Analysis of Fuel-Bundle Radiographs Using Modeling

by

H. B. Demuth
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MASTER
ANALYSIS OF FUEL-BUNDLE RADIOGRAPHS USING MODELING

by

H. B. Demuth

ABSTRACT

It was desired to estimate the thickness of gaps imaged on highly degraded radiographs. A powerful mathematical method for estimating gap widths was developed and applied. This report describes the problem, develops the techniques used to solve the problem, and presents results, conclusions, and suggestions for future work.

I. INTRODUCTION

The Holifield National Laboratory (HNL) presented the Los Alamos Scientific Laboratory (LASL) with 18 radiographs of fuel rod test bundles. The general problem is to estimate the thickness of the gap between some cylindrical rods and a flat wall surface. The edges of the gaps are poorly defined due to finite source size, x-ray scatter, parallax, film grain noise, and other degrading effects.

The radiographs were scanned and the scan-line data were averaged to reduce noise and to convert the problem to one dimension. A model of the ideal gap convolved with an appropriate point-spread function was fit to the averaged data with a least-squares program; and the gap width was determined from the final fitted-model parameters. The least-squares routine did converge and the gaps obtained are of reasonable size. The method is remarkably insensitive to noise.

This report describes the problem, the techniques used to solve it, and the results and conclusions. Suggestions for future work are also given.

II. DISCUSSION OF PROBLEM

A. Objectives

The objectives of this work were threefold: first, to develop a new analytic method for measuring gaps in the HNL radiographs; second, to apply the method to representative radiographs to determine its effectiveness; and third, to find if there were indeed changes in the gaps due to assembly or heating. To achieve these objectives two radiographs would be studied in detail. Mechanical distortion, if present, would be expected to appear as a gradual change in gap width as one traveled the length of the gap.

B. Fuel Rod Test Bundles and Radiographs

A simplified picture of a fuel rod test bundle cross section is shown in Fig. 2-1. The two gaps of one bundle are imaged reasonably well in each radiograph. As shown in Fig. 2-1, the x-ray source is positioned "opposite" the right gap. The geometry is such that the parallax associated with the left gap is severe; and its effects are clearly discernible to the eye in examining the radiographs.

A picture of a typical radiograph is shown in Fig. 2-2. Size reduction has obscured details but Fig. 2-2 does convey some idea of the complexity of the overall object being imaged. The gaps under study are obscured or overlaid with other objects in many places in the radiographs.

Some of the fuel bundles were radiographed when cold and presumably undistorted except through assembly. Other fuel bundles had been heated electrically, and anticipated interior distortions were
unknown. Of the 18 radiographs, Numbers 2 and 5 were chosen as best examples for the work that we were to do. Neither fuel bundle had been heated and these two radiographs were among the best in quality.

C. Ideal Gap and Degrading Effects

A profile of the ideal gap that one would see in the absence of all degrading effects is shown in Fig. 2-3a. This profile can be characterized by six parameters, $P_1$ through $P_6$. The difference $P_4 - P_2$ defines the gap width.

As noted previously, the ideal gap is not imaged clearly for many reasons. First, there may be interference of other physical pieces that overlap the gap image in the radiograph. Second, the radiation source size is fairly large, and this causes blurring. Third, the interaction of Cobalt-60 gamma rays and the fuel bundle will give some scatter and image blurring. Fourth, geometric (parallax) effects will cause still further blurring. The radiation source is parallel to the clamp and bundle on the right side but not on the left side; and there is considerable blurring of the edges of the left gap due to the offset of the source. Fifth, film grain noise is significant in the radiographs and interferes with the interpretation of all details, gap included.

A digital scan across the (degraded) gap as imaged in the radiograph might typically give a film density profile like that shown in Fig. 2-3b. Attempts have been made to guess the gap widths from such data through "eyeballing" a fit to the data; but the errors in such attempts were considerable. Basically, the data is very poor due to known (and perhaps unknown) effects; and some kind of noise reduction, restoration and powerful fitting must be applied to extract the gap edges.

III. SOLUTION OF PROBLEM

A. Scanning

Each of the 18 radiographs was scanned at 26 stations as shown in Fig. 3-1. The vertical distance between stations on the radiograph was chosen at 2.771 cm so that the distance between stations on the fuel bundle is 2.54 cm. The 2.771 enhancement factor is the source-to-film distance (152.4 cm) divided by the source to test bundle distance (139.7 cm). An attempt to determine the enlargement factor by using the 0.61-cm holes in the upper right corner of each radiograph failed. Scans of these holes were noisy and had poorly defined edges.

