GRAPHICAL METHODS FOR THE ANALYSIS OF DATA

by

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PREFACE

The content of this thesis is divided into two parts. Part I consists of a review of graphical methods in data analysis, whilst Part II presents a graphical procedure for identifying growth curves based on the fitting of a polynomial function to sections or "blocks" of the raw data.

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PART I

A REVIEW OF GRAPHICAL METHODS IN DATA ANALYSIS

CHAPTER 1

THE HISTORY OF GRAPHICS

Graphical presentation of statistics was introduced at the end of the eighteenth century. There is some doubt as to whether the "inventor" was William Playfair (1759 - 1823) or A.F.W. Crome (1753 - 1833). Playfair's works on general descriptive economics were illustrated with some extremely good graphs, histograms and pie diagrams, whilst Crome devised charts to describe geographical data of European states, chiefly population figures and areas. Crome justified the use of his geometrical representation as follows:

"The proportions of the different sizes can however be more easily seen and grasped if they are brought before the eye in the form of a drawing, because the imagination is thus stimulated, than if these merely appeared in the form of numbers, especially when these consist of many digits as is often the case with areas of states ..... ." (Crome {10} 1785)

A detailed investigation of the work of Crome and Playfair has been undertaken by Royston {29}.

While holding the part-time appointment of Professor of Geometry at Gresham College (1890-94), Karl Pearson gave a series of twelve lectures under the heading "The Geometry of Statistics." These lectures were mainly concerned with methods of visual presentation of descriptive statistics. The graphical approach was a characteristic feature of Pearson's teaching of

Applied Mathematics and it was only natural that he should extend this approach to Statistics.

In 1915 Fisher {14} used 3-dimensional geometry to describe a mean, a standard deviation, and Student's ratio, and in 1925 wrote:

"The preliminary examination of most data is facilitated by the use of diagrams. Diagrams prove nothing, but bring outstanding features readily to the eye; they are therefore no substitute for such critical tests as may be applied to the data, but are valuable in suggesting such tests, and in explaining the conclusions founded upon them." (Fisher {15})

In 1949 Mosteller and Tukey {25}, in an article on the use of binomial probability paper, drew attention to the advantages of employing graphical methods to analyse data.

"The speed of graphical processes, and the advantages of visual presentation in pointing out facts or clues which might otherwise be overlooked, make graphical analysis very valuable." (Mosteller and Tukey {25})

In the early 1960's, possibly motivated by articles by Tukey {31,32,33} on data analysis, statisticians began detailed investigations into the use of relatively unsophisticated procedures for extracting information from a body of data, in particular the use of graphical procedures. Tukey wrote:

"Procedures of diagnosis, and procedures to extract indications rather than conclusions, will have to play a large part in the future of data analysis. Graphical techniques offer great possibilities in both areas."(Tukey{31})

Wilk and Gnanadesikan, who were to play leading roles in the development of graphical procedures for the analysis of experimental data, also commented on the need for graphics and informal data analytic procedures:

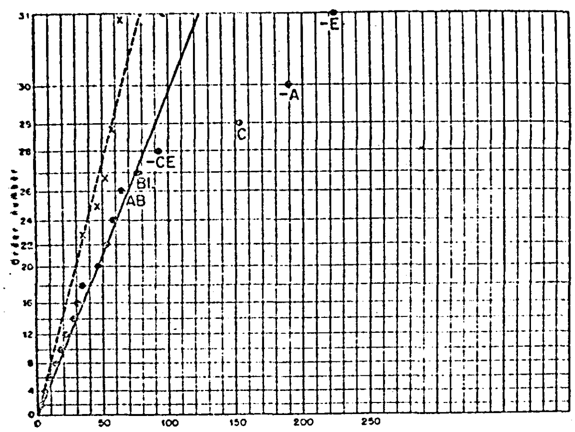
"If statistical methods are to be relevant to the analysis of data, then a major concern of theoretical statistics will have to be the provision of methods which are useful tools for 'learning from' data and for bringing out the latent information in data. There are greater possibilities of gaining insight into data through the use of an informal method, like probability plotting, than through the use of a formal technique like a test of significance." (Gnanadesikan {17})

Tukey was particularly concerned that graphical procedures should involve straight line configurations as often as possible.

"Graphs are most effective ..... when reference situations produce straight lines." (Tukey and Wilk {33})

When comparing data with a fitted curve he advocated improving the histogram by employing, instead, a hanging rootogram (see Figure 1) in which the blocks are attached to the fitted curve (not the base line) and the eye merely has to check on the 'straightness" of the bottom of the rootogram.

The increasing use of computers in data analysis has, in recent years, resulted in the introduction of computerised graphical procedures. This was anticipated



—Half-normal plot of a 2^5 experiment. Dots and solid line-31 contrasts. Crosses and dashed line-24 smallest contrasts.

FIGURE 4

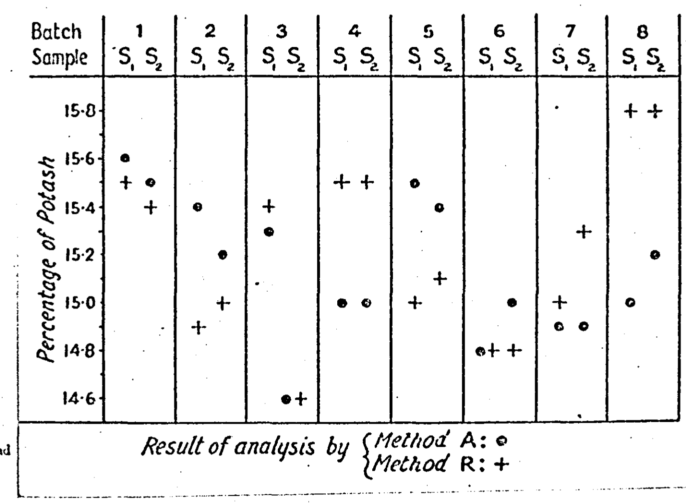


FIGURE 3

ERRORS OF SAMPLING AND ANALYSIS

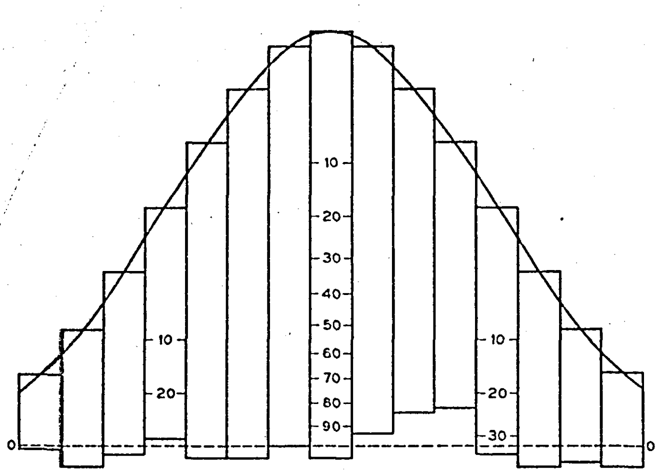


FIGURE 1

HANGING ROOTOGRAM

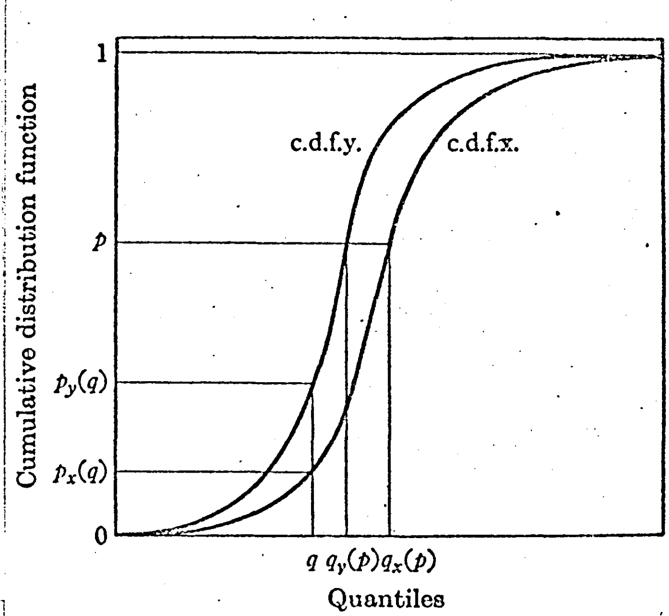


FIGURE 2

ILLUSTRATION FOR P-P AND Q-Q PLOTS

by Tukey:

"Computer-drawn graphs .... are going to be the data analyst's greatest single resource." (Tukey {32}), and is now widely advocated:

"The graphic aspect of the computer can rapidly convey the results of a computation to the man in a form that can be quickly perceived i.e. through the man's visual senses." (Ball and Hall {3}).

"The thorough graphical analysis of residuals as a routine is feasible only with a suitable computer graphical output device." (Cox and Snell {9})

The history of graphics has indicated that only in the last 15 years have the potentials of graphic representation received wide attention. Recent work has tended to concentrate on the data analytic properties of graphics but new techniques are still being devised for the simple presentation of data. Bachi {2} recently proposed a new device - Graphical Rational Patterns - where integers are represented by a pattern of marks enclosed within small square frames, to overcome the inadequacies of common graphical presentation of statistical data.

CHAPTER 2

PROBABILITY PLOTTING

(a) Uses

It is often useful in data analysis to treat a body of data as though it were an unstructured array. A valuable representation of such data is provided by the empirical cumulative distribution function (e.c.d.f.) i.e. a plot of the i'th ordered value as ordinate against $\frac{i - \frac{1}{2}}{n}$ as abscissa ($i = 1, \ldots. n$). Wilk and Gnanadesikan {39} have discussed in detail the advantages of the e.c.d.f., in particular its effectiveness as an indicator of peculiarities e.g. asymmetry. They devised two basic kinds of plots for situations where either (i) two e.c.d.f.'s are to be compared, (ii) an e.c.d.f., is to be compared with a theoretical c.d.f., or (iii) two theoretical c.d.f.'s are to be compared. Their plotting procedures may be described with the aid of Figure 2.

Corresponding to any ordinate value p there are two quantile values $q_x(p)$ and $q_y(p)$. A scatter plot of $q_y(p)$ against $q_x(p)$ for various p, they label a "quantile versus quantile" (Q-Q) plot. Similarly, corresponding to any abscissa value q there are two c.d.f., values $p_x(q)$ and $p_y(q)$. A "percent versus percent" (P-P) plot is just a scatter plot of $p_y(q)$ against $p_x(q)$ for various q.

If the two variables are identically distributed, both the Q-Q plot and the P-P plot will be linear, with slope unity, pointed towards the origin. Q-Q plots are especially sensitive to discrepancies in the tails of the distributions, whilst P-P plots are sensitive to discrepancies in the middles of the distributions.

Wilk and Gnanadesikan mentioned that extensions and hybrids of the P-P and Q-Q plots could be used but suggested that more investigation was required for the applications of these techniques.

Probability plots act as useful, informal aids to inference in data analysis. The essence of such plots is to plot the n ordered "sample" values against some representative values from a presumed standard distribution. There are essentially two choices of representative values:-

(i) corresponding quantiles of the reference distribution such as $\frac{i - \frac{1}{2}}{n}$ or $\frac{i}{n + 1}$ $(i = 1 \ldots\ldots n)$, plotted on the appropriate probability paper,

(ii) expected values of the standard order statistics from the reference distribution.

Under certain null statistical conditions a linear configuration is obtained, passing through the origin. The presence of real effects in a designed experiment, the existence of distributional peculiarities, of outliers, and of heterogeneities of variance all result in distortions of the linear configuration.

Probability plots of the individual residuals in regression studies are informative and sensitive tools. The graphical analysis of residuals will be surveyed in Chapter 5. Probability plots may also be applied to analysis of variance situations and a detailed study of this particular application is made in Chapters 4 and 5.

(b) Choice of Plotting Positions

The choice of plotting positions on probability paper has been investigated by Chernoff and Lieberman {6,7} and Kimball {22}. Chernoff and Lieberman considered the problem of graphically estimating the mean, μ, and standard deviation, σ, of a normal population on the basis of a sample. If x_1, x_2, ... x_n denote the ordered sample values and p_1 p_2, ... p_n the appropriate values on the probability scale, then the problem was, essentially, what values of the p's yield good estimates, $\hat{\mu}$ and $\hat{\sigma}$? In order to translate the process of visually fitting a straight line to the set of plotted points into an analytical process, Chernoff and Lieberman proposed the assumption that the visually fitted line is a very good approximation to the line that would be obtained by minimizing the sum of squares of the deviations (in the x direction) from the line. This process yielded sampling variances of the resulting analytical estimates of the parameters μ and σ.

Their criterion for judging the optimal character of a plotting method was the resulting magnitude of the sampling variances of the parameters, in particular the variance of $\hat{\sigma}$ since this was the more difficult parameter to estimate. Thus they determined values of

p_i $(i = 1, \ldots. n)$, for various n, which minimized the variance of an unbiased estimate of σ. They also showed that a biased estimate of σ with minimum mean square deviation could be found, and the plotting positions for this estimate were given. They concluded that the optimum choice of the $\dot{p}$'s depended upon whether an unbiased estimate was necessary or whether a biased estimate could be tolerated.

Kimball extended the work of Chernoff and Lieberman by pointing out that probability paper was not used merely to estimate parameters. There were two other purposes served in using probability paper, namely, as a test as to whether or not the sample data indicated that the population was of the prescribed type, and for graphical extrapolation at one of the extremes, the purpose most commonly served when plotting data from an extreme-value population.

Kimball considered seven plotting conventions based on the assumption proposed by Chernoff and Lieberman. He applied these conventions to both normal probability paper and extreme-value probability paper. Two of the conventions were those used by Chernoff and Lieberman, namely, the convention which minimized the variance of an unbiased estimate of the scale parameter and the convention which produced a biased estimate of the scale parameter with minimum mean square deviation. Kimball found that both these conventions, when used for plotting data on extreme-value probability paper, gave plotting positions which tended to lie along a curve. He concluded that for both normal and extreme-value populations a convention attributed to Blom {5}, $p_i = \frac{(i - \frac{3}{8})}{(n + \frac{1}{4})}$,

would be satisfactory and simple to use for all three objectives for using probability paper. This convention carried an estimate of the scale parameter with low mean square deviation.

Kimball emphasised that there was need for caution in relying upon any single formula and that, particularly for extrapolation for an extreme-value population, it would be well to supplement the plot using points determined from other conventions.

Blom's convention never seems to be used in practice. Text books tend to use plotting conventions based on order statistics, namely $p_i = \frac{i}{n + 1}$ or $p_i = \frac{i - \frac{1}{2}}{n}$, between which there is no difference except for small values of n. Both Chernoff and Lieberman, and Kimball list the plotting positions for these two conventions, for various values of n.

CHAPTER 3

GRAPHICAL METHODS FOR DISCRETE DATA

(a) Binomial-Like Counts

Dubey {12} proposed a graphical test to determine whether certain experimental data could be described satisfactorily by a binomial distribution. If, in the standard binomial notation,

$$p(i) = \Pr\{X = i\} = \binom{n}{i} \theta^i (1-\theta)^{n-i} \quad (i = 0,1,2, \ldots . n),$$

then

$$\frac{p(i+1)}{p(i)} = -\frac{\theta}{(1-\theta)} + \frac{(n+1)\theta}{(1-\theta)} \cdot \frac{1}{(i+1)} \quad \ldots\ldots\ldots\ldots \quad (3.1)$$

Hence, plotting $\frac{p(i+1)}{p(i)}$ against $\frac{1}{i+1}$ should give a straight line with slope $\frac{(n+1)\theta}{1-\theta}$ and intercept $-\frac{\theta}{1-\theta}$.

This method requires an estimate of the unknown parameter θ in order to calculate $p(i)$. In a later paper Ord {26} noted the relationship $\frac{i\,p(i)}{p(i-1)} = (n+1)\frac{\theta}{1-\theta} - \frac{\theta}{1-\theta} \cdot i \quad (i = 1,2, \ldots . n)$ and suggested that, using the assumption $f_i \alpha\, p(i)$, where the f_i denote frequencies for the cases $X = i$ $(i = 0,1,2, \ldots . n)$, a plot could be made of $\frac{i f_i}{f_{i-1}}$ against i. This should give a straight line with slope $-\frac{\theta}{1-\theta}$ and intercept $\frac{(n+1)\theta}{1-\theta}$.

Gart {16} suggested the simpler relationship

$$\frac{i\ p(i)}{(n-i+1)p(i-1)\ +\ i\ p(i)} = \theta \qquad \text{.......}\ (3.2)$$

and showed how a plotting technique derived from (3.2) is related to estimators and statistical tests of full or nearly full efficiency. Using Ord's assumption that $f_i\ \alpha p(i)$ we have a set of estimators

$\hat{\theta}_i = i\ f_i\{(n-i+1)f_{i-1} + i\ f_i\}^{-1}$ $(i = 1,2,3\ \ldots.\ n)$.

A logical estimator of θ is the weighted mean of the $\hat{\theta}_i$, namely $\hat{\theta} = \dfrac{\sum w_i \hat{\theta}_i}{\sum w_i}$. If $w_i = (n-i+1)f_{i-1} + i\ f_i$ then $\hat{\theta} = \dfrac{\sum i f_i}{n \sum f_i} = \dfrac{\bar{i}}{n}$ which is, of course, the best estimator. If the $\hat{\theta}_i$'s are plotted against i they should cluster around the horizontal straight line with ordinate $\hat{\theta}$.

Gart derived a normal deviate test to test whether any particular $\hat{\theta}_i$ deviated significantly from $\hat{\theta}$. He pointed out that this test did not involve a specific alternative to the binomial distribution and suggested, as a reasonable alternative, the beta-binomial distribution,

$$p(i) = \Pr\{X=i\} = \binom{n}{i} \frac{B(\alpha+i,\beta+n-i)}{B(\alpha,\beta)} \quad (i = 0,1,\ \ldots.\ n)$$

where α and β are positive constants.

Manipulating as in (3.2) we obtain

$$\frac{i\ p(i)}{(n-i+1)p(i-1)+ip(i)} = \frac{\alpha-1}{\alpha+\beta+n-1} + \frac{i}{\alpha+\beta+n-1}$$

$(i=1,2,\ldots.n)$. Following the notation for the binomial analysis, this is equivalent to $\hat{\theta}_i = C + Di$ where C and D are certain constants. If the data deviated from the binomial in the direction of the beta-binomial, the plot of $\hat{\theta}_i$ against i would be linear with positive slope. The hypothesis that the data is binomial as opposed to beta-binomial can be formulated as $H_0 : D = 0$; $H_1 : 0<D<(n-1)^{-1}$. Gart showed that a test based on $\hat{D}$, the weighted least squares estimate of D, is equivalent to the homogeneity χ^2 test. This is the asymptotically locally optimal test for the binomial against the general alternative of θ being itself a random variable. Hence the "best" test of the binomial can be related to a simple and informative graph. The graph may also be used to estimate the parameters of the beta-binomial distribution.

(b) Poisson-Like Counts

Using his ideas set out in the previous section, Dubey proposed a graphical test to determine whether certain experimental data could be described satisfactorily by a Poisson distribution. If, in the standard Poisson notation,

$$p(i) = \Pr\{X=i\} = \frac{e^{-\lambda}\lambda^i}{i!} \quad (i = 0,1,2,\ldots.) \quad (\lambda>0),$$

then

$$\frac{p(i)}{p(i+1)} = \frac{1}{\lambda} + \frac{1}{\lambda}\, i$$

Hence, plotting $\frac{p(i)}{p(i+1)}$ against i should give a straight line with slope $\frac{1}{\lambda}$ and intercept $\frac{1}{\lambda}$. Dubey commented that the method required an estimate of the unknown parameter λ in order to calculate $p(i)$, and Ord later derived an alternative relationship, namely $\frac{ip(i)}{p(i-1)} = \lambda$ ($i = 1,2,3,\ldots.$), from which, using his assumption $f_i \alpha p(i)$, it follows that a plot of $\frac{if_i}{f_{i-1}}$ against i should give a horizontal straight line with ordinate λ.

In a manner similar to his work on binomial-like counts, Gart showed how Ord's plot could be related to estimators and statistical tests. A logical estimator of λ is the weighted mean of the estimators $\hat{\lambda}_i = \frac{if_i}{f_{i-1}}$ i.e. $\hat{\lambda} = \frac{\Sigma w_i \hat{\lambda}_i}{\Sigma_i w_i}$. If $w_i = f_{i-1}$ then $\hat{\lambda}$ takes the value $\bar{i}$ which is the best estimator. Gart's normal deviate test to test whether any particular $\hat{\lambda}_i$ deviated significantly from $\hat{\lambda}$ did not, as in the binomial case, involve a specific alternative to the Poisson distribution. He suggested, as a reasonable alternative, the negative binomial distribution $p(i) = Pr\{X=i\} = \binom{r+i-1}{r-1}\left(\frac{m}{r}\right)^i \left(1 + \frac{m}{r}\right)^{-r-i}$

($i = 0,1,2, \ldots.$) ($m,r>0$).

In a similar manner to the derivation of (3.1), Dubey has shown that

$$\frac{p(i)}{p(i+1)} = \left(\frac{1 + {}^m/r}{{}^m/r}\right) - \left(\frac{(r-1)(1+{}^m/r)}{{}^m/r}\right)\frac{1}{i}$$

and that a plot of $\frac{p(i)}{p(i+1)}$ against $\frac{1}{i}$ should give a straight line with slope $-\left(\frac{(r-1)(1+{}^m/r)}{{}^m/r}\right)$ and intercept

$\left(\frac{1 + {}^m/r}{{}^m/r}\right)$. This however, while providing a useful test in itself, was not directly compatible with plotting techniques used for the Poisson distribution. Gart rectified the situation by noting that Ord had proved the result

$$\frac{i\ p(i)}{p(i-1)} = (r-1)\left(\frac{{}^m/r}{1 + {}^m/r}\right) + \left(\frac{{}^m/r}{1 + {}^m/r}\right) i \quad (i=1,2,\ldots.)$$

which enabled a plot of $\frac{if_i}{f_{i-1}}$ against i to indicate either Poisson or negative binomial. In the latter case this is equivalent to $\hat{\lambda}_i = C + Di$ where C and D are certain constants. Thus, if the data is consistent with the negative binomial, the plot of $\hat{\lambda}_i$ against i would be linear with positive slope.

A test of the deviation of the data from the Poisson assumption in the direction of the negative binomial alternative can be formulated as $H_0 : D = 0$; $H_1 : 0<D<1$. Gart showed that a test based on $\hat{D}$, the weighted least squares estimate of D, is equivalent to the asymptotically locally optimal test of the Poisson distribution against the negative binomial alternative. Hence the "best" test of the Poisson distribution can be related to the graph.

The logarithmic series distribution of Fisher is defined by $p(i) = \Pr\{X=i\} = \frac{\alpha\theta^i}{i}$ $(i = 1,2,3,\ldots.)$

where $\alpha = \frac{1}{\ln(1-\theta)}$ $(0<\theta<1)$. Ord derived a plotting procedure using $\frac{i\ f_i}{f_{i-1}}$ against i which gave a linear configuration with positive slope. This log series plot could possibly be confused with the negative binomial plot, a fact which motivated Gart to investigate other plotting relationships, notably $\frac{i\,p(i)}{(i-1)p(i-1)} = \theta \ (i = 2,3\ldots.)$. The individual estimators of θ are $\hat{\theta}_i = \frac{i\,f_i}{(i-1)f_{i-1}}$ and the $\hat{\theta}_i$'s should cluster around a horizontal straight line when the data fits the log-series model.

(c) General

Grimm {20} showed that the types of some discrete distributions could be readily discerned by plotting data on Poisson cumulative probability paper. Transparent stencils were used to quickly recognize typical curves and to estimate their parameters. The class of compound and generalized Poisson distributions is represented by curves inclined to the right, while the (positive) binomial is versed to the left.

Ord plotted $\frac{i\,p(i)}{p(i-1)}$ against i for several discrete distributions. In the case of the hypergeometric, beta-binomial and beta-Pascal distributions, curves were obtained. Graphs are most effective for identification purposes when linear plots are produced so Gart's work on the derivation of straight line configurations, e.g. beta-binomial distribution, is a welcome extension of Ord's technique.

CHAPTER 4

GRAPHICAL METHODS FOR DATA FROM UNIRESPONSE EXPERIMENTS

(a) Plots of Raw Data

In 1956 Pearson {27}, concerned at the lack of evidence of statisticians "geometrically examining the pattern of their data" before analysing it arithmetically, described simple ways for graphically inspecting data in analysis of variance situations. Figure 3 shows the data from an experiment with eight batches of fertilizer, two independent samples (S_1, S_2) being drawn from each batch, each sample then being divided into two sub-samples, the first analysed by method A, the second by method R. The variable measured was "percentage of potash". Inspection of the plot indicates that with the exception of Batch 3 the difference between the two results for a given batch, using the same method of analysis (either A or R) is small. The determinations by methods A and R, however, differ considerably. Subsequent arithmetical analysis confirmed these findings.

(b) Probability Plots

In 1959 Daniel {11} devised the half-normal plot as a means for detecting real effects in a factorial two-level experiment. Tukey {31} was later to comment "The half-normal plot ..... will have more extensive repercussions than most of us have dreamed of."

Half-normal probability paper is prepared by deleting the probability scale P, for $P < 50\%$, on normal probability paper and replacing each P value by $P' = 2P - 100$, for $P > 50\%$. The absolute value of the i'th smallest contrast is plotted as abscissa, against $P' = \frac{(i - \frac{1}{2})}{n}$ $(i = 1,2,\ldots.n)$ where n is the number of contrasts obtained from the experiment. If there are no real effects then the plotted points follow a straight line with positive slope, passing through the origin. An estimate of the standard error of the contrasts may be obtained from that contrast for which P' is most nearly 68.3%. A particular treatment factor or combination of factors is judged to have a real effect if the corresponding contrast appears to be "too large" relative to the other contrasts in the configuration of the half-normal plot. The plot may then be revised by omitting these contrasts and obtaining a new estimate of the standard error of the remaining contrasts as before (see Figure 4).

In his paper Daniel included some remarks of Tukey's on half-normal plotting. Tukey had prefered a grid that used the logs of the absolute values of the contrasts since the corresponding expansion of the scale for smaller contrasts would be useful. Tukey also suggested inclining the contrast axis at 135^0 to the positive horizontal in order to bring the expected position of the plot for experiments with no real effects to a horizontal straight line. This would be useful in the sense of easier visual identification of real effects but the plot would lose its inherent simplicity.

Daniel added that half-normal plotting could lead to (i) overestimation of the standard error of the contrasts, (ii) the omission of a number of real effects, (iii) faulty identification of real effects and (iv) possible non-detection of "defective" contrasts due to their being masked by real effects. Birnbaum{4} commented that Daniel's graphical method had the advantage that it gained, from the data being analysed, a degree of confirmation for the underlying assumptions used in analysis of factorial experiments, namely, that the contrasts are independent and normally distributed with common variance and that certain high-order interactions are zero. Birnbaum was interested in an alternative to the standard assumptions and developed his own inference procedure for detecting real effects. This could be carried out within Daniel's graphical procedure.

In a series of papers {17,18,34-40} Wilk and Gnanadesikan developed procedures to supplement the analysis of variance table by helping in the following respects: (i) allowing the data themselves to provide guidance in developing an error term, (ii) giving an easily grasped summary with a focus of attention on interesting features such as real effects, and (iii) being self-critical of underlying assumptions. A useful objective of analysis of variance is the joint relative assessment of comparable quantities e.g. a collection of mean squares or contrasts in a 2^n experiment. Wilk and Gnanadesikan labelled procedures which involve the simultaneous comparison of comparable quantities through the use of a statistical measure or standard, "internal comparisons" procedures. They pointed out that Daniel's procedure provided graphical internal comparisons of a set of single-degree-of-freedom contrasts in uniresponse experiments. The graphical nature of the method facilitated the gaining of insight concerning the structure of the data although in this respect they thought it better to include both half and full-normal plots.

Wilk and Gnanadesikan devised graphical internal comparisons methods for analysing experimental data. Their work may be summarized with the aid of the following classifications:-

RESPONSE STRUCTURE

Decomposition of Treatment Structure	Univariate	Multivariate
All 1 d.f.	I	IV
All ν d.f.	II	V
Mixed d.f.	III	VI

Cells IV, V and VI will be discussed in Chapter 5.

Satisfactory procedures for Cell I are full-normal and/or half-normal probability plotting.

Experiments of the type denoted by Cell II are those where the treatment structure is to be analysed in terms of equal (>1) degrees of freedom decompositions e.g. the comparison of all main effects in a three-level factorial experiment. Wilk and Gnanadesikan devised a gamma probability plotting procedure for such data where the n ordered squared contrasts are plotted against appropriate quantiles of the standard gamma distribution (scale parameter, λ,=1) with shape parameter, η, equal to $\frac{1}{2}\nu$.
to calculate an increasing sequence of proportions

What is involved in obtaining such a plot is to calculate an increasing sequence of proportions $\{b_i\}$ $(i = 1,2,\ldots n)$, defined usually as $b_i = \frac{i - \frac{1}{2}}{n}$, and to determine quantiles $\tilde{x}_i$ such that

$$\frac{1}{\Gamma(\eta)} \int_0^{\tilde{x}_i} t^{\eta-1} e^{-t}\, dt = b_i \quad (i = 1,2,\ldots n)$$

Wilk, Gnanadesikan and Huyett {35} provided tables listing $\tilde{x}_i$ for values of η and b_i. The i'th ordered squared contrast is then plotted against $\tilde{x}_i$ on ordinary linear by linear graph paper. Under a null hypothesis of no real effects the squared contrasts may, as a reasonable approximation, be considered as a random sample from a gamma distribution with scale parameter λ unknown. It can easily be shown that, under such an hypothesis, a straight-line configuration should be obtained with intercept 0 and slope $\frac{1}{\lambda}$. The contrasts associated with real effects will appear as "too large" deviations from the straight line pattern (see Figure 5).

Gamma probability plots also serve as important tools for detecting other "peculiarities" in the data such as distortions due to "maverick" observations and bad non-normality of the original data. The gamma distribution has been considered as a model in life-test problems and an evaluation of this assumption, or of an assumption of exponentiality, is possible through a gamma plot of ordered failure times.

Wilk and Gnanadesikan derived a graphical internal comparisons procedure {40} for Cell III of the table i.e. for experiments where the analysis of variance mean squares may have differing degrees of freedom. The procedure consisted of plotting the ordered mean squares against representative values defined as expected values of appropriately conditioned order statistics of standardized mean squares. If the ordered values of the mean squares are denoted by $S_1 \leq S_2 \leq \ldots\ldots\ldots \leq S_K$ with corresponding degrees of freedom $\nu_1, \nu_2 \ldots\ldots \nu_K$ respectively, then the standardized mean squares are such that the i'th ordered standardized mean square, V_i, comes from a $\frac{\chi^2 \nu_i}{\nu_i}$ distribution (i = 1,2,...K). One of the "null" assumptions is that the i'th mean

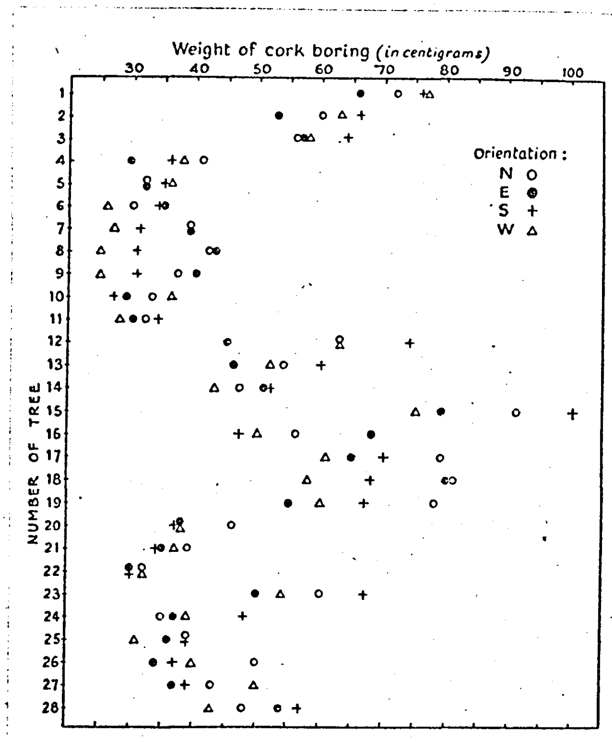


FIGURE 8
MEASUREMENTS OF BARK
ON CORK TREES

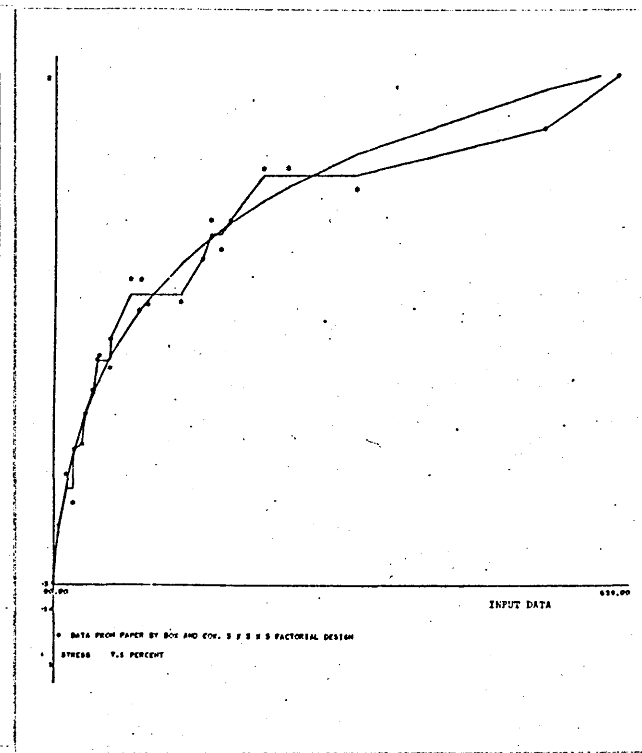


FIGURE 7

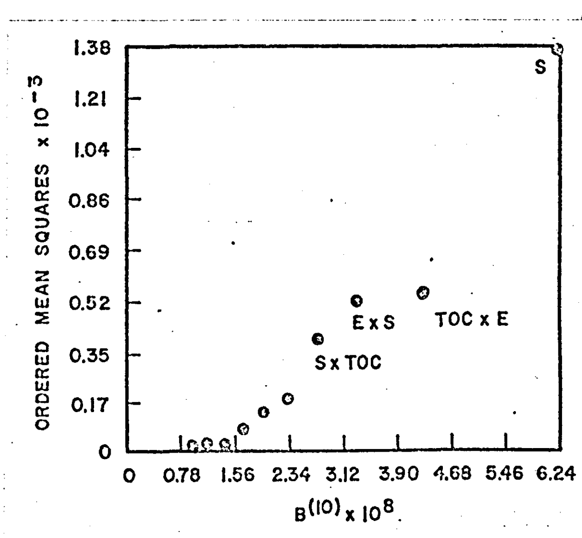


FIGURE 6
GENERALIZED PROBABILITY
PLOT
$(B^{(10)} = f(\theta_i))$

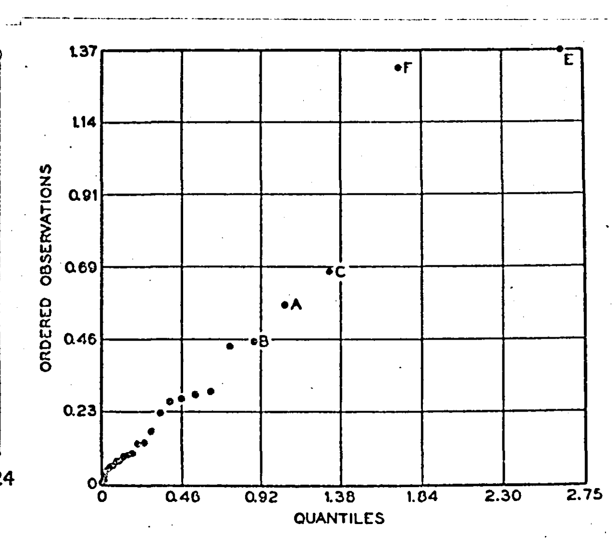


FIGURE 5
GAMMA PLOT

square is distributed (in the absence of real effects) as $\frac{\sigma^2 \chi^2_{\nu_i}}{\nu_i}$ where σ^2 is a presumed common error variance.[1] It follows that $E\{S_i|\nu_1,\nu_2,\ldots.\nu_K\} = \sigma^2 E\{V_i|\nu_1,\nu_2,\ldots.\nu_K\}$ and hence if θ_i = (constant) $E\{V_i|\nu_1,\nu_2,\ldots.\nu_K\}$ then a plot of S_i against θ_i ($i = 1\ldots.K$) would be expected to yield a linear configuration, with a slope which depends on σ^2, when the mean squares do indeed conform to null assumptions. Wilk and Gnanadesikan developed computer programs for calculating the θ_i. With real experimental effects, the associated mean squares would tend to appear as departures from the linear configuration (see Figure 6).

(c) Transformations

An aspect of great importance in data analysis is the transformation of variables. Data from a factorial experiment with large interactions may sometimes be described without interactions if it is first transformed. Kruskal {23} developed a graphical procedure where the data itself indicated the monotone transformation which made the interactions smallest. In the general linear model a set of observations Y_i ($i = 1,\ldots.n$) are such that it is supposed $\dot{y}_i = E\{Y_i\} = \sum_j g_{ij}\beta_j$ where the g_{ij} are known numbers and β_j are unknown parameters. When this model fails to fit the data it may be assumed instead that some appropriate transformation

$Z_i = f(Y_i)$ satisfies the structural relationship,

$z_i = E\{Z_i\} = \sum_j g_{ij}\beta_j$ where the function f must be determined. Kruskal used the quantity

$$S(f,\beta) = \sqrt{\frac{\sum_i (Z_i - z_i)^2}{\sum_i (z_i - \bar{z})^2}}$$

as a measure of disparity between the numbers Z_i and the numbers z_i. Minimising $S(f,\beta)$ over β Kruskal labelled the resulting quantity $S(f)$, the "metric stress" of the numbers Z_i. The "best" monotone function, $\hat{f}$, is defined to be the one which minimizes $S(f)$. $\hat{f}$ is an estimate of the true underlying function f, and is labelled the "minimum stress function". The shape of this function, when plotted, indicates the appropriate transformation.

In Figure 7 the minimum stress function is shown as a jagged curve and is compared with a logarithmic function, the smooth curve. The asterisks show $\beta_i + \gamma_j + \delta_k$ against Y_{ijk} where Y_{ijk} denotes the data and $Z_{ijk} = f(Y_{ijk})$ is such that $E\{Z_{ijk}\} = \beta_i + \gamma_j + \delta_k$.

CHAPTER 5.

GRAPHICAL METHODS FOR MULTIVARIATE DATA

(a) Plots of Raw Data

In a similar manner to his work on univariate data described in the previous chapter, Pearson {27} emphasized the importance of a preliminary graphical study of data when several variables are used. Figure 8 illustrates such a study where the thickness of bark deposit on cork trees is measured for 4 tree orientations, North, South, East and West. Visual examination of the data indicates that, besides the very noticeable between-tree differences, there are differences in pattern associated with the ordering of the trees. It is therefore doubtful whether, without further sub-division, the data would be sufficiently homogeneous to justify any conclusions being drawn using multivariate normal theory.

(b) Probability Plots

In their work on Cell IV in the table in Chapter 4, Wilk and Gnanadesikan developed graphical internal comparisons procedures for analysing 2^n factorial experiments where main effects and interactions are each measured by a single-degree-of-freedom contrast and where several responses (e.g. purity, yield, colour, density, etc.) are generated from the application of a treatment combination to an experimental unit.

If knowledge were available to permit equal weighting to the responses, Wilk and Gnanadesikan suggested that an informal study of the data could be made by conducting a half-normal plot on the absolute values of a variable defined as the sum of the contrasts for each of the responses corresponding to a particular effect.

Roy {28} suggested a way of looking at the multiresponse problem as a sequence of uniresponse problems. If, for example, response D_1 is more important than response D_2, then the bivariate assessments of D_1 and D_2 should be thought of as the sequence of assessments: (i) with respect to D_1 marginally; (ii) with respect to D_2 conditional on D_1. Wilk and Gnanadesikan extended this idea to a graphical procedure involving two half-normal plots, both necessary for a study of the data. One plot used the absolute values of the contrasts for response D_1 only, whilst the other used the contrasts for the "conditional" response "D_2 given D_1". These contrasts are obtained essentially from an analysis of covariance of D_2 with response D_1 as a covariable.

Wilk and Gnanadesikan devised a gamma probability plotting procedure for situations where there is no meaningful basis for ordering the responses. If p responses are observed on each experimental unit then the vector of responses for the i'th treatment combination (i = 1....N, where $N = 2^n$) may be denoted by

$\underline{y}_i' = (y_{i1}, y_{i2}, \dots y_{ip})$. The N x p matrix of observations is then given by

$$\underline{Y} = \begin{pmatrix} \underline{y}_1' \\ \underline{y}_2' \\ \vdots \\ \underline{y}_N' \end{pmatrix}$$

For uniresponse situations, the conventional estimates of the overall mean, main effects and interactions may be viewed as being essentially given by an appropriately chosen orthogonal transformation of the observations. If $\underline{R}$ is the appropriately chosen N x N orthogonal matrix, then, for the multiresponse situation, application of the same transformation $\underline{R}$ to $\underline{Y}$ yields

$$\begin{pmatrix} \underline{m}' \\ \underline{X} \end{pmatrix} = \underline{R}\,\underline{Y} \quad \text{where } \underline{m}' = (m_1, m_2, \dots m_p)$$

is $\sqrt{N}$ times the overall mean vector and $\underline{X} = \{x_{ij}\}$ $(i = 1, \dots N-1;\ j = 1, \dots p)$. The rows of $\underline{X}$ are "single-degree-of-freedom contrast vectors" e.g. the i'th row, denoted by $\underline{x}_i' = (x_{i1}, x_{i2} \dots x_{ip})$, has as elements the contrasts for each of the p responses corresponding to the i'th treatment effect.

Wilk and Gnanadesikan introduced a measure of "size" to go with each of the contrast vectors. For the contrast vector $\underline{x}_i$, they associated the measure of size d_i, defined by $d_i = \underline{x}_i' \underline{A}\, \underline{x}_i$ where $\underline{A}$ is an arbitrary p x p positive semi-definite matrix known as the "compounding" matrix. If $\underline{A}$ was chosen to be the identity matrix then d_i would be the sum of squares of the elements of $\underline{x_i}$. Under a null hypothesis of no real effects the "distances" d_i (≥ 0) ($i = 1, \ldots. N-1$) would be distributed as a linear combination of independent single-degree-of-freedom χ^2 variables and may be expected to behave like a random sample from a gamma distribution with scale parameter λ and shape parameter η unknown.

Before being able to carry out a probability plot of the ordered distances, λ and η need to be estimated. A number L ($\leq$N-1) of contrast vectors which the experimenter is interested in studying comparatively, is chosen, and the associated distances calculated. The inclusion of all these distances, some of which would be associated with contrast vectors that may not satisfy the null assumptions, in the process of estimating the parameters may lead to a masking of the fact that some of these "non null" distances are "too large". A number K ($\leq$L) of contrast vectors which may well not reflect real effects is therefore selected. The M($\leq$K) smallest distances, which are therefore even less likely to reflect real effects, are then considered as the M smallest of a random sample of size K from a gamma distribution.

Wilk, Gnanadesikan and Huyett {36} prepared tables for obtaining the maximum likelihood estimates of λ and η, $\hat{\lambda}$ and $\hat{\eta}$, for the above formulation.

Finally, under a null hypothesis of no real effects, a plot of the L ordered distances against the corresponding quantiles of the standard gamma distribution ($\lambda=1$) with $\eta=\hat{\eta}$ should give a straight line with intercept zero and slope $\frac{1}{\lambda}$. Distances corresponding to real effects tend to appear as deviations from the straight line pattern (see Figure 9).

Discussing their plotting procedure, Wilk and Gnanadesikan pointed out that it would be desirable to try various L,K and M values as well as different compounding matrices. Each distinct plot would give a different insight into the factorial structuring of the data. Replotting after omitting distances corresponding to real effects would also enable one to see other peculiarities in the data. They stressed the fact that their method was not meant to replace preliminary analysis of the separate responses through half-normal plotting. Multi-response analysis could, though, importantly augment the separate uni-response analysis.

In the case of experiments of the type denoted by Cell V, the total set of N degrees of freedom is restructured into k orthogonal sets of ν degrees of freedom each, plus one degree of freedom for the mean. Wilk and Gnanadesikan derived the identity

$$\sum_{i=1}^{N} \underline{y}_i' \underline{A}\, \underline{y}_i = \underline{m}' \underline{A}\, \underline{m} + \sum_{i=1}^{k} \sum_{j=1}^{\nu} \underline{z}_{ij}' \underline{A}\, \underline{z}_{ij}$$

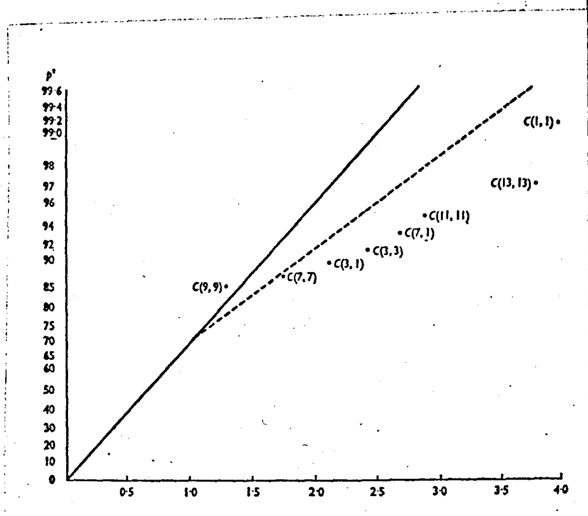


FIGURE 12

A GROUP OF CONTRASTS

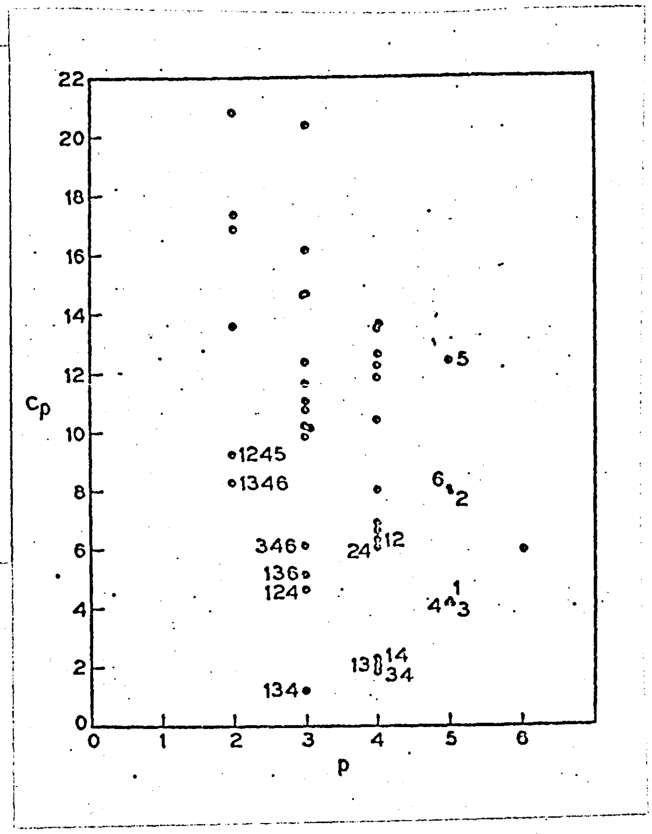


FIGURE 11

C_p PLOT

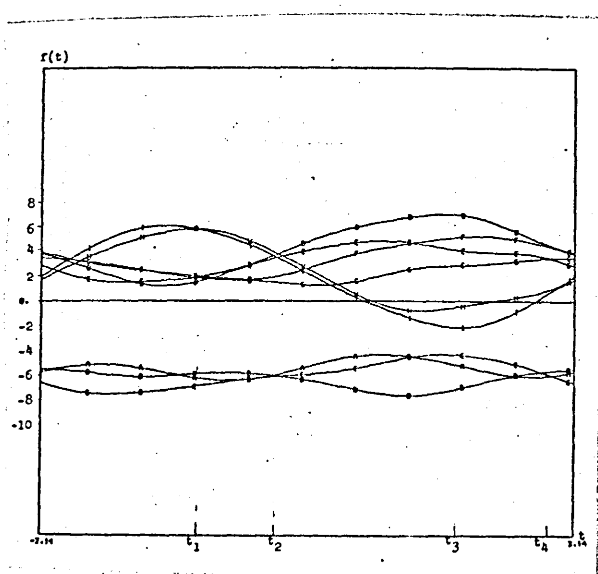


FIGURE 10

8 DIMENSIONAL DATA

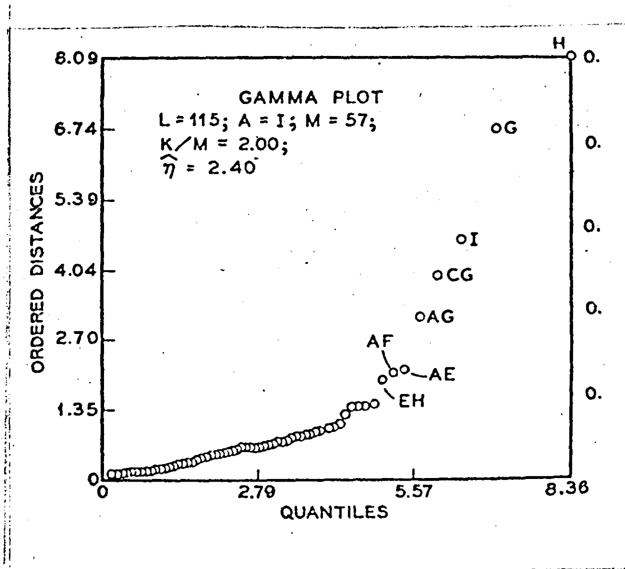


FIGURE 9

GAMMA PLOT

where the $\underline{z_{ij}}$'s are p-dimensional vectors obtained by an appropriate orthogonal transformation of the original observations. Under the null hypothesis of no real effects, they established that "distances" d_i $(i = 1,2,\ldots.k)$, where $d_i = \sum_{j=1}^{\nu} \underline{z_{ij}}' \underline{A}\, \underline{z_{ij}}$, could be considered as a random sample from a gamma distribution with unknown scale and slope parameters. A graphical internal comparisons procedure could then be conducted in the usual manner by plotting the ordered distances against quantiles of the standard gamma distribution using an estimated shape parameter.

