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PEEL - A Program to Perform Exponential "Peeling" (Fitting) On-Line

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Abstract

A program is described which allows interactive data-fitting by a sum of exponential terms. The "peeling" method is used on-line to obtain estimates for the least squares coefficients of each exponential term. The method is described and the program which provides the man-machine interaction is discussed in some detail.

CONTENTS

I. THE "PEELING" METHOD

A) Introduction

Researchers in the fields of Biology and Physics, for example, frequently obtain experimental data in the form of points which they would like to fit by a sum of decaying exponential terms. The least squares criterion is often used to obtain such a fit. Once the coefficients of the exponential terms are determined it is hoped that they will provide some insight into the biological or physical behavior of the system under study.

However, least squares data-fitting by a sum of exponential terms,

$$f(x) = \sum_{i=1}^{m} a_i e^{-b_i x} , \quad b_i \geq 0 \tag{1}$$

is a difficult problem to solve when $m \geq 2$ (see [1]). When only one term is involved ($m = 1$) a least squares fit can be obtained easily by solving a linear system of two equations in two unknowns. However, for the case $m \geq 2$, there is no way to linearize the problem so an iterative scheme of some sort must be employed.

B) The Least Squares Problem

Assume we are given n data points $\left\{(x_\mu, y_\mu)\right\}_{\mu=1}^{n}$ which we are to approximate by a sum of exponential terms (1). Let $a = (a_1 \ldots a_n)$ and $b = (b_1 \ldots b_n)$, $b_i \geq 0$, be vectors in Euclidean n-space, E^n, and define

$$S(a,b) = \sum_{\mu=1}^{n} \left[\sum_{i=1}^{m} a_i e^{-b_i x_\mu} - y_\mu \right]^2 . \tag{2}$$

For given values of the coefficients a and b, S(a,b) represents the sum of squares of the residuals. The least squares problem can now be stated in terms of $S(a,b)$. Find a^* and $b^* \epsilon E^n$ such that for any a and $b \epsilon E^n$ with $b_i \geq 0$,

$$S(a^*, b^*) \leq S(a,b) \ . \tag{3}$$

Alternatively we could state the problem more directly as a minimization problem with constraints:

$$S(a^*,b^*) = \min_{\substack{a,b \,\epsilon E^n \\ b_i \geq 0}} S(a,b) \tag{4}$$

A direct approach to this least squares problem would be to consider $S(a,b)$ as a functional depending on the 2m parameters $\left\{a_i, b_i\right\}_{i=1}^{m}$ and use some minimization algorithm to determine a^* and b^*. If $m = 1$, the approximating function is

$$f(x) = a_1 e^{-b_1 x} \ . \tag{5}$$

By taking the natural logarithm of (5) we have

$$\ln f(x) = \ln a_1 - b_1 x \tag{6}$$

or

$$F(x) = A_1 - b_1 x \ . \tag{7}$$

The coefficients in (7) occur linearly so this function can be used to obtain a least squares fit to $\left\{(\ln y_\mu, x_\mu)\right\}_{\mu=1}^{n}$ by solving a linear system of two equations in two unknowns. It is a simple matter to convert A_1 to the desired coefficient, a_1, since

$$a_1 = e^{A_1} . \tag{8}$$

However, if $m \geq 2$, this linearization of the problem is not possible. We have a non-linear problem which, as pointed out by Lanczos[1], is not well suited to numerical solution. The difficulty in solving this problem is due to the fact that for widely different sets of values for the coefficients $\{a_i, b_i\}_{i=1}^{m}$, we may have nearly identical values for the sum of squares given by (2). This makes it very difficult to locate the absolute minimum of the sum of squares.

One way to circumvent the above mentioned problem is to provide very accurate initial estimates for the values of the coefficients. An iterative scheme for finding the minimum of S(a,b) could then be applied with some degree of confidence that if it locates a local minimum near the initial estimate it is probably the global minimum being sought. Assuming this is true, and that a dependable minimization routine is available, the problem is reduced to that of obtaining accurate initial estimates for the coefficients. The purpose of the method of "peeling" is to provide estimates for the coefficients. Given those initial guesses, an iterative procedure can then be used to refine the least squares solution.

