MATHEMATICAL METHODS OF ANALYSIS AND EXPERIMENTAL DATA PROCESSING (Or Methods of Curve Fitting)

In this chapter, we will examine some methods of analysis and data processing; data obtained as a result of a given experiment. The exposition will begin with the study of simple analytic procedures of construction of empirical functional dependences using the Method of Least Squares.

1. THE METHOD OF LEAST SQUARES.

Let's suppose that as a result of an execution of a series of measurements in a given experiment, the following data table was obtained.

Table 1.

x	x_1	x_2	x_3	...	x_n
$f(x)$	y_1	y_2	y_3	...	y_n

It is required to find a formula that analytically expresses this functional dependence. Of course, we can use Interpolation Methods, for instance, Lagrange's Interpolation Polynomial or Newton's Divided Difference Interpolation Formula, whose values at the interpolation nodes $x_1, x_2,..., x_n$, will match with Table 1's corresponding values of $f(x)$. Nevertheless, occasionally, this function-and-interpolation-value matching at the given nodes could not mean a matching of characters of behavior between $f(x)$ and the interpolation function. The demand that these values should match at the nodes is much more unjustified, if the values of $f(x)$, obtained as a result of the given measurements, are doubtful.

We will formulate the problem so that from the beginning and, for sure, the character of the given function is actually considered, that is, we will find the function of type

$$y = F(x) \qquad (1)$$

at the points $x_1, x_2,..., x_n$, that best "fits" Table 1's $y_1, y_2,..., y_n$ values.

The type of function F that best fits these data can be defined as follows: using Table 1, plot the points of f on a coordinate plane and sketch a smooth curve which reflects better the distribution character of the given points (see Fig. 1). The obtained curve establishes the type of function that best fits these data, that is, the best "curve fitting" for the given data. (It is frequently one of the simple analytic functions)

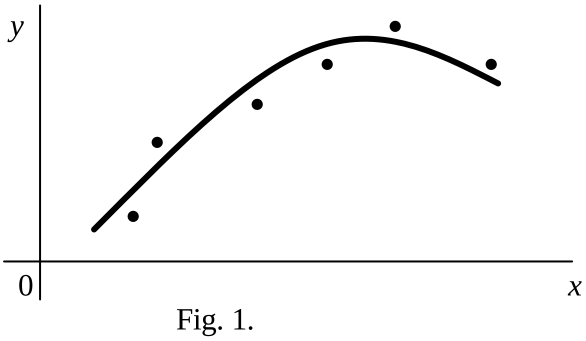

Fig. 1.

It is fair to mention that a rigorous functional dependence for Table 1's experimental data is seldom observed, since each of the involved magnitudes can depend on many random factors. Nevertheless, formula (1) (which is called *empirical formula* or *regression equation* of y on x) is of such a point of interest that allows to find the values of f for values of x that are not in Table 1, fitting in that way the results of the measurements for the corresponding y-magnitude. This approach is justified due to the practical utility of the obtained formula.

We will examine one of the most widespread methods to find formula (1). We will assume that the approximation function F at $x_1, x_2, \ldots, x_n$, has values

$$\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_n. \qquad (2)$$

The demand of proximity of Table 1's $y_1, y_2, \ldots, y_n$ values with values (2) is justified as follows: let's examine the group of Table 1's values and group (2) as the coordinates of two points in an n-dimensional space. Under this assumption, the problem of functional approximation can be formulated as follows: find a function F such that the distance between the points $M(y_1, y_2, \ldots, y_n)$ and $M(\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_n)$ is minimum. Using the metric of an Euclidean Space, it is required that the magnitude

$$\sqrt{(y_1 - \bar{y}_1)^2 + (y_2 - \bar{y}_2)^2 + \ldots + (y_n - \bar{y}_n)^2} \qquad (3)$$

is minimum, which is equivalent to say that the sum of squares

$$(y_1 - \bar{y}_1)^2 + (y_2 - \bar{y}_2)^2 + \ldots + (y_n - \bar{y}_n)^2 \qquad (4)$$

is minimum.

Thus, the problem of approximating function f can now be formulated as follows: for a function f given in Table 1, find a function F of a certain type such that the sum of squares (4) is minimum. This problem is called *Approximation of "f" using "The Method of Least squares"*.