Both gaps were scanned from outside to inside. Thus, the abrupt edge of each gap occurs first as one goes from the beginning to the end of data associated with each gap. There are 500 points on each of the 100 lines scanned at each station. An aperture of 10 um was used.

The data of one scan line were very noisy, as shown in Fig. 3-2. To reduce noise, the 100 lines of data at each station were averaged. The averaged data were recorded on magnetic tape for use by HNL. Averaging reduced the noise considerably but did not eliminate it. A typical picture of averaged data is given in Fig. 3-3.

B. Model and Analysis

It is assumed that the radiograph gap profile can be described by an equation of the form

$$g(x) = \int_{-\infty}^{x} h(x_1)f(x - x_1)dx_1 + n(x), \quad (3.1)$$

where $g$ is the (sampled data) profile recorded on film, $h$ is the point-spread function, $f$ is the "true" profile, and $n$ is the noise. Hopefully the noise is reduced by the averaging described previously.
Fig. 2.2. Radiograph No. 2.
Finite source size, electron scattering and parallax all contribute to the point-spread function (PSF). A PSF whose shape is dependent only on finite source size was chosen for this work. It is a circle with a diameter of approximately 0.0297 cm. The data were averaged in one direction; and averaging the PSF in a similar way produces an $h(x)$ as shown below.

$$h(x) = 2\sqrt{R^2 - x^2}$$

A brief investigation of radiation scatter and parallax shows that it is easy to justify a wider PSF, but fortunately, the gap widths are found not to depend critically on the width of the PSF.

The gap model used is shown below.

The parameters $P_1$ through $P_6$ (and the PSF radius $R = P_7$, if desired) are fit to the data $g(x)$ by a least-squares routine. $P_5$ and $P_6$ allow an arbitrary slope and quadratic term on the tail of the model.

Both $h$ and $f$ are expressible in analytic form. Thus, it was possible to integrate the right side of Eq. (3.1) to give a nonintegral equation

$$g(x) = q(x, P_1, \ldots, P_7).$$

The least-squares procedure was applied to an equation of this form.
C. Least-Squares Solution

The basic equation to be solved is

\[ g(x) = \int_{-R}^{R} h(x_1)f(x - x_1)dx, \quad (3.3) \]

where \( h(x) = 2\sqrt{R^2 - x^2} \) \( (3.4) \)

and

\[ f(x) = \begin{cases} \frac{1}{2} & \text{for } 0 < x < P_2, \\ P_3 & \text{for } P_2 < x < P_4, \\ P_5 + P_3x - P_4P_5 - P_6x^2 + P_5P_6 & \text{for } P_4 < x \end{cases} \quad (3.5) \]

The integral limits are as shown; for outside the range \(-R\) to \(+R\), \( h(x_1) \) is zero.

The function \( h(x_1) \) can overlap \( f(x - x_1) \) in many ways. For instance, if \( x \leq P_2 - R \) then \( h(x_1) \) overlaps \( f(x - x_1) \) entirely to the left of \( P_2 \), and the integral of Eq. (3.3) reduces to

\[ g(x) = \frac{1}{2}\pi R^2. \quad (3.6) \]

However, if \( P_2 - R < x < P_2 + R \)

and \( x \leq P_4 - R \),
then \( h(x) \) overlaps the clamp and gap part of \( f(x-x_1) \)
and Eq. (3.3) integrates to
\[
g(x) = \left( P_3 - P_1 \right) \left( x - P_2 \right)^2 \left[ \frac{R^2 - (x - P_2)^2}{R^2 \sin^2 \left( \sqrt{\frac{x-P_2}{R}} \right)} \right] + \left( P_3 - P_1 \right) \frac{\pi R^2}{2}.
\] (3.7)

So, as \( x \) is varied, \( h(x_1) \) overlaps \( f(x - x_1) \) in different ways and each overlap leads to a unique form of Eq. (3.3). The six possible overlaps and the six equations that result are given in Appendix A.

The least-squares program needs partial derivatives of equation like (3.6) and (3.7). Thus, partials of all six equations for the various overlaps were derived. They are also given in Appendix A. As \( x \) increases, or as \( h(x) \) "travels across" \( f(x) \), the least-squares program determines the overlap and chooses the appropriate partial-derivative equations to use.

Appendix B is a guide to the use of the least-squares system. With it and an appropriate deck of cards one can use the least-squares routine under the KRONOS operating system.

An example of the most important part of the output of the least-squares routine is given in Fig. 3.4.

IV. RESULTS
A. Analytic Method and Its Application

Work with the model and the least-squares routine has been both frustrating and fascinating. A few results and observations are discussed below.