C) Coefficient Estimates by "Peeling"

To illustrate the "peeling" method let us consider an example problem involving two exponential terms. Let

$$f_2(x) = a_1 e^{-b_1 x} + a_2 e^{-b_2 x} \quad (b_1, b_2 \geq 0) , \qquad (9)$$

and assume we have data $\left\{(x_\mu, y_\mu)\right\}_{\mu=1}^{11}$ which can be closely approximated by $f_2(x)$. Let the data be that given in Table 1 and Figure 1. The values shown were obtained by using $a_1 = a_2 = 1.0$, $b_1 = 1.0$ and $b_2 = 0.1$ and evaluating $f_2(x)$ by means of a 5 place table of exponentials. Visual examination of Figure 1 reveals the fact that the contribution to $f_2(x)$ from the first exponential term, $a_1e^{-b_1x}$, is negligible for the last 5 or 6 points since the decay coefficient b_1, is relatively large. Thus, an examination of the points $x = 5$ through $x = 10$ might be expected to provide a good estimate of the 2nd exponential term which dominates $f_2(x)$ for $x > 5.0$.

In Figure 2 we have plotted ln y vs. x. For a range of x over which a single exponential term is dominant, such a plot should be well represented by a straight line. Such a straight line has been drawn on Figure 2 by using a straight edge and visually selecting the line which seems best to "fit" the points at $x = 5$ through $x = 10.0$. The slope and intercept of the line drawn on Figure 2 now provide an estimate of the coefficients of the dominant exponential term in the range indicated. Thus we see that a reasonable estimate for a_2 is $\bar{a}_2 = e^{.1} \approx 1.1$. The estimate for b_2 is obtained from the slope. We have $-\bar{b}_2 = -\frac{1.1}{10.0} = -.11$. We have purposefully drawn the line sloppily in Figure 2 to illustrate the fact that even with errors of some magnitude the method can be used to give useable results.

Since we know that $a_2 = 1.0$ and $b_2 = 0.1$ (these values were used to create the data) we see that the method has given us values with about 10% error.

Now we wish to determine estimates for the coefficients of the first exponential term $a_1e^{-b_1x}$. If we had obtained "exact" values for a_2 and b_2 we could subtract $a_2e^{-b_2x}$ from the data to obtain a new data set

$$x_\mu, \bar{y}_\mu \;{}_{\mu=1}^{11} = x_\mu, y_\mu - a_2 e^{-b_2 x_\mu} \quad . \tag{10}$$

This modified data could then be represented by the term $a_1 e^{-b_1 x}$. In practice we have only approximate values for a_2 and b_2 but they are sufficient for our purposes. Using the approximate values, $\bar{a}_2$ and $\bar{b}_2$, we calculate $\bar{y}_\mu$, $\mu = 1, \ldots, 11$ as

$$\bar{y}_\mu = y_\mu - \bar{a}_2 e^{-\bar{b}_2 x} , \mu=1,\ldots,11 . \tag{11}$$

Figure 3 shows a plot of $\ln (\bar{y}_\mu)$ vs. x. From this we see that the "tail" of the data curve (points $x = 5$ through $x = 10$) is now dominated by the errors made in approximating the second exponential term. The first five points, however, now approximate the straight line as shown. The slope and intercept of this line give approximations for the coefficients of the first exponential term. We obtain as an estimate for a_1, $\bar{a}_1 = e^{-.1} \approx .9$ and for b_1 we obtain $-\bar{b}_1 = \frac{-.4}{5} = -.8$. Table 2 gives in tabular form the data plotted in Figure 3.

The peeling method can be extended to data which is to be represented by more than 2 decaying exponential terms. The algorithm is as follows:

(1) Plot $\ln(y_\mu)$ vs x_μ , $\mu = 1, \ldots, n$.