There has, as yet, been no published work on graphical procedures for Cell VI type experiments.

The probability plotting procedures advocated by Wilk and Gnanadesikan are valuable tools in gaining insight into the structure of the data. No preselection of certain treatment effects for assignment to error is necessary and the procedures assess the consequences, if any, of a breakdown of the assumptions used in generating the plot itself. The data in a sense "analyses itself". Any attempt to interpret these procedures as formal significance testing procedures would be misguided. The data analytic value of these plots is clearly greater than any formal procedure.

Leaving the field of designed experiments, some interesting papers have been written on various graphical techniques for handling multivariate data. Healy {21} described an extension of the normal plot for multivariate situations, in particular for investigating two-dimensional frequency data to see if it indicated bivariate normality. If X and Y denote the two random variables, Healy considered that it would be natural to order the (x,y) points according to their "distance" from the mean point. Under the null hypothesis of bivariate normality, a transformation to new axes and scales may be made in such a way that the bivariate distribution is circular, with equal standard deviations and zero correlation. The squared "distance" of a point (x,y) from the mean (α,β) is given by

$$D^2 = \left(\frac{x-\alpha}{\sigma_x}\right)^2 + \left(\frac{y-\beta}{\sigma_y}\right)^2 - 2\rho\left(\frac{x-\alpha}{\sigma_x}\right)\left(\frac{y-\beta}{\sigma_y}\right)$$

where, in practice, the population parameters σ_x, σ_y and ρ must be replaced by their usual sample estimates. The variable D^2 has a χ^2 distribution with two degrees of freedom, for which the expected order statistics of a sample of size N are given by

$$\frac{2}{N},\ \frac{2}{N} + \frac{2}{N-1},\ \frac{2}{N} + \frac{2}{N-1} + \frac{2}{N-2},\ \ldots.\ \frac{2}{N} + \frac{2}{N-1} + \ldots + \frac{2}{1}$$

A plot of the ordered squared distances against these order statistics, should, in the null situation, give a straight line configuration.

Healy investigated whether or not normal probability paper could be used for a χ^2 plot and concluded that plotting D against expected normal order statistics would detect outliers adequately and would check bivariate normality. Special χ^2 probability paper is now commercially available. His plots could be extended to three or more variables considered simultaneously.

(c) Other Plots

A novel way of plotting multivariate data was developed by Andrews {1}. His idea was to imbed high-dimensional data in an easily visualized space of functions and then to plot the functions. If the data is k-dimensional, each data point $\underline{x}' = (x_1, x_2, \ldots x_k)$ defines a function

$$f_{\underline{x}}(t) = x_1(2)^{-\frac{1}{2}} + x_2 \sin t + x_3 \cos t + x_4 \sin 2t + x_5 \cos 2t + \ldots\ldots,$$

terminating at the x_k term. This function may be plotted over the range $-\pi < t < \pi$ and a function may therefore be drawn for each data point $\underline{x}'$. Close points appear as close functions and distant points as distant functions, so multivariate clusters and outliers may be identified visually from the plot of the functions (see Figure 10). This method has the advantage of being unrestricted as regards the value of k but, for visual purposes, only about ten points may be plotted on the same graph. There is considerable scope for further research into this type of representation, particularly with the use of various $g_i(t)$ forms in the expansion $f_{\underline{x}}(t) = \sum_{i=1}^{k} x_i g_i(t)$.

(d) Plots for Regression Studies

Mallows {24} investigated the problem of deciding how many terms should be included in a regression equation. He was particularly interested in the graphic display of some statistic which would measure the adequacy of any chosen set. One such statistic is the residual mean square. J.W. Gorman, in a private communication, had suggested to Mallows that a plot could be made of residual mean squares in order of size against their ranks in this ordering. Frequently, estimates of residual variance, converge to a stable value as more terms are fitted, leading to a feeling of confidence that a sufficiently complete collection of candidate terms has been specified.

Mallows suggested that a convenient set of displays (one for each candidate term) could be obtained by plotting values of the estimated regression coefficients against the number of terms included in the equation. In favourable cases a horizontal line of points would appear in each display, corresponding to a collection of equations in which the coefficient studied is insensitive to the presence or absence of other terms. Mallows then developed a plot based on a statistic he labelled C_p. This was essentially an estimate of the average predictive mean square error of a fitted p-term equation. If RSS_i denotes the residual sum of squares corresponding to a fitted i-term equation, then Mallows derived the relationship

$$C_p = \frac{(n-k)RSS_p}{RSS_k} - n + 2p$$

where k = total number of candidate terms available, and n = number of data values.
In a plot of values C_p against p, a point lying near the 45^0 line corresponds to an equation in which all the important terms have been included. A point lying some way above the line corresponds to a badly fitting equation. Figure 11 illustrates a C_p plot for data with 6 candidate terms, the points being labelled by terms omitted. It seems clear that terms 1, 3, and 4 are unimportant, both individually and jointly.

The disadvantage of this method is that it requires the specification of a supposedly exhaustive set of candidate terms. In a private communication Tukey suggested using the index $\frac{n+p}{n-p} RSS_p$ in the same way as C_p.

The usefulness of graphical analysis of residuals in regression studies has been discussed by Tukey and Wilk {33}, Wilk and Gnanadesikan {39} and Cox and Snell {9}. All agree that various plots of residuals can be sensitive and informative tools for checking on the adequacy of the model, the appropriateness of independent variables, the existence of outliers, the relevance of extraneous variables and distributional peculiarities. Valuable plots include (i) plots against fitted values for detecting non-constancy of variance, (ii) plots against variables employed in the fit, where a curved relationship would indicate non-linear regression on that variable, (iii) plots against variables not employed in the fit to test the relevance of that variable and (iv) plots of the ordered residuals against the expected order statistics from a standard normal distribution to test for non-normality of the distribution of the errors.

Cox and Snell emphasised that the analysis of residuals would indicate the nature of a departure from an initial model but would not explicitly indicate how to extend or replace the model.

(e) Plots for Contingency Tables and Studies of Association between Variables

A procedure for graphical analysis of large two-way contingency tables was proposed by Fienberg {13}. A certain quantity was added to each cell in the table in order that no zeros would be present, and then, for each cell, a normalised "contrast" was computed, which was a function of the cell frequency and the frequencies of closely neighbouring cells. These contrasts were divided into four groups, so that contrasts within each group were uncorrelated. In order to test the null hypothesis that all interactions between the levels of the two variables are zero, each group of normalised contrasts was plotted separately on half-normal probability paper, assuming that the contrasts within each group formed an independent sample from a normal distribution with zero mean and unit variance. Contrasts deviating significantly from the theoretical unit variance line thus exhibited strong interaction. To separate the strong interaction contrasts from the rest, Fienberg used boundary lines suggested by Daniel {11} and Birnbaum {4} (see Figure 12). He pointed out that his procedure could be extended to handle the analysis of three-way tables and was a development of the procedure presented by Cox and Lauh {8}, who adapted half-normal plotting to the analysis of contingency tables in which there was a binary response variable. A drawback to Cox and Lauh's procedure was the fact that their plotted points were not independent, and thus the results for half-normal plotting were not strictly applicable.

Shahani {30} has given a rather simple graphical procedure for testing association between two random variables. It ignors the points around the central origin of the scatter diagram and involves a test statistic based on the number of points found in four specified regions. The test compares unfavourably with Fisher's Z-transformation but it is much simpler to use.

CHAPTER 6

GRAPHICAL METHODS FOR GROWTH CURVES

Inspection of the preceding chapters reveals problem areas in which no work or very little work has been published concerning the application of graphical methods. One such problem area is growth curves. This is rather surprising since various methods of residual analyses have been successfully applied to model identification in regression studies and these studies have direct analogies in time series models, which take the form of regression models with time as an independent variable.

One graphical approach for identification of growth curves has been advocated by Gregg, Hossell and Richardson {19}. The seven basic growth curves with their characterizing equations are:-

(i) Linear, $y = a + bt$,

(ii) Quadratic, $y = a + bt * ct^2$,

(iii) Exponential, $y = ae^{bt}$,

(iv) Logarithmic Parabola, $y = ae^{bt + ct^2}$,

(v) Simple Modified Exponential, $y = K + ae^{bt}$,

(vi) Gompertz, $y = ae^{be^{ct}}$,

(vii) Logistic, $y = (K + ae^{bt})^{-1}$,

where y denotes the growth variable, t denotes time, and a, b, c and K are parameters.

The following relationships may easily be obtained from the respective characterizing equations:-

(i) Linear, $\frac{dy}{dt}$ is constant,

(ii) Quadratic, $\frac{dy}{dt} = b + 2ct$,

(iii) Exponential, $\left(\frac{1}{y}\right) \frac{dy}{dt}$ is constant,

(iv) Logarithmic Parabola, $\left(\frac{1}{y}\right) \frac{dy}{dt} = b + 2ct$

(v) Simple Modified Exponential, $\log \left(\frac{dy}{dt}\right) = \log (ab) + bt$,

(vi) Gompertz, $\log\left(\frac{1}{y} \cdot \frac{dy}{dt}\right) = \log (bc) + ct$,

and (vii) Logistic, $\log\left(\frac{1}{y^2} \cdot \frac{dy}{dt}\right) = \log (-ab) + bt$.

Using the word "slope" to mean the rate of change $\frac{dy}{dt}$, and estimating the value of y at any point by a moving average (m.a.), Gregg, Hossell and Richardson produced the table below:-

Compute and Plot Against Time:-	If the Plotted points vary about a straight line which is:-	Then the curve suggested is:-
Slope	Horizontal	Linear
Slope	At an angle to the horizontal	Quadratic
Slope/m.a.	Horizontal	Exponential
Slope/m.a.	At an angle to the horizontal	Logarithmic Parabola
log(slope)	Sloping down to the right	Simple modified Exponential
log(slope/m.a.)	Sloping down to the right	Gompertz
$\log\left[\text{slope}/(\text{m.a.})^2\right]$	Sloping down to the right	Logistic

The quantities in column 1 of the table, they labelled "slope characteristics" and their procedure for identification was to plot the slope characteristics of the data and inspect these plots for any indication of a satisfactory model.

This method has two practical difficulties whose importance depends very much on the smoothness of the data available. There is first the problem of measuring the slopes at different times. This can be done approximately by taking first differences and smoothing these with a weighted moving average. Alternatively one can smooth first and then take differences or find the slope of a fitted trend line. Neither approach is very satisfactory. One can similarly question the use of a moving average to estimate the value of y at any point. The second problem comes from the fact that the method depends on an eye comparison of different plots to see which looks most like a straight line. One can, however, be misled in this since the vertical scales are all in different units.

Two other graphical ways of deciding which model is appropriate are (i) plot the data on graph paper using axes designed to give straight lines if the data comes from the appropriate model, (ii) obtain plots using the difference properties of the curves although these plots could vary considerably about their expected configurations because of the large variances involved. Some difference properties are:-

(a) Δy_t is constant for linear data, linear for quadratic data.

(b) $\dfrac{\Delta y_t}{y_t}$ is constant for exponential data.

(c) $\dfrac{\Delta y_t}{\Delta y_{t-1}}$ is constant for linear, exponential and simple modified exponential data.

(d) $\dfrac{\Delta \log y_t}{\Delta \log y_{t-1}}$ is constant for exponential and Gompertz data.

(e) $\Delta\left(\dfrac{1}{y_t}\right) \Big/ \Delta\left(\dfrac{1}{y_{t-1}}\right)$ is constant for exponential and logistic data.

(f) $\Delta \log y_t$ is constant for exponential data, linear for logarithmic parabola data.

(g) $\dfrac{y_t}{y_{t-1}}$ is constant for exponential data.

Both these methods again depend on an eye comparison of different plots whose vertical scales are not alike. In Part II a graphical method is proposed for identifying growth curves which surmounts this deficiency.

PART II

A GRAPHICAL IDENTIFICATION PROCEDURE FOR GROWTH CURVES

CHAPTER 7

FOUNDATION OF THE IDENTIFICATION PROCEDURE

Let the growth data we wish to identify be denoted by $Y_1, Y_2, \ldots\ldots Y_n$, the data being measured at equal intervals of time such that the value Y_i occurs at time $t = i$ $(i = 1,2,\ldots.n)$. The data is divided into overlapping "blocks", each block consisting of a fixed number of consecutive data points, usually between 10 and 25 depending on the magnitude of n. The division is such that each block is comprised of an odd number of data points, say (2m+1), i.e. the k'th block, B_k say, consists of data points Y_k, Y_{k+1}, $\ldots.Y_{k+2m}$ with corresponding time base $t = k$, $t = k+1$, $\ldots.$ $t = k+2m$ $(k = 1,2,\ldots.,n-2m)$. For convenience the time base of each B_k is transformed into (2m+1) equally spaced points in the interval $-1 \leqslant x \leqslant +1$. This is effected for B_k by the transformation

$$T_k : x = \frac{t-k}{m} - 1$$

which also has the property that the natural order of the original time base is preserved and further $k \underset{T_k}{\leftrightarrow} -1$ and $k+2m \underset{T_k}{\leftrightarrow} +1$. We shall use the notation β_k to denote the block B_k transformed by T_k.

To each block β_k we fit the model

$$f(x) = \sum_{r=0}^{r=h} \alpha_r^{(k)} g_r(x)$$

where the $\alpha_r^{(k)}$ are unknown parameters and $g_r(x)$ is a known polynomial of degree r in x which is fixed for the particular data under consideration. In deciding the value of h, the order of the polynomial fit, it was observed that too high a value results not only in computational difficulties but also in a relatively useless oscillatory fit to "noisy" data, while smaller values yield a smoother fit and easier numerical handling. For example, Figure 13 illustrates quite well the difference in smoothness between a seventh order and a fourth order polynomial fitted to a block of "noisy" exponential data. Tests such as that illustrated in Figure 13 together with computational algebraic difficulties encountered in the least squares process (see Chapter 8) led us to accept the value 4 for h as providing an acceptable level of smoothness of fit with a tolerable measure of algebraical and numerical manipulability.

Least squares estimates, $a_0^{(k)}$, $a_1^{(k)}$, $a_2^{(k)}$, $a_3^{(k)}$, $a_4^{(k)}$, of $\alpha_0^{(k)}$, $\alpha_1^{(k)}$, $\alpha_2^{(k)}$, $\alpha_3^{(k)}$, $\alpha_4^{(k)}$ respectively, are obtained for each block β_k. In Chapter 9 we investigate relationships between the estimates or "coefficients" themselves and their dependence on k and so develop some plotting procedures which aim at identification of particular types of growth data. We shall refer to this process as"the sliding block technique." The possible models are restricted to the seven mentioned by Gregg, Hossell and Richardson {19}, namely linear,

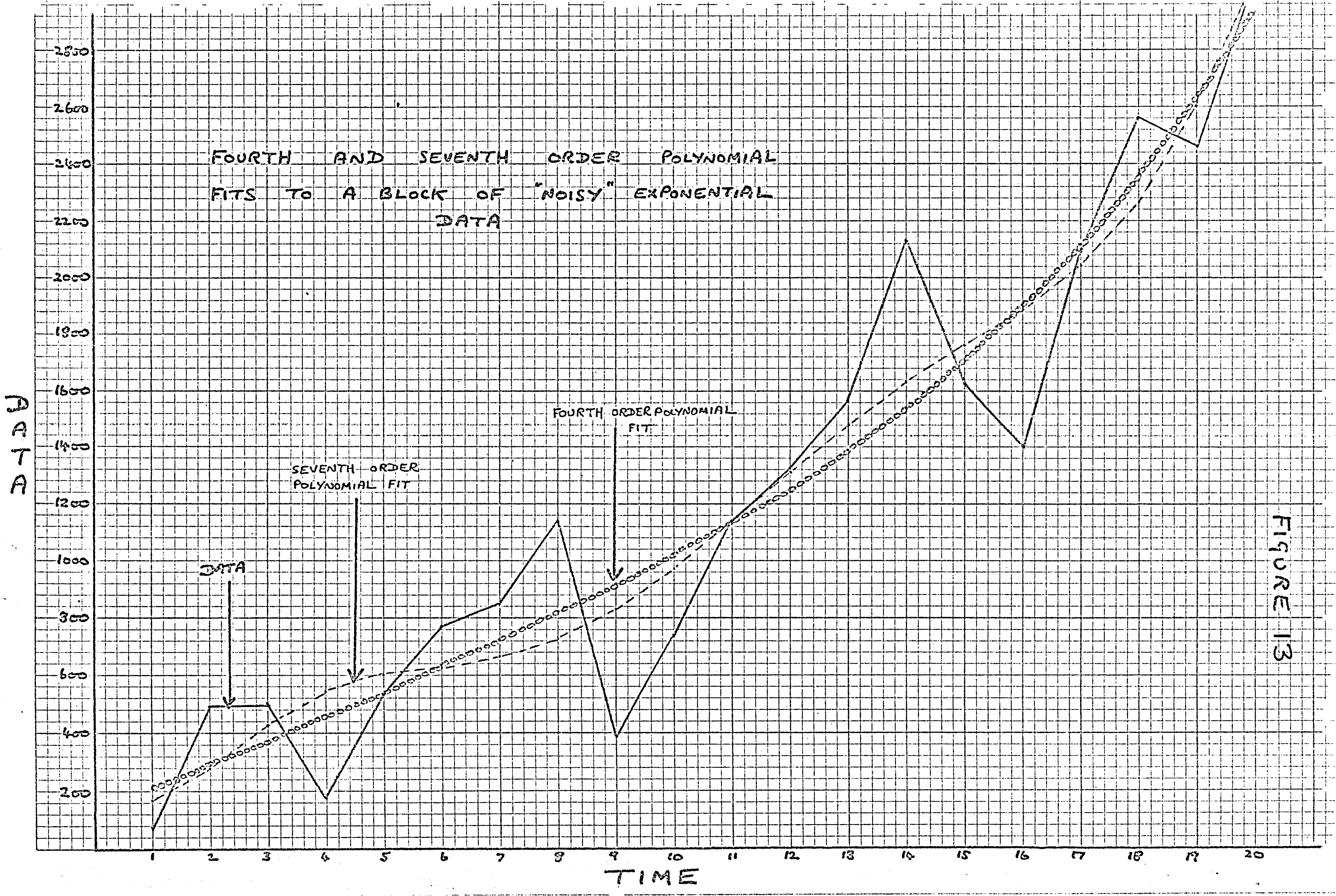

FOURTH AND SEVENTH ORDER POLYNOMIAL FITS TO A BLOCK OF "NOISY" EXPONENTIAL DATA
FOURTH ORDER POLYNOMIAL FIT
SEVENTH ORDER POLYNOMIAL FIT
DATA
DATA
TIME
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20

FIGURE 13

quadratic, exponential, logarithmic parabola, simple modified exponential, Gompertz and logistic.

Much choice is available for the polynomials $g_r(x)$ e.g. the Taylor series (so that $g_r(x) = x^r$), Legendre polynomials, Tchebychef polynomials etc. Each have their own particular advantages (and disadvantages) in fitting procedures. However, in our investigation the $g_r(x)$ are chosen in such a way as to attempt to minimise the ratios of the standard deviations of the coefficients $a_j^{(k)}$ $(j = 0,1,....4)$ to their absolute values, thus obtaining more reliable coefficient plots for identification purposes. While the full details are left until Chapter 10 it should be mentioned that such $g_r(x)$ are tailor-made to a particular set of data but are in no way block dependent.

Finally the identification procedure is tested on artificial growth data, both "clean" and "noisy", and on some real growth data.

CHAPTER 8

THE LEAST SQUARES FITTING PROCESS

In this chapter the general form of the coefficients $a_j^{(k)}$ $(j = 0,1,\ldots 4)$ is obtained by the method of least squares. Throughout Part II of this thesis the notation $\sum_i$ will denote summation over integer values from $i = k$ to $i = k+2m$.

In the k'th block β_k, the data values are Y_k, $Y_{k+1},\ldots Y_{k+2m}$ with corresponding x values $x_k = -\frac{m}{m}$, $x_{k+1} = -\frac{m-1}{m}$, ... $x_{k+m} = 0$, ... $x_{k+2m} = \frac{m}{m}$, so that

$$T_k : t = k + i \longleftrightarrow x = x_{k+i} = -\frac{m-i}{m}$$

To the block β_k we fit the model

$$f(x_i) = \sum_{r=o}^{r=4} \alpha_r^{(k)} g_r(x_i) , \quad (i = k,k+1,\ldots k+2m),$$

where

$$g_r(x_i) = \sum_{j=o}^{j=r} p_{r-j}^{(r)} x_i^j , \quad (r = 0,1,2,3,4),$$

the p's being constants whose values are eventually found in our attempt to minimise $\dfrac{\text{S.Dev.}(a_j^{(k)})}{|a_j^{(k)}|}$ $(j = 0,1,\ldots .4)$ for the data under consideration.

We make the assumptions that $\text{Var}(Y|x=x_i) = \sigma^2$, a constant, and $\text{Cov}(Y_i,Y_j) = 0$ for all i,j $(i \neq j)$.

The least squares estimates $a_0^{(k)}, a_1^{(k)} \ldots . a_4^{(k)}$ of $\alpha_0^{(k)}, \alpha_1^{(k)} \ldots . \alpha_4^{(k)}$ are those values of $\alpha_0^{(k)}, \alpha_1^{(k)} \ldots . \alpha_4^{(k)}$ which minimise the quantity

$$\sum_i (Y_i - \sum_{r=0}^{r=4} \alpha_r^{(k)} g_r(x_i))^2 .$$

If $g(r,s) = \sum_i g_r(x_i) . g_s(x_i)$, then least squares theory gives

$$\begin{pmatrix} g(0,0) & g(0,1) \ldots\ldots & g(0,4) \\ g(1,0) & & \\ \vdots & & \\ g(4,0) & & g(4,4) \end{pmatrix} \begin{pmatrix} \alpha_0^{(k)} \\ \alpha_1^{(k)} \\ \alpha_2^{(k)} \\ \alpha_3^{(k)} \\ \alpha_4^{(k)} \end{pmatrix} = \begin{pmatrix} \sum_i Y_i \; g_0(x_i) \\ \sum_i Y_i \; g_1(x_i) \\ \sum_i Y_i \; g_2(x_i) \\ \sum_i Y_i \; g_3(x_i) \\ \sum_i Y_i \; g_4(x_i) \end{pmatrix} .$$

The calculation of the $g(r,s)$ terms is given in Appendix 1. The inversion process for this matrix is simplified by

(i) putting the terms $p_1^{(1)}, p_1^{(2)}, p_1^{(3)}, p_3^{(3)}, p_1^{(4)}$ and $p_3^{(4)}$ equal to zero as in Tchebychef, Hermite and Legendre polynomials, and (ii) omitting terms of smaller order than $O(m^{-2})$, so forming a "truncated" matrix from the original.

To check that these approximations did not significantly affect the matrix elements a programme was written to calculate the elements of the original matrix above and the "truncated" matrix for values of m from 5 to 13. For convenience the p's were arbitrarily given Taylor series values i.e. $p_o^{(j)} = 1$, $p_r^{(j)} = 0 (r \neq 0)$; $j = 0,1,\ldots.4$.

A typical result (m = 7) was:-

<u>ORIGINAL {g(r,s)} MATRIX</u>

$$\begin{pmatrix} 15.0 & 0 & 5.71428 & 0 & 3.89504 \\ 0 & 5.71428 & 0 & 3.89504 & 0 \\ 5.71428 & 0 & 3.89504 & 0 & 3.14178 \\ 0 & 3.89504 & 0 & 3.14178 & 0 \\ 3.89504 & 0 & 3.14178 & 0 & 2.74317 \end{pmatrix}$$

<u>TRUNCATED FORM OF {g(r,s)} MATRIX</u>

$$\begin{pmatrix} 15.0 & 0 & 5.71428 & 0 & 3.89524 \\ 0 & 5.71428 & 0 & 3.89524 & 0 \\ 5.71428 & 0 & 3.89524 & 0 & 3.14275 \\ 0 & 3.89524 & 0 & 3.14275 & 0 \\ 3.89524 & 0 & 3.14275 & 0 & 2.74587 \end{pmatrix}$$

The largest error in an element due to truncation was 0.01%, a clearly acceptable figure. Similarly acceptable figures were obtained for other values of m.

The inverse of the truncated $\{g(r,s)\}$ matrix is given in Appendix 2. To check the working, a programme was written to compare this inverse with the inverse of the original $\{g(r,s)\}$ matrix obtained by a Fortran subroutine, for values of m from 5 to 13 using Taylor series p values.

A typical result (m=7) was:-

<u>INVERSE OF TRUNCATED $\{g(r,s)\}$ MATRIX AS AS IN APPENDIX 2</u>

$$\begin{pmatrix} 0.237970 & 0 & -1.01195 & 0 & 0.818274 \\ 0 & 1.12743 & 0 & -1.39738 & 0 \\ -1.01195 & 0 & 7.64035 & 0 & -7.30850 \\ 0 & -1.39738 & 0 & 2.05002 & 0 \\ 0.818274 & 0 & -7.30850 & 0 & 7.57098 \end{pmatrix}$$

<u>INVERSE OF ORIGINAL $\{g(r,s)\}$ MATRIX USING FORTRAN SUBROUTINE</u>

$$\begin{pmatrix} 0.239449 & 0 & -1.01132 & 0 & 0.818284 \\ 0 & 1.12946 & 0 & -1.40025 & 0 \\ -1.01132 & 0 & 7.64143 & 0 & -7.31582 \\ 0 & -1.40025 & 0 & 2.05426 & 0 \\ 0.81824 & 0 & -7.31582 & 0 & 7.58154 \end{pmatrix}$$

The largest error in an element is 0.14%. The errors increase with increasing values of m but at a declining rate. The largest error for m = 13 is 0.94%, an acceptable figure.

Denoting the elements of the inverse of the truncated form of the $\{g(r,s)\}$ matrix by $G(r,s)$ $(r=0,1,\ldots.4;\ s=0,1,\ldots.4)$, a good approximation to the coefficients $a_0^{(k)}, \ldots\ldots\ldots a_4^{(k)}$ is given by

$$\begin{pmatrix} a_0^{(k)} \\ a_1^{(k)} \\ a_2^{(k)} \\ a_3^{(k)} \\ a_4^{(k)} \end{pmatrix} = \begin{pmatrix} G(0,0) & G(0,1) & \ldots\ldots\ldots G(0,4) \\ G(1,0) & & \\ \vdots & & \\ G(4,0) & \ldots\ldots\ldots\ldots\ldots & G(4,4) \end{pmatrix}$$

$$\begin{pmatrix} \sum_i Y_i\, p_0^{(0)} \\ \sum_i Y_i\, p_0^{(1)} x_i \\ \sum_i Y_i\, (p_0^{(2)} x_i^2 + p_2^{(2)}) \\ \sum_i Y_i\, (p_0^{(3)} x_i^3 + p_2^{(3)} x_i) \\ \sum_i Y_i\, (p_0^{(4)} x_i^4 + p_2^{(4)} x_i^2 + p_4^{(4)}) \end{pmatrix} \qquad \ldots\ldots \text{(8.1)}$$

where

$$\mathrm{Var}(a_j^{(k)}) = G(j,j)\ .\ \sigma^2,\ (j=0,1,\ldots 4)\ldots \quad (8.2)$$

PLOTS FOR MODEL IDENTIFICATION

In the following sections growth curve models are investigated in order to build up plotting procedures from the "sliding block" technique described in Chapter 7. The procedures are then inspected to see if one in particular would suffice for the identification of the seven basic models.

(a) Linear Data

If the data under inspection was perfectly linear, then, at time t, $Y_t = a + bt$ where a and b are unknown parameters. Applying the transformation T_k to the block B_k we put $t = mx + k + m$, whence in β_k:

$$Y_i = a+b(mx_i+k+m) = (a+bk+bm)+bmx_i, (i=k,k+1,\ldots k+2m).$$

To this data we are fitting the model

$$f(x_i) = \alpha_0^{(k)} p_0^{(0)} + \alpha_1^{(k)} p_0^{(1)} x_i + \alpha_2^{(k)} (p_0^{(2)} x_i^2 + p_2^{(2)}) + \alpha_3^{(k)} (p_0^{(3)} x_i^3 + p_2^{(3)} x_i) + \alpha_4^{(k)} (p_0^{(4)} x_i^4 + p_2^{(4)} x_i^2 + p_4^{(4)}) \ldots (9.1)$$

Equating coefficients we obtain, for non-zero $p_0^{(j)}$, $(j=0,1,\ldots 4)$

$$\alpha_1^{(k)} p_0^{(1)} = bm,$$

$$\alpha_0^{(k)} p_0^{(0)} = a + bk + bm,$$

$$\alpha_2^{(k)} = \alpha_3^{(k)} = \alpha_4^{(k)} = 0.$$

In practice we replace the $\alpha_j^{(k)}$ by their least squares estimate $a_j^{(k)}$. The following plots would be useful as aids to identifying linear data:-

(i) A plot of $a_1^{(k)}$ against k would give a straight line parallel to the k-axis having intercept $\frac{bm}{p_0^{(1)}}$.

(ii) A plot of $a_0^{(k)}$ (vert.) against k (horiz.) would be linear, with slope $\frac{b}{p_0^{(0)}}$ and intercept $\left(\frac{a+bm}{p_0^{(0)}}\right)$.

(iii) A plot of $a_0^{(k)}$ against $a_1^{(k)}$ for increasing k would give a straight line perpendicular to the $a_1^{(k)}$ axis. The plotted points would be equally spaced along this line.

(iv) A plot of $a_0^{(k)}$ against $a_2^{(k)}$ would give a series of points along the $a_0^{(k)}$ axis. Similarly for $a_0^{(k)}$ against $a_3^{(k)}$ or $a_4^{(k)}$.

(v) A plot of $a_1^{(k)}$ against $a_2^{(k)}$ (or $a_3^{(k)}, a_4^{(k)}$) would give a single point on the $a_1^{(k)}$ axis.

(b) Quadratic Data

If the data under inspection was perfectly quadratic, then, at time t, $Y_t = a + bt + ct^2$ where a,b and c are unknown parameters. Transforming as in (a) we obtain for β_k:

$$Y_i = (a+bk+bm+ck^2+2ckm+cm^2) + (bm+2ckm+2cm^2)\, x_i$$
$$+ cm^2x_i^2, \quad (i = k,k+1,\ldots k+2m).$$

Fitting model (9.1) and equating coefficients, we obtain, for non-zero $p_0^{(j)}$ $(j = 0,\ldots 4)$,

$$\alpha_2^{(k)}\, p_0^{(2)} = cm^2,$$

$$\alpha_1^{(k)}\, p_0^{(1)} = bm + 2ckm + 2cm^2,$$

$$\alpha_0^{(k)}\, p_0^{(0)} + \alpha_2^{(k)}\, p_2^{(2)} = a + bk + bm + ck^2 + 2ckm + cm^2,$$

$$\alpha_3^{(k)} = \alpha_4^{(k)} = 0 .$$

Replacement of the $\alpha_j^{(k)}$ by their least squares estimates $a_j^{(k)}$ suggests the following plots as aids to identification:-

(i) A plot of $a_2^{(k)}$ against k would give a straight line parallel to the k-axis having intercept $\dfrac{cm^2}{p_0^{(2)}}$.

(ii) A plot of $a_1^{(k)}$ (vert.) against k (horiz.) would be linear, with slope $\dfrac{2cm}{p_0^{(1)}}$ and intercept $\left(\dfrac{bm+2cm^2}{p_0^{(1)}}\right)$.

(iii) A plot of $a_0^{(k)}$ against $a_2^{(k)}$ for increasing k would give a straight line perpendicular to the $a_2^{(k)}$ axis.

(iv) A plot of $a_1^{(k)}$ against $a_2^{(k)}$ would give a straight line perpendicular to the $a_2^{(k)}$ axis, the points being equally spaced along the line.

(v) A plot of $a_1^{(k)}$ against $a_3^{(k)}$ or $a_4^{(k)}$ would give a series of equally spaced points along the $a_1^{(k)}$ axis.

(vi) A plot of $a_0^{(k)}$ against $a_3^{(k)}$ or $a_4^{(k)}$ would give a series of points along the $a_0^{(k)}$ axis.

(c) Exponential Data

If the data under inspection was perfectly exponential, then, at time t, $Y_t = a\, e^{bt}$ where a and b are unknown parameters. Transforming as in (a) we obtain for β_k:

$$Y_i = a\, e^{b(mx_i+k+m)} \quad .$$

From (8.1) and Appendix 2,

$$a_0^{(k)} = G(0,0) \sum_i Y_i p_0^{(0)} + G(0,2) \sum_i Y_i (p_0^{(2)} x_i^2 + p_2^{(2)})$$

$$+ G(0,4) \sum_i Y_i (p_0^{(4)} x_i^4 + p_2^{(4)} x_i^2 + p_4^{(4)})$$

Hence on substituting for Y_i,

$$a_0^{(k)} = G(0,0).p_0^{(0)}.a.e^{b(k+m)} \sum_i e^{bmx_i} + G(0,2).a.e^{b(k+m)}$$

$$\sum_i e^{bmx_i} (p_0^{(2)} x_i^2 + p_2^{(2)}) + G(0,4).a.e^{b(k+m)} \sum_i e^{bmx_i}$$

$$(p_0^{(4)} x_i^4 + p_2^{(4)} x_i^2 + p_4^{(4)}),$$

i.e. $$a_0^{(k)} = a.e^{b(k+m)} \Big[\sum_i e^{bmx_i} (G(0,0)p_0^{(0)} + G(0,2)p_2^{(2)} + G(0,4)p_4^{(4)}) + \sum_i e^{bmx_i} x_i^2 (G(0,2)p_0^{(2)} + G(0,4)p_2^{(4)}) + \sum_i e^{bmx_i} x_i^4 G(0,4) p_0^{(4)} \Big] .$$

Replacing x_i by its value $\frac{i-k-m}{m}$ and changing the variable of summation to be $r = 0,1,\ldots 2m$, $a_0^{(k)}$ takes the form

$$ae^{bk}\sum_{r=o}^{2m} e^{br}\{(G(0,0)p_0^{(0)}+G(0,2)p_2^{(2)}+G(0,4)p_4^{(4)}) +$$

$$(\frac{r-m}{m})^2(G(0,2)p_0^{(2)}+G(0,4)p_2^{(4)}) + (\frac{r-m}{m})^4 G(0,4)p_0^{(4)}\} ,$$

whence it is easily seen that $\frac{a_0^{(k+1)}}{a_0^{(k)}} = e^b$, a constant.

Similarly it can be shown that $\frac{a_j^{(k+1)}}{a_j^{(k)}} = e^b$ $(j=1,2,3,4)$.

From (8.1) and Appendix 2 we may similarly derive the relationships:

$$a_1^{(k)} = ae^{bk}\sum_{r=o}^{2m} e^{br}\{(G(1,1)p_0^{(1)}+G(1,3)p_2^{(3)})+(\frac{r-m}{m})^3$$

$$G(1,3)p_0^{(3)}\} ,$$

$$a_2^{(k)} = a\ e^{bk}\sum_{r=o}^{2m} e^{br}\{(G(2,0)p_0^{(0)}+G(2,2)p_2^{(2)}+G(2,4)p_4^{(4)})$$

$$+ (\frac{r-m}{m})^2(G(2,2)p_0^{(2)}+G(2,4)p_2^{(4)})+(\frac{r-m}{m})^4 G(2,4)p_0^{(4)}\} ,$$

$$a_3^{(k)} = a\ e^{bk}\sum_{r=o}^{2m} e^{br}\{(G(3,1)p_0^{(1)}+G(3,3)p_2^{(3)})+(\frac{r-m}{m})^3$$

$$G(3,3)p_0^{(3)}\} ,$$

and

$$a_4^{(k)} = a\ e^{bk} \sum_{r=o}^{2m} e^{br}\{(G(4,0)p_0^{(0)}+G(4,2)p_2^{(2)}+G(4,4)p_4^{(4)})$$

$$+\ (\frac{r-m}{m})^2(G(4,2)p_0^{(2)}+G(4,4)p_2^{(4)})+(\frac{r-m}{m})^4 G(4,4)p_0^{(4)}\}.$$

It follows that $\frac{a_r^{(k)}}{a_s^{(k)}}$ $(r = 0,1,2,3,4;\ s = 0,1,2,3,4;$ $r \neq s)$ are constants whose values depend on m, b and the p terms.

The following plots would therefore be useful for identifying exponential data:-

(i) Plots of $\frac{a_j^{(k+1)}}{a_j^{(k)}}$ against k $(j = 0,1,2,3,4)$ would give a straight line parallel to the k-axis having intercept e^b.

(ii) Plots of $a_r^{(k)}$ against $a_s^{(k)}$ $(r \neq s)$ would give straight lines passing through the origin. As k increases the plotted points become increasingly far apart along the lines.

(d) <u>Simple Modified Exponential Data</u>

If the data under inspection was perfectly simple modified exponential, then, at time t, $Y_t = K + a\ e^{bt}$ where a, b and K are unknown parameters. Transforming as in (a) we obtain for β_k:

$$Y_i = K + a\ e^{b(mx_i+k+m)} .$$

From (8.1) and Appendix 2, it follows that

$$a_0^{(k)} = G(0,0)\ \sum_i p_0^{(0)}(K+ae^{b(mx_i+k+m)})+G(0,2)\ \sum_i (p_0^{(2)}x_i^2+p_2^{(2)})(K+ae^{b(mx_i+k+m)}) + G(0,4)\ \sum_i (p_0^{(4)}x_i^4+p_2^{(4)}x_i^2+p_4^{(4)})(K+ae^{b(mx_i+k+m)}),$$

$$\text{i.e. } a_0^{(k)} = K\Big[G(0,0)p_0^{(0)}(2m+1)+G(0,2)(p_0^{(2)}\ \sum_i x_i^2+p_2^{(2)}(2m+1))+G(0,4)(p_0^{(4)}\ \sum_i x_i^4+p_2^{(4)}\ \sum_i x_i^2+p_4^{(4)}(2m+1))\Big]$$

$$+\ a.e^{b(k+m)}\Big[\sum_i e^{bmx_i}(G(0,0)p_0^{(0)}+G(0,2)p_2^{(2)}+G(0,4)p_4^{(4)}) + \sum_i e^{bmx_i}x_i^2(G(0,2)p_0^{(2)}+G(0,4)p_2^{(4)}) + \sum_i e^{bmx_i}\ x_i^4\ G(0,4)p_0^{(4)}\Big] \ldots\ldots\ldots(9.2)$$

In Appendix 3 it is shown that the coefficient of K is non-zero.

Similar relationships may also be obtained for $a_1^{(k)}$, $a_2^{(k)}$, $a_3^{(k)}$ and $a_4^{(k)}$, but these differ from $a_0^{(k)}$ in the essential feature that the coefficient of K is zero, a fact which is established in Appendix 3.

These results indicate that the following plots would be useful for identification of simple modified exponential data:-

(i) Plots of $\dfrac{a_j^{(k+1)}}{a_j^{(k)}}$ against k (j = 1,2,3,4) would give a straight line parallel to the k-axis having intercept e^b. A plot of

$$\frac{a_0^{(k+1)}}{a_0^{(k)}}$$ against k would not take this con-

figuration (since $K \neq 0$).

(ii) Plots of $a_r^{(k)}$ against $a_s^{(k)}$ ($r = 1,2,3,4$; $s = 1,2,3,4$; $r \neq s$) would give straight lines passing through the origin. Since parameter b is negative, the plotted points would become increasingly close as k increased.

(iii) Plots of $a_0^{(k)}$ against $a_j^{(k)}$ ($j = 1,2,3,4$) would give straight lines not passing through the origin.

(e) Sigmoid Data; Gompertz and Logistic

If the data under inspection was perfectly Gompertz or logistic, the theoretical forms of the coefficients $a_j^{(k)}$ ($j = 0,..4$) become too complicated for any immediate plotting procedure to emerge. We can, however, reason what should happen if we bear in mind that we are in practice moving "along" the s-shaped trend curve as we pass from block to block.

There are three distinct phases:

(i) Growth is relatively slow at first and then begins to rise exponentially. The first few blocks will, in fact, be composed solely of such data and we might expect plotting procedures applied to these blocks to give results consistent with exponential data.

(ii) In the middle of the trend curve there is a point of inflection. Blocks composed of data points in this region would be expected to give plots indicating linear data.

(iii) There is, finally, a relative decline in growth as the trend rises to an upper asymptote. Plotting procedures applied to blocks composed of data at this "top end" of the curve would be expected to give results consistent with simple modified exponential data.

Plots involving the coefficients $a_j^{(k)}$ $(j = 0,\ldots 4)$, when applied to perfect sigmoid data, would therefore give patterns indicating a merging of exponential, linear and simple modified exponential data. It does, however, appear that we shall be unable to distinguish between Gompertz data and logistic data.

(f) Logarithmic Parabolic Data

If the data under inspection was a perfect logarithmic parabola, then, at time t, $Y_t = a\,e^{bt+ct^2}$ where a, b and c are unknown parameters. The theoretical forms of the coefficients $a_j^{(k)}$ $(j = 0,1,\ldots 4)$ again become too complicated for any immediate plotting procedure to emerge. It is possible, however, that if c is small, plots would give configurations similar to those expected from exponential data. The best course seems to be to apply plotting procedures to artificial logarithmic parabolic data once the p terms have been fixed and see if these result in distinct configurations. This is done in Chapter 11.

Summary

In order to avoid having to make an eye comparison of different plots, with possibly different scales, when identifying the growth model, it is desirable that one particular plot involving some (or all) of the coefficients $a_j^{(k)}$ $(j = 0,1,...4)$ should give markedly different configurations for the various models. It is also desirable that as many of these configurations as possible are straight line configurations since, as Tukey has remarked in {33}, a straight line is most easily discernible by the eye.

A plot that satisfies these requirements is the plot of $a_1^{(k)}$ against $a_2^{(k)}$. Determination of the p terms (see Chapter 10) and subsequent application of the "sliding block" technique (see Chapter 11) showed that coefficients $a_1^{(k)}$ and $a_2^{(k)}$ are positive for perfect exponential data whilst $a_2^{(k)}$ is negative for perfect simple modified exponential data. The centre column of Figure 14 illustrates the configurations that a plot of $a_1^{(k)}$ against $a_2^{(k)}$ would take for the various growth curve models. We can clearly distinguish between the models and therefore surmount the principle deficiency of the slope characteristics method advocated by Gregg, Hossell and Richardson{19} since we do not have to make an eye comparison of different plots each possessing a different scale.

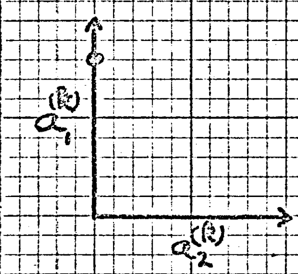
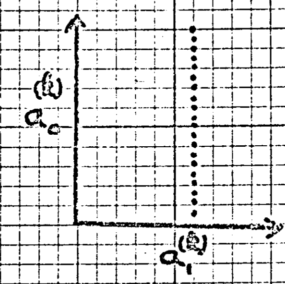
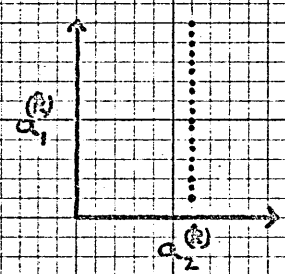
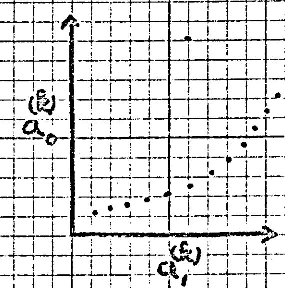
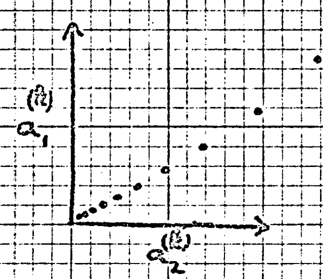
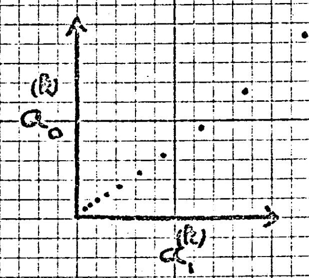
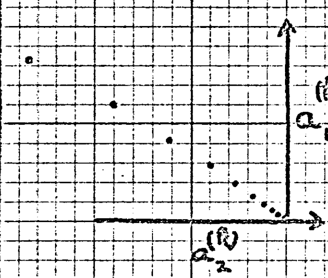
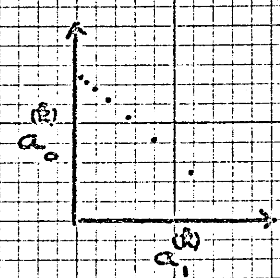
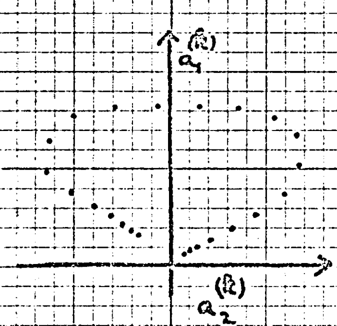
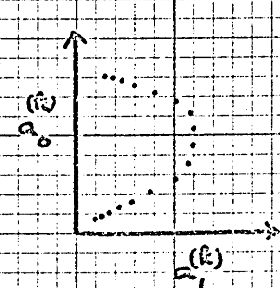
MODEL	CONFIGURATION OF $a_1^{(k)}$ AGAINST $a_2^{(k)}$ PLOT	CONFIGURATION OF $a_0^{(k)}$ AGAINST $a_1^{(k)}$ PLOT
LINEAR		
QUADRATIC		
EXPONENTIAL		
SIMPLE MODIFIED EXPONENTIAL		
SIGMOID [GOMPERTZ OR LOGISTIC]		

FIGURE 14

Another plot which would distinguish between the growth curve models is the plot of $a_0^{(k)}$ against $a_1^{(k)}$, although this is not quite as efficient as the previous plot since all the configurations are in the same quadrant and one configuration is a quadratic curve. It nevertheless has the advantage of greater accuracy in one of the coefficients (see Chapter 11). Appendix 3 shows that the coefficient of K in (9.2) is positive and since parameter K is positive for simple modified exponential data it is easily shown that the configuration for this model is a straight line cutting the positive $a_0^{(k)}$ axis. The right - hand column of Figure 14 illustrates the configurations for this plot.

CHAPTER 10

CHOOSING THE "p" TERMS

Since some (or all) of the coefficients $a_j^{(k)}$ $(j = 0,\dots 4)$ will be used in plotting procedures, it is desirable that the variances of these coefficients be small. Consider, for example, coefficient $a_1^{(k)}$. From (8.2) and Appendix 2 the standard deviation of $a_1^{(k)}$ is

$$\left[p_0^{(1)}p_0^{(3)}\right]^{-1}.B^{-\frac{1}{2}}.\left[p_0^{(3)2}J+2p_0^{(3)}p_2^{(3)}D+p_2^{(3)2}E\right]^{\frac{1}{2}}\sigma. \quad \dots\dots(10.1)$$

We could reduce this standard deviation by increasing $p_0^{(1)}$, but since, from (8.1),

$$\begin{aligned}a_1^{(k)} &= G(1,1)p_0^{(1)}\sum_i Y_i x_i + G(1,3)p_0^{(3)}\sum_i Y_i x_i^3 + G(1,3)p_2^{(3)}\sum_i Y_i x_i \\ &= \left[p_0^{(1)}p_0^{(3)2}B\right]^{-1}\Big[(p_0^{(3)2}J+2p_0^{(3)}p_2^{(3)}D+p_2^{(3)2}E)\sum_i Y_i x_i \\ &\quad + (-p_0^{(3)2}D-p_0^{(3)}p_2^{(3)}E)\sum_i Y_i x_i^3 + (-p_0^{(3)}p_2^{(3)}D-p_2^{(3)2}E)\sum_i Y_i x_i\Big] \\ &= \left[p_0^{(1)}p_0^{(3)}B\right]^{-1}\Big[p_0^{(3)}(-D\sum_i Y_i x_i^3 + J\sum_i Y_i x_i) + p_2^{(3)}(-E\sum_i Y_i x_i^3 + \\ &\quad D\sum_i Y_i x_i)\Big], \quad \dots\dots\dots\dots\dots\dots\dots\dots(10.2)\end{aligned}$$

this action would also reduce $a_1^{(k)}$ in the same proportion. Hence lowering the standard deviation by increasing $p_0^{(1)}$ would only result, in effect, in a different scale on the $a_1^{(k)}$ axis of a plot and would not make the calculated coefficient more reliable for any given block of data points. It would be rather like a confidence interval for a parameter being altered from 10 ± 1 to $5 \pm \frac{1}{2}$.

We could, however, manipulate the terms $p_0^{(1)}$ $p_0^{(3)}$ and $p_2^{(3)}$ in order to minimise the ratio of the standard deviation to the absolute value of the calculated value of the coefficient. From (10.1) and and (10.2) this ratio is given by

$$\frac{\text{S.Dev.}(a_1^{(k)})}{|a_1^{(k)}|} = \frac{\left[p_0^{(3)^2}J+2p_0^{(3)}p_2^{(3)}D+p_2^{(3)^2}E\right]^{\frac{1}{2}} . B^{\frac{1}{2}} . \sigma}{\left|p_0^{(3)}(-D\sum_i Y_i x_i^3+J\sum_i Y_i x_i)+p_2^{(3)}(-E\sum_i Y_i x_i^3+D\sum_i Y_i x_i)\right|} .$$

The quantity B depends only on the block size and is therefore constant for a fixed value of m. The quantity σ is a constant and we might note that even the estimate of σ, obtained from the squared residuals of the polynomial fit to the data, is unaffected by choice of individual p terms, provided we always use a fixed order polynomial.

