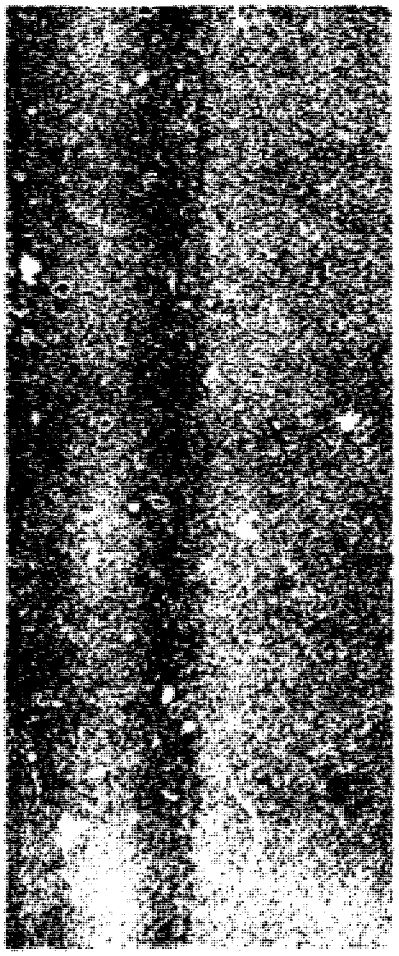
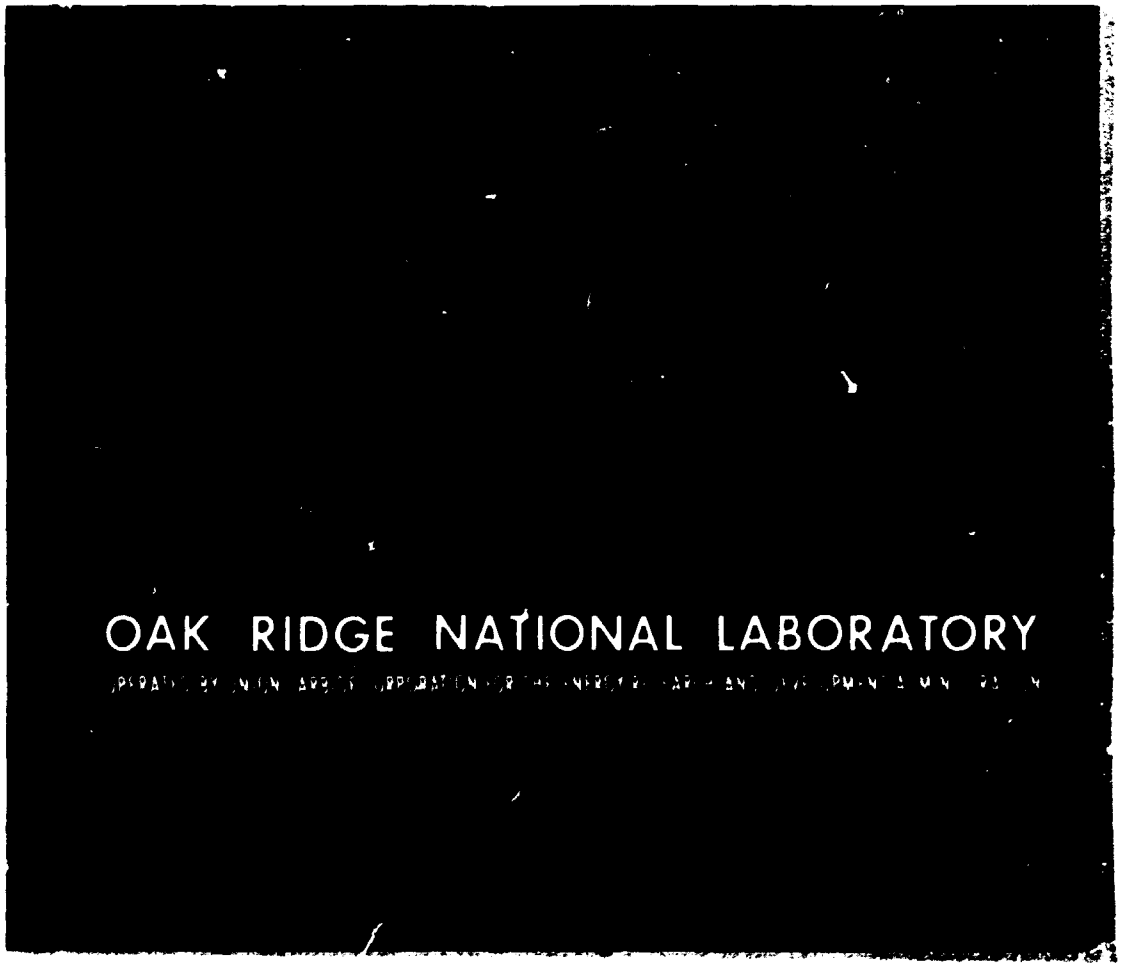
MATHEMATICS and STATISTICS RESEARCH DEPARTMENT

PROGRESS REPORT
for Period Ending June 30, 1976





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MATHEMATICS AND STATISTICS RESEARCH DEPARTMENT PROGRESS REPORT

for Period Ending June 30, 1976

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PART D. PRESENTATION OF RESEARCH RESULTS

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Preface

Undoubtedly, a highlight of the year's activities of the Mathematics and Statistics Research Department was the Visiting Mathematicians Program. Several distinguished mathematicians and statisticians visited the department to talk about our research, and theirs, and to participate in our seminar programs. Spending a full week with us were Richard Barlow of the University of California and Florida State University, Ralph Bradley of Florida State University, Walter Gautschi of Purdue University, Paul Halmos of Indiana University, Pete Stewart of the University of Maryland, Richard Varga of Kent State University, and Eugene Wachspress of the Knolls Atomic Power Laboratory. Several other mathematicians and statisticians of note visited the department for one to three days. Many of these visitors participated in a new venture, the Mathematics Colloquium Series, sponsored jointly by the department and the University of Tennessee's Department of Mathematics. A list of these speakers and their topics is given in Part C.

The department was pleased to have Sherwood F. Ebey of the University of the South and Douglas S. Robson of Cornell University spend parts of their sabbatical leaves with us. Sherwood Ebey worked with the Statistics Section on a number of statistical problems and helped administer the Southern College University Union Science Semester. Douglas Robson participated in the biostatistics program and contributed to the solution of a number of important problems in the ORNL Biology and Environmental Sciences Division.

Robert C. Meacham joined the department from the University of Tennessee. He complements the Computing Support Section, which was reorganized under the direction of William Lever.

For part of the year Toby Mitchell was on leave. He spent five months with the Department of Statistics at the University of Wisconsin, Madison, and five months at the National Institute of Environmental Health Sciences at the Research Triangle in North Carolina.

The department is proud to acknowledge a singular honor conferred upon one of its members: V. R. R. Uppuluri was elected to membership in the International Statistical Institute in recognition of his contributions to statistical research.

Part A. Mathematical and Statistical Research

1. Statistical Estimation

K. O. Bowman J. E. Cope[1] D. S. Robson B. W. Rust[1] D. G. Wilson

DISTRIBUTIONAL PROPERTIES OF MAXIMUM LIKELIHOOD ESTIMATORS OF THE PARAMETERS OF A MIXTURE OF TWO NORMALS

An investigator may believe that certain data are a sample from a mixture of two or more normal distributions. This belief may come from observing a bimodal or multimodal curve obtained by plotting the data or from a knowledge of the population that generated the data. As a trivial example, height measurements of adult human beings appear to come from a mixture of two normal distributions, one for the female portion of the population and one for the male. Nontrivial examples abound and range from the distribution of DNA (deoxyribonucleic acid) content of megakaryocyte cells to the distribution of fish lengths in a commercial fisherman's catch. Experimental biologists and commercial fisheries alike wish to estimate the parameters and the proportions of the underlying distributions without attempting to classify each observation. In addition, they would like to obtain reliable estimates at the least cost, that is, from as few observations as possible.

The problem is, then, to devise an economical scheme for estimating the means, standard deviations, and proportions associated with a sample from a mixture of normal distributions and to determine the effect of sample size on the reliability of these estimates.

Bowman and Shenton[2] have investigated these questions for the moment estimators of the five parameters of a mixture of two normal distributions. We are now investigating them for the maximum likelihood estimators.

Part of the motivation for this work is the desire to solve a frequently occurring practical problem, but in addition we expect to extend statistical theory. Maximum likelihood estimators have been widely used for estimating the parameters of distributions because their asymptotic properties have been extensively studied. However, for finite sample sizes their properties are unknown. Our study will contribute to a better understanding of the maximum likelihood estimators for small sample sizes.

Given a data set $\bar{x} = \{x_i\}$, $i = 1, \ldots, n$, which is assumed to come from a mixture of two normal distributions, the maximum likelihood estimators are the values $(\hat{\mu}_1, \hat{\sigma}_1, \hat{\mu}_2, \hat{\sigma}_2, \hat{p})$ of the five parameters which maximize the likelihood function $L(\mu_1, \sigma_1, \mu_2, \sigma_2, p, \bar{x})$ defined by

$$L = \prod_{i=1}^{n} \left\{ \frac{p}{\sqrt{2\pi}\sigma_1} \exp[-(x_i - \mu_1)^2/(2\sigma_1^2)] + \frac{1-p}{\sqrt{2\pi}\sigma_2} \exp[-(x_i - \mu_2)^2/(2\sigma_2^2)] \right\}.$$

Setting the partial derivative of L with respect to each of the five parameters equal to zero gives five coupled, nonlinear, homogeneous equations for the estimators. The mathematical questions are: When do these equations have no solution, exactly one solution, or many solutions; assuming that a solution does exist, how does one go about finding one; and how does the sample size influence the answers to the two previous questions?

We have developed an iterative scheme for solving the nonlinear equations. Using the computer program

1. Computing Applications Department.

2. K. O. Bowman and L. R. Shenton, "Space of Solutions for a Normal Mixture," *Biometrika* **60**, 629–36 (1973).

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implementing this scheme, we are conducting a Monte Carlo investigation of the effect of sample size on the computed estimators. We repeatedly generate a specified number of samples from a known mixture of two normal distributions and compute the maximum likelihood estimators. After a specified number of repetitions, we compute the first four moments of the distribution of estimators. The means of the estimator values are compared with the parameter values used to generate the samples. This is a rather time-consuming investigation, and although it is well under way, it is not nearly completed.

Preliminary indications are that the maximum likelihood estimators are not noticeably better for "small" sample sizes than are the moment estimators, but we cannot yet make a quantitative statement.

SUBOPTIMAL CONSTRAINED INTERVAL ESTIMATION BY MEANS OF LINEAR PROGRAMMING

The numerical solution of Fredholm integral equations of the form

$$\int_a^b K(t, s)x(s)\,ds = \hat{y}(t) + \hat{\epsilon}(t) ,$$

where $K(t, s)$ and $\hat{y}(t)$ are known functions and $\hat{\epsilon}(t)$ is a stochastic measuring error, is an important problem in many physical situations. The usual approach is to replace the integral equation by a corresponding linear system,

$$K\mathbf{x} = \mathbf{y} + \boldsymbol{\epsilon} , \tag{1}$$

and to assume that the stochastic error vector $\boldsymbol{\epsilon}$ is chosen from a joint normal distribution with variance matrix S^{-2}, which, without loss of generality, can be assumed to be diagonal. To estimate any integral quantity of the form

$$\phi = \int_a^b w(s)x(s)\,ds ,$$

where $w(s)$ is a known function, one seeks to estimate the approximating linear functional

$$\phi = \mathbf{w}^T\mathbf{x}$$

subject to the constraints imposed by (1). The system (1) is almost always very poorly conditioned, so it is possible to obtain physically meaningful solutions only by applying a priori constraints on the problem. An often very powerful and almost always physically justified constraint is that the solution $\mathbf{x}$ be non-negative.

In solving such constrained estimation problems it is important to calculate confidence-interval estimates to get an idea of the amount of uncertainty in the answer. Rust and Burrus[3] have shown that the confidence-interval bounds ϕ^{lo} and ϕ^{up} can be obtained as the roots of the equation

$$L(\phi) = \mu^2 ,$$

where μ is a constant corresponding to the desired confidence level and $L(\phi)$ is the piecewise quadratic functional

$$L(\phi) = \min_{\mathbf{x}} \left\{ (K\mathbf{x} - \mathbf{y})^T S^{-2} (K\mathbf{x} - \mathbf{y}) \mid \mathbf{x} \geq 0 ,\ \mathbf{w}^T\mathbf{x} = \phi \right\} .$$

A computational procedure for computing these roots would involve parametric quadratic programming, which is difficult and very expensive. An alternate approach[4] is to calculate suboptimal approximations to ϕ^{lo} and ϕ^{up}, using various linear programming approximations. These approximations are obtained by replacing the 2-norm constraint,

$$(K\mathbf{x} - \mathbf{y})^T S^{-2} (K\mathbf{x} - \mathbf{y}) \leq \mu^2 , \tag{2}$$

with either an ∞-norm constraint,

$$\max_i \left\{ |S^{-1}(K\mathbf{x} - \mathbf{y})|_i \right\} \leq \mu , \tag{3}$$

or a 1-norm constraint,

$$|\mathbf{e}^T S^{-1} (K\mathbf{x} - \mathbf{y})| \leq \mu , \tag{4}$$

where $\mathbf{e}^T = (1, 1, \ldots, 1)$. We have developed and tested a number of strategies for reducing these approximating problems to a standard linear programming tableau; one strategy uses both (3) and (4) to give a

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3. B. W. Rust and W. R. Burrus, *Mathematical Programming and the Numerical Solution of Linear Equations*, American Elsevier, New York, 1972, pp. 162–72.

4. B. W. Rust and W. R. Burrus, *Suboptimal Methods for Solving Constrained Estimation Problems*, DASA-2604 (January 1971).

better approximation to the ellipsoidal constraint region defined by (2). The linear programming problems corresponding to this last strategy can be written

$$\phi^{\{\text{up}\}}_{\{\text{lo}\}} = \{^{\max}_{\min}\} \left\{ (\mathbf{w}^T, 0^T)\begin{pmatrix}\mathbf{x}\\ \mathbf{p}\end{pmatrix} : \begin{pmatrix}\mathbf{x}\\ \mathbf{p}\end{pmatrix} \geq 0 , \right.$$

$$\left. \begin{pmatrix} K & -I \\ -K & -I \\ 0 & \mathbf{e}^T S^{-1} \\ 0 & S^{-1} \end{pmatrix} \begin{pmatrix}\mathbf{x}\\ \mathbf{p}\end{pmatrix} \leq \begin{pmatrix} \mathbf{y} \\ -\mathbf{y} \\ \mu\sqrt{m} \\ \mu\mathbf{e} \end{pmatrix} \right\} .$$

where m is the number of rows in K, I is the mth order identity matrix, and $\mathbf{p}$ is a dummy vector defined by $\mathbf{p} = |K\mathbf{x} - \mathbf{y}|$.

We are currently studying the following extensions of this work:

1. improving the bounds by prerotating the constraint region by means of the singular value decomposition,
2. allowing the incorporation of other kinds of a priori constraints,
3. allowing for errors in the matrix K,
4. computing the bounds corresponding to directly constructed polytope confidence regions.

RANDOMIZED SAMPLING RATES IN SPARSELY SAMPLED STRATA

Any stratification plan can ordinarily be improved for purposes of sampling and estimation by further partitioning the population into finer classes of even greater homogeneity. The requirement that every stratum be represented in the sample, however, limits the number of strata to, at most, the number of elements in the proposed sample. The need for a standard error estimate from the sample further reduces the possible number of strata to, at most, half of the proposed sample size, since each stratum must be sampled at least twice to provide within-strata estimates of variance. This latter need conflicts with the primary objective of stratification and is commonly circumvented by the post facto pairing of singly sampled strata for purposes of variance estimation.

Randomization of sampling rates among sparsely sampled strata offers an honest means of circumventing the "two per stratum" requirement. An extreme form of such a scheme would allow all but one stratum to be singly sampled, provided that this stratum is randomly picked. More generally, if k out of K strata are singly sampled and the remaining $K - k$ are (say) doubly sampled, then an unbiased estimator of sampling error variance exists when the choice of the k strata to be singly sampled is a random choice. The variance of a stratified sample estimate

$$\bar{y}_{\text{strat}} = \sum_{h=1}^{K} W_h \bar{y}_h$$

in this case becomes

$$\text{var}(\bar{y}_{\text{strat}}) = \sum_{h=1}^{K} W_h^2 \left(\frac{K+k}{2K} - \frac{1}{N_h} \right) S_h^2 ,$$

where S_h^2 is the variance among the N_h elements in the hth stratum. An unbiased estimator of this sampling error variance is then

$$\text{var}(\bar{y}_{\text{strat}}) = \frac{K}{K-k} \sum W_h^2 \left(\frac{K+k}{2K} - \frac{1}{N_h} \right) s_h^2 ,$$

where the sum now extends only over those $K - k$ doubly sampled strata where variance estimates s_h^2 are available.

The concept of randomized sampling rates applies also to multistage sampling designs and adapts to more general probability sampling schemes for randomizing the rates. Its primary utility, however, appears to reside in the common situation of sparsely sampled strata.

2. Statistical Testing

J. J. Beauchamp K. O. Bowman F. L. Miller, Jr. D. S. Robson
L. R. Shenton[1] M. Sobel[2] V. R. R. Uppuluri

EFFECT OF NONNORMALITY ON THE DISTRIBUTION OF THE *t* STATISTIC

Preliminary results from the investigation of the effect of nonnormality upon the distribution of the *t* statistic are given in a previous report.[3] Table I gives the combinations of skewness ($\sqrt{\beta_1}$) and kurtosis (β_2) values for three of the distributions being considered. Since the $\sqrt{\beta_1}$ and β_2 values for the gamma and Weibull distributions are related to the parameters of their respective distribution functions, we are considering a meaningful range of parameter values for these two distributions. In particular, for the gamma probability density function, we consider

$$f_g(x) = \frac{x^{\rho-1}}{\Gamma(\rho)} \exp(-x), \quad x > 0,$$

where

$$2\beta_2 - 3\beta_1 - 6 = 0,$$

and for the Weibull probability density function, we consider

$$f_w(x) = cx^{c-1} \exp(-x^c), \quad x > 0,$$

where

$$2\beta_2 - 3\beta_1 - 6 < 0.$$

The range of the parameters is $\rho = 1(1)10, 15, 25$, and $c = 1.2(0.2)4.0$. Sample sizes of 25, 50, 75, and 100 are being used in calculating the higher moments of the distribution of the *t* statistic for each of the assumed nonnormal parent distributions. An ongoing study to apply new methods of evaluating summations will make it possible to extend the range of sample sizes to values much less than 25. The basic parent distributions under investigation cover a wide range of practical statistical distributions in the life and physical sciences.

Although the determination of the higher moments of the *t* statistic from different parent distributions is helpful in evaluating the effect of nonnormality, a more practical consideration is to have knowledge about the level of significance expected when tabled *t* values are used on samples from nonnormal distributions. A program by Amos and Daniel[4] allows us to determine specific percentage points of interest from the distribution of the *t* statistic. We have been able to examine the contours for particular levels of significance in the $(\sqrt{\beta_1}, \beta_2)$-space from the results of the above calculations. Figure 1 shows the actual level of significance achieved on the distribution of the *t* statistic when the underlying distribution is a type I or A distribution and the tabled 95% *t* value ($t = 1.711$) is used for a sample size of 25. We may conclude from an examination of this figure that if an experimenter is sampling from a type I or A distribution and is using the tabled *t* statistic for a one-sided test at the 5% level of significance, then the actual level of significance would be between 3 and 7% for a sample size of 25.

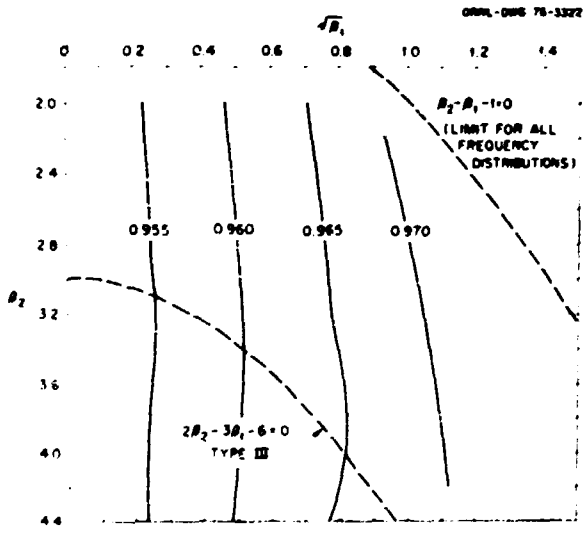

Fig. 1. Percentage contours for $t_{n\ 25} = 1.711$.

1. University of Georgia.
2. University of California at Santa Barbara.
3. "Effect of Nonnormality on the Distribution of the *t* Statistic," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCCND/CSD-18, pp. 4–5 (October 1975).
4. D. E. Amos and S. L. Daniel, *Tables of Percentage Points of Standardized Pearson Distributions*, SC RR-71 0348, Sandia Laboratories (1971).

Table 1. Combinations of $\sqrt{b_1}$, b_2 considered

	$\sqrt{b_1}$														
b_2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
2.0	1.3[a]	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3						
2.2	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3					
2.4	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3				
2.6	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3			
2.8	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3		
3.0	1.3	1.3	1.3	1.3	1.3	1.3	1	1.3	1.3	1.3	1.3	1.3	1.3	1.3	
3.2	1.2	1.2	1	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	
3.4	1.2	1.2	1	1	1	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3
3.6	1.2	1.2	1.2	1.2	1	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3
3.8	1.2	1.2	1.2	1.2	1.2	1	1	1	1.3	1.3	1.3	1.3	1.3	1.3	1.3
4.0	1.2	1.2	1.2	1.2	1.2	1.2	1	1	1	1.3	1.3	1.3	1.3	1.3	1.3
4.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1	1	1.3	1.3	1.3	1.3	1.3	1.3
4.4	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1	1	1	1	1	1	1

[a] 1 = mixture of normal distributions.
2 = Gram-Charlier type A distribution.
3 = Pearson type I distribution.

NEW SYSTEM OF BIVARIATE MODEL FOR THE DISTRIBUTION OF TWO PARAMETERS

Bowman and Shenton[5] have constructed a set of contours for the $\sqrt{b_1}$ and b_2 joint distributions by transforming each variate to a normal variate, using Johnson's system of transformations. Although this set of contours shows a 90, 95, and 99% region of true contents of distributions and a good practical use for simplicity, it does not contain the smallest region, nor does it represent the equiprobability of a true bivariate distribution of $\sqrt{b_1}$ and b_2.