(2) Fit a straight line to the "tail". The tail is those points at the end (largest abscissa values) which appear to represent a straight line.

(3) Subtract the exponential term represented by the line obtained in (2) from all the data ordinate values.

(4) Ignore (lop off) the tail used in step (2).

(5) Using the data as modified in steps (3) and (4) go back to step (1).

Steps (1) through (5) are repeated for as many exponential terms as appropriate. The number of exponential terms may be pre-specified by some a priori knowledge of that data or by arbitrary choice or it may be determined empirically as the algorithm is executed.

II. PEEL - AN INTERACTIVE PROGRAM FOR PEELING

A program for performing on-line peeling with graphic display has been written for the IBM 360/91 and IBM 2250 display unit at SLAC. The program allows a user to make initial guesses for the exponential parameters by performing peeling on-line and then allows him to select one of various methods of refining the parameter values.

A) On-Line Peeling

There are two steps involved for the determination of each exponential term. First, a straight line is "fit" to the tail of the log-linear plot of the data and secondly a point must be selected at which the tail is cut off before proceeding with the determination of the next exponential term. Both of these steps are accomplished by a single interactive display shown on the 2250 screen. Figure 4 illustrates this display. The function of the various light pen options is given as follows:

<u>Adjustment of the straight line</u>

There are two ways to adjust the straight line until it best "fits" the tail of the displayed data points. The slope and the intercept can both be changed by light pen commands. In each case the value can be increased or decreased by a given increment which is indicated by lines on the display.

TILT --- allows slope changes as follows:

* UP	makes the slope more positive by the given increment
* DOWN	makes the slope more negative by the given increment
* DOUBLE	doubles the given increment of slope change
* HALVE	halves the given increment of slope change

VERTICAL POSITION --- Allows intercept changes as follows:

* RAISE	raises the intercept value (and the line) by the given increment
* LOWER	lowers the intercept value (and the line) by the given increment
* DOUBLE	doubles the given increment of intercept change
* HALVE	halves the given increment of intercept change

Cutting off the tail

A vertical line displayed on the screen marks the current value of the cutoff point. This marker can be moved left or right by light pen command to choose the desired point.

* MOVE LEFT	moves the cutoff marker to the next data point to the left
* MOVE RIGHT	moves the cutoff marker to the next data point to the right

Going on to the next exponential term

After the straight line and the cutoff point have been adjusted to the desired positions, a light pen command activates the necessary calculation and display updating procedures.

* GO ON TO NEXT EXPONENTIAL

  Subtracts out the chosen straight line and changes the number of points to be plotted so as to cut off the tail as indicated

Updating the display

After the chosen straight line has been subtracted and the number of points to be displayed has been reduced according to the cutoff value, the display is updated. The updating consists of saving and displaying tabularly the coefficients of all exponential terms already estimated, making initial guesses for the slope and intercept of the next straight line, making an initial guess for the next cutoff point, and displaying the plot of the modified data with the initial guesses displayed. The initial guesses are crudely made by the PEEL program and serve only to provide a starting point for the user's adjustments.

The above process is repeated for each exponential term. When all terms have been estimated, a light pen command will cause a different display to be presented. This display allows a choice of several methods of parameter improvement.

B) Least Squares Improvement and Result Comparison

When the second display appears it shows four sets of exponential coefficients and an option to enter coefficents numerically from the 2250 keyboard. The four sets of coefficients are the following:

(i) Interactive peeling

These are the coefficients just selected by the on-line peeling.

(ii) Automatic peeling

These coefficients are also selected by peeling but the choice of straight lines and cutoff points is made by an automatic procedure. The criteria for selecting the lines and cutoff points are somewhat arbitrarily preset in this automatic method so these results will in general be somewhat different from those in (i).

