

PHYS416- Computer Applications in Physics

Homework 5 – Nonlinear Least Squares Curve Fitting

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I pledge that I worked entirely alone on this homework and will not share information about any aspect of this homework with any other persons.

Signature: _____

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import numpy as np

import matplotlib.pyplot as plt

from scipy.optimize import curve_fit

volume = np.array([0.5, 0.8, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0])
pressure = np.array([48.9, 31.2, 24.4, 16.3, 12.3, 9.8, 8.2, 7.0, 6.2, 5.5, 4.9])
R, T = 0.0831446, 300

def van_der_waals(V, a, b):
    return (R * T) / (V - b) - a / (V**2)

params, covariance = curve_fit(van_der_waals, volume, pressure, p0=[1.0, 0.1], bounds=([0,
0], [np.inf, np.inf]), maxfev=10000)

a_fit, b_fit = params

print(a_fit)

print(b_fit)

volume_fine = np.linspace(b_fit + 0.01, max(volume), 500)
pressure_fit = van_der_waals(volume_fine, a_fit, b_fit)

plt.scatter(volume, pressure, color='blue', s=60)
plt.plot(volume_fine, pressure_fit, 'r-', linewidth=3)
plt.xlabel('Volume (L/mol)')
plt.ylabel('Pressure (bar)')
plt.xlim(0, 5.5)
plt.ylim(0, 55)
plt.grid(True, linestyle='--', alpha=0.7)
plt.show()

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a: 1.17085083

b: 0.03498359