We attempt, therefore, to fix the terms $p_0^{(3)}$ and $p_2^{(3)}$ at those values which minimise the expression

$$\frac{\left[p_0^{(3)^2}J+2p_0^{(3)}p_2^{(3)}D+p_2^{(3)^2}E\right]^{\frac{1}{2}}}{\left|p_0^{(3)}(-D\sum_i Y_i x_i^3+J\sum_i Y_i x_i)+p_2^{(3)}(-E\sum_i Y_i x_i^3+D\sum_i Y_i x_i)\right|} \quad .....(10.3)$$

In general, we aim to fix all the p terms of the polynomials to be those values which minimise the ratios

$$\frac{\text{S.Dev. } (a_j^{(k)})}{|a_j^{(k)}|} \quad , \quad (j = 0,1,\ldots 4).$$

In reality, we shall find that this is impossible without choosing different values of the p terms for each block. The plotting procedures described in Chapter 9 however, hold only if the p terms are constant for each block of the data under investigation. We show however, that using constant p terms, we still obtain a close approximation to the true minimum for each block.

(a) <u>Minimisation for Coefficient $a_4^{(k)}$</u>

From (8.2) and Appendix 2,

$$\text{S.Dev. } (a_4^{(k)}) = \left[p_0^{(4)}\right]^{-1} . \; Z^{-\frac{1}{2}} . \; A^{\frac{1}{2}} . \; \sigma.$$

From (8.1), manipulating as in (10.2), we obtain

$$a_4^{(k)} = \left[p_0^{(4)} Z\right]^{-1} \left[B\sum_i Y_i - C\sum_i Y_i x_i^2 + A\sum_i Y_i x_i^4\right].$$

There are, therefore, no p terms we can adjust to minimise the ratio of S.Dev.$(a_4^{(k)})$ to $|a_4^{(k)}|$, i.e. the ratio is independent of the p terms.

(b) <u>Minimisation for Coefficient $a_3^{(k)}$</u>

From (8.2) and Appendix 2,

$$\text{S.Dev. } (a_3^{(k)}) = \left[p_0^{(3)}\right]^{-1} . \; B^{-\frac{1}{2}} . \; E^{\frac{1}{2}} . \; \sigma .$$

From (8.1), manipulating as in (10.2), we obtain

$$a_3^{(k)} = \left[p_0^{(3)} B\right]^{-1} \left[E \sum_i Y_i x_i^3 - D \sum_i Y_i x_i\right].$$

The ratio of S.Dev.$(a_3^{(k)})$ to $|a_3^{(k)}|$ is, therefore, also independent of the p terms.

(c) Minimisation for Coefficient $a_2^{(k)}$

From (8.2) and Appendix 2,

$$\text{S.Dev.}\ (a_2^{(k)}) = \left[p_0^{(2)} p_0^{(4)}\right]^{-1} . Z^{-\frac{1}{2}} . \left[-p_0^{(4)2} H + p_2^{(4)2} A + 2 p_2^{(4)} p_0^{(4)} C\right]^{\frac{1}{2}} . \sigma .$$

From (8.1), manipulating as in (10.2), we obtain

$$a_2^{(k)} = \left[p_0^{(2)} p_0^{(4)}\right]^{-1} . Z^{-1} . \left[p_0^{(4)} (-C \sum_i Y_i x_i^4 - H \sum_i Y_i x_i^2 + F \sum_i Y_i)\right.$$

$$\left. + p_2^{(4)} (-A \sum_i Y_i x_i^4 + C \sum_i Y_i x_i^2 - B \sum_i Y_i)\right] .$$

If

$$r = -C \sum_i Y_i x_i^4 - H \sum_i Y_i x_i^2 + F \sum_i Y_i ,$$

and

$$s = -A \sum_i Y_i x_i^4 + C \sum_i Y_i x_i^2 - B \sum_i Y_i$$

then

$$\frac{\text{S.Dev.}(a_2^{(k)})}{|a_2^{(k)}|} = \frac{\left[-p_0^{(4)2} H + p_2^{(4)2} A + 2 p_2^{(4)} p_0^{(4)} C\right]^{\frac{1}{2}} . Z^{\frac{1}{2}} . \sigma}{|p_0^{(4)} r + p_2^{(4)} s|}$$

We require, therefore, the values of $p_0^{(4)}, p_2^{(4)}$ which minimise

$$Q = \frac{\left[-p_0^{(4)^2}H + p_2^{(4)^2}A + 2p_2^{(4)}p_0^{(4)}C\right]^{\frac{1}{2}}}{|p_0^{(4)}r + p_2^{(4)}s|} ,$$

where H, A and C depend solely on the block size, which is fixed, and r and s depend on the data values for the particular block and the block size.

If $\theta = \frac{p_0^{(4)}}{p_2^{(4)}}$, then

$$Q = \frac{\left[-H\theta^2 + 2C\theta + A\right]^{\frac{1}{2}}}{|r\theta + s|} . \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (10.4)$$

In practice both Q and θ are real, hence the equation $Q^2(r\theta+s)^2 = -H\theta^2+2C\theta+A$ or

$$\theta^2(r^2Q^2+H)+\theta(2rsQ^2-2C)+(s^2Q^2-A) = 0 \quad \ldots\ldots\ldots\ldots (10.5)$$

has real roots in θ; consequently

$$(2rsQ^2-2C)^2 \geq 4(r^2Q^2+H)\ (s^2Q^2-A), \quad \ldots\ldots\ldots\ldots\ldots (10.6)$$

i.e.

$$4Q^2(r^2A-s^2H-2rsC) \geq -4C^2-4HA,$$

i.e.

$$Q^2 \geq \frac{-HA-C^2}{r^2A-s^2H-2rsC} . \qquad \ldots\ldots\ldots\ldots\ldots\ldots (10.7)$$

The minimum value of Q^2 occurs at equality in (10.7), i.e. when inequality (10.6) becomes an equality. Solving equation (10.5) for θ we obtain

$$\theta = \frac{-(2rsQ^2-2C)\pm\left[(2rsQ^2-2C)^2-4(r^2Q^2+H)(s^2Q^2-A)\right]}{2(r^2Q^2+H)} .$$

With (10.6) as an equality, the value of θ which minimises Q^2, say θ_{min}, is given by

$$\theta_{min} = \frac{C - rsQ^2}{r^2Q^2+H} \quad .$$

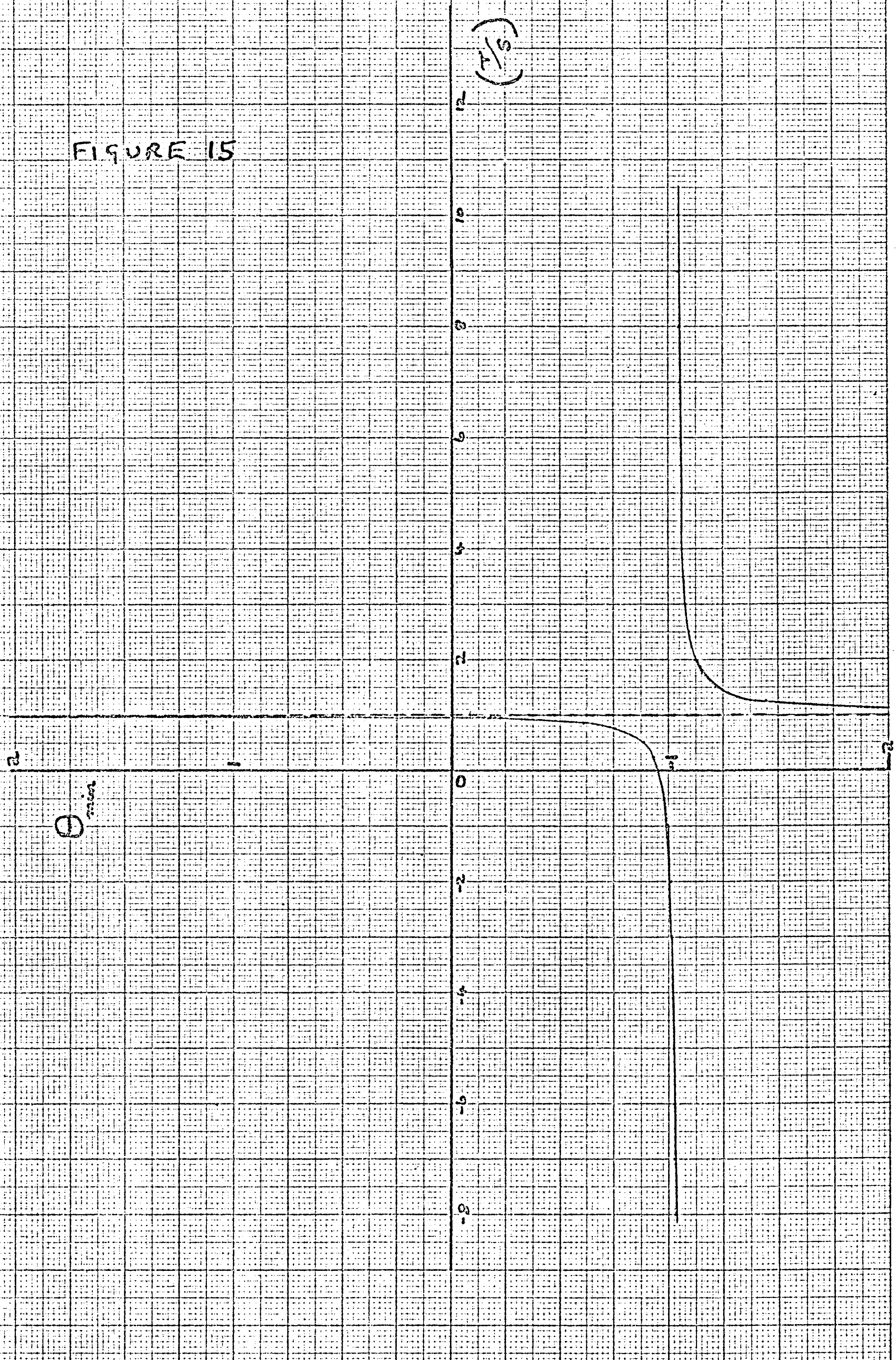
Substituting for the minimum value of Q^2 obtained from (10.7) we obtain

$$\theta_{min} = \frac{C - (r/s)A}{H+(r/s)C} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(10.8)$$

The value of $\dfrac{p_0^{(4)}}{p_2^{(4)}}$ which minimises $\dfrac{S.Dev.(a_2^{(k)})}{|a_2^{(k)}|}$

is thus a function of the quantity (r/s) and therefore varies from block to block. We need a fixed value of $\dfrac{p_0^{(4)}}{p_2^{(4)}}$ in order to apply the plotting procedures described in Chapter 9. Study of diagrams like Figure 15, in which θ_{min} is plotted against (r/s) for the case m = 7, indicates that a suitable fixed value to take would be the asymptotic value of θ_{min}, $-\frac{A}{C}$. A programme was written to calculate (r/s) for blocks of all types of data and it was found that, in practice, (r/s) took values anywhere between $\pm\infty$, so endorsing the view that θ_{min} should take this value.

FIGURE 15



Using $-\frac{A}{C}$ instead of the true θ_{min} to determine the ratio $\frac{p_0^{(4)}}{p_2^{(4)}}$, we must check that the value of Q obtained, denoted by Q_{asy} say, is reasonably close to the true minimum of Q denoted by Q_{min}. From (10.7)

$$Q_{min} = \frac{\left[-HA-C^2\right]^{\frac{1}{2}}}{|s|\left[(r/s)^2A-H-2(r/s)C\right]^{\frac{1}{2}}},$$

whence on substituting $-\frac{A}{C}$ for θ in (10.4), we obtain

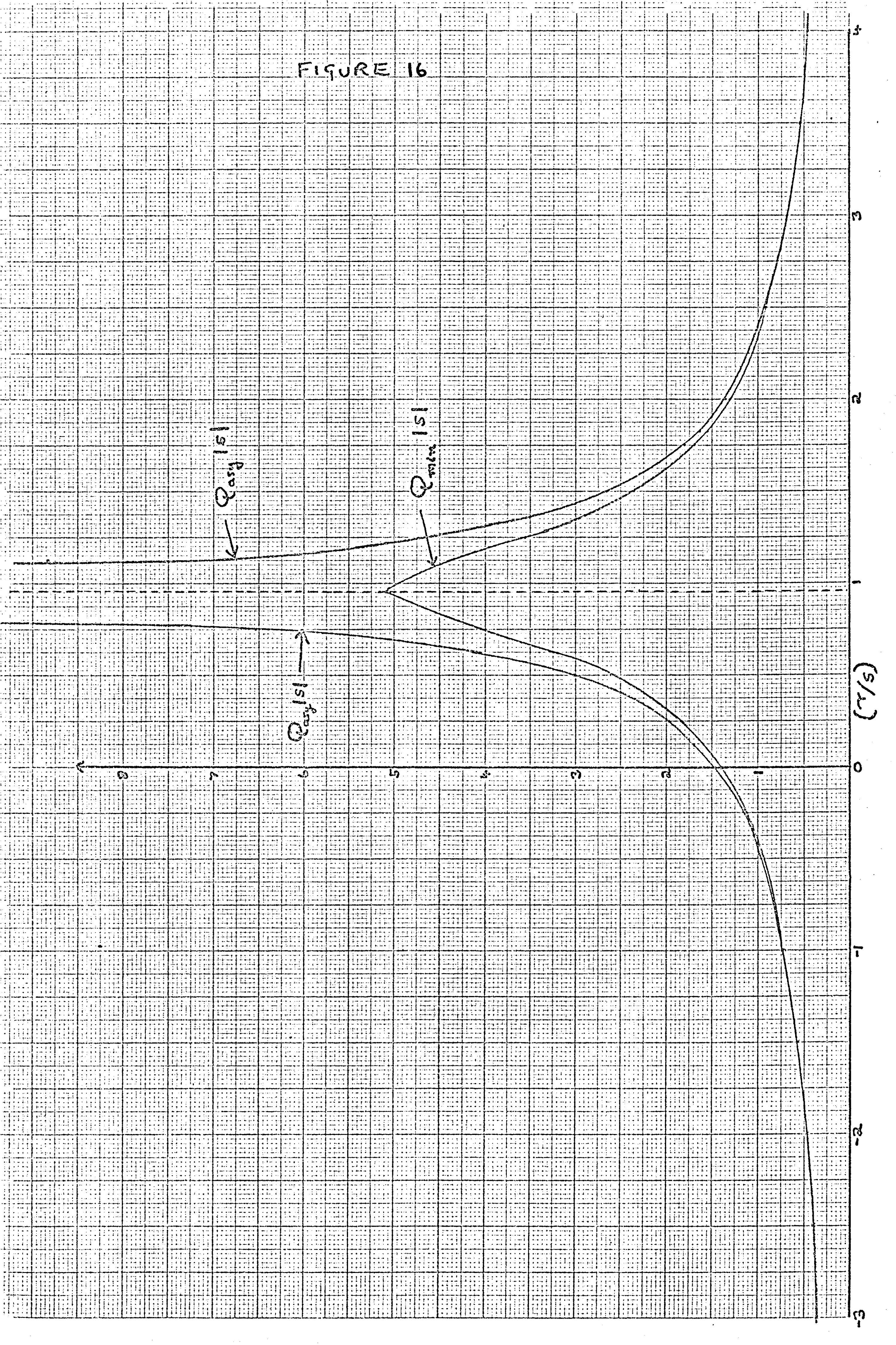
$$Q_{asy} = \frac{[A]^{\frac{1}{2}}\left[-HA-C^2\right]^{\frac{1}{2}}}{|s|\ |C-A(r/s)|}.$$

Figure 16 shows plots of $Q_{min}|s|$ and $Q_{asy}|s|$ against (r/s). The two Q's are close except for the range of (r/s) values where $Q_{asy}|s| \to \infty$ and $Q_{min}|s|$ remains finite. Since $p_0^{(2)}$ is constant in this analysis,

$$a_2^{(k)} \propto r + s\left(\frac{p_2^{(4)}}{p_0^{(4)}}\right) = s(r/s + 1/\theta)$$

whence $a_2^{(k)} = 0$ if $\frac{r}{s} = -\frac{1}{\theta}$. Since we are taking the value $-\frac{A}{C}$ for θ, $a_2^{(k)} = 0$ if $\frac{r}{s} = \frac{C}{A}$, which is the value (r/s) takes at the discontinuity

FIGURE 16



shown in Figure 16. Hence the range of (r/s) values for which $Q_{asy}|s| \to \infty$ corresponds to blocks for which $a_2^{(k)}$ is approximately zero. These blocks will still be reliable for plotting purposes since, with the p terms fixed, the standard deviation of $a_2^{(k)}$ is invariant from block to block.

The ratio $\dfrac{p_0^{(4)}}{p_2^{(4)}}$, now being fixed at the value $-\dfrac{A}{C}$, is m dependent. The table below gives values of $\dfrac{p_0^{(4)}}{p_2^{(4)}}$ for values of m from 5 to 12.

m	$\dfrac{p_0^{(4)}}{p_2^{(4)}}$	m	$\dfrac{p_0^{(4)}}{p_2^{(4)}}$
5	-0.9986	9	-1.0597
6	-1.0195	10	-1.0686
7	-1.0358	11	-1.0762
8	-1.0489	12	-1.0827

The error in the calculated values of $\dfrac{p_0^{(4)}}{p_2^{(4)}}$ is derived in Appendix 4. This error is of the order $\pm$ 0.0002.

An interesting point emerges from the above analysis. For Tchebychef polynomials, $\dfrac{p_0^{(4)}}{p_2^{(4)}} = -1$, and substitution of -1 for θ in (10.4) would give a quantity we may label Q_{Tcheb} in accordance with our previous notation. It was found that Q_{Tcheb} was marginally closer to Q_{min} than Q_{asy} only for $0 < (r/s) < 1$. In using $-\frac{A}{C}$ for $\frac{p_0^{(4)}}{p_2^{(4)}}$ our polynomials are therefore generally better than Tchebychef polynomials in the sense of minimising $\frac{S.Dev.(a_2^{(k)})}{|a_2^{(k)}|}$.

(d) Minimisation for Coefficient $a_1^{(k)}$

If

$$u = -D\Sigma_i Y_i x_i^3 + J\Sigma_i Y_i x_i$$

and

$$v = -E\Sigma_i Y_i x_i^3 + D\Sigma_i Y_i x_i$$

then, from (10.3), we require the values of $p_0^{(3)}$, and $p_2^{(3)}$ which minimize

$$Q' = \frac{\left[p_0^{(3)2}J+2p_0^{(3)}p_2^{(3)}D+p_2^{(3)2}E\right]^{\frac{1}{2}}}{|p_0^{(3)}u + p_2^{(3)}v|}$$

where J, D and E depend on the block size only, and u and v depend on the data values for the particular block and the block size.

If $\lambda = \frac{p_0^{(3)}}{p_2^{(3)}}$, then proceeding as in the previous section, the value of λ which minimises Q'^2, i.e. λ_{min}, is given by

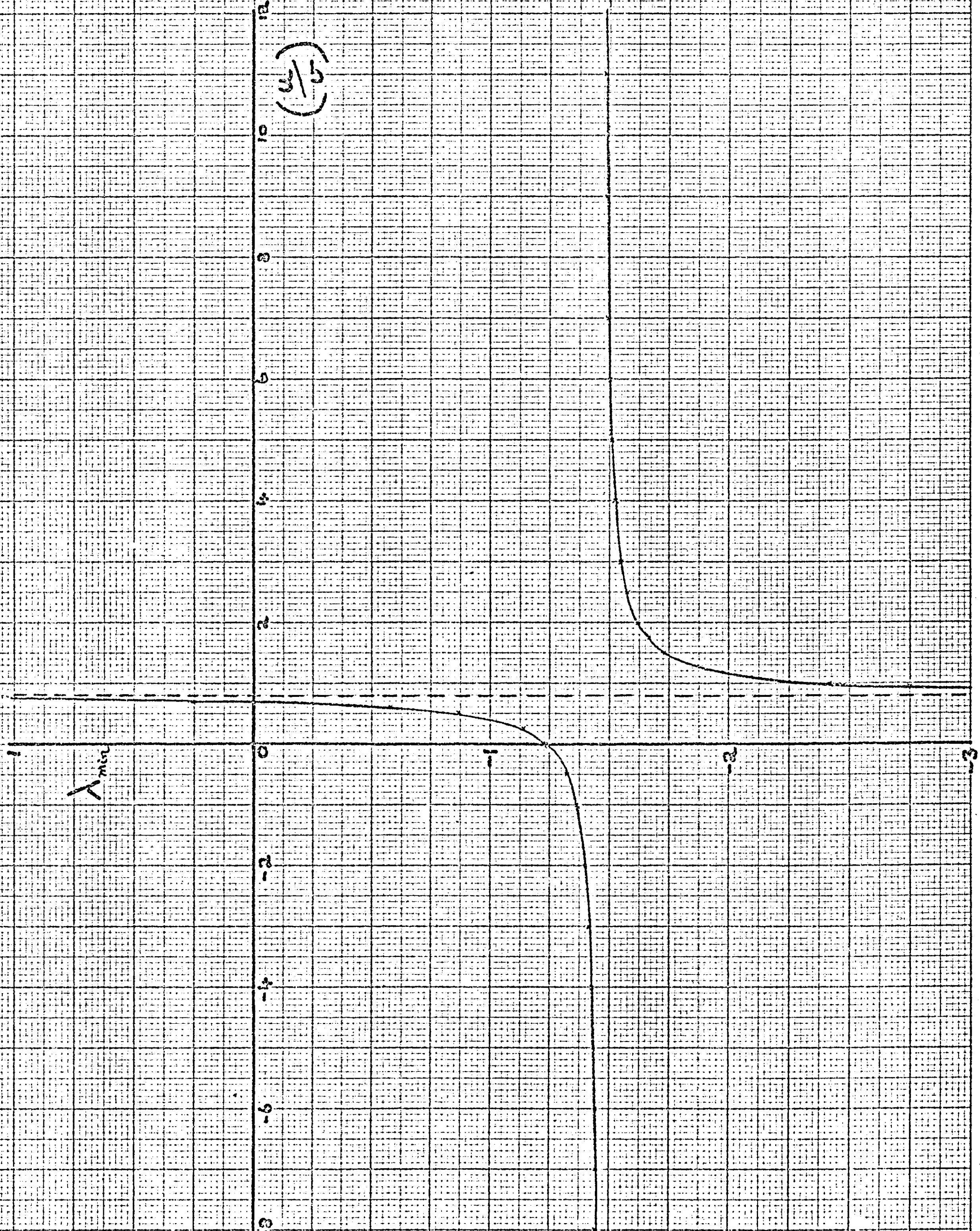
$$\lambda_{min} = \frac{D - (u/v)E}{-J+(u/v)D} \quad \ldots\ldots\ldots\ldots\ldots (10.10)$$

Figure 17 shows a plot of λ_{min} against (u/v) for the case $m = 7$. With reasoning similar to the previous section, the value of λ_{min} was fixed at its asymptotic value, $-\frac{E}{D}$, this decision being endorsed by the results of a programme which showed that, in practice, (u/v) took values anywhere between $\pm\infty$ for data blocks.

We may similarly compare the true minimum of Q', denoted by Q'_{min}, with the value of Q' obtained by using $-\frac{E}{D}$ instead of λ_{min}, Q'_{asy} say. Figure 18 shows plots of $Q'_{min}|v|$ and $Q'_{asy}|v|$ against (u/v). The two Q's are again close except for the range of (u/v) values where $Q'_{asy}|v| \to \infty$ whilst $Q'_{min}|v|$ remains finite. This range corresponds to blocks for which $a_1^{(k)}$ is approximately zero, as was the case with $a_2^{(k)}$ in the previous section, these blocks still being reliable for plotting purposes because of the invariance of S.Dev. $(a_1^{(k)})$.

The ratio $\frac{p_0^{(3)}}{p_2^{(3)}}$, if fixed at the value $-\frac{E}{D}$, is m dependent. The table overleaf gives values of $\frac{p_0^{(3)}}{p_2^{(3)}}$ for values of m from 5 to 12.

FIGURE 17



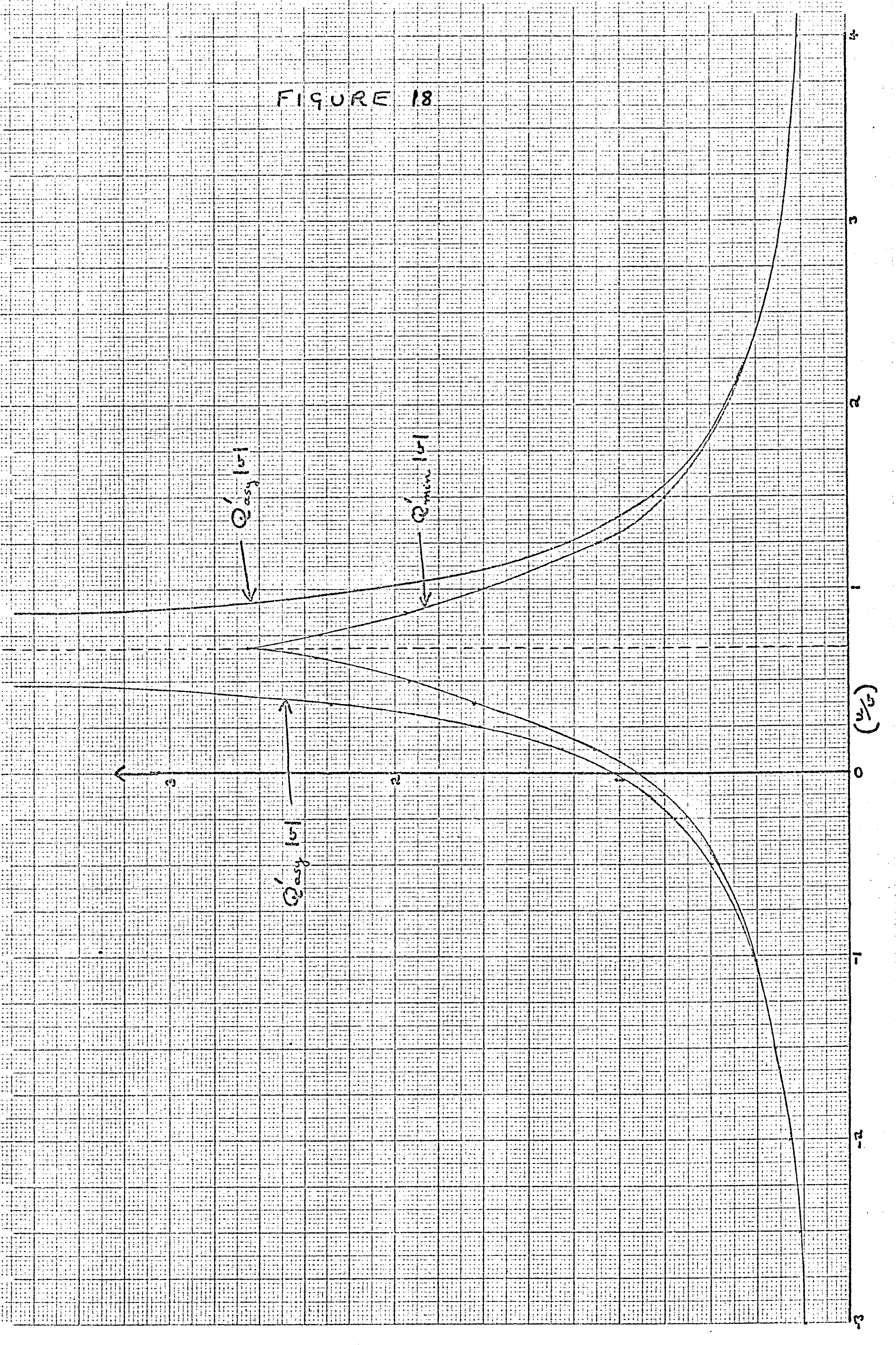


FIGURE 18

m	$\dfrac{p_0^{(3)}}{p_2^{(3)}}$	m	$\dfrac{p_0^{(3)}}{p_2^{(3)}}$
5	-1.4043	9	-1.5056
6	-1.4399	10	-1.5198
7	-1.4670	11	-1.5317
8	-1.4884	12	-1.5418

Appendix 4 shows the error in the calculated values of $\dfrac{p_0^{(3)}}{p_2^{(3)}}$ to be of the order $\pm$ 0.0001.

It is interesting to note that, for Tchebychef polynomials, $\dfrac{p_0^{(3)}}{p_2^{(3)}} = -1.3333$ and substitution of this value in (10.9) gives Q'_{Tcheb} which is marginally closer to Q'_{min} than Q'_{asy} only for $-\frac{1}{4} < (u/v) < \frac{3}{4}$ In using $-\frac{E}{D}$ for $\dfrac{p_0^{(3)}}{p_2^{(3)}}$ our polynomials are therefore generally better than Tchebychef polynomials in the sense of minimising $\dfrac{\text{S.Dev.}(a_1^{(k)})}{|a_1^{(k)}|}$.

(e) Minimisation for Coefficient $a_0^{(k)}$

If $w = B\sum_i Y_i x_i^4 + F\sum_i Y_i x_i^2 + L\sum_i Y_i$,

$$\rho = \frac{p_2^{(2)}}{p_0^{(2)}}, \quad \nu = \frac{p_2^{(2)}p_2^{(4)} - p_4^{(4)}p_0^{(2)}}{p_0^{(2)}p_0^{(4)}},$$

then from (8.1), (8.2) and Appendix 2 it can be shown that

$$\frac{\text{S.Dev.}(a_0^{(k)})}{|a_0^{(k)}|} = \frac{\left[-H\rho^2+A\nu^2-2F\rho+2B\nu+2C\rho\nu+L\right]^{\frac{1}{2}} \cdot Z^{\frac{1}{2}}.\sigma}{|-r\rho - s\nu + w|}$$

where r and s are the quantities given in section (c). We require, therefore, the values of ρ and ν which minimise

$$Q'' = \frac{\left[-H\rho^2+A\nu^2-2F\rho+2B\nu+2C\rho\nu+L\right]^{\frac{1}{2}}}{|-r\rho - s\nu + w|}$$

where
$$Q'' = \frac{\text{S.Dev.}(a_0^{(k)})}{Z^{\frac{1}{2}}\sigma\ |a_0^{(k)}|} .$$

Section (i) of Appendix 5 shows that this equation may be written in the form

$$Q''(\eta,T) = \frac{\left[c_1\eta^2 + c_2T^2 + c_3\right]^{\frac{1}{2}}}{|c_4\eta + c_5T + c_6|} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (10.11)$$

where

$Q''(\eta,T) = Q''$,

$c_1 = -H$,

$c_2 = A + C^2/H$,

$$c_3 = \frac{HAL+2BCF+F^2A-HB^2+LC^2}{AH + C^2},$$

$c_4 = -r$,

$$c_5 = -s - \frac{C}{H}.r ,$$

$$c_6 = \frac{r(BC+FA)+s(BH-FC)+w(AH+C^2)}{AH + C^2},$$

$$\eta = \rho - \frac{C\nu}{H} + \left(\frac{BC+FA}{AH+C^2}\right) - \left(\frac{C}{H}\right)\left(\frac{BH-FC}{AH+C^2}\right)$$

and

$$T = \nu + \left(\frac{BH-FC}{AH+C^2}\right)$$

We require the values of η and T which minimise (10.11). Keeping T fixed and letting η vary we obtain, in a similar manner to (10.7),

$$Q''^2(\eta,T) \geqslant \frac{c_1(c_2T^2 + c_3)}{\left[c_4^2(c_2T^2+c_3)+c_1(c_5T+c_6)^2\right]} \quad \ldots\ldots\ldots\ldots(10.12)$$

The minimum value of $Q''^2(\eta,T)$ for a particular T and variable η occurs when (10.12) is an equality. Hence if $Q''^2_{min}(T)$ denotes this minimum,

$$T^2\left[(c_4^2c_2+c_1c_5^2).Q''^2_{min}(T)-c_1c_2\right] + T\left[2c_1c_5c_6Q''^2_{min}(T)\right]$$

$$+\left[(c_4^2c_3+c_1c_6^2)Q''^2_{min}(T)-c_1c_3\right] = 0 \quad \ldots\ldots\ldots\ldots(10.13)$$

This must have real roots in T for a particular minimum $Q''_{min}(T)$, whence

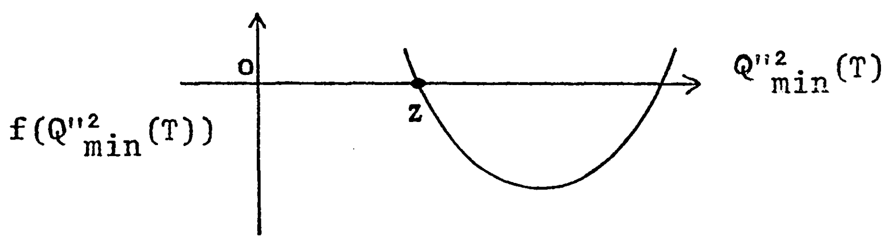
$$(2c_1c_5c_6Q''^2_{min}(T))^2 \geqslant 4\left[(c_4^2c_2+c_1c_5^2)Q''^2_{min}(T)-c_1c_2\right].$$

$$\left[(c_4^2c_3+c_1c_6^2)Q''^2_{min}(T)-c_1c_3\right]$$

i.e. $\left[(c_4^2c_2+c_1c_5^2)(c_4^2c_3+c_1c_6^2)-c_1^2c_5^2c_6^2\right]Q''^4_{min}(T)$

$$-\left[c_1c_2(c_4^2c_3+c_1c_6^2)+c_1c_3(c_4^2c_2+c_1c_5^2)\right]Q''^2_{min}(T)+c_1^2c_2c_3 \leqslant 0 \quad ..(10.14)$$

We shall denote the L.H.S. of (10.14) by $f(Q''^2_{min}(T))$. Equation (10.14) gives the full range of possible values of $Q''^2_{min}(T)$ for $-\infty \leqslant T \leqslant \infty$. It follows that the minimum value of $Q''(\eta,T)$, being the minimum value of $Q''_{min}(T)$, is given by the smallest real value of $Q''^2_{min}(T)$ to satisfy $f(Q''^2_{min}(T)) \leqslant 0$. Section (ii) of Appendix 5 shows that both the coefficient of $Q''^4_{min}(T)$ and the last term in $f(Q''^2_{min}(T))$ are positive. The quadratic $f(Q''^2_{min}(T))$ must therefore have the shape indicated in the diagram below:



The minimum value Q''^2_{min} of Q''^2 is given by $Q''_{min} = \sqrt{Z}$.

If we now keep η fixed and let T vary, then by an exactly similar procedure we may derive the inequality:

$$\left[(c_5^2c_1+c_2c_4^2)(c_5^2c_3+c_2c_6^2) - c_2^2c_4^2c_6^2\right] Q''^4_{min}(\eta)$$

$$-\left[c_2c_1(c_5^2c_3+c_2c_6^2)+c_2c_3(c_5^2c_1+c_2c_4^2)\right] Q''^2_{min}(\eta)+c_2^2c_1c_3 \leqslant 0 \quad ..(10.15)$$

where $Q''^2_{min}(\eta)$ is the minimum value of Q''^2 for a particular η and variable T. Applying a similar argument to $Q''_{min}(\eta)$ as for $Q''_{min}(T)$ we see that Q''^2_{min} is the smallest value of $Q''^2_{min}(\eta)$ to satisfy (10.15) and is thus the smallest root of (10.15) considered as an equality. It is therefore evident that (10.14) and (10.15), when considered as equalities, have a common root which may be found by simple algebra and in fact is given by

$$Q''^2_{min} = \frac{c_1 c_2 c_3}{c_1 c_2 c_6^2 + c_1 c_3 c_5^2 + c_2 c_3 c_4^2} \quad \ldots\ldots\ldots\ldots(10.16)$$

Substituting this value in (10.13) and recalling that $Q''^2_{min}(T) = Q''^2_{min}$ satisfies the equality (10.14) we obtain

$$T_{min} = \frac{c_3 c_5}{c_2 c_6} \quad \ldots\ldots\ldots\ldots(10.17)$$

Substituting (10.16) into the corresponding equation to (10.13) for $Q''^2_{min}(\eta)$, and remembering that (10.15) is an equality, we obtain

$$\eta_{min} = \frac{c_3 c_4}{c_1 c_6} \quad \ldots\ldots\ldots\ldots(10.18)$$

T_{min} and η_{min} are those values of T and η which minimise (10.11). Since

$$\nu = T - \frac{BH - FC}{AH + C^2} \quad ,$$

from equation (10.17) and the transformation equations for the "c" terms, it follows that the value of ν which minimises Q'' is given by:

$$\overset{\vee}{\nu}_{min} = \frac{-r\left[(BH-FC)(BC+AF)-C\Delta\right] - s\left[(BH-FC)^2 - H\Delta\right] + w\left[(BH-FC)(-AH-C^2)\right]}{-r\left[(-AH-C^2)(BC+AF)\right] - s\left[(-AH-C^2)(BH-FC)\right] + w\left[(-AH-C^2)^2\right]}$$

$$\ldots\ldots\ldots(10.19)$$

where $\Delta = HB^2 - HAL - 2BCF - F^2A - LC^2$.

Similarly,

$$\rho = \eta + \frac{C}{H}\nu - \left(\frac{BC+FA}{AH+C^2}\right) + \left(\frac{C}{H}\right)\left(\frac{BH-FC}{AH+C^2}\right),$$

so that from (10.18),(10.19) and the transformation equations for the "c" terms, it can be shown that the value of ρ which minimises Q'' is given by

$$\rho_{min} = \frac{-r\left[(BC+AF)^2+\Delta A\right] - s\left[(BC+AF)(HB-FC)-\Delta C\right] + w\left[(BC+AF)(-AH-C^2)\right]}{-r\left[(-AH-C^2)(BC+AF)\right] - s\left[(-AH-C^2)(HB-FC)\right] + w\left[(-AH-C^2)^2\right]}$$

..........(10.20)

Both these equations are of the form

$$\frac{z_1 + (s/r)\, z_2 + (w/-r)\, z_3}{z_4 + (s/r)\, z_5 + (w/-r)\, z_6}$$

where the "z" terms can be obtained from (10.20) and depend solely on the block size.

By putting

$$\left(\frac{s}{r}\right)^* = \left(\frac{s}{r}\right) - \frac{z_4z_3 - z_1z_6}{z_2z_6 - z_5z_3}$$

and

$$\left(\frac{w}{-r}\right)^* = \left(\frac{w}{-r}\right) - \frac{z_4z_2 - z_1z_5}{z_3z_5 - z_6z_2}$$

both (10.19) and (10.20) may be reduced to the form

$$\frac{z_2 + z_3\ (w/-r)^*/(s/r)^*}{z_5 + z_6\ (w/-r)^*/(s/r)^*}$$

where w, r and s depend on the data values for the particular block and the block size.

Figures 19 and 20 show the plots of ν_{min} and ρ_{min} against $(w/-r)^*/(s/r)^*$ for $m = 7$. The values of ν_{min} and ρ_{min} must be constant for all blocks i.e. for all values of w, r and s, so they were fixed at their asymptotic values z_3/z_6, as was done with θ_{min} and λ_{min} in sections (c) and (d). The asymptotic values of ν_{min} and ρ_{min} are, from (10.19) and (10.20), $\frac{BH-FC}{-AH-C^2}$ and $\frac{BC+AF}{-AH-C^2}$ respectively. A programme written to calculate $(w/-r)^*/(s/r)^*$ for data blocks again endorsed the choice of these asymptotic values by showing that this quantity in practice took values anywhere between $\pm\infty$.

The true minimum of Q" i.e. Q''_{min}, may be compared with the value of Q" obtained by using these asymptotic values, Q''_{asy} say. Figure 21 shows plots of $Q''_{min}|r|$ and $Q''_{asy}|r|$ against values of (s/r) and (w/-r) for the case $m = 7$. The two Q's are close except for the range of (s/r) and (w/-r) values where $Q''_{asy}|r| \to \infty$. This range corresponds to blocks for which $a_0^{(k)}$ is approximately zero, as was the case with $a_2^{(k)}$ and $a_1^{(k)}$ in previous sections. These blocks will still be reliable for plotting purposes because of the invariance of S.Dev.$(a_0^{(k)})$.

The ratios $\frac{p_2^{(2)}p_2^{(4)} - p_4^{(4)}p_0^{(2)}}{p_0^{(2)}p_0^{(4)}}$ and $\frac{p_2^{(2)}}{p_0^{(2)}}$, if fixed respectively at the values $\frac{BH-FC}{-AH-C^2}$ and $\frac{BC+AF}{-AH-C^2}$, are m-dependent only and are shown for

FIGURE 19

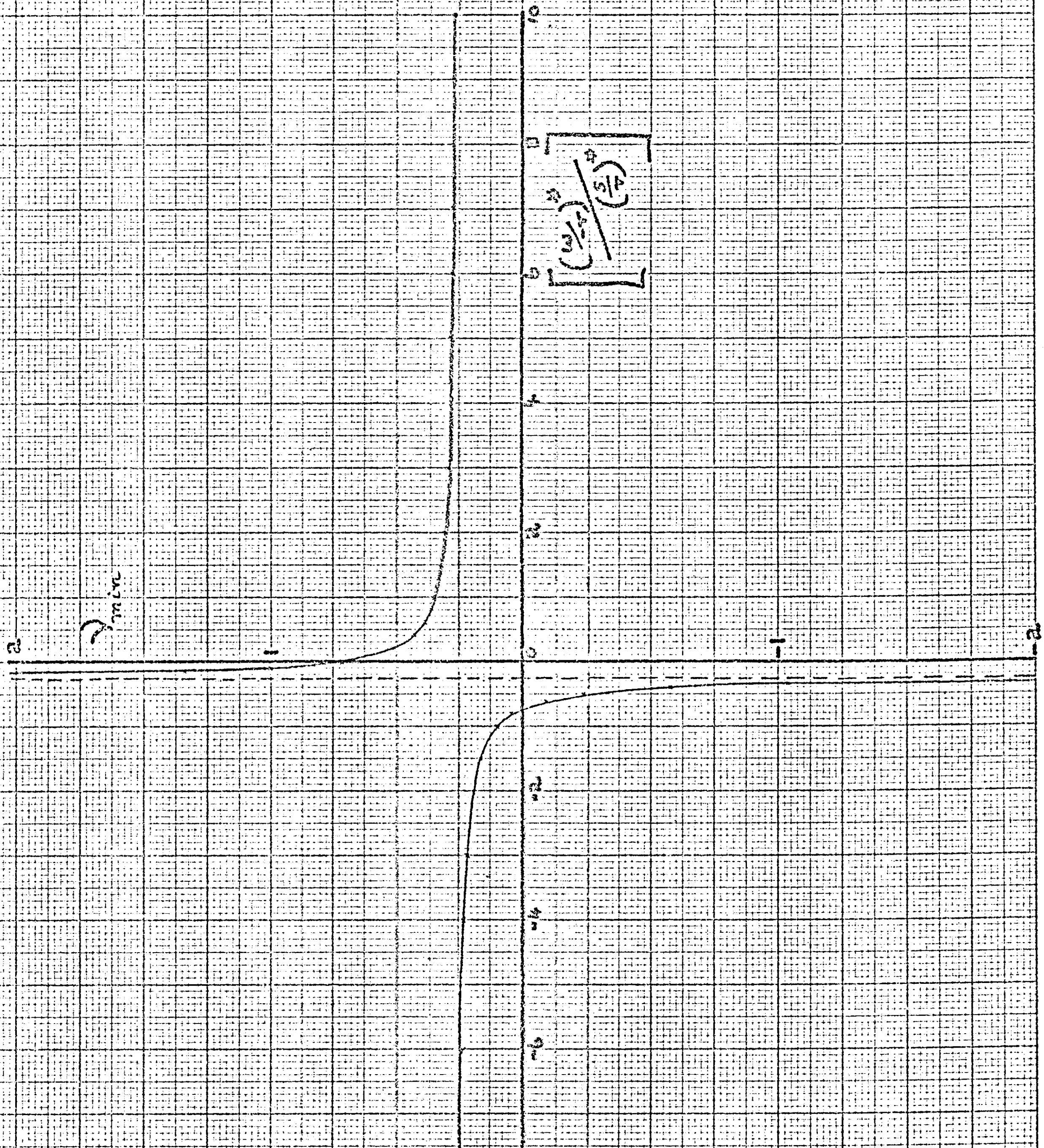


FIGURE 20

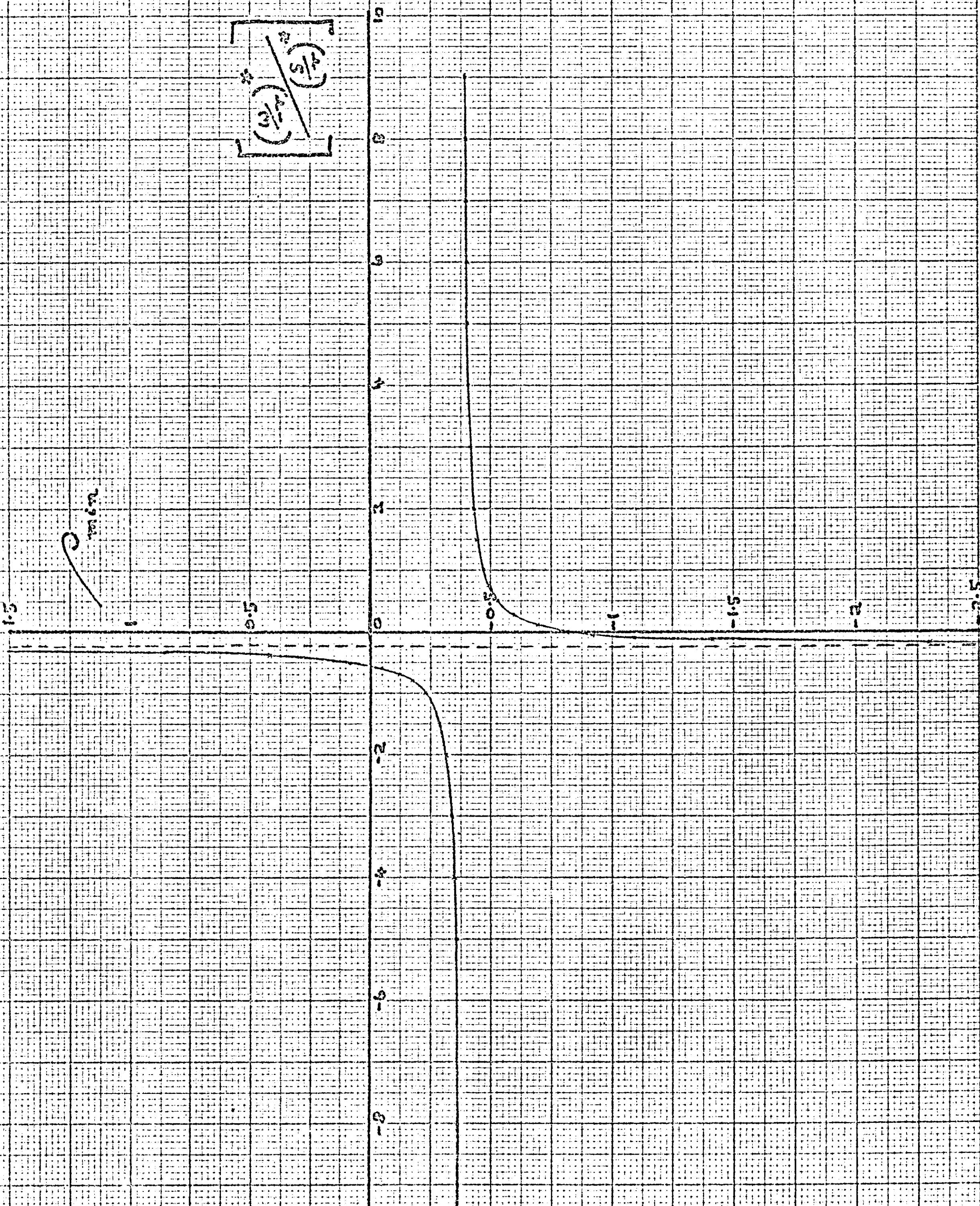
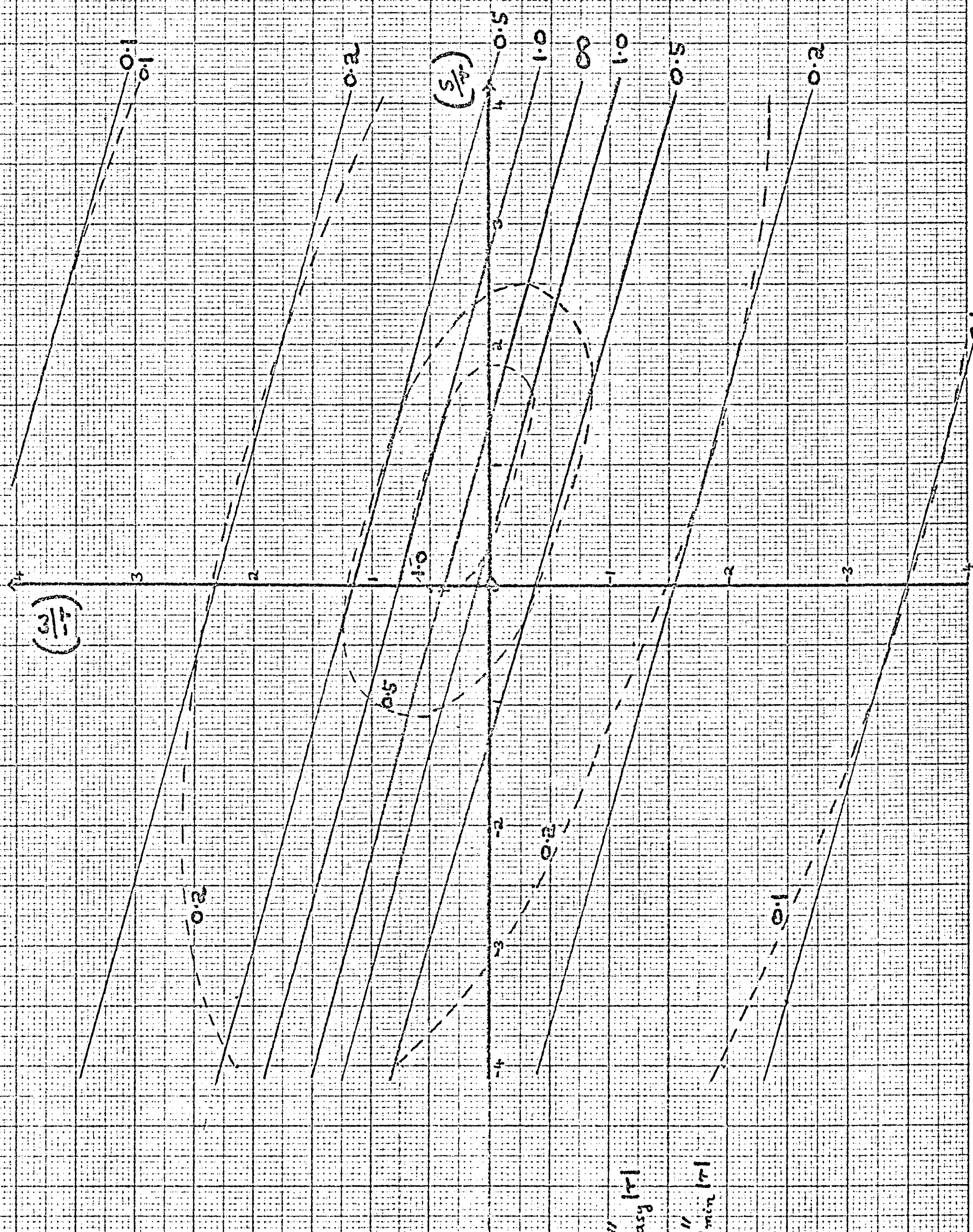


FIGURE 21



m = 5(1)12 in the table below:

m	$\dfrac{p_2^{(2)}p_2^{(4)}-p_4^{(4)}p_0^{(2)}}{p_0^{(2)}p_0^{(4)}}$	$p_2^{(2)}/p_0^{(2)}$
5	0.2843	-0.3995
6	0.2695	-0.3883
7	0.2590	-0.3804
8	0.2513	-0.3744
9	0.2453	-0.3697
10	0.2406	-0.3660
11	0.2367	-0.3629
12	0.2335	-0.3604

Appendix 4 shows the errors in the calculated values of the two ratios to be of the orders $\pm$ 0.0047 and $\pm$ 0.0054 respectively. We should, therefore, only work to 3 decimal places when using these quantities.