(iii) Interactive peeling with Least Squares improvement

The coefficients shown here are based on those of (i). The exponential coefficients, $\{b_i\}$ are identical to those of (i) but the linear coefficients $\{a_i\}$, which multiply each exponential term have been improved by a least squares technique. This is easily accomplished by solving a set of simultaneous linear equations which give the solution to the following problem in the notation of Section I.

Find $a^* \epsilon E^n$ such that for any $a \epsilon E^n$

$$S(a^*,b) \leq S(a,b) .$$

Note that b is held fixed at the values given in (i).

(iv) Automatic peeling with Least Squares improvement

The coefficients given here are based on those of (ii) in the same way (iii) is based on (i). The b coefficients are identical to those of (ii) whereas the a coefficients have been improved by least squares as discussed for (iii).

The display showing all these various sets of coefficients also shows the sum of squares calculated with each set of coefficients. This allows a user to choose which set of exponential terms best represents the data in the least squares sense.

At this point further refinement (improvement) of the exponential fit is available to the user. He may choose any of the five (including keyboard entered values) sets of coefficients as starting values for a "direct search"[2] minimization of the sum of squares. This is done by selecting one of the columns of coefficients by pointing the light pen at its heading.

While the direct search minimization is taking place a message to that effect is displayed on the screen. When the minimization is finished, the sum of squares at the located minimum is displayed for comparison to the starting value. At this point another set of coefficients may be selected for direct search treatment.

Finally after improving the exponential fit by direct search for all sets of coefficients, the set giving the smallest sum of squares can be selected as that giving the best fit. In practice not all sets are treated by direct search since the sum of squares displayed on the screen may indicate that certain sets are far better than others. However the option exists to treat all sets if so desired.

After all desired direct search improvements have been made a light pen command causes a new set of data to be read in. The new data is then plotted in a log-linear fashion on the display allowing peeling and the whole process may be repeated.

III. DECK SETUP FOR USING PEEL

To use PEEL on the IBM 360/91 at SLAC the following deck setup is required.

- -

Job card

EXEC card

LKED cards bringing in data sets from disk

PUB.LBS. SCP	}	These contain routines used to produce the displays
PUB.LBS. XD5		
PUB.LBS. PEEL	-	This contains the routines specific to the PEELing program

Object cards (if necessary for A050, A058, etc.)

GO. cards

Data cards (several sets of data may be included)

- -

Each data set consists of the following:

1st card Number of data points in col 5 (I5)

2nd
3rd
.
.
.
n + 1st } Each card contains one data point, (x_i, y_i), in Format 2E 10.4 .

REFERENCES

1. Lanczos, C. Applied Analysis, Prentice Hall, Englewood Cliffs, N.J. (1956).

2. Hooke, R. and T. A. Jeeves. "Direct search" solution of numerical and statistical problems. Journal of the ACM, 8, 2 (1961) 212-229.

EXPONENTIAL DATA

x	$y = e^{-x} + e^{-0.1x}$ (from 5 place table)
0.0	2.0
1.0	1.27272
2.0	.95407
3.0	.79061
4.0	.68864
5.0	.61327
6.0	.55129
7.0	.49750
8.0	.44967
9.0	.40669
10.0	.36793

Table 1

EXPONENTIAL DATA WITH ONE APPROXIATED EXPONENTIAL TERM

SUBTRACTED OUT

x	$\bar{y} = y - 1.1\, e^{-.11x}$	$\ln \bar{y}$
0.0	1.0	0.0
1.0	.37689	-0.976
2.0	.15155	-1.885
3.0	.07169	-2.64
4.0	.04460	-3.11
5.0	.03632	-3.33
6.0	.03444	-3.35
7.0	.03449	-3.35
8.0	.03489	-3.34
9.0	.03511	-3.34
10.0	.03506	-3.34

