AD-A014 917

TECHNIQUES OF RESPONSE SURFACE
ESTIMATION, WITH APPLICATIONS IN
COMPUTER SIMULATION

Michael A. Crane

Control Analysis Corporation

20000801161

Prepared for:

Office of Naval Research

August 1975
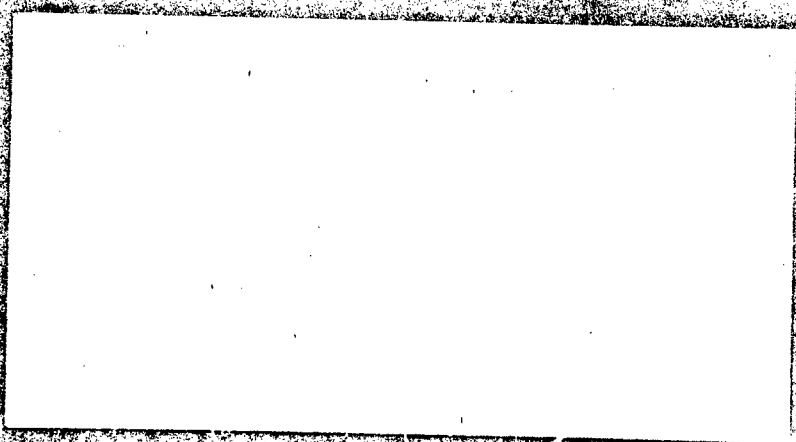
Reproduced From
Best Available Copy

control analysis corporation

800 welch road • palo alto, california 94304
telephone (415) 326 2100

DOCUMENT CONTROL DATA - R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1 ORIGINATING ACTIVITY (Corporate author)	2a. REPORT SECURITY CLASSIFICATION
CONTROL ANALYSIS CORPORATION 800 Welch Road - Palo Alto, CA 94304	Unclassified 2b GROUP

3 REPORT TITLE

Techniques of Response Surface Estimation, With Applications in Computer Simulation

4 DESCRIPTIVE NOTES *(Type of report and inclusive dates)*

Technical Report

5. AUTHOR(S) *(Last name, first name, initial)*

Michael A. Crane

6. REPORT DATE	7a TOTAL NO. OF PAGES	7b. NO. OF REFS
August 1975	21	10

8a CONTRACT OR GRANT NO. N00014-72-C-0086	9a. ORIGINATOR'S REPORT NUMBER(S)
b. PROJECT NO. NR-047-106	Technical Report No. 86-19
c.	9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*
d.	

10. AVAILABILITY/LIMITATION NOTICES

Distribution of this document is unlimited

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
	Operations Research Program Office of Naval Research Arlington, VA 22217

13. ABSTRACT

A technique is presented for obtaining confidence intervals and confidence bands for a one-dimensional response surface which is assumed to be a general-order polynomial. Specifically, suppose that λ is an input parameter for an experiment and that estimates for an output $g(\lambda)$ are desired, where g is an $(n-1)^{th}$-order polynomial over an interval $a_0 \le \lambda \le a_{n+1}$. If observations are made at n distinct values $\lambda = a_i$, $1_0 \le i \le n$, then under certain conditions confidence intervals may be obtained for $g(\lambda)$, $a_0 \le \lambda \le a_{n+1}$, and a confidence band may be obtained for the entire function over this interval. The basic requirement for these results is that central limit theorems exist which permit confidence interval estimation at the n points $\lambda = a_i$. Two illustrations are given which satisfy this requirement, including an application of the regenerative approach in steady-state simulation analysis.

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Simulation						
Statistical analysis of simulations						
Confidence intervals in simulations						
Response surface estimation						
Confidence intervals for polynomials						
Confidence bands for polynomials						
Polynomial approximation						
Bounds for polynomials						
Regenerative Approach in simulation						

INSTRUCTIONS

1. ORIGINATING ACTIVITY: Enter the name and address of the contractor, subcontractor, grantee, Department of Defense activity or other organization (corporate author) issuing the report.

2a. REPORT SECURITY CLASSIFICATION: Enter the overall security classification of the report. Indicate whether "Restricted Data" is included. Marking is to be in accordance with appropriate security regulations.

2b. GROUP: Automatic downgrading is specified in DoD Directive 5200.10 and Armed Forces Industrial Manual. Enter the group number. Also, when applicable, show that optional markings have been used for Group 3 and Group 4 as authorized.

3. REPORT TITLE: Enter the complete report title in all capital letters. Titles in all cases should be unclassified. If a meaningful title cannot be selected without classification, show title classification in all capitals in parenthesis immediately following the title.

4. DESCRIPTIVE NOTES: If appropriate, enter the type of report, e.g., interim, progress, summary, annual, or final. Give the inclusive dates when a specific reporting period is covered.

5. AUTHOR(S): Enter the name(s) of author(s) as shown on or in the report. Enter last name, first name, middle initial. If military, show rank and branch of service. The name of the principal author is an absolute minimum requirement.

6. REPORT DATE: Enter the date of the report as day, month, year; or month, year. If more than one date appears on the report, use date of publication.

7a. TOTAL NUMBER OF PAGES: The total page count should follow normal pagination procedures, i.e., enter the number of pages containing information.

7b. NUMBER OF REFERENCES: Enter the total number of references cited in the report.

8a. CONTRACT OR GRANT NUMBER: If appropriate, enter the applicable number of the contract or grant under which the report was written.