1. The initial value of \( D = 2R = 0.0297 \) cm in the point-spread function \( h \) is too small to allow a reasonable fit of data on the left side of the gap. If \( R \) is allowed to vary, the program finds it larger by a factor of 2 or 3. This is understandable, for the true width of the point-spread function is the sum of the widths due to many effects; and the effects are such that one could justify almost any \( D \) larger than 0.0297 cm.

2. The values of \( P_2 \) and \( P_4 \) and the gap width are not critically dependent on \( R \).

3. The least-squares solution proceeds better with \( R \) fixed because other parameters are closely correlated with \( R \). We picked \( R = 303 \mu m \) for much of the work.
4. The least-squares program develops singularities if \( P_2 \) or \( P_4 \) wander past the data bounds. Thus, \( P_2 \) and \( P_4 \) have been constrained to stay within the data.

5. The least-squares program has apoplexy if \( P_2 \) gets bigger than \( P_4 \). Thus, \( P_2 \) has been constrained to be less than \( P_4 \).

6. The least-squares iteration process may develop huge and disastrous "corrections" in \( P_2 \) or \( P_4 \) without much notice. Thus, the change in \( P_2 \) or \( P_4 \) on any iteration is confined to be

\[
\varepsilon = 500 \, \text{m.}
\]

where \( \varepsilon \) is the iteration number.

7. Inclusion of too much data on the tail of the model leads the program to fit a "lurgy" nonlinear tail on the right side.

8. The computing time required to do the fit is small. Typically, fits to 10 stations takes about a minute of 7600 time.

The "fits" to the data produced by the model look reasonably good. An example is given in Fig. 4-1. More examples are shown in Appendix C.

Fig. 4-1. Typical fit of model to data points.

Fig. 4-2. Calculated gap edges and gap width of Radiograph No. 2 (Runs 1FR, 1VG).

B. Measurements*

Fig. 4-2 is a plot of the measured values of \( P_2 \) and \( P_4 \) for Stations 1 to 13 of Radiograph 2. These two parameters define the edges of the gap. Their difference, the gap width, is also shown in Fig. 4-2. Figure 4-3 shows similar results for Stations 14 to 26 of Radiograph 2. Figure 4-4 presents a plot of the sums of the gaps found in Radiograph 2. Figures 4-5 through 4-7 show results for Radiograph 5 like those shown in Figs. 4-2 through 4-4 for Radiograph 2.

A few general comments are in order before proceeding to a detailed examination of the results shown in Figs. 4-2 through 4-7. First, the sets of

*All measurements discussed here are those made on the original radiograph, expressed in um.
points representing the gap edges $P_2$ and $P_4$ generally have a slope due to the fact that the scan lines were not precisely perpendicular to the gap. Second, most $P_2$ and $P_4$ point sets are reasonably smooth, as expected, with gradual changes that might well be caused by bending; but occasional outlying points away from a smooth course are seen. These could be due to obfuscation of the gap at that point by other physical parts imaged in the radiograph. Third, it was hypothesized that the gap widths not only would vary smoothly but that, for any one radiograph, the sums of the gaps would be a constant of the order of 1500 µm.

Figures 4-2 and 4-5 show particularly good definition of the sharp edge $P_2$ on the nonparallax (right) gap of the radiographs. The $P_2$ edges on the left gaps of the radiographs, where the parallax is severe, are also well defined. The $P_4$ edges of the gaps, as found by the least-squares routine, show more variance; but if allowance is made for exclusion of some outlying points, even these edges can be fit by smooth curves. $P_4$ in Radiograph 5 is a possible exception. It shows considerably more scatter than the other $P_4$ edges.

Smooth curves drawn through the $P_2$, $P_4$ measurements lead one to believe that there was indeed some bending of the physical pieces in the fuel element assembly. For example, $P_2$ of Fig. 4-2 indicates that that "edge" is bent, for it slopes off sharply and uniformly to the left. A similar bend can be visualized in $P_4$ of Fig. 4-3. In contrast, $P_2$ of Fig. 4-6 would appear to show a number of gradual deformations. The extent to which these data reflect real changes is not known and probably will not be known: for a disassembly for investigative purposes presumably would induce additional changes. It is the author's feeling that smooth curves drawn through the best of the data do represent the "edges" of the gap quite well, and that deviations from a straight line do reflect physical changes.