Table 2

Exponential Data

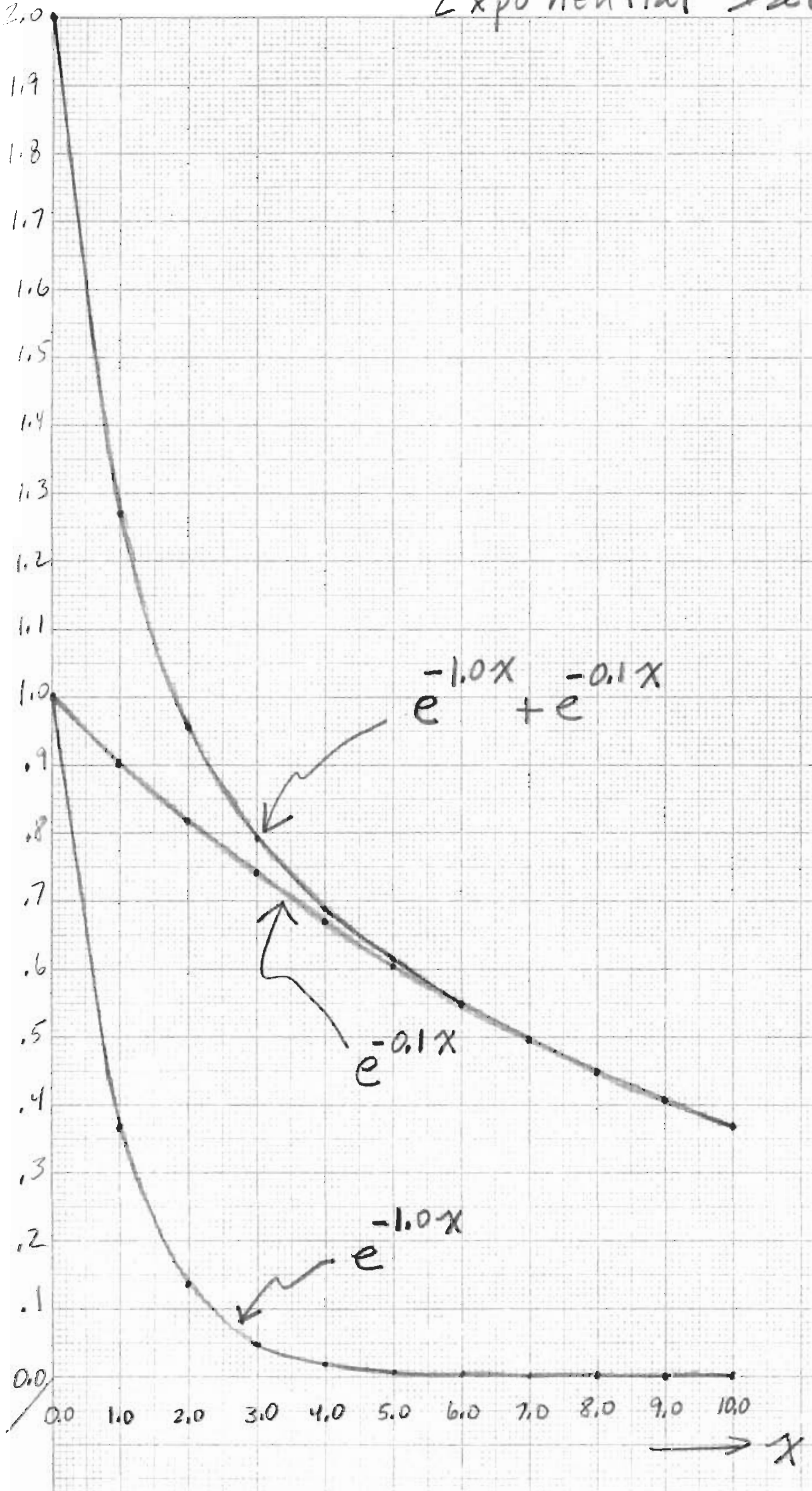

Figure 1.