We have developed a new model for the general sampling of two parameters

$$f(\sqrt{b_1}, b_2) = w(\sqrt{b_1})g(b_2 \mid \sqrt{b_1}), \qquad (1)$$

where $w(\cdot)$ refers to the S_U approximation to the marginal probability density function and $g(\cdot \mid \cdot)$ refers to a conditional gamma distribution. Thus,

$$w(\sqrt{b_1}) = [\delta/(2\pi)^{1/2}] \left\{1/[\lambda^2 + (\sqrt{b_1} - \xi)^2]^{1/2}\right\} \times \exp\left(-\tfrac{1}{2}\left\{\gamma + \delta \sinh^{-1}[(\sqrt{b_1} - \xi)/\lambda]\right\}^2\right),$$

$$g(b_2 \mid \sqrt{b_1}) = \frac{k[k(b_2 - 1 - b_1)]^{p(\sqrt{b_1})-1}}{\Gamma[p(\sqrt{b_1})]} \times \exp[-k(b_2 - 1 - b_1)],$$

where $k > 0$, $p(\sqrt{b_1}) > 0$, and $\xi, \lambda, \gamma, \delta$ are found in Johnson's table.[6]

We have shown that the new set of contours constructed by using the new bivariate distribution, $f(\sqrt{b_1}, b_2)$, approximates almost precisely the true equiprobability of the joint distribution $\sqrt{b_1}$ and b_2.[7] Further, the new model can be extended by utilizing a variety of univariate distributions to approximate a function of any two parameters x and y. For example:

a. Instead of the gamma density in Eq. (1), we may use a Weibull component. Thus,

$$f(x, y) = [w(x)e^{-X(x)k}]\{p(x)[k(y - 1 - x^2)]^{p(x)-1}\},$$

where

$$X(x) = [k(y - 1 - x^2)]^{p(x)}$$

for $k > 0$, $p(x) > 0$, $y > 1 + x^2$.

If fitted by moments, quadrature methods would be required.

b. Another possibility is to use the F-ratio density instead of the gamma. Thus,

$$f(x, y) = w(x)\frac{a^{q+1}(y - 1 - x^2)^{p-1}\Gamma(p + q + 1)}{(a + y - 1 - x^2)^{p+q+1}\Gamma(p)\Gamma(q + 1)}$$

for $-\infty < x < \infty$ and $y > 1 + x^2$.

5. K. O. Bowman and L. R. Shenton, "'Omnibus' Test Contours for Departures from Normality Based on $\sqrt{b_1}$ and b_2," *Biometrika* **62**, 243–50 (1975).

6. E. S. Pearson and H. O. Hartley, *Biometrika Tables for Statisticians*, vol. 2, Cambridge University Press, London, 1972.

7. L. R. Shenton and K. O. Bowman, "A Bivariate Model for the Distribution of $\sqrt{b_1}$ and b_2," *J. Am. Stat. Assoc.*, to be published.

where $a > 0$, $p > 0$, $q >$ 1, and a, p, and q may be taken as functions of x.

c. Interchange the roles of x and y and use Johnson's S_I for the marginal of y and a beta distribution for the conditional. Thus,

$$f(y, x) = w(y) \frac{\Gamma(p+q)}{\Gamma(p)\Gamma(q)} \times \frac{|\sqrt{(y-1)} - x|^{p-1} |\sqrt{(y-1)} + x|^{q-1}}{2^{p+q-1}(y-1)^{1/2(p+q-1)}},$$

where $p > 0$, $q > 0$, $x^2 <$ y 1, and the indices p and q are functions of y.

MARGINAL SIZE OF THE ONE-SIDED FISHER EXACT TEST

Discreteness of the hypergeometric distribution produces small sample irregularities in the operating characteristics of a one-sided Fisher Exact Test for a 2 × 2 table. Numerical exploration of the power surface has revealed anomalies such as decreasing power with increasing sample size. Power characteristics may be substantially improved by allowing the conditional size of the test to increase while retaining control over a marginal size.

In the context of one-sided, two-sample tests of homogeneity, only the two sample sizes (row totals n_1 and n_2, say) are predetermined by the experimenter, who is therefore justified in dropping the condition of fixed column totals in order to achieve nominal test size conditioned only on sample sizes. One way of achieving this end is to retain the structure of the Fisher Exact Test but to implement the test at a predetermined conditional significance level α_c, exceeding the nominal target level α. This conditional size α_c is calculated as the tail probability of the hypergeometric distribution determined by both row and column totals. The value of α_c is chosen, however, to ensure only that the H_0-average tail probability exceeds α when conditioned on just the row totals.

HYPOTHESIS TESTING

Sobel and Uppuluri[8] have developed a sparse- and crowded-cell test for the hypothesis that a set of data may be described as coming from a specified distribution. Miller and Quesenberry[9] have evaluated several statistics for testing uniformity, and the sparse- and crowded-cell test has been applied to the alternative distributions of the report in order to see whether it is a worthwhile competitor. The sparse- and crowded-cell test is easy to apply in practice because of its simplicity of computation. One merely counts the number of cells with less than a given number of occupants or more than another given number. If this number is greater than some predetermined constant, the hypothesis is rejected. The above assumes that the interval is divided into cells of equal probability.

For the first member of family 1 of the report,[9] the power of the sparse- and crowded-cell test for samples of size 50 can be as high as 82%, depending on the criteria for sparseness and crowdedness. For comparison, the Watson U^2 statistic has power 85%, the Cramer von Mises statistic has power 98%, and the Anderson-Darling statistic has power 99%.

The test is appealing both from the viewpoint of ease of computation and how much power you can get from such a relatively coarse classification procedure. We are trying to improve the power of the test, while not overly complicating the computation, by considering also the number of runs of sparse and crowded cells. This addition of "neighbor" information will hopefully sharpen the test.

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8. M. Sobel and V. R. R. Uppuluri, "Sparse and Crowded Cells and Dirichlet Distributions," *Ann. Stat.* 2, 977–87 (1974).

9. F. L. Miller, Jr., and C. P. Quesenberry, *Statistics for Testing Uniformity on the Unit Interval*, UCCND/CSD-12 (April 1975).

3. Experimental Design

J. A. John[1] M. D. Morris[3]
H. M. McClellan[2] D. S. Robson
T. J. Mitchell R. C. Ward

OPTIMAL INCOMPLETE BLOCK DESIGNS

One of the most effective techniques for increasing the precision of an experiment is "blocking," that is, the grouping of the experimental units into relatively homogeneous blocks, within each of which a subset of the experimental treatments is then applied. The problem is to determine the best way of assigning treatments to blocks. The classical approach to this problem has been to place certain requirements of "balance" on the design and to devise algebraic or geometric methods for constructing designs that satisfy these requirements. In this research, we take a somewhat different approach, based on the application of some well-established optimality criteria.

We shall assume that r replications of each of v treatments are to be sorted into b blocks of size k, where $k < v$. We restrict consideration to designs in which every pair of treatments appears together in either λ_1 or λ_2 blocks, where $\lambda_2 = \lambda_1$ or $\lambda_2 = \lambda_1 + 1$. Extensive computer work[4] has previously implied that optimum incomplete block designs should have this form.

In a previous report,[5] we described a method for constructing designs of this type that are D-optimum, that is, designs that minimize the determinant of the variance-covariance matrix Ω of the treatment parameters. This method utilized a relationship between Ω and the incidence matrix of a regular graph of degree t with v vertices, where t is related to the design parameters by

$$r(k-1) = m(v-1) + t,$$

where m is an integer. A rather elaborate computer program was written to construct the complete set of regular graphs for all $v \le 12$, except for the case $(v, t) = (12, 5)$, which was too extensive to handle. For every parameter set (v, k, r) we then searched the set of regular graphs with the appropriate degree t to find those that yielded the optimum Ω. Using the algorithm described by John,[6] we then attempted to construct the design itself. If no design was found to exist for the optimum Ω, we then considered the second best, third best, and so forth.

This procedure was applied using three different definitions of optimality, all of which, roughly speaking, have to do with minimizing the variances of the estimated treatment effects:

1. D-optimality: minimize the determinant of Ω.
2. A-optimality: minimize the trace of Ω.
3. E-optimality: minimize the maximum eigenvalue of Ω.

Occasionally, the E-optimal design differed from the D- and A-optimal designs, but in all cases the D- and A-optimal designs were the same.

We have compiled a list of these optimal designs and their properties[7] for all cases in which $v \le 12$ and $r \le 10$ [except for the seven cases corresponding to $(v, t) = (12, 5)$]. For the 33 cases in which the optimum design appears to be new, we have presented it in full.

A_2-OPTIMAL DESIGNS

Experimenters are frequently interested in determining, in a least squares sense, the coefficients of a polynomial of order r in k variables that approximate a set of n observations. For example, an experimenter may want to approximate the observations y by the second-order polynomial in two variables x_1 and x_2:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_{1,2} + \beta_{12} x_{1,1} + \beta_{22} x_{2,2},$$

where $x_{i,j}$ is the vector whose pth component is the product of the pth components of the x_i and x_j vectors. The unknown quantities to be determined are

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1. University of Southampton
2. SCUC Science Semester Student Participant, University of the South
3. ORAU Laboratory Graduate Participation Fellow, Virginia Polytechnic Institute and State University
4. T. J. Mitchell, "Computer Construction of 'Small D-optimal' Incomplete Block Designs," *Proc. 39th Session ISI*, 732–38 (1974).
5. "Construction of D-optimal Incomplete Block Designs," *Math Stat Res Dep Prog Rep June 01 19** J*, ORNL-4989, pp. 10–11 (December 1974).
6. J. A. John, "Computer Construction of Binary Incomplete Block Designs," submitted to *Appl. Stat.*
7. T. J. Mitchell and J. A. John, *Optimal Incomplete Block Designs*, ORNL CSD-8 (1976).

the β_i's. This problem can be restated as the problem of *determining* a real m-vector β^*, *minimizing* the Euclidean length of $X\beta - y$, given the real $n \times m$ matrix X and the real n-vector y. The symbolism $X\beta \cong y$ will denote this linear least squares problem.

Since the experimenter can frequently choose the values of the dependent variables at which the observations are taken, these values (design points) should be chosen such that the resulting answers are optimal in some sense. One such design criterion with statistical motivation is the criterion of "*D*-optimality." A *D*-optimal design which minimizes the volume of the joint confidence region for the least squares estimators of β is based on maximizing the determinant of $X'X$ and has been investigated by several statisticians. We have begun an investigation of a different design criterion called "K_2-optimality." Specifically, a K_2-optimal design minimizes the spectral condition number of X. The motivation for this criterion is based on perturbation results for the least squares problem. These results indicate that the magnitude of the relative error in the solution vector is essentially bounded by the sum of the magnitude of the relative errors in the X matrix and y vector magnified by the condition number of the X matrix. Thus if the condition number is minimized, the bound on the solution's relative error is minimized.

The spectral condition number of X, $K_2(X)$, is defined by

$$K_2(X) \equiv \| X \|_2 \, \| X^+ \|_2 \, ,$$

where X^+ is the Moore-Penrose generalized inverse of X and $\|\cdot\|_2$ is the spectral norm (2-norm). For our purposes, a better characterization of the spectral condition number of X is given by the singular values of X, which are the positive square roots of the eigenvalues of $X'X$. This characterization defines $K_2(X)$ as the ratio of the largest singular value to the smallest singular value. From this we can easily determine that $K_2(X) \geq 1$ and $K_2(X) = 1$ only when the columns of X are orthogonal, that is, only when X represents an orthogonal design. Thus, minimizing the spectral condition number of X is an attempt to make X represent more closely an orthogonal design.

We are in the initial phases of this research and have written a computer subroutine K2MIN that attempts to determine K_2-optimal designs with the variables x_i restricted to the unit cube $-1 \leq x_i \leq 1$, $i = 1, 2, \ldots, k$. K2MIN uses a transformation technique and Zangwill's modification of Powell's conjugate direction algorithm to find a local minimum of $K_2(X)$ inside the constrained region. Since K2MIN determines only a local minimum, there is no guarantee that the returned design points yield the global minimum for the constrained region. However, the possibility of not finding the global minimum can be reduced by performing the minimization several times, using widely separated initial design points.

Using K2MIN, we have constructed a design for a second-order model in two variables with six design points. The design has points at (1, 1), (0.1, 0.1), (0.915, 0.915), (−0.915, 0.915), (1, −0.465), and (−0.465, −1) and has a $K_2(X)$ value of 4.63. These design points are similar to those produced by Box and Draper[8] for a *D*-optimal design. The *D*-optimal design has points at (1, 1), (0.1315, 0.1315), (1, −1), (−1, 1), (−1, 0.3945), and (−0.3945, −1). This similarity as well as other properties of K_2-optimal designs are expected to be studied in the near future.

FACTORIAL DESIGNS FOR DETECTION OF MODEL INADEQUACIES

In the analysis of factorial experiments, a linear model containing only the mean and main effects is often assumed to be adequate. This procedure involves a tacit assumption that the main effects do not interact, or that interactions are negligible. While there may be some evidence to support this assumption, an additional test for model adequacy is often desirable.

In the context of analysis of variance, a test for lack of fit can be made, based on a noncentral χ^2 or noncentral F statistic. In each case the power of the test to detect nonnegligible interactions is a monotonically increasing function of a quadratic form

$$\beta_2' L \beta_2 \, .$$

where β_2 is a vector of interaction terms, and L is a positive semidefinite matrix determined by the experimental design. Therefore, by control of the experimental design, and hence the form of L, the experimenter can control (to some extent) the power properties of this test.

We are concerned with the selection of design classes and particular designs for which the power to detect nonnegligible two-factor interactions is high. The principal criterion for design selection has been the trace of L, $\mathrm{tr}(L)$; maximizing this quantity is equivalent

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8. M. J. Box and N. R. Draper, "Factorial Designs, the $|X'X|$ Criterion, and Some Related Matters," *Technometrics* 13, 731–42 (1971).

to maximizing the average value of $\beta_2' I \beta_2$ in an appropriate region of the β_2 space. We have shown for certain design sizes that a design is tr(I)-optimal if and only if it is orthogonal and of resolution IV. Design sizes for which these conditions exist have been derived.

For design sizes which do not allow construction of orthogonal resolution IV designs, various techniques have been used to find optimal or near optimal designs. For 2^k experiments, the class of fold-over designs has provided excellent results for designs with $2k$ to $3k$ points. (For a discussion of fold-over designs, see Box and Hunter.[9]) In the case of 3^k experiments, two classes of designs have been investigated. One is the class of designs generated by balanced arrays. This class was introduced and first studied by Chakravarti.[10] Another similar class, which we have formulated specifically for this problem, is under investigation. Computer searches and optimization routines are used to find optimal designs within each design class.

Designs which we find to be optimal or near optimal with respect to the tr(I) measure will be further examined with regard to more classical measures of design optimality.

OPTIMAL DESIGN FOR MEASURING SIMPLE EXPONENTIAL DECAY WITH POISSON SAMPLING ERROR

If $Y(T_1), \ldots, Y(T_k)$ are independent Poisson variables with mean values $E[Y(T)] = \alpha \exp(-\beta T)$, then for a sampling design with $n_i = np_i$ independent replicates at T_i, the variance of the maximum likelihood estimator of β is (asymptotically)

$$\operatorname{var}(\hat{\beta}) = \left[n\alpha T_{1/2}^2 \sum_{i=1}^{k} p_i 2^{-t_i} (t_i - \bar{t})^2 \right]^{-1}.$$

The variate $t_i = T_i / T_{1/2}$ is measured in "half-life" units of time:

$$T_{1/2} = (\ln 2)/\beta,$$

and $\bar{t}$ is the weighted mean:

$$\bar{t} = \frac{\sum_{i=1}^{k} p_i t_i 2^{-t_i}}{\sum_{i=1}^{k} p_i 2^{-t_i}}.$$

The (unique) optimal design for minimizing $\operatorname{var}(\hat{\beta})$ is a two-point design with np replicates at $t = 0$ and $n(1 - p)$ at $t = 2\xi = 3.688$, where ξ is the zero of $1 + 2^{-\xi} - \xi \ln 2$ and $p = (1 + 2^{\xi})^{-1}$. This design achieves

$$\bar{t} = 2^{-\xi+1} \ln 2,$$

$$\operatorname{var}(\hat{\beta}) = \left[n\alpha (\bar{t} T_{1/2})^2 \right]^{-1}.$$

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9. G. E. P. Box and J. S. Hunter, "The 2^{k-p} Fractional Factorial Designs, Part I," *Technometrics* 3, 311–51 (1961).

10. I. M. Chakravarti, "On Some Methods of Construction of Partially Balanced Arrays," *Ann. Math. Stat.* 32, 1181–85 (1961).

4. Probability

R. R. Coveyou S. A. Patil[1] M. Sobel[2] V. R. R. Uppuluri

MINIMAL SUFFICIENT CHARACTERIZATIONS OF UNIFORMITY

From the viewpoint of applications of the theory of stochastic processes to physical processes, for example, the analysis by the Monte Carlo method of neutron and other particle transport problems or of other physical (and social or biological) problems, the so-called uniform distribution on the real unit interval is of basic importance.

For many reasons, and in particular, because of the already wide use and even wider applicability of the Monte Carlo method to the solution of physical and other problems arising from nuclear and other energy programs, it would seem that a deeper understanding of this basic probability distribution is of great potential relevance.

A careful study of this distribution has been made. In particular, several results are obtained (some of which are presented below) which characterize this distribution by sets of conditions which are, in some sense, as weak as possible.

Let M denote a random variable with values in the real unit interval $[0, 1)$, and let U denote the random variable uniformly distributed on $[0, 1)$. Let D denote the "degenerate" random variable on this interval: $\text{Prob}[D = 0] = 1$. For each real x, let $x = [x] + \cdot x \cdot$, with $[x]$ an integer and $\cdot x \cdot \in [0, 1)$. For random variables M_1 and M_2, let $M_1 \overset{d}{=} M_2$ mean that M_1 and M_2 have the same distribution.

If, for each $u \in [0, 1)$,

$$(*)\quad M \overset{d}{=} \{M + u\},$$

then

$$M \overset{d}{=} U.$$

Also, if, for each integer $n \neq 0$,

$$(**)\quad M \overset{d}{=} \{nM\},$$

then M is a mixture of U and D.

We have shown that it is not necessary that (*) should hold for each $u \in [0, 1)$. In fact, if (*) holds for a single irrational $u \in [0, 1)$, the conclusion follows.

We have also shown that it is not necessary that (**) should hold for each $n \neq 0$. In fact, if (**) holds for each prime integer, then the conclusion follows.

Neither of these hypotheses can be further weakened.

Some applications of these results are to the field of random number generation and testing.

INFERENCES ABOUT RARE EVENTS

According to Weaver,[3] a small probability event, or an improbable event, is called a rare event. He observes that rare events are often, though not always, interesting. He also introduces the concept of a surprising event, which implies that the event is rare, though a rare event need not be surprising. This idea is illustrated in terms of dealing a bridge hand (13 playing cards) and tossing a metal disk with three possible outcomes. At a bridge table, when a hand of 13 spades is dealt, one may say that an improbable but not a surprising event occurred, since a dull hand is as likely (or unlikely) as any of the possible alternative outcomes of the dealing process. However, for the toss of a metal disk, standing on the edge would be a surprising event, since the probability of standing on the edge is very small in comparison with the other two alternatives.

In diverse fields of scientific studies, there is interest in understanding and making inferences about rare events. If observations are made at discrete time intervals, a rare event may not appear even once. In such a situation one problem of interest is to give confidence limits for the probability p of observing the rare event at any trial. A procedure based on a heuristic analysis, along with a set of tables and a few well-thought examples, is suggested by Gardiner in an unpublished memorandum.[4] One can justify this rigorously as follows.

One cannot obtain confidence limits on p from the theory of the binomial distribution, since the estimate

1. Tennessee Technological University
2. University of California at Santa Barbara.

3. W. Weaver, "Probability, Rarity, Interest and Surprise," *Sci. Mon.* 67, 390–92 (1948).
4. D. A. Gardiner, personal communication (1971).

$\hat{p}$ (of p) is zero. By studying the problem of rare events in the context of the phenomena of waiting times and frequencies of events, one can surpass this difficulty. As a matter of fact, one can find a waiting time W_1 (random variable) associated with the binomial distribution. Since W_1 has a geometric distribution with the same parameter p, we can obtain the confidence limits on p.

In a discrete time process, let N_n denote the frequency of rare events observed during $[0, n\Delta t]$ and W_1 denote the trial at which we observe the first rare event. Then we have

$$\text{Prob}[N_n = 0] = \text{Prob}[W_1 > n] = (1 - p)^n ,$$

which leads to

$$\text{Prob}[W_1 = n] = p(1 - p)^{n-1} , \qquad n = 1, 2, \ldots .$$

In order to find confidence limits for p at a significance level α, we look for a probability statement involving p and W_1. Using the relations

$$\text{Prob}[W_1 \leq n] = \text{Prob}[W_1 \ln(1 - p) \geq n \ln(1 - p)] = 1 - \alpha ,$$

we obtain

$$\text{Prob}[p \leq 1 - \alpha^{1/W_1}] = 1 - \alpha .$$

Since $W_1 > n$, it is reasonable to suggest $0 \leq p \leq 1 - \alpha^{1/n}$ as a $(1 - \alpha)$ confidence interval for p. This is the interval suggested by Gardiner as a confidence interval for p. More details may be found in the report by Uppuluri and Patil.[5]

We shall now discuss a discrete time version of the "waiting time paradox." This is in direct analogy with the waiting time paradox discussed by Feller[6] in the case of exponential waiting times and Poisson frequencies.

Suppose in a discrete time process events occur in accordance with a geometric process where the expected time between consecutive events is equal to $1/p$. Say we observe the system at an arbitrary but fixed instant of time t. We discuss the following question: What is the expectation $E(W_t)$ of the waiting time W_t for the next event? It is understood that the epoch t is independent of the times of occurrence of the events. As in the waiting time paradox for buses which arrive in accordance with a Poisson process, two contradictory answers stand to reason. The two answers are $1/p$ and $[1 + (1/p)] = E(1 + W_1)$. The paradox can be understood in terms of the following:

Proposition. Let the discrete random variables $X_1, X_2, \ldots$ be mutually independent with a common geometric distribution

$$\text{Prob}[X_i = x] = p(1 - p)^{x-1} , \quad x = 1, 2, \ldots .$$

Let $0 < t$ be a fixed natural number (though arbitrarily chosen), and let $S_k = X_1 + X_2 + \cdots + X_k$. The element X_k satisfying $S_{k-1} < t \leq S_k$ has the probability density function

$$f_t(x) = \begin{cases} p^2 x q^{x-1} , & x = 1, 2, \ldots, t \\ p^2 t q^{x-1} + p q^{x-1} , & x = t + 1, t + 2, \ldots . \end{cases}$$

The mean of this distribution is given by

$$\sum_{x=1}^{\infty} x f_t(x) = \frac{2}{p} - 1 - \frac{1}{p} q^{t+1} .$$

For proof, one may refer to the report by Uppuluri and Patil.[5]

WAITING TIMES AND INCOMPLETE DIRICHLET INTEGRALS

The incomplete Dirichlet integral of type I is introduced in a previous report[7] as a generalization of the incomplete beta function in the following way:

$$I_p^{(h)}(r, n) = \frac{\Gamma(n + 1)}{\Gamma^h(r)\Gamma(n - hr + 1)} \times \int_0^p \cdots \int_0^p (1 - x_1 - \cdots - x_h)^{n - hr} \prod_{a=1}^{h} x_a^{r-1} \, dx_a$$

for integers n, r, and h and for $0 < p < 1/h$. It can be seen[8] that this integral is equal to the probability that

5. V. R. R. Uppuluri and S. A. Patil, *Inferences About Rare Events*, ORNL/CSD-12, (June 1976).

6. W. Feller, *An Introduction to Probability Theory and Its Applications*, II, 2d ed., Wiley, New York, 1971.

7. "Generating Functions of Generalized Incomplete Dirichlet Integrals," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCCND/CSD-18, p. 12 (October 1975).