As noted previously, it was thought that the sum of left and right gap widths taken along a line perpendicular to the length of the gaps would be a constant. This "constant" was 0.14224 (1 ± 0.1) cm, which, taking 9% enlargement into account, converts to 1550 (1 ± 0.1) µm. The sums of the gaps, the 1550 µm line, and lines representing a ±10% change from 1550 µm are shown in Figs. 4-4 and 4-7. The gap sums for Radiograph 2 tend to fall substantially above the anticipated sum, while those for Radiograph 5 fall fairly well within the bounds anticipated despite the fact that $P_4$ in Fig. 4-6 is quite "noisy." The author does not know why the gap sums for Radiograph 2 are so great, but it would appear that at least some of the contribution comes from a leveling-out of $P_4$ as one goes from left to right in Fig. 4-3. The $P_4$ data fit a smooth curve rather well, and the author has no particular reason to doubt that this edge does curve up toward the right side.

![Fig. 4-3. Calculated gap edges and gap width of Radiograph No. 2 (Runs 1VK, 1PH).](image-url)
V. CONCLUSIONS

A. Analytical Methods

The idea of using a model of the gap and applying a least-squares fit to determine the parameters of the model has worked well. The methods developed were easy to use, required little computer time, and were remarkably insensitive to noise and other degradations.

B. Fuel Bundle Gaps

The fuel bundle gap edges found in this study show bending of various kinds. The statistical parameters associated with the fits to data at various stations indicate that the fits are indeed good, that the results are reliable, and that the smooth bending of the gap edges, as observed, is actually present.

VI. FUTURE WORK

The investigation reported here has suggested a variety of paths for future work. For instance, the computer runs took little time but were done in a batch mode. If the runs could be done in an interactive mode, it would be possible to optimize the choice of data bounds, model (linear or nonlinear tail), free parameters, convergence criteria, etc. With such optimization, the results might improve considerably. Better results might also be obtained with a point-spread function that had a different shape; and an improved understanding of the effects of parallax on the left side might well produce better results there.

*Results were relatively insensitive to point-spread function width, but the effect of PSF shape is unknown.

The general approach of fitting a model of few parameters to low quality images is an interesting area for future research. It is, in essence, the epitome of parameter reduction in which only a few "answers" are desired from a wealth of data. It has the potential of being applied to any case in which an object of "known" geometry is imaged but in which the orientation, size, etc., are not known. For such cases, the model/point-spread function/least-squares fit methods used here offer a great deal; and research in the area would be worthwhile.

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APPENDIX A

SIX CASES OF OVERLAP

The material shown below illustrates the six possible ways in which \( h(x) \) and \( f(x) \) can overlap. The results obtained on integrating

\[
g(x) = \int_{-R}^{R} h(x_1) f(x - x_1) \, dx_1
\]

in each case are also given.

The partial differentials of the equations for each case are needed for use in the least-squares program. These differentials are shown in the last part of this appendix.

1. Six Possible Overlaps

Case I: \( x \leq P_2 - R \)

\[
h(x) = \begin{cases} 1 & x-R \leq x < P_2 \\ \frac{x-P_2}{P_2} & x = P_2 \\ 0 & P_2 < x \leq P_4 \end{cases}
\]

Case II: \( P_2 - R < x \leq P_2 + R \) and \( x \leq P_4 - R \)

\[
h(x) = \begin{cases} \frac{1}{2} & x-R \leq x < P_2 \\ \frac{x-P_2}{P_2} & x = P_2 \\ \frac{1}{2} & P_2 < x \leq P_4 \end{cases}
\]

Case III: \( P_2 + R < x \leq P_4 - R \)

\[
h(x) = \frac{1}{x-R} \begin{cases} 1 & x-R \leq x < P_2 \\ \frac{x-P_2}{P_2} & x = P_2 \\ 0 & P_2 < x \leq P_4 \end{cases}
\]

Case IV: \( P_4 - R < x \leq P_4 + R \) and \( x > P_2 + R \)

\[
h(x) = \frac{1}{x-R} \begin{cases} \frac{1}{2} & x-R \leq x < P_2 \\ \frac{x-P_2}{P_2} & x = P_2 \\ \frac{1}{2} & P_2 < x \leq P_4 \end{cases}
\]

Case V: \( x > P_4 + R \)

\[
h(x) = \begin{cases} 1 & x-R \leq x < P_2 \\ \frac{x-P_2}{P_2} & x = P_2 \\ 0 & P_2 < x \leq P_4 \end{cases}
\]

