_i - (a_1 x_i + a_0)]^2$$

Para el conjunto $\{(x_i, y_i)\}_{i=1}^{m}$, **minimizar** respecto de a_0, a_1:

$$E \equiv E_2(a_0, a_1) = \sum_{i=1}^{m} [y_i - (a_1 x_i + a_0)]^2$$

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$$\frac{\partial E}{\partial a_0} = 0 \quad \text{y} \quad \frac{\partial E}{\partial a_1} = 0$$

Esto es:

$$0 = \frac{\partial}{\partial a_0} \sum_{i=1}^{m} [y_i - (a_1 x_i + a_0)]^2 = 2 \sum_{i=1}^{m} (y_i - a_1 x_i - a_0)(-1)$$

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Ecuaciones normales:

$$a_0 \cdot m + a_1 \sum_{i=1}^{m} x_i = \sum_{i=1}^{m} y_i$$

$$a_0 \sum_{i=1}^{m} x_i + a_1 \sum_{i=1}^{m} x_i^2 = \sum_{i=1}^{m} x_i \, y_i$$

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Solución:

$$a_0 = \frac{\sum_{i=1}^{m} x_i^2 \sum_{i=1}^{m} y_i - \sum_{i=1}^{m} x_i y_i \sum_{i=1}^{m} x_i}{m \left(\sum_{i=1}^{m} x_i^2 \right) - \left(\sum_{i=1}^{m} x_i \right)^2}$$

$$a_1 = \frac{m \sum_{i=1}^{m} x_i y_i - \sum_{i=1}^{m} x_i \sum_{i=1}^{m} y_i}{m \left(\sum_{i=1}^{m} x_i^2 \right) - \left(\sum_{i=1}^{m} x_i \right)^2}$$

Ejemplo: Encontrar la recta de mínimos cuadrados:

x_i	y_i	x_i^2	$x_i y_i$	$P(x_i) = 2.437x_i + 3.903$
1	7.07	1	7.07	6.34
2	6.99	4	13.97	8.78
3	11.37	9	34.10	11.21
4	14.73	16	58.92	13.65
5	16.03	25	80.14	16.09
6	18.02	36	108.10	18.52
7	21.69	49	151.85	20.96
8	23.94	64	191.52	23.40
9	25.07	81	225.62	25.83
10	28.15	100	281.49	28.27
55	173.04	385	1152.77	$E \approx 6.62$

Ejemplo: Encontrar la recta de mínimos cuadrados:

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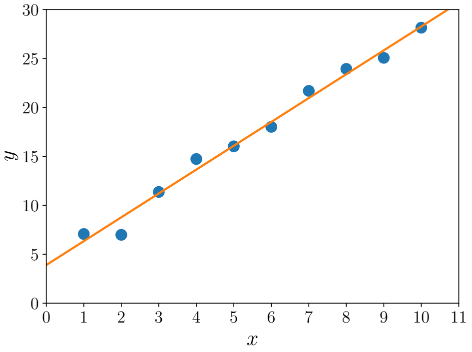
55	173.04	385	1152.77	$E \approx 6.62$

$$a_0 = \frac{385(173.04) - 55(1152.77)}{10(385) - 55^2} = 3.903$$

$$a_1 = \frac{10(1152.77) - 55(173.04)}{10(385) - 55^2} = 2.437$$



Mínimos cuadrados polinomiales:

$$P_n(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$$

$\{(x_i, y_i)\}, i = 1, \ldots m$, $n < m - 1$. Minimizar:

$$\begin{aligned}
E &= \sum_{i=1}^{m} [y_i - P_n(x_i)]^2 \\
&= \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m} P_n(x_i) y_i + \sum_{i=1}^{m} [P_n(x_i)]^2 \\
&= \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m} \left(\sum_{j=0}^{n} a_j x_i^j\right) y_i + \sum_{i=1}^{m} \left(\sum_{j=0}^{n} a_j x_i^j\right)^2 \\
&= \sum_{i=1}^{m} y_i^2 - 2\sum_{j=0}^{n} a_j \left(\sum_{i=1}^{m} y_i x_i^j\right) + \sum_{j=0}^{n}\sum_{k=0}^{n} a_j a_k \left(\sum_{i=1}^{m} x_i^{j+k}\right)
\end{aligned}$$

