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THE LEAST-SQUARES FITTING METHOD IN THE UNDERGRADUATE PHYSICS LABORATORIES

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INTRODUCTION

The main purpose of the first Physics lab is to teach students good lab practices, including data analysis. We introduce regression analysis (least squares) in a first lab for Physics courses that may be either calculus or noncalculus based. We apply least squares to a series of experiments used for teaching data fitting via the computer and that allow the study of more complicated physical phenomena than a lab usually covers.

We insist that, before students use the computer, they should plot their "n" data and determine by eyesight if all or part of it can be fit by a straight line, potential, polynomial or exponential relation. By eyesight, they draw the best curve through this data.

When the graphical analysis is complete, the data are entered as "n" pairs of (x,y) data into a computer program (NUMERAL[1]) that permits to choose the regression: potential, exponential or polynomial relation. Values for parameters, correlation coefficient R^2, variance (σ) and errors of parameters are obtained. The best data adjustment is achievement, if they evaluated the variance and the effective errors associated to the estimated parameters.

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LEAST-SQUARES ANALYSIS NONCALCULUS

In the first course of physics lab, we teach least-squares fitting method non-calculus, we establish nemotechnics rules.
The present paper deals with the use of linear, potential, polynomial least squares analysis in fitting experimental results in which the independent variables are not subject to errors of measurement.