8. M. Sobel and V. R. R. Uppuluri, "Sparse and Crowded Cells and Dirichlet Distributions," *Ann. Stat.* 2, 977–87 (1974).

in a multinomial experiment with $b + 1$ cells (b cells each with probability p and one cell with probability $1 - bp$), the minimum frequency in the b cells is at least r in n independent trials. One way to generalize this integral is by the introduction of the parameter j as follows:

$$I_p^{(b,j)}(r,n) = \frac{(p^r/r!)\Gamma(n+1)}{\Gamma^b(r)\Gamma(n-br+1)} \times \int_0^p \cdots \int_0^p \left(1 - jp - \sum_{\alpha=1}^{b} x_\alpha\right)^{n-br} \times \prod_{\alpha=1}^{b} x_\alpha^{r-1}\, dx_\alpha .$$

This is a $(b-j)$-fold integral which, when $j = 0$, gives $I_p^{(b)}(r,n)$ and, when $j = 1$, has a probabilistic interpretation for the following waiting-time random variable. In the multinomial problem discussed above, let $v_{b,r}$ denote the trial at which every one of the b cells has at least r balls in each cell (for the first time). Then we have the equality of the following probabilities:

$$\text{Prob}[v_{b,r} \le n] = \text{Prob}[\min(N_1, N_2, \ldots, N_b) \ge r] = I_p^{(b)}(r,n).$$

After some integration, one can show

$$\text{Prob}[v_{b,r} = n] = (rb/n) I_p^{(b,1)}(r,n).$$

The ascending factorial moment generating function of $v_{b,r}$ is defined by

$$\phi(t) = E[t^{v_{b,r}}] = \sum_{n=br}^{\infty} t^n \,\text{Prob}[v_{b,r} = n],$$

which reduces to

$$\phi(t) = b!\left(\frac{p}{1+p-t}\right)^r C_p^{(b-1)}(r, r),$$

where

$$C_a^{(b)}(r,M) = \int_0^a \cdots \int_0^a g(x_1, \ldots, x_b) \prod_{\alpha=1}^{b} dx_\alpha .$$

$$g(x_1, \ldots, x_b) = \frac{\Gamma(M+br)}{\Gamma^b(r)\Gamma(M)} \frac{\prod_{\alpha=1}^{b} x_\alpha^{r-1}}{(1+x_1+\cdots+x_b)^{M+br}}, \quad x_\alpha > 0.$$

The function $C_a^{(b)}(r,M)$ is referred to as the incomplete Dirichlet integral of type II. From $\phi(t)$, one can show that the jth ascending factorial moment of $v_{b,r}$ is equal to

$$E\left[v_{b,r}^{[j]}\right] = \frac{b!}{b^j} \frac{\Gamma(r+j)}{\Gamma(r)} C_1^{(b-1)}(r, r+j).$$

where

$$E\left[v_{b,r}^{[j]}\right] = b[v_{b,r}(v_{b,r}+1)\cdots(v_{b,r}+j-1)].$$

In the special case $r = 1$, the random variable $v_{b,1}$ denotes the variable associated with the coupon collector's problem.[9] The moments of the waiting time $v_{b,1}$ are known to be related to the harmonic series. Thus we have new representations such as

$$\sum_{\alpha=1}^{b} \frac{1}{\alpha} = b\, C_1^{(b-1)}(1,2).$$

$$\sum_{\alpha=1}^{b} \frac{1}{\alpha^2} = 2b\, C_1^{(b-1)}(1,3) - b^2[C_1^{(b-1)}(1,2)]^2 .$$

An associated waiting-time random variable arises in the case of sampling without replacement from a finite population with b categories. Let there be N objects in each category, and let $T_{b,d}$ denote the number of draws necessary to obtain d objects from each class. For $d = 1$ it can be shown that

$$\text{Prob}[T_{b,1} > t] = \sum_{\alpha=1}^{\min(Nb-t,\,N)} (-1)^{\alpha+1} \binom{b}{\alpha} \frac{[N(b-\alpha)]![(Nb-t)!]}{[N(b-\alpha)-t]![Nb!]},$$

and the expected values are given by

$$E[T_{b,1}] = \sum_{\alpha=1}^{b} (-1)^{\alpha+1} \binom{b}{\alpha} \frac{Nb+1}{N\alpha+1}.$$

For $d = 1$ and small values of b and N, the probability distribution and moments of $T_{b,d}$ were tabulated with the help of Keaven Anderson. For large values of b and N, one can use the results of the previous paragraphs as approximations.

9. W. Feller, *An Introduction to Probability Theory and Its Applications*, Wiley, New York, 1957.

5. Continuum Mechanics

S. J. Cuang E. H. Lee[1] D. N. Robinson[2] G. C. Smith[2] L. J. Zapas[3]

CONSTITUTIVE LAWS FOR ELASTIC-PLASTIC MEDIUM

Hill[4] considers a rate- or flow-type constitutive law for elastic-plastic rate-independent medium of the form

$$\dot{s}_{ij} = \frac{\partial \dot{F}}{\partial(\partial v_i / \partial X_j)},$$

where the X_j are rectangular Cartesian coordinates in the initial or reference configuration, the rate potential $\dot{F}$ is a homogeneous function of degree 2 in the velocity gradients $\partial v_i / \partial X_j$, and $\dot{s}_{ij}$ is the partial time derivative of the first Kirchhoff stress with fixed X. Choosing the reference state to be the current state and using curvilinear convected coordinates ξ^α, it can be shown that the above constitutive law follows from the existence of an associated potential $F(\epsilon_{\alpha\beta})$ of the strain rate components

$$\epsilon_{\alpha\beta} = \frac{1}{2}(v_{\alpha|\beta} + v_{\beta|\alpha}).$$

In the above equation, v is the velocity vector in the deforming body, and the comma denotes covariant differentiation. The second Kirchhoff stress is assumed to be derivable from the potential F by

$$\tau^{\alpha\beta} = \frac{\partial F}{\partial(\epsilon_{\alpha\beta})}.$$

Using the relation

$$\dot{\tau}^{\alpha\beta} = \dot{\tau}^{\alpha\beta} + \tau^{\alpha\gamma} v^{\beta}_{,\gamma},$$

we obtain

$$\dot{\tau}^{\alpha\beta} v_{\beta|\alpha} = \frac{\partial F}{\partial(\epsilon_{\alpha\beta})} \epsilon_{\alpha\beta} + \tau^{\alpha\gamma} v^{\beta}_{,\gamma} v_{\beta|\alpha}.$$

Since the constitutive law is rate independent, $F(\epsilon_{\alpha\beta})$ is a homogeneous function of degree 2. Hence the above expression is reduced to

$$\dot{\tau}^{\alpha\beta} v_{\beta|\alpha} = 2F(\epsilon_{\alpha\beta}) + \tau^{\alpha\gamma} v^{\beta}_{,\gamma} v_{\beta|\alpha}.$$

This implies Hill's relation,

$$\dot{\tau}^{\alpha\beta} = \frac{\partial \dot{E}}{\partial(v_{\beta|\alpha})}$$

in terms of convected coordinates with

$$2E(v_{\beta|\alpha}) = 2F(\epsilon_{\alpha\beta}) + \tau^{\alpha\gamma} v^{\beta}_{,\gamma} v_{\beta|\alpha}.$$

With $\tau^{\alpha\gamma}$ known, this establishes that E is a homogeneous function of degree 2 in $v_{\beta|\alpha}$.

Since the laws of plasticity must apply in the presence of rotations, their influence must not affect the stress rate term in the constitutive relation; hence, a Jaumann or spin-invariant stress rate is appropriate. We use the configuration at t as the reference configuration and utilize Cartesian coordinates x. It can be shown that

$$\frac{D^J \tau_{ij}}{Dt} = \dot{\tau}_{ij} + \sigma_{ik} D_{jk} + \sigma_{kj} D_{ik},$$

where D/Dt denotes the Jaumann derivative and

$$D_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right).$$

In the above equation, τ_{ij} is defined to be $\tau_{ij} = J\delta_{ij}$, where δ_{ij} is the Cauchy stress in Cartesian coordinates x and where J is the density ratio. Previously the quantity τ_{ij} has been introduced by Lee[5] to express the yield condition in his finite elastic-plastic theory. With $F(D_{ij})$ homogeneous of second order in the strain

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1 Stanford University

2 Reactor Division, ORNL

3 National Bureau of Standards

4 R. Hill, "Some Basic Principles in the Mechanics of Solids without a Natural Time," *J. Mech. Phys. Solids* 7, 209–25 (1959).

5 E. H. Lee, "Elastic-Plastic Deformation at Finite Strains," *J. Appl. Mech.* 36, 1–6 (1969).

rates, it follows that

$$\frac{\partial \dot{U}_{ij}}{\partial t} D_{ij} = 2\dot{F} + 2\sigma_{jk} D_{ij} D_{ik} .$$

Thus, if we define

$$G = F + \sigma_{jk} D_{ij} D_{ik} ,$$

a third rate potential G is generated as follows:

$$\frac{\partial \dot{U}_{ij}}{\partial t} = \frac{\partial \dot{G}}{\partial D_{ij}} .$$

ELASTIC WAVE DIFFRACTION BY HALF-INFINITE CRACKS

For reactor design calculations, we are interested in the problem of diffraction of a plane elastic wave by a half-infinite crack located on the positive x axis in a two-dimensional elastic medium. Further, we want to use the solution of this problem to calculate the secondary diffraction by a different and parallel half-infinite crack. Previously we have studied a finite crack problem that can be considered as the interaction of two half-infinite-crack problems.[6]

Since the governing equations of dynamic elasticity can be decomposed into several wave equations with distinct wave speeds, the mathematical techniques for the wave equation can be borrowed in dealing with the elastic wave problems. It is known that the half-plane diffraction problem of a scalar wave equation can be solved by means of the Wiener-Hopf technique. A different approach to this problem has been proposed as the ray theory. As an extension, the uniform asymptotic theory of edge diffraction has been developed by Ahluwalia, Lewis, and Boersma.[7] Recently the scalar wave diffraction by two parallel half-planes has been studied by Jones[8] using the Wiener-Hopf technique. Jones's result indicates that, in certain circumstances, the solution based on the uniform asymptotic theory shows slight discrepancy to the exact solution. An improvement of the uniform theory has been made by Boersma.[9] We are interested in the corresponding problem of elastic wave diffraction.

The problem of elastic wave diffraction by a half-infinite crack can be solved by the method of Wiener-Hopf, as outlined below, using the following definitions and notation. The one-sided Laplace transform in time is defined by

$$\bar{f}(p) = \int_0^\infty f(t) e^{-pt} dt .$$

and the two-sided Laplace transform in x is defined by

$$g^*(p\eta) = \int_{-\infty}^{\infty} e^{-p\eta x} g(x) dx .$$

The subscript + or − with the superscript * is defined by

$$g_+^* = \int_0^\infty e^{-p\eta x} g(x) dx .$$

$$g_-^* = \int_{-\infty}^0 e^{-p\eta x} g(x) dx .$$

On the boundary, stresses of given magnitude are applied on both surfaces of the crack. By symmetry, the displacement is zero along the negative x axis. Thus the Laplace transforms of the boundary conditions can be reduced to a relation between the unknowns $\bar{\tau}_{xy}^*$ and $\bar{v}_+^*$, where

$$\bar{\tau}_{xy}^* = \int_{-\infty}^0 e^{-p\eta x} \tau_{xy}(x) dx ,$$

$$\bar{v}_+^* = \int_0^\infty e^{-p\eta x} \bar{v}(x) dx .$$

In the above integrals, the stress component in the direction of the y axis $\tau_{xy}(x)$ and the vertical displacement $\bar{v}(x)$ are unknown in their ranges of integration. The Wiener-Hopf equation relating $\bar{\tau}_{xy}^*$ and $\bar{v}_+^*$ is

$$2\mu p \left(\frac{s_T^2 - s_L^2}{s_T^2} \right) \left(\frac{\eta^2 - s_L^2}{\gamma_L} \right) K(\eta) \bar{v}_+^* = \bar{\tau}_{xy}^- + \tau_{xy+}^* .$$

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6. S. J. Chang, "Diffraction of Plane Dilatational Waves by a Finite Crack," *Q. J. Mech. Appl. Math.* 24, 423–43 (1971).

7. D. S. Ahluwalia, R. M. Lewis, and J. Boersma, "Uniform Asymptotic Theory of Diffraction by a Plane Screen," *SIAM J. Appl. Math.* 16, 783–807 (1966).

8. D. S. Jones, "Doubled Knife-Edge Diffraction and Ray Theory," *Q. J. Mech. Appl. Math.* 26, 1–18 (1973).

9. J. Boersma, "Diffraction by Two Parallel Half-Planes," *Q. J. Mech. Appl. Math.* 28, 405–19 (1975).

where s_T, s_L, and s_k are constants determined by the wave speeds and $\gamma_L^2 = (s_L^2 - \eta^2)$. The function $K(\eta)$ in the above equation is related to the speed of the Rayleigh surface wave. Both $\bar{\sigma}_+^*$ and $\bar{\tau}_+^*$ can be solved from the above equation by arguments from the theory of functions of a complex variable.

The transformed stress components can be expressed in terms of $\bar{\sigma}_+^*$, and the problem reduces to the inversion of the Laplace transforms. These inversions have integrals of the type

$$I = \frac{1}{2\pi i}\int_{\eta_1}^{\eta_2}\int_{t=0}^{t=\infty} F(x, y, \eta) \times \exp\{-p[(s^2 - \eta^2)^{1/2} y - \eta x]\}\, d\eta,$$

where η is a complex variable. If we introduce in the integrand a variable t, where

$$t = (s^2 - \eta^2)^{1/2} y - \eta x,$$

and consider the deformation of the contour of integration, we have

$$\bar{I}_L = \int_{s_T}^{\infty} D(r, \theta, t) e^{-pt}\, dt + R.$$

where the polar coordinates r and θ are used. The inversion of I_L can then be obtained immediately.

COMPARISON OF A GENERAL RATE FLUID AND THE BKZ FLUID

After the basic formulation was set forth by Oldroyd,[10] many constitutive equations for viscoelastic fluids were proposed. Because the differential types have suffered various drawbacks, great interest has been shown in integral types of constitutive equations to describe the nonlinear rheological phenomena such as non-Newtonian viscosity, normal stress, stress overshoot, etc., for different flow histories. An interesting question is how the integral types compare in predicting nonlinear phenomena. In this study, we simply want to point out some obvious differences between BKZ[11] theory and the rate theory represented as a generalized version of the one proposed by Bird.[12] Yamamoto[13] has observed the inaccuracy of rate theory to predict certain types of rheological phenomena and has questioned its more restricted relaxation spectrum. We analyze rate theory from its general representation. It appears that many results can be obtained equally well without using the special spectrum of the rate theory. We conclude, therefore, that if a rate model is inaccurate to describe certain rheological phenomenon, it is not in general due to its special spectrum but is a general character of the rate-dependent kernel function.

The constitutive equations for the incompressible BKZ fluid[11] are expressed by

$$\sigma_{ij}(t) = p\delta_{ij} + \int_{-\infty}^{t} \{U_{I_1}[I_1(t, \tau), I_2(t, \tau), t - \tau] B_{ij}(t, \tau) - U_{I_2}[I_1(t, \tau), I_2(t, \tau), t - \tau] B_{ij}^{-1}(t, \tau)\}\, d\tau,$$

where σ_{ij} denotes the stress tensor, p is the hydrostatic pressure, and U is the BKZ potential. If we define $II(t)$ as the second invariant of the rate of deformation tensor, then the constitutive equations for the rate fluid are defined by

$$\sigma_{ij}(t) = p\delta_{ij} + \int_{-\infty}^{t} \mu[t - \tau, II(\tau)] \left\{\left(1 + \frac{\epsilon}{2}\right)[c_{ij}^{-1}(t, \tau) - \delta_{ij}] + \frac{\epsilon}{2}[c_{ij}(t, \tau) - \delta_{ij}]\right\} d\tau,$$

where μ is a kernel function.

The difference between the two constitutive models is reflected from their kernel functions. For BKZ theory the kernel function depends on the two invariants I_1 and I_2 of deformation, whereas for rate theory, it depends on the invariant of the rate of deformation. Furthermore, BKZ theory is expressed in terms of the potential U.

For the flow history of stress relaxation after the stoppage of steady shear, we have derived two rheological relations corresponding to the two different

10 J. G. Oldroyd, "On the Formulation of Rheological Equations of State," *Proc. R. Soc.* A200, 45–63 (1950).

11 B. Bernstein, E. Kearsley, and L. Zapas, "A Study of Stress Relaxation with Finite Strain," *Trans. Soc. Rheol.* 7, 391 (1963).

12 R. B. Bird and P. J. Carreau, "A Nonlinear Viscoelastic Model for Polymer Solutions and Melts," *Chem. Eng. Sci.* 23, 427–34 (1968).

13 M. Yamamoto, "Rate Dependent Relaxation Spectra and Their Determination," to be published.

constitutive equations. By a rheological relation, we mean a condition that is true only to a specific rheological model for a specific flow history and is independent of the material property. The rheological relation for the BKZ theory is obtained as

$$\frac{\partial \sigma_{1n}}{\partial t} = -\eta \left(1 + \eta \frac{\partial}{\partial \eta}\right)\sigma_s ,$$

where σ_s is the shear stress, η is the shear rate, and σ_{1n} is the first normal stress difference. Similarly, we have obtained for the rate theory

$$\frac{\partial \sigma_{1n}}{\partial t} = -2\eta\sigma_s ,$$

which was also obtained by Yamamoto using a modified relaxation spectrum of μ. The two relations are equal if

$$\eta \frac{\partial \sigma_s}{\partial \eta} = \sigma_s ,$$

which gives

$$\sigma_s(t, \eta) = C(t)\eta .$$

But, in general, σ_s is not linearly proportional to η.

As a different flow history, we have considered the example of suddenly applied steady shear. A rheological relation for the BKZ fluid derived by Bernstein[14] is

$$\frac{\partial}{\partial \eta}\left(\frac{1}{\eta}\frac{\partial \sigma_{1n}}{\partial t} - t\frac{\partial \sigma_s}{\partial t}\right) = \frac{t}{\eta}\frac{\partial \sigma_s}{\partial t} .$$

The corresponding rheological relation for the rate model, obtained by eliminating the function μ from the shear stress σ_s and the first normal stress difference σ_{1n}, is given by

$$\frac{\partial^2}{\partial \eta^2}\left(\frac{1}{\eta}\frac{\partial \sigma_{1n}}{\partial t} - t\frac{\partial \sigma_s}{\partial t}\right) = 0 .$$

It is seen that the difference between the two relations is

$$\frac{1}{\eta}\frac{\partial \sigma_s}{\partial t} = \frac{\partial}{\partial \eta}\left(\frac{\partial \sigma_s}{\partial t}\right)$$

or that the rate of change of shear stress is directly proportional to the shear rate η.

$$\frac{\partial \sigma_s}{\partial t} = B(t)\eta ,$$

which cannot be true in general.

Further, for suddenly applied shear the difference in predicting shear stress by the two models is

$$\Delta_s = -\int_t^{\infty} K_*(\eta t, \xi)\, d\xi - \int_t^{\infty} \eta t\, \mu(\xi, 0)\, d\xi ,$$

where $K_*(\eta t, \xi)$ is the specific kernel function for BKZ theory, and $\mu(t, 0)$ is the limiting value of $\mu(t, 2\eta^2)$ for $\eta \to 0$; that is,

$$\mu(t, 0) = \lim_{\eta \to 0} \frac{-1}{\eta t} K_*(\eta t, t) = \dot{G}(t) .$$

The deviation between the two models is therefore not zero unless η is small, corresponding to the linear case.

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14. B. Bernstein, "Time Dependent Behavior of an Incompressible Elastic Fluid," *Acta Mech.* 2, 239–54 (1966).

6. Functional Integration

L. J. Gray T. Kaplan[1]

OFF-DIAGONAL DISORDER IN RANDOM SUBSTITUTIONAL ALLOYS

A theory for elementary excitations in random substitutional alloys with off-diagonal as well as diagonal disorder has been developed. The theory parallels Mookerjee's[2,3] treatment of alloys with diagonal disorder only. It can be divided into two parts: (1) construction of a new (nonrandom) Hamiltonian such that configuration averages in real space are equal to inner products in what we shall refer to as the augmented space and (2) evaluation of the Green's function in the augmented space by applying a recursion method[4] to the new Hamiltonian. Transformation to the augmented space (which we shall define shortly) allows one to evaluate the configurationally averaged, real-space Green's function directly by computing the Green's function of the transformed Hamiltonian. This method has many advantages over other theories for disordered systems. Besides including off-diagonal disorder correctly, it works well in both the short and long mean-free-path regions, and it generates a translationally invariant Green's function that is always analytic. The essential difference between our treatment and Mookerjee's involves writing both the diagonal and off-diagonal elements of the Hamiltonian matrix in terms of functions of an appropriate set of independent random variables and applying the transformation to the augmented space in its most general form. In general, the matrix elements of the Hamiltonian in real space must be represented by functions that involve products of Kronecker delta functions. By treating the Kronecker delta function as the limit of an exponential function, the transformation to the augmented space can be easily handled.

The theory is quite general and can be applied equally well to phonons, excitons, magnons, etc. In order to be more specific, we investigate the electronic properties of a binary A-B alloy with a nearest-neighbor, single-band, tight-binding Hamiltonian. The Hamiltonian, H, is given by the relation

$$H_{ij} = \epsilon_i \delta_{ij} + W_{ij} . \tag{1}$$

The diagonal element ϵ_i equals either ϵ_A or ϵ_B, and the off-diagonal element W_{ij} takes on the values W'_{AA}, W'_{BB}, or $W'_{AB} = W'_{BA}$, depending on the occupation of sites i and j. Also, $W_{ij} = 0$ if $i = j$ or if i and j are not nearest neighbors. The relative concentrations of the A and B constituents are denoted by c_A and $c_B = 1 - c_A$ respectively. The theory treats the diagonal element ϵ_i as an independent random variable with probability distribution $p(\epsilon_i)$. Then W_{ij} can be written explicitly as a function of ϵ_i and ϵ_j as

$$\begin{aligned} W_{ij} = {} & W'_{AA}\delta(\epsilon_i - \epsilon_A)\delta(\epsilon_j - \epsilon_A) \\ & + W'_{AB}\delta(\epsilon_i - \epsilon_A)\delta(\epsilon_j - \epsilon_B) \\ & + W'_{BA}\delta(\epsilon_i - \epsilon_B)\delta(\epsilon_j - \epsilon_A) \\ & + W'_{BB}\delta(\epsilon_i - \epsilon_B)\delta(\epsilon_j - \epsilon_B) . \end{aligned} \tag{2}$$

where $\delta(\epsilon_i - \epsilon_A)$ is the Kronecker delta function.

We want to evaluate the configurationally averaged Green's function $\overline{G_{ij}(\epsilon)}$, which is given by the relation

$$\overline{G_{ij}(\epsilon)} = \int\int\cdots\int \langle \omega_i | (\epsilon I - H(\{\epsilon_k\}))^{-1} | \omega_j \rangle \times p(\epsilon_1) p(\epsilon_2) \cdots p(\epsilon_k) \cdots d\epsilon_1\, d\epsilon_2 \cdots d\epsilon_k \cdots . \tag{3}$$

where ω_i is the vector defined such that $H_{ij} = \langle \omega_i | H | \omega_j \rangle$.