As functions of approximation, depending on the graphical character of the points of function f, are usually used the following ones:

1. $y = ax + b$ (**Linear Regression**).
2. $y = ax^2 + bx + c$ (**Regression of Degree Two**).
3. $y = ax^m$ (**Power Function or Geometric Regression**).
4. $y = a.e^{mx}$ (**Exponential Function**).
5. $y = 1/(ax + b)$ (**Linear Rational Function**).
6. $y = a.\ln x + b$ (**Logarithmic Function**).
7. $y = (a/x) + b$ (**Hyperbola**).
8. $y = x/(ax + b)$ (**Rational Function**).

Where a, b, c, m are parameters. When the type of approximation function is established, the problem is reduced to finding the values of these parameters.

Let's examine the method of finding the parameters of an approximation function in the general case of an approximation function with three parameters,

$$y = F(x, a, b, c). \qquad (5)$$

Thus $F(x_i, a, b, c) = \overline{y}_i$, $i = 1, 2,..., n$. The sum of the square differences for the corresponding values of *f* and *F* can be written as

$$\sum_{i=1}^{n} [y_i - F(x_i, a, b, c)]^2 = \Phi(a, b, c).$$

This sum is a function $\Phi(a, b, c)$ of three variables: the parameters *a*, *b*, *c*. Thus, the problem is reduced to searching a minimum. We will use the necessary condition for the existence of an optimum:

$$\partial\Phi/\partial a = 0, \quad \partial\Phi/\partial b = 0, \quad \partial\Phi/\partial c = 0,$$

that is,

$$\begin{aligned} &\sum_{i=1}^{n} [y_i - F(x_i, a, b, c)]\, F_a^{'}(x_i, a, b, c) = 0, \\ &\sum_{i=1}^{n} [y_i - F(x_i, a, b, c)]\, F_b^{'}(x_i, a, b, c) = 0, \\ &\sum_{i=1}^{n} [y_i - F(x_i, a, b, c)]\, F_c^{'}(x_i, a, b, c) = 0. \end{aligned} \qquad (6)$$

Resolving this system of three equations with three unknowns; the parameters *a*, *b*, *c*, we will obtain a concrete type of the search function $F(x, a, b, c)$. Note that the change of the number of parameters does not alter the essence of approaching the problem, and it is expressed only in the change of the number of equations of system (6). It is natural to expect that the values of the found function $F(x, a, b, c)$ at the points $x_1, x_2,..., x_n$ will be different of Table 1's $y_1, y_2,..., y_n$ values. The values of the differences

$$y_i - F(x_i, a, b, c) = \varepsilon_i \quad (i = 1, 2,...,n) \qquad (7)$$

are called *deflections* (or *deviations*) of the measured *y*-values in relation to those ones calculated using formula (5). For the found empirical formula (5) and in accordance with Table 1, the sum of the square deflections can be expressed as

$$s = \sum_{i=1}^{n} e_i^2, \qquad (8)$$

which, according to The Method of Least Squares for the given type of approximation function and the values found for parameters *a*, *b*, *c*, must be minimum.

Of two different approximations of the same tabulated function using The Method of Least Squares, it is considered better that one for which the sum (8) has a minimum value.

2. FINDING THE TYPE OF APPROXIMATION FUNCTIONS CALLED LINEAR REGRESSION AND REGRESSION OF DEGREE TWO.

Let's determine the approximation function called Linear Regression,

$$F(x, a, b) = ax + b. \qquad (9)$$

The partial derivatives with respect to the parameters are

$$\partial F/\partial a = x, \quad \partial F/\partial b = 1.$$

The system of type (6) can be written as

$$\sum (y_i - ax_i - b)x_i = 0,$$
$$\sum (y_i - ax_i - b) = 0.$$

(In the sum $\sum$, index i varies from 1 to n). Thus we get:

$$\sum x_i y_i - a\sum x_i^2 - b\sum x_i = 0, \qquad (10)$$
$$\sum y_i - a\sum x_i - nb = 0,$$

and dividing each equation by n,

$$\left(\frac{1}{n}\sum x_i^2\right) a + \left(\frac{1}{n}\sum x_i\right) b = \frac{1}{n}\sum x_i y_i,$$
$$\left(\frac{1}{n}\sum x_i\right) a + b = \frac{1}{\mathrm{n}}\sum y_i.$$