Case VI: \( x \leq P_2 + R \) and \( x \geq P_4 + R \)

\[
h(x) = \begin{cases} 1 & x-R \leq x < P_2 \\ \frac{x-P_2}{P_2} & x = P_2 \\ 0 & P_2 < x \leq P_4 \end{cases}
\]
\((x-P_4)\sqrt{R^2-(x-P_4)^2}\)
\[\frac{5}{4}(x-P_4) + \frac{6}{4}(x^2-P_4^2) + \frac{1}{2}P_6R^2\]

\[+ R^2\sin^{-1}\left(\frac{x-P_4}{R}\right)\left[p_5(x-P_4) + p_6(x^2-P_4^2) + \frac{1}{4}P_6R^2\right] + \frac{3}{2}\left[\frac{2}{3}P_5 + \frac{4}{3}P_6x - \frac{1}{2}P_6(x-P_4)\right]\]

\[3. \text{ Partials Needed by Least-Squares Program}\]

\text{Case I: } x \leq P_2 - R

\[\frac{3g}{\partial P_1} = R^2\pi\]

\text{Case II: } P_2 - R < x \leq P_2 + R

\[\frac{3g}{\partial P_2} = -2(P_3-P_1)\sqrt{R^2-(x-P_2)^2}\]

\text{Case III: } P_2 + R < x \leq P_4 - R

\[\frac{3g}{\partial P_3} = R^2\pi\]

\text{Case IV: } P_4 - R < x \leq P_4 + R \text{ and } x > P_2 + R

\[\frac{3g}{\partial P_4} = [p_5 - 2P_4P_6]R^2\sin^{-1}\left(\frac{x-P_4}{R}\right)\]

\[\frac{3g}{\partial P_5} = R^2\pi\left[p_5(x-P_4) + p_6(x^2-P_4^2) + \frac{1}{4}P_6R^2\right] + \frac{3}{2}\left[p_5 + \frac{4}{3}P_6x - \frac{1}{2}P_6(x-P_4)\right]\]

\[x-P_4\right)^2\sqrt{R^2-(x-P_4)^2} + R^2\sin^{-1}\left(\frac{x-P_4}{R}\right)\]

\[\frac{3g}{\partial P_6} = R^2\pi\left[p_5(x-P_4) + p_6(x^2-P_4^2) + \frac{1}{4}P_6R^2\right] + \frac{3}{2}\left[p_5 + \frac{4}{3}P_6x - \frac{1}{2}P_6(x-P_4)\right]\]

\[\frac{3g}{\partial R} = -2(P_3-P_1)\sqrt{R^2-(x-P_2)^2}\]

\text{Case V: } P_4 + R < x

\[\frac{3g}{\partial P_4} = R^2\pi\left[-p_5 - 2P_4P_6\right] + \frac{3}{2}\left[p_5 + \frac{4}{3}P_6x - \frac{1}{2}P_6(x-P_4)\right]\]

\[\frac{3g}{\partial P_6} = R^2\pi\left[p_5(x-P_4) + p_6(x^2-P_4^2) + \frac{1}{4}P_6R^2\right] + \frac{3}{2}\left[p_5 + \frac{4}{3}P_6x - \frac{1}{2}P_6(x-P_4)\right]\]

\[\frac{3g}{\partial R} = R^2\pi\left[\frac{x^2-P_4^2 + \frac{1}{4}R^2}{R}\right] + \frac{3}{2}\left[p_5 + \frac{4}{3}P_6x - \frac{1}{2}P_6(x-P_4)\right]\]
I. BACKGROUND

LSMFT is a collection of programs combined into a system to permit a general approach to least-squares problems. Written for the CDC 6600 and 7600 computers, LSMFT is designed to accept free-format input of problem specification and data, choice of prewritten or user-specified functions, choice of optimizing algorithm, and selected output with various graphical displays.

LSMFT has been designed so that it probably will never be declared "finished." That is, as new minimizing algorithms are developed, as new display methodology appears, and as interactive computing grows at LASL, LSMFT can be expected to form the basis of adapting these new features to the matter of least-squares analysis.

II. SOME MATHEMATICAL FORMULATIONS

Consider a collection of N points, each point having M elements. Let $X_n = (X_{n1}, X_{n2}, \ldots, X_{nM})$ denote the nth such point. Then the entire collection can be represented by an NxM matrix, $X = (X_{nm})$, $n = 1, 2, \ldots, N$ and $m = 1, 2, \ldots, M$.

Consider next a function of M variables and P parameters, say $f_n(z_1, z_2, \ldots, z_M; \alpha_1, \alpha_2, \ldots, \alpha_P) = 0$. If $f_n(z;\alpha) = 0$ is chosen properly and the vector $X_n$ is "perfect," it is reasonable that $f_n(X_n;\alpha) = 0$ be satisfied for all N functions and vectors $X_n$.