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$$\begin{aligned} E &= \sum_{i=1}^{m} [y_i - P_n(x_i)]^2 \\ &= \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m} P_n(x_i) y_i + \sum_{i=1}^{m} [P_n(x_i)]^2 \\ &= \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m} \left(\sum_{j=0}^{n} a_j x_i^j\right) y_i + \sum_{i=1}^{m} \left(\sum_{j=0}^{n} a_j x_i^j\right)^2 \\ &= \sum_{i=1}^{m} y_i^2 - 2\sum_{j=0}^{n} a_j \left(\sum_{i=1}^{m} y_i x_i^j\right) + \sum_{j=0}^{n}\sum_{k=0}^{n} a_j a_k \left(\sum_{i=1}^{m} x_i^{j+k}\right) \end{aligned}$$

Minimización: $\partial E/\partial a_j = 0, j = 0, 1, \ldots n$.

$$0 = \frac{\partial E}{\partial a_j} = -2\sum_{i=1}^{m} y_i x_i^j + 2\sum_{k=0}^{n} a_k \sum_{i=1}^{m} x_i^{j+k}$$

$(n+1)$ **ecuaciones normales**:

$$\sum_{k=0}^{n} a_k \sum_{i=1}^{m} x_i^{j+k} = \sum_{i=1}^{m} y_i x_i^j, \; j = 0, 1, \ldots n$$

$$
\begin{aligned}
a_0 \sum_{i=1}^{m} x_i^0 + a_1 \sum_{i=1}^{m} x_i^1 + a_2 \sum_{i=1}^{m} x_i^2 + \cdots + a_n \sum_{i=1}^{m} x_i^n &= \sum_{i=1}^{m} y_i x_i^0 \\
a_0 \sum_{i=1}^{m} x_i^1 + a_1 \sum_{i=1}^{m} x_i^2 + a_2 \sum_{i=1}^{m} x_i^3 + \cdots + a_n \sum_{i=1}^{m} x_i^{n+1} &= \sum_{i=1}^{m} y_i x_i^1 \\
&\vdots \\
a_0 \sum_{i=1}^{m} x_i^n + a_1 \sum_{i=1}^{m} x_i^{n+1} + a_2 \sum_{i=1}^{m} x_i^{n+2} + \cdots + a_n \sum_{i=1}^{m} x_i^{2n} &= \sum_{i=1}^{m} y_i x_i^n
\end{aligned}
$$

Solución única: $x_i \neq x_j \quad \forall i \neq j$.

Ejemplo:

i	x_i	y_i
1	0	1.0000
2	0.25	1.2840
3	0.50	1.6487
4	0.75	2.1170
5	1.00	2.7183

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$n = 2, m = 5$

$$5a_0 + 2.5a_1 + 1.875a_2 = 8.7680$$

$$2.5a_0 + 1.875a_1 + 1.5625a_2 = 5.4514$$

$$1.875a_0 + 1.5625a_1 + 1.3828a_2 = 4.4015$$

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Solución:

$$a_0 = 1.005,\ a_1 = 0.8642,\ a_2 = 0.8437$$

$$P_2(x) = 1.005 + 0.8642x + 0.8437x^2$$

Error total:

$$E = \sum_{i=1}^{5} [y_i - P_2(x_i)]^2 = 2.74 \times 10^{-4}$$

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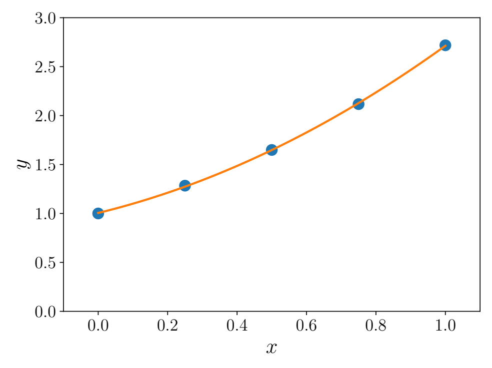


Relación exponencial:

$$y = b\,e^{ax}$$

Minimizar:

$$E = \sum_{i=1}^{m} (y_i - be^{ax_i})^2$$

Ecuaciones normales:

$$0 = \frac{\partial E}{\partial b} = 2\sum_{i=1}^{m} (y_i - be^{ax_i})(-e^{ax_i})$$

$$0 = \frac{\partial E}{\partial a} = 2\sum_{i=1}^{m} (y_i - be^{ax_i})(-bx_i e^{ax_i})$$