Keeping in mind the following designations:

$$\frac{1}{n}\sum x_i = M_x, \ \frac{1}{\mathrm{n}}\sum y_i = M_y,$$
$$\frac{1}{n}\sum x_i y_i = M_{xy}, \ \frac{1}{\mathrm{n}}\sum x_i^2 = M_{x^2}. \qquad (11)$$

We conclude that the last system can be written as

$$M_{x^2} a + M_x b = M_{xy}, \qquad (12)$$
$$M_x a + b = M_y.$$

The coefficients M_x, M_y, M_{x^2}, M_{xy} of system (12) are numbers that in each concrete problem of approximation can easily be calculated using formulae (11), where x_i, y_i are the values in Table 1.

Let's determine the Second Degree Approximation Function or Regression of Degree Two,

$$F(x, a, b, c) = ax^2 + bx + c. \qquad (13)$$

Its partial derivatives are

$$\partial F/\partial a = x^2, \quad \partial F/\partial b = x, \quad \partial F/\partial c = 1.$$

Thus, the system of type (6) can be written as

$$\begin{gathered} \sum (y_i - ax_i^2 - bx_i - c)x_i^2 = 0, \\ \sum (y_i - ax_i^2 - bx_i - c)x_i = 0, \\ \sum (y_i - ax_i^2 - bx_i - c) = 0. \end{gathered}$$

After a series of transformations, we get a system of three linear equations with unknowns a, b, c. The system's coefficients, as in the case of a linear regression, are calculated using Table 1's known data,

$$\begin{gathered} M_{x^4}\, a + M_{x^3}\, b + M_{x^2}\, c = M_{x^2y}, \\ M_{x^3}\, a + M_{x^2}\, b + M_x\, c = M_{xy}, \qquad (14) \\ M_{x^2}\, a + M_x\, b + c = M_y. \end{gathered}$$

Here, we have used (11) and also the following designations:

$$\frac{1}{n}\sum x_i^{\,4} = M_{x^4}, \ \frac{1}{\mathrm{n}}\sum x_i^{\,3} = M_{x^3}, \ \frac{1}{n}\sum x_i^{\,2} y_i = M_{x^2y}. \qquad (15)$$

3. FINDING THE OTHER TYPES OF APPROXIMATION FUNCTIONS.

We will show that the problem of finding approximation functions $F(x, a, b)$ with two parameters of the type of the eight ones listed above can be reduced to finding the parameters of a linear function.

3.1. Power Function (Geometric Regression).

Find an approximation function of type

$$F(x, a, m) = ax^m. \qquad (16)$$

Suppose that in Table 1, both x-values and y-values are positive. Extracting the natural logarithm to (16), assuming $a > 0$, we get:

$$\ln F = \ln a + m \ln x. \qquad (17)$$

Since function F is an approximation function for function f, function $\ln F$ will be an approximation for $\ln f$. Let's make the substitution $u = \ln x$. Thus, as it follows from (17), $\ln F$ will be a function of u, say $\Phi(u)$.

Making

$$m = A, \quad \ln a = B, \qquad (18)$$

equation (17) can be expressed as

$$\Phi(u, A, B) = Au + B, \qquad (19)$$

that is, the problem is reduced to finding an approximation function of linear type.

Keeping in mind the above conditions, in order to find the required approximation function, we will proceed as follows:

1. In accordance with Table 1, construct a new table which contains the natural logarithms of both x and y.
2. Using this new table, find the parameters A and B (see Paragraph 2) of the approximation function of type (19).
3. Using formulae (18), find the values of parameters a, m, and substitute them in (16).

3.2. Exponential Function.

Suppose that Table 1 is such that its approximation function is of exponential type:

$$F(x, a, m) = a^x \exp(mx), \; a > 0. \qquad (20)$$

Extracting the natural logarithm to (20), we get:

$$\ln F = \ln a + mx. \qquad (21)$$

According to (18), equation (21) can be expressed as

$$\ln F = Ax + B. \qquad (22)$$

Consequently, to find the approximation function of type (20), it is required to extract the natural logarithms to the values of f in Table 1 and considering them along with its x-values, construct for this new table of values a function of type (22). After that and according to designations (18), it only remains to obtain the values of the search parameters *a*, *b*, and to substitute them in formula (20).