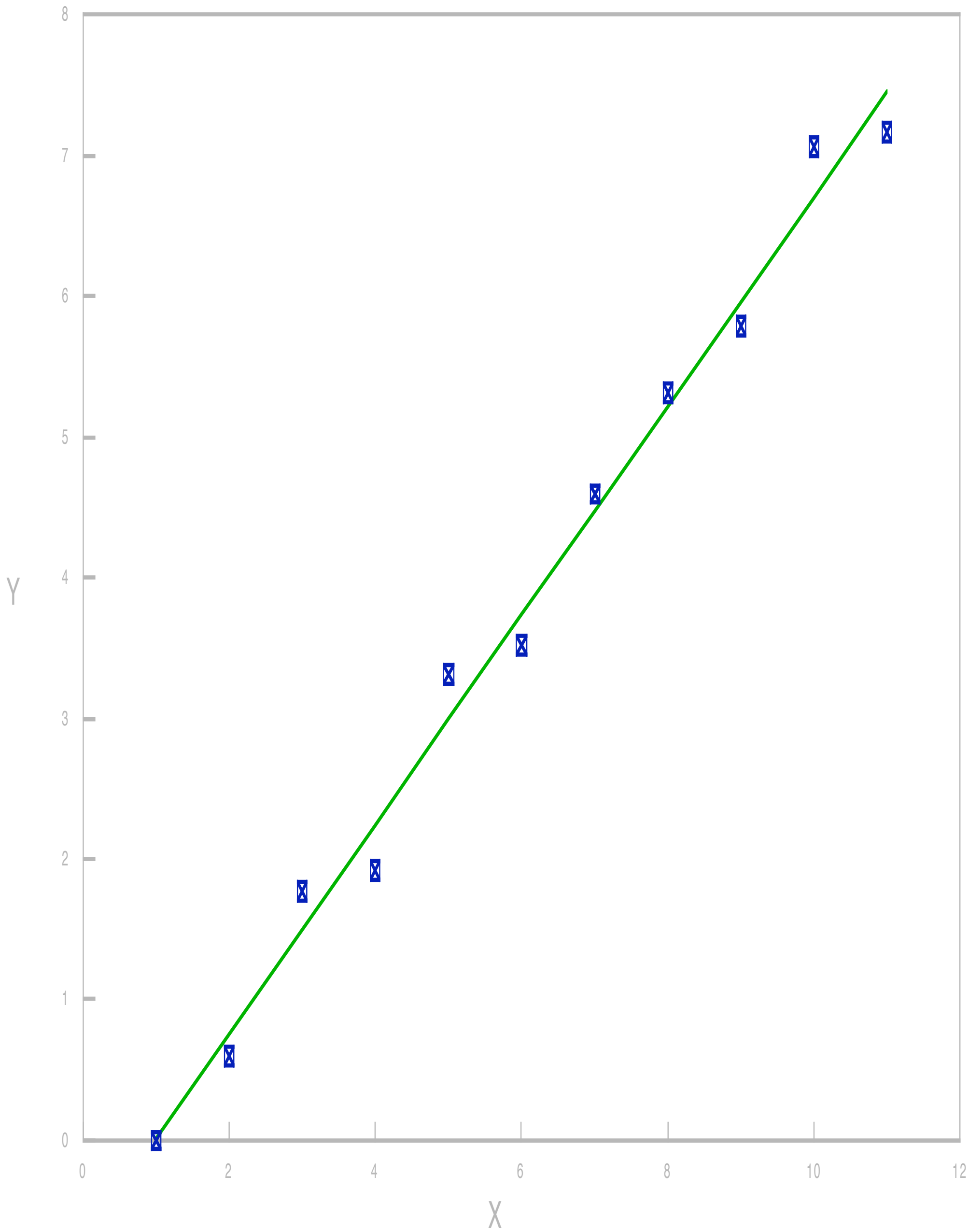

Fig. 1. Plot y vs x showing the experimental points through of the squares. The dashed curve is the standard least-squares plot, y vs x, assuming all $\delta x_i = 0$.

It is asumed here that a number of sets of measurables (X_1,Y_1), $(X_2,Y_2),...,(X_i,Y_i),...(X_n,Y_n)$ has been obtained experimentally, and that the experimenter has reasons to believe that there exists a functional relation among these variables of the form **Y= m X + b**, that would correspond exactly with the observed data if the measurment errors did not exist:

$$
\begin{array}{l}
Y_1 \neq m\,X_1 + b = Y_{1t} \\
\quad " \qquad\quad " \qquad " \qquad " \\
Y_i \neq m\,X_i + b = Y_{it} \\
\quad " \qquad\quad " \qquad " \qquad " \\
Y_n \neq m\,X_n + b = Y_{nt}
\end{array}
\tag{1}
$$

where Y_{it} is the theoretical value of Y_i.

To determinate the values of the coefficients m and b the discrepancy between the values of our measurements Y_i and the corresponding values Y_{it} given by equation (1) should be minimized. We cannot determine exactly the coefficients with only a finite number of observations, but we do want to extract from these data the most probable estimates for the coefficients. The problem is to establish criteria for minimizing the discrepancy and optimizing the estimates of the coefficients. The deviation $\Delta Y_i=Y_i-(mx_i+b)$ should be relatively small $\Delta Y_i \to 0$. The sum of these deviation for i=1,..,n with $\Delta Y_i \simeq 0$ we led to

$$\sum_i^n Y_i = m\sum_i^n X_i + nb \tag{2}$$

multiplying (1) for X_i, the deviation $\Delta(X_i Y_i) = X_i Y_i - m X_i^2 - bX$ is similary small (there are not error in X_i), then $\Delta X_i Y_i \simeq 0$, of the sum of these deviation we obtain

$$\sum_{i=1}^{n} X_i Y_i = m \sum_{i=1}^{n} X_i^2 + b \sum_{i=1}^{n} X_i \tag{3}$$

we wish to solve equations (2-3) for the coefficients m and b.
Suppose our data (X_i, Y_i) were not fit well by straight line. We might construct a more complex function which includes curvature and determine the coefficients of this function to fit the data . The useful function for such a fit is a $\mathbf{Y=a_0+a_1X+a_2X^2}$ then

$$\begin{aligned}
Y_1 &\neq a_0 + a_1 X_1 + a_2 X_1^2 = Y_{1t} \\
&\qquad\quad '' \qquad\quad '' \\
Y_i &\neq a_0 + a_1 X_i + a_2 X_i^2 = Y_{it} \\
&\qquad\quad '' \qquad\quad '' \\
Y_n &\neq a_0 + a_1 X_n + a_2 X_n^2 = Y_{nt}
\end{aligned} \tag{4}$$

we can determine the coefficients $\mathbf{a_0}$**,** $\mathbf{a_1}$ **and** $\mathbf{a_2}$ minimizing the discrepancy between Y_i and $Y_{it} = a_0 + a_1 X_i + a_2 X_i^2$. The deviation $\Delta Y_i \equiv (Y_i - (a_0 + a_1 X_i + a_2 X_i^2)) \to 0$ then of the sum of this deviation we obtain

$$\sum_{i=1}^{n} Y_i = n a_0 + a_1 \sum_{i=1}^{n} X_i + a_2 \sum_{i=1}^{n} X_i^2 \tag{5}$$

