UNIVERSIDAD DE GUANAJUATO

Universidad de Guanajuato, División de ciencias e ingenierías, Campus León.

Ingeniería Química Sustentable.

Métodos numéricos.

TAREA: Ajuste mínimos cuadrados

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PYTHON

```
[1]
✓ 1s
import pandas as pd
import numpy as np
from scipy.optimize import curve_fit
import matplotlib.pyplot as plt
```

```
[2]
✓ 0s
file_path = "/content/Experimental water adsorption isotherms.xlsx"
df = pd.read_excel(file_path)
```

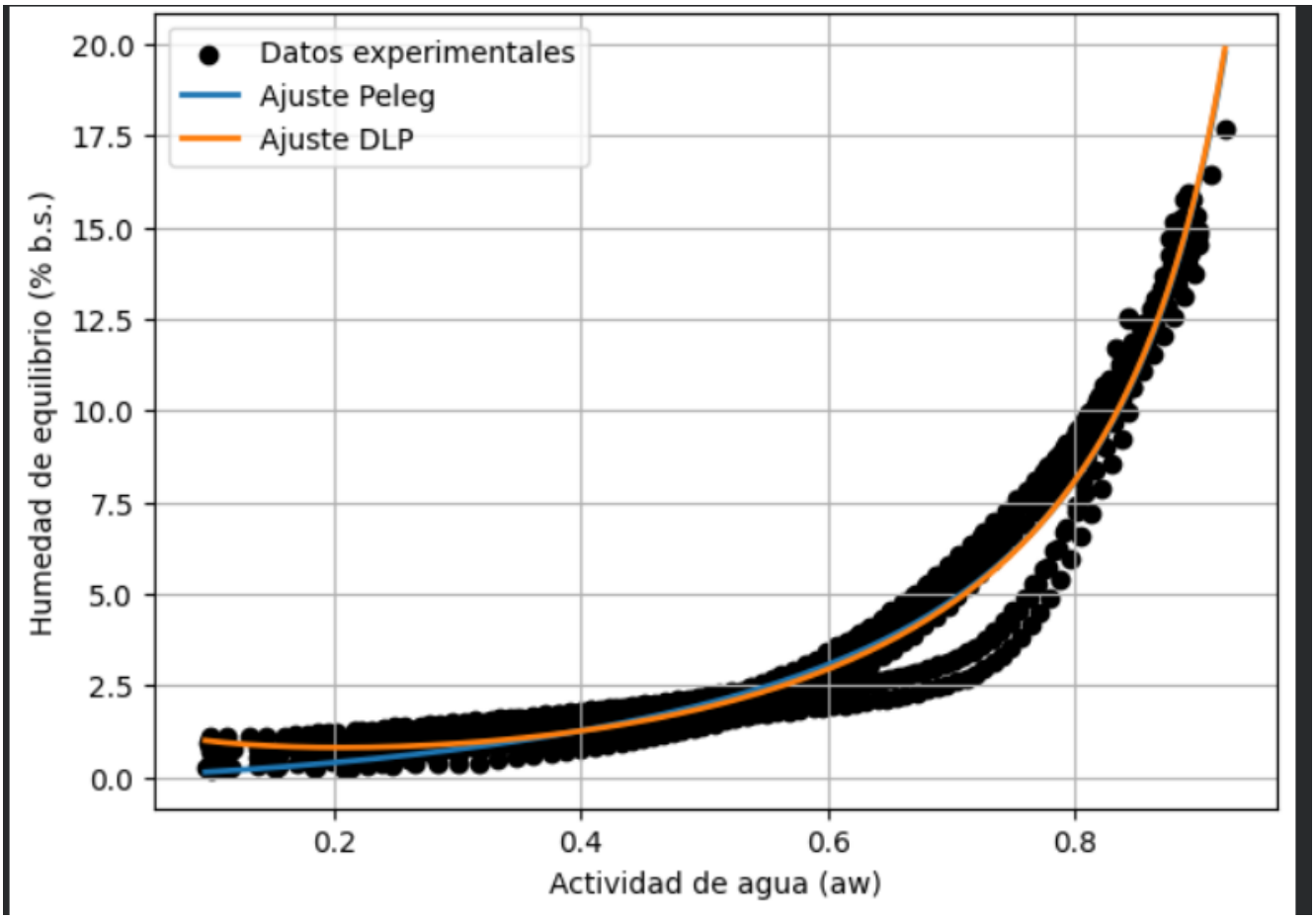
```
[4]
✓ 0s
def peleg_model(aw, b0, b1, b2, b3):
    return (b0 * aw**b1) / (b2 + b3 * aw**b1)

def dlp_model(aw, b0, b1, b2, b3):
    x = np.log(-np.log(aw))
    return b0 + b1*x + b2*x**2 + b3*x**3
```

```
]
0s
types = df["Type"].unique()
for t in types:

    data = df[df["Type"] == t]
    aw = data["Water activity"].values
    Xe = data["Moisture content (% dry basis)"].values
    p0_peleg = [1, 1, 1, 1]
    popt_peleg, _ = curve_fit(peleg_model, aw, Xe, p0=p0_peleg)

    p0_dlp = [1, 1, 1, 1]
    popt_dlp, _ = curve_fit(dlp_model, aw, Xe, p0=p0_dlp)