8b, 8c, & 8d. PROJECT NUMBER: Enter the appropriate military department identification, such as project number, subproject number, system numbers, task number, etc.

9a. ORIGINATOR'S REPORT NUMBER(S): Enter the official report number by which the document will be identified and controlled by the originating activity. This number must be unique to this report.

9b. OTHER REPORT NUMBER(S): If the report has been assigned any other report numbers (either by the originator or by the sponsor), also enter this number(s).

10. AVAILABILITY/LIMITATION NOTICES: Enter any limitations on further dissemination of the report, other than those imposed by security classification, using standard statements such as:

(1) "Qualified requesters may obtain copies of this report from DDC."

(2) "Foreign announcement and dissemination of this report by DDC is not authorized."

(3) "U. S. Government agencies may obtain copies of this report directly from DDC. Other qualified DDC users shall request through

_____."

(4) "U. S. military agencies may obtain copies of this report directly from DDC. Other qualified users shall request through

_____."

(5) "All distribution of this report is controlled. Qualified DDC users shall request through

_____."

If the report has been furnished to the Office of Technical Services, Department of Commerce, for sale to the public, indicate this fact and enter the price, if known.

11. SUPPLEMENTARY NOTES: Use for additional explanatory notes.

12. SPONSORING MILITARY ACTIVITY: Enter the name of the departmental project office or laboratory sponsoring (paying for) the research and development. Include address.

13. ABSTRACT: Enter an abstract giving a brief and factual summary of the document indicative of the report, even though it may also appear elsewhere in the body of the technical report. If additional space is required, a continuation sheet shall be attached.

It is highly desirable that the abstract of classified reports be unclassified. Each paragraph of the abstract shall end with an indication of the military security classification of the information in the paragraph, represented as (TS), (S), (C), or (U).

There is no limitation on the length of the abstract. However, the suggested length is from 150 to 225 words.

14. KEY WORDS: Key words are technically meaningful terms or short phrases that characterize a report and may be used as index entries for cataloging the report. Key words must be selected so that no security classification is required. Identifiers, such as equipment model designation, trade name, military project code name, geographic location, may be used as key words but will be followed by an indication of technical context. The assignment of links, roles, and weights is optional.

CONTROL ANALYSIS CORPORATION

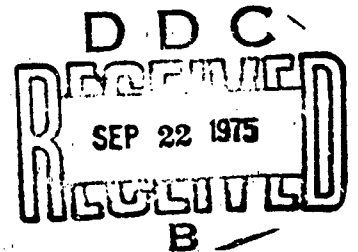800 Welch Road

Palo Alto, California 94304

Technical Report No. 86-19

TECHNIQUES OF RESPONSE SURFACE ESTIMATION,

WITH APPLICATIONS IN COMPUTER SIMULATION

by

Michael A. Crane

August 1975

D D C

SEP 22 1975

B

ABSTRACT

A technique is presented for obtaining confidence intervals and confidence bands for a one-dimensional response surface which is assumed to be a general-order polynomial. Specifically, suppose that λ is an input parameter for an experiment and that estimates for an output $g(\lambda)$ are desired, where g is an $(n-1)^{th}$-order polynomial over an interval $a_0 \leq \lambda \leq a_{n+1}$. If observations are made at n distinct values $\lambda = a_i$, $1_0 \leq i \leq n$, then under certain conditions confidence intervals may be obtained for $g(\lambda)$, $a_0 \leq \lambda \leq a_{n+1}$, and a confidence band may be obtained for the entire function over this interval. The basic requirement for these results is that central limit theorems exist which permit confidence interval estimation at the n points $\lambda = a_i$. Two illustrations are given which satisfy this requirement, including an application of the regenerative approach in steady-state simulation analysis.

TECHNIQUES OF RESPONSE SURFACE ESTIMATION,

WITH APPLICATIONS IN COMPUTER SIMULATION*

by

Michael A. Crane

1. Introduction

In this paper a method is presented for one-dimensional response surface estimation when it is assumed that the response surface has a general-order polynomial form. In particular, it is shown that if the response is of order $n-1$ and if observations are taken at n distinct values for the input or "treatment" variable, then under general conditions it is possible to obtain large-sample confidence intervals for the response at any value of the input variable. Additionally, large-sample confidence bands for the entire response function may be obtained.

Specifically, suppose that λ is an input parameter for a statistical experiment and that estimates for an unknown output function $g(\lambda)$ are desired, where g is an $(n-1^{th})$-order polynomial over an interval $a_0 \leq \lambda \leq a_{n+1}$. Suppose further that observations are made for n distinct values of λ, namely, $\lambda = a_i$, $1 \leq i \leq n$ with $a_0 \leq a_1 < \ldots < a_n \leq a_{n+1}$. In Section 2, conditions are given which allow one to compute confidence intervals for $g(\lambda)$ at any point $a_0 \leq \lambda \leq a_{n+1}$. In Section 3, confidence bands for the function $g(\lambda)$ over $a_0 \leq \lambda \leq a_{n+1}$ are derived. The basic requirement for these results is that central limit theorems exist which permit confidence interval estimation at the n points $\lambda = a_i$.

-1-

The methods are illustrated in Section 4, where two examples are provided which satisfy this requirement. The first example is the typical case where the experiment at $\lambda = a_i$ consists of a sample of independent and identically distributed variates from a population with mean $g(a_i)$. In the second example, the observations at $\lambda = a_i$ are based on random tours in an application of the regenerative approach in simulation analysis; see [4, 5, 6, 7, 10].