For Tchebychef polynomials $\dfrac{p_2^{(2)}p_2^{(4)}-p_4^{(4)}p_0^{(2)}}{p_0^{(2)}p_0^{(4)}} = 0.375$ and $p_2^{(2)}/p_0^{(2)} = -0.5$. Substitution of these values in (10.11) gives Q''_{Tcheb}, which is marginally closer to Q''_{min} than Q''_{asy} only for a small range of (s/r) and (w/-r) values. Our Polynomials are therefore generally better than Tchebychef polynomials in the sense of minimising

$$\frac{S.Dev.(a_0^{(k)})}{|a_0^{(k)}|}.$$

(f) The Form of the Polynomials $g_j(x)$ $(j=0,1,\ldots 4)$.

For a given value of m we now have values of

$$\frac{p_0^{(4)}}{p_2^{(4)}}, \quad \frac{p_0^{(3)}}{p_2^{(3)}}, \quad \frac{p_2^{(2)}p_2^{(4)}-p_4^{(4)}p_0^{(2)}}{p_0^{(2)}p_0^{(4)}} \quad \text{and} \quad \frac{p_2^{(2)}}{p_0^{(2)}}$$

which are approximately "best" in the sense of minimizing the ratios $\dfrac{\text{S.Dev.}(a_j^{(k)})}{|a_j^{(k)}|}$ $(j = 0,1,\ldots 4)$.

We have no information on $p_0^{(0)}$ and $p_0^{(1)}$; these two terms will, therefore, be fixed at unity as is the case with Legendre and Tchebychef polynomials. Consider the case for m = 5. We know that $\dfrac{p_0^{(4)}}{p_2^{(4)}} = -0.9986$,

$$\frac{p_0^{(3)}}{p_2^{(3)}} = -1.4043 \quad \text{and} \quad \frac{p_2^{(2)}}{p_0^{(2)}} = -0.400.$$

Now $$\frac{p_2^{(2)}p_2^{(4)}-p_4^{(4)}p_0^{(2)}}{p_0^{(2)}p_0^{(4)}} = \left(\frac{p_2^{(2)}}{p_0^{(2)}}\right)\left(\frac{p_2^{(4)}}{p_0^{(4)}}\right) - \frac{p_4^{(4)}}{p_0^{(4)}} = 0.284$$

Hence $$\frac{p_4^{(4)}}{p_0^{(4)}} = (-0.400)(-0.9986)^{-1}-0.284 = 0.116\pm 0.001$$

Hence the "best" polynomial to fit to the data blocks is $f(x) = \alpha_0+\alpha_1 x+\alpha_2(x^2-0.400)+\alpha_3(1.4043\ x^3-x)$

$$+\ \alpha_4(0.9986x^4-x^2+0.116)$$

Similar calculations lead to the following "best" polynomials for the cases m = 6 to m = 12:

m = 6

$$f(x) = \alpha_0+\alpha_1 x+\alpha_2(x^2-0.388) + \alpha_3(1.4399x^3-x)$$

$$+ \alpha_4(1.0195x^4-x^2+0.114)$$

m = 7

$$f(x) = \alpha_0+\alpha_1 x+\alpha_2(x^2-0.380) + \alpha_3(1.4670x^3-x)$$

$$+ \alpha_4(1.0358x^4-x^2+0.112)$$

m = 8

$$f(x) = \alpha_0+\alpha_1 x+\alpha_2(x^2-0.374) + \alpha_3(1.4884x^3-x)$$

$$+ \alpha_4(1.0489x^4-x^2+0.111)$$

m = 9

$$f(x) = \alpha_0+\alpha_1 x+\alpha_2(x^2-0.370) + \alpha_3(1.5056x^3-x)$$

$$+ \alpha_4(1.0597x^4-x^2+0.110)$$

m = 10

$$f(x) = \alpha_0+\alpha_1 x+\alpha_2(x^2-0.366) + \alpha_3(1.5198x^3-x)$$

$$+ \alpha_4(1.0686x^4-x^2+0.109)$$

m = 11

$$f(x) = \alpha_0+\alpha_1 x+\alpha_2(x^2-0.363) + \alpha_3(1.5317x^3-x)$$

$$+ \alpha_4(1.0762x^4-x^2+0.108)$$

m = 12

$$f(x) = \alpha_0+\alpha_1 x+\alpha_2(x^2-0.360)+\alpha_3(1.5418x^3-x)$$

$$+ \alpha_4(1.0827x^4-x^2+0.108)$$

To apply the identification procedure we need to chose the value of m for the data under investigation and then fit the appropriate polynomial to each block, recording the coefficients $a_0^{(k)} \ldots a_4^{(k)}$.

CHAPTER 11

RESULTS AND CONCLUSIONS

The p terms having been fixed, application of the "sliding block" technique to all types of data showed that $a_0^{(k)}$ was the most "accurate" coefficient in the sense of having the smallest standard deviation and a relatively large magnitude.
For example, with m = 9, we obtain, from (8.2),

$$\text{S.Dev}\,(a_0^{(k)}) = 0.2294\ \sigma$$
$$\text{S.Dev}\,(a_1^{(k)}) = 0.3770\ \sigma$$
$$\text{S.Dev}\,(a_2^{(k)}) = 0.6954\ \sigma$$
$$\text{S.Dev}\,(a_3^{(k)}) = 0.8739\ \sigma$$
$$\text{S.Dev}\,(a_4^{(k)}) = 2.3876\ \sigma$$

It would therefore be desirable for the identification procedure to involve coefficient $a_0^{(k)}$ but, as shown in Figure 14, the $a_1^{(k)}$ against $a_2^{(k)}$ plot produces, for the various models, configurations more disparate than the $a_0^{(k)}$ against $a_1^{(k)}$ plot.

It is proposed, therefore, that the identification procedure should consist of:-

(i) deciding the value of m for the investigation,

(ii) plotting both $a_1^{(k)}$ against $a_2^{(k)}$ and $a_0^{(k)}$against $a_1^{(k)}$ these plots supplementing each other in indication of the growth model.

The choice of m depends on how many data values are available. It would be desirable for the plots to consist of at least ten to fifteen points so the value of m should be fixed accordingly. If there are n data values then there will be (n-2m) blocks. A rough criterion would be $m \leqslant (n/2 - 6)$.

The following results were obtained using two computer programmes, one which generated data from the seven growth curve models, adding, if necessary, a random component, and one which fitted the polynomials derived in Chapter 10 to blocks of the data, recording the $a_j^{(k)}$ $(j = 0,1,\ldots 4)$ for each block.

For reference purposes, the plots are arranged in "book" fashion e.g. all those plots relating to artificial linear data, both "clean" and "noisy" are in the Linear Book. Similarly for the other models.

(a) <u>Form of the Plots for "Clean" Data</u>

The first two figures in each book show the configurations obtained by plotting $a_1^{(k)}$ against $a_2^{(k)}$ and $a_0^{(k)}$ against $a_1^{(k)}$ for "clean" data generated from the seven growth curve models. The plotted points are labelled by their block number, k. Two interesting facts arise:-

(i) The plots do not distinguish between Gompertz and logistic data although these sigmoid curves exhibit configurations markedly different from the other curves.

(ii) Logarithmic parabolic data gives a configuration almost identical to exponential data except for a very slight curve, extremely difficult to detect visually. It would appear that, in practice, we shall be unable to distinguish between these two models and should perhaps discard the logarithmic parabola model since it is the least common of the two.

(b) Form of the Plots for "Noisy" Data

The plots behave as indicated by the theory of Chapter 9 when the data is "clean", but we must expect deviations from the configurations for "noisy" data. Data was generated from the growth curve models with (a) a small normally distributed random component, and (b) a large normally distributed random component added. Figures 22 and 23 show respectively, the resulting data values, and the standard deviation of the random component. Logarithmic parabolic data was excluded from this exercise for reasons given in the previous section, and sigmoid data was generated only from the logistic model since we cannot distinguish this from the Gompertz model. The coefficient plots for the data are shown in the graph books.

It is still possible to identify the underlying model from these plots, particularly if we remember that it is important to study the pattern

FIGURE 22

DATA WITH A SMALL RANDOM COMPONENT

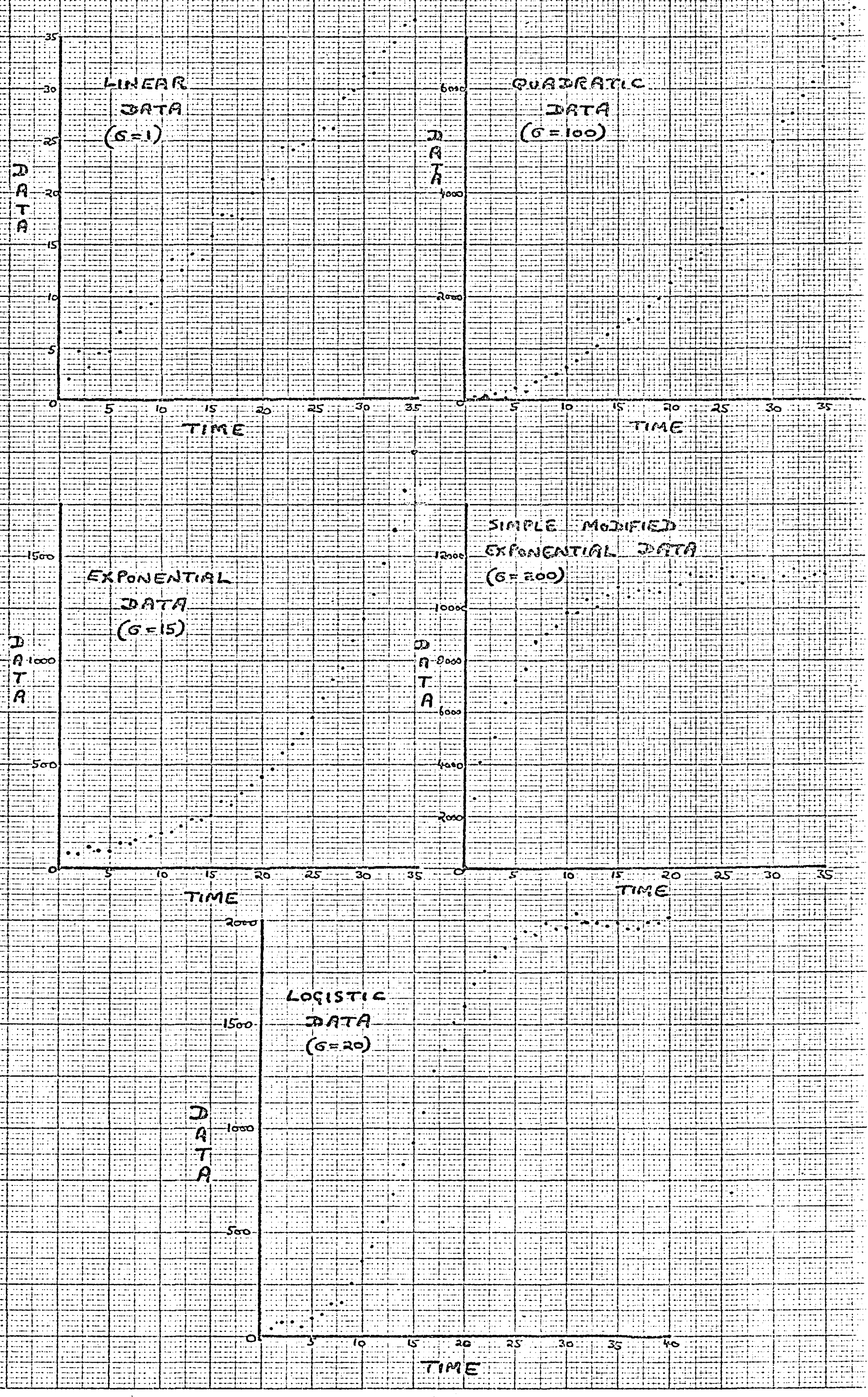
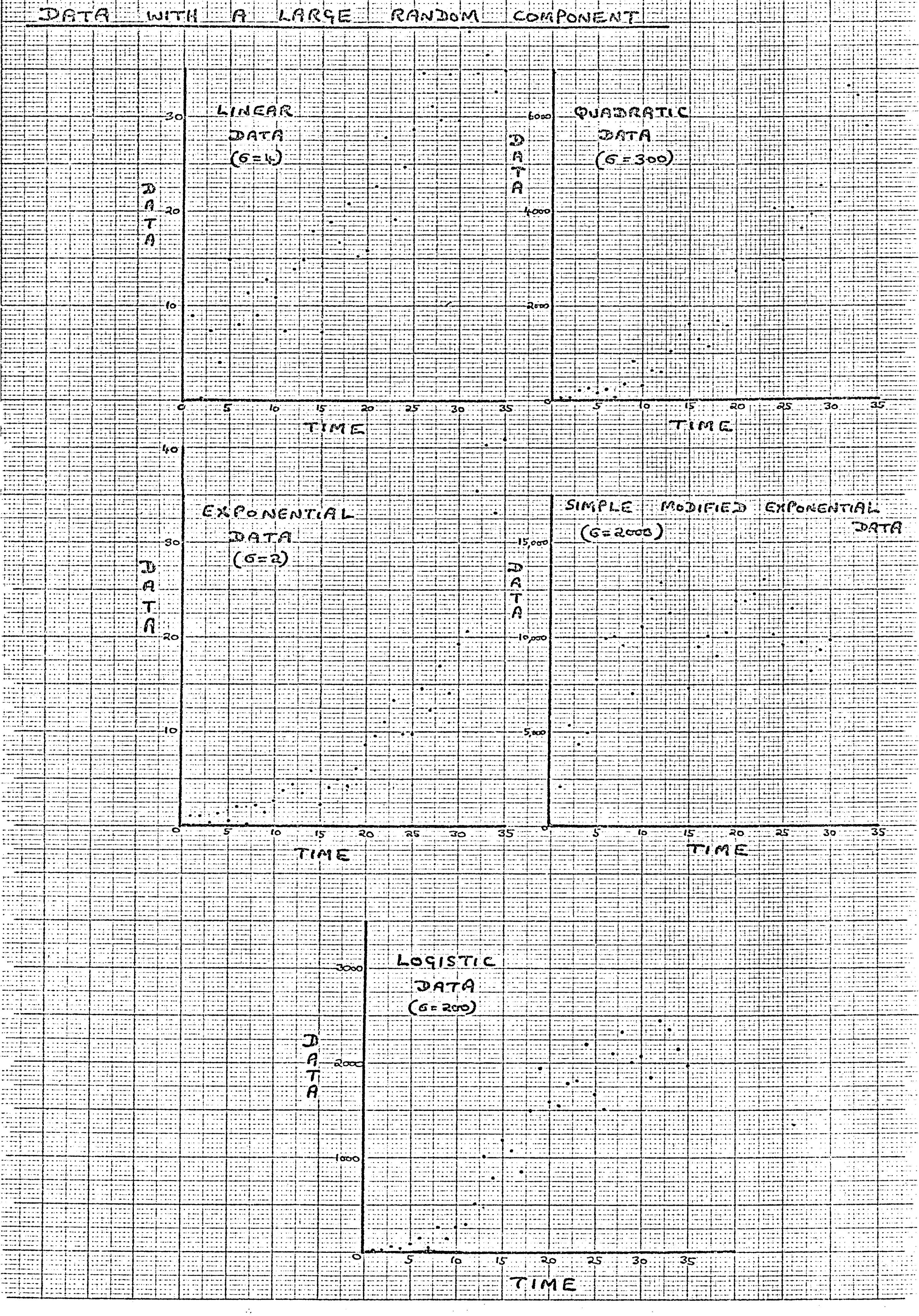


FIGURE 23

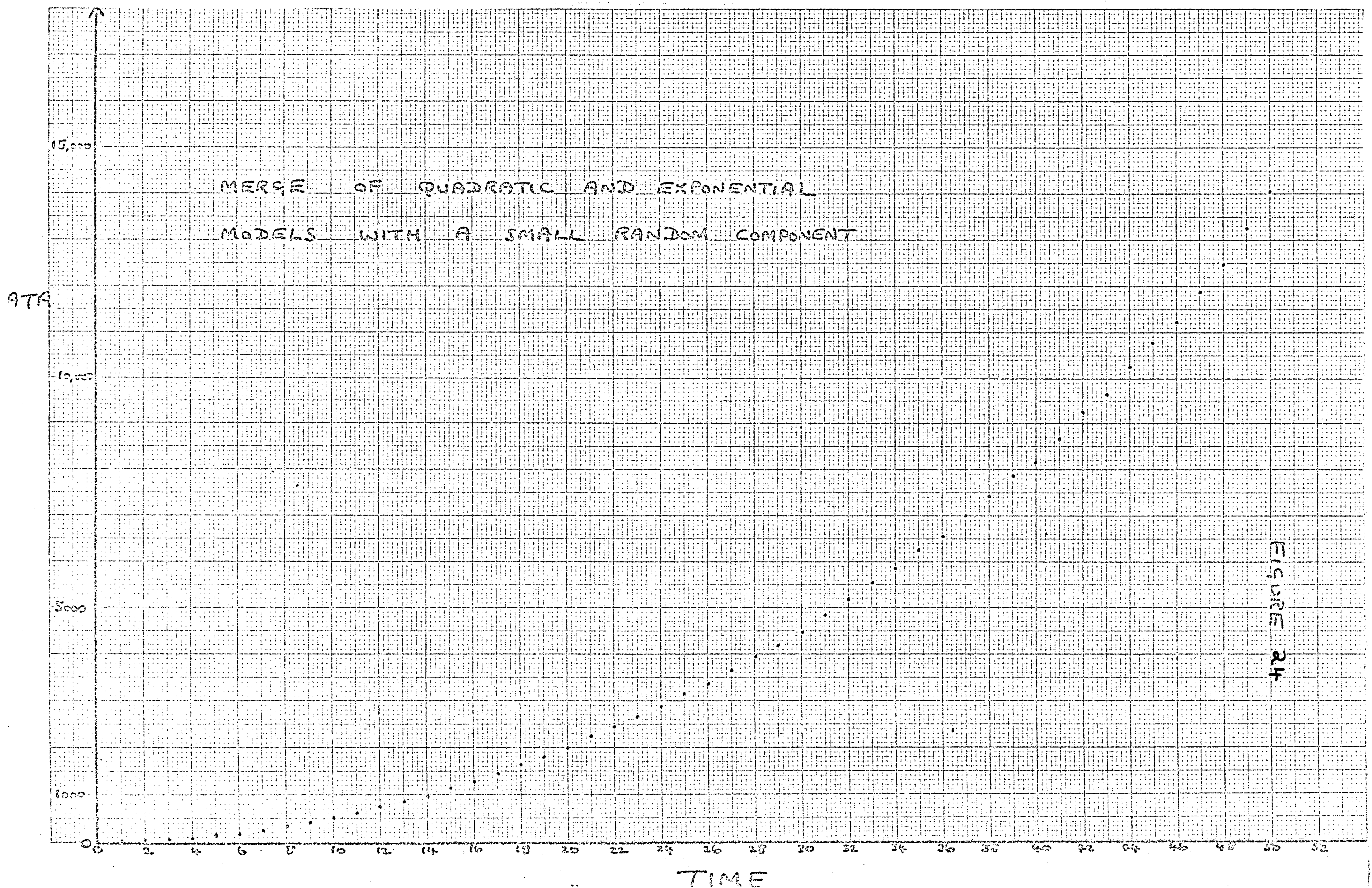

DATA WITH A LARGE RANDOM COMPONENT
LINEAR DATA (σ=4)
QUADRATIC DATA (σ=300)
EXPONENTIAL DATA (σ=2)
SIMPLE MODIFIED EXPONENTIAL DATA (σ=2000)
LOGISTIC DATA (σ=200)
DATA
TIME
0 5 10 15 20 25 30 35
10 20 30 40
2000 4000 6000
5,000 10,000 15,000
1000 2000 3000

of the block numbers. This pattern is unique for each of the five basic configurations. The identification of the model becomes increasingly difficult as the data becomes "noisier". We thus have a limitation on the identification procedure in that for very "noisy" data accurate identification is not possible, although an approximate indication of the underlying model could be given.

Because of the "movement" along the data as we go from block to block, the identification procedure is efficient in detecting changes in the underlying model. Data from quadratic and exponential models with a small random component added, was carefully merged to give the data values depicted in Figure 24. It is impossible to detect by eye that the data consists of these two models yet application of the identification procedure results in a firm conclusion that we have quadratic data merged with exponential data (see Figures 25 and 26).

(c) Estimation of the Model Parameters

The "sliding block" technique is designed primarily to identify growth models, not to estimate their parameters. However, as indicated in Chapter 9, it is possible to acquire quite reasonable estimates of some of the parameters for some of the models.



MERGE OF QUADRATIC AND EXPONENTIAL
MODELS WITH A SMALL RANDOM COMPONENT
DATA
15,000
10,000
5000
1000
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
34
36
38
40
42
44
46
48
50
52
TIME

FIGURE 24

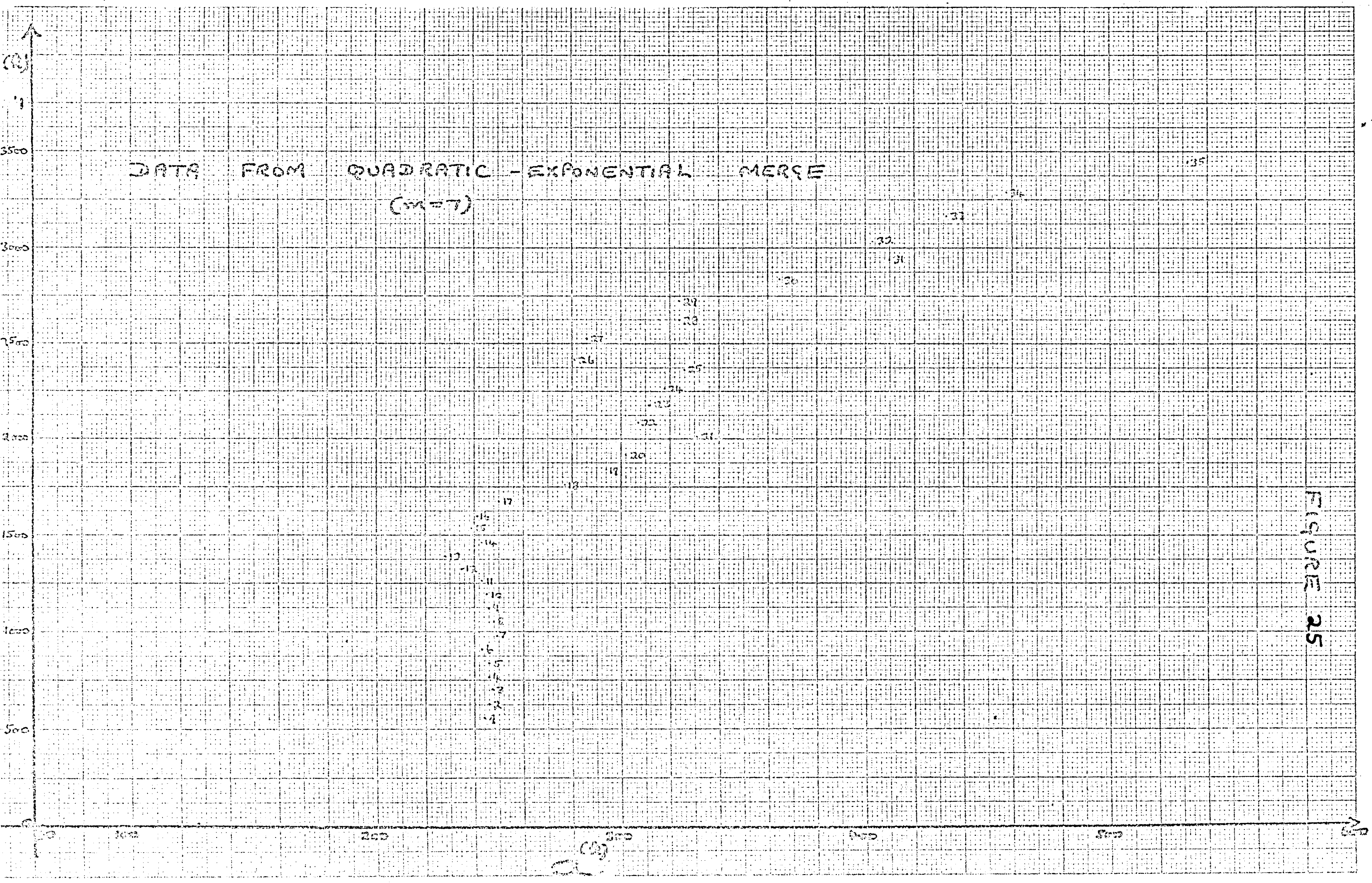
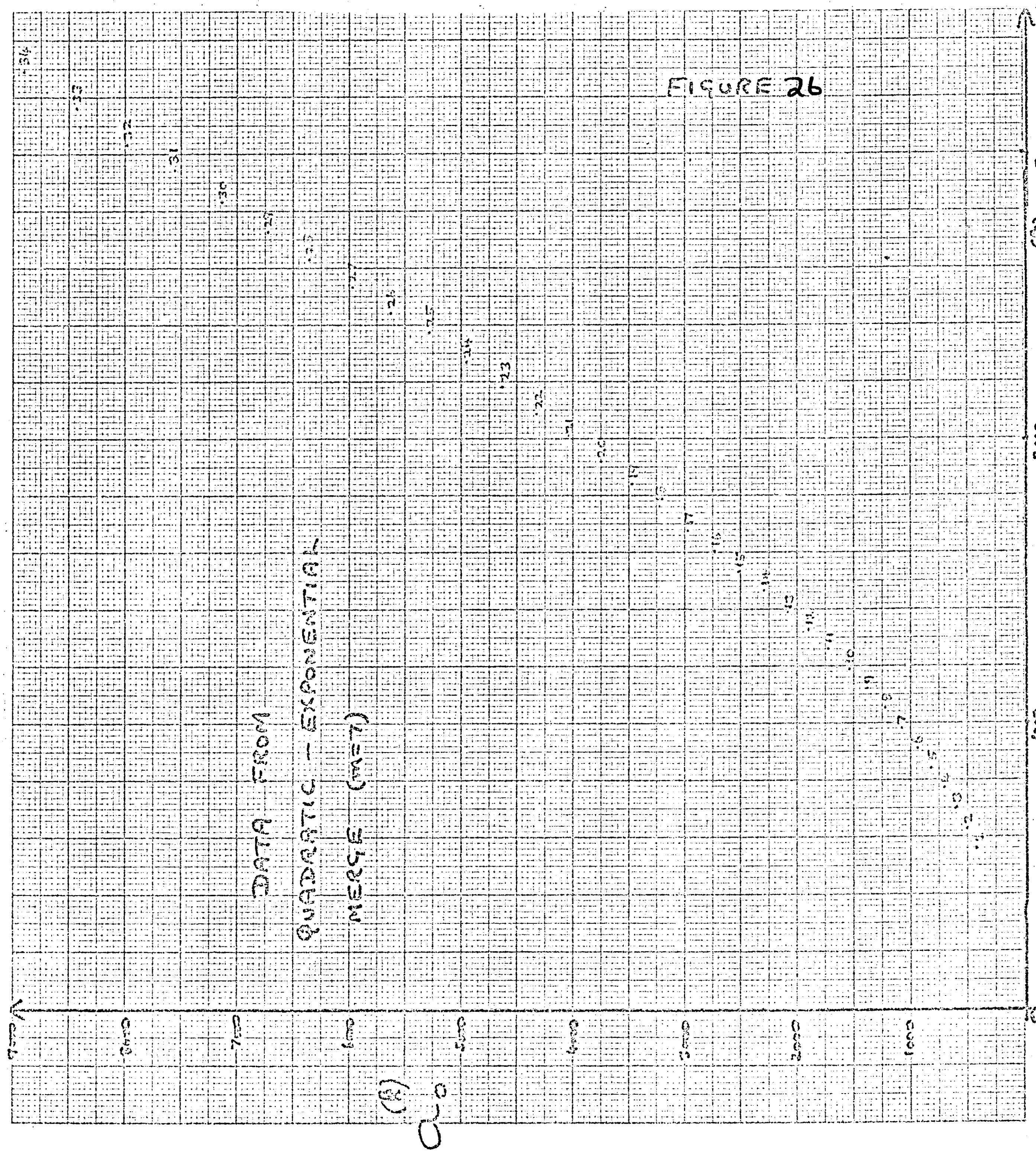

DATA FROM QUADRATIC - EXPONENTIAL MERGE
(m=7)
3500
3000
2500
2000
1500
1000
500

FIGURE 25

FIGURE 26



(i) Linear Data

For linear data ($Y_t = a + bt$), parameter "b" is estimated by the quantity $a_1^{(k)}/m$. Also $a_0^{(k)} = (a + bm) + bk$, so a plot of $a_0^{(k)}$ against k would give a straight line with slope "b" and intercept $(a + bm)$. These estimates were found to be accurate for "clean" data but became increasingly poor for "noisy" data. The last two figures in the linear book (L.7 and L.8) show $a_0^{(k)}$ plotted against k for the linear data shown, respectively, in Figures 22 and 23. The underlying model was $Y_t = 1 + t$. The estimates of "a" and "b" from Figure L.7 are 0.845 and 1.006 respectively, whilst the estimates of "a" and "b" from Figure L.8 are -0.054 and 1.08 respectively. The estimates of "b" obtained by dividing the average value of $a_1^{(k)}$ by m are 1.01 and 0.98 respectively. It would appear, therefore, that parameter "b" can be estimated quite accurately even with very "noisy" data, but not so parameter"a".

(ii) Quadratic Data

For quadratic data ($Y_t = a + bt + ct^2$), parameter "c" is estimated by the quantity $a_2^{(k)}/m^2$. Also $a_1^{(k)} = (bm + 2cm^2) + 2cmk$, so a plot of $a_1^{(k)}$ against k would give a straight line with slope 2cm and intercept $(bm + 2cm^2)$. The estimates of both "c" and "b" would be needed for an estimate of "a", and as this would involve fitting a quadratic to a plot of $a_0^{(k)}$ against k it is unlikely that the estimate of "a" eventually obtained would be reliable. The last two figures in the quadratic book (Q.7 and Q.8) show $a_1^{(k)}$ plotted against k for the quadratic data depicted, respectively, in Figures 22 and 23. The underlying model was $Y_t = 60 + 10t + 5t^2$. The estimates of "b" and "c" from Figure Q.7 are 5.93 and 5.06 respectively, whilst the estimates of "b" and "c" from Figure Q.8 are -27.52 and 6.26 respectively. The estimates of "c" obtained by dividing the average value of $a_2^{(k)}$ by m^2 are 4.83 and 6.02 respectively. It therefore appears that reasonable estimates of parameter "c" may be obtained provided that the data is not too "noisy", but estimates of parameter "b" are not reliable.

(iii) Exponential Data

For exponential data ($Y_t = ae^{bt}$), parameter "b" may be estimated from the relationship $a_j^{(k+1)}/a_j^{(k)} = e^b$ $(j = 0,1, \ldots 4)$. Using the ratio $a_0^{(k+1)}/a_0^{(k)}$, since $a_0^{(k)}$ is the most reliable of the coefficients, estimates of "b" for the exponential data depicted in Figures 22 and 23, where "b" was set at 0.1, are 0.1 and 0.1 respectively, a result which indicates that we may obtain a good estimate of parameter "b" even for "noisy" data.

(iv) Simple Modified Exponential Data

We may similarly use the ratio $a_1^{(k+1)}/a_1^{(k)}$ to estimate the parameter "b" for simple modified exponential data ($Y_t = K + ae^{bt}$), but the realibility of this estimate becomes poor as the data becomes increasingly "noisier". With "b" set at -0.1825 in the data depicted in Figure 22, the average $a_1^{(k+1)}/a_1^{(k)}$ ratio gave an estimate of -0.294. With "b" set at -0.2 in the data depicted in Figure 23, the average ratio gave an estimate of -0.55.

(d) Some Results with "Real" Data

(i) Gregg, Hossell and Richardson {19} use data they label "Commodity A" to illustrate their slope characteristic procedure. The data is S-shaped (see Figure 27) but because their slope characteristics for Gompertz and logistic models show small regions of non-linearity for years 7 to 9, they are wary of fitting one of these models to the entire period. Figures 28 and 29 show the coefficient plots for this data with m fixed at 5. Both plots suggest that a sigmoid curve could be fitted to the data; indeed there is very little deviation from the standard sigmoid configuration.

(ii) In a paper in J.R.S.S.(C), volume 19, number 1, F.R. Oliver estimated the parameters of an exponential growth model by direct least squares

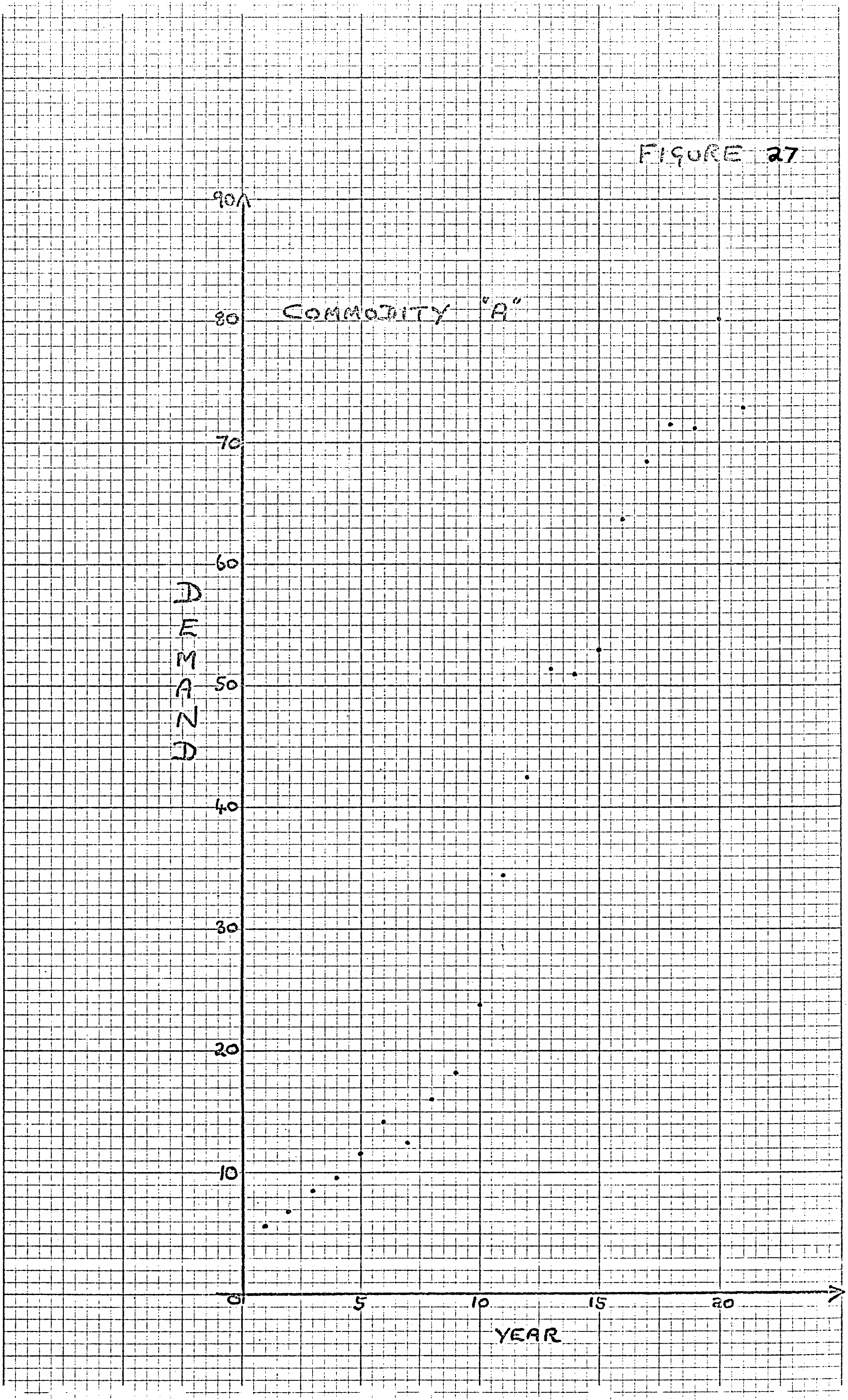
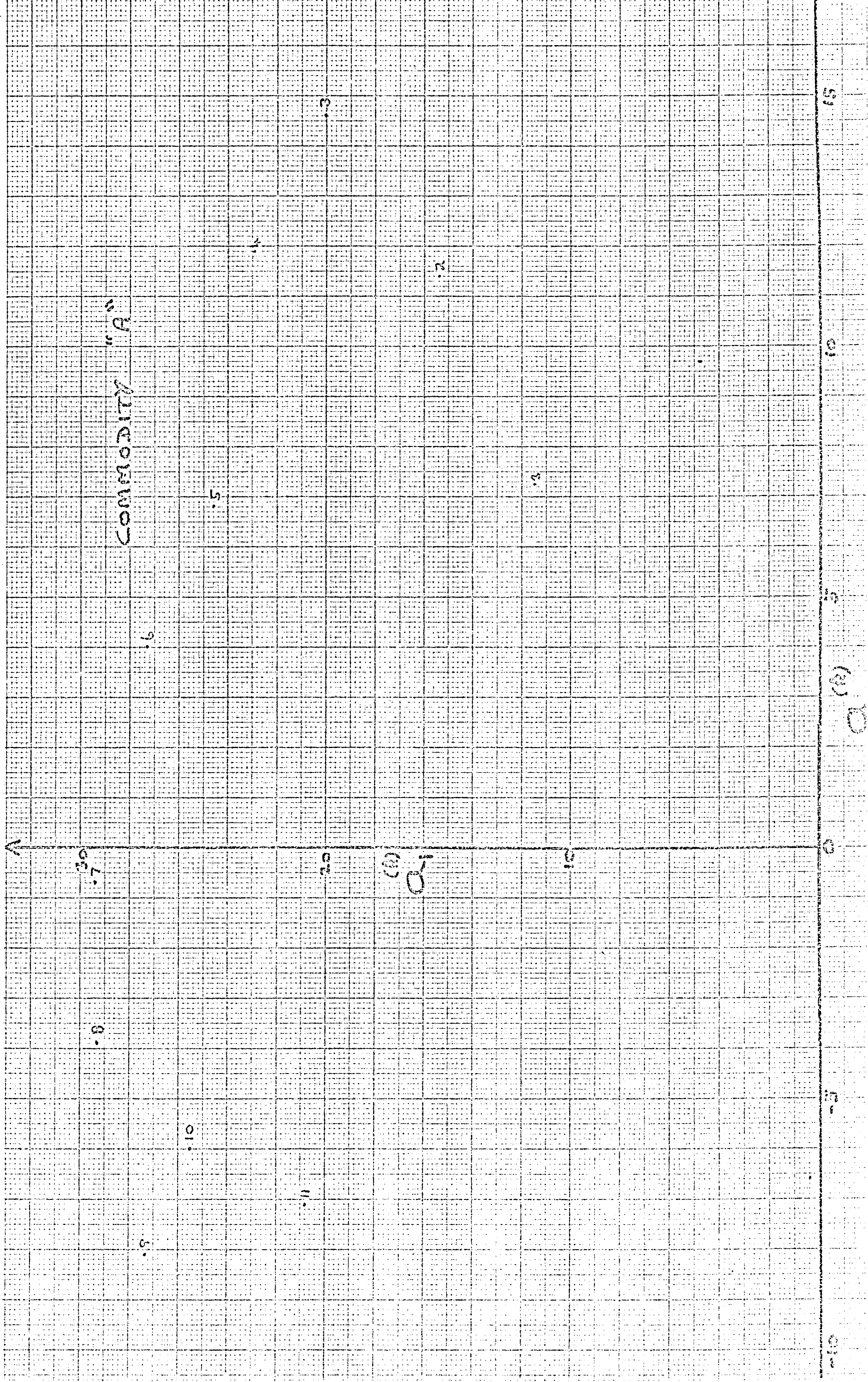


FIGURE 27
COMMODITY "A"
DEMAND
YEAR
0
5
10
15
20
10
20
30
40
50
60
70
80
90

FIGURE 28



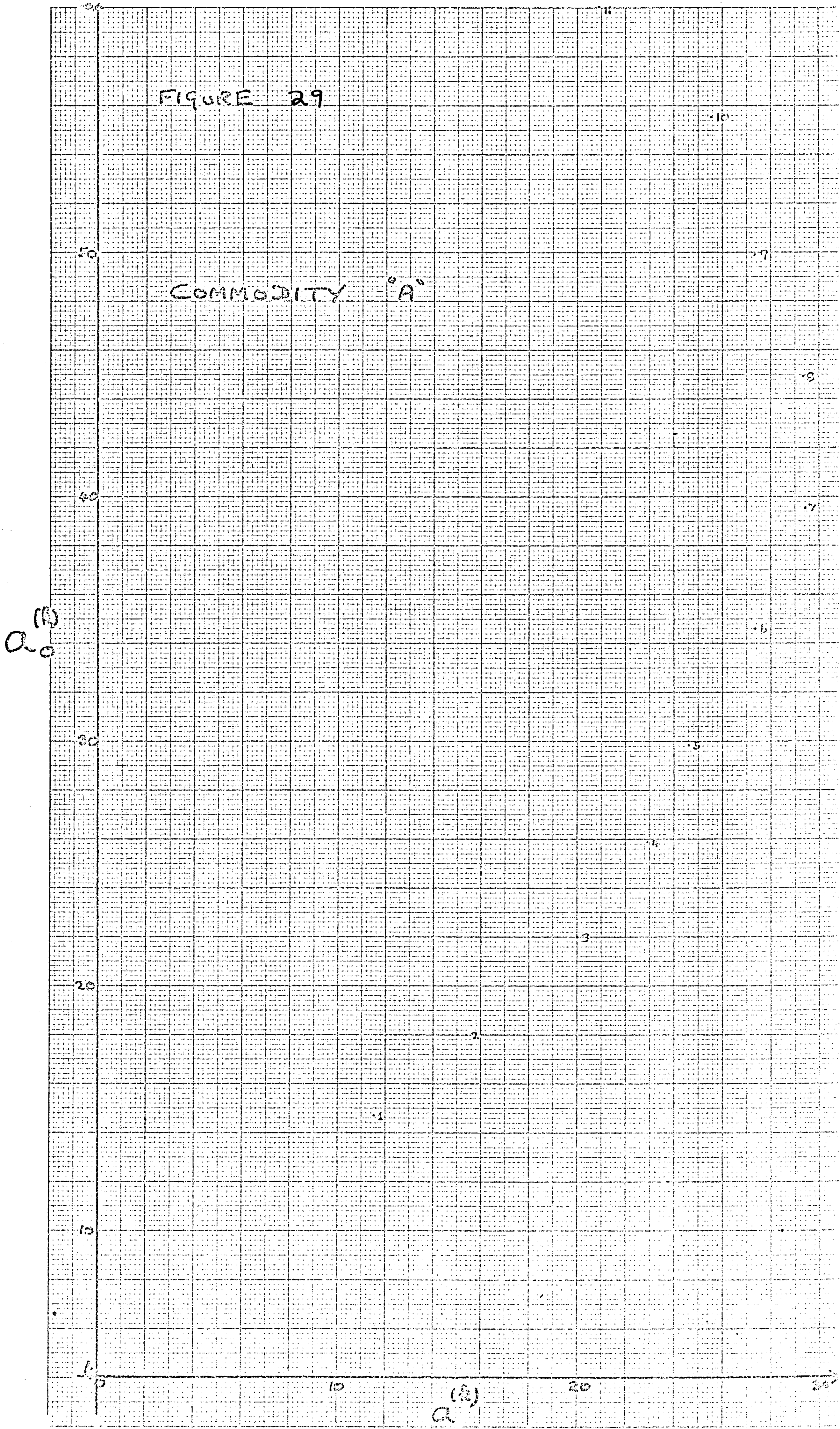


FIGURE 29
COMMODITY "A"
50
40
30
20
10
0
10
20
30

and compared his results with the estimates obtained by taking logarithms and then applying least squares. The estimates of parameter "b" were:-

Direct Least Squares	Logarithmic Least Squares
0.081441	0.084102

The average of the $a_0^{(k+1)}/a_0^{(k)}$ ratios from an application of the identification procedure to his data gave an estimate of "b" as 0.0815.

(iii) Experiments on rats at the M.R.C. unit, Middlewood Hospital, Sheffield, required the rats to be under constant conditions. The rats needed a time to acclimatize after arriving and the length of the acclimatization period was the subject of some research. One variable used to measure this period was the daily fluid intake of the rats. Once the rats become acclimatized this intake becomes constant. Figure 30 shows the data for the first 33 days of acclimatization for Rat C118. There was doubt as to whether the fluid intake curve could be adequately fitted by a sigmoid curve, a simple modified exponential curve or two straight lines. Figures 31 and 32, obtained directly from a graph plotter, show the coefficient plots for the data. They show that there is some initial linearity, a marked simple modified exponential region and then several blocks of linear data indicating linearity from day 10 onwards. There is no suggestion of an S-shaped trend.