3.3. Linear Rational Function.

Find an approximation function of type

$$F(x, a, b) = 1/(ax + b). \qquad (23)$$

Formula (23) can be expressed as

$$1/[F(x, a, b)] = ax + b.$$

Keeping in mind the last expression, to find the values of parameters *a*, *b* and in accordance with Table 1, it is required to construct a new table in which its *x*-values remain unchanged, and those ones of *f* are substituted by their reciprocals. After that and in accordance with the new obtained table, one can find the approximation function *ax* + *b*. The search parameters *a*, *b* are then substituted in formula (23).

3.4. Logarithmic Function.

Suppose that we want to find an approximation function of type

$$F(x, a, b) = a \cdot \ln x + b. \qquad (24)$$

In order to transform (24) into a linear function, it is enough to make the substitution ln *x* = *u*. So, to determine the values of *a* and *b*, it is necessary to extract the natural logarithm to Table 1's *x*-values and examining the obtained results along with those ones of function *f*, find, for the new obtained table, the approximation function of linear type. The coefficients *a*, *b* of the search function should be substituted in formula (24).

3.5. Hyperbola.

If the graph of points plotted according to Table 1 turns out to be the branch of a hyperbola, the approximation function has the form

$$F(x, a, b) = (a/x) + b. \qquad (25)$$

For its transformation into a linear function, we make the substitution $u = 1/x$.

$$\Phi(u, a, b) = a \cdot u + b. \qquad (26)$$

So, to determine the approximation function of type (26), Table 1's *x*-values should be substituted by their reciprocals and then, for the new table, find the approximation (26) of linear type. The coefficients *a*, *b* of the obtained function are then substituted in formula (25).

3.6. Rational Function.

Suppose that the approximation function has the form

$$F(x, a, b) = x/(ax + b). \qquad (27)$$

Thus, we get:

$$1/[F(x, a, b)] = a + (b/x),$$

so, the problem turns out to be one of the same form of the previous case. In fact, if in Table 1 we change the values of both x and y by their reciprocals then, according to the formulae $z = 1/x$, $u = 1/y$, we find for the new table of values an approximation function of type $u = bz + a$. The values of a, b are then substituted in formula (27).

Example. Construct an approximation function using the Method of Least Squares for the functional dependence given by the following table:

Table 2.

x	1.1	1.7	2.4	3.0	3.7	4.5	5.1	5.8
y	0.3	0.6	1.1	1.7	2.3	3.0	3.8	4.6

The graph of points is shown in Fig. 2. To compare the quality of this approximation, consider, at the same time, two approximation curves for the given function: the linear regression $y = ax + b$ and the power fitting $y = cx^m$. After finding the values for parameters a, b, c, and m, the sum of the square deflections (8) can be found to establish which of these two approximations is better.

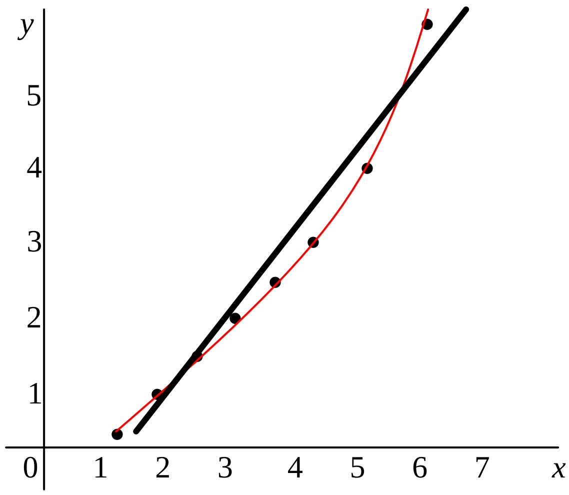

Fig. 2.

In the case of the linear regression, the values of parameters a, b are found using system (12), whose coefficients are calculated according to Table 1's data and in accordance with designations (11). In order to compute the coefficients of the given system, keep in mind Table 2 and construct an auxiliary table (Table 3) whose last row corresponds to the values of the sums of the terms of the corresponding column.