In the absence of "perfection" of the data and the functions and knowledge of the values of the elements of the parameter vector $\alpha$, consider the problem of finding a vector, say $\alpha^*$, such that $\alpha^*$ is, in some sense, "best" for the choice of the N functions and the given matrix of data.

LSMFT is designed to find $\alpha^*$ by the method of least squares. That is, $\alpha^*$ is the choice of $\alpha$ such that the quadratic form

$$S(\alpha) = \sum_{n=1}^{N} \sum_{n'=1}^{N} w_{nm} f_n(X_n;\alpha) f_n(X_{n'};\alpha)$$

is smaller when $\alpha = \alpha^*$ than for any other choice of $\alpha$. The scalars $w_{nm}$ are elements of a "weight matrix," say $W = (w_{nm})$, $n, n' = 1, 2, \ldots, N$.

If $F(X;\alpha)$ is an N-element vector whose nth element is $f_n(X_n;\alpha)$ and $F'(X;\alpha)$ denotes its transpose, then $S(\alpha)$ can be written

$$S(\alpha) = F'(X;\alpha) W F(X;\alpha).$$

When W is a diagonal matrix and $F(X;\alpha)$ is linear in the elements of $\alpha$, the solution is found by solving the P linear "normal equations" which are obtained by differentiating $S(\alpha)$ with respect to each of the elements of $\alpha$. Some arbitrariness is involved, of course, should the number of parameters be larger than the number of functions or should the normal equations be singular or should W be singular, but various conventions exist for resolving these difficulties.

When, however, any one $f_n(X_n;\alpha)$ is nonlinear in at least one of the parameters, the normal equations are nonlinear and special algorithms must be employed. These may range from simple searches of
the P-dimensional parameter space to sophisticated mathematically-based procedures.

III. SOME ILLUSTRATIVE EXAMPLES

Most problems will not employ the basic LSMFT least-squares formulation outlined in Section II. The following examples are intended to illustrate how some of the more conventional least-squares problems may be stated in terms of LSMFT conventions.

Example 1: The straight line. Suppose N pairs of observed data are available, denoted \((x_n, y_n), n = 1, 2, \ldots, N\). Let \(f_n(z_1, z_2; \beta_1, \beta_2) = y_n - \beta_1 - \beta_2 x_n = 0\) be the function of interest. Let the weight matrix \(W\) be the identity matrix. Then the function to be minimized can be written

\[
S(\beta) = \sum_{n=1}^{N} (y_n - \beta_1 - \beta_2 x_n)^2,
\]

exactly the sum of squares found in most first encounters with least squares. In this formulation \(y\) often is called the dependent variable and \(x\) is the independent variable, while \(\beta_1\) is the intercept and \(\beta_2\) is the slope of the line. Once \(\hat{\beta}\) is found by solving the 2x2 linear system of normal equations, \(\hat{\beta} = (X'X)^{-1}X'y\), \(\hat{\beta}_1\) and \(\hat{\beta}_2\) are the estimated slope and intercept obtained by using the particular set of \(N\) pairs of observed data at hand.

For LSMFT the matrix \(Y\) has \(N\) rows and 2 columns. One column is designated the dependent variable, the other is designated the independent variable. Unless otherwise specified by the user, LSMFT is designed to use the first column of \(X\) as the dependent variable. Thus, the sum of squares can be written

\[
S(\beta) = \sum_{n=1}^{N} (x_n - \hat{\beta}_1 - \hat{\beta}_2 x_n)^2.
\]

Example 2: General linear hypothesis model of full rank. The function to be fitted is linear in all \(P\) parameters. A matrix \(Z\) is set up by augmenting a vector of 1's with the matrix \(X\), where \(X\) has dimensions \(N\) and \(M = (P-1)\). Again assuming that \(W\) is the identity matrix, the function to be minimized is

\[
S(\hat{\beta}) = (Y - Z\hat{\beta})'(Y - Z\hat{\beta}),
\]

where \(Y\) is an \(N\)-element vector of observations of the dependent variable. The minimizing value of \(\hat{\beta}\) is given by

\[
\hat{\beta} = (Z'Z)^{-1}Z'Y.
\]

In LSMFT terminology, \(f_n(x_n; \beta) = x_n_1 - \beta_1 - \beta_2 x_n + \beta_3 x_n^2 = 0\) is the function of interest for \(n = 1, 2, \ldots, N\). Only the matrix \(X\) need be stored, since the first column of \(1's\) is taken care of in the formulation of the function.