Alternativa:

$$\ln y = \ln b + ax$$

Relación potencial:

$$y = b\,x^a$$

Minimizar:

$$E = \sum_{i=1}^{m} (y_i - bx_i^a)^2$$

Ecuaciones normales:

$$0 = \frac{\partial E}{\partial b} = 2\sum_{i=1}^{m} (y_i - bx_i^a)(-x_i^a)$$

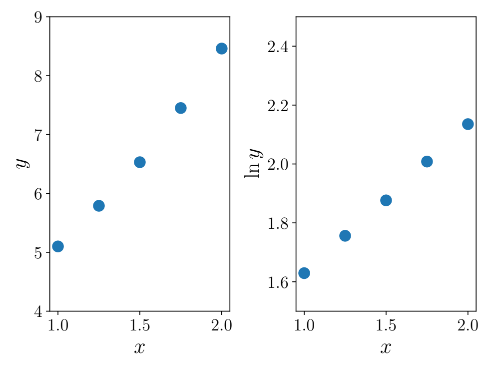
$$0 = \frac{\partial E}{\partial a} = 2\sum_{i=1}^{m} (y_i - bx_i^a)[-b\ln(x_i)x_i^a]$$

Alternativa:

$$\ln y = \ln b + a\ln x$$

Ejemplo:

i	x_i	y_i	$\ln y_i$	x_i^2	$x_i \ln y_i$
1	1.00	5.10	1.63	1.00	1.63
2	1.25	5.79	1.76	1.56	2.20
3	1.50	6.53	1.88	2.25	2.81
4	1.75	7.45	2.01	3.06	3.51
5	2.00	8.46	2.14	4.00	4.27
	7.50		9.41	11.88	14.42



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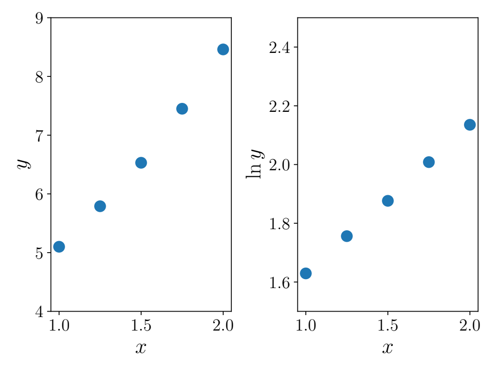

$$y = be^{ax} \Rightarrow \ln y = \ln b + ax$$

$$a = \frac{5(14.42) - (7.5)(9.41)}{5(11.88) - (7.5)^2} = 0.5057$$

$$\ln b = \frac{(11.88)(9.41) - (14.42)(7.5)}{5(11.88) - (7.5)^2} = 1.122$$

$$\ln b = 1.122 \to b = e^{1.122} = 3.071$$

$$y = 3.071e^{0.5056x}$$

Ejemplo:

i	x_i	y_i	$\ln y_i$	x_i^2	$x_i \ln y_i$
1	1.00	5.10	1.63	1.00	1.63
2	1.25	5.79	1.76	1.56	2.20
3	1.50	6.53	1.88	2.25	2.81
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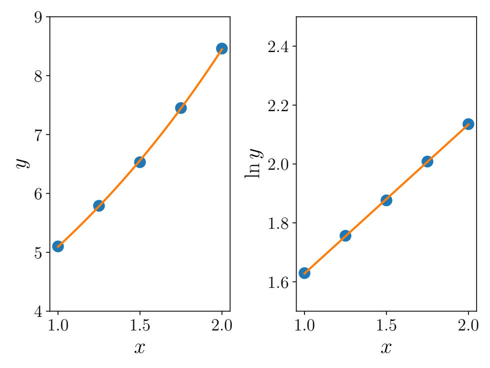

$$y = be^{ax} \Rightarrow \ln y = \ln b + ax$$

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$$\ln b = \frac{(11.88)(9.41) - (14.42)(7.5)}{5(11.88) - (7.5)^2} = 1.122$$

$$\ln b = 1.122 \rightarrow b = e^{1.122} = 3.071$$

$$y = 3.071e^{0.5056x}$$

Python: ejemplo 1

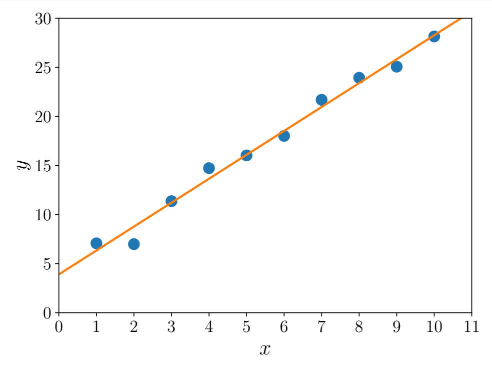
```python
import numpy as np

rng = np.random.default_rng(14)

delta = 5.5
x = np.linspace(1, 10, 10)
y = 2.5 * x + delta * rng.random(x.size)
z = np.polyfit(x, y, 1)
p = np.poly1d(z)
print(p)
print(f"a_0 = {p[0]:.5f}, a_1 = {p[1]:.5f}")
```

```
$ ./ejemplo-01.py

2.437 x + 3.903
a_0 = 3.90314, a_1 = 2.43661
```



