

polFIT – Polynomial Regression and Gibbs–Helmholtz Curve as a Function of Temperature

José Maurício Schneedorf Ferreira da Silva

2026-02-13

Gibbs–Helmholtz curves, or stability curves as a function of temperature, are important in studies of folding, denaturation, and biomolecular interactions (Licata and Liu, 2011). Unlike the linear Van’t Hoff profile, they indicate changes in the heat capacity of the system and exhibit a curvilinear behavior that can be modeled using polynomial fitting.

The *polFIT* program performs polynomial regression using data provided as lists and a user-defined polynomial degree, presenting statistical fitting parameters as well as the scatter plot with the fitted curve superimposed.

1 Equation

Considering a general second-degree polynomial:

$$y = a + bx + cx^2$$

It is possible to approximate the thermodynamic quantities ΔH (enthalpy), ΔS (entropy), and ΔC_p (heat capacity) that describe the phenomenon as a function of temperature using the relationships below (Waelbroeck and Van Obberghen, 1979):

$$\Delta G = a + bT + cT^2$$

$$\Delta S = - \left(\frac{\partial \Delta G}{\partial T} \right)_p = -(b + 2cT)$$

$$\Delta H = \left(\frac{\partial(\Delta G/T)}{\partial(1/T)} \right)_p = \Delta G + T \Delta S = a - cT^2$$

$$\Delta C_p = \left(\frac{\partial \Delta H}{\partial T} \right)_p = -2cT$$

Thus, by solving for the polynomial coefficients, the thermodynamic quantities involved in the process can be obtained.

2 Files

1. Main program
2. Scatter plot program
3. Residuals plot program
4. Example
5. Source code
6. This tutorial

3 Usage and example

From a list of x values, a list of y values, and the polynomial degree, *polFIT* returns several fitting parameters. Two additional programs, *polPlot* and *polRes*, generate respectively the scatter plot with the fitted curve and the regression residual plot. The program requires the following data to be entered sequentially on the stack:

```
# Input:
```

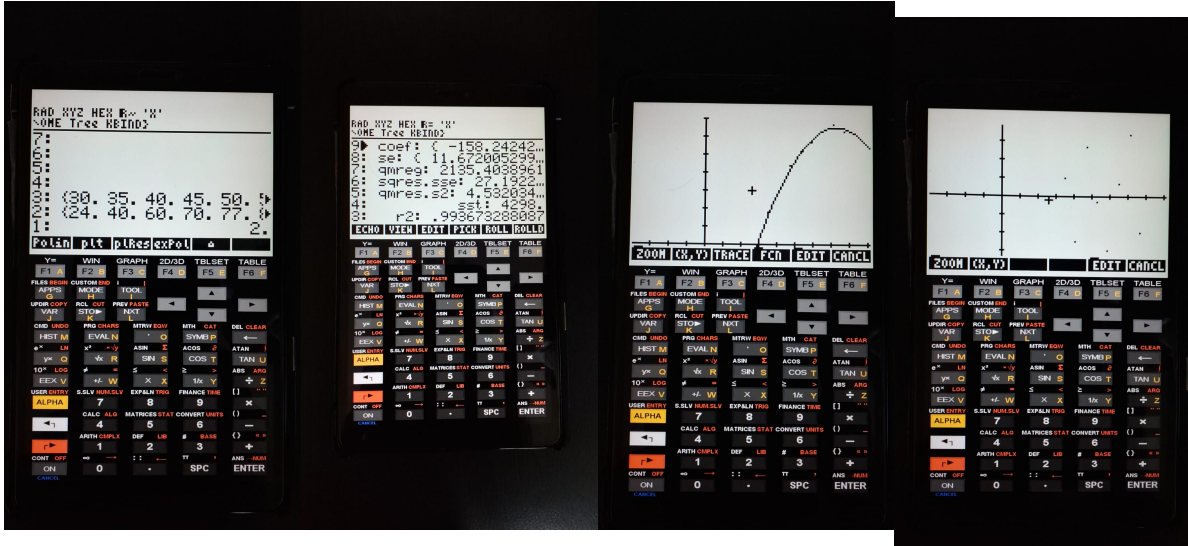
1. List of "x" values;
2. List of "y" values;
3. Polynomial degree.

When running *polFIT*, the following outputs are generated:

Output:

1. coef: polynomial coefficients;
2. se: standard errors of the coefficients;
3. qmreg: mean square of the regression;
4. sqres.sse: sum of squared errors (SSE);
5. qmres.s2: mean square of residuals;
6. sst: total sum of squares;
7. r2: coefficient of determination;
8. F: Snedecor's F value;
9. pval: p-value of the regression.

The polynomial fitting of the example data yields the quantities and graphical profiles illustrated below.



(a) Input of example data. (b) Resulting statistical parameters. (c) Scatter plot with fitted curve. (d) Residual plot.

Figure 1: Execution of the *polFIT* program applied to the example, illustrating data input, statistical results, fitted curve, and residual analysis.

For the second-degree polynomial fit, the estimated coefficients were $a = -158.24$, $b = 7.99$, and $c = -6.5 \times 10^{-2}$. Substituting these values into the equations above, the thermodynamic quantities at 50 K are $\Delta H = -20.1$ kJ/mol, $\Delta S = 1.5$ J/mol/K, and $\Delta C_p = 6.5$ J/mol.

References

1. Licata, V. J., & Liu, C. C. (2011). Analysis of free energy versus temperature curves in protein folding and macromolecular interactions. In *Methods in Enzymology* (Vol. 488, pp. 219–238). Academic Press.
2. Waelbroeck, M., Van Obberghen, E., & De Meyts, P. (1979). Thermodynamics of the interaction of insulin with its receptor. *Journal of Biological Chemistry*, 254(16), 7736–7740.

José Maurício Schneedorf Ferreira da Silva
Dept. Biochemistry, Institute of Biomedical Sciences
Federal University of Alfenas - UNIFAL-MG, Brazil
Email: jose.dasilva@unifal-mg.edu.br

Site: <https://bioquanti.netlify.app>
Lattes: <http://lattes.cnpq.br/0436922594542722>
ORCID: 0000-0002-2031-6315