The same method aplying to fitting a straight line is adopting, multiplying (4) for X_i and since there are not error in X_i

$$\sum_{i=1}^{n} X_i Y_i = a_0 \sum_{i=1}^{n} X_i + a_1 \sum_{i=1}^{n} X_i^2 + a_2 \sum_{i=1}^{n} X_i^3 \qquad (6)$$

similarly multiplying (4) for X_i^2 , we obtain

$$\sum_{i=1}^{n} X_i^2 Y_i = a_0 \sum_{i=1}^{n} X_i^2 + a_1 \sum_{i=1}^{n} X_i^3 + a_2 \sum_{i=1}^{n} X_i^4 \qquad (7)$$

we find a_0, a_1 and a_2 resolving the equations system (5,6,7).

The extrapolation of these nemotechnics rule to higher-order polynomials is straightforward. If we consider an nth degree polynomial,

$$Y=a_0+a_1X+a_2X^2+...+a_nX^n \qquad (8)$$

then we obtain n+1 equations in n+1 coefficients. The terms on the left sides of the equations range from $\sum Y_i$ to $\sum X_i^n Y_i$ and the terms on the right sides range from "n" to $\sum X_i^{2n}$.

LEAST-SQUARES ANALYSIS WITH CALCULUS

In this section, we discuss the problem of least-squares approximation by polynomials. We propose

$$y = \sum_i A_i f_i(x) \tag{9}$$

where the $f_i(x)$ are an a priore select set of function ($f_i(x)$ imply the construction of a mathematical model), and the A_i are parameters which must be determined. The general idea is to choose A_i so that the deviations

$$(\Delta y)^2 = \sum_{k=1}^{n} (y_k - y_c)^2 \tag{10}$$

are simultaneously made as small as possible (where y_k is the experimental variable), if one to minimize $(\Delta y)^2$ then

$$\sum_j \frac{\partial (\Delta y)^2}{\partial A_j} \delta A_j = \sum_j 2(Y_k - \sum_i A_i f_i(x_k)) \sum_j (-f_j(x_k)) = 0 \tag{11}$$

it is

$$\sum_{kij} x_k f_j(x_k) = \sum_{kij} A_i f_i(x_k) f_j(x_k) \tag{12}$$

this equation in matricial form, we conduce to

$A=(TT^t)^{-1}T$

where

$$T=\begin{pmatrix} f_{11}f_{12}\cdots f_{1n} \\ f_{21}f_{22}\cdots f_{2n} \\ . \quad . \quad . \\ f_{n1}\,f_{n2}\cdots f_{nn} \end{pmatrix}, y=\begin{pmatrix} y_1 \\ y_2 \\ . \\ y_n \end{pmatrix}$$

with T^t the transpose of T.

In like manner we calculation the errors in A_i, the effective variance method we conduce to [2]

$$\delta(A_i)=\frac{\sigma(A_i)}{\sqrt{n}}\equiv\frac{\sigma y(TT^t)_{ii}^{-1}}{\sqrt{n}}$$

where σy is the variance of y, and where the (ii) is the diagonal entries of the matrix.

THE MODEL SELECTION PROBLEM

The aim of FIMAS projet is to design teaching strategies in order to improve students understanding the application of the method the least-squares fitting. The problem of selecting an effective or good or best model arises in a wide variety of problems. Engineering models frequently require functional representations of empirical data that may be defined at arbitrary intervals. A least-squares fitted polynomial provides a simple approach to the problem. Using least-squares fitting, students study physics systems.