The problem as stated above has been studied previously in the context of linear regression analysis. The interval estimation problem is discussed, for example, in Graybill [8, pp. 121-122], and confidence bands for a general linear model are obtained by Bowden [2]. However, the results presented here are to be distinguished from the linear regression models in that

1) the confidence interval and confidence band derivations do not require distributional assumptions,

2) the variances at $\lambda = a_i$ are unknown and no relationship among the variances is assumed,

3) the response surface is a general polynomial, and

4) it is not essential that all observations be independent, only that n independent experiments be conducted and that a central limit theorem be applicable for the observations in each experiment.

2. Confidence Interval Estimation

Suppose that λ is an input parameter or "treatment" variable for a statistical experiment and that we wish to estimate some output parameter $g(\lambda)$ which is an unknown $(n-1)^{th}$-order polynomial function of λ over an interval $a_0 \leq \lambda \leq a_{n+1}$, i.e.,

$$g(\lambda) = z_1 + z_2 \lambda + \ldots + z_n \lambda^{n-1}, \quad a_0 \leq \lambda \leq a_{n+1}$$

-2-

where the coefficients $z_1, z_2, \ldots, z_n$ are unknown. Independent experiments resulting in statistical observations are made at n particular parameter settings $\lambda = a_i$, $1 \le i \le n$, with $a_0 \le a_1 < a_2 < \cdots < a_n \le a_{n+1}$. At the parameter setting $\lambda = a_i$, the experiment produces N_i observations resulting in sample statistics $\hat{r}(a_i, N_i)$ and $\hat{\eta}(a_i, N_i)$. For example, the N_i observations might be independent and identically distributed sample variates from a population with mean $g(a_i)$, and $\hat{r}(a_i, N_i)$ and $\hat{\eta}(a_i, N_i)$ might be the sample mean and sample standard deviation, respectively. Alternatively, the observations might be based on random tours in an application of the regenerative approach in simulation analysis. See Section 4 for details.

The function g may be expressed in terms of its values at the n points $a_1, a_2, \ldots, a_n$, as follows:

$$g(\lambda) = \Psi(\lambda) \begin{bmatrix} g(a_1) \\ \cdot \\ \cdot \\ \cdot \\ g(a_n) \end{bmatrix} , \quad a_0 \le \lambda \le a_{n+1}$$

where

$$\Psi(\lambda) = (1 \ \lambda \ \cdots \ \lambda^{n-1}) \begin{bmatrix} 1 & a_1 & \cdots & a_1^{n-1} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ 1 & a_n & \cdots & a_n^{n-1} \end{bmatrix}^{-1}$$

Let $\Psi_i(\lambda)$ denote the ith component of $\Psi(\lambda)$. Note that the matrix to be inverted is the Vandermonde matrix, and its inverse is well-known, cf. [a] pp. 124-125.

The following proposition forms a basis for a method to compute confidence intervals for $g(\lambda)$ where $a_0 \leq \lambda \leq a_{n+1}$. Let a double arrow denote convergence in distribution and let $N(\mu, \sigma)$ denote a normally distributed random variable with mean μ and standard deviation σ.

PROPOSITION 1. <u>Suppose there esist</u> $\eta(a_i)$ <u>such that</u> $\hat{\eta}(a_i, N_i) \rightarrow \eta(a_i)$ <u>in probability as</u> $N_i \rightarrow \infty$, $i = 1, 2, \ldots, n$. <u>Suppose further that</u>

$$N_i^{\frac{1}{2}}[\hat{r}(a_i, N_i) - g(a_i)]/ \eta(a_i) \Longrightarrow N(0, 1)$$

<u>as</u> $N_i \rightarrow \infty$, $i = 1, 2, \ldots, n$. <u>Then for</u> $a_0 \leq \lambda \leq a_{n+1}$,

$$[\hat{r}(\lambda, N_1, \ldots, N_n) - g(\lambda)]/ \hat{\upsilon}(\lambda, N_1, \ldots, N_n) \Longrightarrow N(0, 1)$$

<u>as</u> $N_1 \rightarrow \infty$ <u>and</u> $N_i = [C_i N_1]$ (integer part) $i = 2, \ldots, n$, <u>where</u> $C_2, \ldots, C_n$ <u>are arbitrary positive constants,</u>

$$\hat{r}(\lambda, N_1, \ldots, N_n) = \Psi(\lambda) \begin{bmatrix} \hat{r}(a_1, N_1) \\ \cdot \\ \cdot \\ \cdot \\ \hat{r}(a_n, N_n) \end{bmatrix},$$

<u>and</u>

$$\hat{\upsilon}(\lambda, N_1, \ldots, N_n) = \left\{ \sum_{i=1}^{n} \Psi_i^2(\lambda) \hat{\eta}^2(a_i, N_1)/N_1 \right\}^{1/2}.$$

<u>Proof.</u> From the conditions of the proposition, we may write

$$[C_i N_1]^{1/2} [\hat{r}(a_i, N_1) - g(a_i)] \Longrightarrow N(0, \eta(a_i)), \quad i = 1, \ldots, n$$

as $N_1 \rightarrow \infty$ and $N_i = [C_i N_1]$, where we have set $C_1 = 1$.