Fitting the "Tail" by a Straight Line

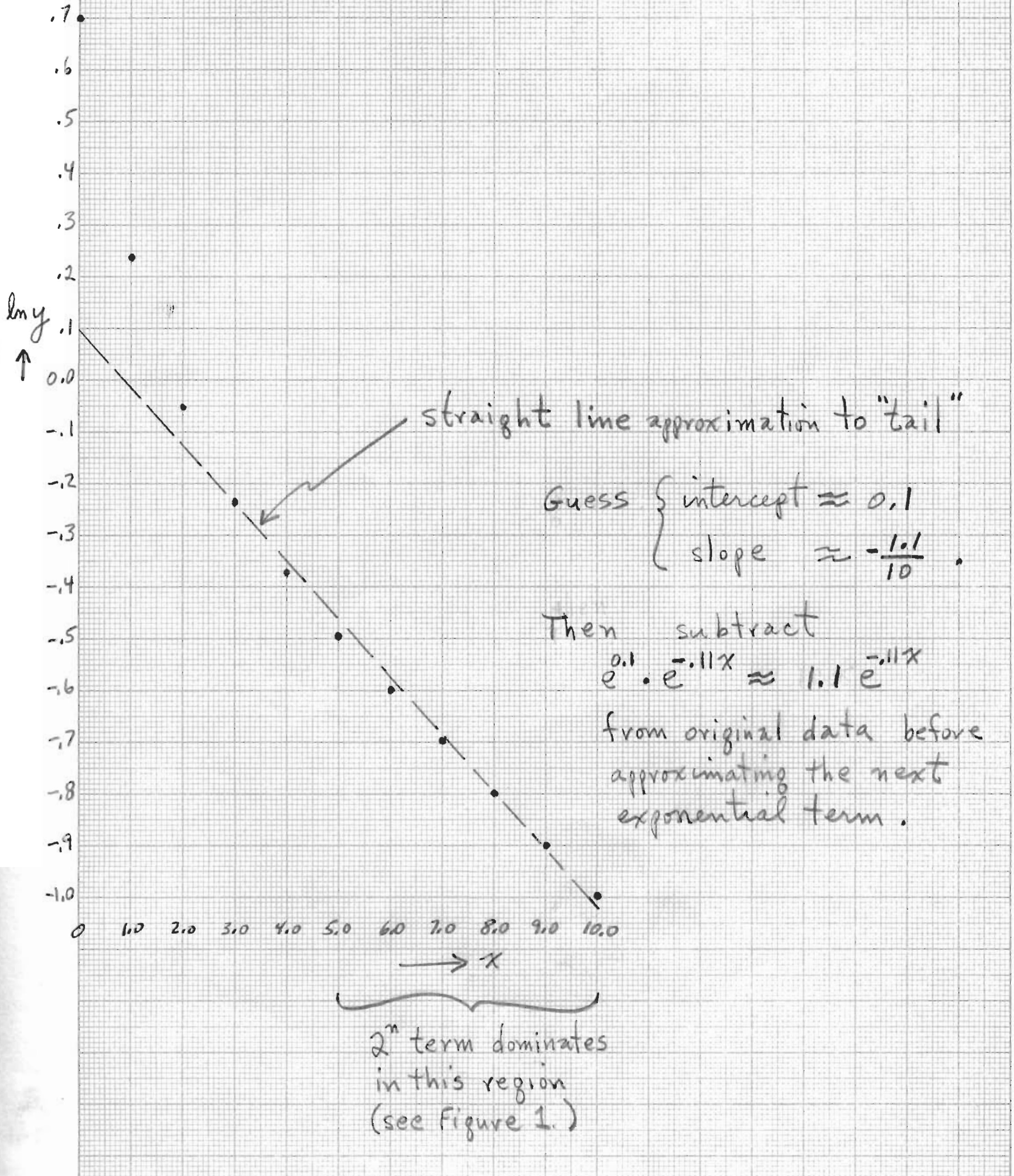

Figure 2.