Example 3: Multiple regimes. The notation \(f_n(X_n; \beta)\) may seem redundant for most least-squares problems, because the model usually is the same for each vector \(X_n\). However, some problems require the more general notation.

Consider \(N = n_1 + n_2\) observations. For \(1 \leq n \leq n_1\), the function of interest is \(f_n(X_n; \beta) = x_n_1 - \beta_1 - \beta_2 x_n = 0\), and for \(n_1 + 1 \leq n \leq N\), the function is \(f_n(X_n; \beta) = x_n_1 - \beta_1 - \beta_2 x_n + \beta_3 x_n^2 = 0\). These represent two parallel lines. If each were fitted alone, the equality of the slopes could not be assured.

More complicated multiple regime problems can be treated with LSMFT. It is not necessary that the data and functions match sequentially, as in the parallel line example. Sometimes the choice of function for a particular \(X_n\) can be made by an indicator variable in one column of the data matrix \(X\).

IV. USE OF LSMFT

LSMFT is available as a CROS cafeteria batch job using Class 2 resident fileset and on KRONOS either in batch mode or through a remote keyboard terminal. In either case, a preprocessor sets minimum array sizes needed to run and sets calls to subroutines and library functions. The main program CCPROC calls PACKALG to fit the data to the selected function, calls OUTPACK to print answers, then calls PLTPACK if requested.

Users of the old PACKAGE routines will find the preprocessor solves the problem of exceeding code dimension sizes, but the new code will not count data points. A subroutine can be written to do this, however, if you set the number of points to a reasonable upper limit for the preprocessor to use.

*CROS is a LASL 7600 operating system.
and then reset the number of points to the exact value in the subroutine. It is possible to add a dummy variable by reading it in as an extra independent variable, then resetting the number of variables appropriately. The new code does not calculate the variance of the predicted mean.

APPENDIX C

This Appendix contains (1) various parts of run 1VG, including all of the printing associated with Station 1, Radiograph 2, and (2) all the fits for Stations 1 through 13, Radiograph 2.

```
SET NPTS=21 NVR=2 NPARAH=0 UERVAN=1 INVAR=2 NệmLIN=100
SET FItASIC=1.273x
READ INPUT=MAN
+0.045 ZER 0.0006 30.3 110. 150.
SET FItVARAN=7
CALL SIMGEN
READ INPUT=TITLE
1 FILE 1 LIN AL TAIL + FIXU
SET DPARAH=
FIT ALGONPACKALG FUNCUNIT1 DFUNCUNIT1
READ INPUT=TITLE
FILE 1, LINEAL TAIL + FIXEU
READ INPUT=TITLE
X=AXIS
READ INPUT=LINEAL Y=AXIS
PLOT ULTRA=TRUE PLOT=THRU
RESET
SET NPTS=21 NVR=2 NPARAH=0 UERVAN=1 INVAR=2 NĖMELIN=100
SET FItASIC=1.273x
READ INPUT=MAN
+0.045 ZER 0.0006 30.3 110. 150.
SET FItVARAN=7
CALL SIMGEN
READ INPUT=TITLE
1 FILE 2 LIN AL TAIL + FIXU
SET DPARAH=
FIT ALGONPACKALG FUNCUNIT1 DFUNCUNIT1
READ INPUT=TITLE
FILE 2, LINEAL TAIL + FIXEU
READ INPUT=TITLE
X=AXIS
READ INPUT=LINEAL Y=AXIS
PLOT ULTRA=TRUE PLOT=THRU
RESET
SET NPTS=21 NVR=2 NPARAH=0 UERVAN=1 INVAR=2 NĖMELIN=100
SET FItASIC=1.273x
HEAD INPUT=MAN
+0.045 ZER 0.0006 30.3 110. 150.
SET FItVARAN=7
CALL SIMGEN
READ INPUT=TITLE
1 FILE 3 LIN AL TAIL + FIXU
SET DPARAH=
FIT ALGONPACKALG FUNCUNIT1 DFUNCUNIT1
READ INPUT=TITLE
FILE 3, LINEAL TAIL + FIXEU
READ INPUT=TITLE
X=AXIS
READ INPUT=LINEAL Y=AXIS
PLOT ULTRA=TRUE PLOT=THRU
RESET
SET NPTS=21 NVR=2 NPARAH=0 UERVAN=1 INVAR=2 NĖMELIN=100
SET FItASIC=1.273x
READ INPUT=MAN
+0.045 ZER 0.0006 30.3 110. 150.
SET FItVARAN=7
CALL SIMGEN
READ INPUT=TITLE
1 FILE 4 LIN AL TAIL + FIXU
SET DPARAH=
FIT ALGONPACKALG FUNCUNIT1 DFUNCUNIT1
```
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<th>Step Size</th>
<th>Sum of Squares</th>
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<td>1.6099130E-01</td>
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</tr>
<tr>
<td>Iteration 14</td>
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<td>Iteration 15</td>
<td>1.000000E+00</td>
<td>1.2867834E-01</td>
</tr>
</tbody>
</table>