    aw_fit = np.linspace(min(aw), max(aw), 200)
    Xe_peleg = peleg_model(aw_fit, *popt_peleg)
    Xe_dlp = dlp_model(aw_fit, *popt_dlp)
```

```
chi2_peleg = np.sum((Xe - peleg_model(aw, *popt_peleg))**2)
chi2_dlp = np.sum((Xe - dlp_model(aw, *popt_dlp))**2)

print(f"\n===== {t} =====")
print("PELEG PARAMETERS:", popt_peleg)
print("Chi² Peleg:", chi2_peleg)
print("DLP PARAMETERS:", popt_dlp)
print("Chi² DLP:", chi2_dlp)
```

```
...
===== Ground-Fine =====
PELEG PARAMETERS: [ 1.47950179  1.40248032  0.44159964 -0.42022536]
Chi² Peleg: 455.05812335472183
DLP PARAMETERS: [ 1.11527588 -1.42121882  1.73581049 -0.27330228]
Chi² DLP: 423.34953819066254
```

```python
plt.figure(figsize=(7,5))
plt.scatter(aw, Xe, label="Datos experimentales", color="black")
plt.plot(aw_fit, Xe_peleg, label="Ajuste Peleg", linewidth=2)
plt.plot(aw_fit, Xe_dlp, label="Ajuste DLP", linewidth=2)
plt.title(f"Isoterma - {t}")
plt.xlabel("Actividad de agua (aw)")
plt.ylabel("Humedad de equilibrio (% b.s.)")
plt.legend()
plt.grid(True)
plt.show()
```