Since $[C_i N_1]^{1/2} / (C_i N_1)^{1/2} \rightarrow 1$ we have

$$(C_i \, N_1)^{1/2} \left[\hat{r}(a_i, \, N_i) - g(a_i) \right] \Longrightarrow N\left(0, \, \eta(a_i)\right), \quad i = 1, \ldots n$$

or

$$N_1^{1/2} \left[\hat{r}(a_i, \, N_i) - g(a_i) \right] \Longrightarrow N\left(0, \, \eta(a_i) / C_i^{1/2}\right), \quad i = 1, \ldots, n.$$

Since $\hat{r}(a_i, \, N_i)$, $i = 1, \ldots, n$ are independent, we have, by Theorem 3.2 of [1], convergence of the vector process

$$\begin{bmatrix} N_1^{1/2} [\hat{r}(a_1, \, N_1) - g(a_1)] \\ \cdot \\ \cdot \\ \cdot \\ N_1^{1/2} [\hat{r}(a_n, \, N_n) - g(a_n)] \end{bmatrix} \Rightarrow \begin{bmatrix} N(0, \, \eta(a_1)/C_1^{1/2}) \\ \cdot \\ \cdot \\ \cdot \\ N(0, \, \eta(a_n)/C_n^{1/2}) \end{bmatrix}$$

where the limit random variables are independent. Using the Continuous Mapping Theorem, cf. [1] Theorem 5.1, we have

$$\psi(\lambda) \begin{bmatrix} N_1^{1/2}[\hat{r}(a_1, \, N_1) - g(a_1)] \\ \cdot \\ \cdot \\ \cdot \\ N_1^{1/2}[\hat{r}(a_n, \, N_n) - g(a_n)] \end{bmatrix} \Longrightarrow N[0, \, (\sum_{i=1}^{n} \psi_i^2(\lambda) \, \eta^2(a_i)/C_i)^{1/2}]$$

or

$$N_1^{1/2}[\hat{r}(\lambda, \, N_1, \ldots, N_n) - g(\lambda)] / [\sum_{i=1}^{n} \psi_i^2(\lambda)\eta^2(a_i)/C_i]^{1/2} \Rightarrow N(0, 1).$$

Since $[C_i \, N_1]/C_i \, N_1 \to 1$ and $\hat{\eta}(a_i, \, N_i) \to \eta(a_i)$ in probability,

this implies

$$[\hat{r}(\lambda, \, N_1, \ldots, N_n) - g(\lambda)] / [\sum_{i=1}^{n} \psi_i^2(\lambda) \, \hat{\eta}^2(a_i, \, N_i)/[C_i \, N_1]]^{1/2} \Rightarrow N(0, 1)$$

or

$$[\hat{r}(\lambda, N_1, \ldots, N_n) - g(\lambda)]/\hat{v}(\lambda, N_1, \ldots, N_n) \Rightarrow N(0, 1)$$

which is the desired result.

The above proposition allows one to obtain an approximate $100(1 - \gamma)\%$ confidence interval for $g(\lambda)$ as follows. For N_i sufficiently large, $i = 1, \ldots, n$,

$$P\left\{-\phi^{-1}(1 - \gamma/2) \leq [\hat{r}(\lambda, N_1, \ldots, N_n) - g(\lambda)]/\hat{v}(\lambda, N_1, \ldots, N_n) \leq \right.$$

$$\left. \phi^{-1}(1 - \gamma/2)\right\} \cong 1 - \gamma .$$

This may be rewritten as

$$P\left\{\hat{r}(\lambda, N_1, \ldots, N_n) - \hat{v}(\lambda, N_1, \ldots, N_n)\, \phi^{-1}(1 - \gamma/2) \leq g(\lambda) \leq \right.$$

$$\left. \hat{r}(\lambda, N_1, \ldots, N_n) + \hat{v}(\lambda, N_1, \ldots, N_n)\, \phi^{-1}(1 - \gamma/2)\right\} \cong 1 - \gamma$$

giving the desired confidence interval.

Note that the confidence interval obtained at $\lambda = a_i$ reduces to

$$\hat{r}(a_i, N_i) \pm N_i^{-\frac{1}{2}} \hat{h}(a_i, N_i)\, \phi^{-1}(1 - \gamma/2) ,$$

which is exactly the same confidence interval which could be obtained based on the N_i observations at $\lambda = a_i$. Letting $\hat{\ell}(\lambda, N_1, \ldots, N_n)$ denote the length of the confidence interval obtained at λ, we see that

$$\hat{\ell}(\lambda, N_1, \ldots, N_n) = 2\, \hat{v}(\lambda, N_1, \ldots, N_n)\, \phi^{-1}(1 - \gamma/2)$$

$$= 2\left\{\sum_{i=1}^{n} \psi_i^2(\lambda)\, \hat{h}^2(a_i, N_i)/N_i\right\}^{\frac{1}{2}} \phi^{-1}(1 - \gamma/2)$$

$$= \left\{\sum_{i=1}^{n} \psi_i^2(\lambda)\, \hat{\ell}^2(a_i, N_i)\right\}^{\frac{1}{2}}$$

where $\ell(a_i, N_i)$ is the length obtained at $\lambda = a_i$.