Python: ejemplo 2

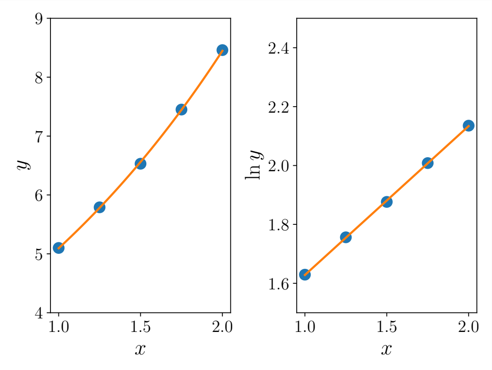
```python
from math import exp
import numpy as np

x = np.array([1.00, 1.25, 1.50, 1.75, 2.00])
y = np.array([5.10, 5.79, 6.53, 7.45, 8.46])
ly = np.log(y)

z = np.polyfit(x, ly, 1)
p = np.poly1d(z)
print(p)
print(f"ln(b) = {p[0]:.5f}, a = {p[1]:.5f}")
```

```
$ ./ejemplo-02.py

0.5057 x + 1.122
ln(b) = 1.12249, a = 0.50572
```



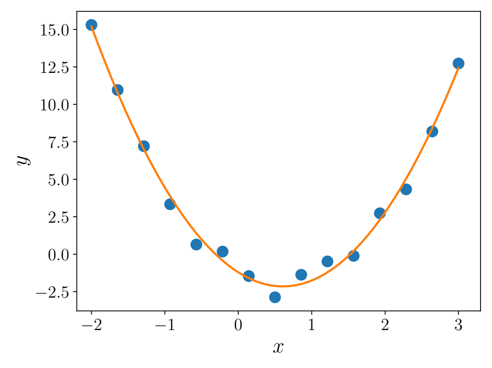
Python: ejemplo 3

```python
import numpy as np

rng = np.random.default_rng(13)

delta = 1.5
x_0, x_1, n = -2, 3, 15
x = np.linspace(x_0, x_1, n)
y = 2.5 * x**2 - 3 * x - 2 + delta * rng.random(x.size)
z = np.polyfit(x, y, 2)
p = np.poly1d(z)
print(p)
print(f"a_0 = {p[0]:.5f}, a_1 = {p[1]:.5f}, a_2 = {p[2]:.5f}")
```

```
$ ./ejemplo-03.py
      2
2.55 x - 3.099 x - 1.205
a_0 = -1.20479, a_1 = -3.09868, a_2 = 2.54970
```



Python: ejemplo 4

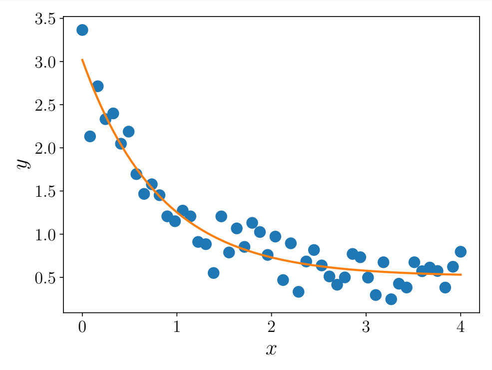
```python
import numpy as np
from scipy.optimize import curve_fit

def modelo(x, a, b, c):
    return a * np.exp(-b * x) + c

rng = np.random.default_rng(13)
x_datos = np.linspace(0, 4, 50)
y = modelo(x_datos, 2.5, 1.3, 0.5)
y_ruido = 0.2 * rng.normal(size=x_datos.size)
y_datos = y + y_ruido

popt, pcov = curve_fit(modelo, x_datos, y_datos)
print(popt)
```

```
> ./ejemplo-04.py
[2.50685815 1.21831291 0.51137751]
```



Lecturas recomendadas I

- R.L. Burden, D.J. Faires y A.M. Burden. *Análisis numérico*. 10.ª ed. Mexico: Cengage Learning, 2017. Capítulo 8.
- E. Kreyszig, H. Kreyszig y E.J. Norminton. *Advanced Engineering Mathematics*. Hoboken, USA: John Wiley & Sons, Inc, 2011. Capítulo 25.9.