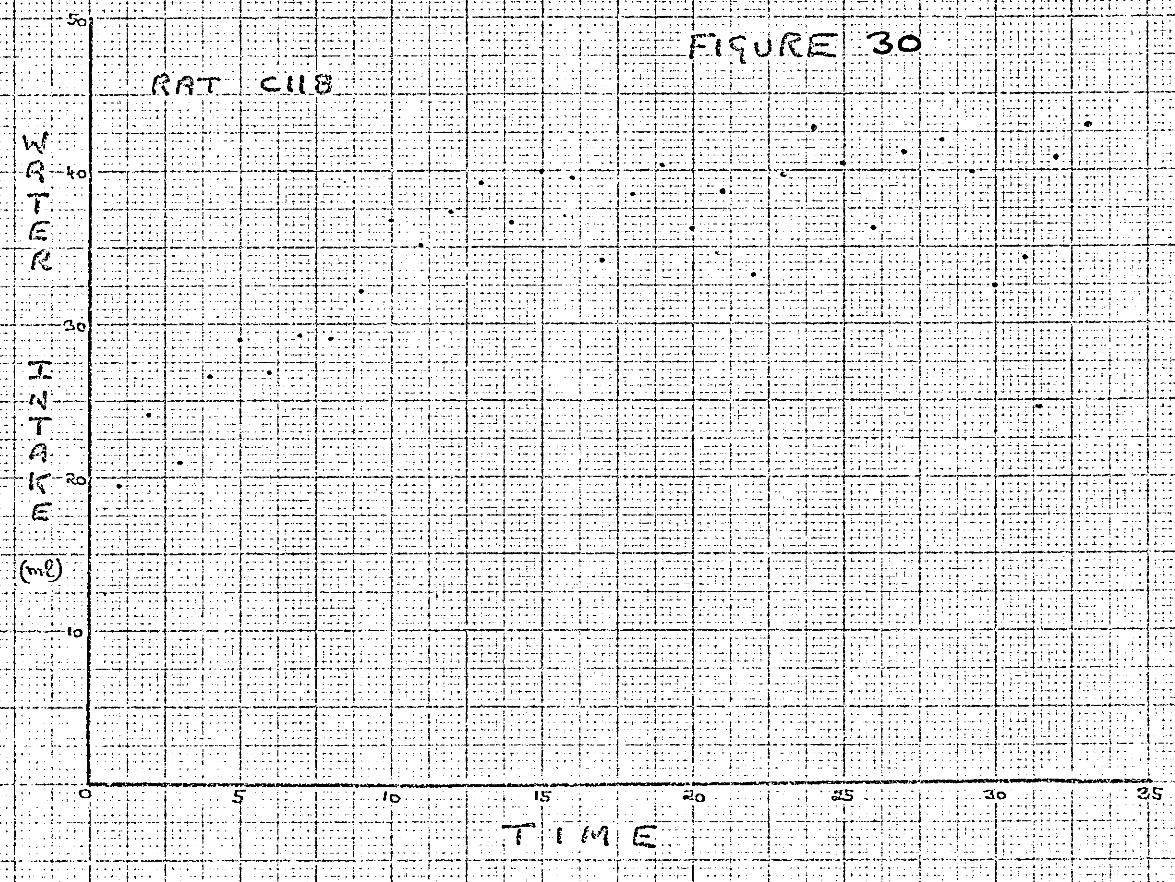


FIGURE 30

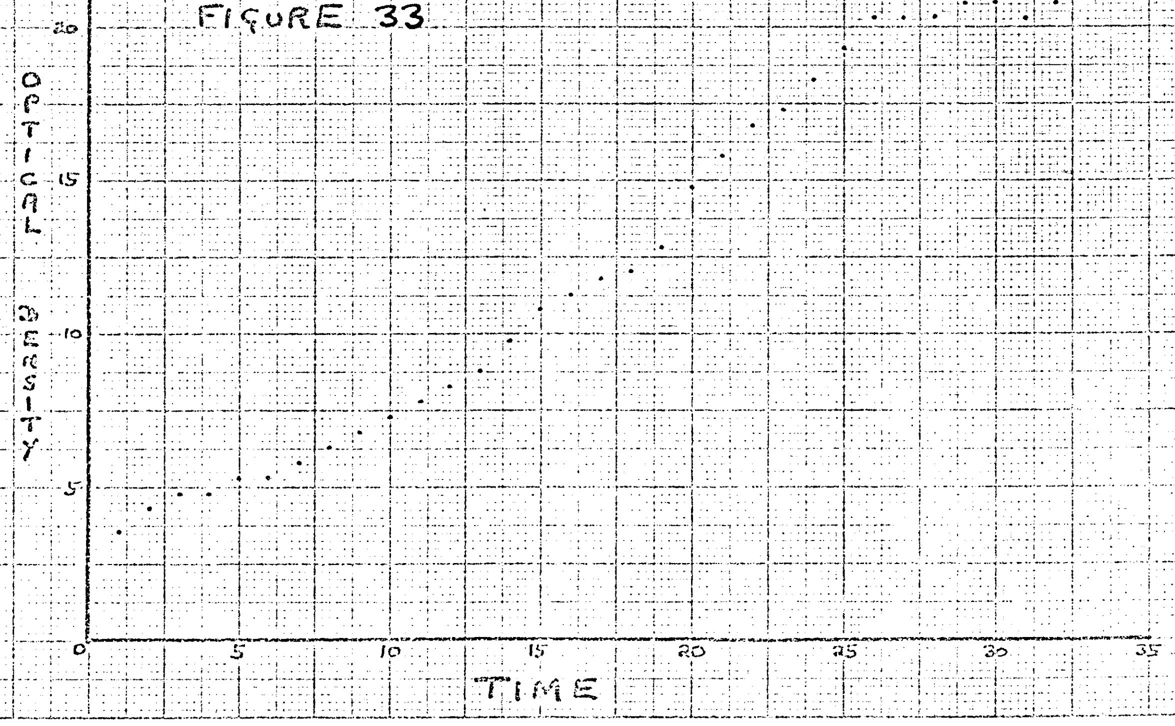


FIGURE 33

FIGURE 31

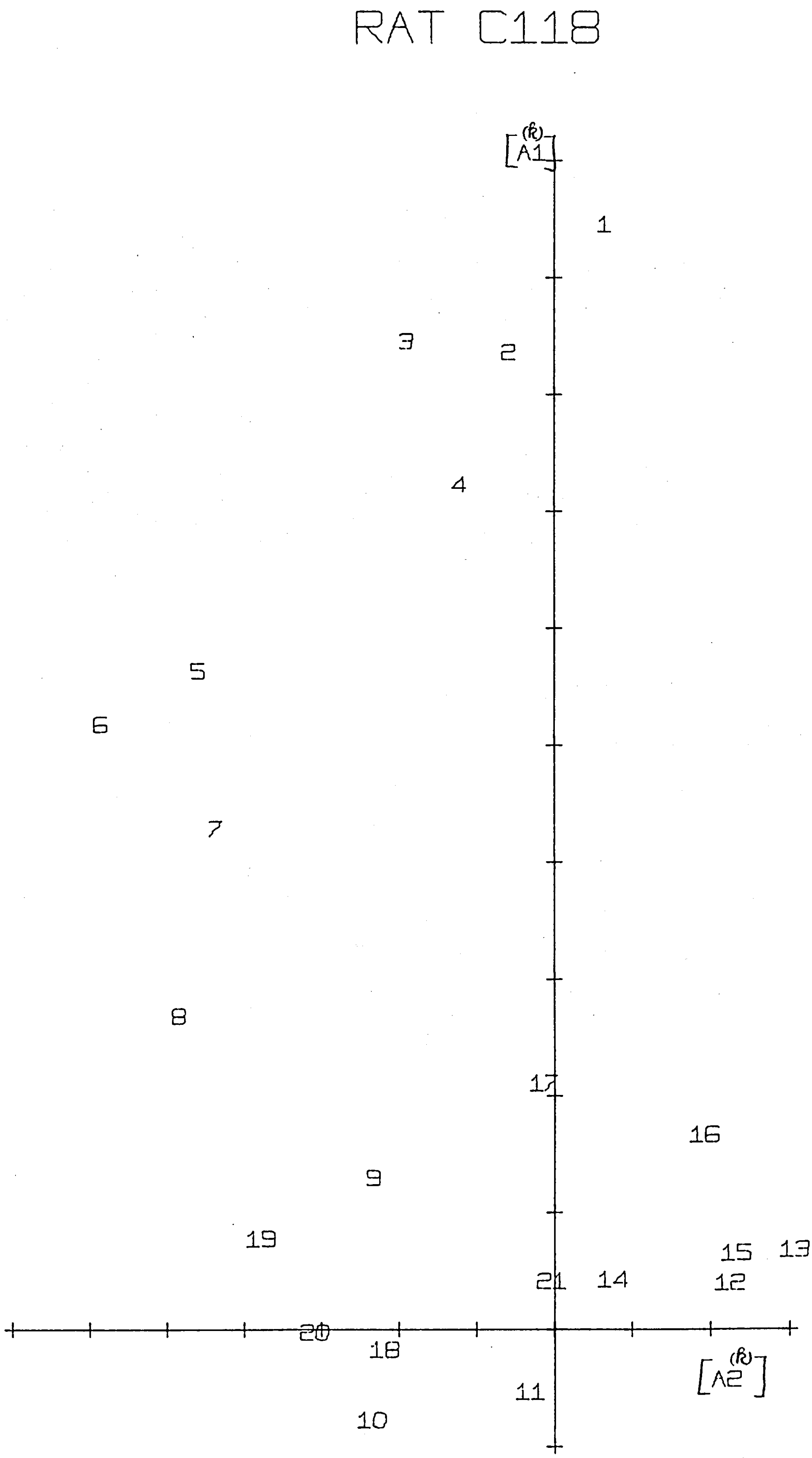
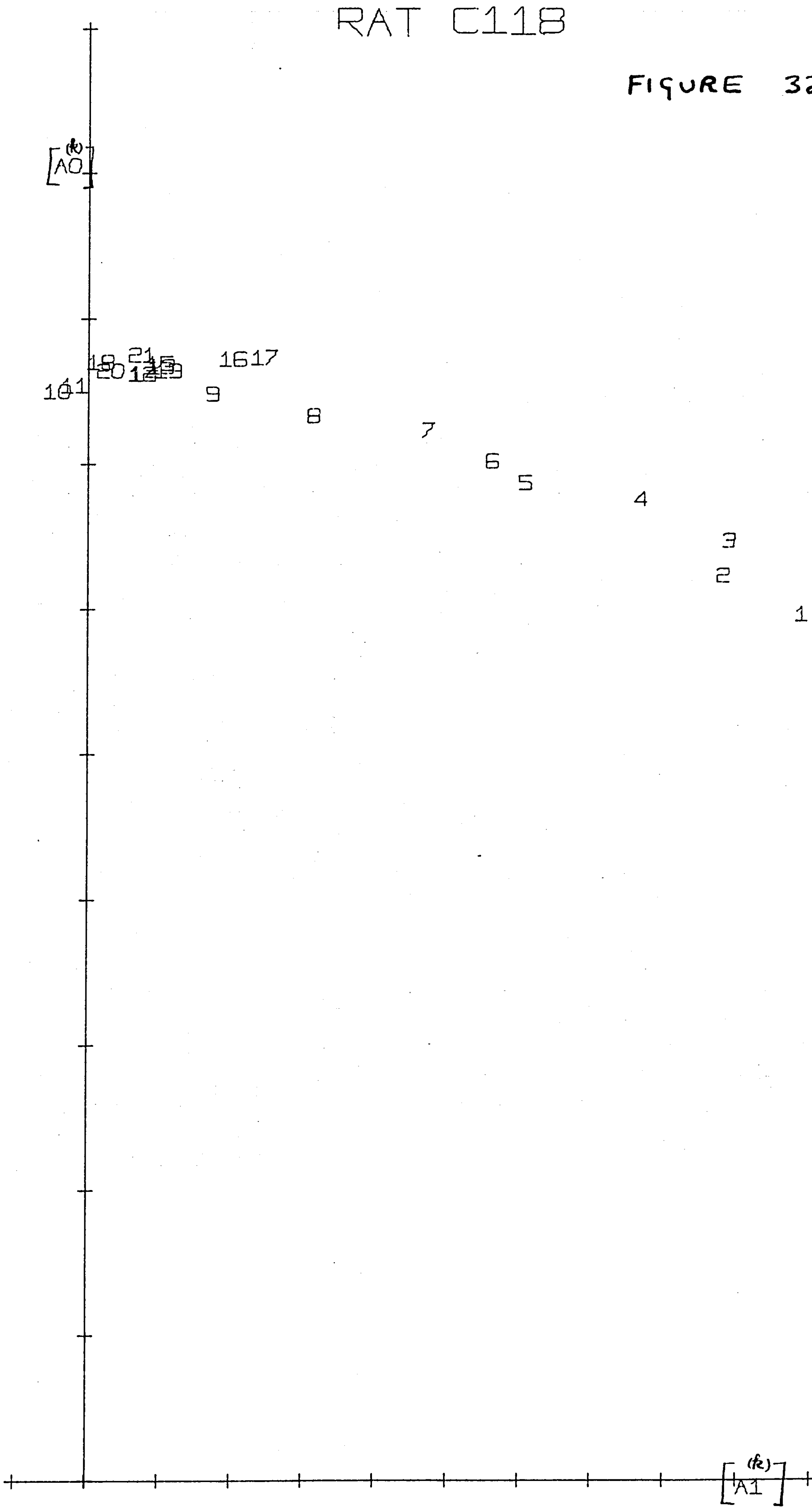
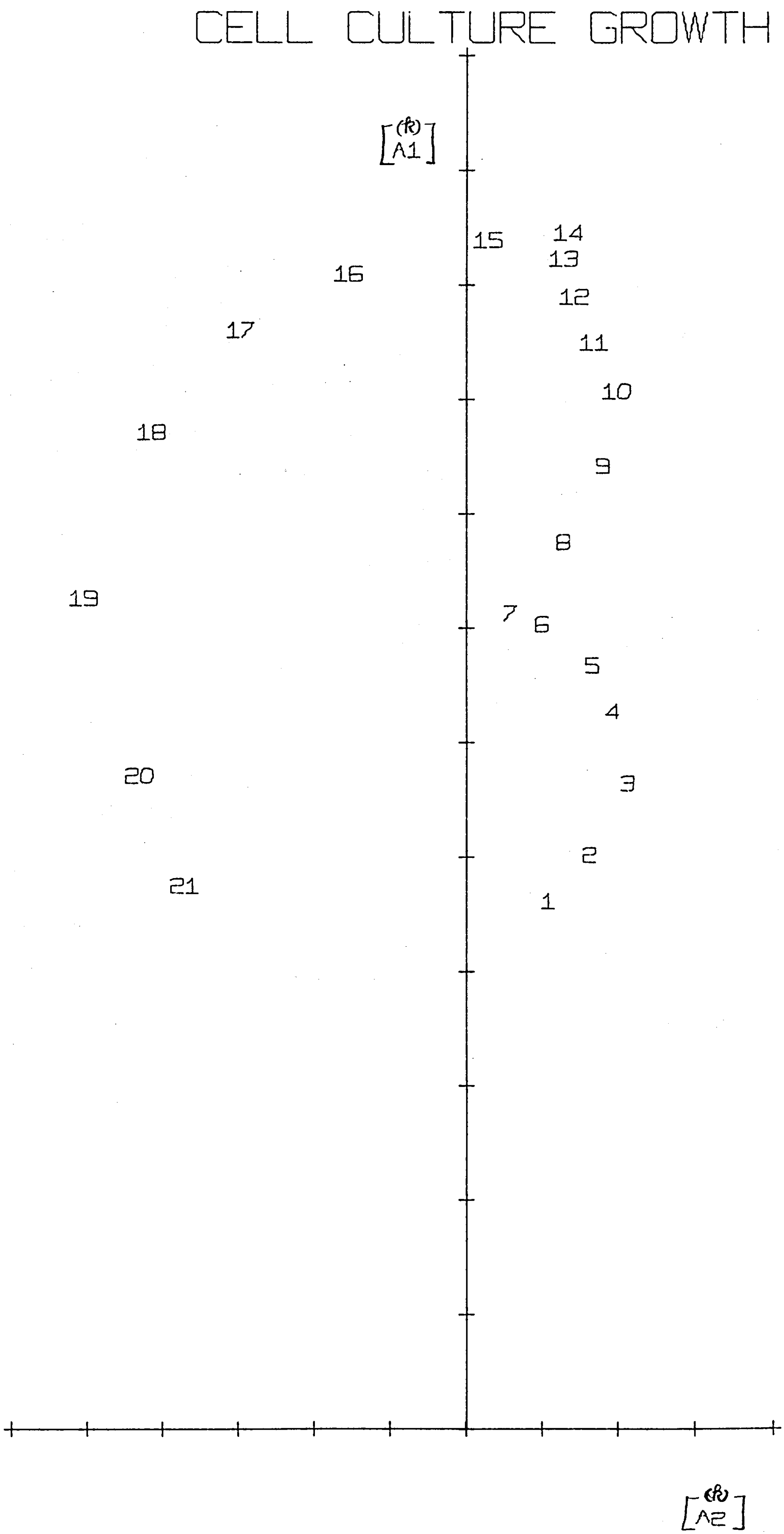


FIGURE 32

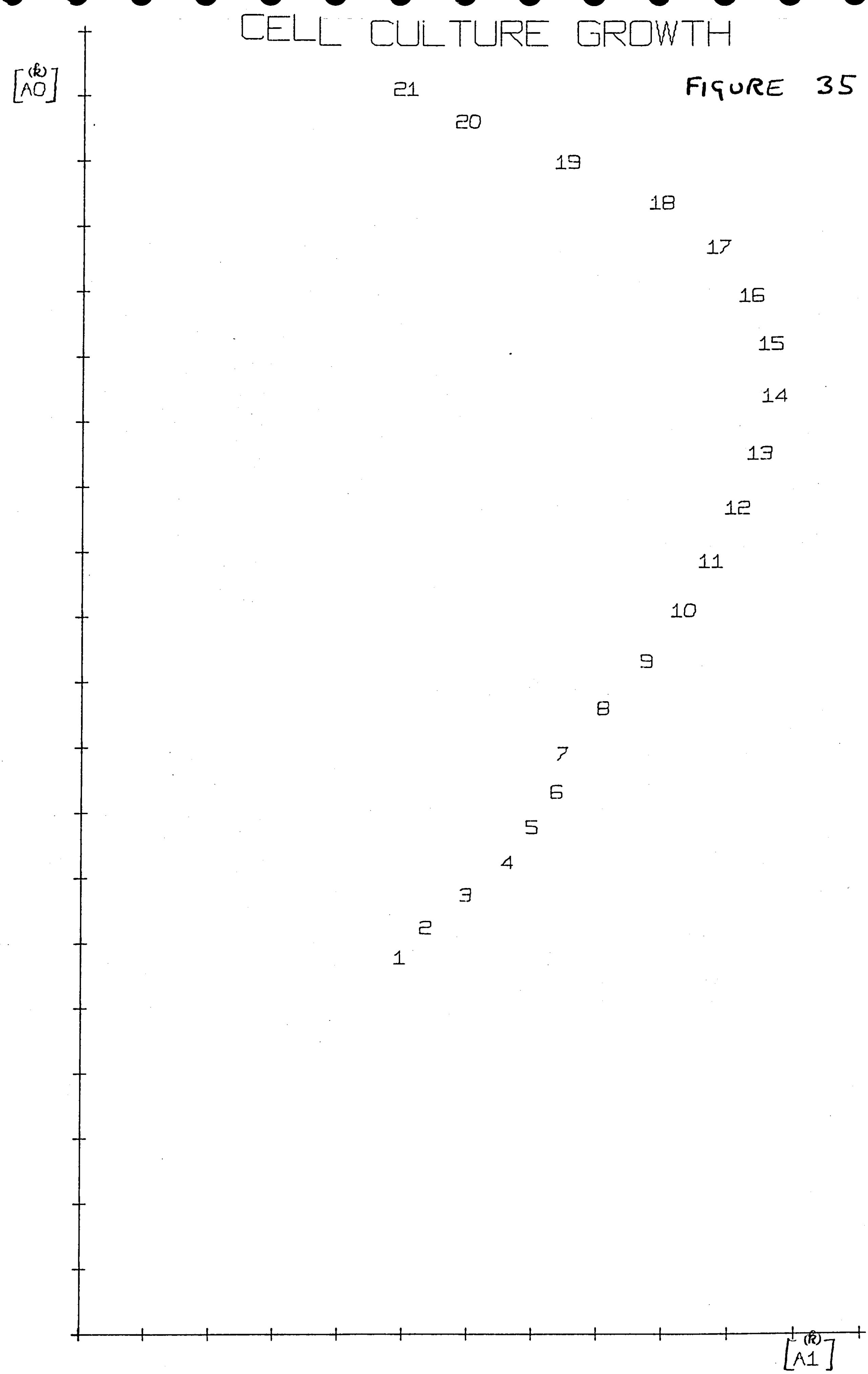


(iv) In an experiment conducted by the Department of Chemistry and Biology at Sheffield Polytechnic, a known concentration of organisms was placed in a culture medium, the whole being incubated at 37°c. Samples were taken from the flask at equal time intervals and the optical density of the samples was measured in the appropriate units. The data is shown in Figure 33. To identify the growth data obtained, coefficient plots were produced by a graph plotter (see Figures 34 and 35). These indicate that the data has a sigmoid trend up to the nineteenth reading and then, surprisingly, follows a new sigmoid trend. An experimental explanation offered by the Department was that there could have been a temperature fluctuation.

FIGURE 34



CELL CULTURE GROWTH
[A1 (k)]
[A2 (k)]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21


CELL CULTURE GROWTH
FIGURE 35
[AO]^(k)
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
[A1]^(k)

CHAPTER 12

AREAS FOR FURTHER RESEARCH

The development and application of the coefficient plots suggests areas that lend themselves to further study. These are:-

(i) Several "p" terms were set equal to zero in Chapter 8 for computational reasons and because these terms are zero for polynomials such as Tchebychef, Hermite and Legendre. The polynomials derived in Chapter 10 might be improved if these "p" terms were evaluated in the same manner as the remaining terms.

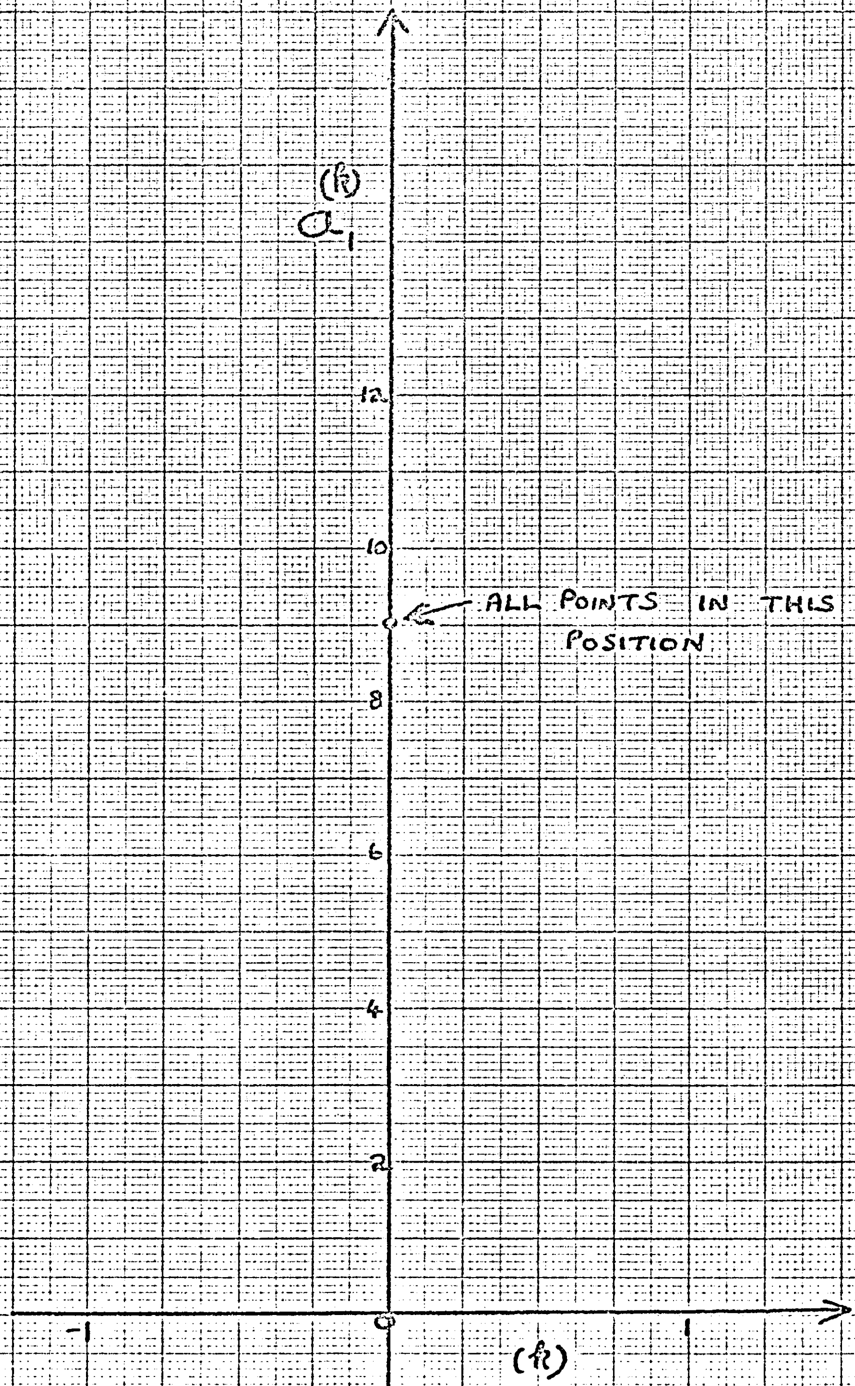
(ii) Orders other than a fourth-order polynomial fit could be investigated and in fact h could be chosen to further improve the ratio S.Dev.$(a_j^{(k)})/|a_j^{(k)}|$ $(j = 0,1....h)$, especially for the small values 0,1,2,... of j.

(iii) A deep mathematical treatment of the logarithmic parabola, logistic and Gompertz models might indicate useful plots for identification purposes.

(iv) The $g_r(x)$ in the fitted model could be varied; a chain of exponential functions suggests itself. There might, indeed, be some optimum form of the $g_r(x)$ for the purpose of identification of growth curves.

FIGURE L.1

CLEAN LINEAR DATA (m=9)



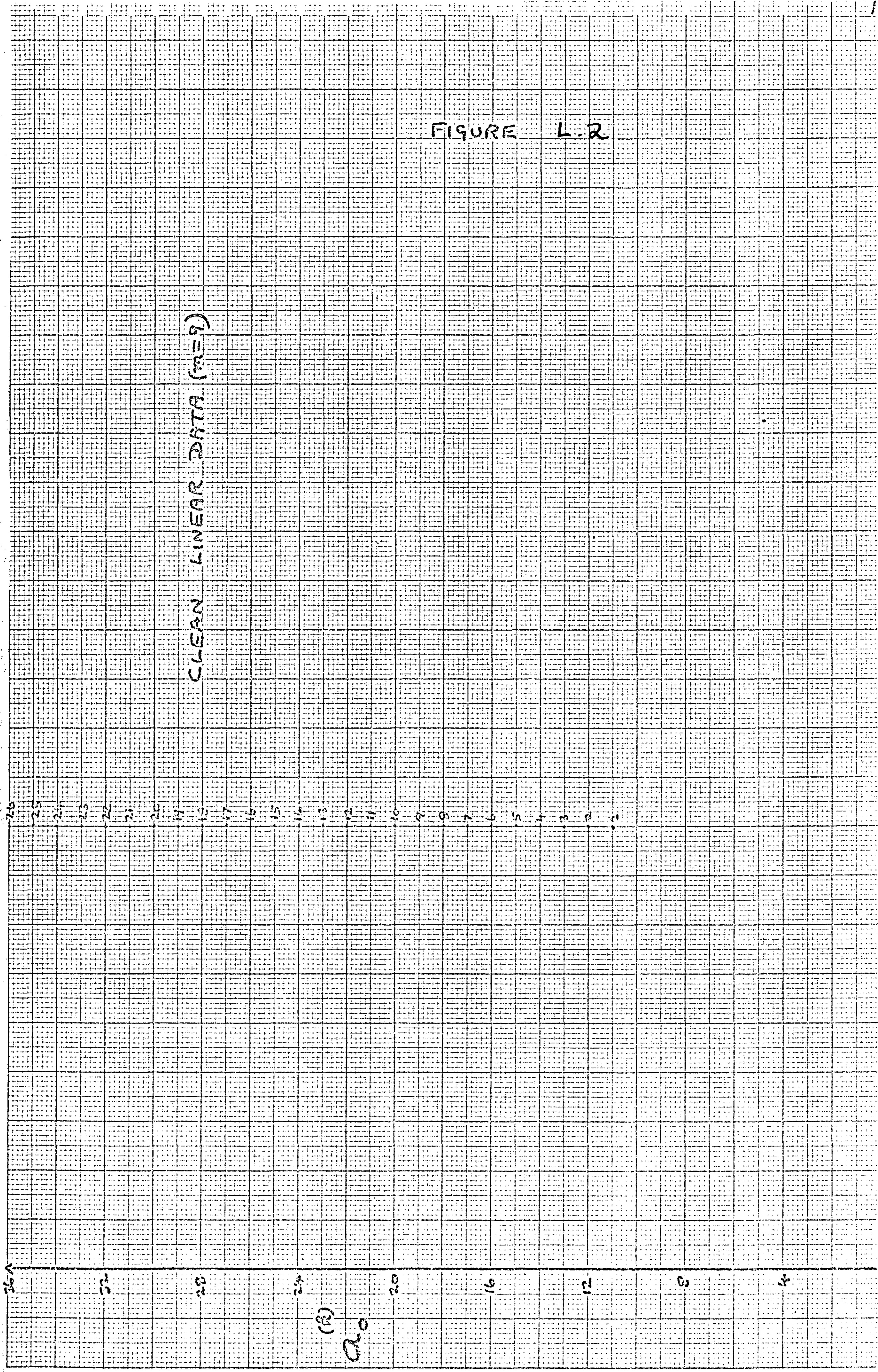


FIGURE L.2

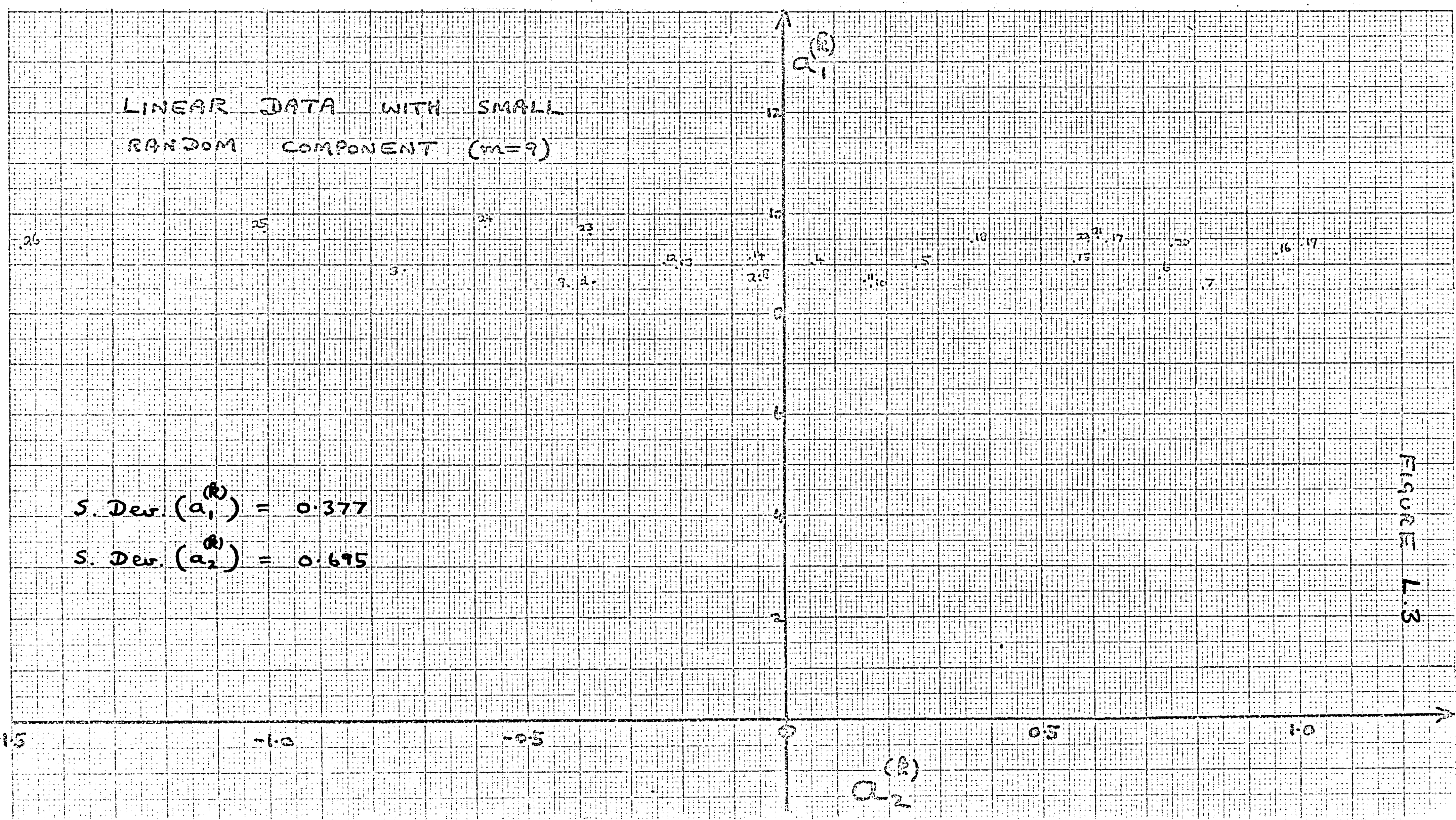
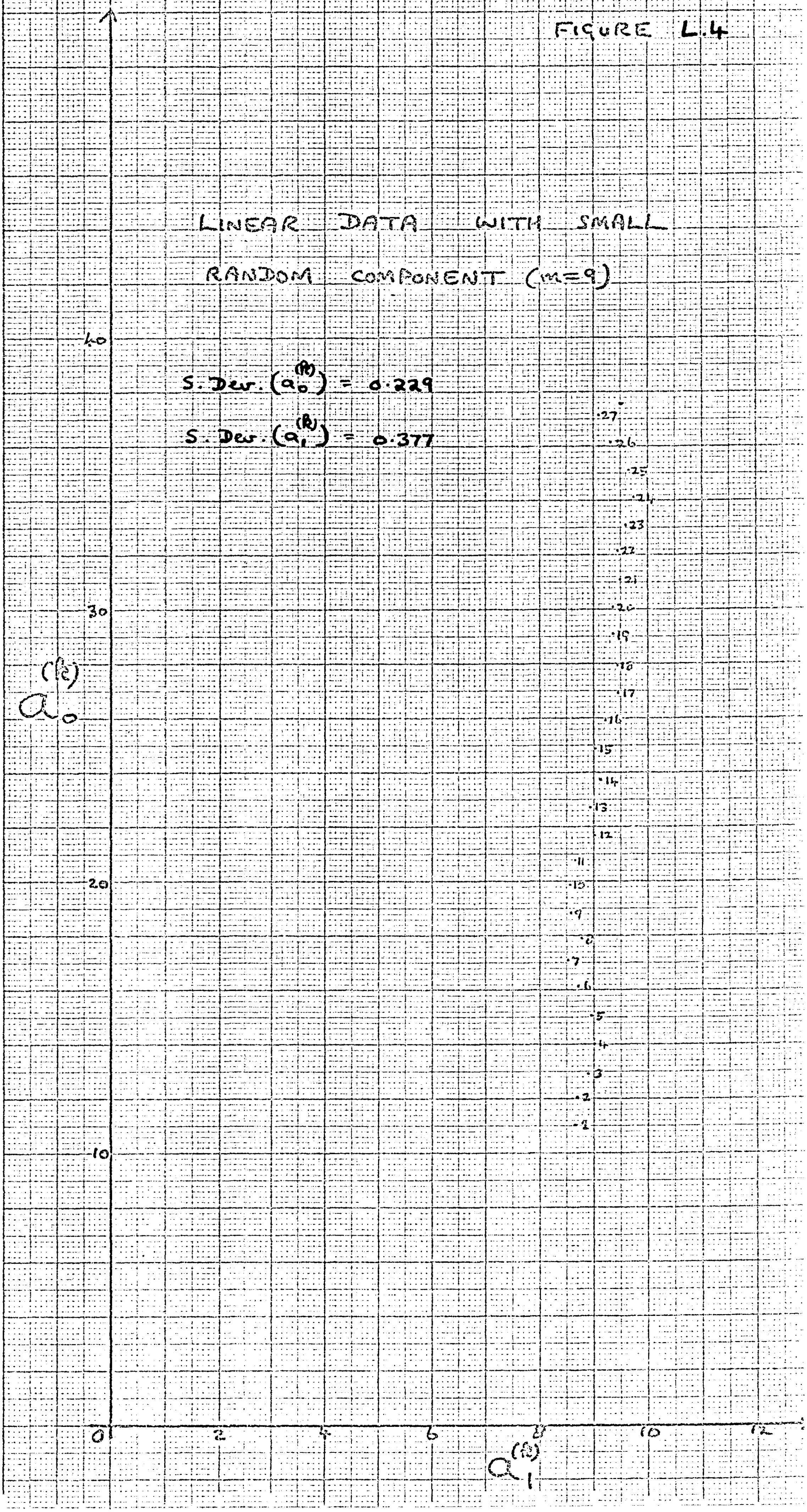

LINEAR DATA WITH SMALL
RANDOM COMPONENT (m=9)
S. Dev. $(a_1^{(k)})$ = 0·377
S. Dev. $(a_2^{(k)})$ = 0·695
$a_1^{(k)}$
$a_2^{(k)}$
-1·5
-1·0
-0·5
0
0·5
1·0

FIGURE L.3

FIGURE L.4


LINEAR DATA WITH SMALL
RANDOM COMPONENT (m=9)
S. Dev. $(a_0^{(k)})$ = 0.229
S. Dev. $(a_1^{(k)})$ = 0.377
$a_0^{(k)}$
$a_1^{(k)}$
0
2
4
6
8
10
12
10
20
30
40

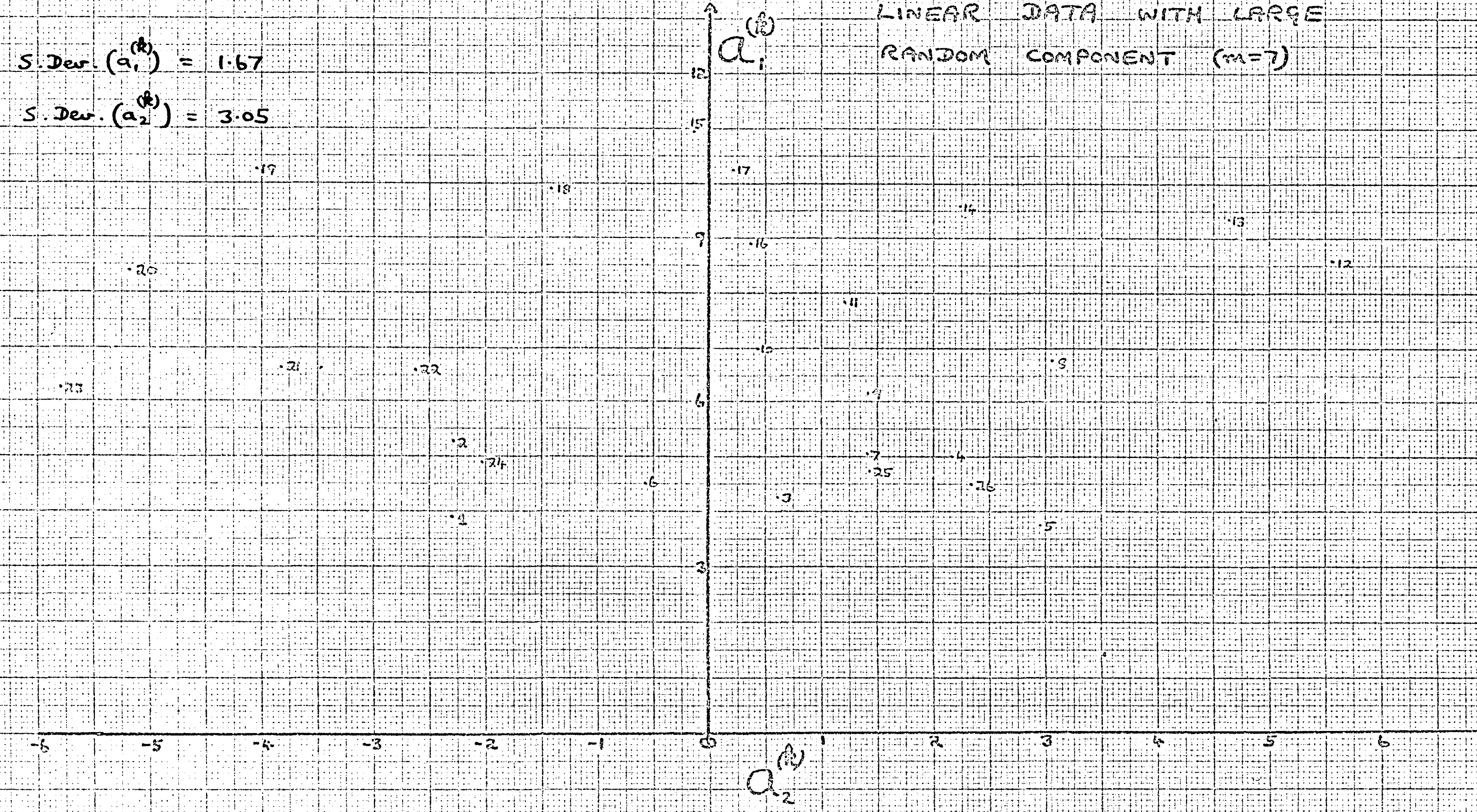
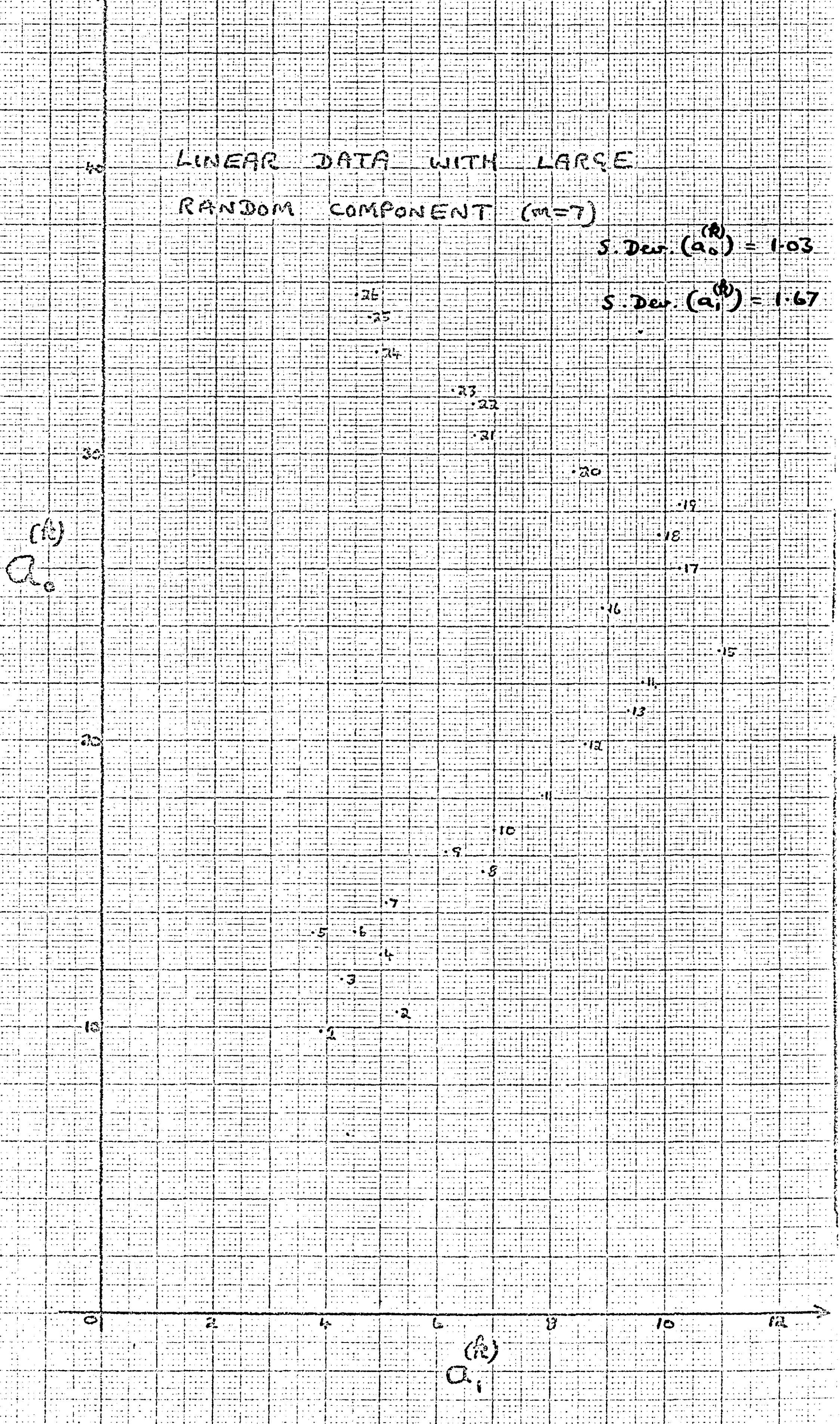

LINEAR DATA WITH LARGE
RANDOM COMPONENT (m=7)
S. Dev. $(a_1^{(k)})$ = 1.67
S. Dev. $(a_2^{(k)})$ = 3.05
$a_1^{(k)}$
$a_2^{(k)}$

FIGURE L.5

FIGURE L.6


LINEAR DATA WITH LARGE RANDOM COMPONENT (m=7)
S. Dev. $(a_0^{(k)}) = 1.03$
S. Dev. $(a_1^{(k)}) = 1.67$
$a_0^{(k)}$
$a_1^{(k)}$
10
20
30
40
0
2
4
6
8
10
12
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26

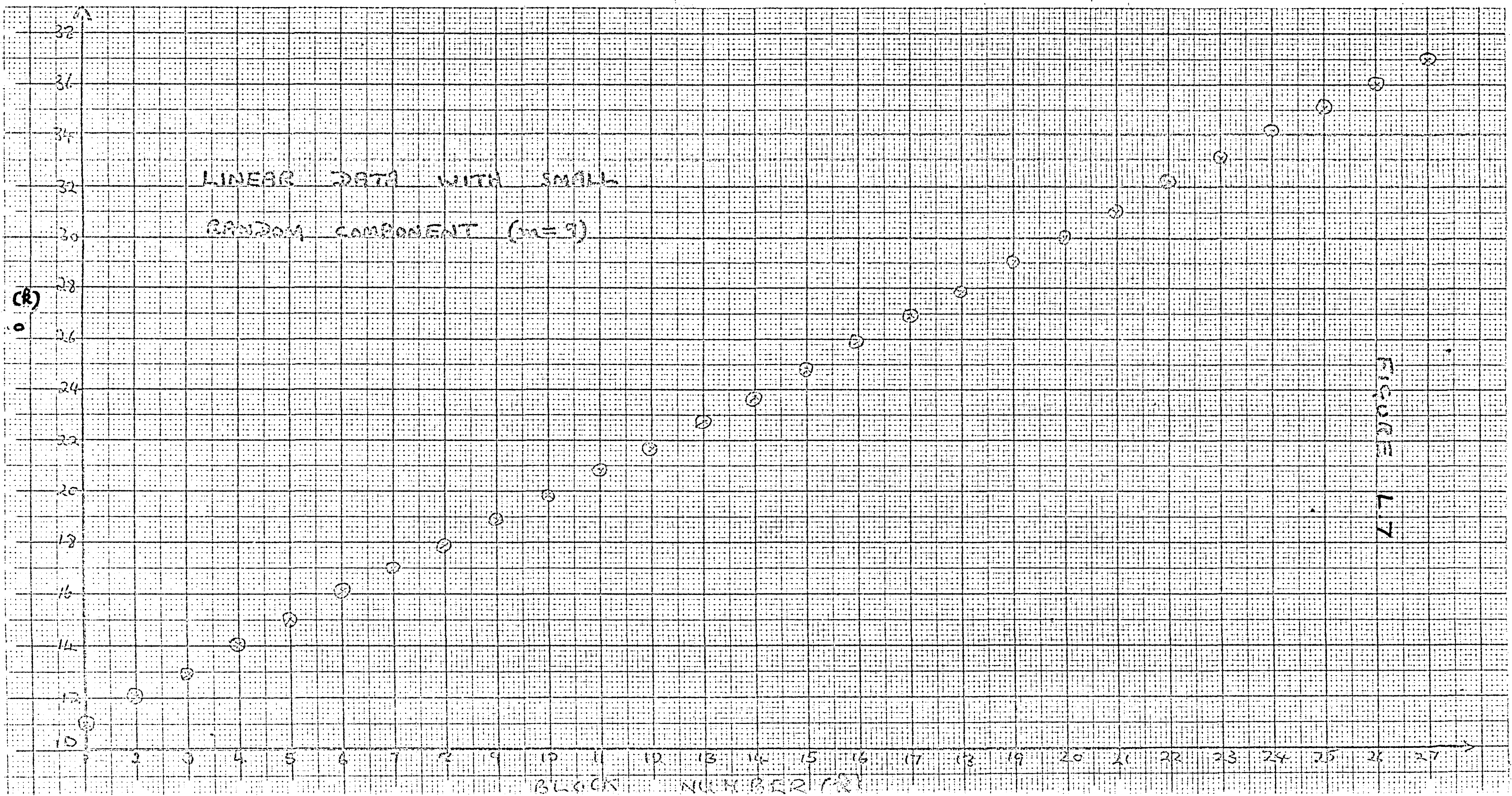

LINEAR DATA WITH SMALL
RANDOM COMPONENT (m=9)
(k)
BLOCK NUMBER
32
31
30
28
26
24
22
20
18
16
14
12
10
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27