3. Confidence Band Estimation for the Function $g(\lambda)$

As noted in Section 2, we may obtain approximate $100(1 - \gamma_i)\%$ confidence intervals $[A_i^1, A_i^2]$ for $g(\lambda)$ at $\lambda = a_i$, $i = 1, \ldots, n$:

(1) $A_i^1 \leq g(a_i) \leq A_i^2$ with probability $(1 - \gamma_i)$, $i = 1, \ldots, n$,

where $A_i^1 = \hat{r}(a_i, N_i) - N_i^{-\frac{1}{2}} \hat{\eta}(a_i, N_i) \Phi^{-1}(1 - \gamma_i/2)$ and

$A_i^2 = \hat{r}(a_i, N_i) + N_i^{-\frac{1}{2}} \hat{\eta}(a_i, N_i) \Phi^{-1}(1 - \gamma_i/2)$. Proposition 1

enables one to obtain confidence *intervals* for $g(\lambda)$ at any point $a_0 \leq \lambda \leq a_{n+1}$.
In this section, we show how (1) may be used to obtain a confidence *band*
for the entire function $g(\lambda)$ over $a_0 \leq \lambda \leq a_{n+1}$.

Before stating the result, we shall need some additional notation.
Define the column vectors $\underset{\sim}{A}^1(m)$ and $\underset{\sim}{A}^2(m)$, $m = 0, 1, \ldots, n$ as follows.
For $1 \leq j \leq n$, the jth components of $\underset{\sim}{A}^1(m)$ and $\underset{\sim}{A}^2(m)$ are, respectively,

$$\underset{\sim j}{A}^1(m) = \begin{cases} A_j^1 & \text{if } j \leq m \text{ and } m-j \text{ is even} \\ & \text{or } j > m \text{ and } j-m \text{ is odd,} \\ A_j^2 & \text{if } j \leq m \text{ and } m-j \text{ is odd} \\ & \text{or } j > m \text{ and } j-m \text{ is even,} \end{cases}$$

$$\underset{\sim j}{A}^2(m) = \begin{cases} A_j^2 & \text{if } j \leq m \text{ and } m-j \text{ is even} \\ & \text{or } j > m \text{ and } j-m \text{ is odd,} \\ A_j^1 & \text{if } j \leq m \text{ and } m-j \text{ is odd} \\ & \text{or } j > m \text{ and } j-m \text{ is even.} \end{cases}$$

The following proposition gives the desired confidence band for the function
$g(\lambda)$. With the stated probability, the inequalities in the proposition hold

simultaneously for all values $a_0 \leq \lambda \leq a_{n+1}$, given that (1) holds.

PROPOSITION 2. <u>With probability</u> $(1 - \gamma_1)(1 - \gamma_2) \ldots (1 - \gamma_n)$,

(2) $\qquad\qquad \Psi(\lambda) \underset{\wedge}{A}^1(m) \leq g(\lambda) \leq \Psi(\lambda) \underset{\wedge}{A}^2(m)$

<u>for</u> $a_m \leq \lambda \leq a_{m+1}$ <u>and</u> $m = 0, 1, 2, \ldots, n$.

<u>Proof.</u> Since the experiments at $\lambda = a_i$, $i = 1, \ldots, n$ are independent, all the inequalities (1) hold simultaneously with probability $(1 - \gamma_1)(1 - \gamma_2) \ldots (1 - \gamma_n)$. It is easy to see that the inequalities (2) imply the inequalities (1), since $\Psi(a_m) \underset{\wedge}{A}^k(m) = A_m^k$ for $k = 1, 2$ and $1 \leq m \leq n$. It is therefore sufficient to show that (1) imply (2). This fact, however, is proved in an earlier result by the author; see [3].

The above proposition may be interpreted as follows. For $1 \leq m \leq n - 1$ and $a_m \leq \lambda \leq a_{m+1}$, the bounds for $g(\lambda)$ are obtained by forming two $(n-1)^{\text{th}}$-order polynomials passing through subsets of the points $A_1^1, \ldots, A_n^1$ and $A_1^2, \ldots, A_n^2$. The upper bound polynomial is the unique polynomial passing through A_m^2, A_{m+1}^2, and A_j^k, $1 \leq j \leq m-1$, $m + 2 \leq j \leq n$, where k alternates between 1 and 2 for each integer step away from the interval $[m, m + 1]$, starting with $k = 1$ for $j = m - 1$ or $j = m + 2$. Similarly, the lower bound polynomial is the unique polynomial passing through A_m^1, A_{m+1}^1 and alternating values for A_j^k, $1 \leq j \leq m - 1$, $m + 2 \leq j \leq n$, starting with $k = 2$ for $j = m - 1$ or $j = m + 2$. For $a_0 \leq \lambda \leq a_1$, the upper bound is the polynomial passing through $A_1^2, A_2^1, A_3^2, A_4^1$, etc., whereas the lower bound polynomial passes through $A_1^1, A_2^2, A_3^1, A_4^2$, etc. Similarly, for $a_n \leq \lambda \leq a_{n+1}$, the upper bound polynomial passes through $A_n^2, A_{n-1}^1, A_{n-2}^2, A_{n-3}^1$, etc.,

whereas the lower bound polynomial passes through A_n^1, A_{n-1}^2, A_{n-2}^1, A_{n-3}^2, etc.