Exponential Data with one Approximated Term subtracted out ("Peeled off")

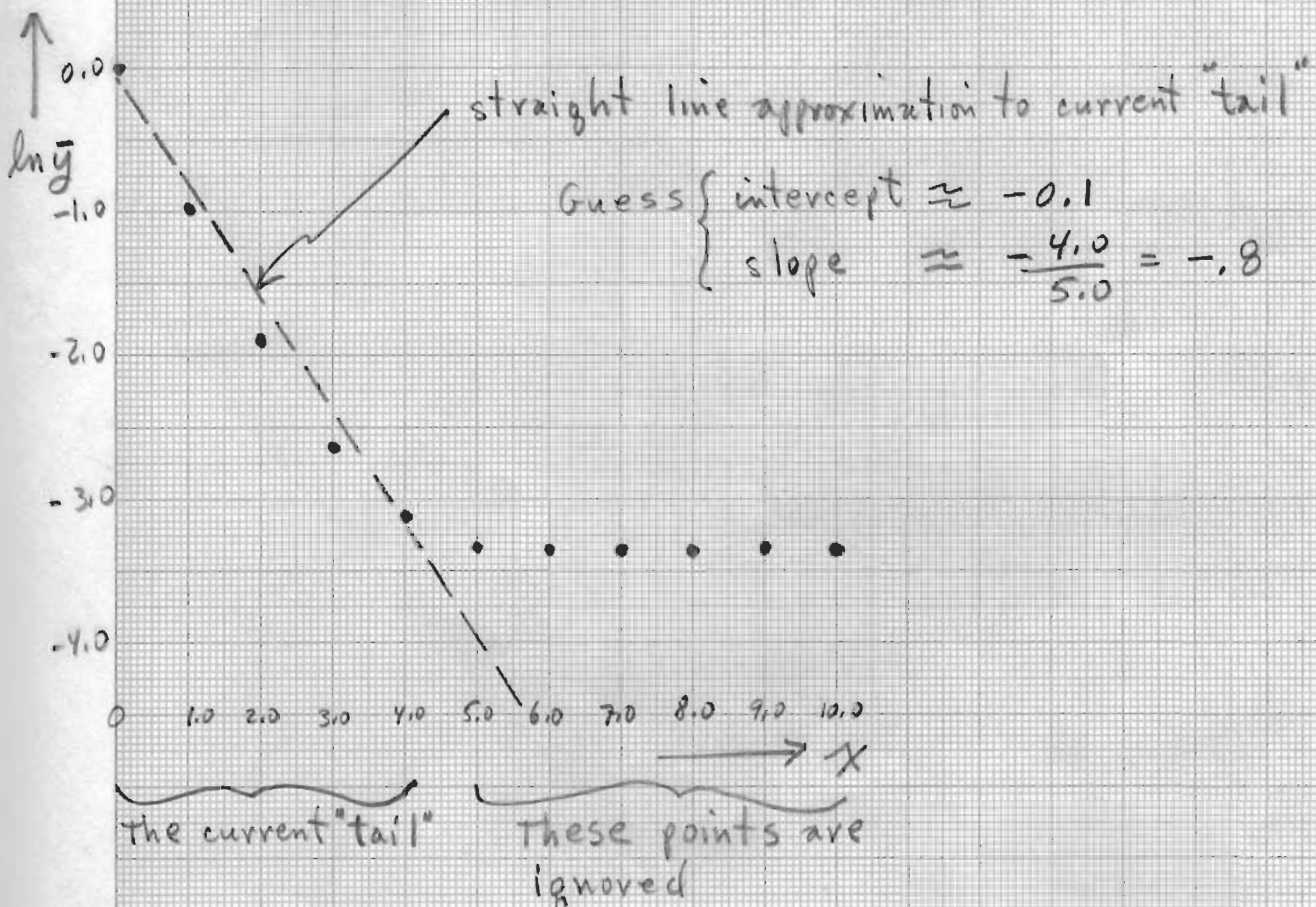