One of the experiments that the students do in the lab is to determinate the wavelength of light with a ruler [Shalow]. In the figure 2. we plot

$$Y = \frac{d}{2}\frac{Dy_n{}^2 - Dy_0{}^2}{X_0^2} \quad \text{versus "n"}$$

$$\frac{d}{2}\frac{Dy_n{}^2 - Dy_0{}^2}{X_0^2} = \lambda n$$

If the data set have a polynomial regression, what it is the best polynomial?. The answer for this question is to determinate the variance and the effective errors associated to the estimated parameters . We analyse the local minimums of the variance plot versus polynomial order, then the best polynomial is those with minimums errors parameters.

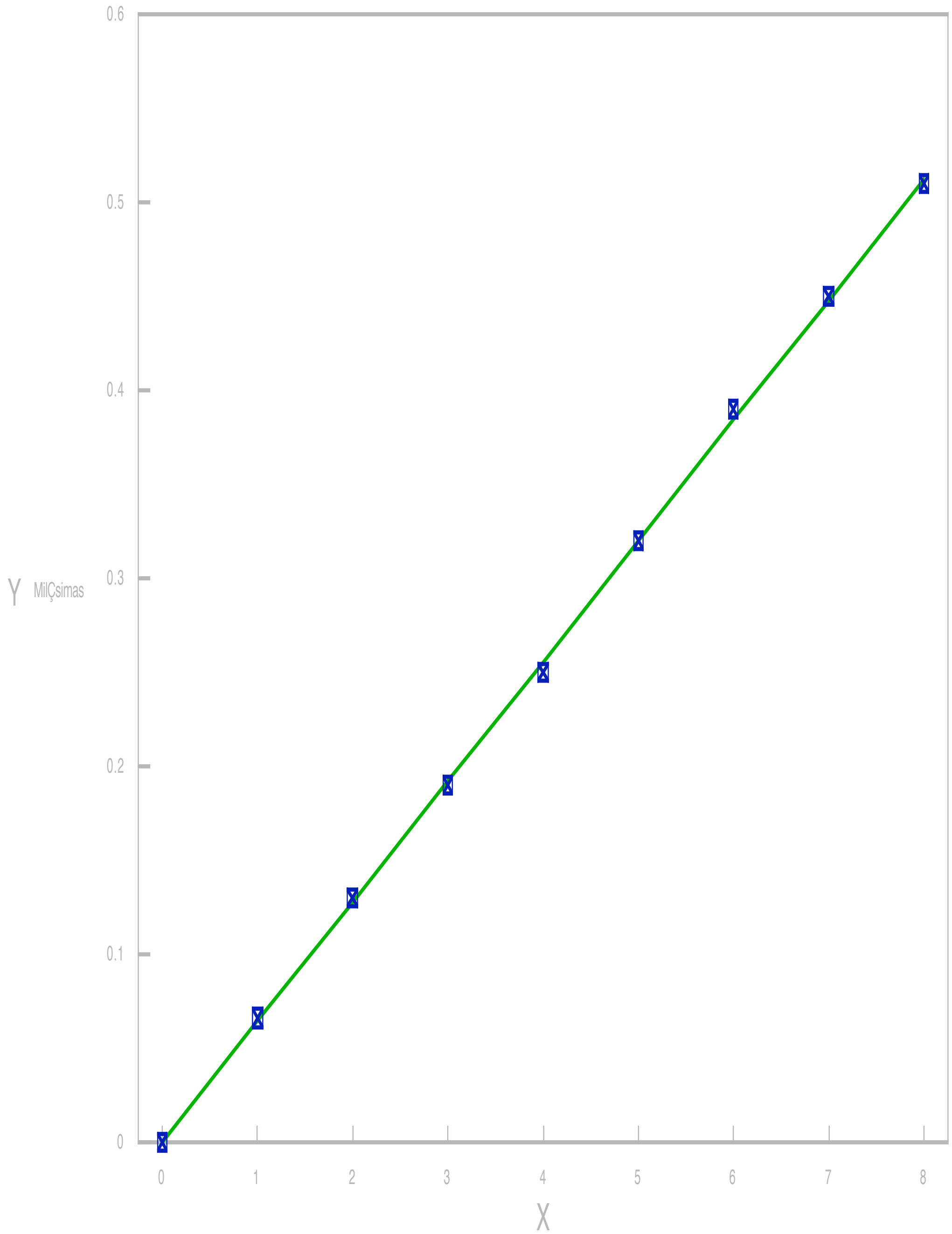

Fig. 2. Determination the wave length of light with a ruler.