4. Applications

The most straightforward application of Propositions 1 and 2 is the situation where the N_i observations at $\lambda = a_i$ are independent and identically distributed sample variates $X_{i1}, \ldots, X_{iN_i}$ from a population with mean $g(a_i)$ and standard deviation $\eta(a_i)$. Letting

$$\hat{f}(a_i, N_i) = \frac{1}{N_i} \sum_{j=1}^{N_i} X_{ij}$$

and

$$\hat{\eta}(a_i, N_i) = \left[\frac{1}{N_i - 1} \sum_{j=1}^{N_i} (X_{ij} - \hat{f}(a_i, N_i))^2 \right]^{1/2}$$

we know from the Central Limit Theorem and the Law of Large Numbers that

$$N_i^{1/2} [\hat{f}(a_i, N_i) - g(a_i)]/\eta(a_i) \rightarrow N(0, 1)$$

and

$$\hat{\eta}(a_i, N_i) \longrightarrow \eta(a_i) \quad \text{in probability}$$

as $N_i \longrightarrow \infty$, thus satisfying the hypotheses in Proposition 1. Similarly, Proposition 2 may be applied once confidence intervals are obtained at $g(a_i)$, $i = 1, \ldots, n$.

We shall devote the remainder of this section to a second application which is based on the regenerative approach for analyzing computer simulation experiments. (References [4, 5, 6, 7, 10] may be consulted for more details on the regenerative method.) A basic statistical problem in simulations is to estimate the quantity $g(\lambda) = E\left\{ f(\underline{X}(\lambda)) \right\}$ where f is a general real-valued function, λ is an input parameter, and $\underline{X}(\lambda)$ is the stationary random vector associated with $\left\{ \underline{X}(s, \lambda) : s \geq 0 \right\}$, the process being simulated.

-9-

In the regenerative method, we observe the process $\{\underset{\sim}{X}(s, \lambda):s \geq 0\}$ in random cycles of lengths $\alpha_1(\lambda)$, $\alpha_2(\lambda)$, ..., $\alpha_N(\lambda)$ and record in each cycle the values $Y_1(\lambda)$, $Y_2(\lambda)$, ..., $Y_N(\lambda)$ where $Y_k(\lambda)$ is the area under the curve $f(\underset{\sim}{X}(s,\lambda))$ in the kth cycle. The crucial conditions required for the regenerative method to be used are that the N pairs $\{(Y_k(\lambda), \alpha_k(\lambda))$ $k = 1, 2, \ldots, N\}$ are independent and identically distributed and that $g(\lambda) = E\{Y_1(\lambda)\}/E\{\alpha_1(\lambda)\}$. These conditions hold, for example, in simulating a GI/G/S queue with traffic intensity less than 1, letting cycles be defined in terms of the beginning of successive busy periods.

Now define the column vector $\underset{\sim}{U}_k(\lambda) = (Y_k(\lambda), \alpha_k(\lambda))$ and let

$$\underset{\sim}{\Sigma}(\lambda) = \begin{pmatrix} \alpha_{11}(\lambda) & \alpha_{12}(\lambda) \\ \alpha_{12}(\lambda) & \alpha_{22}(\lambda) \end{pmatrix} .$$

denote the covariance matrix for $\underset{\sim}{U}_k(\lambda)$. Denote the sample mean by

$$\underset{\sim}{\bar{U}}(\lambda, N) = \begin{pmatrix} \bar{Y}(\lambda, N) \\ \bar{\alpha}(\lambda, N) \end{pmatrix} = \frac{1}{N} \sum_{k=1}^{N} U_k(\lambda)$$

and the sample covariance by

$$\underset{\sim}{s}(\lambda, N) = \begin{pmatrix} s_{11}(\lambda, N) & s_{12}(\lambda, N) \\ s_{21}(\lambda, N) & s_{22}(\lambda, N) \end{pmatrix} = \frac{1}{N-1} \sum_{k=1}^{N} [\underset{\sim}{U}_k(\lambda) - \underset{\sim}{\bar{U}}(\lambda, N)][\underset{\sim}{U}_k(\lambda) - \underset{\sim}{\bar{U}}(\lambda, N)]'$$

where the prime denotes transpose. Next, define point estimates for $g(\lambda)$ as follows:

-10-

(1) Classical estimator

$$\hat{r}_c(\lambda, N) = \frac{\bar{Y}(\lambda, N)}{\bar{\alpha}(\lambda, N)} \quad ;$$

(2) Beale estimator

$$\hat{r}_b(\lambda, N) = \frac{\bar{Y}(\lambda, N)}{\bar{\alpha}(\lambda, N)} \cdot \frac{[1 + s_{12}(\lambda, N)/N\,\bar{Y}(\lambda, N)\ \bar{\alpha}(\lambda, N)]}{[1 + s_{22}(\lambda, N)/N\,\bar{\alpha}^2(\lambda, N)]} \quad ;$$

(3) Tin estimator

$$\hat{r}_t(\lambda, N) = \frac{\bar{Y}(\lambda, N)}{\bar{\alpha}(\lambda, N)} \left[1 + \left(\frac{s_{12}(\lambda, N)}{\bar{Y}(\lambda, N)\,\bar{\alpha}(\lambda, N)} - \frac{S_{22}(\lambda, N)}{\bar{\alpha}^2(\lambda, N)} \right) N^{-1} \right] \quad ;$$

(4) Jacknife estimator

$$\hat{r}_J(\lambda, N) = \frac{1}{N} \sum_{k=1}^{N} \theta_k(\lambda, N)$$

where $\theta_k(\lambda, \cdot) = N[\bar{Y}(\lambda, N)/\bar{\alpha}(\lambda, N)] - (N - 1) [\sum_{j \neq k} Y_j(\lambda)/ \sum_{j \neq k} \alpha_j(\lambda)]$.