Table 3.

x	y	xy	x^2
1.1	0.3	0.33	1.21
1.7	0.6	1.02	2.89
2.4	1.1	2.64	5.76
3.0	1.7	5.10	9.00
3.7	2.3	8.51	13.69
4.5	3.0	13.50	20.25
5.1	3.8	19.38	26.01
5.8	4.6	26.68	33.64
27.3	17.4	77.16	112.45

Dividing the obtained sums by the number of elements $n = 8$, in accordance with formulae (11), we get:

$$M_x = 3.412,\ M_y = 2.175,$$
$$M_{xy} = 9.645,\ M_{x^2} = 14.056.$$

Let's form now the system of type (12):

$$14.056a + 3.412b = 9.645$$
$$3.412a + b = 2.175.$$

Its solution, applying Cramer's Rule, is $a = 0.921$, $b = -0.968$. Thus, the approximation function $y = F(x, a, b)$ can be written as

$$y = 0.921x - 0.968. \qquad (28)$$

To determine the values of the parameters c, m of the power fitting, as it follows from Paragraph 3.1, a new table with the natural logarithms of both the x-values and y-values must be constructed. Denote the values of the new corresponding variables u and z by $u = \ln x$, $z = \ln y$. According to the new table's numerical data, form the system of equations of type (12):

$$M_{u^2} A + M_u B = M_{uz} \qquad (29)$$
$$M_u A + B = M_z,$$

whose coefficients are the numbers calculated using the new table and formulae (11), while unknowns A and B are related to the search parameters by the correlations

$$A = m,\ B = \ln c.$$

Table 4.

u	z	uz	u^2
0.095	-1.204	-0.114	0.009
0.531	-0.511	-0.271	0.282
0.875	0.095	0.083	0.766
1.099	0.531	0.584	1.208
1.308	0.833	1.090	1.711
1.504	1.099	1.653	2.262
1.629	1.335	2.175	2.654
1.758	1.526	2.683	3.091
8.799	3.704	7.883	11.983

To find the coefficients of system (29), construct an auxiliary table (Table 4). Dividing the values of the last row of Table 4 by 8, we obtain:

$$M_u = 1.1,\ M_z = 0.463,\ M_{uz} = 0.985,\ M_{u^2} = 1.498.$$

Let's form the system of type (29):

$$\begin{aligned} 1.498A + 1.1B &= 0.985 \\ 1.1A + B &= 0.463. \end{aligned}$$

Its solution is

$$A = 1.656,\ B = -1.359.$$

Let's find now the values of parameters c and m:

$$m = 1.656,\ c = \exp(-1.359) = 0.257.$$

Therefore, the power fitting can be expressed as

$$y = 0.257x^{1.656}. \qquad (30)$$

Table 5.

x	y	$0.921x$-0.968	ε_1	ε_1^2	$0.257x^{1.656}$	ε_2	ε_2^2
1.1	0.3	0.0451	0.2549	0.0650	0.3009	-0.0009	0.0000
1.7	0.6	0.5977	0.0023	0.0000	0.6188	-0.0188	0.0004
2.4	1.1	1.2424	-0.1424	0.0203	1.0954	0.0046	0.0000
3.0	1.7	1.7950	-0.0950	0.0090	1.5851	0.1149	0.0132
3.7	2.3	2.4397	-0.1397	0.0195	2.2432	0.0568	0.0032
4.5	3.0	3.1765	-0.1765	0.0312	3.1021	-0.1021	0.0104
5.1	3.8	3.7291	0.0709	0.0050	3.8165	-0.0165	0.0003
5.8	4.6	4.3738	0.2262	0.0512	4.7225	-0.1225	0.0150
				0.2012			0.0425

To compare the quality of the approximations (28) and (30), calculate the sum of the square deflections (see Table 5). It follows from Table 5 that the sum of the square deflections for the linear regression is $\sigma = 0.2012$ and for the power fitting is $\sigma = 0.0425$. Comparing the quality of these two approximations, (in the sense of The Method of Least Squares) we can conclude that the power fitting is better.

The previous example shows that to solve the approximation problem of a function using The Method of Least Squares, it is required to carry out a significant amount of calculations along with the use of a large amount of numerical values, which are essentially originated in the own process of calculation. It is evident that, in this case, the most appropriate instrument of calculation should be a computer.

Below, for the interested reader, we have listed a Pascal program for simulating the values of the parameters of a regression equation for each of the following three types: $y = ax + b$, $y = ax^m$, $y = ae^{mx}$. Pascal was chosen as the programming language because of its clarity and readability. In Pascal, the information occurring between brackets {} is commentary and is not read by the computer.