To construct the augmented space as described by Mookerjee,[2] proceed as follows. First, choose a Hilbert space ϕ_k, a unit vector v_0^k in ϕ_k, and a self-adjoint operator M^k such that

$$p(\epsilon_k) = -\frac{1}{\pi} \lim_{\epsilon \to \epsilon_k + i\delta} \operatorname{Im} \langle v_0^k | (\epsilon I - M^k)^{-1} | v_0^k \rangle . \tag{4}$$

Such a relation can always be found for any positive integrable function p. If the Hamiltonian is originally defined on the Hilbert space Ω, then construct a new Hilbert space which is the direct product of the spaces of the random variables and Ω. This space is the augmented space and is defined as

$$\Psi = \Omega \otimes \phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_k \cdots = \Omega \otimes \Phi . \tag{5}$$

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1. Solid State Division, ORNL.
2. A. Mookerjee, "A New Formalism for the Study of Configuration-Averaged Properties of Disordered Systems," *J. Phys. C* 6, 1205 (1973).
3. A. Mookerjee, "Averaged Densities of States in Disordered Systems," *J. Phys. C* 6, 1340 (1973).
4. R. Haydock, V. Heine, and M. J. Kelly, "Electronic Structure Based on the Local Atomic Environment for Tight-Binding Bands: II," *J. Phys. C* 8, 2591 (1975).

where $\bullet$ indicates the direct product. In this space, we define the operator

$$\tilde{H} = \sum_i P_i \bullet Q_i + \sum_{ij} T_{ij} \bullet R_{ij} . \tag{6}$$

where P_i is the projection operator onto the site i, T_{ij} is the projection operator onto the pair of nearest-neighbor sites i and j.

$$Q_i = I \bullet I \bullet \cdots \bullet I \bullet M^i \bullet I . \tag{7}$$

$$\begin{aligned} R_{ij} = {} & W_{AA}(I \bullet I \bullet \cdots \bullet f_A{}^i \bullet \cdots \bullet f_A{}^j \bullet I \bullet \cdots) \\ & + W_{AB}(I \bullet I \bullet \cdots \bullet f_A{}^i \bullet \cdots \bullet f_B{}^j \bullet I \bullet \cdots) \\ & + W_{BA}(I \bullet I \bullet f_B{}^i \bullet \cdots \bullet f_A{}^j \bullet I \bullet \cdots) \\ & + W_{BB}(I \bullet I \bullet \cdots \bullet f_B{}^i \bullet \cdots \bullet f_B{}^j \bullet I \bullet \cdots) . \end{aligned} \tag{8}$$

$$f_A{}^i = \delta(\epsilon_A I, M^i) , \quad f_B{}^i = \delta(\epsilon_B I, M^i) . \tag{9}$$

The superscript i on M^i and f^i indicates that these operators appear in the same position in the direct-product definitions of Q_i and R_{ij} as ϕ_i appears in the definition of Φ given in Eq. (5). For a binary alloy, each ϕ_k has dimension 2 and

$$M = \begin{bmatrix} a & b \\ b & c \end{bmatrix} . \tag{10}$$

where

$$a = \epsilon_A c_A + \epsilon_B c_B ,$$

$$b = [\epsilon_A - \epsilon_B]\sqrt{c_A c_B} ,$$

$$c = \epsilon_A + \epsilon_B - a ,$$

$$v_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} .$$

We approximate the Kronecker delta as the limit as $\sigma \to 0$ of the exponential

$$\delta(\epsilon_A I, M^i) = f_A{}^i = \lim_{\sigma \to 0} \exp[-(\epsilon_A I - M^i)^2/\sigma^2] \tag{11}$$

and find that

$$f_A = \begin{bmatrix} c_A & \sqrt{c_A c_B} \\ \sqrt{c_A c_B} & c_B \end{bmatrix} .$$

$$f_B = \begin{bmatrix} c_B & -\sqrt{c_A c_B} \\ -\sqrt{c_A c_B} & c_A \end{bmatrix} . \tag{12}$$

In the augmented space formalism we then have

$$\overline{G_{ij}(\epsilon)} = \langle \omega_i \bullet \gamma_0 | (\epsilon I - \tilde{H})^{-1} | \omega_j \bullet \gamma_0 \rangle . \tag{13}$$

where

$$\gamma_0 = v_0{}^1 \bullet v_0{}^2 \bullet \cdots \bullet v_0{}^k \bullet \cdots . \tag{14}$$

We have defined the augmented space and the relation between the averaged Green's function and the matrix elements in this new space. Everything to this point is exact. The approximation is introduced when the Green's function in the augmented space is evaluated. We choose to use the recursion method of Haydock, Heine, and Kelly[4] as did Mookerjee in his theory for diagonal disorder. This method generates a continued-fraction approximation to the Green's function. The accuracy of the approximation is determined by the number of levels of the continued fraction which are evaluated exactly. For n levels the contributions from the first $2n$ moments are included exactly, while the effects of larger moments are approximated as a background effect. This method is particularly attractive, since it always generates an analytic Green's function.

As an example, we have calculated the density of states of a one-dimensional binary alloy with $\epsilon_A = 2.5$,

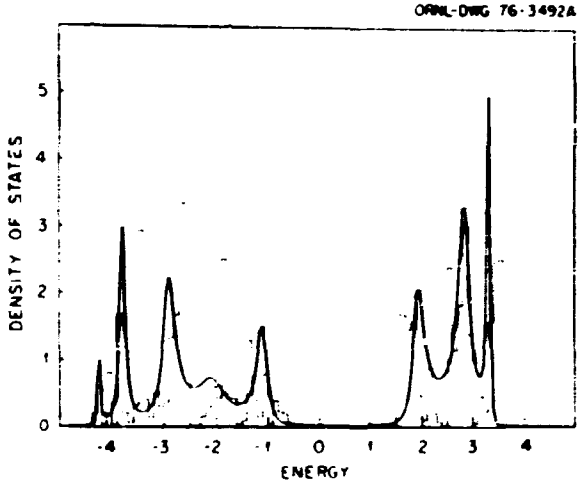

Fig. 2. Calculation of the density of states by the augmented space theory with a recursion level of 9 (smooth line) and exact results (histogram) for a one-dimensional electronic alloy with $\epsilon_A = -\epsilon_B = 2.5$, $W_{AA} = 0.5$, $W_{AB} = W_{BA} = 0.8$, $W_{BB} = 1.0$, and $C_A = C_B = 0.5$.

$\epsilon_B = 2.5$, $W'_{AA} = 0.5$, $W'_{AB} = W'_{BA} = 0.8$, $W'_{BB} = 1.0$, and $c_A = c_B = 0.5$, using the augmented space theory with a recursion level of 9. The results of these calculations are shown in Fig. 2, where they are compared with essentially exact results obtained using the Schmidt method.[5] Note that with only nine levels in the recursion approximation, the theory agrees reasonably well with the exact results, even for this split-band case. The theory correctly predicts some of the major peaks in the density of states and approximately matches the unequal band widths of the two bands. For a similar three-dimensional system, the exact density of states is considerably smoother, and even fewer levels in the recursion method should be needed.

One final comment is necessary. Mookerjee[6] has also attempted to include off-diagonal disorder, using the augmented space formalism. As he noted, he failed to include the correlations between sites correctly. He simply replaced the hopping integrals randomly and thus neglected to note that if site i contains an A atom, then W'_{ij} must equal W'_{AA} or W'_{AB} for all j coupled to i. Similarly, if site i contains a B atom, W'_{ij} must be W'_{BA} or W'_{BB}. The theory we have presented here properly accounts for these correlations between sites.

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5. H. Schmidt, "Disordered One-Dimensional Crystals," *Phys. Rev.* **105**, 425 (1957).

6. A. Mookerjee, "Fermion-Field Theory and Configuration Averaging: III. Off Diagonal Disorder and Band CPA," *J. Phys. C* **8**, 2943 (1975).

7. Matrices and Other Operators

R. E. Cline[1] R. E. Funderlic[2] L. J. Gray R. C. Ward

RANK AND DECOMPOSITION OF THE DIFFERENCE OF MATRICES AND GENERALIZED INVERSES

Several results in matrix theory have been obtained which relate to the problem of solving ank (A S) = rank(A) + k for the integer k. We have shown[3] how this problem is closely related to the Moore-Penrose generalized inverse of A S. These results are important because of their relation to ill-posed and singular problems which have recently generated much interes' Least squares and the method of modification for matrices of defective rank are also related. This work has unified and generalized several areas in the theory of matrices. Many special cas·, for the generalized inverse of A S appear in the literature. We include all of these under a unified approach based on our results concerning rank (A S).

BIQUASITRIANGULAR OPERATORS

Let H be a complex separable Hilbert space and $B(H)$ the collection of all bounded operators on H. If $T^n = 0$ for $T \in B(H)$ and some integer n, T is called nilpotent; we denote by N the collection of all nilpotent operators and by N_0 those nilpotents T for which T^k has closed range for all k. Recently,[4] we and, independently, Apostol and Stampfli[5] and Williams[6] have shown that every $T \in N_0$ is similar to a Jordan operator. Thus, $T = XSX^{-1}$, where $S = \sum_j S_j$ and each S_j operates on C^{n_j}, $0 < n_j < \infty$, by the matrix

$$\begin{bmatrix} 0 & 1 & 0 & & 0 \\ 0 & 0 & 1 & & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & & & 1 & 0 \\ 0 & & & & 1 \\ 0 & & & & 0 \end{bmatrix}$$

An operator X is called *triangular* (respectively quasitriangular) if there exists a sequence of finite rank projections E_n converging strongly to the identity such that $\|XE_n - E_nXE_n\| = 0$ (respectively $\|XE_n - E_nXE_n\| \to 0$). Call X *bitriangular* (respectively biquasitriangular) if both X and X^* are triangular (respectively quasitriangular). The above result implies that every $T \in N_0$ is bitriangular. In this study we have shown that N_0 is norm dense in N. Using a result of Voiculescu,[7] we then derive that the norm closure of the set of bitriangular operators equals the set of biquasitriangular operators. The corresponding result for triangular and quasitriangular operators was first proved by Halmos[8] and later by Apostol, Foias, and Voiculescu.[9]

ON THE EQUATION $\delta_A(X) = \delta_{f(A)}(X)$

If A is an $n \times n$ matrix, denote by $\delta_A(X)$ the matrix $AX - XA$; δ_A is called the inner derivation induced by A. The range of the derivation δ_A, $R[\delta_A]$, consists of all matrices Z such that $Z = \delta_A(X)$ for some X. It is known that if $f(z)$ is analytic on an open set containing the spectrum of A, then $R[\delta_{f(A)}] \subseteq R[\delta_A]$. If A is an operator, $R[\delta_{f(A)}] \subseteq \text{clw}\{R[\delta_A]\}$, where clw indicates the closure in the weak operator topology. These facts also follow from an interesting formula

$$\delta_A(\partial f(A)/\partial a_{ij}) = \delta_{f(A)}(S_{ij}),$$

where S_{ij} denotes the matrix with 1 in the (i, j) location and zero elsewhere and

$$\frac{\partial f(A)}{\partial a_{ij}} = \lim_{h \to 0} \frac{1}{h}[f(A + hS_{ij}) - f(A)].$$

It is hoped that this formula will aid in understanding derivation range.

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1. University of Tennessee
2. Computing Applications Department
3. R. E. Cline and R. E. Funderlic, *Differences of Matrices. I. The Rank of a Difference of Matrices*, CS-75-11, University of Tennessee (1975).
4. L. J. Gray, "Jordan Representation for a Class of Nilpotent Operators," *Indiana Univ. J. of Math.*, to be published.
5. C. Apostol and J. G. Stampfli, "On Derivation Ranges," to be published.
6. J. Williams, "Similarity Invariants for a Class of Nilpotent Operators," to be published.
7. D. Voiculescu, "Norm-Limits of Algebraic Operators," *Rev. Roum. Math. Pures et Appl.* 29, 371–78 (1974).
8. P. R. Halmos, *Invariant Subspaces*, Lecture Notes, Quelqus Brasilero de Matematica, 1969.
9. C. Apostol, C. Foias, and D. Voiculescu, "Some Results on Non-Quasitriangular Operators II," *Rev. Roum. Math. Pures Appl.* 18, 159–81 (1973).

8. Mathematical Software

K. O. Bowman J. R. Shenton[1] R. C. Ward

ALGORITHMS FOR SUMMING DIVERGENT SERIES WITH PARTICULAR REFERENCE TO STATISTICAL SAMPLING MOMENTS

During the past 12 years, Shenton and Bowman have made an extensive study of moments of statistics that are functions of sample moments. For example, for a statistic b we have developed the expansion $\mathrm{var}(b) = a_0 + a_1/n + a_2/n^2 + \cdots$ in terms of sample size n. The series may continue as far as n^{-5} in a number of cases and to n^{-10} in a few. The Padé approach along with pattern recognition are the current main approaches for summing a divergent series. An algorithm has been developed to compute and evaluate a function, $F_r(n)$, approximating the divergent series. This approximating function is of the form

$$F_r(n) = n\left[\Psi_{r,\,r-1}(n)\right] + \gamma_r(n)R(n),$$

where $\Psi_{r,\,r-1}(\cdot)$ and $\gamma_r(\cdot)$ are real polynomials of degrees $r-1$ and r, respectively, and $R(n)$ is a given summable Stieltjes series with a corresponding convergent continued fraction. The $2r+1$ unknown coefficients in the approximating function are determined from the coefficients of n^0 through n^{-2r} in the given divergent series and are related to the convergents of the continued fraction development of $R(n)$. There is also an interfacing function relating the Stieltjes series and the orthogonal system associated with the continued fraction denominators. There are, for any one given divergent series, an infinite number of choices of $R(n)$ which need not correspond to a well-known closed form. Questions regarding the asymptotic value of contributory terms to the algorithm are considered along with formal relations between the series $R(n)$ and the interfacing functions.

If the divergence of a series is more rapid than $(2s)!$, then generalized Borel-Padé summational techniques are needed. With a view to retrieving more information from divergent statistical series, studies are under way involving algorithms based on approximations of the form

$$F_r^*(n) = \Pi^*(n) + \Pi_r(n)\omega_{s,\,r-1}(n) + \hat{\Pi}_r(n)\omega_s(n).$$

where $\Pi^*(\cdot)$, $\Pi(\cdot)$, and $\hat{\Pi}(\cdot)$ are real polynomials in n and

$$\omega_s(n) = \int_0^\infty \frac{t^s e^{-t}\,dt}{1 + kt^2/n}, \quad k > 0.$$

The parameters are again determined from the equivalence of coefficients of powers of n in $F_r^*(n)$ and the given divergent series. The algorithm is sensitive to round-off errors, therefore, computations require precision of 70 to 100 significant digits. We have utilized the set[2] of subroutines that will permit arithmetic operations using a greater number of significant digits than are provided in the machine instructions of the IBM 360.

The algorithms may also apply to solving a problem arising in a physical model which involves infinite series.

NORM REDUCTION IN THE MATRIX EXPONENTIAL ALGORITHM PADE8

In the original version of the algorithm[3] PADE8 for computing the exponential of a matrix A, the algorithm shifted the origin by the average eigenvalue and then scaled the matrix by a power of 2. This resulted in a shifted normalized matrix with its norm bounded above by 1. That is, m was determined such that

$$\left\|A - \frac{\mathrm{trace}(A)}{n} I\right\|_\infty 2^{-m} \le 1.$$

A rounding and truncation error analysis indicated that the a priori bound for the norm of the relative error in the exponential of the shifted normalized matrix was extremely small. However, a reasonable a priori bound was not obtained for the error in removing the scaling factor 2^{-m} by successive squaring. Therefore, the error was monitored during this step. This original version of PADE8 was extensively tested. The results of these tests were favorable and also indicated that most of the error occurs in the squaring process. Thus, additional techniques for reducing the norm of A before scaling were investigated.

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1. University of Georgia.
2. J. G. Sullivan, *Multiple Precision Arithmetic*, ORNL-TM-68-4-16 (May 7, 1968).
3. "Numerical Computation of the Matrix Exponential," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCSD-CSD-18, pp. 18–19 (October 1975).

In addition to shifting the origin by the average eigenvalue, the revised version of PADE8 attempts to *minimize* the 1-norm of A over all possible diagonal similarity transformations, that is, $\min_{D \in \mathcal{D}} \|D^{-1}AD\|_1$, where $\mathcal{D}$ is the set of all $n \times n$ nonsingular diagonal matrices and $\|B\|_1 = \max_{1 \le j \le n} (\sum_{i=1}^{n} |b_{ij}|)$. Parlett and Reinsch[4] describe an algorithm called BALANCE which attempts this minimization over the set $\mathcal{D}_\beta$ after some preliminary similarity permutations are made. The set $\mathcal{D}_\beta$ is the set of all $n \times n$ nonsingular diagonal matrices with entries restricted to integer powers of the machine base β. This set is used in BALANCE to prevent rounding errors during the execution of this process. It has been determined that the reduction in the scaling factor parameter m is much more important than the absence of rounding errors in this step in the computation of the matrix exponential. Therefore, the minimization in PADE8 is over the set $\mathcal{D}_2$, which may be significantly different from $\mathcal{D}_\beta$ on some computers, such as the IBM 360 series.

The error analysis has been revised to reflect these additional steps in the algorithm. PADE8 continues to return to the user an estimate for the minimum number of accurate digits in the norm of the computed exponential matrix. An estimate for the actual number of accurate digits is also returned.

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4. B. N. Parlett and C. Reinsch, "Balancing a Matrix for Calculation of Eigenvalues and Eigenvectors," *Numer. Math.* 13, 293–304 (1969).

Part B. Statistical and Mathematical Collaboration

The mathematics and Statistics Research Department collaborates with many divisions of Oak Ridge National Laboratory and other UCCND and ERDA installations. Each quarter the individual statisticians and mathematicians report and document major collaborations, which are listed in Table 2 by division for fiscal year 1976. Some of these activities are summarized in this part of the report.

Table 2. Tabulation of collaborations by statisticians and mathematicians during fiscal year 1976

Division	Number
Biology, ORNL	30
Metals and Ceramics, ORNL	26
Environmental Sciences, ORNL	18
Y-12 Plant	13
Computer Sciences Division	8
Institute for Energy Analysis	6
Health Physics, ORNL	5
Reactor, ORNL	5
Uranium Resources Evaluation Project	5
Analytical Chemistry, ORNL	4
Thermonuclear, ORNL	4
Directors, ORNL	3
Solid State, ORNL	3
Tennessee Valley Authority	3
Chemistry, ORNL	2
Comparative Animal Research Laboratory	2
Oak Ridge Associated Universities, Medical Division	2
Energy Research and Development Administration	2
Energy, ORNL	2
Neutron Physics, ORNL	2
Chemical Technology, ORNL	1
Nuclear Safety Information Center	1
Physics, ORNL	1
Oak Ridge Gaseous Diffusion Plant	1

9. Analytical Chemistry

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SIMULTANEOUS CONFIDENCE LIMITS FOR COMPARING SMOKING MACHINES

Comparisons of the amounts of tar, total particulate matter, nicotine, and water from seven smoking machines were made to detect significant differences in the chemical measurements. There were four types of one-lung smoking machines, two types of Walton smoking machines, and a Phipps and Bird smoking machine. Comparisons were made among the one-lung smoking machines and between the Walton smoking machines, while the Phipps and Bird machine was compared with each of the other six smoking machines.

Two problems arise when calculating confidence intervals and making comparisons for these data. The first problem arises from the necessity to calculate seven confidence intervals and two sets of six paired comparisons for each of the four chemical measurements. When calculating a large number of confidence intervals and comparisons, the confidence statement claimed for the overall confidence interval and comparisons is less than that for each individual confidence statement. For example, if 95% confidence intervals are calculated individually for each of seven means, the probability that the means will *simultaneously* be in their confidence interval will be less than 95%. Therefore, a simultaneous procedure is needed, so if a 95% confidence statement is claimed for the means or the comparisons, then each individual confidence statement on a mean or a comparison is at least a 95% confidence statement.

The second problem is due to the unequal number of observations made on the different smoking machines. The unbalanced data cause problems in calculating the distributional properties of the test statistics.

A simultaneous procedure for unbalanced data is the studentized maximum modulus statistic.[2] The studentized maximum modulus $(1 - \alpha)\%$ confidence interval for the mean of the ith machine (i.e., $\bar{Y}_i$, $i = 1, \ldots, 7$) is

$$\bar{Y}_i \pm |m|^{\alpha}_{K,\nu} S_E / \sqrt{N_i}, \; i = 1, \ldots, K ,$$

where $|m|^{\alpha}_{K,\nu}$ is the upper α point of the studentized maximum modulus distribution with parameters $K = 7$ and ν degrees of freedom. The variance of $\bar{Y}_i$ is estimated by $S_E / \sqrt{N_i}$, in which S_E is the pooled estimate of error from the seven machines and N_i is the number of measurements taken on the ith machine. The 95% confidence interval for the difference of two means is

$$\bar{Y}_i - \bar{Y}_j \pm |m|^{0.95}_{7,\nu} S_E (1/\sqrt{N_i} + 1/\sqrt{N_j}) .$$

HTGR INTERLABORATORY COMPARISON PROGRAM

The Analytical Chemistry Division with six other chemical laboratories participated in an interlaboratory program to determine the "state-of-the-art" measurement of uranium and thorium in HTGR fuel materials. Ten sample sets, each consisting of four sample types, were analyzed. One set was analyzed each month for a period of ten months. Our data were sent to New Brunswick Laboratory (NBL) and will be compared with data received from the other laboratories.

Statistical evaluation of the data leads to the following conclusions:

1. The analytical procedure for the determination of uranium is quite satisfactory. The precision among replicate determinations (within the month) is adequate for uranium accountability. The precision among the same sample types on a month-to-month basis is not as good but is still sufficient.
2. The analytical procedure for thorium determinations is not as good as desired. The precision is poorer than that of the uranium determinations, both on replicates and on a month-to-month basis. Again, the within-month precision is better than the month-to-month precision.
3. Sample preparation, the conversion of the sample to a solution form amenable to heavy-metal assay, is extremely important. The poorer precision observed for both the uranium and thorium determinations on a month-to-month basis indicates errors arising from difficulties in sample preparation.

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1. Analytical Chemistry Division, ORNL.
2. R. G. Miller, Jr., *Simultaneous Statistical Inference*, McGraw-Hill, New York, 1966.

VARIATION IN BATCH CORRELATION COEFFICIENTS

Low and high doses of smoke condensate are painted on the skins of mice to determine whether skin tumors develop. Visual and histopathological measurements of this biological activity are then reported as probabilities (PF) that a skin-painted mouse will *not* develop skin tumors in 546 days. To relate the biological activity to the chemical components in cigarettes, the correlation coefficients (ρ's) between the PF values and the concentrations of different chemical components are estimated by sample correlation coefficients (r's).

The concentration of a chemical component in a batch of smoke condensate is measured as the average of the determinations made on several samples taken from the batch. Batches of condensate are prepared periodically, and a selection of four batches is sent to ORNL for chemical analyses. The four batches are identified as two bioassay batches (B1 and B2), a composite batch (C), and an analytical batch (A). The two bioassay batches are prepared at two different times for skin painting, the composite batch is an accumulation of condensates from each production batch, and the analytical batch is condensate generated specifically for chemical analyses. Usually four determinations are made on each batch for each cigarette and chemical constituent.