Finally, define

$$\hat{\eta}_c(\lambda, N) = [s_{11}(\lambda, N) - 2\hat{r}_c(\lambda, N)\, s_{12}(N) + \hat{r}_c^2(\lambda, N)\, s_{22}(\lambda, N)]/\bar{\alpha}(\lambda, N)$$

and

$$\hat{\eta}_J(\lambda, N) = \left\{ \sum_{k=1}^{N} [\theta_k(\lambda, N) - \hat{r}_J(\lambda, N)]^2/(N-1) \right\}^{1/2} \quad .$$

Now let

$$Z_k(\lambda) = Y_k(\lambda) - g(\lambda)\, \alpha_k(\lambda)$$

and note that $E\{ Z_k(\lambda) \} = 0$ and define $\sigma^2(\lambda) = \mathrm{var}\left\{ Z_k(\lambda) \right\}$. Since

the vectors $\left\{ U_k(\lambda), k \geq 1 \right\}$ are i.i.d., it follows that $\left\{ Z_k(\lambda), k \geq 1 \right\}$

are i.i.d. By the central limit theorem for partial sums of i.i.d. random variables, it follows that

$$\sum_{k=1}^{N} z_k(\lambda)/N^{1/2} \; \sigma(\lambda) \implies N(0, 1)$$

as $N \longrightarrow \infty$, which may be rewritten

$$N^{1/2}[\hat{r}_c(\lambda, N) - g(\lambda)] \; \bar{\alpha}(\lambda, N)/ \; \sigma(\lambda) \implies N(0, 1) \; .$$

Since $\bar{\alpha}(\lambda, N) \longrightarrow E\{\alpha_1(\lambda)\}$ a.e., it follows that

$$N^{1/2}[\hat{r}_c(\lambda, N) - g(\lambda)]/\eta(\lambda) \implies N(0, 1) \; ,$$

where $\eta(\lambda) = \sigma(\lambda)/E\{\alpha_1(\lambda)\}$. Now it may be shown that

$$N^{1/2}[\hat{r}_c(\lambda, N) - \hat{r}_b(\lambda, N)] \longrightarrow 0 \quad \text{a.e.,}$$

$$N^{1/2}[\hat{r}_c(\lambda, N) - \hat{r}_t(\lambda, N)] \longrightarrow 0 \quad \text{a.e.,}$$

$$N^{1/2}[\hat{r}_c(\lambda, N) - \hat{r}_J(\lambda, N)] \longrightarrow 0 \quad \text{a.e.,}$$

and that $\hat{\eta}_c(\lambda, N) \longrightarrow \eta(\lambda)$ and $\hat{\eta}_J(\lambda, N) \longrightarrow \eta(\lambda)$ in probability as $N \longrightarrow \infty$. Hence, the conditions of Proposition 1 are satisfied with any of the following substitutions:

$$\hat{r}_c(a_i, N_i), \; \hat{r}_b(a_i, N_i), \; \hat{r}_t(a_i, N_i) \quad \text{or} \quad \hat{r}_J(a_i, N_i)$$

substituted for $\hat{r}(a_i, N_i)$, $i = 1, 2, \ldots, n$;

$\hat{\eta}_c(a_i, N_i)$ or $\hat{\eta}_J(a_i, N_i)$ substituted for $\hat{\eta}(a_i, N_i)$, $i = 1, 2, \ldots, n$.

To illustrate the application of Propisitions 1 and 2, consider a

simulation of the customer waiting time process $\{W_n, n \geq 1\}$ in a GI/G/1 queue. Suppose we wish to study the sensitivity of the mean stationary waiting time $\beta(\lambda) = E\{W(\lambda)\}$ to the arrival rate λ over the range $2 \leq \lambda \leq 6$, with the service rate $\mu = 10$. In what follows, we shall illustrate the proposition for this simulation using the "classical" estimators $\hat{r}_c$ and $\hat{\eta}_c$, though we could have chosen any of the estimators given above.

In the queueing simulation, we say that the kth busy cycle is initiated with the arrival of the kth customer to find an empty queue. Suppose that simulation runs consisting of $N_1 = N_2 = N_3 = 10,000$ busy cycles are made at parameter settings $\lambda = a_1 = 3$, $\lambda = a_2 = 4$, and $\lambda = a_3 = 5$. Let $\alpha_k(\lambda)$ denote the number of customers served in the kth busy cycle, and let $Y_k(\lambda)$ be the sum of the waiting times for those customers. Then it may be shown, cf. [4], that $\{(Y_k(\lambda), \alpha_k(\lambda), k \geq 1\}$ are independent and identically distributed, and $E\{W(\lambda)\} = E\{Y_1(\lambda)\}/E\{\alpha_1(\lambda)\}$. Hence, it is appropriate to apply the regenerative method as discussed above. In particular, we can compute, for $i = 1, 2, 3$, $\bar{Y}(a_i, N_i)$, $\bar{\alpha}(a_i, N_i)$, $s_{11}(a_i, N_i)$, $s_{12}(a_i, N_i)$, and $s_{22}(a_i, N_i)$ and from these we can compute $\hat{r}_c(a_i, N_i)$ and $\hat{\eta}_c(a_i, N_i)$ as defined avove.