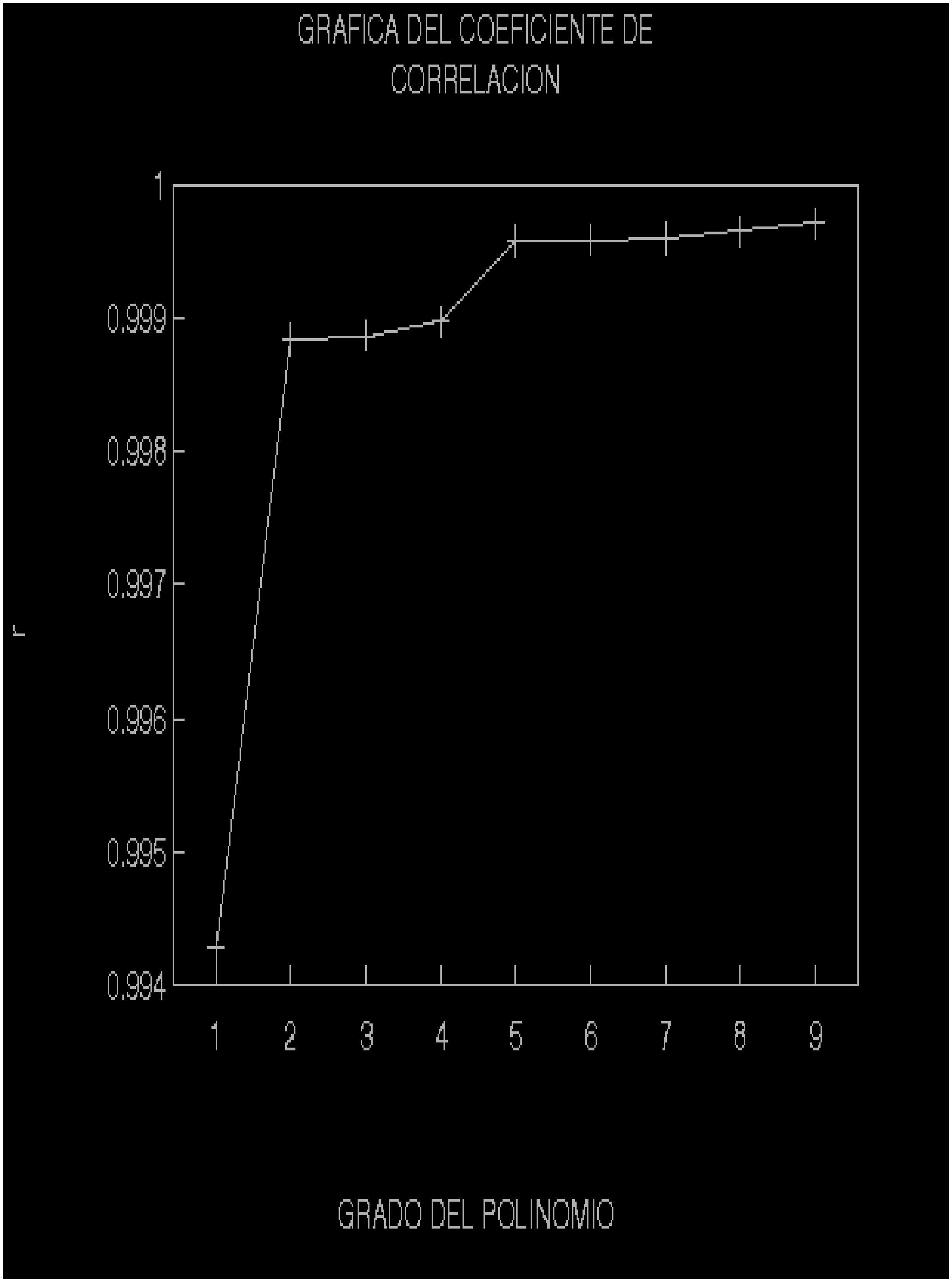

Fig. 3. "r" versus polynomials order, anomaly behavior.