The means of the chemical determinations for the batches have been shown to be significantly different at the 1% significance level for the 16 chemicals listed in Table 3. The question under investigation is whether the significant difference among chemical means implies a significant difference among correlation coefficients calculated for each batch.

The sample correlation coefficients can be used to test the null hypothesis that the correlation coefficients for all four batches are equal, H_0: $\rho_1 = \rho_2 = \rho_3 = \rho_4$, against the alternative hypothesis that at least two of the correlation coefficients are unequal, H_1: $\rho_i \neq \rho_j$ for some i and j. To test the null hypothesis, the correlation coefficients are converted to a random variable by Fisher's z transformation, $z = 0.5[\ln(1 + r) - \ln(1 - r)]$, which is approximately normally distributed with an approximate mean and a variance of $0.5[\ln(1 + \rho) - \ln(1 - \rho)]$ and $1/(n - 3)$. The chi-square test statistic,

$$\chi^2(3) = (n - 3)\sum_{i=1}^{4} (z_i - \bar{z})^2 ,$$

Table 3. Chemical constituents used to study variations in correlations

1.	Total alkaloids (wt % TPM)[a]
2.	Nicotine (wt % TPM)
3.	Benz[*a*]anthracene (μg/g)
4.	Benzo[*a*]pyrene (μg/g)
5.	*o*-Cresol (mg/g)
6.	*m*- + *p*-Cresol (mg/g)
7.	Phenol (mg/g)
8.	Phenol + cresol (mg/g)
9.	pH
10.	Weak acids (meq)
11.	Very weak acids (meq)
12.	Total weak acids (meq)
13.	Free fatty acids (mg/g)
14.	Oleic-linoleic-linolenic acids (mg/g)
15.	Palmitic acid (mg/g)
16.	Stearic acid (mg/g)

[a]Total particulate matter.

is then used to test the null hypothesis with

$$\bar{z} = \sum_{i=1}^{4} z_i/4$$

and three degrees of freedom.

For example, the correlation values between benz[*a*]anthracene and the low-dose visual PF values give a chi-square value of $\chi^2(3) = 3.47$. The probability that a chi-square random variable is greater than the value of the chi-square test statistic is $\text{Prob}(\chi^2 > 3.47) = 0.32$. This probability indicates that the null hypothesis would not be rejected at any significance level less than 32%.

The value of the chi-square test statistic for benz[*a*]anthracene and the low-dose visual PF values was the largest test-statistic value for all 16 constituents and all four types of PF values. Therefore, none of the correlation coefficients between different batches are significant at a 32% significance level or less.

Inferences from these results imply that fewer batches need to be chemically analyzed for determining correlations between chemical and biological data. However, frequent chemical analysis on different batches of smoke condensate is necessary to determine the batch-to-batch variation of a chemical constituent and a better approximation of the true concentration.

10. Biological Research

J. J. Beauchamp, S. F. Ebey, D. G. Gosslee, E. Leach, R. C. Meacham, F. L. Miller, Jr., T. J. Mitchell, D. S. Robson, J. E. Tobias, J. Trent, D. G. Wilson, E. B. Darden[1], F. Finamore[2], M. Francis[2], J. M. Holland[2], A. W. Hsie[2], M. C. Jernigan[2], A. Li[2], P. Mazur[2]

SPECIFIC DISEASE INCIDENCE IN MICE

The odds ratio analysis described previously[3] has been applied to data from an experiment to study the effects of prepubertal ovariectomy on survival and specific diseases in female RFM mice given 300 R of x rays. The four experimental "treatments" were

1. control (no x ray, no ovariectomy),
2. x ray alone,
3. ovariectomy alone,
4. x ray + ovariectomy.

Fourteen specific diseases were analyzed.

The data were grouped into 50-day intervals based on age at death. For each disease D, a distinction was made between lethal occurrences – deaths *from D* – and incidental occurrences – deaths *with D*. To compare any two experimental groups, two 2 × 2 tables were constructed for each time interval. In one of these, the frequency of death *from D* relative to the number of animals at risk at the start of the interval was recorded for both groups. In the other, the frequency of deaths *with D*, but not caused by D, relative to the number of deaths without the disease was recorded. The entire set was then analyzed by the odds ratio method.

In particular, tests were made of the hypothesis that both groups are the "same" with respect to D; that is, the odds for the disease in one group are the same as those in the other group in all of the 2 × 2 tables. The maximum likelihood estimate of the log odds ratio λ was obtained with approximately 95% confidence limits. The computer program was also extended to give a likelihood ratio test of the constancy of λ over all intervals.

Although the extremely high incidence of thymic lymphoma, especially in the irradiated groups, tended to mask other effects of the experimental treatments, there were several instances in which a significant effect of ovariectomy (or ovariectomy combined with irradiation) on disease incidence was noted, in addition to the expected effects of radiation alone.

ODDS RATIO COMPARISONS OF RADIATION-INDUCED LIFE SHORTENING

The odds ratio analysis developed last year was utilized to compare radiation-induced life-shortening effects in a 2 × 2 factorial treatment design. Posttreatment life span of the cohort of experimental mice was divided into 50-day intervals, and for any treatment group a, the odds for dying in the ith interval were defined as the ratio of the mortality rate, p_{ai}, to the survival rate, $q_{ai} = 1 - p_{ai}$, for that interval. Pairwise comparison of two treatment groups, say a and b, was then based upon the assumption that the odds ratio, $\alpha_{abi} = p_{ai}q_{bi}/p_{bi}q_{ai}$, was constant over the life span of the cohort, and maximum likelihood estimates of $\alpha_{abi} = \alpha_{ab}$ were computed for each of the six pairwise treatment comparisons.

The assumption $\alpha_{abi} = \alpha_{ab}$ was tested by the likelihood ratio method and was rejected in five of the six cases. This result led to closer scrutiny of the model and to the conclusion that if risk of death changes with age, then a constant odds ratio can be obtained only with intervals of infinitesimal length, and then only with Lehmann-type alternatives. An instantaneous odds ratio is the ratio of hazard functions, and if this ratio is constant, then the distributions $F_a(x)$ and $F_b(x)$ of posttreatment survival time x are related by

$$1 - F_a(x) = [1 - F_b(x)]^{\alpha_{ab}} .$$

A k-sample distribution-free analysis and goodness-of-fit test are therefore being developed for this continuous-time model.

EFFECT OF AGE ON RED-BLOOD-CELL CLEARING RATE

An experiment was performed on mice to test the hypothesis that red blood cells (RBC) are retained

1. Comparative Animal Research Laboratory.
2. Biology Division, ORNL.
3. "Likelihood Inference for the Log Odds Ratio in Survival Experiments," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCCND/CSD-18, pp. 1–2 (October 1975).

longer in older animals. Blood was taken from each of seven old and seven young mice, labeled with Cr^{51} and partitioned into four lots, which were then injected intravenously into two young and two old recipient mice per donor. Recipients were bled from the tail twice weekly for four weeks, and a corrected 5-min count was recorded at each bleeding. A circulating RBC half-life of approximately 14 days was predicted from earlier work.

The intended response variable was the logarithmic rate of RBC clearance as measured by the absolute slope of the linear regression of log count on post-injection time. A maximum likelihood estimate of the slope was iteratively calculated for each recipient on the tested assumption of only independent Poisson errors in the counts at each bleeding. Young recipients showed no effect of donor age on this response variable, while in old recipients the RBC from young donors had a significantly shorter half-life than old donor cells when tested by an analysis of variance.

These counter-intuitive results in both young and old recipients appear to be artifactual consequences of nonstationarity in the logarithmic rate of RBC clearance. Departure from linearity of regression, though minor for any individual mouse, exhibited consistent and statistically significant patterns within young and old recipient categories. The pattern of residuals indicates a two-phase clearance which operates differentially in young and old recipients. These data will next be fitted to a two-compartment model by iterative methods to test for donor by recipient age effects.

ENZYME KINETICS

The mechanism of the phosphorylation of histone, using an enzyme from Chinese hamster ovary cells, is to be determined experimentally. The reaction equations for several mechanisms each imply differential equations, which have been solved in terms of the initial velocity of the enzymatic reaction.[4] Statistical methods are used to determine the mechanism by testing the models. The initial velocity of the reaction, that is, rate of formation of the end product, is a function of the concentrations of the substrates. This rate is estimated from observations on the amount of labeled substrate incorporated into the product of the reaction at successive times early in the reaction.

The choice of concentrations of the substrates histone (H) and adenosine 5'-triphosphate (ATP) was critical. Statistical principles and biological knowledge were required to allow the dilutions of the substrates to be prepared accurately and to ensure that the levels of concentration for each substrate, to be used in factorial combination, efficiently included the range of the design space without exceeding the limits of validity of the models.

The equation

$$r = \frac{VAH}{K_{ia}K_h + K_hA + K_aH + AH}$$

is a rate equation which includes several bireactant mechanism models expressing the initial velocity r as a function of the concentrations of histone (H) and ATP (A). The constants describing different mechanisms are V, the maximum velocity of the reaction, and the Ks, which are functions of the rate constants in the reaction equations.

The model was linearized in the reciprocals of the variables:

$$\frac{1}{r} = \frac{1}{V} + \frac{K_a}{V}\left(\frac{1}{A}\right) + \frac{K_h}{V}\left(\frac{1}{H}\right) + \frac{K_{ia}K_h}{V}\left(\frac{1}{AH}\right).$$

Weighted least-squares procedures were used, since the errors in estimating $1/r$ are large relative to $1/r$ and are not homogeneous. The variances are approximately proportional to $1/r^2$; therefore, weights proportional to the estimate $\hat{r}^2$ lead to efficient estimates of the parameters. These analyses are extremely sensitive to the weights, which is not the case with many other types of statistical analyses.

The significance of the product term, $1/AH$, in the linearized model led to the conclusion that the class of the mechanism is one of three sequential models. The analyses further suggested that the correct model is the special case in which $K_{ia} = K_a$. Additional statistical analyses of the four experiments are in progress to obtain a more conclusive test of the three models. The analyses will include refined estimates of the weights as well as a combined analysis of the four experiments.

ESTIMATING THE VOLUME OF A CELL

A step in the preservation of fertilized ova is to replace the water in the cell with glycerin. Because of the difference in their molecular weights, water passes

4. W. W. Cleland, "Steady State Kinetics," pp. 1–65 in *The Enzymes*, 3d ed., vol. 2, ed. by P. D. Boyer, Academic Press, New York, 1970.

out through the cell membrane more readily than glycerin enters the cell. This causes a rapid decrease in cell volume, followed by a slower increase to the original volume. In order to characterize the dynamics of cell-volume change, the process is interrupted, and photographs are taken of the largest area seen while the focusing plane of a microscope is shifted through the cell.

We assume that this largest cross section, or slice, contains the center of the cell. Further we assume that the noncircularities observed on the slice are representative of those that would be found by taking any other slice through the center of the cell. Given the above, the first step of the algorithm developed is to find the center of mass of the largest slice. This is done by use of the Stokes theorem, a device for converting area integrals into line integrals around the boundary. We have an estimate of the boundary obtained by use of a digitizer to find coordinates of points spaced around the outside of the cell. The coordinates are then shifted so that the center of mass is at (0, 0). Several diameters are then found, and the volumes computed from these diameters are averaged to give the final estimated volume. Another way to compute the volume, which may be slightly more accurate but also more expensive, is to compute the volume of solids of revolution of several "semicircles" and then to average these volumes. This will be tested if the volume obtained by using diameters is not sufficiently accurate.

LENS OPACITY STUDY

Preliminary results from the analysis of data from extensive experiments on the effect of different types of radiation upon the eyes of mice have been summarized.[5] The time-percent-lens-opacity relation previously presented[5] made it possible to compare the different types of radiation as well as the two methods of delivering this radiation, that is, in one intense dose (acute) or in dose segments over a period of time (chronic). During this period it was found that the estimated percent lens opacity at 300 days posttreatment was a biologically meaningful "response" to use in deriving a dose-response relationship for each radiation group. A linear relation in log radiation and log estimated response at 300 days posttreatment was found to be adequate for describing the dose-response phenomenon for each combination of radiation type and method of radiation delivery. A measure of the relative biological effectiveness (RBE) of the acute neutron and x-ray radiation groups was found by examining the ratio of doses for the two groups that yield equal responses. The dependence of this RBE measure upon dose was found, and an approximate expression for the variance of RBE as a function of dose was also derived. Additional comparisons among the regression coefficients were used to compare other experimental treatment groups.

5. "Lens Opacity Study," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCCND/CSD-18, p. 32 (October 1975).

CHOLESTEROL IN RABBITS

An experiment on rabbits was conducted to measure the effectiveness of ascorbic sulfate in reversing the formation of cholesterol deposits (plaques) on the inner walls of blood vessels. The normal diet of rabbits contains no cholesterol; after seven weeks on a high-cholesterol diet, 3 of 23 rabbits died. The remaining 20 rabbits were paired on the basis of biweekly serum cholesterol levels, and ascorbic sulfate injections were given daily to one member of each pair beginning in the tenth week. Biweekly serum cholesterol readings were continued, and after an additional ten weeks, the surviving rabbits were sacrificed for plaque measurements.

Mortality occurred during the course of this experiment, and though cholesterol could not be directly implicated through pathology in each instance, there was a definite association between serum cholesterol level and mortality. A rank sum test of this association was devised in order to avoid parametric assumptions. If the N_i rabbits alive at the ith bleeding are ranked with respect to cumulative serum cholesterol and if S_i is the sum of the ranks of the d_i rabbits that then die before the $(i + 1)$th bleeding, then the expectation and variance of S_i under the hypothesis of no effect are

$$E_{H_0}(S_i) = d_i(N_i + 1)/2 ,$$

$$V_{H_0}(S_i) = d_i(N_i - d_i)(N_i + 1)/12 .$$

A normal score value of

$$\sum[S_i - E_{H_0}(S_i)] / \sqrt{\sum V_{H_0}(S_i)} = 2.88$$

was calculated for the 11 deaths among the 23 rabbits. Thus the association between serum cholesterol and mortality was significant at a probability of 0.002.

There was no significant difference in the number of deaths in the treated and control groups. Treatment comparison will be completed when the plaque measurements become available.

11. Chemistry and Physics Research

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MATRIX STORAGE REDUCTION IN CALCULATION OF THE DENSITY OF STATES

One step in the calculation of the density of states for random substitutional alloys with off-diagonal and diagonal disorder is the computation of all the eigenvalues of a large, sparse matrix. To use the most stable numerical technique for this task, one is currently required to store the matrix in some compact form in order to concurrently have all the necessary information about the matrix elements in central memory. Two of the most common compact forms are the bandwidth and the profile storage schemes.

Recently, a new efficient algorithm[4] for reducing the bandwidth and the profile of a sparse matrix by permuting the rows and columns was obtained. This algorithm was used to reduce the storage required by the matrix generated in calculating the density of states of a body-centered cubic alloy composed of potassium and rubidium. The original matrix was of order 459 and had a bandwidth of 244, which would have required 896K bytes of storage with the bandwidth storage scheme and 480K bytes with the profile scheme. The algorithm, which effectively renumbers the atoms in the cubic alloy, reduced the bandwidth to 77, requiring only 283K bytes of storage with the bandwidth scheme and 178K bytes with the profile scheme. This reduced the amount of central memory used for matrix storage by a factor of about 3.

AN EIGENVALUE PROBLEM IN ELECTRON SCATTERING CALCULATIONS

In the development of fusion reactors like the Tokamak, energy levels and lifetimes or cross sections of the gas containing the plasma, as well as the plasma itself, are of interest to thermonuclear researchers. It is through this information that energy losses and energy transfers along with the mechanisms involved in these changes of energy state are studied. One of the techniques used to calculate cross sections of atoms involves calculations of electron scattering.

A promising method for calculations of elastic and inelastic electron scattering of atoms is the matrix variational method described by Nesbet.[5] In this method the external orbitals, as well as the target states, are represented by expansions in known functions. This replaces the solution of a system of coupled integrodifferential equations in the close-coupling method (a popular method for electron scattering calculations) by some algebraic matrix manipulations. A crucial step in these manipulations is the determination of m linearly independent solution vectors of an $N \times N$ homogeneous linear system of equations representing the asymptotic partial wave functions. The OAF (optimized anomaly-free) variational method is used to determine these solutions and the associated variational coefficient and reactance matrices.

In the first step of the OAF method, the $N \times N$ linear system must be transformed by a unitary similarity transformation into an upper quasi-triangular matrix with the diagonal blocks, which must be dimensioned either 1×1, corresponding to a real eigenvalue, or 2×2, corresponding to a complex conjugate pair of eigenvalues, ordered by increasing eigenvalue magnitude down the diagonal. Since the matrix is not always diagonalizable, an eigenvalue-eigenvector decomposition of the matrix cannot be used to accomplish this task. Also, standard eigenvalue algorithms for matrices that are not diagonalizable transform the matrix into an upper quasi-triangular matrix with the diagonal blocks unordered. There exist some extremely slow algorithms, like the unshifted QL algorithm, which produce the desired results, but these are completely unacceptable because of their inefficiency. Thus, new efficient mathematical software has been developed to accomplish this numerical task.

The following five subroutines are required to produce the desired results: ORTHES, ORTRAN, SCHUR, SORTEV, and SWAP. The first two subroutines are

1. Chemistry Division, ORNL.
2. Solid State Division, ORNL.
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4. Norman E. Gibbs, William G. Poole, Jr., and Paul K. Stockmeyer, "An Algorithm for Reducing the Bandwidth and Profile of a Sparse Matrix," *SIAM J. Numer. Anal.* **13**, 236–50 (1976).
5. R. K. Nesbet, "Matrix Variational Method," *Comput. Phys. Commun.* **6**, 275–87 (1974).

from the Argonne eigenvalue-eigenvector package EISPACK. SCHUR is a modification of subroutine HQR2, which is also from EISPACK. SCHUR reduces an upper Hessenberg matrix to upper quasi-triangular form with the diagonal blocks unordered, but does not compute the eigenvectors of the matrix as does HQR2. SORTEV and SWAP are new subroutines developed for this project. Subroutine SORTEV determines which two adjacent diagonal blocks should be interchanged to achieve the end result of having the eigenvalues ordered in increasing magnitude down the diagonal. Subroutine SWAP, which is the heart of the ordering algorithm, actually performs the interchange.

Subroutine SWAP interchanges diagonal blocks and uses only unitary similarity transformations. To interchange a 1 X 1 block with a 1 X 1 (2 X 2) block, one (two) rotation(s) is (are) required, as expected. But to interchange a 2 X 2 block with another 2 X 2 block, a different approach is required. The double-shift QR iteration is used to accomplish this interchange. Theoretically, one double-shift QR iteration using the upper 2 X 2 diagonal block as the shift should result in interchanging the two diagonal blocks. Because of rounding error, it is possible, but unlikely, that two iterations may be required. SWAP performs one iteration and performs a second iteration if it is required. Each iteration requires three elementary unitary transformations; three permutations are required as a preliminary step before the first iteration. Thus, six unitary transformations are usually required for this interchange, and there exists a possibility of nine such transformations being required.

Calculations by the matrix variational method of both elastic and inelastic electron scattering of hydrogen have been made, using the above subroutines. These subroutines are performing their function accurately and efficiently, and the final calculations are in good agreement with known data.

HYDRATION AND DEHYDRATION ON THE SURFACE OF METAL CRYSTALS

The chemical process by which water reacts with metal ions on the surface of a metal crystal has suggested several interesting problems concerning probabilities.

The idealized physical situation consists of a square, bounded, two-dimensional lattice in which the points of the lattice represent metal ions. The lattice point is said to be closed if it has an attached hydroxyl ion. If the metal ion lacks an attached hydroxyl, the lattice point is said to be open. The process by which hydroxyl ions are attached to the metal ions involves the reaction of a water molecule with a pair of adjacent metal ions. It is assumed that there is always an oxygen ion available on the surface to combine with the H_2O molecule to produce a pair of hydroxyls attached to the lattice at adjacent points. Further assumptions are that the process begins with all points open and that there is sufficient water available so that eventually all sites (a site is a pair of adjacent points) will be approached by a water molecule. The order in which sites are approached by water molecules is completely random. Because the reaction must occur at a pair of adjacent open points, there will exist isolated open points when the process is complete. The following problem is of interest: What is the average (expectation) of the fraction of closed points at the end of the process?

As a preliminary step, the assumption was made that all reactions would occur on SW-NE diagonal lines of the lattice. This situation is mathematically more tractable and apparently is of some chemical significance. This reduces the problem to a process occurring on a one-dimensional lattice.

Let u_n denote the average number of reactions (each involving a pair of open points) that will occur in a one-dimensional lattice of n points. The sequence u_n was found to satisfy the recursion formula

$$(n-1)u_n = (n-2)u_{n-1} + 1 + 2u_{n-2} . \qquad (1)$$

with initial conditions $u_0 = u_1 = 0$. This recursion formula was used to obtain a table of the expectations u_n for values of n from 1 to 100.

By defining the generating function

$$U(t) = \sum_{n=0}^{\infty} u_n t^n ,$$

the recursion formula (1) implies that $U(t)$ satisfies the differential equation

$$t^2 \frac{d}{dt}\left[\frac{U(t)}{t}\right] = t^3 \frac{d}{dt}\left[\frac{U(t)}{t}\right] + \frac{t^2}{1-t} + 2t^2 U(t) . \qquad (2)$$

Let $g(t) = U(t)/t$. Then (2) becomes

$$g'(t) = t[g'(t)] + \frac{1}{1-t} + 2t[g(t)] . \qquad (3)$$

The initial conditions imply $g(0) = 0$. The solution to (3) is

$$g(t) = \frac{1}{2(1-t)^2}(1 - e^{-2t}).$$

It follows that

$$U(t) = \frac{t}{2(1-t)^2}(1 - e^{-2t}).$$

If $U(t)$ is expanded in powers of t, u_n can be written

$$u_n = \sum_{k=1}^{n-1} \frac{(-1)^{k-1}(n-k)2^{k-1}}{k!}, \quad n = 2, 3, \ldots, \quad (4)$$

where $u_0 = u_1 = 0$.

From (4) we can deduce that

$$\lim_{n\to\infty} \frac{u_n}{n} = 0.5(1 - e^{-2}),$$

which is approximately equal to 0.4323. The physical meaning of this is that for n large, about 86.46% of the metal ions in a row of length n would be expected to have a hydroxyl ion attached at the completion of the process when no further bonds are possible. A similar situation exists in polymer chemistry. The limit e^{-2} for the fraction of isolated open points had been previously obtained by Flory[6] and again by Cohen and Reiss.[7] This work provides an alternate mathematical approach to the problem.

Obviously, the reverse process of dehydration of the surface involves the same mathematical model. The project will continue with the study of the process of applying hydration and dehydration alternately and in succession several times. There is interest in studying the kinetics of this process and in determining the expectation of the fraction of closed points on the genuinely two-dimensional lattice. The problem will also be studied by using other plane lattices, such as a hexagonal lattice. Where analytical methods fail to provide an exact answer, the process will be studied by Monte Carlo techniques.

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6. P. J. Flory, "Intramolecular Reaction between Neighboring Substituents of Vinyl Polymers," *J. Am. Chem. Soc.* **61**, 1518 (1939).