Suppose that, as a result of these computations for a simulation run,

$$\hat{r}_c(a_1, N_1) = .04 \qquad \hat{\eta}_c(a_1, N_1) = .20$$

$$\hat{r}_c(a_2, N_2) = .06 \qquad \hat{\eta}_c(a_2, N_2) = .30$$

$$\hat{r}_c(a_3, N_3) = .10 \qquad \hat{\eta}_c(a_3, N_3) = .50$$

Recall that approximate $100(1 - \gamma)\%$ confidence intervals at $\lambda = a_i$ are given by $\hat{r}_c(a_i, N_i) \pm \hat{\eta}_c(a_i, N_i) \phi^{-1}(1 - \gamma/2)/N_i^{1/2}$. For example, if

95% confidence intervals are desired, these would be

$$.03608 \leq g(3) \leq .04392 \quad \text{with 95\% confidence}$$

$$.05412 \leq g(4) \leq .06588 \quad \text{with 95\% confidence}$$

$$.09020 \leq g(5) \leq .10980 \quad \text{with 95\% confidence.}$$

Now assume that $g(\lambda) = E\{W(\lambda)\}$ is approximately quadratic for $2 \leq \lambda \leq 6$. From Proposition 1, an approximate $100(1-\gamma)\%$ confidence interval at λ is given by $\hat{r}(\lambda, N_1, N_2, N_3) \pm \hat{v}(\lambda, N_1, N_2, N_3) \, \Phi^{-1}(1 - \gamma/2), \quad 2 \leq \lambda \leq 6,$ where

$$\hat{r}(\lambda, N_1, N_2, N_3) = \Psi(\lambda) \begin{bmatrix} .04 \\ .06 \\ .10 \end{bmatrix}$$

$$\hat{v}(\lambda, N_1, N_2, N_3) = \left\{ \Psi_1^2(\lambda)(.20)^2 + \Psi_2^2(\lambda)(.30)^2 + \Psi_3^2(\lambda)(.50)^2 \right\}^{1/2} / 100$$

and

$$\Psi(\lambda) = (1 \quad \lambda \quad \lambda^2) \begin{bmatrix} 1 & 3 & 9 \\ 1 & 4 & 16 \\ 1 & 5 & 25 \end{bmatrix}^{-1} = (1 \quad \lambda \quad \lambda^2) \begin{bmatrix} 10 & -15 & 6 \\ -9/2 & 8 & -7/2 \\ 1/2 & -1 & 1/2 \end{bmatrix} .$$

Thus, for example, a 95% confidence interval for $g(3.5)$ is

$$.04269 \leq g(3.5) \leq .05231 \quad \text{with 95\% confidence.}$$

Finally, using Proposition 2 together with the above confidence intervals at $\lambda = 3, 4,$ and 5, we obtain a $100(.95)^3\%$ confidence band for the function $g(\lambda)$ over $2 \leq \lambda \leq 6$:

$$\Psi(\lambda) \, A^1(m) \leq g(\lambda) \leq \Psi(\lambda) A^2(m)$$

for $a_m \leq \lambda \leq a_{m+1}$ and $m = 0, 1, 2, 3$, where

$$A^1(0) = \begin{bmatrix} .03608 \\ .06588 \\ .09020 \end{bmatrix} \qquad A^2(0) = \begin{bmatrix} .04392 \\ .05412 \\ .10980 \end{bmatrix} \qquad A^1(1) = \begin{bmatrix} .03608 \\ .05412 \\ .10980 \end{bmatrix} \qquad A^2(1) = \begin{bmatrix} .04392 \\ .06588 \\ .09020 \end{bmatrix}$$

$$A^1(2) = \begin{bmatrix} .04392 \\ .05412 \\ .09020 \end{bmatrix} \qquad A^2(2) = \begin{bmatrix} .03608 \\ .06588 \\ .10980 \end{bmatrix} \qquad A^1(3) = \begin{bmatrix} .03608 \\ .06588 \\ .09020 \end{bmatrix} \qquad A^2(3) = \begin{bmatrix} .04392 \\ .05412 \\ .10980 \end{bmatrix} .$$

REFERENCES

[1] BILLINGSLEY, P. (1968, Convergence of Probability Measures: John Wiley, New York.

[2] BOWDEN, D.C.. (1970), Simultaneous Confidence Bands for Linear Regression Models, J. Am. Stat. Assoc. 65, 413-421.

[3] CRANE, M.A. (1975), A Bounding Technique for Polynomial Functions, SIAM J. Applied Math. 29.

[4] CRANE, M.A. and IGLEHART, D.L. (1974). Simulating stable stochastic systems, I: General multi-server queues. J.Assoc. Comput. Mach. 21, 103-113.

[5] CRANE, M.A. and IGLEHART, D.L.(1974). Simulating stable stochastic systems, II: Markov chains. J.Assoc. Comput. Mach. 21, 114-123.

[6] CRANE, M.A. and IGLEHART, D.L. (1974). Simulating stable stochastic systems, III: Regenerative processes and discrete-event simulations. Operations Res. 23, 33-45.

[7] CRANE, M.A. and IGLEHART, D.L. (1974). Simulating stable stochastic systems, IV: Approximation techniques. Management Sci. 21, 1215-1224.

[8] GRAYBILL, F.A. (1961). An Introduction to Linear Statistical Models, McGraw-Hill, New York.

[9] HAMMING, R.W. (1962). Numerical Methods for Scientists and Engineers, McGraw-Hill, New York.

[10] IGLEHART, D.L. (1974). Simulating stable stochastic systems, V: Comparison of ratio estimators. To appear in Naval Research Logistics Quarterly.