Figure 3

ON-LINE PEELING DISPLAY

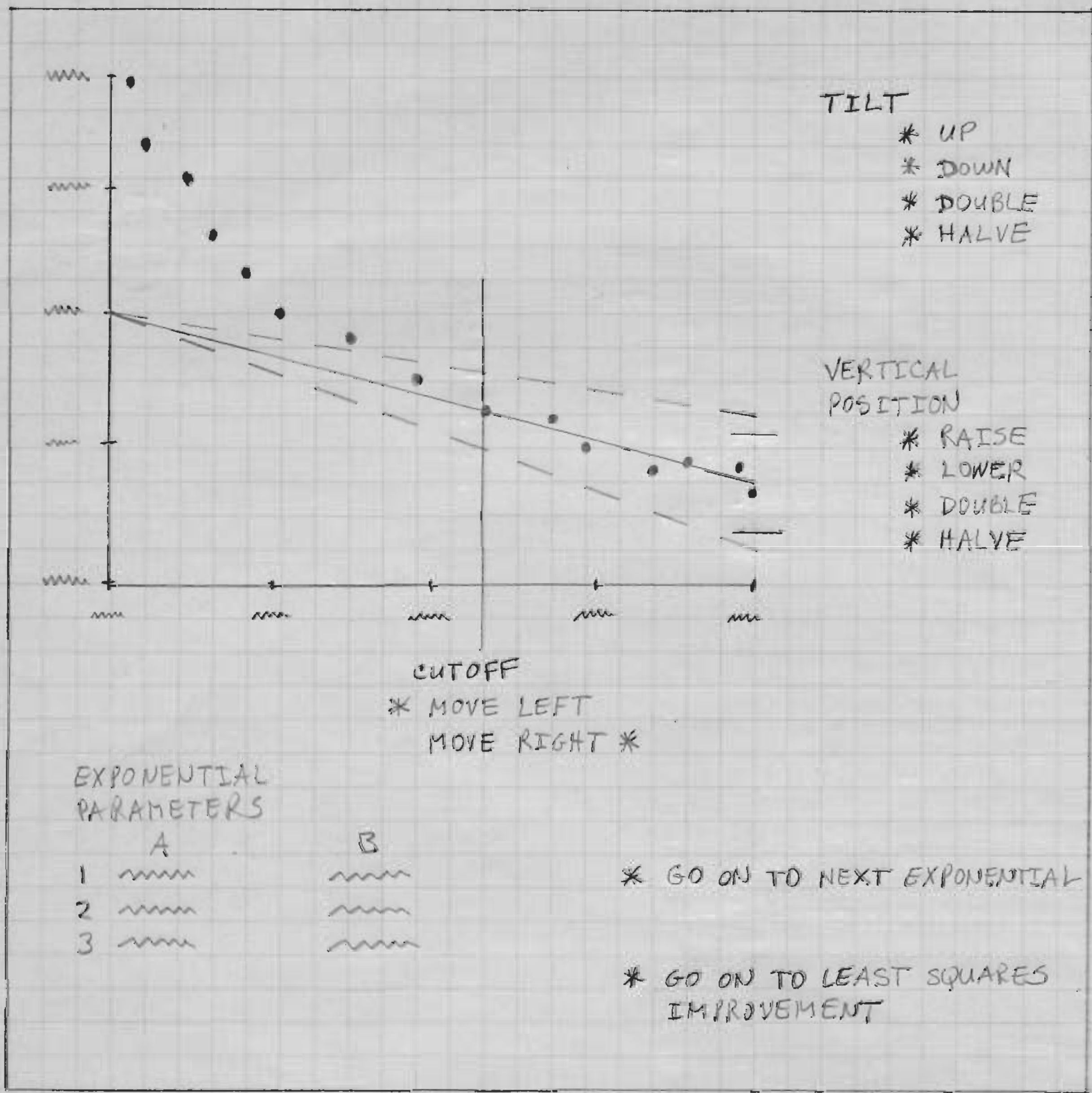

Figure 4