7. E. R. Cohen and H. Reiss, "Kinetics of Reactant Isolation: One-Dimensional Problems," *J. Chem. Phys.* **38**, 680 (1963).

12. Energy Research

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ENERGY MODELING AND ANALYSIS

For an economic model, a homogeneous function F of energy, labor, and capital variables, which satisfies a linear system of first-order partial differential equations, was sought. Algebraic manipulation reduced the equations to

$$u\partial_x F = v\partial_y F = w\partial_z F = F ,$$

where u, v, and w are functions whose form is not completely specified. That is, the functions which combine to make up u, v, and w are to be chosen so that the original equations represent plausible economic activity.

For the equations to have a continuously differentiable solution, the mixed partial derivatives of F must be equal. This requirement imposes the following conditions on the functions u, v, and w:

$$\partial_x(1/v) = \partial_y(1/u) ;$$

$$\partial_x(1/w) = \partial_z(1/u) ;$$

$$\partial_y(1/w) = \partial_z(1/v) .$$

If these conditions are satisfied, then the solution can be obtained by a straightforward sequence of integrations. Unfortunately the underlying functions that were the investigators' first choice gave rise to u, v, and w functions which did not satisfy the necessary conditions. The search for acceptable constituent functions was reinitiated with these criteria in mind.

EFFECT OF ENERGY DECISIONS ON THE ECONOMY

Von Neumann's uniform growth model of an economy results in a generalized eigenvalue problem $Ax = \lambda Bx$. The elements of the A and B matrices represent input-output coefficients and capital equipment coefficients respectively. These coefficients indicate the amount of various raw materials, manufactured products, and capital equipment that is necessary to produce a particular item in the economy per unit time. The growth rate of the economy is given by the largest eigenvalue of the problem. This eigenvalue will be real, simple, and positive. Before decisions are made concerning energy-related problems, one would like to predict the effect of these decisions upon the economy. The results of this project will give such a prediction.

The mathematical problem can be formulated as the problem in perturbation theory of determining the largest eigenvalue of $(A + \epsilon E)x = \lambda(B + \epsilon F)x$, where $\|E\|$ is approximately equal to $\|A\|$ and $\|F\|$ is approximately equal to $\|B\|$. Denoting the largest eigenvalue of $Ax = \lambda Bx$ by λ_1, there exists, for sufficiently small ϵ, a simple eigenvalue λ_1' which is the largest eigenvalue of $(A + \epsilon E)x = \lambda(B + \epsilon F)x$ and can be represented by the convergent power series

$$\lambda_1' = \lambda_1 + k_1\epsilon + k_2\epsilon^2 + \dots .$$

By algebraic manipulations and the use of known linear-algebra theorems, expressions can be found for the first- and second-order perturbations of λ_1. Denoting $y_i^T Bx_i$ by g_i and $y_i^T(E - \lambda_1 F)x_j$ by γ_{ij1}, where x_i and y_i are the right and left eigenvectors, respectively, of the eigenvalues λ_i of the problem $Ax = \lambda Bx$, these expressions are

$$k_1 = \frac{\gamma_{111}}{g_1} .$$

$$k_2 = \frac{1}{g_1}\left[\sum_{r=2}^{n} \frac{\lambda_{r11}\lambda_{1r1}}{g_r(\lambda_r - \lambda_1)}\right] - \frac{\lambda_{111}}{g_1^2}\, y_1^T F x_1 .$$

Currently, algorithms are being developed and modified to compute k_1 efficiently. These algorithms are the combination shift QZ algorithm to compute the eigenvalues and the inverse iteration algorithm to compute both the left and right eigenvectors. If the value of k_2 is required, algorithms will be developed or modified to determine this value.

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13. Environmental Research

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THERMAL RESISTANCE OF JUVENILE CRAYFISH

Three groups of juvenile crayfish, which were representative samples from a larger population of interest, were acclimated at 15, 20, or 25°C respectively. A random sample of ten crayfish was taken from each group, subjected to an elevated test temperature for a predetermined length of time, and returned to the original acclimation temperature for a period of 72 hr, at which time the number of dead crayfish was recorded. This procedure was repeated for different combinations of elevated test temperatures and exposure times. Two goals were achieved in the analysis of the resulting 72-hr mortality data, utilizing the linear logistic model[3]:

1. characterization of the distribution of the mortality data,
2. determination of the influence of exposure time and elevated test temperature on the mortality observations within an acclimation temperature group.

The maximum likelihood estimates of the parameters in the model were used to estimate the expected frequencies of crayfish dying at different test temperature–exposure time configurations. From the expected frequencies a goodness-of-fit chi-square statistic was used to evaluate the adequacy of the model. The results of this test for each acclimation temperature group indicated that the linear logistic model accurately described the data. The estimated parameters in the logistic model were utilized to construct, within each acclimation temperature group, contours of constant mortality as a function of elevated temperature and exposure time. These contours furnished a visual comparison of the acclimation temperature groups and demonstrated the influence of elevated test temperature and exposure time upon mortality as well. The results of this analysis will be valuable in the design of future experiments.

1. Environmental Sciences Division, ORNL.
2. Reactor Division, ORNL.
3. D. R. Cox, *Analysis of Binary Data*, Methuen, London, 1970.

INFLUENCE OF ADULT DENSITY ON A CALANOID COPEPOD ZOOPLANKTER

Zooplankton play a major role in aquatic ecosystems, serving as a link in the food chain between primary producers and fish. Although research has been conducted on external environmental parameters that regulate populations of zooplankton, little effort has been expended on internal mechanisms of population control. Our purpose of this project was to take the data[4] on density of adult organisms and to determine whether this parameter affected the number of young (clutch size) produced. A study[5] on the population dynamics of *Diaptomus clavipes* found reproduction to be an area of the life cycle requiring further study.

The data consisted of observations on clutch size, female size, adult density, and water temperature from samples collected in a pond, representing a closed ecosystem, during a full year's reproductive cycle. Regression analyses revealed that adult density does have a significant effect ($P < 0.05$) upon clutch size during the entire reproductive cycle. A linear regression model used to approximate the observed clutch size contained terms related to adult density, water temperature, and female size. The initial number of 28 parameters in the model was reduced by more than 50% through a statistical variable selection procedure without significantly reducing the multiple correlation coefficient R^2. Various partitions of the data set over density values and seasonal periods yielded additional insight on the influence of density. The statistical analysis indicated that adult density values greater than 2.25 adults/liter do have a significant effect ($P < 0.05$) upon the clutch size during late winter as well as early spring. These results have been useful in the design of laboratory experiments to further examine the role of density in regulating clutch size by giving an indication of (1) factors to be considered, (2) basic variation to be expected, and (3) density range to be examined.

4. C. W. Gehrs, "Aspects of the Population Dynamics of the Calanoid Copepod, *Diaptomus clavipes* Schacht," Ph.D. Thesis, University of Oklahoma, 1972.
5. C. W. Gehrs and A. Robertson, "Use of Life Tables in Analyzing the Dynamics of Copepod Populations," *Ecology* **56**, 665–72 (1975).

NATURAL CONCENTRATIONS OF TRACE ELEMENTS IN AQUATIC ORGANISMS

Environmental contamination from toxic trace elements has emphasized the need for baseline data on concentrations of elements in biological compartments of natural systems. Larvae of a detritus-feeding aquatic insect, collected from an unpolluted spring stream, were analyzed for 30 elements before and after gut evacuation to determine the concentrations in the gut relative to whole-body concentrations. Linear regressions of the concentration of each element on mean dry weight per individual were calculated for larvae with the gastrointestinal (GI) tract both filled and evacuated in order to test for significant relationships between organism size and concentration. The analyses for the chromium and aluminum concentrations with GI tracts evacuated resulted in significantly ($P < 0.01$) negative relationships. However, there was a significantly ($P < 0.01$) negative slope estimate for the chromium concentration with GI tracts filled. No other slopes were significantly different from zero ($P > 0.05$). Changes in chromium and aluminum concentrations with gut evacuation as a function of initial dry weight were also calculated. Regression analysis was used to show that the change in chromium concentration with gut evacuation was not significantly different from zero ($P > 0.05$) over the entire size range of individuals. However, for aluminum there was a highly significant ($P < 0.01$) decrease in concentration over the entire range of larvae analyzed. The percentage of element body burden associated with gut contents was calculated as the ratio of gut burden to initial whole-body burden. Initial body burden of chromium and aluminum was based on an individual of the same initial dry weight, using the final concentrations as calculated from previously mentioned regression equations. Approximations to the variance of this ratio were made by using the information on the individual variance components.

INCORPORATION OF CHROMIUM BY SOYBEANS

Incorporation of chromium derived from cooling tower drift was studied in vegetation along root uptake and foliar absorption pathways. Uptake and translocation to nonroot parts was determined from soybeans cultured in a potting medium contaminated with cooling water from tower basins at the Oak Ridge Gaseous Diffusion Plant (treatment 1). Translocation from foliage to stems and roots was determined similarly from plants subjected to foliar contamination (treatment 2). In addition, control plants were subjected to contamination at only normal background levels (treatment 3).

The data consisted of measured chromium concentrations in the foliage and roots of soybean plants sampled from each of the three treatment groups during the experimental period. However, no observations were available from the foliar component of plants in treatment 2. The dry weight of the foliage from each sampled plant was also recorded. A linear regression model was found to be adequate for describing the logarithm of the observed chromium concentration as a function of "days since treatment" (X_1) and "foliar dry weight" (X_2). The adequacy of the model was determined from lack-of-fit tests on the observed concentrations for each plant component and treatment group combination. Regression analyses were used to test for significant effects of the variables X_1 and X_2 upon the observed chromium concentrations. The statistical analyses detected differences in the behavior of chromium concentration from the foliar and root components of soybeans as well as differences in the level of chromium concentration for different modes of contamination.

SPATIAL AND TEMPORAL VARIATIONS IN CO_2 EFFLUX BY WHITE OAK ROOTS

An experiment has been conducted to examine the release of $^{14}CO_2$ by the root system of a ^{14}C-sucrose-tagged white oak tree. The CO_2, which evolved from the forest floor, was measured as an indication of variations in root distribution and substrate movement. During a 30-day interval, CO_2 (^{14}C and ^{12}C) efflux was measured at six sampling stations in each of three concentric circles (with radii 0.5, 1.0, and 1.5 m). The purpose of analyzing these data was (1) to determine the dependence of CO_2 efflux upon sampling time, station location, and other biologically meaningful factors; (2) to examine the variation among the CO_2 efflux observations for significant changes; and (3) to use the above information to recommend sample sizes for future experiments.

Nonparametric statistical procedures were used to determine that the CO_2 efflux *level* did change significantly ($P < 0.01$) over the experimental period analyzed. However, the only significant ($P < 0.10$) location effect upon the CO_2 efflux level was the distance from the sample tree.

The *variation* among the observations at a fixed distance from the sample tree on a particular date was not found to be a function of distance from the sample

tree. However, there was a significant ($P < 0.01$) change in this variation over the experimental period. These analyses were used to estimate the number of samples needed to estimate the CO_2 efflux level expected within specified limits as a function of the variation among the observed CO_2 efflux values.

A linear regression model formulated to describe the CO_2 efflux data accounted for 67% of the total variation in CO_2 efflux with a coefficient of variation of 29%. The model expresses CO_2 efflux as a function of the effects of other vegetation, moisture, and biologically meaningful interactions. The original model, which contained 16 terms, was reduced to 12 terms by applying a forward-selection procedure using a 0.25 level of significance. The final regression model was used to construct contours of constant estimated CO_2 efflux as a function of location relative to the sample tree. The statistical analyses have been used in planning experiments related to forest floor respiration.

LARVAL FISH, POWER PLANTS, AND BUFFON'S NEEDLE PROBLEM

Electrical power producing plants, both nuclear and nonnuclear, use large volumes of water for cooling in the condensation portion of the power production cycle. The water is usually taken from an adjacent body of water into the plant by means of intake pumps which have impeller blades that determine the rate of flow and volume of water being used. The water may contain small larval fish that pass through the preliminary screening devices and are then possibly killed if hit by one of the impeller blades.

The study of the effects of power plants upon aquatic life is of major importance, and plans are in progress at ORNL to build a working model of the power plant condensation cycle in order to study these effects through controlled experiments. Our goal was to construct a mathematical model to predict the probability of a larval fish being killed due to impingement upon the impeller blades.

The problem was formulated as a Buffon needle-type problem by considering a fish as a line segment and projecting this line segment onto a cross section of the intake tube. The geometry for a four-blade pump is depicted in Fig. 3.

The inner circle of this figure represents the hub of the impeller. The four radial segments represent the cutting edges of the impeller blades. The probability that a fish dies was defined as the probability that a random line segment falls on one of the radial segments.

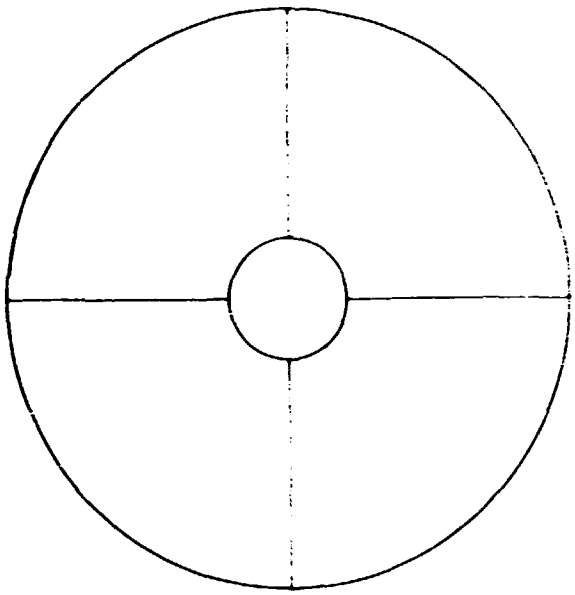

Fig. 3. Cross section of the intake tube.

There were four random variables to consider: two locate the center of gravity of the fish in the cross-sectional plane, and two determine its spatial orientation. We assumed that the location and spatial orientation variables were uniformly and independently distributed. Thus the sample space was a region of four-dimensional space, and it was possible to derive an integral for the probability of the fish being killed by hitting one of the impeller blades. The integral depended upon the following parameters: R_0, the radius of the hub; R, the radius of the tube; L, the length of the larval fish; and n, the number of blades. In attempting to calculate the desired probability, we needed to evaluate an integral of the form

$$\int_0^L \int_0^{\pi/2} \sin^{-1}\left(\frac{x \sin\Theta}{2R}\right) d\Theta\, dx .$$

The diameter of the experimental tube is 12 in. The diameter of the tube in power plants is two to three times larger. Since the length of larval fish would range between 0.25 and 0.5 in., $L/2R$ would be small; hence, we can replace $\sin^{-1}[(x \sin\Theta)/2R]$ with the linear approximation $(x \sin\Theta)/2R$. The solution for the probability of a fish being killed by the impeller blades reduced to

$$P = 4nL/\pi(R + R_0) .$$

where R, R_m, I, and n are the parameters defined above.

The validity of this mathematical model for describing the probability of mortality due to the impeller blades will be tested experimentally at ORNL.

JOINT ACTION OF TOXIC SUBSTANCES

The effect of resorcinol and 6-methylquinoline on the mortality of *Daphnia magna* has been evaluated from the results of an experiment using several concentrations of these organics applied jointly.

The basic experimental procedure was to subject a known number of *Daphnia magna* to a toxic environment and observe the mortality after a 48-hr period. The toxic environments were dilutions (6, 8, 10, 12, 14, and 16%) of a toxic mixture in water. There were five toxic mixtures: pure resorcinol, pure 6-methylquinoline, and mixtures of resorcinol and 6-methylquinoline in the ratios 1:3, 1:1, and 3:1. The range of dilutions, 6 to 16%, was selected to cover the expected 48-hr LC_{50} value, that is, the concentration for which it would be expected that 50% of the animals would be dead in 48 hr.

Probit analysis was used to estimate the LC_{50}'s and their 95% confidence intervals for each of the five toxic mixtures. The analysis indicated that mixtures of the compounds in the ratios of 1:3, 1:1, and 3:1 were less toxic than either of the pure compounds. Also, it was determined that the effects of the concentrations of the compounds were not additive—that antagonistic interactions occur when resorcinol is dominant and that infra-additive interactions occur when 6-methylquinoline is dominant.

An alternative analysis using the linear logistic model is now in progress. In this analysis the probability that an organism dies is approximated by the following function of the resorcinol concentration (x_1) and the 6-methylquinoline concentration (x_2):

$$\frac{\exp M}{1 + \exp M} ,$$

where

$$M = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{1,1} x_1^2 + \beta_{2,2} x_2^2 + \beta_{1,2} x_1 x_2 .$$

It is hoped that this model will be general enough to allow specific hypotheses to be tested about the presence or absence of antagonistic or synergistic interactions.

14. Health Physics Research

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LEUKEMIA INCIDENCE IN HIROSHIMA AND NAGASAKI

A new set of radiation dose estimates has been computed for Hiroshima and Nagasaki blast survivors in the Radiation Effects Research Foundation sample. These estimates are for bone marrow dose and are more useful than the Tentative 1965 Dosimetry, T65D, estimate of skin dose for determining the relationship between radiation insult and leukemia incidence.

Certain empirical functions have been used in prior studies to describe the relationship between leukemia incidence and skin dose as estimated from the T65D data. These same functions have now been used to describe the relationship between leukemia incidence and estimates of bone marrow dose. From these relationships have come new estimates of risk, expressed as expected number of leukemia cases per rad of exposure, which agree more closely with other risk estimates such as those obtained from ankylosing spondylitics.

RADIATION SYMPTOM INCIDENCE IN BLACK-RAIN VICTIMS

Some residents of Hiroshima and Nagasaki were subjected to a black, oily rain which fell shortly after the explosions. A report[2] was written detailing the increased incidence (relative to a control group maintained by the Radiation Effects Research Foundation) of radiation-induced symptoms among these people.

When the victims and the controls were further categorized according to the amount of blast dose received, the ratios of the number of victims to the number of controls differed markedly from one blast dose category to another. That is, the black-rain factor and the blast dose factor were confounded with one another.

In an attempt to isolate the effect of black rain from the effect of blast dose, the expected numbers of symptom incidences were computed for each of 26 symptoms under the hypothesis that black rain had no effect. In 25 of the 26 cases the observed incidence exceeded the expected.

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1. Health Physics Division, ORNL.
2. H. Yamada and T. D. Jones, *An Examination of A Bomb Survivors Exposed to Fallout Rain and a Comparison to a Similar Control Population*, ORNL TM-4017 (October 1975).

15. Materials Research

C. K. Bayne, T. L. Hebble, E. Leach, W. E. Lever, R. C. Meacham, J. Trent, D. A. Canonico[1], A. J. Caputo[1], J. V. Cathcart[1], D. P. Edmonds[1], G. M. Goodwin[1], L. A. Harris[1], W. L. Harper[2], R. L. Huddleston[2], W. J. Lackey, Jr.[1], P. Patriarca[1], R. E. Pawel[1], R. A. Perkins[1], V. K. Sikka[1], W. F. Thompson[2], G. J. Yurek[1]

ANALYSIS OF DIFFUSIVITY DATA

Measurements of the diffusivity of oxygen in β-Zircaloy have been made to estimate the constant D_0 and the activation energy Q for the oxidation rate model

$$D = D_0 e^{-Q/RT} , \qquad (1)$$

where D is the oxidation rate constant (cm^2 sec), R is the gas constant (1.987 cal mole^{-1} K^{-1}), and T is temperature (°K). The oxidation rate model is linearized by taking logarithms to get $\ln D = \ln D_0 - Q(1/RT)$, and estimates of $\ln D_0$ and Q are obtained by the methods of least squares.

The least-squares estimators $\ln \hat{D}_0$ and $\hat{Q}$ are unbiased estimators of $\ln D_0$ and Q, but $\hat{D}_0 = \exp(\ln \hat{D}_0)$ is a biased estimator of D_0. Even if $\hat{D}_0$ was corrected to be an unbiased estimator and both the unbiased estimators for D_0 and Q were substituted into Eq. (1), the resulting estimate of the oxidation rate constant would be a biased estimate because of the correlation between the two estimates, $\hat{D}_0$ and $\hat{Q}$. Unbiased estimates of the oxidation rate constant can be made from the predicted values of the linearized model. To estimate the values of D from the predicted values, $\ln \hat{D}$, we use the fact that $\ln \hat{D}$ is normally distributed under the assumption that the logarithms of the observations are normally distributed. Hence, $\exp(\ln \hat{D})$ has a log-normal distribution with mean $D \exp[\mathrm{var}(\ln \hat{D})/2]$. Then the unbiased estimate of D at the $(1/T)_k$ temperature is

$$\hat{D}_k = \exp(\ln \hat{D}_k) \cdot \exp[-\mathrm{var}(\ln \hat{D}_k)/2] .$$

VARIABILITY OF VOLUME PERCENT ESTIMATES OF PYRITE IN COAL

The precision of estimates of the volume percent of pyrite in a specially prepared coal specimen was investigated to determine the degree of effort required to obtain precise estimates from subsequent specimens. The estimates were obtained by image analysis, using a Quantimet. The Quantimet measures volume percent by projecting a magnified image of a linear surface area onto a picture tube with 500,000 picture points and by counting the number of picture points of pyrite, coal, and the epoxy binder projected. The estimate of the volume percent for the area is the ratio of the number of pyrite points to the number of pyrite plus coal points.

As a base measurement, approximately 4800 areas were measured on the specimen, yielding an estimate of 0.1315 vol % of pyrite in the coal. Since the general purpose of the study was to recommend the number of areas to be measured to obtain precise estimates, a map of the results of the 4800 point count measurements was sampled to obtain estimates based on much smaller sets of area measurements. A series of samples taken from the center of the map produced disappointing results, with an estimate of 0.0784 vol % for 225 areas and estimates of 0.1068 and 0.1508 vol % for about 700 areas each.

In addition to this sampling study, the coal specimen was cut in half and a new series of estimates was obtained, using both the previous and newly cut surfaces, based on 800 and 400 areas. The estimates based on 800 areas varied from 0.0473 to 0.1420 vol %, while the estimates based on 400 areas varied from 0.0974 to 0.2478 vol %.

As a result of the variation in these estimates, the measurement tapes of the point counts were reexamined to test the assumption that the pyrite was randomly distributed throughout the coal specimen. This investigation indicated that the assumption was false and that the pyrite tended to occur in varying size clumps, with over half the areas containing no pyrite.

Since the magnitude of an estimate was found to depend almost solely on the number of the sparsely distributed large clumps of pyrite which appeared in the sample of areas measured and since the major cost of the measurement process is the setup cost, the

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recommendation was to completely survey the surfaces of subsequent coal specimens of similar sparse pyrite content, as was initially done with the specimen in question.

VARIATION AMONG HEATS OF TYPES 304 AND 316 STAINLESS STEEL TUBE

The large heat-to-heat variation associated with mechanical properties of steels is of growing concern among metallurgists. Of current interest are materials such as types 316 and 304 stainless steel and 2¼ Cr 1 Mo alloy steel, which are used in steam generators for nuclear reactors. To understand this variation among heats better and to emphasize the need for properly designed experiments, Japanese data[3,4] were selected for analysis.