Once the program is executed, you could enter, for example, Table 2's data.

We know that with certain data transformations, the calculation of the parameters of the power and exponential fittings is reduced to calculating the parameters of the linear regression, that is, to solving the system of type (12). For this reason, the fundamental steps of carrying this algorithm out can be described as follows:

1. Enter the given data.
2. Choose the type of curve fitting.
3. Transform the data into the functional dependence of linear type.
4. Obtain the parameters of the regression equation.
5. Transform conversely the data and find the square deflections of the found values of the function related to the data.
6. Print the output results.

```
{Curve Fitting}
uses crt;

var A,B,D,s,s1,s2,s3,s4       : real;
    N,i,k                     : integer;
    X,Y,U,V                   : array[0..50] of real;

begin
  clrscr;
  writeln('Enter the number of ordered pairs in the table:');
  readln(N);
  writeln('Enter the values of X:');
    begin
      for i:=1 to N do
        readln(X[i]);
    end;
  writeln('Enter the values of Y:');
    begin
      for i:=1 to N do
        readln(Y[i]);
    end;
```

```
writeln('Choose the type of curve fitting:');
writeln('1: y=a*x+b');
writeln('2: y=a*x^m');
writeln('3: y=a*exp(m*x)');
writeln('Enter the number of the required equation:');
readln(k);
s1:=0; s2:=0; s3:=0;
for i:=1 to N do
  begin
    if k=1 then
      begin U[i]:=X[i]; V[i]:=Y[i]; end;
    if k=2 then
      begin U[i]:=Ln(X[i]); V[i]:=Ln(Y[i]); end;
    if k=3 then
      begin U[i]:=X[i]; V[i]:=Ln(Y[i]); end;
    s1:=s1+U[i]; s2:=s2+V[i]; s3:=s3+U[i]*V[i];
    s4:=s4+U[i]*U[i];
  end;
D:=N*s4-s1*s1;
A:=(N*s3-s1*s2)/D;
B:=(s4*s2-s1*s3)/D;
s:=0;
for i:=1 to N do
   begin
     V[i]:=A*U[i]+B;
     if (k=2) or (k=3) then V[i]:=Exp(V[i]);
     writeln(V[i]);
     s:=s+Sqr(Y[i]-V[i]);
   end;
 writeln('Equation of the regression curve:');
 if k=1 then
   begin writeln('Y = ',A,'*X + ',B); writeln('S = ',s); end;
 if k=2 then
   begin writeln('Y = ',Exp(B),'*X^',A); writeln('S = ',s); end;
 if k=3 then
   begin writeln('Y = ',Exp(B),'*exp(',A,'*X)');
                                       writeln('S = ',s); end;
end.
```

In the previous Pascal program, to save the data, we use the 1-dimensional arrays *X* and *Y*. The transformed data are then saved, respectively, in the arrays *U* and *V*.

Executing the calculations for Table 2’s data when using this program, to the request “Choose the type of curve fitting” and, keeping in mind that, the underlined command in the program allows the output of the values of the calculated function in accordance with the obtained regression equation, we get:

0.043082107412
0.59622837143
1.2415656795
1.7947119435
2.4400492515
3.1775776035
3.7307238676

4.3760611756
Equation of the regression curve:
Y = 0.92191044004*X + -0.97101937663
S = 0.20112760029.

For k = 2, the program gives:

Equation of the regression curve:
Y = 0.25804799057*X^1.6524291053
S = 0.0392269377,

and for k = 3:

Equation of the regression curve:
Y = 0.24039914766*exp(0.55338299484*X)
S = 2.3419773528.

Exercise: Fit Table 6's data using the approximation functions of linear, power, exponential, and logarithmic types. Determine which fitting is better and why.

Table 6.

x	0.2	0.5	0.9	1.3	1.7	1.8	1.9	2.2
y	0.66	0.95	1.61	2.72	4.55	5.2	5.92	8.73

Solution:

k = 1: Y = 3.7115290839*X + - 1.0788819226
S = 5.8293104842.

k = 2: Y = 2.6140639311*X^1.0708222005
S = 8.829323519.

k = 3: Y = 0.503046564*exp(1.2967166974*X)
S = 0.0006294117834.