FIGURE L.7

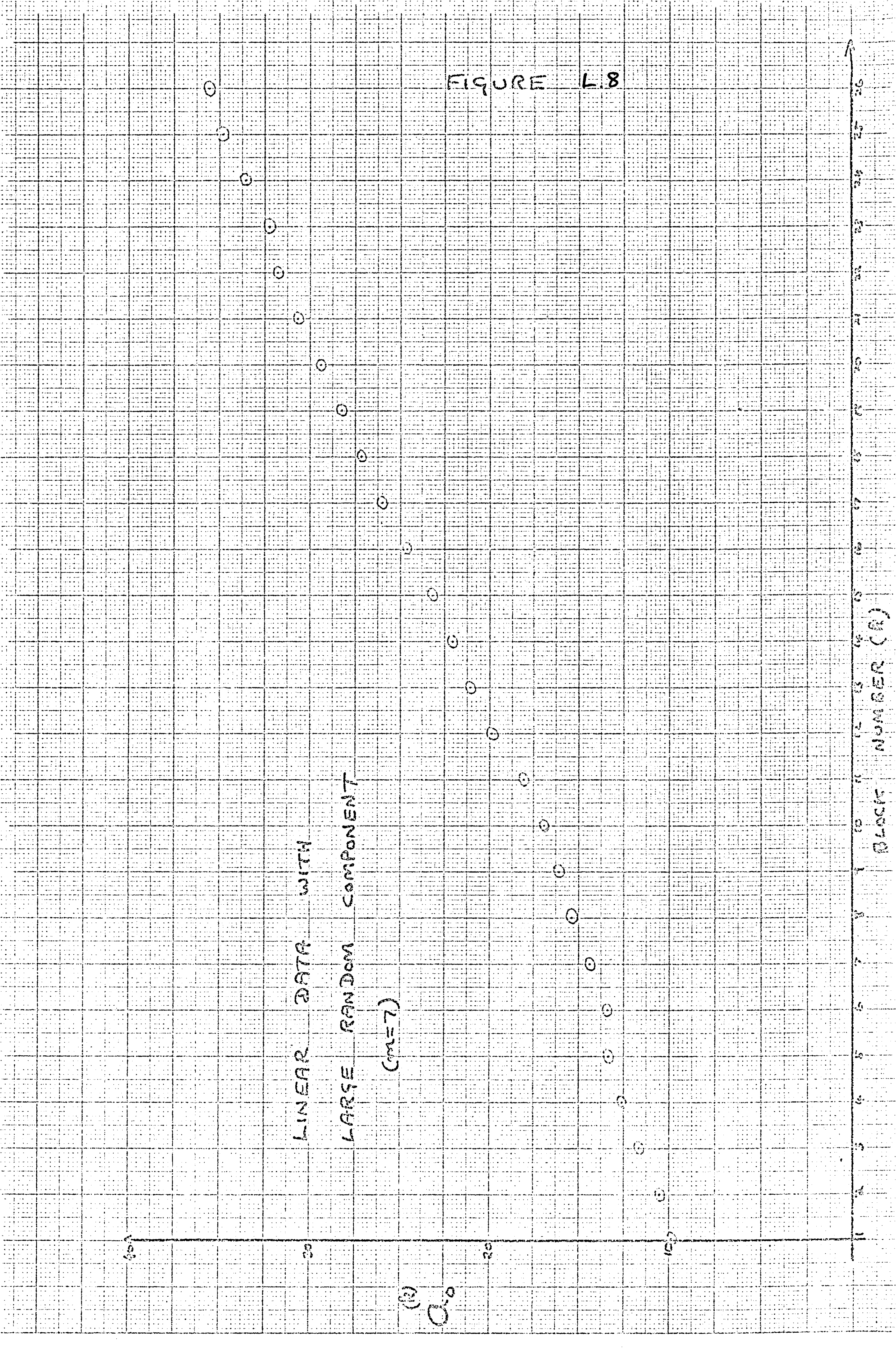


FIGURE L.8
LINEAR DATA WITH
LARGE RANDOM COMPONENT
(m=7)
BLOCK NUMBER (k)

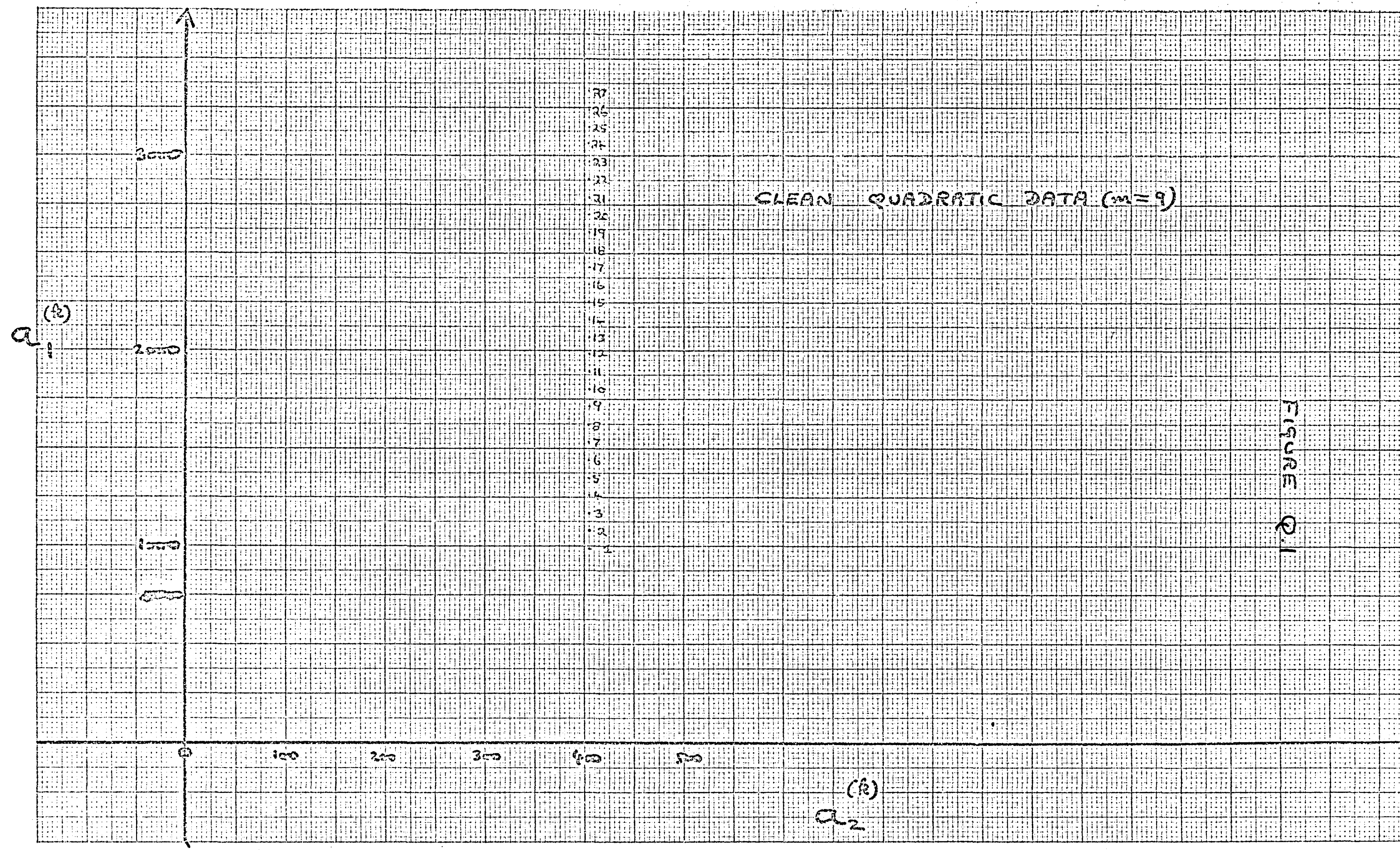

CLEAN QUADRATIC DATA (m=9)
3000
2000
1000
0
100
200
300
400
500
$a_1^{(k)}$
$a_2^{(k)}$

FIGURE Q.1

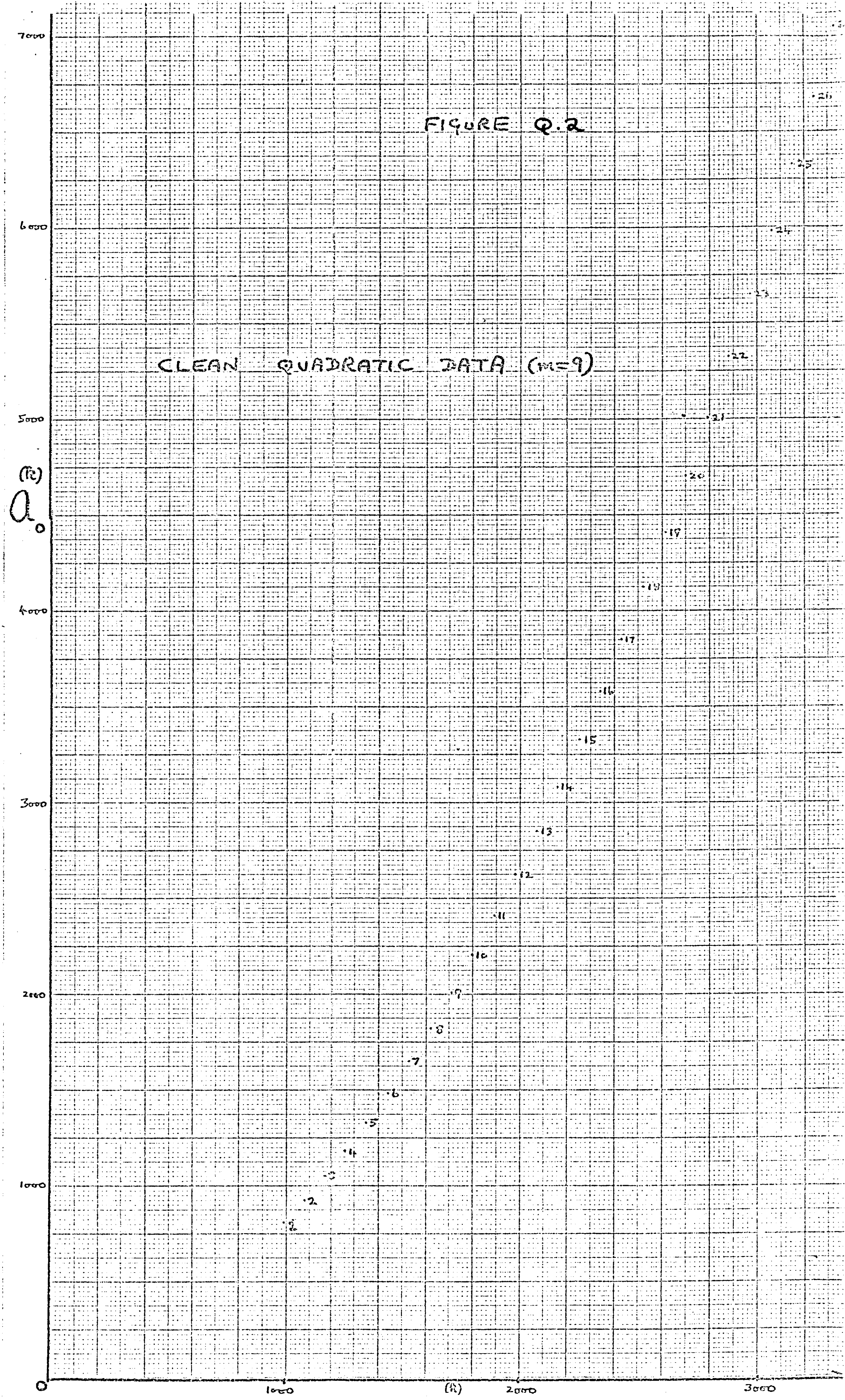


FIGURE Q.2
CLEAN QUADRATIC DATA (m=9)
(k)
a_0
(k)
0
1000
2000
3000
4000
5000
6000
7000

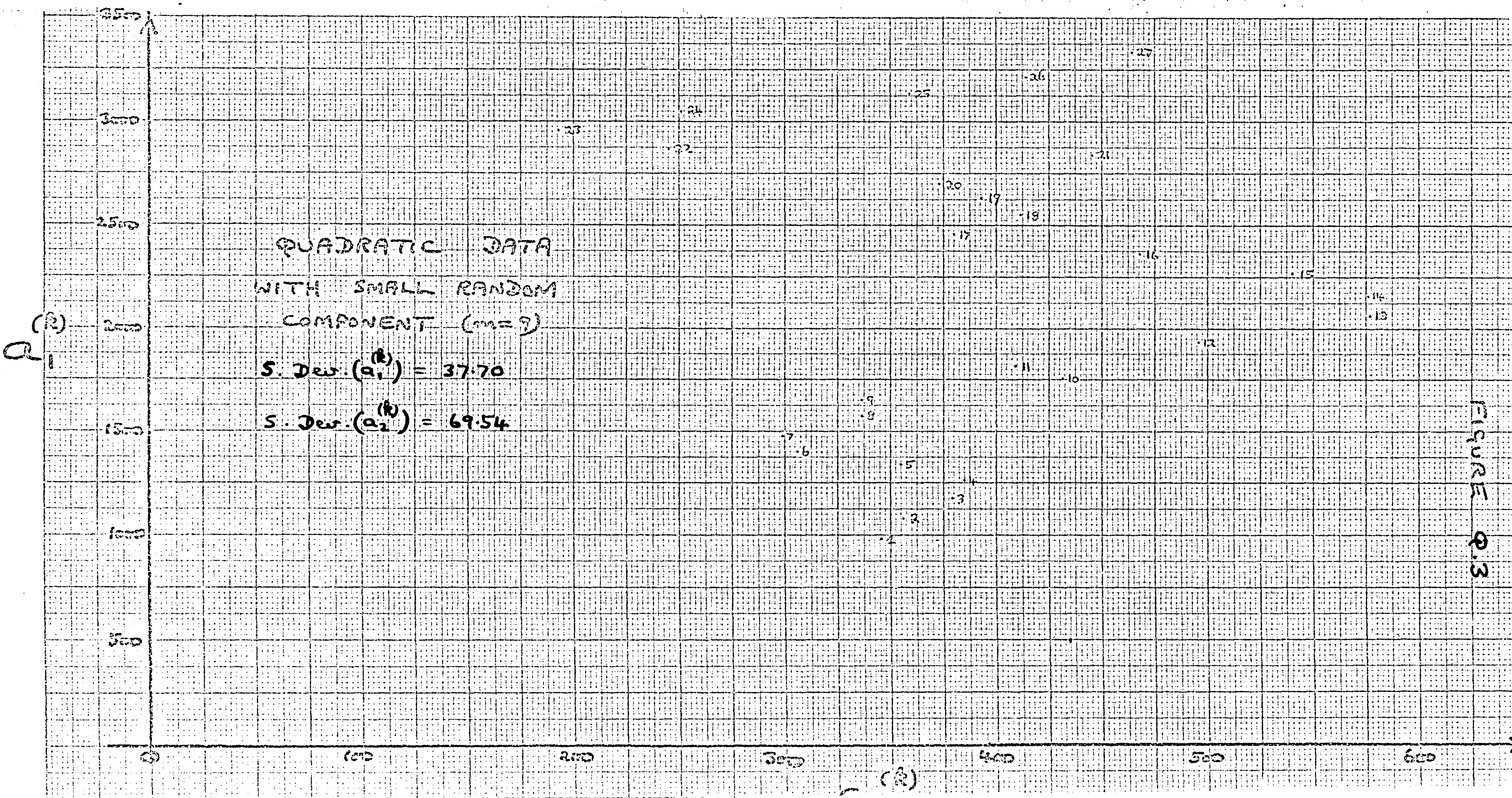

QUADRATIC DATA
WITH SMALL RANDOM
COMPONENT (m=9)
S. Dev. $(a_1^{(k)}) = 37.70$
S. Dev. $(a_2^{(k)}) = 69.54$
$a_1^{(k)}$
3500
3000
2500
2000
1500
1000
500
0
100
200
300
400
500
600
(k)

FIGURE Q.3

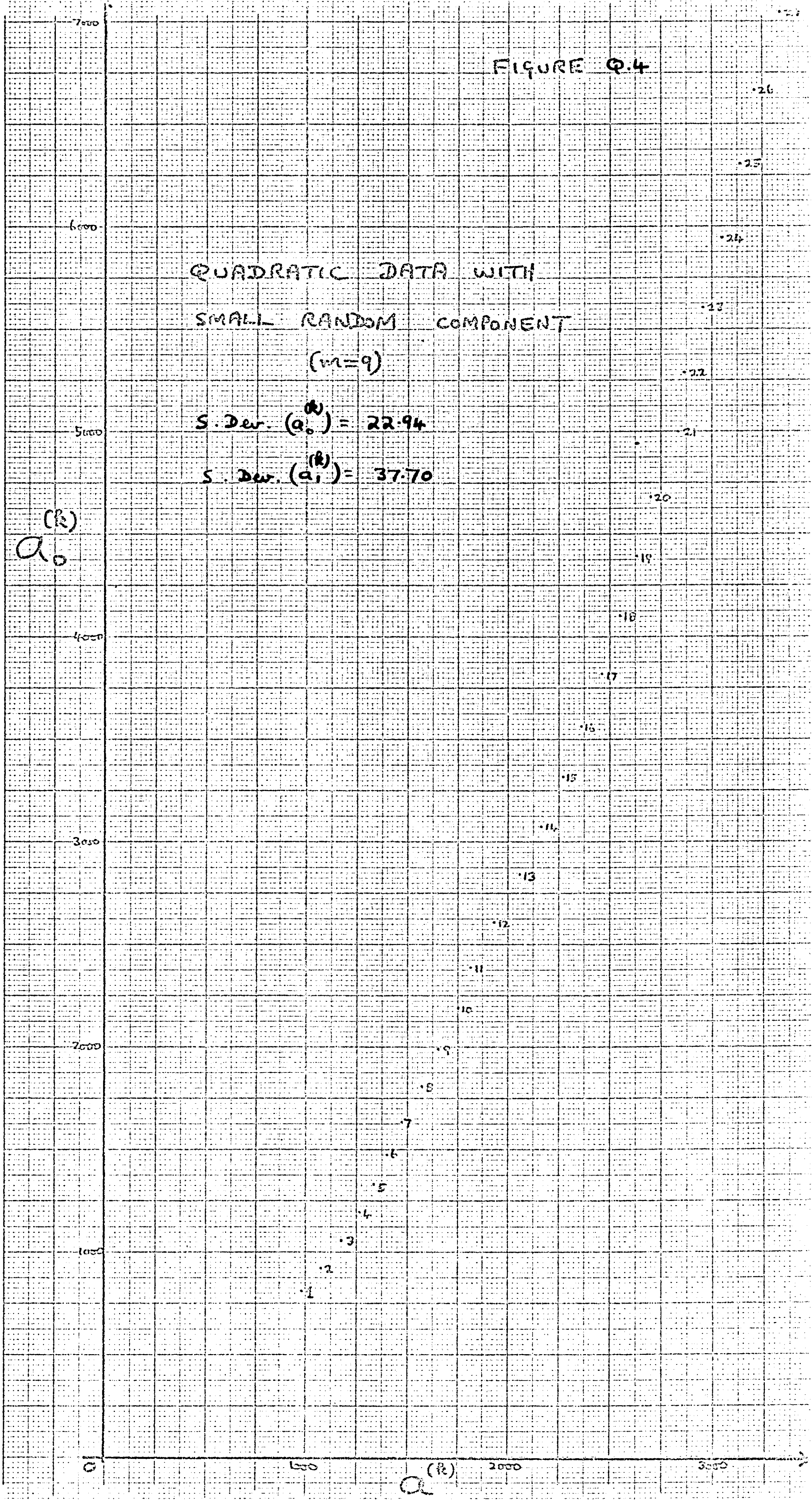


FIGURE 9.4
QUADRATIC DATA WITH
SMALL RANDOM COMPONENT
(m=9)
S. Dev. $(a_0^{(k)})$ = 22.94
S. Dev. $(a_1^{(k)})$ = 37.70
$a_0^{(k)}$
$a^{(k)}$
7000
6000
5000
4000
3000
2000
1000
0
1000
2000
3000

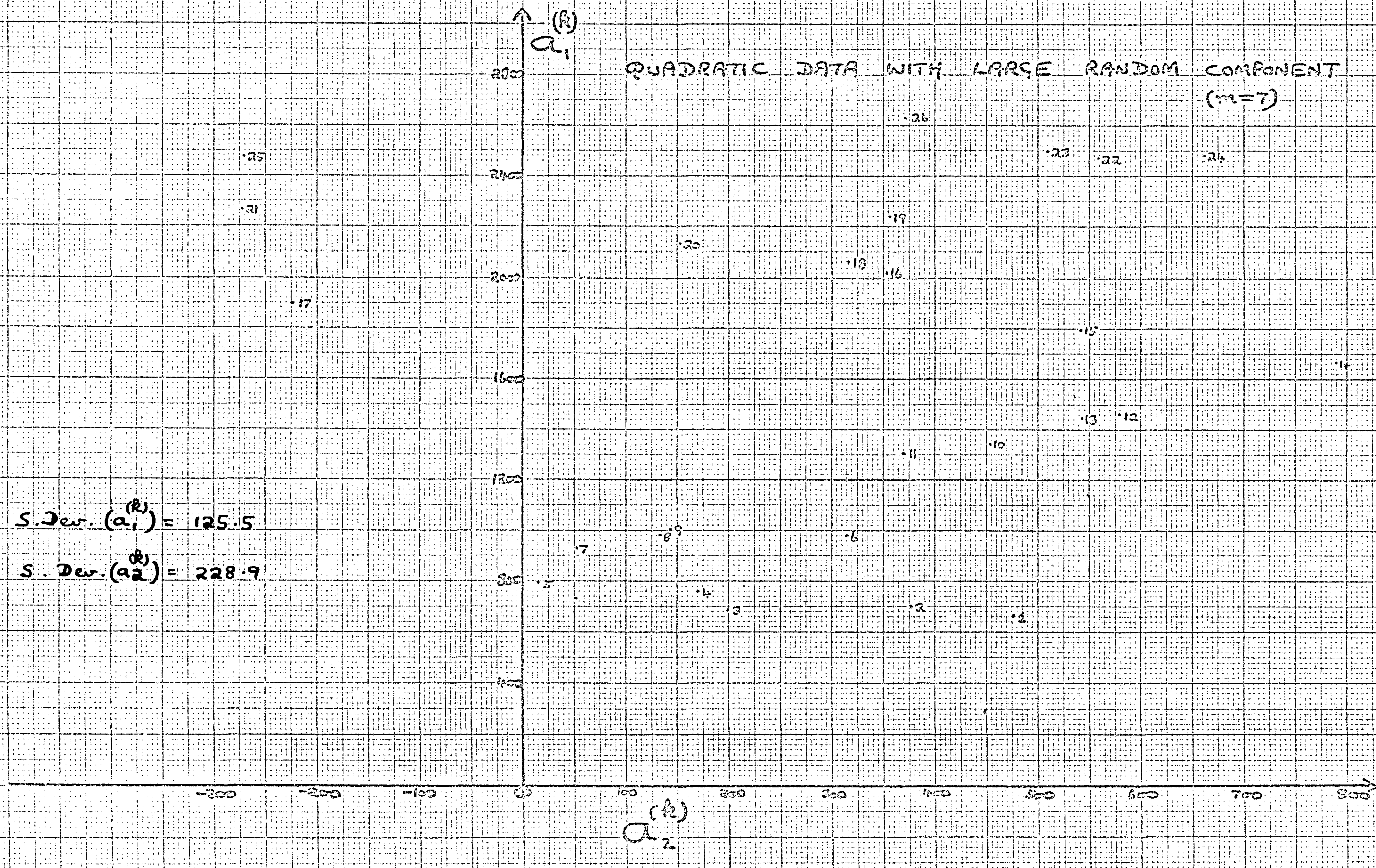

QUADRATIC DATA WITH LARGE RANDOM COMPONENT
(m=7)
$a_1^{(k)}$
$a_2^{(k)}$
S. Dev. $(a_1^{(k)}) = 125.5$
S. Dev. $(a_2^{(k)}) = 228.9$
2800
2400
2000
1600
1200
800
400
-300
-200
-100
0
100
200
300
400
500
600
700
800

FIGURE Q.5

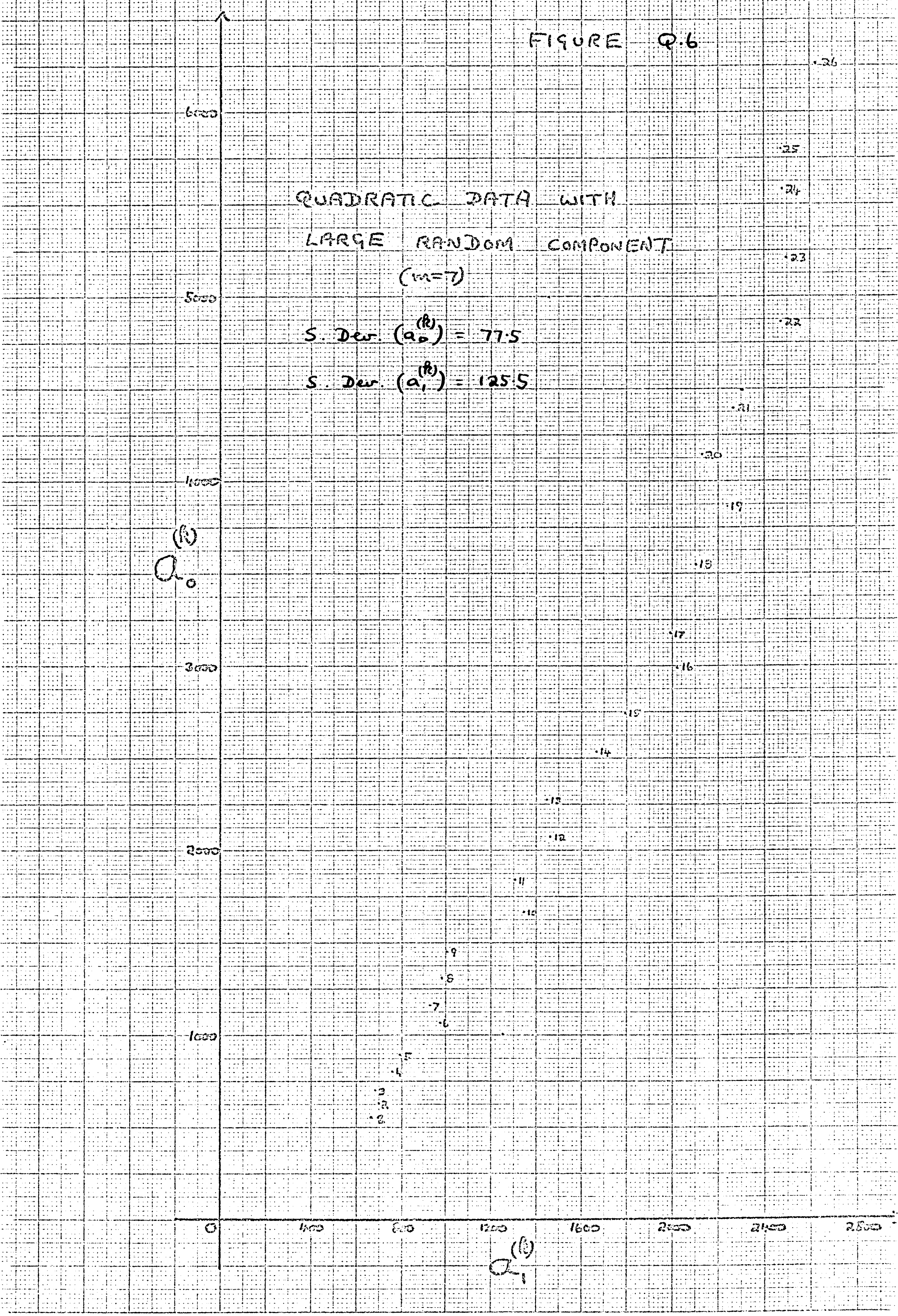
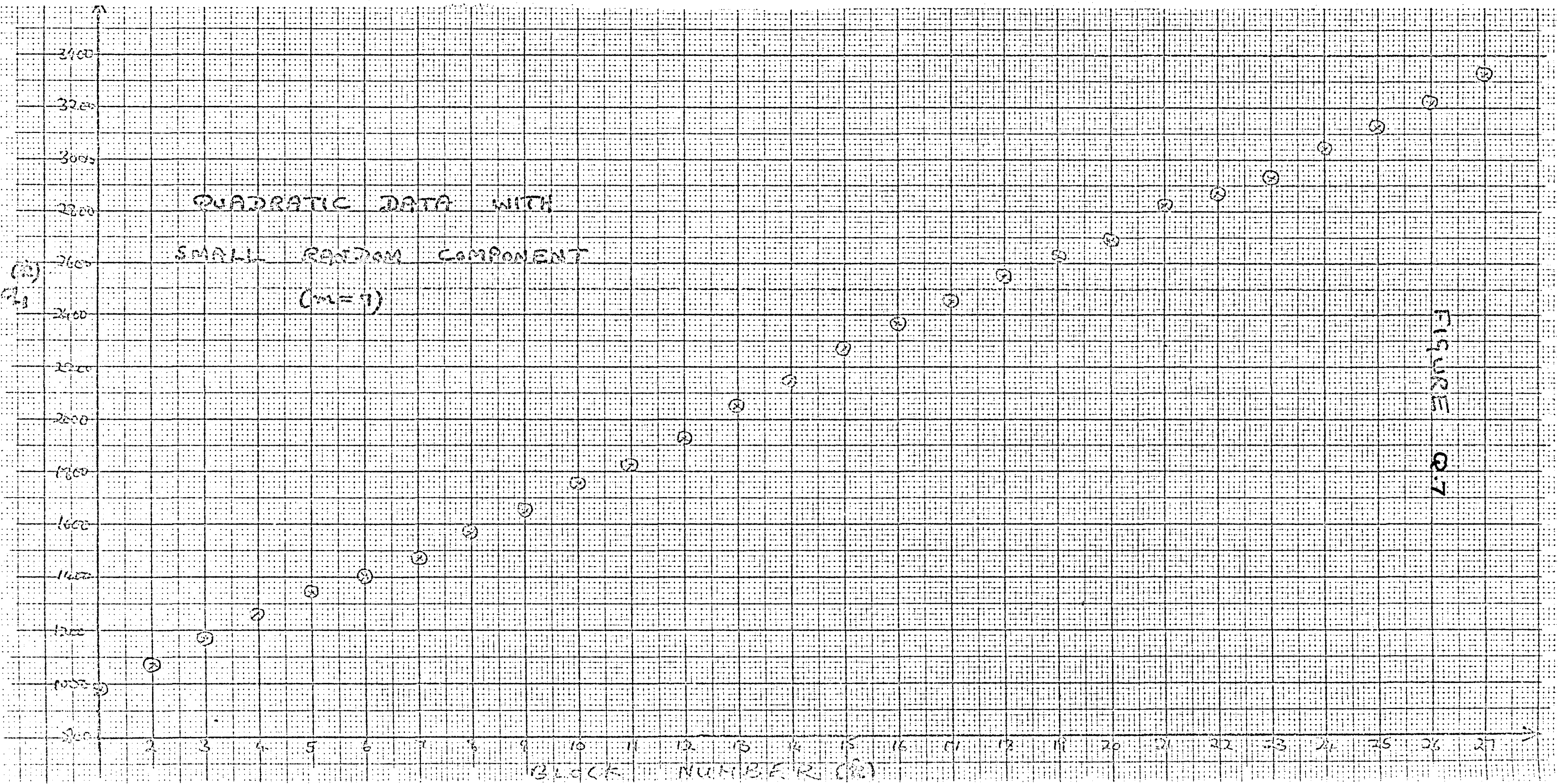


FIGURE Q.6
QUADRATIC DATA WITH
LARGE RANDOM COMPONENT
(m=7)
S. Dev. $(a_0^{(k)})$ = 77.5
S. Dev. $(a_1^{(k)})$ = 125.5
$a_0^{(k)}$
$a_1^{(k)}$
6000
5000
4000
3000
2000
1000
0
400
800
1200
1600
2000
2400
2800


QUADRATIC DATA WITH
SMALL RANDOM COMPONENT
(m=7)
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27
BLOCK NUMBER
FIGURE Q.7

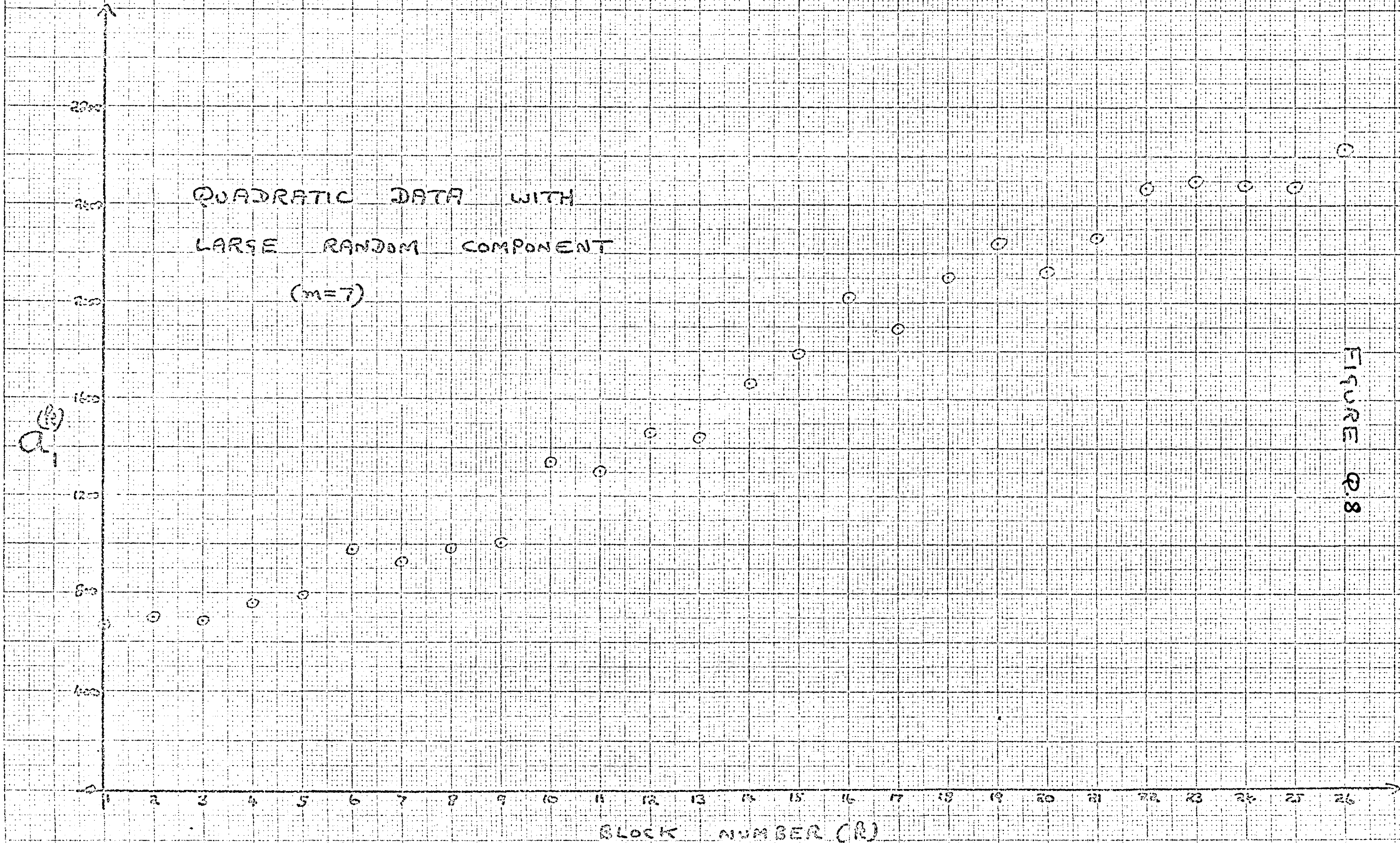

QUADRATIC DATA WITH
LARGE RANDOM COMPONENT
(m=7)
$a_1^{(k)}$
0
400
800
1200
1600
2000
2400
2800
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26
BLOCK NUMBER (k)

FIGURE Q.8

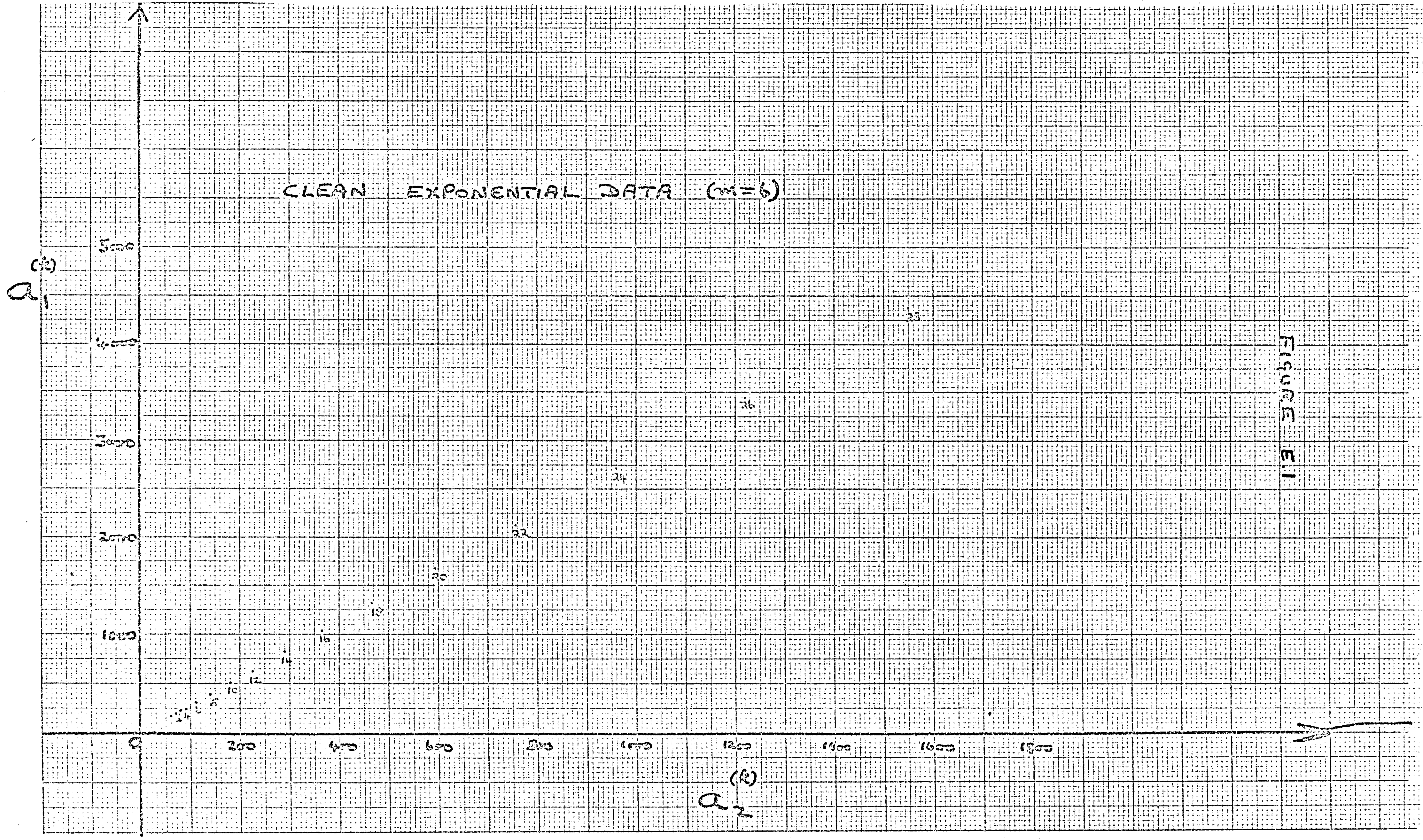

CLEAN EXPONENTIAL DATA (m=6)
$a_1^{(k)}$
5000
4000
3000
2000
1000
0
200
400
600
800
1000
1200
1400
1600
1800
$a_2^{(k)}$

FIGURE E.1

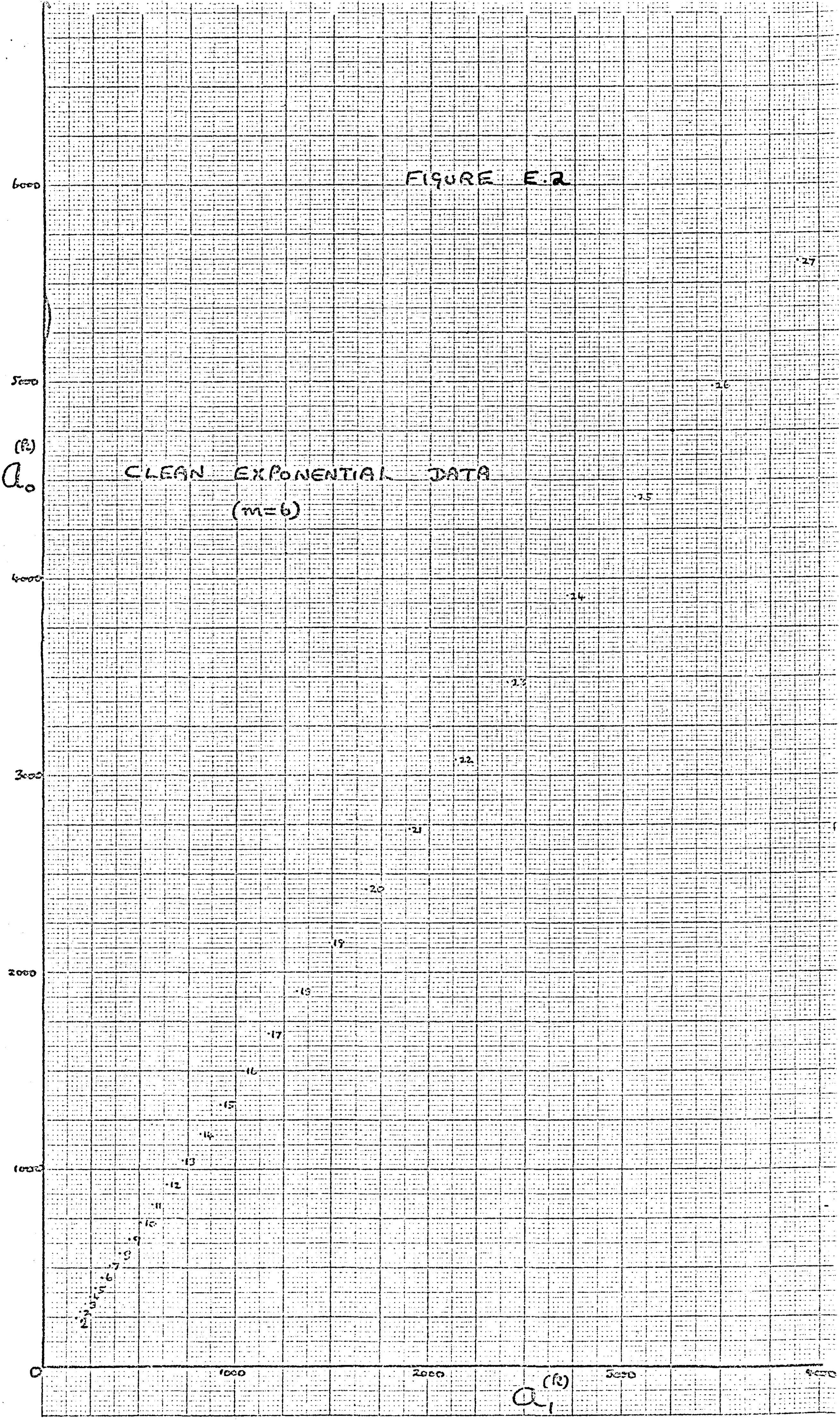


FIGURE E.2
CLEAN EXPONENTIAL DATA
(m=6)
$a_0^{(k)}$
$a_1^{(k)}$
0
1000
2000
3000
4000
5000
6000

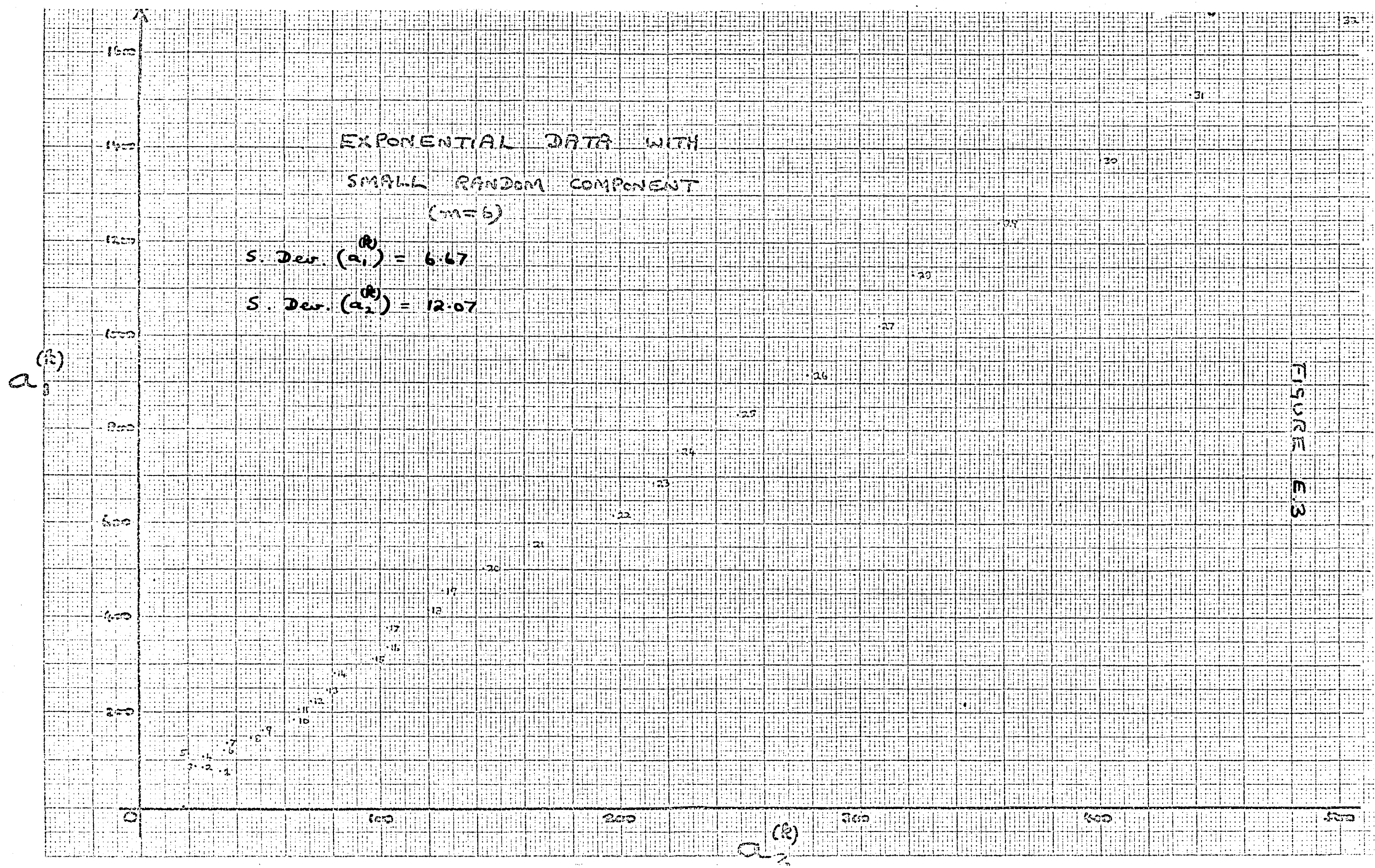

EXPONENTIAL DATA WITH
SMALL RANDOM COMPONENT
(m=6)
S. Dev. $(a_1^{(k)})$ = 6.67
S. Dev. $(a_2^{(k)})$ = 12.07
$a_3^{(k)}$
$a_2^{(k)}$
0
100
200
300
400
500
200
400
600
800
1000
1200
1400
1600

FIGURE E.3

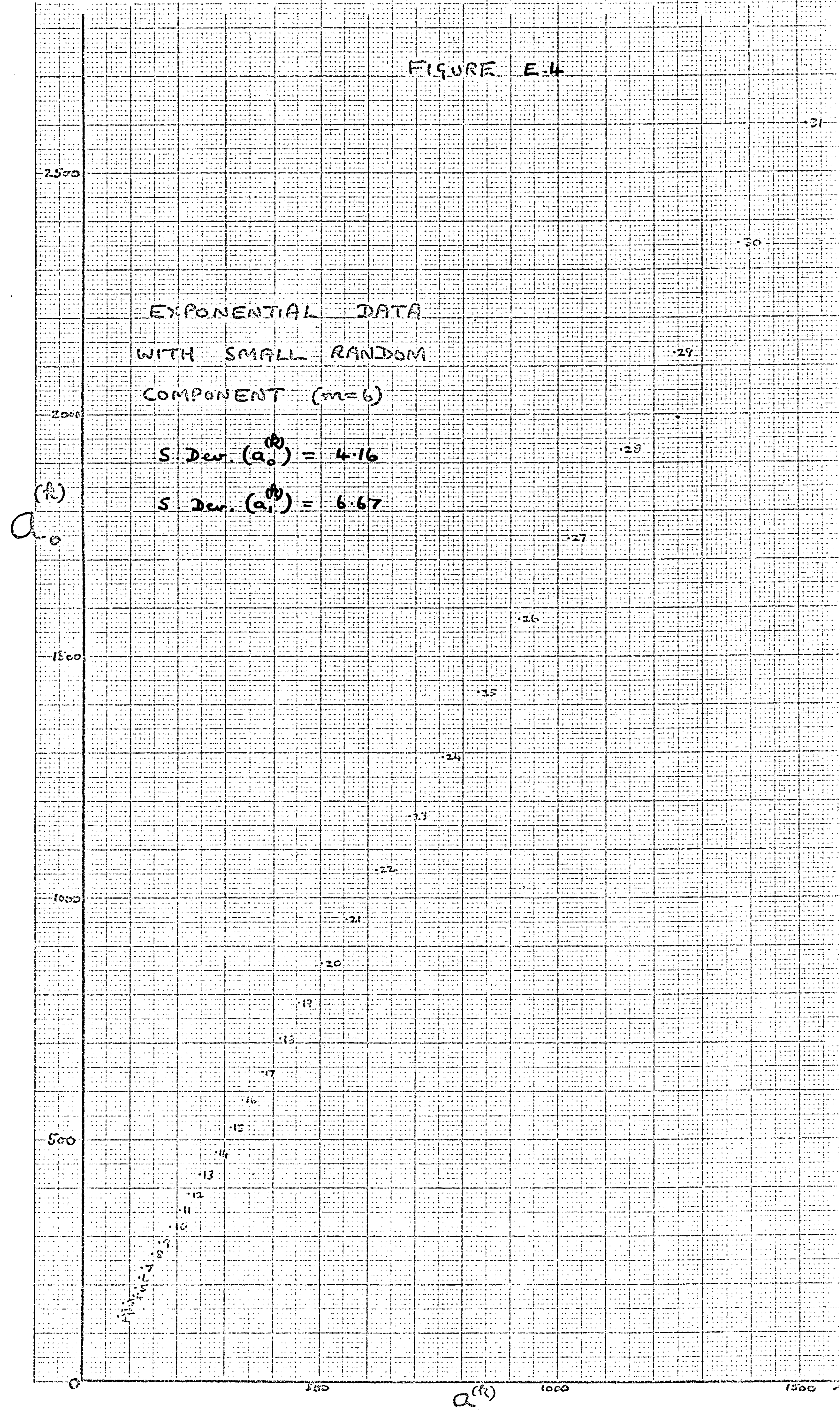


FIGURE E.4
EXPONENTIAL DATA
WITH SMALL RANDOM
COMPONENT (m=6)
S. Dev. $(a_0^{(k)})$ = 4.16
S. Dev. $(a_1^{(k)})$ = 6.67
$a_0^{(k)}$
$a^{(k)}$
2500
2000
1500
1000
500
0
500
1000
1500