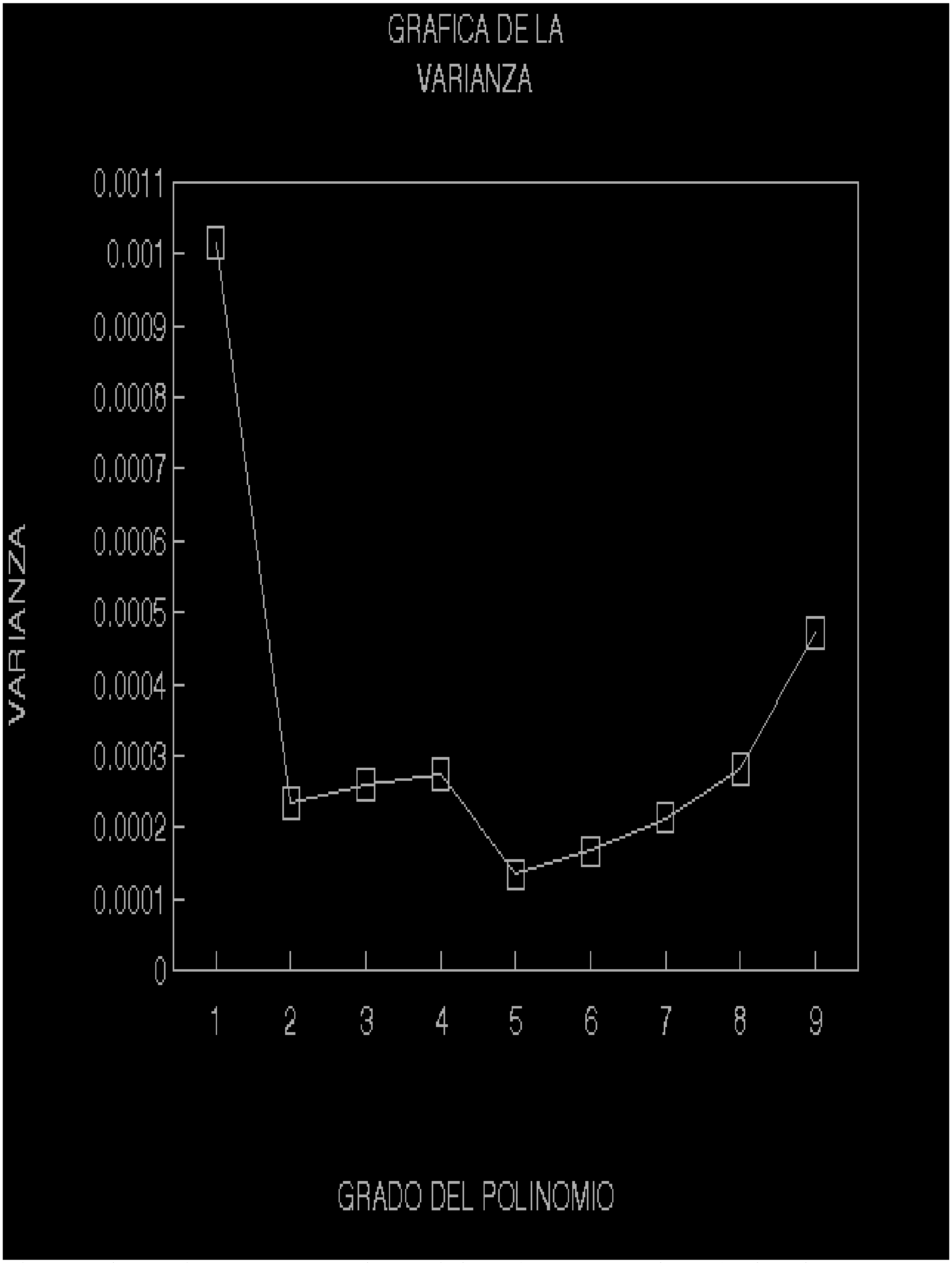

Fig. 4. Plot variance versus polynomials order. We analyse the local minimums.