Using analysis of variance techniques, an estimate of heat-to-heat variation, denoted σ_H^2, from nine heats of material was calculated for tensile and creep properties of types 304 and 316 stainless steel. In this section we discuss the tensile properties, yield strength (YS, kg/mm^2) and ultimate tensile strength (UTS, kg mm^2), and the logarithm of the creep property, rupture life (t_r, hr).

The expected mean square (EMS) for the random effect of heat on tensile properties is

$$\text{EMS} = \sigma^2 + n_t \sigma_H^2 ,$$

where

n_t = number of temperature levels,

σ^2 = error variance.

This EMS is based on the assumption that tensile properties are an additive function of a fixed temperature effect and a random heat effect. The corresponding EMS for the logarithm of rupture life is

$$\text{EMS} = \sigma^2 + n_t n_s \sigma_H^2 ,$$

where n_s = number of stress levels and σ^2, n_t, and σ_H^2 are as defined above. In this case the logarithm of rupture life is assumed to be an additive function of a fixed temperature effect, a fixed stress (within temperature) effect, a random heat effect, and a temperature-by-heat interaction. Estimates of the mean squares for heats and of the heat-to-heat variation are listed in Table 4.

To illustrate the effect of heats on the uncertainty of the true value, we omit σ^2 and compute the 95% confidence interval about a single test based solely on heat-to-heat variation.

$$\text{mechanical property} \pm t_{0.95} \sqrt{\sigma_H^2} ,$$

where $t_{0.95}$ is the critical t value at the 0.95 confidence level for an appropriate number of degrees of freedom. Also a similar expression is used for the ($P = 0.90$, $\lambda = 0.95$) tolerance limits to reflect the scatter in data due solely to variation among heats

$$\text{mechanical property} \pm K \sqrt{\sigma_H^2} ,$$

where K is the tolerance factor based on the proportion P, the confidence level λ, and an appropriate number of degrees of freedom. Results of these calculations are given in Table 5.

DELTA-FERRITE IN PRODUCTION STAINLESS STEEL PIPE WELDS

Numerical and pictorial summaries were used to analyze 1449 paired ferrite measurements collected by

3. *Data Sheets on the Elevated Temperature Properties of 18 Cr 8 Ni Stainless Steel for Boiler and Heat Exchanger Seamless Tubes*, SUS 27 HTB, NRIM Creep Data Sheet No. 4, National Research Institute for Metals, Tokyo, Japan (1972).

4. *Data Sheets on the Elevated Temperature Properties of 18 Cr 12 Ni Mo Stainless Steel for Boiler and Heat Exchanger Seamless Tubes*, SUS 32 HTB, NRIM Creep Data Sheet No. 6, National Research Institute for Metals, Tokyo, Japan (1972).

Table 4. Estimates of mean squares and heat-to-heat variation

	Type 304 stainless steel tube		Type 316 stainless steel tube	
	Mean square	σ_H^2	Mean square	σ_H^2
UTS (kg mm^2)[a]	16.737	1.457	18.205	1.598
YS (kg mm^2)[b]	23.593	2.069	35.886	3.181
$\log t_r$[c]	0.6493	0.05270	0.1453	0.01120

[a] UTS, ultimate tensile strength

[b] YS, yield strength

[c] t_r, rupture life.

Table 5. Confidence limits and tolerance limits

Type 304 stainless steel tube	Type 316 stainless steel tube
Confidence limits based on heat-to-heat variation	
UTS = [illegible] kg/mm² ([illegible] ksi)[a]	UTS = [illegible] kg/mm² ([illegible] ksi)
YS = [illegible] kg/mm² ([illegible] ksi)[b]	YS = [illegible] kg/mm² ([illegible] ksi)
[illegible]	[illegible] 0.244
Tolerance limits based on heat-to-heat variation	
UTS = [illegible] kg/mm² ([illegible] ksi)	UTS = [illegible] kg/mm² ([illegible] ksi)
YS = [illegible] kg/mm² ([illegible] ksi)	YS = [illegible] kg/mm² ([illegible] ksi)
[illegible]	[illegible]

[a] UTS = ultimate tensile strength.
[b] YS = yield strength at 2 [illegible] offset.
[c] [illegible] rupture life.

the Joint Task Group on Control of Stainless Steel Welding Materials. The purpose of this study was to compare delta-ferrite content as measured by ferrite number in the filler metal weld pad (FW) with that in the resultant production weld (PW).

Three welding processes were used to join several forms and combinations of types 304, 308, and 316 stainless steel. FW values ranged from 5 to 15, while ferrite content for the base metal weldments ranged from 2.3 to 17.5. For FW values less than 14, the median PW number corresponded reasonably well to the FW number, although there exists a wide scatter of PW results at each FW level. This is illustrated in Fig. 4 with "box and whisker" plots suggested by Tukey[5] for displaying data.

These plots are created by first determining the median and hinges (see Fig. 4b) from an ordered set of data and then finding the "whisker" and extreme points accordingly. The median is the middle value of the order set, while the hinges correspond to the middle values between the median and extremes. Thus, at most, 50% of the data fall inside the interval spanned by the H-spread. If hinge points are included, then at least 50% of the observations are contained in the interval. All points that fall outside the H-spread plus 1 step are plotted. Unusual plots, such as in Fig. 4 under FW 13, call attention to, and summarize important distributional aspects of, the observations. Here, no upper "whisker" is shown, because at least 25% of the data are equal to 17. In this situation the upper hinge and the maximum value within one step of the upper hinge are both equal to 17. In the extreme case, where all values in a data set are the same, there is no "box" or "whisker," just a median.

Measurement techniques were completely confounded with differences between ferrite filler and production numbers. That is, two techniques (magne-gage and chemical analysis, Schaeffler diagram) were used solely for FW measurements, while the remaining three techniques (severn gage, elcometer, and ferrite scope) were used solely for PW measurements. Also, these methods were partially confounded with data source and thickness of metal.

Results from the "range reading" severn gage and "dial reading" elcometer and ferrite scope methods were compared separately with results from the dial-reading magne-gage and the empirically determined Schaeffler diagram. This comparison is made by looking at the distribution of differences given in Fig. 5. As expected, the dial-reading results (Fig. 5c) exhibited less scatter.

DETECTING A DEFECT BY VARIANCE COMPONENTS

While analyzing the variation of thicknesses in a diffusion experiment, a large variance component due to sample position in the experimental apparatus was detected. Subsequent experiments to explain this position variation indicated that certain regions of the experimental apparatus were not heating properly.

In an oxidation rate experiment, the thicknesses of the oxide layer and alpha layer are measured r times at each of m positions on a zirconium tube. An initial position on the zirconium tube is chosen randomly, and the tube is rotated θ° to each new position.

The values for r and m can be chosen to control the variance of the average of the thickness measurements for each experiment. If the variance of the individual measurements increases with temperature, a reasonable number of additional measurements may be made with increasing temperatures to ensure that the variances of the averages are constant over all temperatures. The number of additional measurements will depend on the rate of increase of the variances.

The variance components of y_{ijk} are examined by using the analysis-of-variance (ANOVA) model

$$y_{ijk} = \mu + F_i + P_{j(i)} + e_{ijk} , \qquad (1)$$

where

$i = 1, \ldots, t, j = 1, \ldots, m, k = 1, \ldots, r$.

[5] J. W. Tukey, *Exploratory Data Analysis*, Addison-Wesley, Reading, Mass., 1970.

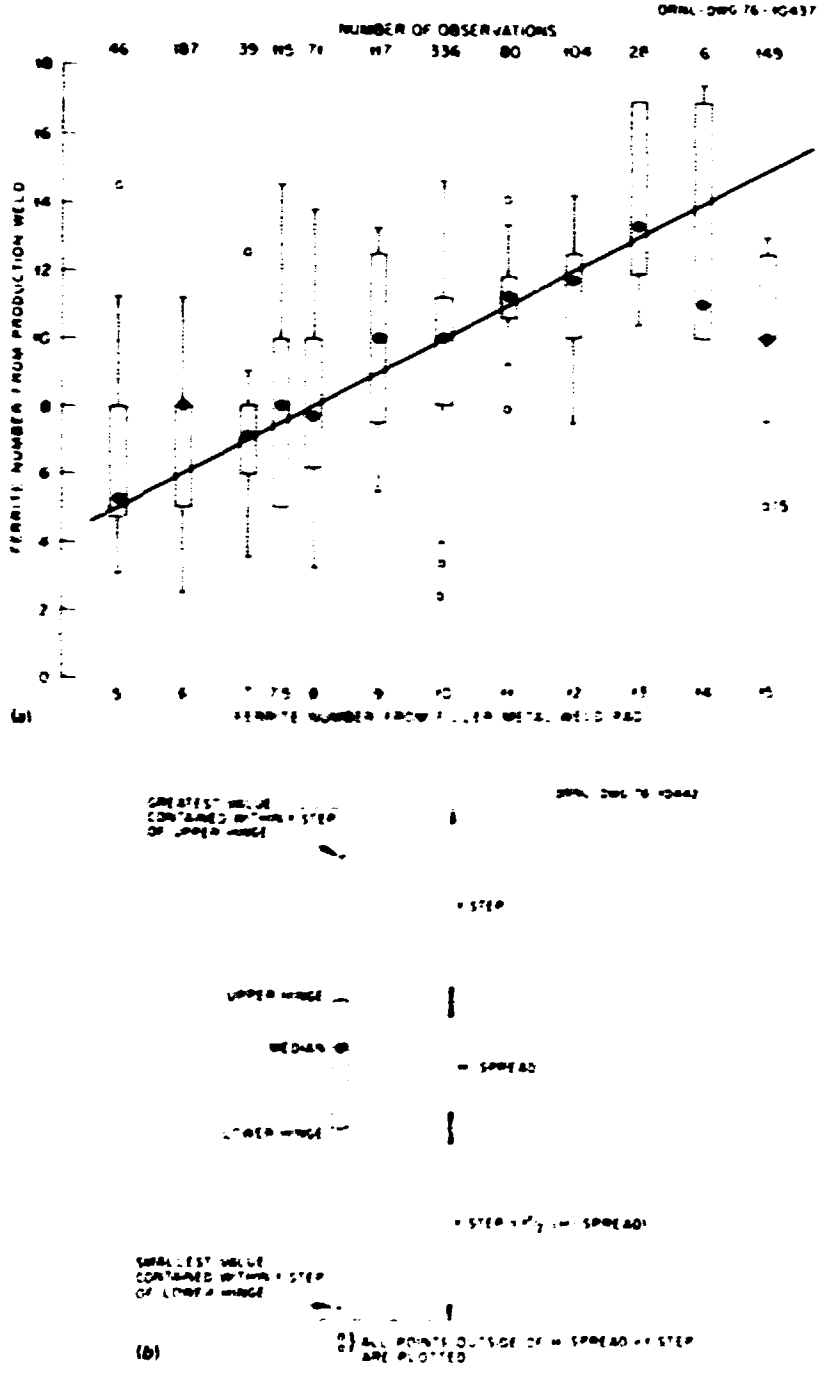

Fig. 4. Distribution of ferrite numbers on production welds. (a) Distribution. (b) Key

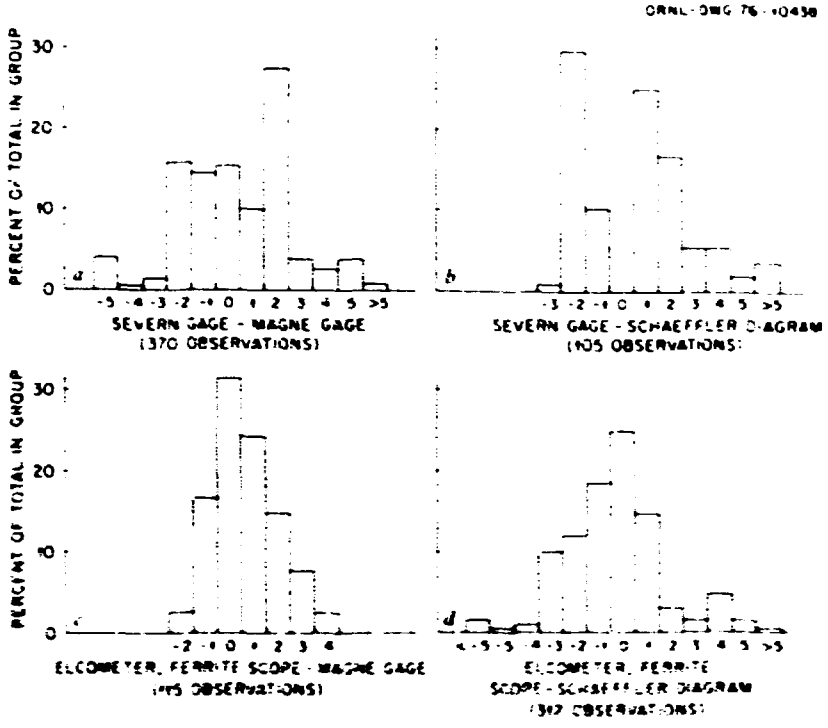

Fig. 5. Distribution of differences (PW-FW).

Table 6. ANOVA for the variance component model

Source of variation	Degrees of freedom	Mean squares	Expected mean squares
Experiment	$r-1$	MSEXP	$\sigma_\epsilon^2 + n\sigma_{P(E)}^2 + mn\sigma_E^2$
Position within experiment	$r(m-1)$	MSPOS	$\sigma_\epsilon^2 + n\sigma_{P(E)}^2$
Error	$rm(n-1)$	MSERR	σ_ϵ^2
Total	$rmn-1$		

The estimated variance components are $\hat{\sigma}_\epsilon^2$ = MSERR, $\hat{\sigma}_{P(E)}^2$ = (MSPOS − MSERR)/n, $\hat{\sigma}_E^2$ = (MSEXP − MSPOS)/mn.

In the model, each measurement Y_{ijk} is the sum of an overall mean, μ, a random component due to the ith experiment, E_i, a random component due to the jth position within the ith experiment, $P_{j(i)}$, and a random error component, ϵ_{ijk}. The random components, E_i, $P_{j(i)}$, and ϵ_{ijk}, are assumed to be mutually independent with mean zero and variances σ_E^2, $\sigma_{P(E)}^2$, and σ_ϵ^2 respectively. The variance components are estimated by equating the expected mean squares,[6] EMS, to the corresponding mean squares in the ANOVA (Table 6) derived from the model.

6. S. R. Searle, *Linear Models*, Wiley, New York, 1971.

Measurements were made on the thickness of the oxide and alpha layers on ten experiments at 900°C and 15 experiments at 1300°C. For each experiment two measurements were made at each of four positions. The estimates of each variance component are summarized in Table 7.

The estimates of the experimental variance component $\hat{\sigma}_E^2$ are much larger than the estimates of the other two variance components. The larger value is to be expected, because each experiment represents the oxidation accumulated over a given period of time.

The estimate for the position variance component $\hat{\sigma}_{P(E)}^2$ represents the variation in thickness at different

Table 7. Variance component estimates

Variance component	Oxide at 900°C	Oxide at 1340°C	Alpha at 900°C	Alpha at 1340°C
$\hat{\sigma}^2_E$	7.1144	264.286	38.2620	4901.4452
$\hat{\sigma}^2_{P(E)}$	0.0715	3.9770	0.1850	9.8434
$\hat{\sigma}^2_t$	0.2596	0.1643	0.3611	0.7261

positions around the zirconium tubing. Although this variation is not zero at 900°C, it is smaller than the estimated measurement variation $\hat{\sigma}^2_t$ for both the oxide thickness and alpha thickness. For 1300°C the estimated position variations for both the oxide thickness and alpha thickness are considerably larger than the estimated measurement variation. The explanation for this increase with an increase in temperature is not clear.

To investigate the position variation, an experiment was conducted at 1300°C in which thickness measurements were made on a number of different positions corresponding to the zirconium sample orientation in the furnace. By plotting thickness vs furnace position, two cold spots relative to the nominal temperature were identified at the hinges and opening of the furnace. Subsequent thickness measurements were eliminated from these two areas in order to reduce the position variation. Therefore, by analyzing the components of variation in the thickness measurements, a defect in the experimental apparatus was found and accounted for in subsequent measurements.

AMERICAN WELDING SOCIETY MEMBERSHIP SURVEY

A survey is being conducted to better understand the makeup of the American Welding Society membership. Preliminary results from an initial response of 220 members in the Houston area are being analyzed. During June 1976 a revised questionnaire will be distributed to 300 members in another region. Results from these initial mailings will be used to prepare a questionnaire for distribution to the Society's 28,000 members.

VARIATIONS IN OXIDATION RATES DUE TO TEMPERATURE VARIATIONS

For a fixed temperature T the oxide thickness ξ of Zircaloy is assumed to be related to the time t of exposure to steam by the equation

$$\xi^2 = K(T)t + \alpha . \qquad (1)$$

The intercept α is a constant, and the slope $K(T)$ is a function of temperature given by

$$K(T) = Ae^{-Q/RT},$$

where A, Q, and R are constants and T is temperature. The slope is a constant for a fixed temperature; however, if temperature cannot be measured exactly, the slope will vary from experiment to experiment. The effect of temperature variations on estimating the slope and intercept in Eq. (1) is a difficult problem to solve analytically. An approximate solution can be obtained by simulating random temperatures in the range of $T \pm 10$ and then calculating the corresponding slopes and intercepts.

This was done by generating normally distributed random temperatures with mean T and standard deviation 10/1.96 for ten different times (t_i, $i = 1, 2, \ldots, 10$) and then estimating the slope and intercept by the least-squares method. One thousand slopes and intercepts were generated in this manner for each of the seven temperatures, 900, 1000, 1100, 1200, 1300, 1400, and 1500°C. The results of this simulation show that the estimated slopes do not vary much with temperature variations but that the estimated intercepts do vary appreciably, especially at the lower temperatures.

PERMEABILITY OF HTGR GRAPHITE BLOCKS

During the fabrication of fuel rods for the HTGR, pitch in the matrix of the fuel rods volatilizes and diffuses through the webbing of the graphite block (see Fig. 6) into the coolant holes. If the permeability of the webbing is too low, the pitch materials cannot escape, and this results in a high pitch-coke yield for the fuel rod. Therefore, the pitch-coke yield is related to the permeability properties of the graphite block.

To study these permeability properties, air flow measurements were made on 146 holes in ten different graphite blocks. An analysis of this data indicated a wide variation in the permeability values among the blocks. Within each block, variation in permeability values can be attributed to two factors. The dominant

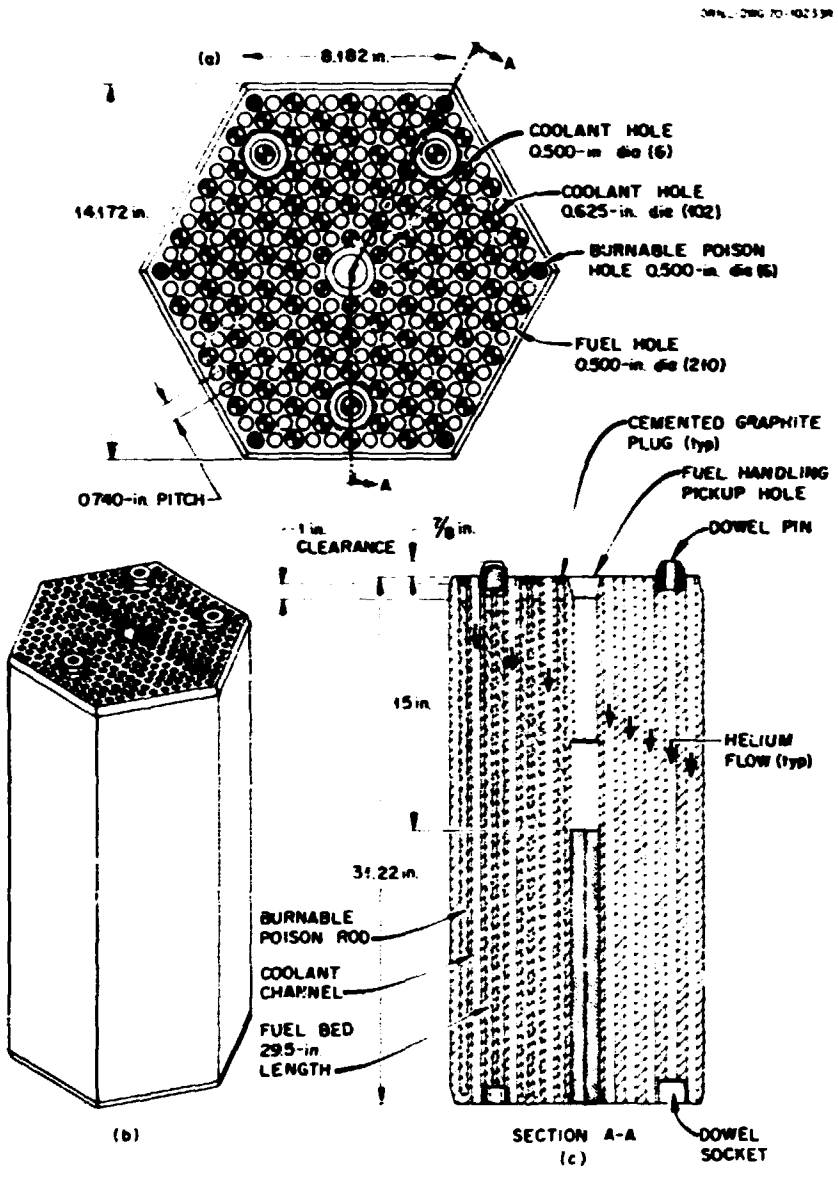

Fig. 6. Fort St. Vrain fuel element.

factor is the position of a fuel hole in the graphite block, and the second factor is the geometry of a fuel hole in the graphite block. The geometry effect is the relation of a fuel hole to its surrounding coolant holes and other fuel holes. Five different types of geometry are identified.

The statistical analysis of the permeability measurements on ten graphite blocks indicated four sources of permeability variation, which account for 97% of the variation of the measurements from an overall mean. The four sources: (1) block-to-block variation, (2) geometry-type variation, (3) hole location variation, and (4) block and type interaction variation were all significant at the 1% level for the combined data set of the ten blocks.

Each individual block was then analyzed to study the effect of the geometry type and hole location. The geometry-type effect was significant at the 1% level in all but one block. An estimate of the sum of the geometry effect and the overall mean was made for each type. These estimates are called adjusted geometry-type means and represent the permeability

response due to different geometry types without the influence of hole location.

Hole location effects are represented by contours of fixed values of the permeability response. These contours indicate that the responses are slightly elliptical but are not centered in the middle of the block. The values of the permeability responses decrease in a nonuniform manner as the holes are located farther from the center of the block.

EVALUATION OF CHARACTERISTICS OF KELVAR YARN

An experimental design has been devised to evaluate the uniformity of denier and tensile strength within and among spools of Kelvar yarn. The design calls for four spools of yarn to be selected at random from the lot of spools, for ten lengths to be selected at random within each spool, and for five measurement regions to be defined within each length for a total of 200 measurements each for denier and tensile strength. The design was constructed to give 95% power of detecting a substantial excess of among-spool, over within-spool, variability when testing equality of variance at the 5% level of significance.

In addition to the evaluation of the denier and tensile strength variability, a preliminary evaluation of chemical variability is required. The design for the chemical analysis was constructed as a subsample of the primary design and utilized only four lengths per spool and two measurement regions per length for a total of 32 sets of chemical measurements.