C

```
#include <stdio.h>
#include <math.h>

#define MAX 500
#define LR 0.00000001
#define ITER 40000

double aw[MAX], Xe[MAX];
int N;

double peleg(double aw, double b0, double b1, double b2, double b3) {
   double t = pow(aw, b1);
   double denom = b2 + b3 * t;

   if (fabs(denom) < 1e-9)
      denom = (denom < 0 ? -1e-9 : 1e-9);

   return (b0 * t) / denom;
}

double dlp(double aw, double b0, double b1, double b2, double b3) {
if (aw <= 0 || aw >= 1) return 0;
double x = log(-log(aw));
return b0 + b1*x + b2*x*x + b3*x*x*x;
}
```

```
double chi2_peleg(double b0, double b1, double b2, double b3) {
double sum = 0;
for(int i=0; i<N; i++) {
double pred = peleg(aw[i], b0, b1, b2, b3);
sum += pow(Xe[i] - pred, 2);
}
return sum;
}

double chi2_dlp(double b0, double b1, double b2, double b3) {
double sum = 0;
for(int i=0; i<N; i++) {
double pred = dlp(aw[i], b0, b1, b2, b3);
sum += pow(Xe[i] - pred, 2);
}
return sum;
}

int main() {

//Leer datos de archivo externo
FILE *f = fopen("datos.csv", "r");
if(!f) {
  printf("No se pudo abrir datos.csv\n");
  return 1;
```

```
}

N = 0;
while(!feof(f)) {
  fscanf(f, "%lf,%lf", &aw[N], &Xe[N]);
  N++;
}
fclose(f);

printf("Se leyeron %d datos.\n", N);

//Modelo Peleg
double b0 = 0.1;
double b1 = 0.1;
double b2 = 0.5;
double b3 = 0.1;

for(int it=0; it<ITER; it++) {

  double d0=0, d1=0, d2=0, d3=0;

  for(int i=0; i<N; i++) {

    double t = pow(aw[i], b1);
    double denom = b2 + b3 * t;
```

```
      if (fabs(denom) < 1e-12) denom = 1e-12;

      double p = peleg(aw[i], b0, b1, b2, b3);
      double e = Xe[i] - p;
      double dp_db0 = t / denom;
      double dp_db1 = (b0 * t * log(aw[i]) * b2) / (denom * denom);
      double dp_db2 = -(b0 * t) / (denom * denom);
      double dp_db3 = -(b0 * t * t) / (denom * denom);

      d0 += -2 * e * dp_db0;
      d1 += -2 * e * dp_db1;
      d2 += -2 * e * dp_db2;
      d3 += -2 * e * dp_db3;
    }

    b0 -= LR * d0;
    b1 -= LR * d1;
    b2 -= LR * d2;
    b3 -= LR * d3;
  }

  printf("MODELO PELEG \n");
  printf("b0 = %lf\n", b0);
  printf("b1 = %lf\n", b1);
  printf("b2 = %lf\n", b2);
  printf("b3 = %lf\n", b3);
```

```
printf("Chi2 final = %lf\n", chi2_peleg(b0,b1,b2,b3));


//Modelo DLP
double c0 = 2.0, c1 = 0.5, c2 = 0.1, c3 = 0.05;


for(int it=0; it<ITER; it++) {


  double d0=0, d1=0, d2=0, d3=0;


  for(int i=0; i<N; i++) {


    if (aw[i] <= 0 || aw[i] >= 1) continue;


    double x = log(-log(aw[i]));
    double p = dlp(aw[i], c0, c1, c2, c3);
    double e = Xe[i] - p;


    double dp_dc0 = 1;
    double dp_dc1 = x;
    double dp_dc2 = x*x;
    double dp_dc3 = x*x*x;


    d0 += -2 * e * dp_dc0;
    d1 += -2 * e * dp_dc1;
    d2 += -2 * e * dp_dc2;
    d3 += -2 * e * dp_dc3;
```

```
    }

    c0 -= LR * d0;
    c1 -= LR * d1;
    c2 -= LR * d2;
    c3 -= LR * d3;
}

printf("MODELO DLP\n");
printf("c0 = %lf\n", c0);
printf("c1 = %lf\n", c1);
printf("c2 = %lf\n", c2);
printf("c3 = %lf\n", c3);
printf("Chi2 final = %lf\n", chi2_dlp(c0,c1,c2,c3));

return 0;

}
```

```
Se leyeron 32 datos.
MODELO PELEG
b0 = 1.#QNAN0
b1 = 1.#QNAN0
b2 = 1.#QNAN0
b3 = 1.#QNAN0
Chi2 final = 1.#QNAN0
MODELO DLP
c0 = 2.015865
c1 = 0.482288
c2 = 0.119386
c3 = 0.026214
Chi2 final = 15.694638
```