**Notes:**
- The table lists iterations with their corresponding step sizes and sum of squares values.
- The values in the table are in scientific notation.
- The sum of squares values are all below 1.0E-01, indicating a good fit or convergence criterion.
- The step sizes vary, with some iterations showing slight variations.
ITERATION NO. 19
STEP SIZE = 1.000000E+00 WEIGHTED SUM OF SQUARES = 1.2867834E+01 SUM OF SQUARES = 1.2867834E+01
1 1.65000000E+03 1.2623313E+03 1.0290398E+03 9.3554826E+00
2 6.50000000E+02 2.6753386E+02 3.9270592E+02 2.8978758E+02
3 1.80000000E+02 1.3737295E+02 1.3737295E+02 6.1429976E+02
4 1.70000000E+00 1.747701E+00 1.747701E+00 7.7350549E+00
5 0
6 0
7 3.030000E+00 0.000000E+00
ITERATION NO. 20
STEP SIZE = 1.000000E+00 WEIGHTED SUM OF SQUARES = 1.2867834E+01 SUM OF SQUARES = 1.2867834E+01
1 1.65000000E+03 1.2623313E+03 1.0290398E+03 9.3554826E+00
2 6.50000000E+02 2.6753386E+02 3.9270592E+02 2.8978758E+02
3 1.80000000E+02 1.3737295E+02 1.3737295E+02 6.1429976E+02
4 1.70000000E+00 1.747701E+00 1.747701E+00 7.7350549E+00
5 0
6 0
7 3.030000E+00 0.000000E+00
ITERATION NO. 21
STEP SIZE = 1.000000E+00 WEIGHTED SUM OF SQUARES = 1.2867834E+01 SUM OF SQUARES = 1.2867834E+01
1 1.65000000E+03 1.2623313E+03 1.0290398E+03 9.3554826E+00
2 6.50000000E+02 2.6753386E+02 3.9270592E+02 2.8978758E+02
3 1.80000000E+02 1.3737295E+02 1.3737295E+02 6.1429976E+02
4 1.70000000E+00 1.747701E+00 1.747701E+00 7.7350549E+00
5 0
6 0
7 3.030000E+00 0.000000E+00
ITERATION NO. 22
STEP SIZE = 1.000000E+00 WEIGHTED SUM OF SQUARES = 1.2867834E+01 SUM OF SQUARES = 1.2867834E+01
1 1.65000000E+03 1.2623313E+03 1.0290398E+03 9.3554826E+00
2 6.50000000E+02 2.6753386E+02 3.9270592E+02 2.8978758E+02
3 1.80000000E+02 1.3737295E+02 1.3737295E+02 6.1429976E+02
4 1.70000000E+00 1.747701E+00 1.747701E+00 7.7350549E+00
5 0
6 0
7 3.030000E+00 0.000000E+00
FILE i: LINEAR TAIL. A FIXED
10/25/74 17:42:30
THIS PROBLEM CONTAINS 241 DATA POINTS, OF 2 VARIABLES
THERE ARE 7 PARAMETERS
FREE PARAMETERS ARE 1 2 3 4 5
CONVERGED IN 22 ITERATIONS

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THIS PARAMETER WAS HELD FIXED

FILE j: LINEAR TAIL. A FIXED
10/25/74 17:42:30
THIS PROBLEM CONTAINS 241 DATA POINTS, OF 2 VARIABLES
THERE ARE 7 PARAMETERS
FREE PARAMETERS ARE 1 2 3 4 5
CONVERGED IN 22 ITERATIONS

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<th>GRADIENT OF G-FUNCTION SHOULD BE ZERO</th>
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THIS PARAMETER WAS HELD FIXED
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FILE 2, LINEAR TAIL, R FIXED

FILE 3, LINEAR TAIL, R FIXED

FILE 4, LINEAR TAIL, R FIXED
FILE 5, LINEAR TAIL, R FIXED

FILE 6, LINEAR TAIL, R FIXED

FILE 7, LINEAR TAIL, R FIXED

X-AXIS

Y-AXIS

100 160 220 280 340 400

X-AXIS

Y-AXIS

100 160 220 280 340 400

X-AXIS

Y-AXIS

100 160 220 280 340 400