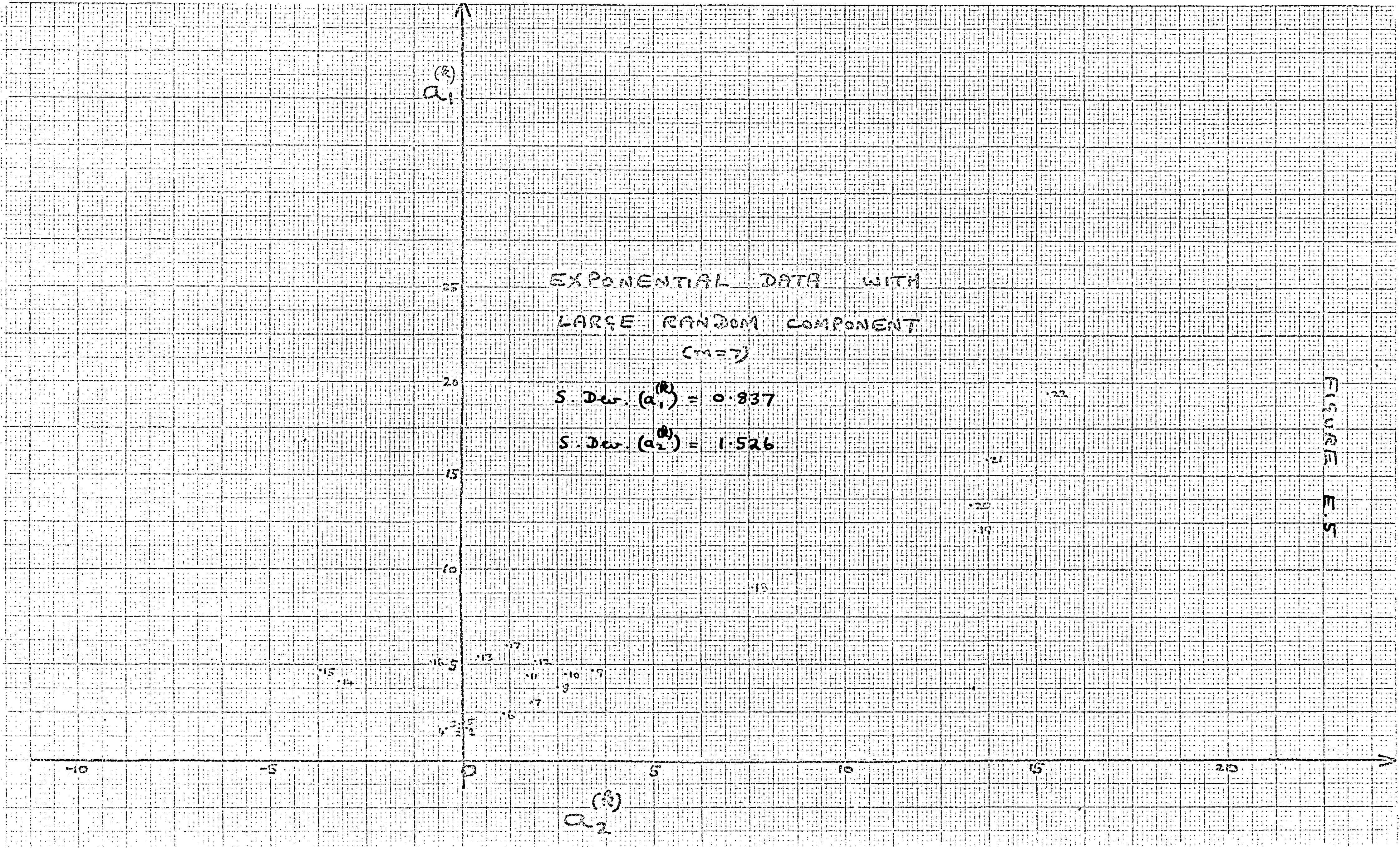

EXPONENTIAL DATA WITH
LARGE RANDOM COMPONENT
(m=7)
S. Dev. $(a_1^{(R)})$ = 0·837
S. Dev. $(a_2^{(R)})$ = 1·526
$a_1^{(R)}$
$a_2^{(R)}$

FIGURE E.5

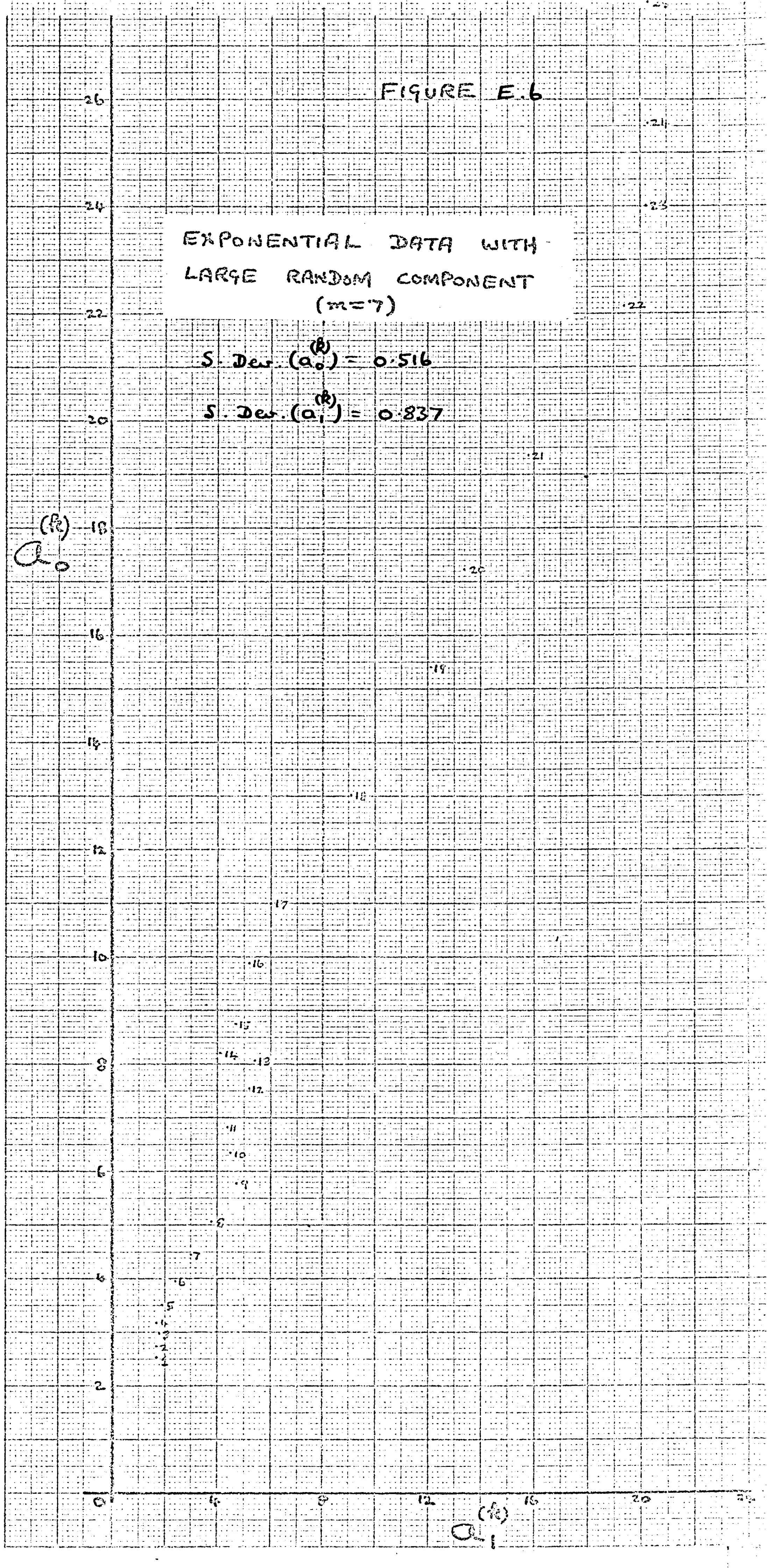


FIGURE E.6
EXPONENTIAL DATA WITH
LARGE RANDOM COMPONENT
(m=7)
S. Dev. $(a_0^{(k)})$ = 0.516
S. Dev. $(a_1^{(k)})$ = 0.837
$a_0^{(k)}$
$a_1^{(k)}$
0
2
4
6
8
10
12
14
16
18
20
22
24
26

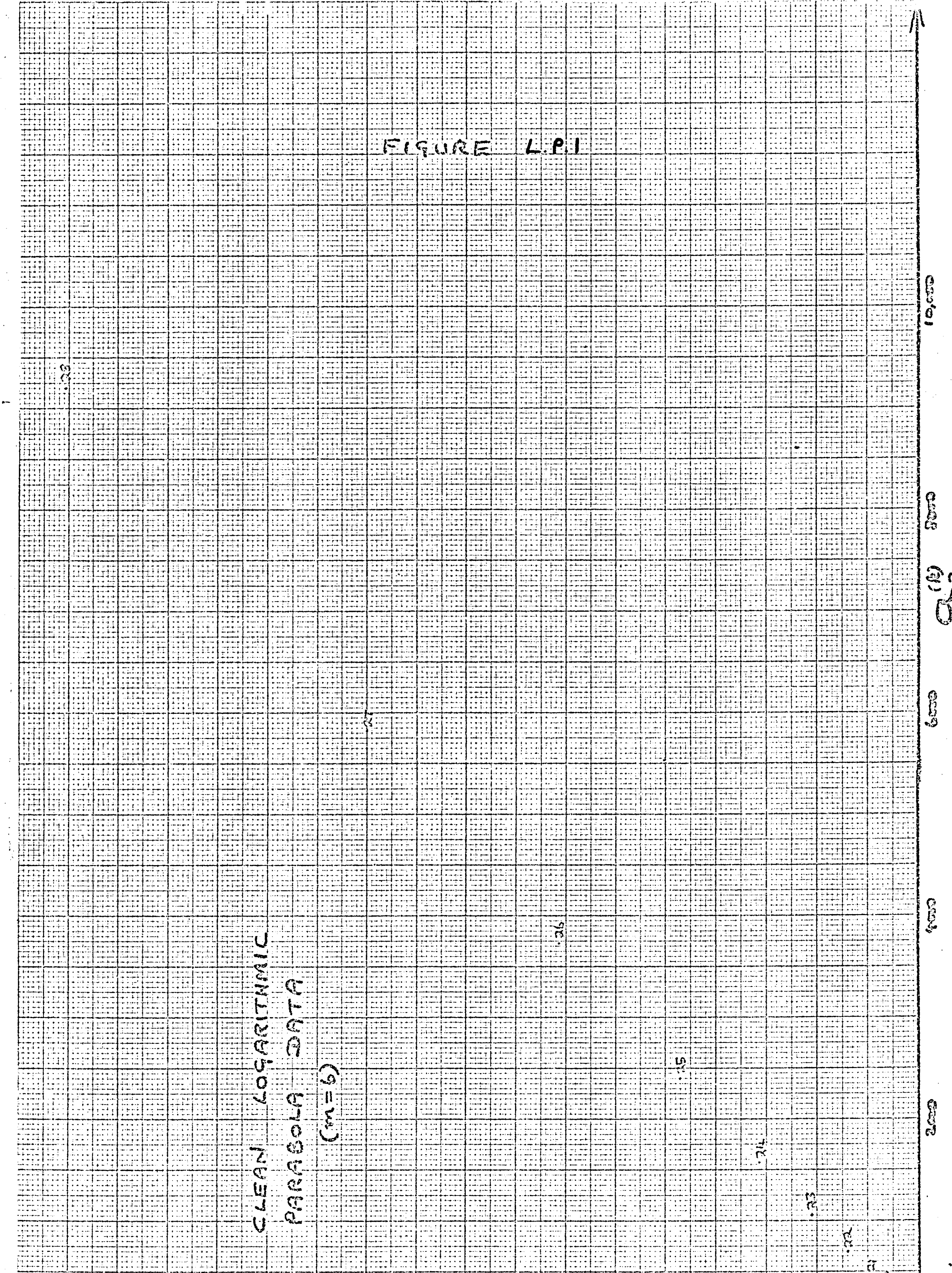
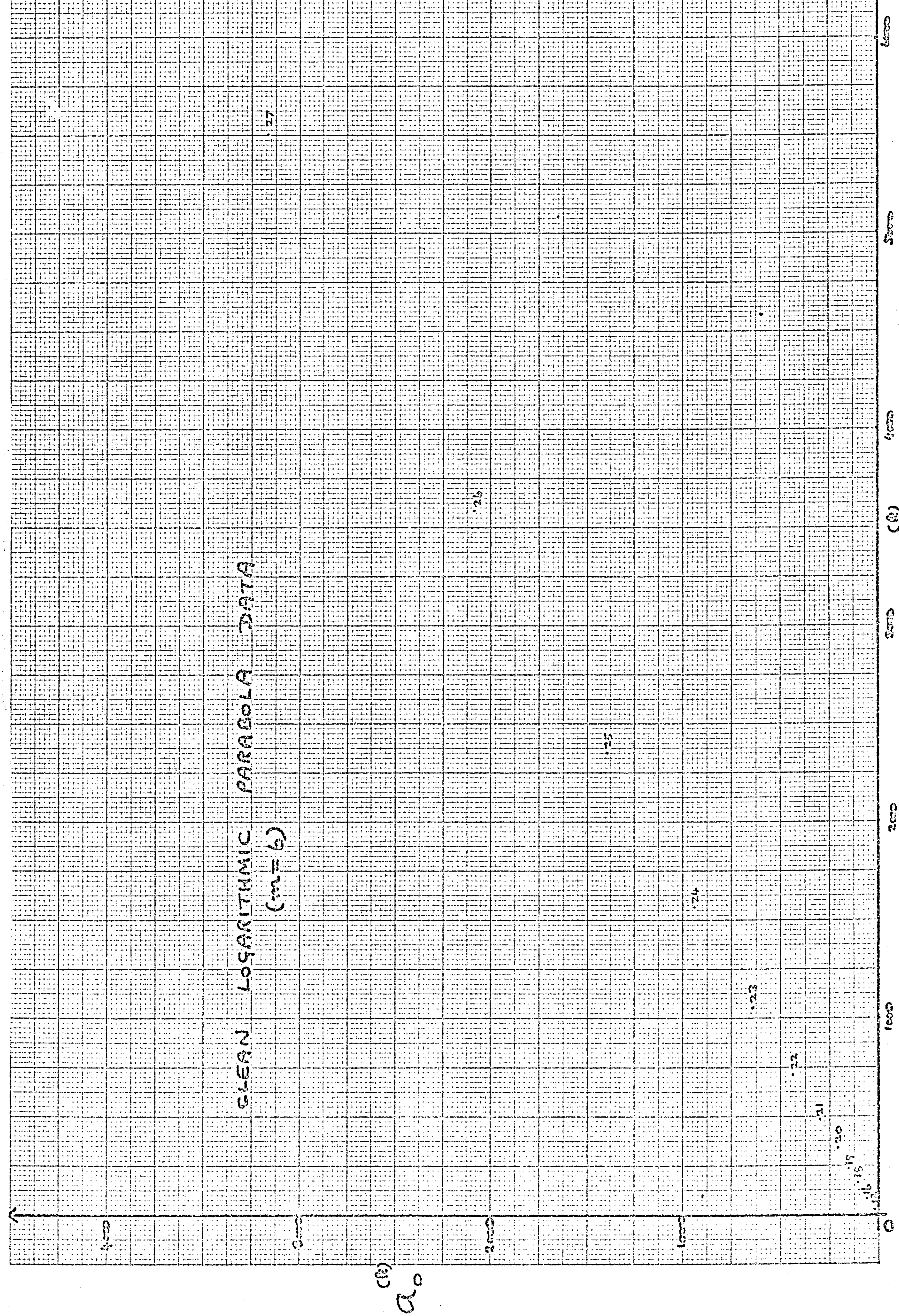
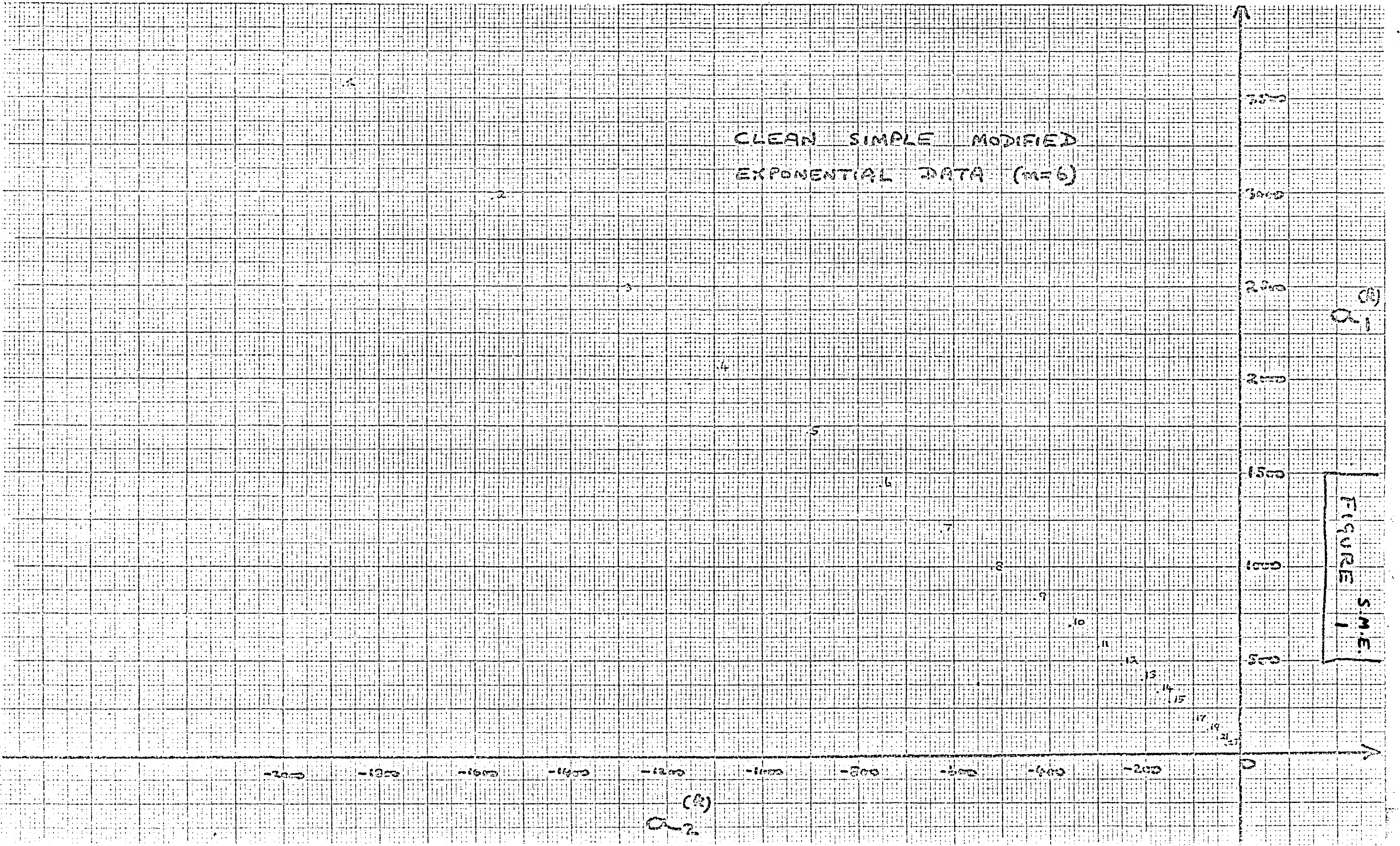


FIGURE LP.1
CLEAN LOGARITHMIC
PARABOLA DATA
(m=6)
10,000
8000
6000
4000
2000
0

FIGURE L.P.2


CLEAN LOGARITHMIC PARABOLA DATA
(m=6)
$a_1^{(l)}$
$a_0^{(l)}$
0
1000
2000
3000
4000
5000
6000
.15
.16
.19
.20
.21
.22
.23
.24
.25
.26
.27

<u>SIMPLE MODIFIED EXPONENTIAL GRAPH BOOK</u>


CLEAN SIMPLE MODIFIED
EXPONENTIAL DATA (m=6)
FIGURE S.M.E. 1
(R)
σ1
3500
3000
2500
2000
1500
1000
500
0
-2000
-1800
-1600
-1400
-1200
-1000
-800
-600
-400
-200
(R)
σ2

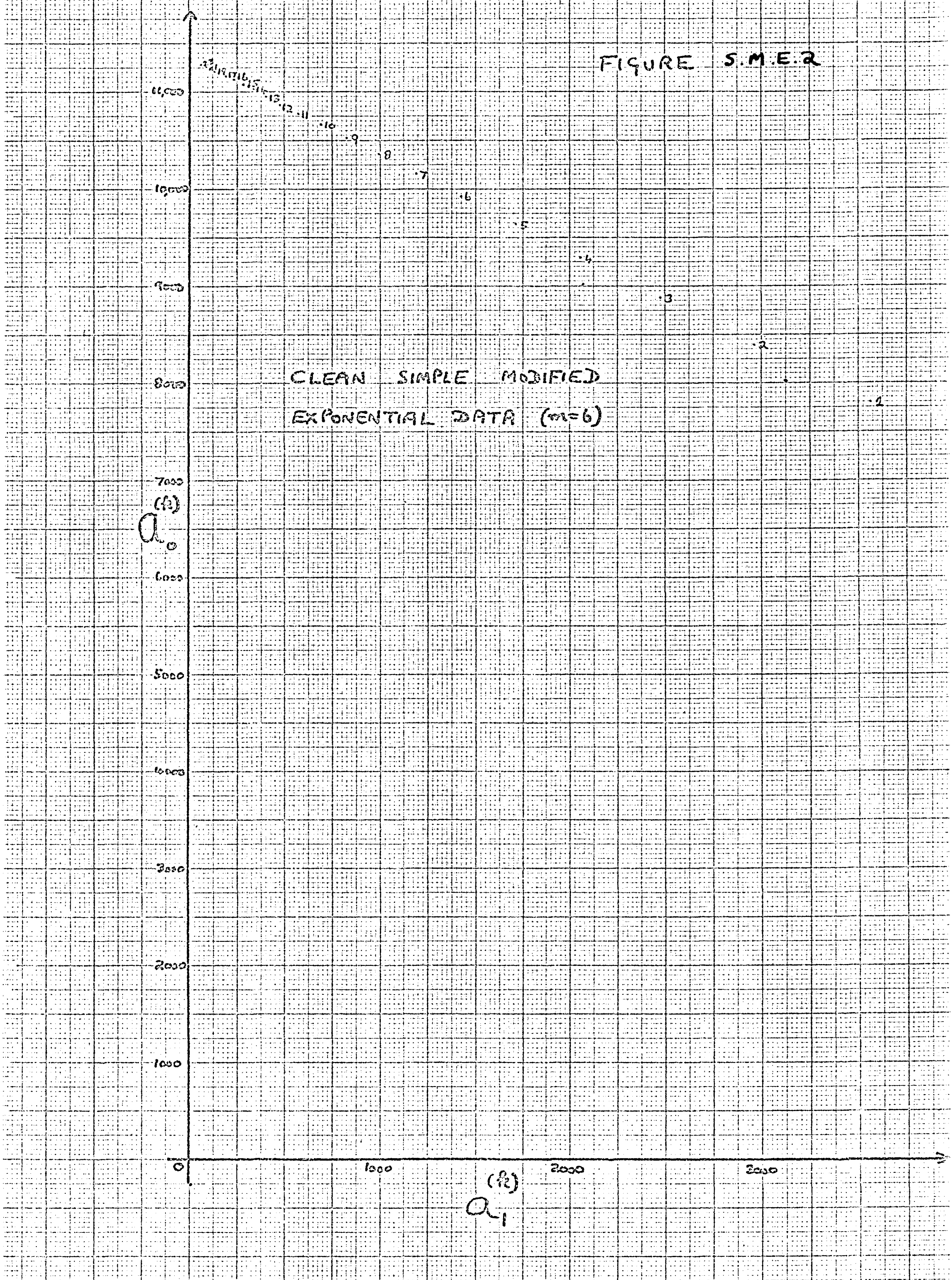


FIGURE S.M.E.2
CLEAN SIMPLE MODIFIED
EXPONENTIAL DATA (m=6)
11,000
10,000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
1000
2000
3000
(ft)
a_0
a_1

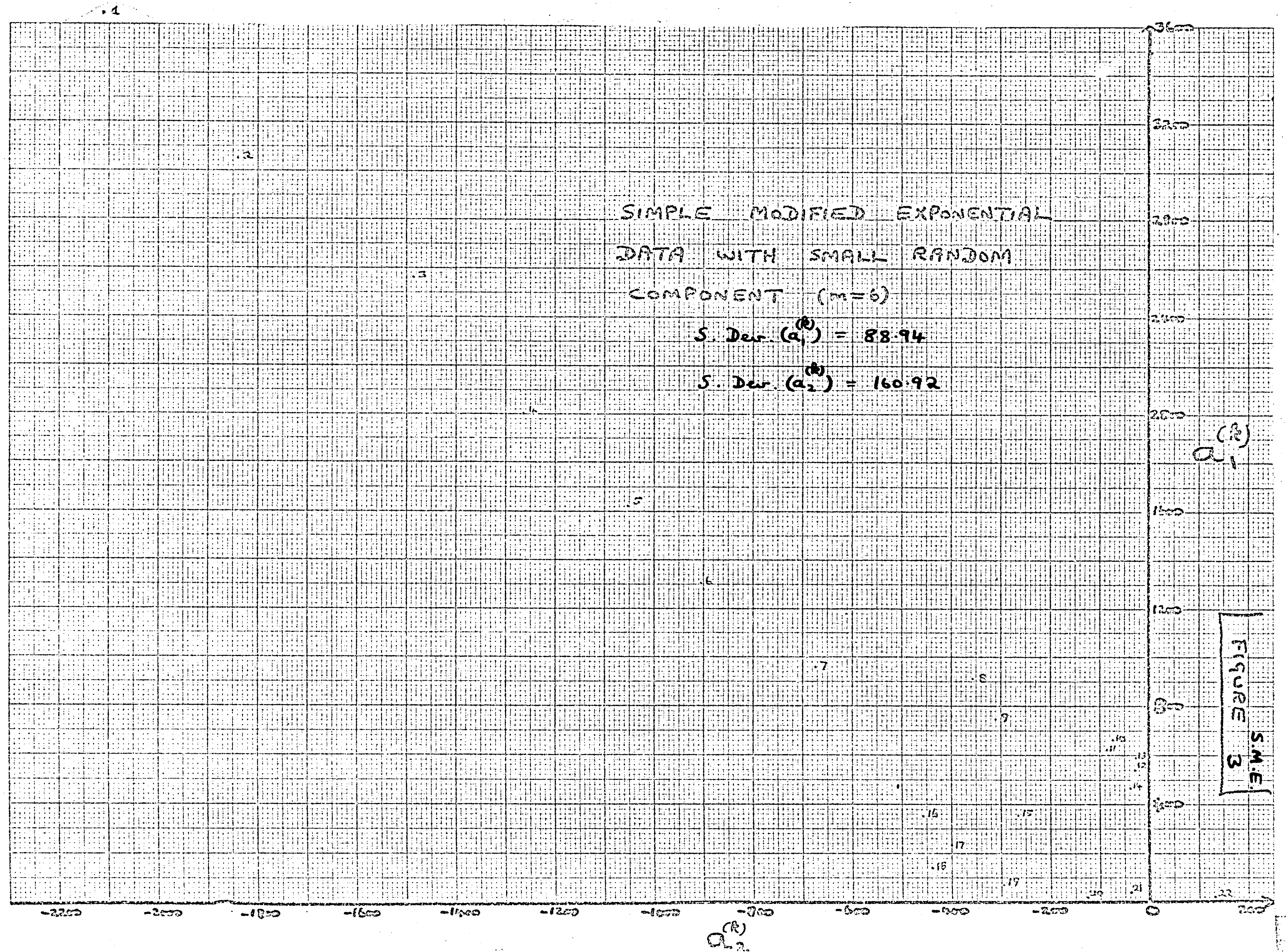
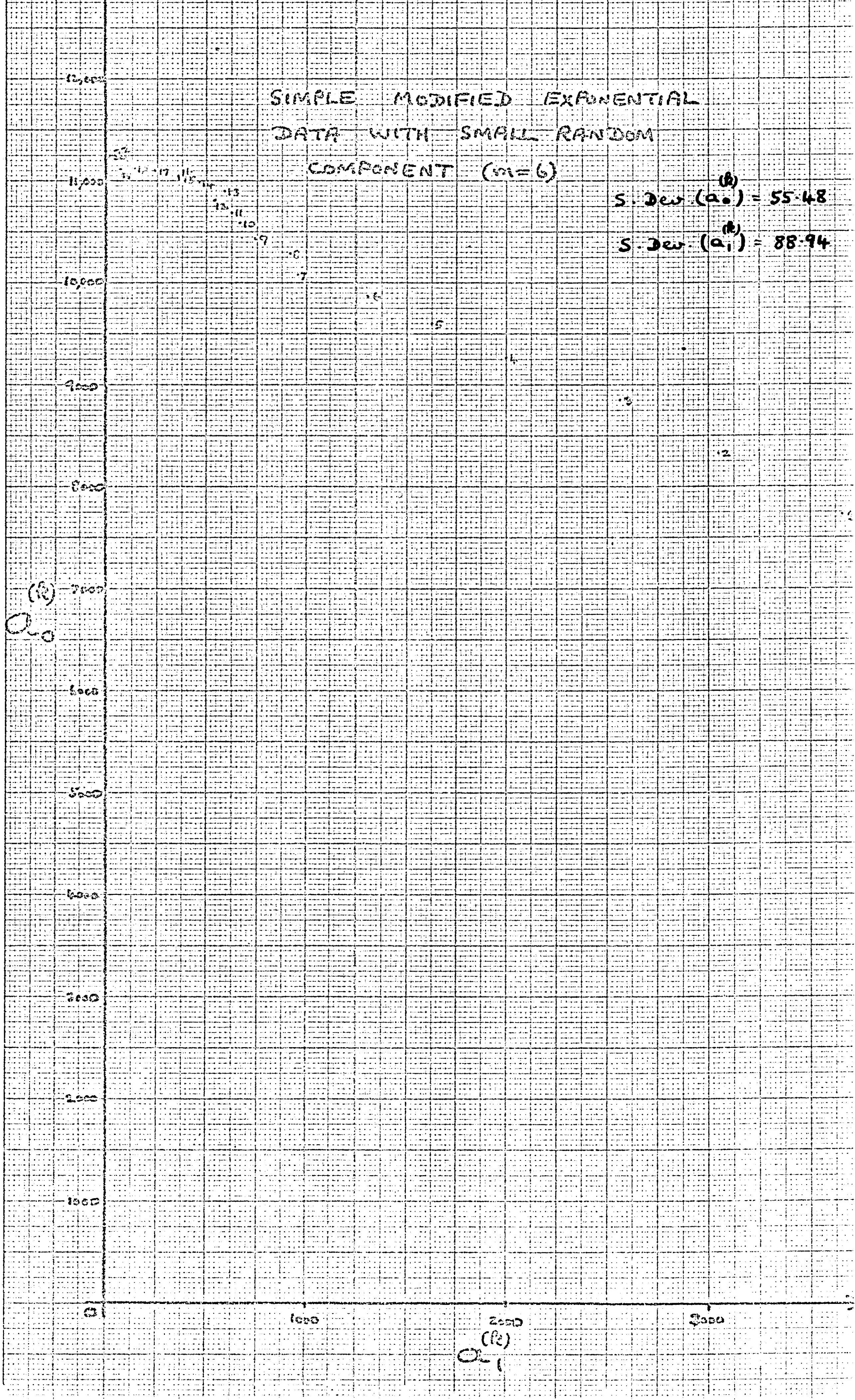

SIMPLE MODIFIED EXPONENTIAL
DATA WITH SMALL RANDOM
COMPONENT (m=6)
S. Dev. ($a_1^{(k)}$) = 88·94
S. Dev. ($a_2^{(k)}$) = 160·92
FIGURE 3
S.M.E.
$a_1^{(k)}$
$a_2^{(k)}$
3600
3200
2800
2400
2000
1600
1200
800
400
0
-2200
-2000
-1800
-1600
-1400
-1200
-1000
-800
-600
-400
-200
200

FIGURE S.M.E. 4



SIMPLE MODIFIED EXPONENTIAL DATA WITH SMALL RANDOM COMPONENT (m=6)
S. Dev. $(a_0^{(k)}) = 55.48$
S. Dev. $(a_1^{(k)}) = 88.94$
12,000
11,000
10,000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
1000
2000
3000
$a_0^{(k)}$
$a_1^{(k)}$

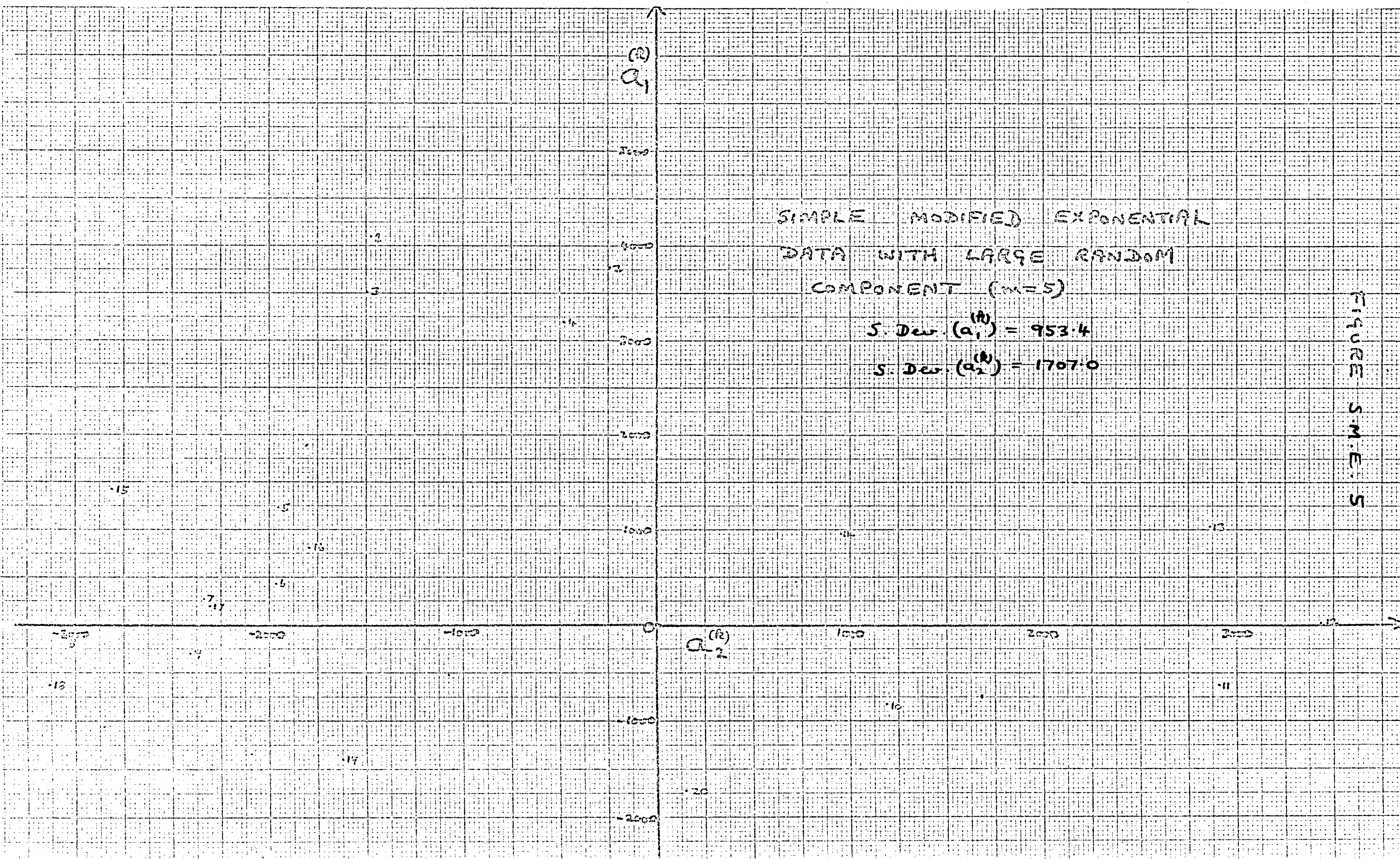

SIMPLE MODIFIED EXPONENTIAL
DATA WITH LARGE RANDOM
COMPONENT (m=5)
$S.\ Dev.\ (a_1^{(R)}) = 953.4$
$S.\ Dev.\ (a_2^{(R)}) = 1707.0$
$a_1^{(R)}$
$a_2^{(R)}$
0
1000
2000
3000
-1000
-2000
-3000

FIGURE S.M.E. 5

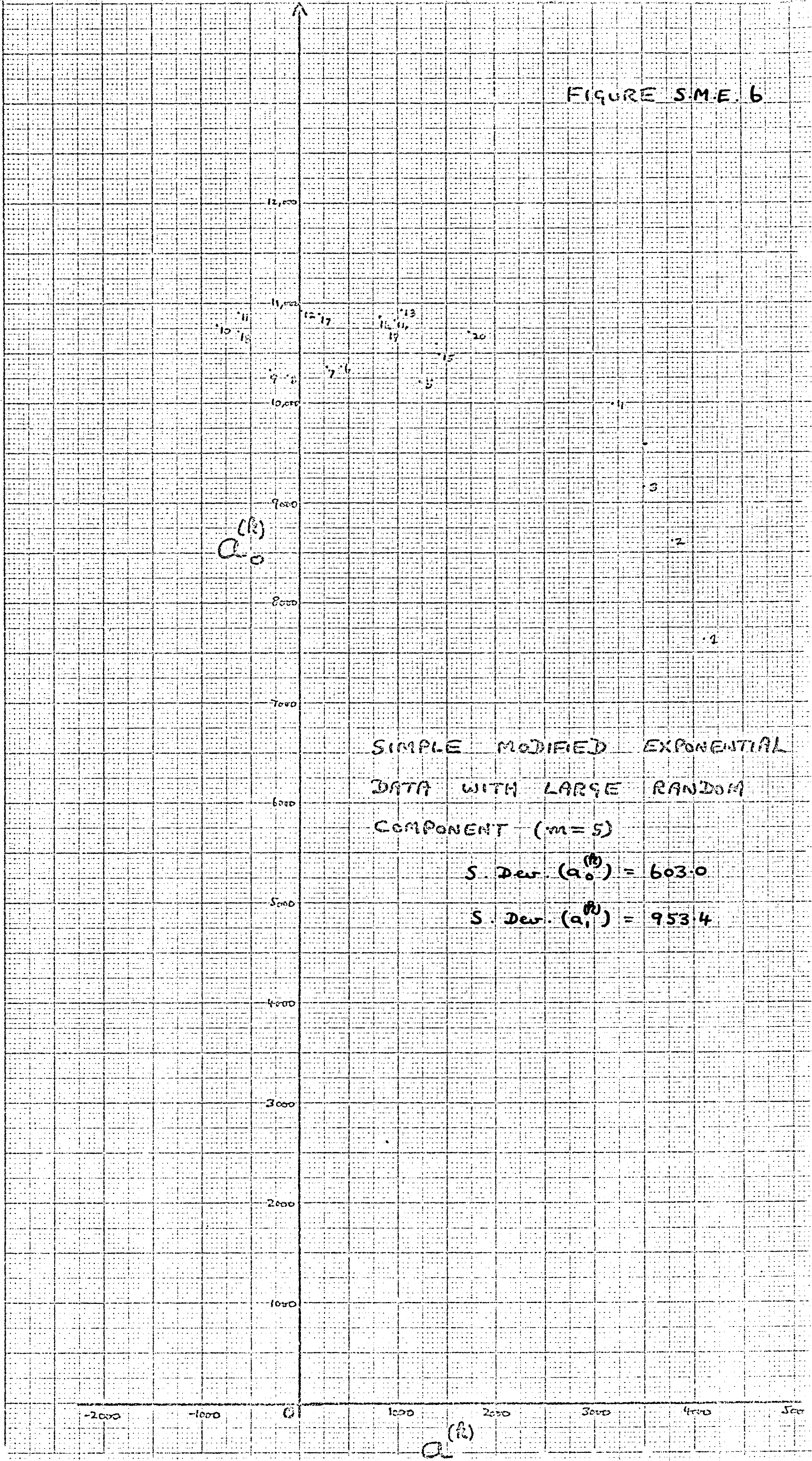
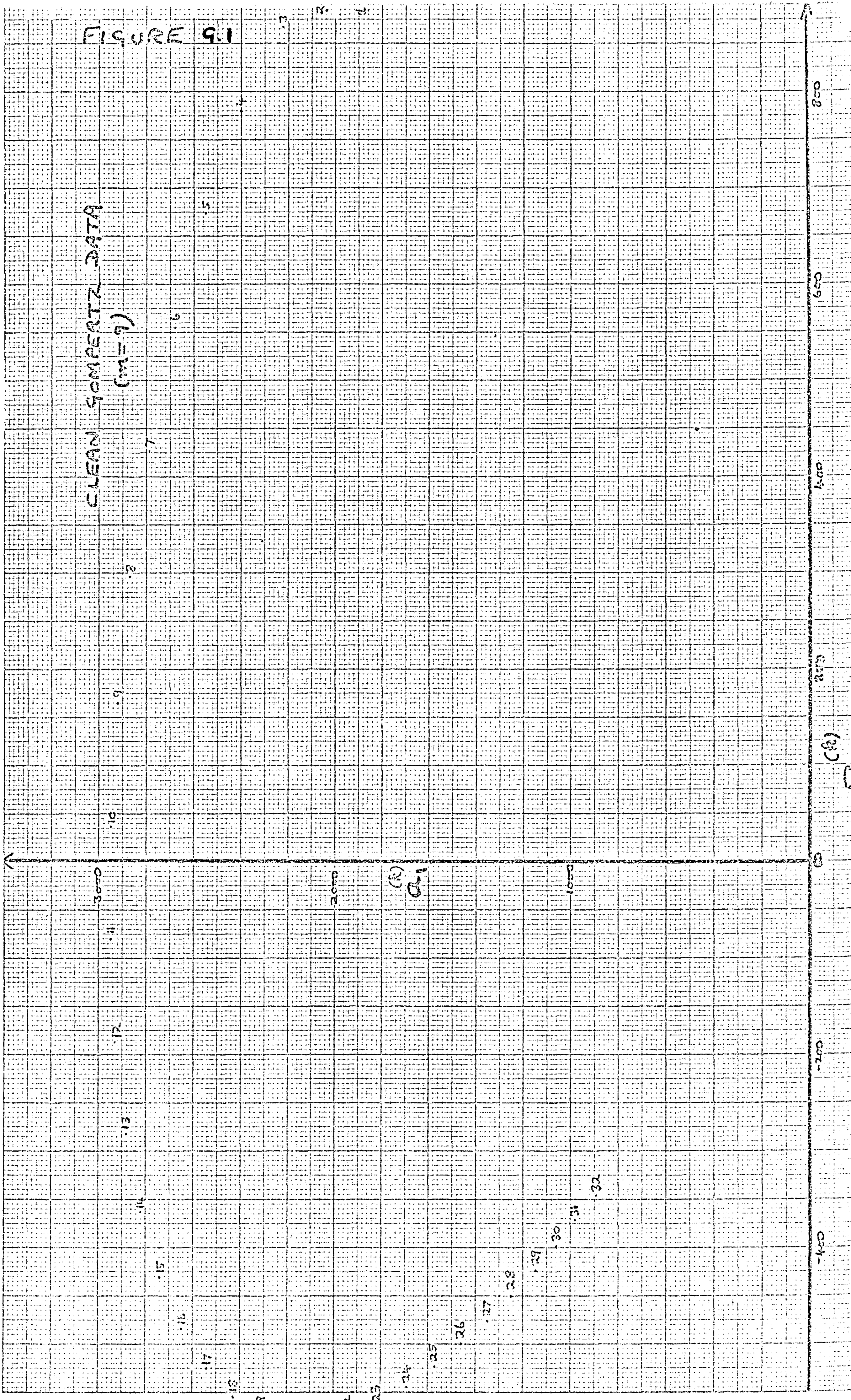


FIGURE S.M.E. 6
SIMPLE MODIFIED EXPONENTIAL DATA WITH LARGE RANDOM COMPONENT (m = 5)
S. Dev. $(a_0^{(k)})$ = 603.0
S. Dev. $(a_1^{(k)})$ = 953.4
$a_0^{(k)}$
$a_1^{(k)}$
12,000
11,000
10,000
9000
8000
7000
6000
5000
4000
3000
2000
1000
-2000
-1000
0
1000
2000
3000
4000
5000

FIGURE 9.1


CLEAN GOMPERTZ DATA
(m=9)
3000
2000
1000
0
(R)
a_1
800
600
400
200
-200
-400
(θ)
b_2

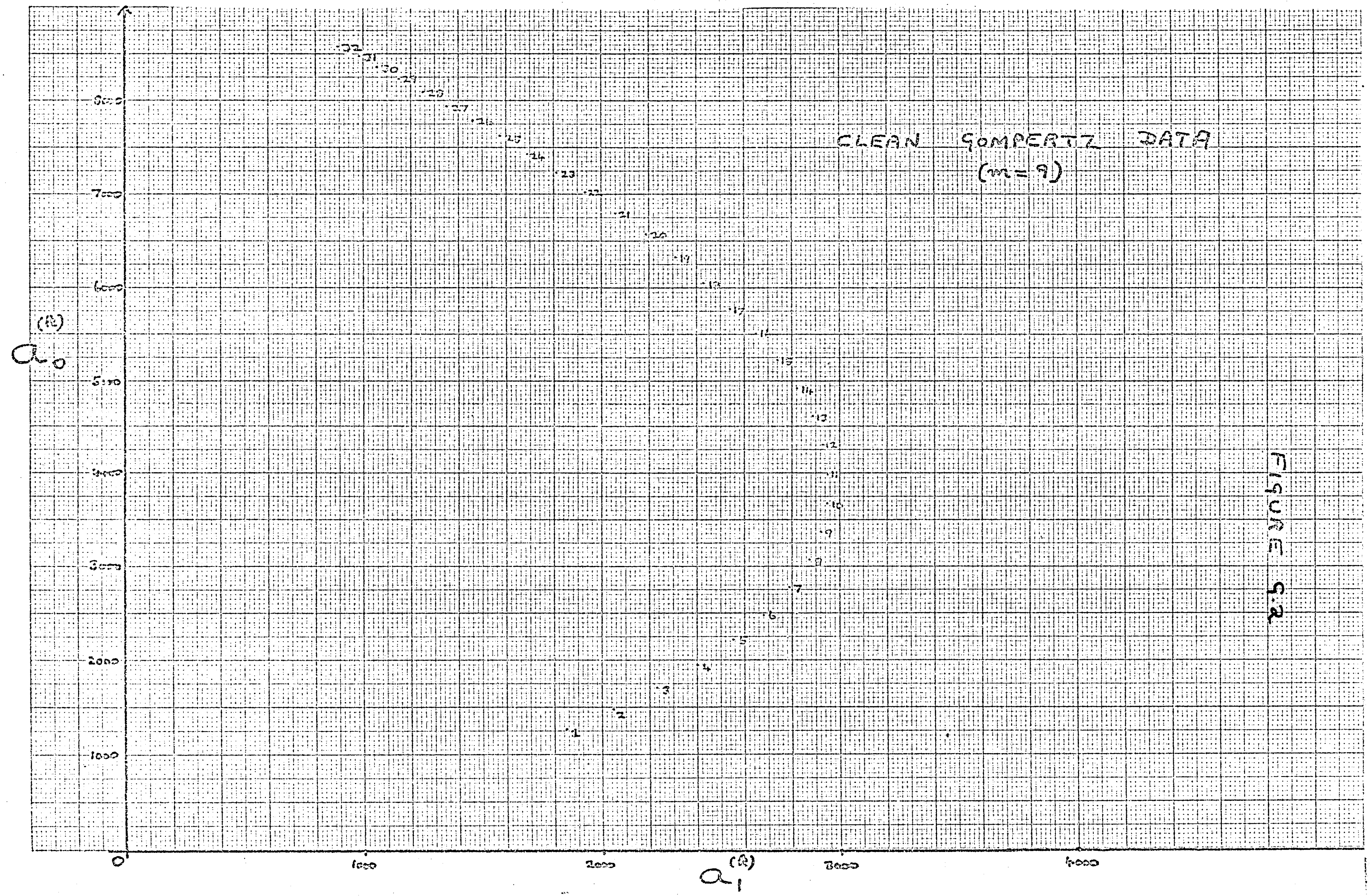

CLEAN GOMPERTZ DATA
(m=9)
(R)
a0
(R)
a1
0
1000
2000
3000
4000
5000
6000
7000
8000

FIGURE 9.2

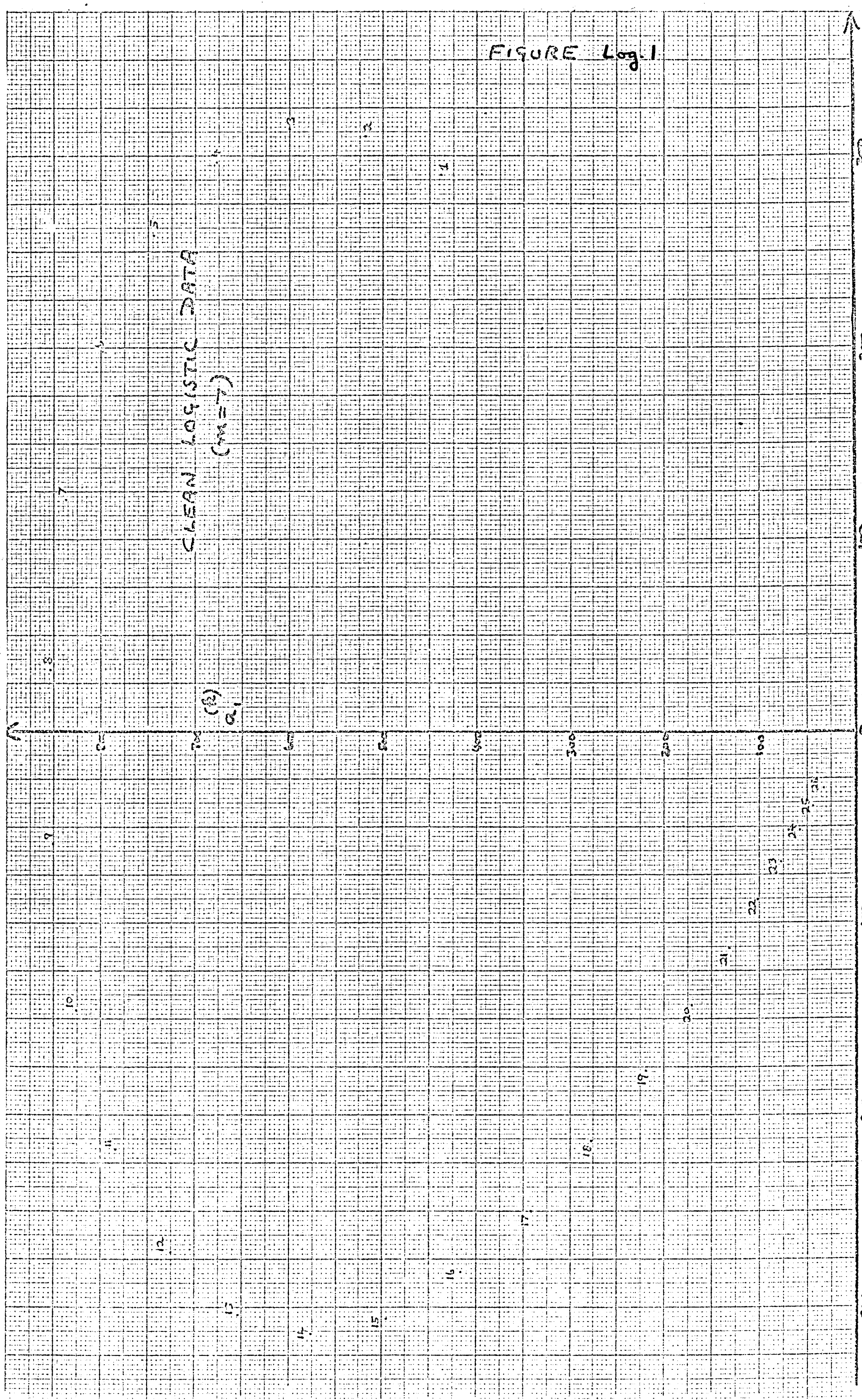


FIGURE Log.1

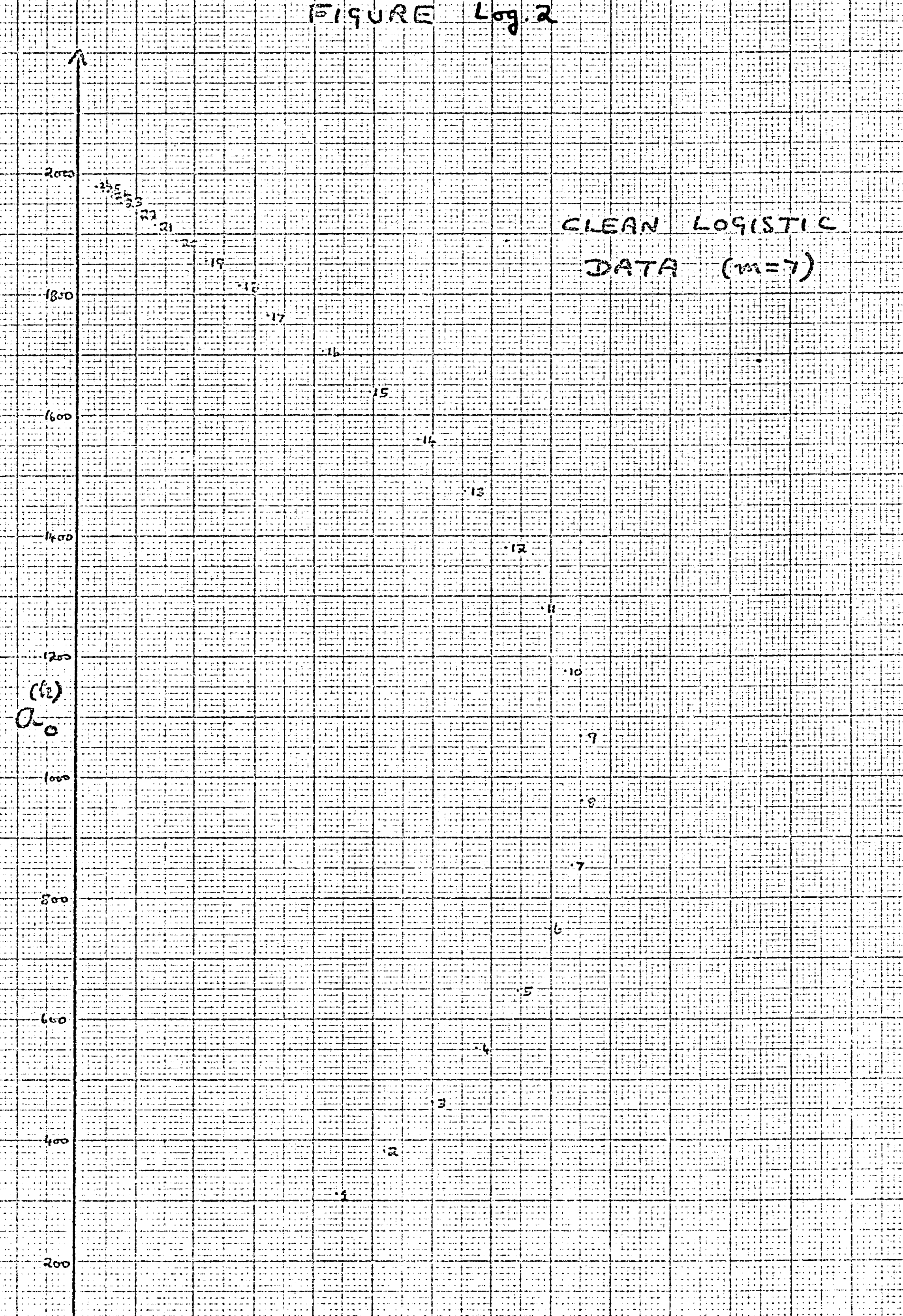


FIGURE Log.2
CLEAN LOGISTIC DATA (m=7)
a_0 (k)
a_1 (k)
2000
1800
1600
1400
1200
1000
800
600
400
200
0
200
400
600
800
1000

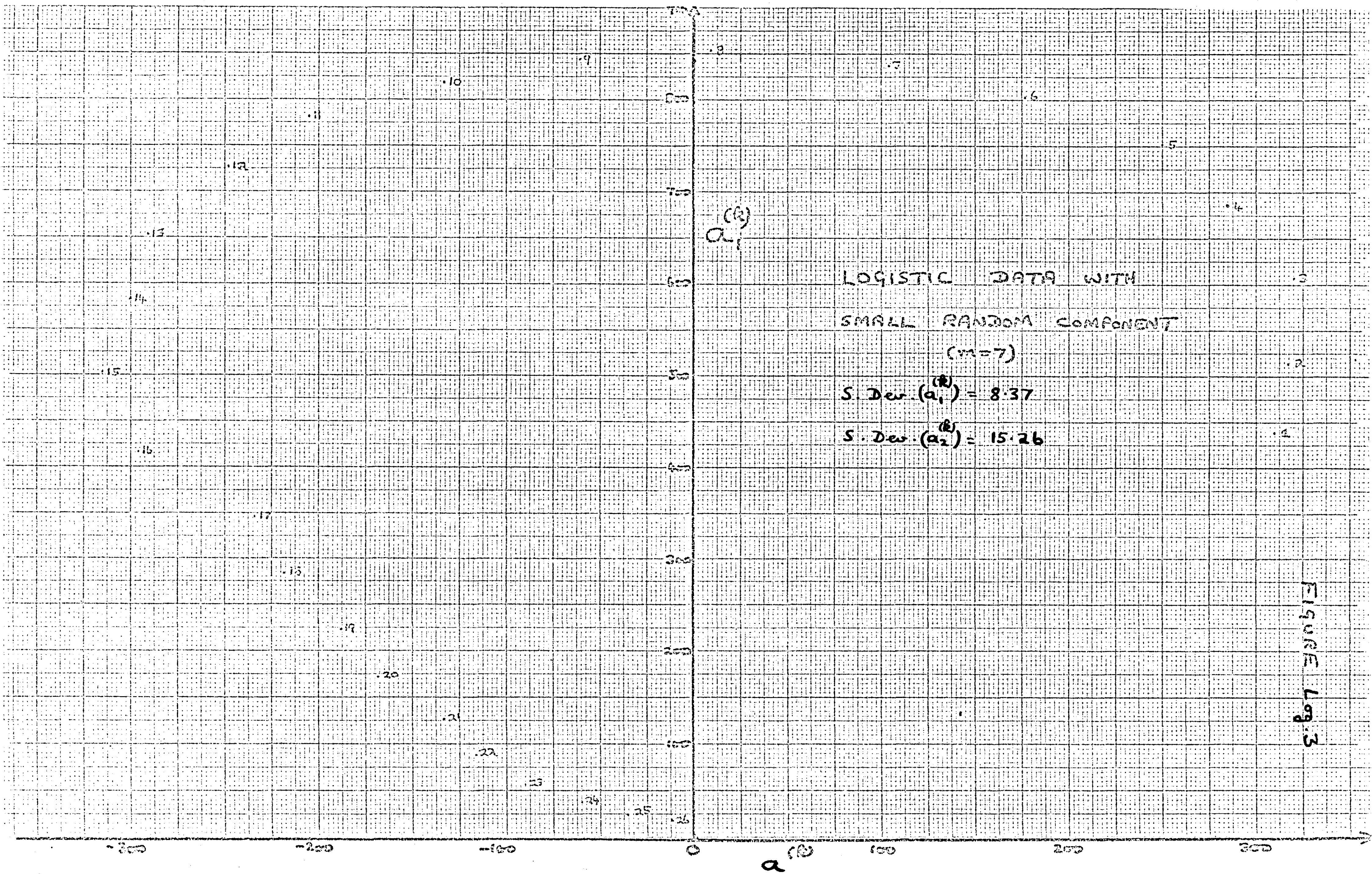

LOGISTIC DATA WITH
SMALL RANDOM COMPONENT
(m=7)
S. Dev. $(a_1^{(k)})$ = 8.37
S. Dev. $(a_2^{(k)})$ = 15.26
$a_1^{(k)}$
$a^{(k)}$
-300
-200
-100
0
100
200
300
400
500
600
700
800

FIGURE Log.3

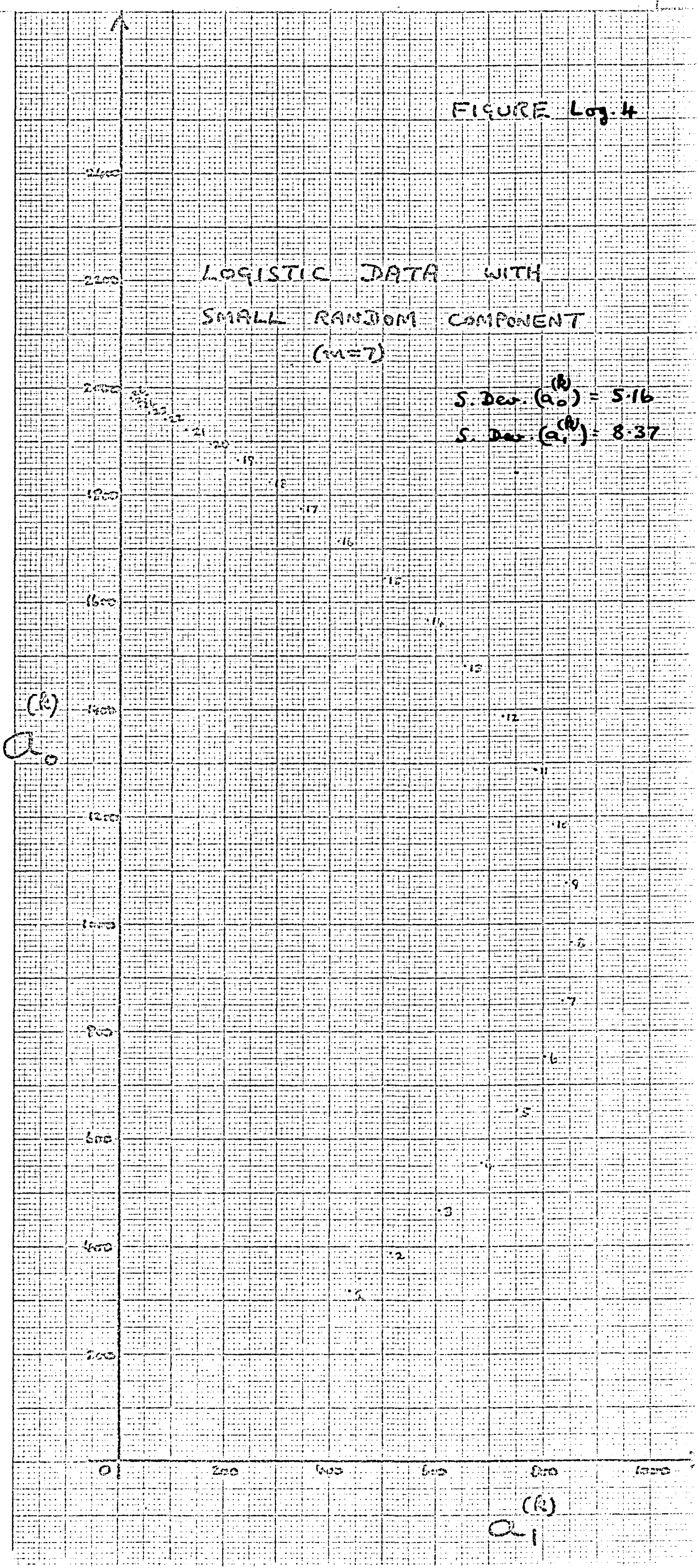


FIGURE Log.4
LOGISTIC DATA WITH
SMALL RANDOM COMPONENT
(m=7)
S. Dev. $(a_0^{(k)}) = 5.16$
S. Dev. $(a_1^{(k)}) = 8.37$
$a_0^{(k)}$
$a_1^{(k)}$

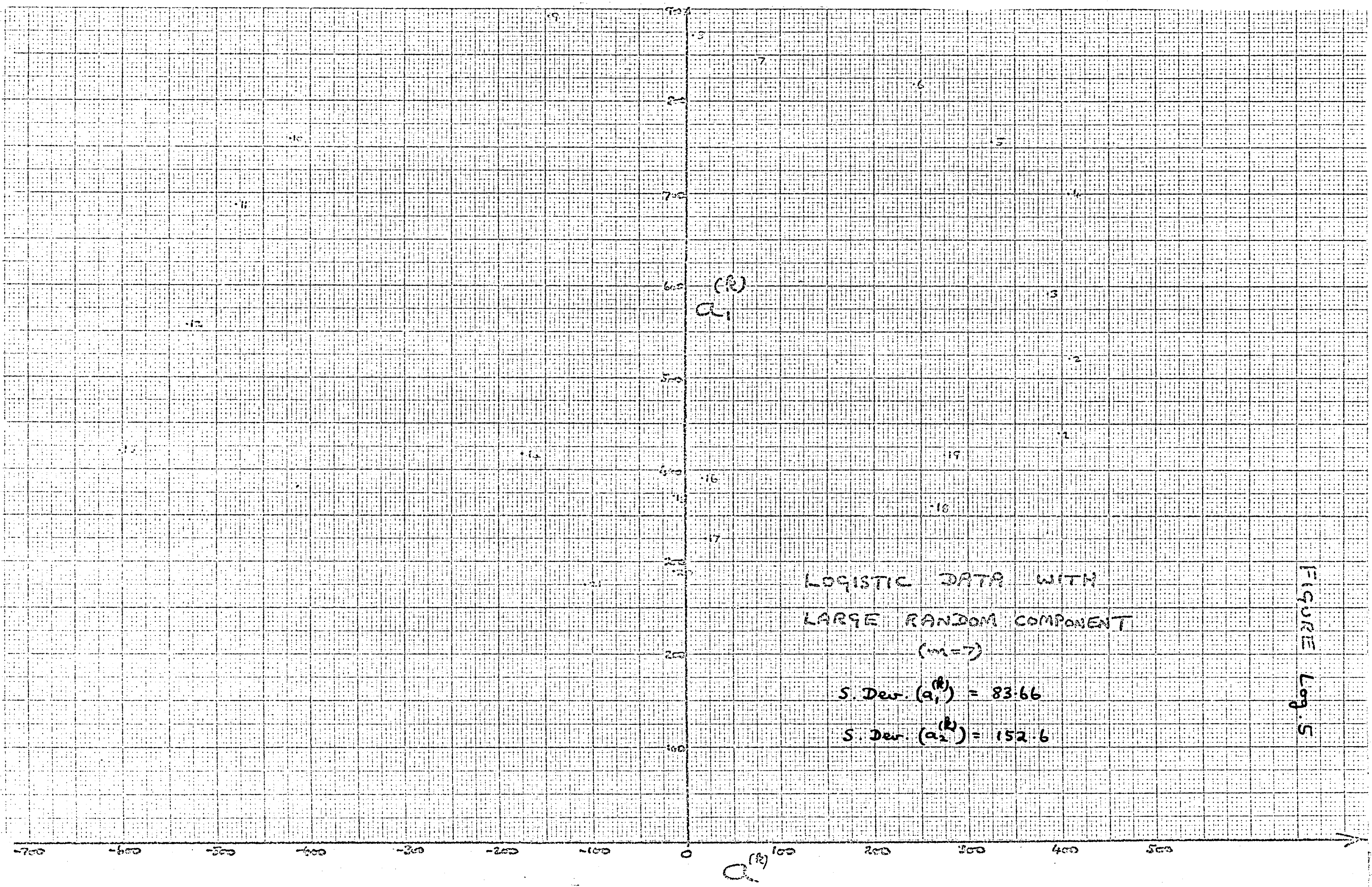


FIGURE Log.5
LOGISTIC DATA WITH
LARGE RANDOM COMPONENT
(m=7)
S. Dev. $(a_1^{(k)})$ = 83.66
S. Dev. $(a_2^{(k)})$ = 152.6
$a_1^{(k)}$
$a^{(k)}$
-700
-600
-500
-400
-300
-200
-100
0
100
200
300
400
500

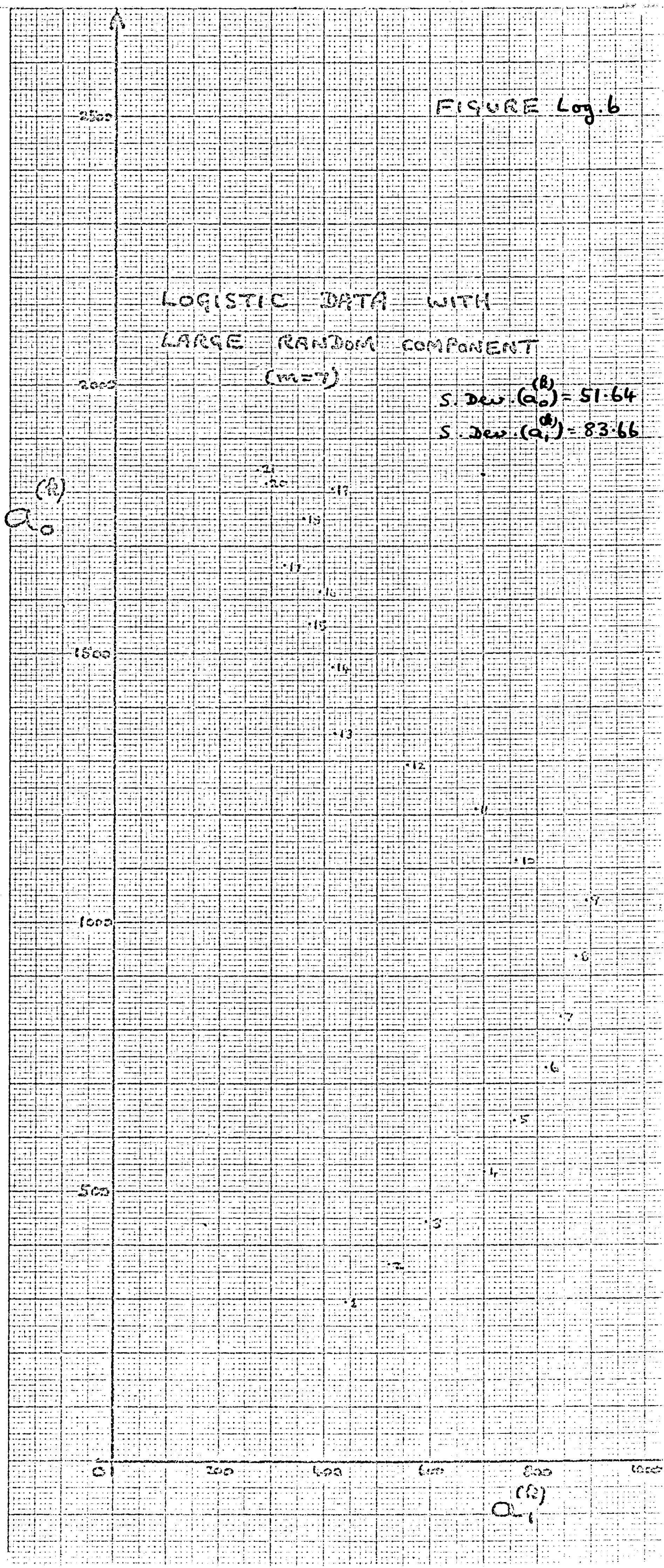


FIGURE Log.6
LOGISTIC DATA WITH
LARGE RANDOM COMPONENT
(m=7)
S. Dev. $(a_0^{(k)})$ = 51·64
S. Dev. $(a_1^{(k)})$ = 83·66
$a_0^{(k)}$
$a_1^{(k)}$
2500
2000
1500
1000
500
0
200
400
600
800
1000

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APPENDIX 1

DETERMINATION OF THE g(r,s) TERMS IN THE LEAST SQUARES FIT

To determine the elements of the g(r,s) matrix $(r = 0,\ldots 4)$; $(s = 0,\ldots 4)$, we use the following identities. For ease of reading the quantities $\alpha,\beta,\gamma,\delta$ and ε are defined as shown:

$$\sum_{i=k}^{i=k+2m} 1 = (2m+1) = \alpha$$

$$\sum_{i=k}^{i=k+2m} x_i^2 = 2\sum_{j=1}^{j=m}\left(j^2/m^2\right) = \frac{2}{m^2}\cdot\frac{1}{6}\,m(m+1)(2m+1)$$

$$= \frac{2}{3}m + 1 + \frac{1}{3m} = \beta$$

$$\sum_{i=k}^{i=k+2m} x_i^4 = \frac{2}{5}m + 1 + \frac{2}{3m} - \frac{1}{15m^3} = \gamma$$

$$\sum_{i=k}^{i=k+2m} x_i^6 = \frac{2}{7}m + 1 + \frac{1}{m} - \frac{1}{3m^3} + \frac{1}{21m^5} = \delta$$

$$\sum_{i=k}^{i=k+2m} x_i^8 = \frac{2}{9}m + 1 + \frac{4}{3m} - \frac{14}{15m^3} + \frac{4}{9m^5} - \frac{1}{15m^7} = \varepsilon$$

Also, $$\sum_{i=k}^{i=k+2m} x_i = \sum_{i=k}^{i=k+2m} x_i^3 = \sum_{i=k}^{i=k+2m} x_i^5 = \sum_{i=k}^{i=k+2m} x_i^7 = 0$$

Application of these identities gives:-

$g(0,0) = \alpha\, {p_0^{(0)}}^2$

$g(0,1) = g(1,0) = \alpha\, p_0^{(0)} p_1^{(1)}$,

$g(0,2) = g(2,0) = \beta\, p_0^{(0)} p_0^{(2)} + \alpha\, p_0^{(0)} p_2^{(2)}$

$$g(0,3) = g(3,0) = \beta\ p_0^{(0)}p_1^{(3)} + \alpha\ p_0^{(0)}p_3^{(3)}$$

$$g(0,4) = g(4,0) = \gamma p_0^{(0)}p_0^{(4)}+\beta p_0^{(0)}p_2^{(4)}+\alpha p_0^{(0)}p_4^{(4)}$$

$$g(1,1) = \beta\ p_0^{(1)^2}+\alpha\ p_1^{(1)^2}$$

$$g(1,2) = g(2,1) = \beta(p_0^{(1)}p_1^{(2)}+p_1^{(1)}p_0^{(2)})+\alpha p_1^{(1)}p_2^{(2)}$$

$$g(1,3) = g(3,1) = \gamma p_0^{(1)}p_0^{(3)}+\beta(p_1^{(1)}p_1^{(3)}+p_0^{(1)}p_2^{(3)})+\alpha p_1^{(1)}p_3^{(3)}$$

$$g(1,4)=(g4,1)=\gamma(p_0^{(1)}p_1^{(4)}+p_1^{(1)}p_0^{(4)})+\beta(p_0^{(1)}p_3^{(4)}+p_1^{(1)}p_2^{(4)})+$$
$$\alpha p_1^{(1)}p_4^{(4)}$$

$$g(2,2) = \gamma\ p_0^{(2)^2} + \beta(2p_0^{(2)}p_2^{(2)}+p_1^{(2)^2}) + \alpha p_2^{(2)^2}$$

$$g(2,3) = g(3,2)=\gamma\ p_0^{(2)}p_1^{(3)}+p_1^{(2)}p_0^{(3)})+\beta(p_0^{(2)}p_3^{(3)}+p_1^{(2)}p_2^{(3)}+$$
$$p_2^{(2)}p_1^{(3)}) + \alpha\ p_2^{(2)}p_3^{(3)}$$

$$g(2,4)=g(4,2)=\delta p_0^{(2)}p_0^{(4)}+\gamma(p_0^{(2)}p_2^{(4)}+p_1^{(2)}p_1^{(4)}+p_2^{(2)}p_0^{(4)})$$
$$+\beta(p_0^{(2)}p_4^{(4)}+p_1^{(2)}p_3^{(4)}+p_2^{(2)}p_2^{(4)}) + \alpha p_2^{(2)}p_4^{(4)}$$

$$g(3,3)=\delta p_0^{(3)^2}+\gamma(2p_0^{(3)}p_2^{(3)}+p_1^{(3)^2})+\beta(2p_1^{(3)}p_3^{(3)}+p_2^{(3)^2}) +\alpha p_3^{(3)^2}$$

$$g(3,4)=g(4,3)=\delta(p_0^{(3)}p_1^{(4)}+p_1^{(3)}p_0^{(4)})+\gamma(p_0^{(3)}p_3^{(4)}+p_1^{(3)}p_2^{(4)} +$$
$$p_2^{(3)}p_1^{(4)}+p_3^{(3)}p_0^{(4)})+\beta(p_1^{(3)}p_4^{(4)}+p_2^{(3)}p_3^{(4)}+p_3^{(3)}p_2^{(4)})+\alpha p_3^{(3)}p_4^{(4)}$$

$$g(4,4) = \varepsilon p_0^{(4)^2}+\delta(2p_2^{(4)}p_0^{(4)}+p_1^{(4)^2})+\gamma(2p_0^{(4)}p_4^{(4)}+2p_1^{(4)}p_3^{(4)}+$$
$$p_2^{(4)^2})+\beta(2p_2^{(4)}p_4^{(4)}+p_3^{(4)^2})+\alpha p_4^{(4)^2}$$

APPENDIX 2

THE INVERSE OF THE TRUNCATED $[g(r,s)]$ MATRIX

Let the elements of the inverse of the truncated $[g(r,s)]$ matrix be denoted by

$G(r,s)$ $(r = 0,1,2,3,4\ ;\ s = 0,1,2,3,4)$.

Let $A = 0.3556m^2+1.0667m+0.8890-0.1111m^{-2}$

$B = 0.0305m^2+0.1524m+0.2285-0.1112m^{-2}$,

$C = 0.3047m^2+1.2190m+1.4222-0.2222m^{-2}$,

$D = 0.4000m+1+0.6667m^{-1}$,

$E = 0.6667m+1+0.3333m^{-1}$,

$F = -0.0338m^2-0.2032m-0.3725+0.2223m^{-2}$,

$H = -0.2842m^2-1.4224m-2.1330+0.4443m^{-2}$,

$J = 0.2857m+1+m^{-1}$,

$L = 0.0073m^2+0.0508m+0.1101-0.1111m^{-2}$,

and

$Z = 0.0042m^3+0.0312m^2+0.0714m+0.0025-0.0959m^{-1}$.

These quantities occur during the inversion process and are related to the truncated form of quantities $\alpha,\beta,\gamma,\delta$ and ε of Appendix 1 as follows:-

$A = \alpha\gamma-\beta^2$; $B = \beta\delta-\gamma^2$; $C = \alpha\delta-\beta\gamma$; $D = \gamma$;

$E = \beta$; $F = \delta\gamma-\beta\varepsilon$; $H = \gamma^2-\alpha\varepsilon$; $J = \delta$;

$L = \gamma\varepsilon-\delta^2$; $Z = 2\beta\delta\gamma-\beta^2\varepsilon + \alpha\gamma\varepsilon - \alpha\delta^2 - \gamma^3$

Inversion of the truncated $g(r,s)$ matrix gives:

$$G(0,0) = \left[p_0^{(0)2}p_0^{(2)2}p_0^{(4)2}Z\right]^{-1}\Big[p_0^{(2)2}p_0^{(4)2}L - p_2^{(2)2}p_0^{(4)2}H + (p_2^{(2)}p_2^{(4)}-p_4^{(4)}p_0^{(2)})^2A+2p_0^{(2)}p_0^{(4)}(p_2^{(2)}p_2^{(4)}-p_4^{(4)}p_0^{(2)})B - 2p_2^{(2)}p_0^{(2)}p_0^{(4)2}F+2p_2^{(2)}p_0^{(4)}(p_2^{(2)}p_2^{(4)}-p_4^{(4)}p_0^{(2)})C\Big],$$

$$G(0,2) = G(2,0) = \left[p_0^{(0)} p_0^{(2)^2} p_0^{(4)^2} Z\right]^{-1} \left[(p_0^{(2)} p_0^{(4)^2} F - p_0^{(2)} p_0^{(4)} p_2^{(4)} B + p_0^{(4)} (p_0^{(2)} p_4^{(4)} - 2p_2^{(2)} p_2^{(4)}) C + p_2^{(4)} (p_0^{(2)} p_4^{(4)} - p_2^{(2)} p_2^{(4)}) A + p_2^{(2)} p_0^{(4)^2} H\right],$$

$$G(0,4) = G(4,0) = \left[p_0^{(0)} p_0^{(2)} p_0^{(4)^2} Z\right]^{-1} \left[(p_2^{(2)} p_2^{(4)} - p_0^{(2)} p_4^{(4)}) A + p_0^{(2)} p_0^{(4)} B + p_2^{(2)} p_0^{(4)} C\right],$$

$$G(1,1) = \left[p_0^{(1)^2} p_0^{(3)^2} B\right]^{-1} \left[p_0^{(3)^2} J + 2p_0^{(3)} p_2^{(3)} D + p_2^{(3)^2} E\right],$$

$$G(1,3) = G(3,1) = \left[-p_0^{(1)} p_0^{(3)^2} B\right]^{-1} \left[p_0^{(3)} D + p_2^{(3)} E\right],$$

$$G(2,2) = \left[p_0^{(2)^2} p_0^{(4)^2} Z\right]^{-1} \left[-p_0^{(4)^2} H + p_2^{(4)^2} A + 2p_2^{(4)} p_0^{(4)} C\right],$$

$$G(2,4) = G(4,2) = \left[p_0^{(2)} p_0^{(4)^2} Z\right]^{-1} \left[-p_0^{(4)} C - p_2^{(4)} A\right],$$

$$G(3,3) = \left[p_0^{(3)^2} B\right]^{-1} . E,$$

$$G(4,4) = \left[p_0^{(4)^2} Z\right]^{-1} . A.$$

Also

$$G(0,1) = G(1,0) = G(0,3) = G(3,0) = G(1,2) = G(2,1)$$

$$= G(1,4) = G(4,1) = G(2,3) = G(3,2) = G(3,4) = G(4,3) = 0$$

APPENDIX 3

SOME RESULTS CONCERNING THE COEFFICIENTS $a_j^{(k)}$ (j=0,1....4) FOR SIMPLE MODIFIED EXPONENTIAL DATA

(a) Coefficient $a_4^{(k)}$.

From (8.1) and Appendix 2, the theoretical form of $a_4^{(k)}$ for perfect simple modified exponential data is given by

$$a_4^{(k)} = K\Big[G(4,0)p_o^{(0)}(2m+1)+G(4,2)(p_o^{(2)}\sum_i x_i^2+p_2^{(2)}(2m+1))$$
$$+G(4,4)(p_0^{(4)}\sum_i x_i^4+p_2^{(4)}\sum_i x_i^2+p_4^{(4)}(2m+1))\Big]$$
$$+\ a.e^{b(k+m)}\Big[\sum_i e^{bmx_i}(G(4,0)p_0^{(0)}+G(4,2)p_2^{(2)}+G(4,4)p_4^{(4)})$$
$$+\sum_i e^{bmx_i}x_i^2(G(4,2)p_0^{(2)}+G(4,4)p_2^{(4)})+\sum_i e^{bmx_i}x_i^4G(4,4)p_0^{(4)}\Big],$$

where a,b and K are unknown parameters.

Consider the coefficient of K above.

This can be written as

$$G(4,0)p_0^{(0)}\alpha+G(4,2)p_0^{(2)}\beta+G(4,2)p_2^{(2)}\alpha+G(4,4)p_0^{(4)}\gamma+G(4,4)p_2^{(4)}\beta+$$
$$G(4,4)p_4^{(4)}\alpha$$

where $G(4,0)=\left[p_0^{(0)}p_0^{(2)}p_0^{(4)2}Z\right]^{-1}\Big[(p_2^{(2)}p_2^{(4)}-p_0^{(2)}p_4^{(4)})A+$
$p_0^{(2)}p_0^{(4)}B+p_2^{(2)}p_0^{(4)}C\Big]$,

$$G(4,2) = \left[p_0^{(2)} p_0^{(4)^2} Z\right]^{-1} \left[-p_0^{(4)} C - p_2^{(4)} A\right],$$

$$G(4,4) = \left[p_0^{(4)^2} Z\right]^{-1} . A .$$

Hence the coefficient of K has the value

$$\left[p_0^{(0)} p_0^{(2)} p_0^{(4)^2} Z\right]^{-1} \left[p_0^{(0)} p_2^{(2)} p_2^{(4)} A\alpha - p_0^{(0)} p_0^{(2)} p_4^{(4)} A\alpha + \right.$$

$$p_0^{(0)} p_0^{(2)} p_0^{(4)} B\alpha + p_0^{(0)} p_2^{(2)} p_0^{(4)} C\alpha - p_0^{(0)} p_0^{(2)} p_0^{(4)} C\beta$$

$$- p_0^{(0)} p_0^{(2)} p_2^{(4)} A\beta - p_0^{(0)} p_2^{(2)} p_0^{(4)} C\alpha - p_0^{(0)} p_2^{(2)} p_2^{(4)} A\alpha$$

$$\left. + p_0^{(0)} p_0^{(2)} p_0^{(4)} A\gamma + p_0^{(0)} p_0^{(2)} p_2^{(4)} A\beta + p_0^{(0)} p_0^{(2)} p_4^{(4)} A\alpha \right]$$

i.e.

$$\left[p_0^{(0)} p_0^{(2)} p_0^{(4)^2}\right]^{-1} \left[p_0^{(0)} p_0^{(2)} p_0^{(4)} (B\alpha - C\beta + A\gamma)\right] .$$

But, from Appendix 2, $B = \beta\delta - \gamma^2$; $C = \alpha\delta - \beta\gamma$; $A = \alpha\gamma - \beta^2$ from which it follows that $B\alpha - C\beta + A\gamma = 0$

Hence the coefficient of K, for $a_4^{(k)}$, equals zero.

(b) Coefficient $a_3^{(k)}$

From (8.1) and Appendix 2, the coefficient of K for $a_3^{(k)}$, when $Y_i = K + ae^{b(mx_i + k + m)}$, is given by the term

$$G(3,1) p_0^{(1)} \sum_i x_i + G(3,3) (p_0^{(3)} \sum_i x_i^3 + p_2^{(3)} \sum_i x_i) .$$

But $\sum_{i=k}^{i=k+2m} x_i = \sum_{i=k}^{i=k+2m} x_i^3 = 0,$

hence the coefficient of K, for $a_3^{(k)}$, equals zero.

(c) Coefficients $a_2^{(k)}$ and $a_1^{(k)}$

The coefficient of K, for $a_2^{(k)}$, is given by the term

$$G(2,0)p_0^{(0)}\alpha+G(2,2)p_0^{(2)}\beta+G(2,2)p_2^{(2)}\alpha+G(2,4)p_0^{(4)}\gamma+$$
$$G(2,4)p_2^{(4)}\beta+G(2,4)p_4^{(4)}\alpha$$

In a manner exactly similar to section (a) of this Appendix, the above expression can be shown to equal zero.

The coefficient of K, for $a_1^{(k)}$, is given by the term

$$G(1,1)p_0^{(1)}\sum_i x_i + G(1,3)(p_0^{(3)}\sum_i x_i^3 + p_2^{(3)}\sum_i x_i)$$

from which it follows, as in section (b) of this Appendix, that this coefficient is also equal to zero.

(d) Coefficient $a_0^{(k)}$

From (9.2) the coefficient of K, for $a_0^{(k)}$, is given by the term

$$G(0,0)p_0^{(0)}\alpha+G(0,2)p_0^{(2)}\beta+G(0,2)p_2^{(2)}\alpha+G(0,4)p_0^{(4)}\gamma+G(0,4)$$
$$p_2^{(4)}\beta+G(0,4)p_4^{(4)}\alpha$$

Proceeding as in section (a) of this Appendix we can reduce this expression to the form

$$\left[p_0^{(0)^2}p_0^{(2)^2}p_0^{(4)^2}Z\right]^{-1}\left[p_0^{(0)}p_0^{(2)^2}p_0^{(4)^2}(L\alpha+F\beta+B\gamma)\right]$$

From Appendix 2,

$$L\alpha+F\beta+B\gamma=2\beta\delta\gamma-\gamma^3-\alpha\delta^2-\beta^2\varepsilon+\alpha\gamma\varepsilon$$

which, from Appendix 1, equals

$0.00082m^3+0.0136m^2+0.0564m+0.0508-0.0116m^{-1}-0.0508m^{-2}$,

omitting terms of smaller order than $O(m^{-2})$.

Our plotting procedure restricts us to positive, integer values of m so the above expression is non-zero. Hence the coefficient of K for $a_0^{(k)}$ is non-zero.

APPENDIX 4

ERROR ANALYSIS FOR THE ASYMPTOTIC VALUES OF θ_{min}, λ_{min}, ν_{min} and ρ_{min}.

In the following sections we use the terms "absolute error modulus" and "relative error". If R is the approximate value of a quantity whose exact value (not necessarily known) is R* then the absolute error modulus of R is $|r|$ where $r = R-R^*$. The relative error is $\frac{|r|}{|R^*|}$ or, for practical purposes, $\frac{|r|}{|R|}$.

(a) θ_{min}

The asymptotic value of θ_{min} is $-\frac{A}{C}$, where A and C are given in Appendix 2. We will consider the case for m=8, a value in the middle of the likely range of m values.

The absolute error modulus in A does not exceed

$$(\tfrac{1}{2}\text{x}10^{-4}\text{x}m^2) + (\tfrac{1}{2}\text{x}10^{-4}\text{x}m) + (\tfrac{1}{2}\text{x}10^{-4}) + (\tfrac{1}{2}\text{x}10^{-4}\text{x}m^{-2})$$

$$= 36.5078 \text{ x}10^{-4}.$$

Similarly, the absolute error modulus in C does not exceed $36.5078\text{x}10^{-4}$. Now $A = 32.1721$, $C = 30.6715$, whence the relative error in A/C does not exceed

$$\frac{36.5078\text{x}10^{-4}}{32.1721} + \frac{36.5078\text{x}10^{-4}}{30.6715}$$

$$= 2.3250\text{x}10^{-4}.$$

Therefore the absolute error modulus in A/C does not exceed

$$1.0489 \times 2.3250 \times 10^{-4}$$

$$= 2.4387 \times 10^{-4}.$$

Hence $-\frac{A}{C}$ certainly lies in the range -1.0489 ± 0.0002.

Other values of m give a similar order of error.

(b) $\underline{\lambda_{min}}$

The asymptotic value of λ_{min} is $-\frac{E}{D}$, where E and D are given in Appendix 2. With m=8, the absolute error modulus in E does not exceed

$$(\tfrac{1}{2} \times 10^{-4} \times m) + (\tfrac{1}{2} \times 10^{-4} \times m^{-1})$$

$$= 4.0625 \times 10^{-4}.$$

Similarly, the absolute error modulus in D does not exceed

$$\frac{1}{2} \times 10^{-4} \times m^{-1} = 0.0625 \times 10^{-4}.$$

Since E = 6.3753 and D = 4.2833, the relative error in E/D does not exceed

$$\frac{4.0625 \times 10^{-4}}{6.3753} + \frac{0.0625 \times 10^{-4}}{4.2833}$$

$$= 0.6518 \times 10^{-4}.$$

Whence the absolute error modulus in E/D does not exceed

$$1.4884 \times 0.6518 \times 10^{-4}$$

$$= 0.9701 \times 10^{-4}.$$

Thus -E/D certainly lies in the range -1.4884 ± 0.0001

Other values of m give a similar order of error.

(c) $\underline{\nu_{min}}$

From Chapter 10, section (e), the asymptotic value of ν_{min} is $\frac{BH-FC}{-AH-C^2}$. For m=8, the absolute error moduli in B,H,F,C and A do not exceed 36.5078×10^{-4}, from section (a) of this appendix. The relative errors in B,H,F,C and A do not exceed, respectively, 10.7440×10^{-4}, 1.1519×10^{-4}, 8.7805×10^{-4}, 1.1903×10^{-4} and 1.1348×10^{-4}.

Hence the relative errors in BH, FC, AH and C^2 do not exceed, respectively, 11.8959×10^{-4}, 9.9708×10^{-4}, 2.2867×10^{-4} and 2.3806×10^{-4}.

The absolute error moduli in BH, FC, AH and C^2 do not exceed, respectively, 1281.132×10^{-4}, 1271.536×10^{-4}, 2331.670×10^{-4} and 2239.528×10^{-4}.

Hence the absolute error moduli in (BH-FC) and ($-AH-C^2$) do not exceed, respectively, 2552.668×10^{-4} and 4571.198×10^{-4}. The relative errors in (BH-FC) and ($-AH-C^2$) do not exceed 128.723×10^{-4} and 57.9183×10^{-4} respectively, hence the relative error in $\frac{BH-FC}{-AH-C^2}$ does not exceed 186.641×10^{-4}, whence the absolute error modulus in $\frac{BH-FC}{-AH-C^2}$ does not exceed

$$0.2513 \times 186.641 \times 10^{-4}$$

$$= 46.90 \times 10^{-4}.$$

Thus $\frac{BH-FC}{-AH-C^2}$ certainly lies in the range 0.2513 ± 0.0047. Other values of m give a similar order of error.

(d) ρ_{min}

From Chapter 10, section (e), the asymptotic value of ρ_{min} is $\frac{BC+AF}{-AH-C^2}$. Using the results from the previous section for m=8, the relative errors in BC and AF do not exceed 11.9343×10^{-4} and 9.9153×10^{-4} respectively. The absolute error moduli in BC and AF do not exceed 1243.799×10^{-4} and 1326.322×10^{-4} respectively, hence the absolute error modulus in (BC+AF) does not exceed 2570.121×10^{-4}.

The relative error in (BC+AF) does not exceed 86.9911×10^{-4}, hence, using results from the previous section, the relative error in $\frac{BC+AF}{-AH-C^2}$ does not exceed 144.9094×10^{-4}. The absolute error modulus in $\frac{BC+AF}{-AH-C^2}$ does not exceed, therefore,

$$0.3744\times144.9094\times10^{-4}$$

$$= 54.24 \times 10^{-4}.$$

Thus $\frac{BC+AF}{-AH-C^2}$ certainly lies in the range -0.3744 ± 0.0054. Other values of m give a similar order of error.

APPENDIX 5

SOME RESULTS IN THE MINIMIZATION PROCEDURE FOR COEFFICIENT $a_0^{(k)}$

(i) Reduction of the Quadratic Form in Q''

From section (e) of Chapter 10,

$$\frac{\text{S.Dev.}(a_0^{(k)})}{Z^{\frac{1}{2}}\sigma|a_0^{(k)}|} = Q'' = \frac{\left[-H\rho^2+A\nu^2-2F\rho+2B\nu+2C\rho\nu+L\right]^{\frac{1}{2}}}{|-r\rho-s\nu+w|} .$$

The quadratic form in the numerator may be reduced by means of the substitutions $\rho = P + p$, $\nu = V + v$. Making these substitutions and equating the coefficients of P and V to zero, we obtain

$$p = \frac{BC+FA}{-HA-C^2}$$

and

$$v = \frac{BH-FC}{-HA-C^2} .$$

The numerator is then of the form

$$\left[-HP^2+AV^2+2CPV+(HAL+2BCF+F^2A-HB^2+LC^2)(AH+C^2)^{-1}\right]^{\frac{1}{2}} .$$

This may be rearranged to the form

$$\left[-H(P-\frac{C}{H}V)^2+(A+\frac{C^2}{H})V^2+(HAL+2BCF+F^2A-HB^2+LC^2)(AH+C^2)^{-1}\right]^{\frac{1}{2}}$$

i.e. $\left[c_1\eta^2+c_2T^2+c_3\right]^{\frac{1}{2}}$

where

$$c_1 = -H,$$

$$c_2 = A + \frac{C^2}{H} ,$$

$$c_3 = (HAL+2BCF+F^2A-HB^2+LC^2)(AH+C^2)^{-1},$$

$$\eta = P - \frac{C}{H}V ,$$

and $T = V.$

Substituting

$$\rho = P + \frac{BC+FA}{-HA-C^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (A5.1)$$

and

$$\nu = V + \frac{BH-FC}{-HA-C^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (A5.2)$$

into the denominator of Q", we obtain the expression

$$\left| -r(P-\frac{C}{H}V)+(-s-\frac{C}{H}r)V+(r(BC+FA)+s(BH-FC)+w(AH+C^2))(AH+C^2)^{-1} \right|$$

i.e. $\quad |c_4\eta + c_5T + c_6|$,

where

$$c_4 = -r$$

$$c_5 = -s-\frac{C}{H}r$$

and

$$c_6 = (r(BC+FA)+s(BH-FC)+w(AH+C^2))(AH+C^2)^{-1} .$$

Hence Q" may be written as

$$Q'' = \frac{\left[c_1\eta^2 + c_2T^2 + c_3\right]^{\frac{1}{2}}}{|c_4\eta + c_5T + c_6|} .$$

Note that from (A5.1) and (A5.2) η and T may be expressed as

$$\eta = \rho - \frac{C}{H}\nu + \left(\frac{BC+FA}{AH+C^2}\right) - \left(\frac{C}{H}\right)\left(\frac{BH-FC}{AH+C^2}\right) ,$$

$$T = \nu + \frac{BH-FC}{AH+C^2} .$$

(ii) <u>The Coefficient Properties of $f(Q''^2_{min}(T))$</u>

Consider the quadratic $f(Q''^2_{min}(T))$ from inequality (10.14) of Chapter 10. The last term in this quadratic is $c_1{}^2c_2c_3$. Noting that

$$c_2 = A + \frac{C^2}{H} = \frac{1}{H}(HA+C^2) ,$$

and applying Appendix 2 to establish that

$HA+C^2=-0.0082m^4-0.0659m^3-0.1755m^2-0.0723m+0.1265$,

(where we have omitted terms of order $O(m^{-1})$) we see that for positive, integer values of m, $HA+C^2$ is negative, and since H itself is negative, the term c_2 is positive.

Consider the numerator for the term c_3 . From Appendix 2 it can be shown that

$$\begin{aligned}HAL+2BCF+F^2A-HB^2+LC^2 = &-0.0000175m^6-0.0002596m^5\\ &-0.0015672m^4-0.0044835m^3\\ &-0.0044635m^2+0.0056138m\\ &+0.0130478,\end{aligned}$$

where terms of order $O(m^{-1})$ have been omitted. For positive, integer values of m this expression is negative, and since the denominator for c_3 is also negative the term c_3 itself is positive, hence the term $c_1{}^2c_2c_3$ is positive.

The coefficient of $Q''^4_{min}(T)$ in equation (10.14) is

$$c_4{}^4c_2c_3 + c_4{}^2c_1c_2c_6{}^2 + c_1c_5{}^2c_4{}^2c_3 .$$

Since c_1, c_2 and c_3 are positive, this coefficient is itself positive.

Similar results hold for the equivalent quadratic in $Q''^2_{min}(\eta)$.