This configuration will have 95% power of detecting among-spool variability 2.5 times as large as within-spool variability when equality of variance is tested at the 5% level of significance.

The spools to be sampled have been designated, a procedure has been established for the random selection of the lengths within the spools for the denier and tensile strength evaluation, and the subsample has been specified for the preliminary chemical variability evaluation.

The implementation of the experimental design has been scheduled, and the statistical analysis of the subsequent data will follow the completion of the study.

16. Reactor and Thermonuclear Research

S. J. Chang D. G. Wilson H. R. Hicks[1] D. N. Robinson[2]

A MAGNETOHYDRODYNAMICS PROBLEM

We have obtained a solution for a time-independent magnetohydrodynamics problem posed in a torus of rectangular cross section. Our motivation was a desire to broaden the class of time-independent problems for which closed-form solutions exist as well as a need to generate initial values for computer codes to solve time-independent problems with similar geometry. The problem consisted of partial differential equations for pressure and magnetic field: grad $p = (\text{curl } \vec{B}) \times \vec{B}$, div $\vec{B} = 0$ in cylindrical polar coordinates for (r, ϕ, z) interior to the torus – that is,

$$r_0 - a < r < r_0 + a, \quad 0 \le \phi < 2\pi, \quad -b < z < b;$$

and boundary conditions:

$$p(r_0 \pm a, \phi, z) = p(r, \phi, \pm b) = 0,$$

$$B_r(r_0 \pm a, \phi, z) = B_z(r, \phi, \pm b) = 0.$$

A number of assumptions, motivated by the physics of the problem, reduced the equations to a single second-order linear partial differential equation in two variables with homogeneous boundary conditions. This equation in turn separated into two second-order ordinary differential equations similar to that for a harmonic oscillator. One of these was immediately solvable, and the other yielded to a finite difference scheme. In this respect we fell somewhat short of the goal, to obtain a closed-form solution, but a usable computational solution was obtained.

CREEP POTENTIAL FOR TIME-DEPENDENT INELASTIC DEFORMATION

In his formulation of inelastic stress-strain relations for metals, Rice[3] has proposed that the inelastic strain can be expressed from a potential function Ω, the creep potential, as

$$\dot{E}^p_{ij} = \frac{\partial \Omega}{\partial \Sigma_{ij}},$$

where $\dot{E}^p_{ij}$ and Σ_{ij} are inelastic strain rate and stress tensors respectively. In the above expression, Ω is a function of the stress tensor Σ_{ij} and the past strain history. The existence of the potential Ω can be deduced from the microstructure of the metal. A sample of material is known to be composed of microscopic grains, randomly oriented. Inelastic deformation of the solid may be determined by the inelastic deformation of the grains. Suppose that the sample is subject to a homogeneous stress state Σ. The macroscopic strain tensor E associated with the displacement u is defined by requiring that $\Sigma^*_{ij}E_{ij}$ be the specific work corresponding to the given surface displacement of the sample for any stress state Σ^*_{ij}; that is,

$$(\Sigma^*_{ij}E_{ij})V = \int_A (\Sigma^*_{ij}n_j)u_i \, dA, \tag{1}$$

where V is the volume of the small sample with surface A and where n_j is the direction cosine of the normal to the surface. Equation (1) can be reduced to

$$E_{ij} = \frac{1}{V}\int_A \tfrac{1}{2}(n_i u_j + n_j u_i)\, dA. \tag{2}$$

Independent of the given stress Σ^*, Eq. (2) can be regarded as the volume average of the microstrains of the grains within the sample.

From the reciprocal theorem in elasticity, the work of load set (*) on displacement set (**) equals the work of load set (**) on displacement set (*), where (*) and (**) denote any two solutions of the elastic field equations. Hence,

$$(\Sigma^*_{ij}E^{**}_{ij})V - \int_{A\,(\text{slip})} \sigma^*_{ij}n_j \Delta u^{**}_i \, dA = (\Sigma^{**}_{ij}E^*_{ij})V - \int_{A\,(\text{slip})} \sigma^{**}_{ij}n_j \Delta u^*_i \, dA.$$

where Δu denotes the inelastic slip of the grain. Let us take (*) as the elastic field associated with Σ^*, so that $\Delta u^* = 0$. We choose (**) as the residual field left on unloading; that is, $\Sigma^{**} = 0$ and $E^{**} = E^p$. The right side of the above equation is zero, and we therefore have

$$\Sigma^*_{ij}E^p_{ij} = \frac{1}{V}\int_{A\,(\text{slip})} \sigma^*_{ij}n_j \Delta u_i \, dA$$

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1. Computing Applications Department.
2. Reactor Division, ORNL.
3. J. R. Rice, "On the Structure of Stress-Strain Relations for Time-Dependent Plastic Deformation in Metals," *J. Appl. Mech.* 37, 728–37 (1970).

for arbitrary elastic Σ_{ij}^{*} and its associated σ_{ij}^{*}. Since the plastic deformation for each grain is due to shearing strain, the above equation can be reduced to

$$\Sigma_{ij}\dot{E}_{ij}^{p} = \frac{1}{V}\int_{V\,(\text{slip})} \tau\gamma\, dV .$$

where τ and γ are shearing stress and strain respectively.

Physical considerations of dislocation suggest that

$$\dot{\gamma} = \dot{\gamma}\ (\tau, \text{current state}) .$$

We obtain, therefore,

$$\dot{E}_{ij}^{p}(\Sigma)\, d\Sigma_{ij} = \frac{1}{V}\int_{V\,(\text{slip})} [\dot{\gamma}(\tau)\, d\tau]\, dV .$$

whence the existence of Ω can be derived; that is,

$$\dot{E}_{ij}^{p} = \frac{\partial \Omega}{\partial \Sigma_{ij}} .$$

In the above equation,

$$\Omega(\Sigma) = \frac{1}{V}\int_{V\,(\text{slip})} \omega(\tau)\, dV ,$$

$$\omega(\tau) = \int_{0}^{\tau} \dot{\gamma}(\tau)\, d\tau .$$

With the existence of creep potential, the known results in time-independent plasticity can be consistently generalized to the time-dependent case. Using this formulation, further understanding of the plastic deformation of metals can be expected.

17. Sampling Inspection, Quality Control, and Life Testing

C. K. Bayne W. E. Lever J. E. Tobias C. E. Knight, Jr.[1] D. R. Johnson[2]

ACCELERATED LIFE TEST

An accelerated life test was designed to yield an estimate of the probability that a unit will survive to at least a specified time T under an operating stress which is a small fraction of the failure stress. The test will be conducted under a series of stresses that are much greater than the operating stress but are still only a fraction of the failure stress. The failure stress is defined as the mean stress required to cause immediate failure of the unit when that level of stress is applied.

A literature search indicated the Weibull distribution,

$$F(t; S, m, \lambda_S) = 1 - \exp[-(\lambda_S t)^m] ,$$

would be a reasonable choice for the time-to-failure distribution when the shape parameter m is constant over all test stresses S and the scale parameter λ_S is a function of the ratio of the test stress S to the failure stress S_0. Two models proposed for λ_S were

$$\lambda_S = kP^n \text{ (power law model)} ,$$

$$\lambda_S = k \exp(nP) \text{ (exponential model)} ,$$

where $P = S/S_0$.

While few data were available for the unit in question, data on the time to failure were available for a similar unit for stresses in the range of 60 to 90% of failure stress. The time-to-failure distribution of the similar unit is believed to be of the same type as that of the unit in question but with at least a 10% shorter mean time to failure.

A method proposed by Nelson[3] was used to estimate the parameters m, k, and n and to test the fit for both the power law and exponential models. For the range of stresses in which data were available, statistical tests indicated that both models fit the data. In addition, both models predicted that at least 95% of the units would last longer than the specified time T with 95% confidence under the low operating stress, but the exponential model produced more conservative predictions.

Utilizing the data available on the similar units, an accelerated life test was designed, assuming the time-to-failure distribution is the Weibull distribution with a constant shape parameter for all stresses less than the failure stress and with a scale parameter of the exponential model form. The design allocates the test units budgeted for the study equally among five equally spaced stress ratios.

This design does not meet a recently proposed optimality criterion,[4] since that criterion calls for only two stress ratios, one of which would likely require a test period much longer than the three-year period proposed for this test. In addition, the proposed optimum test would not allow a comparison between the two models proposed for the scale parameter.

The test units are to be manufactured and tested according to the specifications of the experimental design, with subsequent statistical analysis of the data following the completion of the test period.

LIMITS ON FUEL ROD LENGTHS

The tolerance limits of the lengths of fuel rods are $L \pm \Theta$ (in inches). A number, n, of these fuel rods are stacked so that the total length is within a tolerance of $nL \pm \delta$ (in inches). It is necessary to estimate the value of Θ for a given value of δ so that the total length of the stack is within the interval $nL \pm \delta$, with a probability of $1 - \alpha$, for small values of α.

We assume that the lengths of fuel rods are independent and normally distributed with an expected value L. In addition, we assume that a proportion, at least $1 - \gamma$, of the fuel rods have lengths which fall within the interval $(L - \Theta, L + \Theta)$; that is,

$$\text{Prob}\{L - \Theta < L_i < L + \Theta\} = 1 - \gamma, \quad i = 1, 2, \ldots, n .$$

From this second assumption we can derive Θ in terms of the standard deviation σ of the process

$$\Theta = \sigma Z_{\gamma/2} , \qquad (1)$$

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1. Y-12 Development.
2. Metals and Ceramics Division, ORNL.
3. W. B. Nelson, *Statistical Methods for Accelerated Life Test Data — The Inverse Power Law Model*, No. 71-C-011, General Electric Company Technical Information Series (1970).
4. W. Q. Meeker and W. B. Nelson, *Charts for Optimum Accelerated Life Tests for the Weibull and Extreme Value Distributions*, No. 74CRD247, General Electric Company Technical Information Series (1974).

where $Z_{\gamma/2}$ is the quantile of the standardized normal variate such that

$$\text{Prob}\{Z > Z_{\gamma/2}\} = \gamma/2 .$$

From the first assumption of normality, the random variable

$$\left(\sum_{i=1}^{n} L_i - nL\right)/\sigma\sqrt{n}$$

is also a normally distributed random variable with a mean of zero and a variance of one. Using this random variable, the $1 - \alpha$ confidence interval for the total length is derived from

$$\text{Prob}\{nL - Z_{\alpha/2}\sigma\sqrt{n} < TL < nL + Z_{\alpha/2}\sigma\sqrt{n}\} = 1 - \alpha .$$

This implies that the standard deviation of the process is

$$\sigma = \delta/(Z_{\alpha/2}\sqrt{n}) . \tag{2}$$

Substituting Eq. (2) into Eq. (1), we find Θ for known values of γ, α, and δ by

$$\Theta = (\delta Z_{\gamma/2})/(Z_{\alpha/2}\sqrt{n}) . \tag{3}$$

For example, we plan to stack 15 fuel rods of length $2 \pm \Theta$ inches. We know that only γ ($\gamma = 0.05, 0.01, 0.001$) of the fuel rods will be rejected if they have lengths greater than $2 + \Theta$ inches or less than $2 - \Theta$ inches. We require values of Θ such that

$$\text{Prob}\{30 - \delta < \sum_{i=1}^{n} L_i < 30 + \delta\} = 1 - \alpha ,$$

when $\alpha = 0.05, 0.01$, and 0.001.

The Θ values are listed in Table 8 as a function of δ. For example, if $\delta = 0.15$, $\gamma = 0.001$, and $\alpha = 0.01$, then $\Theta = 0.329\delta = 0.329(0.15) = 0.0494$. That is, the length of each fuel rod must be within a tolerance of ± 0.0494 in. We should note that if $\alpha = \gamma$, then $\Theta = \delta\sqrt{15} = 0.258\delta$, which is independent of the size of the confidence intervals. Under the normality assumption, if we have a high degree of confidence that the lengths of the fuel rods will be within the tolerance range of $2 \pm 0.258\delta$, then we have the same high degree of confidence that the total length will be within the tolerance range $30 \pm \delta$.

Table 8. Values of Θ for various values of α and γ

γ	α = 0.05	α = 0.01	α = 0.001
0.05	0.258δ	0.196δ	0.154δ
0.01	0.340δ	0.258δ	0.203δ
0.001	0.433δ	0.329δ	0.258δ

AVERAGE OUTGOING QUALITY FOR MODIFIED CONTINUOUS SAMPLING PLANS

The Oak Ridge Y-12 Plant uses modified versions of Dodge and Torrey's CSP-1 and CSP-3 sampling plans in some of their quality control programs. Since the exact versions were not used, the average outgoing quality (AOQ) and the average fraction of units inspected (AFI) functions were not known. The forms of these functions are required to correctly estimate the effect of this phase of the quality control program.

The modified version of the CSP-1 plan used by the Y-12 Plant is as follows:

1. *Qualifying period*: Inspect 100% of the units consecutively as produced until i units in succession are found free of the defect of interest.
2. *Normal inspection period*: When i units in succession are found free of the defect of interest, discontinue 100% inspection and randomly inspect only a fraction f of the units, but do not allow uninspected sequences greater than k units. That is, if an uninspected sequence of k units occurs, the $k + 1$ unit will be inspected.
3. If a unit is found to have the defect of interest during the normal inspection period (2), revert to the qualifying period (1).

The modified plan differs from the CSP-1 plan because of the restriction forbidding uninspected sequences greater than k. The Y-12 plan can be described as an $i + k + 1$ state Markov process, where $i + 1$ states are inspection states and k states are uninspected states. The transition matrix M associated with the process is of the form

$$M = \begin{bmatrix} q\underline{1}_i & p\underline{I}_i & \underline{0} & \underline{0} \\ q\underline{1}_1 & \underline{0} & p\underline{1}_1 & \underline{0} \\ fq\underline{1}_k & \underline{0} & pf\underline{1}_k & (1 - f)\underline{I}_k \\ q\underline{1}_1 & \underline{0} & p\underline{1}_1 & \underline{0} \end{bmatrix} .$$

where $q = 1 - p$ is the probability a unit comes to the inspection station with the defect of interest, I_s is an identity matrix of rank s, $\underline{1}_s$ is a unit column vector of length s, and $\underline{0}$ is a matrix of zeros of the appropriate dimensions.

The matrix M is ergodic, and the forms of the AOQ and AFI functions can be found in terms of q from the steady-state probability vector associated with M. The AOQ function is found by summing the steady-state probabilities of the uninspected states and multiplying this sum by the probability q that a unit has the defect of interest.

The steady-state probability vector $\underline{\beta}$ is found by solving the equation $\underline{\beta} = \underline{\beta}M$. Let $\underline{\beta} = (\underline{\beta}_1, \underline{\beta}_2)$, where $\underline{\beta}_1 = (\beta_{1,0}, \ldots, \beta_{1,i-1})$ are the probabilities associated with the qualifying period (1) and $\underline{\beta}_2 = (\beta_{2,0}, \ldots, \beta_{2,k})$ are the probabilities associated with the normal inspection period (2). Then the states associated with all of $\underline{\beta}_1$ and $\beta_{2,0}$ are the inspection states, and the remaining states are the noninspection states. So the AOQ is of the form

$$\mathrm{AOQ}(q) = q\sum_{j=1}^{k} \beta_{2,j} .$$

The equations for the steady-state probabilities are found to be

$$\beta_{1,0} = q\left\{1 - p^i + p^i\left[\frac{1-(1-f)^{k+1}}{f}\right]\right\}^{-1},$$

$$\beta_{1,j} = p^j\beta_{1,0}, \quad j = 1, \ldots, i-1,$$

$$\beta_{2,0} = p^i\beta_{1,0}/q,$$

$$\beta_{2,j} = (1-f)^j\beta_{2,0}, \quad j = 1, \ldots, k,$$

$$1 = \sum_{j=0}^{i-1} \beta_{1,j} + \sum_{j=0}^{k} \beta_{2,j} .$$

Then

$$\sum_{j=1}^{k}\beta_{2,j} = \beta_{2,0}\sum_{j=1}^{k}(1-f)^j = \frac{p^i(1-f)[1-(1-f)^k]/f}{1+p^i(1-f)[1-(1-f)^k]/f}.$$

Thus the forms of the AOQ and AFI functions in terms of q can be seen to be

$$\mathrm{AOQ}(q) = \frac{qp^i(1-f)[1-(1-f)^k]/f}{1+p^i(1-f)[1-(1-f)^k]/f},$$

$$\mathrm{AFI}(q) = 1 - \mathrm{AOQ}(q)/q .$$

The modified version of the CSP-3 plan used by the Y-12 Plant is as follows:

1. and 2. are as in CSP-1.

3. *Conditional requalifying period*: If a unit is found to have the defect of interest during the normal inspection period, revert to 100% inspection until x units in succession are found to be clear of the defect of interest. However, if a unit is found with the defect of interest, revert immediately to the qualifying period (1).

4. *Conditional normal inspection period*: If the next x units are found to be free of the defect of interest, revert to normal inspection as in (2), but if any of the next y units inspected have the defect of interest, revert immediately to the qualifying period (1).

5. If the next y units inspected are free of the defect of interest, then revert to the normal inspection period (2) without restriction.

The Y-12 version of the CSP-3 plan differs from the regular CSP-3 plan in two ways: (1) the restriction forbids uninspected sequences greater than k, as in the Y-12 version of CSP-1; (2) the conditional requalifying period has been altered to allow the x units to be inspected sequentially, with a decision to be made after each inspection. The CSP-3 plan calls for the x units to be inspected as a batch, and a decision is made only after all x units have been inspected, regardless of the results of the individual inspections.

The Y-12 sampling plan can be described as an $i + k + x + y(k + 1) + 1$ state Markov process with $i + x + y + 1$ inspection states and $k(y + 1)$ states in which units are not inspected for the defect of interest. The transition matrix M associated with the process is of the following form:

$$M = \begin{bmatrix}
q\underline{1}_{i-1} & p\underline{I}_{i-1} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} \\
q\underline{1}_i & \underline{0} & p\underline{1}_i & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} \\
\underline{0} & \underline{0} & fp\underline{1}_k & (1-f)\underline{I}_k & fq\underline{1}_k & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} \\
\underline{0} & \underline{0} & p\underline{1}_i & \underline{0} & q\underline{1}_i & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} \\
q\underline{1}_x & \underline{0} & \underline{0} & \underline{0} & \underline{0} & p\underline{I}_x & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} \\
qf\underline{1}_k & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & (1-f)\underline{I}_k & p\underline{I}_k & \underline{0} & \underline{0} & \underline{0} \\
q\underline{1}_i & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & p\underline{1}_i & \underline{0} & \underline{0} & \underline{0} \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
qf\underline{1}_k & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & (1-f)\underline{I}_k & p\underline{I}_k & \underline{0} \\
q\underline{1}_i & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & p\underline{1}_i & \underline{0} \\
qf\underline{1}_k & \underline{0} & fp\underline{1}_k & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & (1-f)\underline{I}_k \\
q\underline{1}_i & \underline{0} & p\underline{1}_i & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0} & \underline{0}
\end{bmatrix}$$

The matrix M is again ergodic, so forms of the AOQ and AFI functions can again be found in terms of q from the steady-state probability vector $\underline{\beta}$, where $\underline{\beta} = \underline{\beta}M$.

Let $\underline{\beta} = (\underline{\beta}_1, \underline{\beta}_2, \underline{\beta}_3, \underline{\beta}_{3+1}, \ldots, \underline{\beta}_{3+y})$, where $\underline{\beta}_1 = (\beta_{1,0}, \ldots, \beta_{1,i-1})$ is associated with the qualifying period (1), $\underline{\beta}_2 = (\beta_{2,0}, \ldots, \beta_{2,k})$ is associated with the normal inspection period (2), $\underline{\beta}_3 = (\beta_{3,0}, \ldots, \beta_{3,x-1})$ is associated with the conditional requalifying period (3), and the $\underline{\beta}_{3+l} = (\beta_{3+l,0}, \ldots, \beta_{3+l,k})$, where $l = 1, \ldots, y$, are associated with the y phases of the conditional normal inspection period (4).

The states associated with all $\beta_1, \beta_3, \beta_{2,0}$, and $\beta_{3+l,0}$, where $l = 1, \ldots, y$, are the inspection states, and the remaining states are the noninspection states. So the AOQ is of the form

$$\mathrm{AOQ}(q) = q\left(\sum_{j=1}^{i} \beta_{2,j} + \sum_{l=1}^{y}\sum_{j=1}^{k} \beta_{3+l,j}\right).$$

The equations for the steady-state probabilities are found to be

$$\beta_{1,0} = q(1-p^{x+y})$$

$$\vdots$$

$$\left((1-p^{i})(1-p^{x+y}) + p^{i}\left\{\left[\frac{1-(1-f)^{k+1}}{f}\right](1+p^{x}-p^{x+y}) + (1-p^{x})\right\}\right);$$

$$\beta_{1,j} = p^{j}\beta_{1,0},\ j = 1, \ldots, i-1;$$

$$\beta_{2,0} = p^{i}\beta_{1,0}\{q(1-p^{x+y})\};$$

$$\beta_{2,j} = (1-f)^{j}\beta_{2,0},\ j = 1, \ldots, k;$$

$$\beta_{3,0} = q\beta_{2,0};$$

$$\beta_{3,j} = qp^{j}\beta_{2,0},\ j = 1, \ldots, x-1;$$

$$\beta_{3+1,0} = qp^{x}\beta_{2,0};$$

$$\beta_{3+1,j} = (1-f)^{j}qp^{x}\beta_{2,0},\ j = 1, \ldots, k;$$

$$\beta_{3+l,0} = qp^{x+l-1}\beta_{2,0},\ l = 2, 3, \ldots, y;$$

$$\beta_{3+l,j} = (1-f)^{j}qp^{x+l-1}\beta_{2,0},\ \begin{cases} j = 1, \ldots, k; \\ l = 2, 3, \ldots, y; \end{cases}$$

$$1 = \sum_{j=0}^{i-1}\beta_{1,j} + \sum_{j=0}^{k}\beta_{2,j} + \sum_{j=0}^{x-1}\beta_{3,j} + \sum_{l=1}^{y}\sum_{j=0}^{k}\beta_{3+l,j}.$$

By summing the noninspection probabilities we find that

$$\mathrm{AOQ}(q) = q\left\{(1-f)\left[1-(1-f)^{k}\right]/f\left\{p^{i}(1+p^{x}-p^{x+y}) \vdots \left((1+p^{i}-p^{x+y}) + \left\{(1-f)\left[1-(1-f)^{k}\right]/f\right\}p^{i}(1+p^{x}-p^{x+y})\right)\right.\right.$$

$$\mathrm{AFI}(q) = 1 - \mathrm{AOQ}(q)/q.$$

18. Uranium Resource Evaluation Research

V. E. Kane

URANIUM RESOURCE EVALUATION PROGRAM

The Union Carbide Uranium Resource Evaluation (URE) Program is part of an ERDA national study to evaluate the uranium potential of the United States. For the Union Carbide study, approximately 130,000 stream sediment, stream water, groundwater, and botanical samples from a 12-state region in the central United States are collected. The statistical support for this program encompasses the entire effort: field data collection, laboratory method studies, and the data interpretation necessary for the formulation of regional geochemical models.

The basic URE sampling design consists of pilot survey studies, sampling wide-spaced regions (100 sq miles), and selected sampling of close-spaced regions (10 sq miles). The data interpretation must address two main questions in the justification of the sampling design. First, is the sequential sampling approach an effective design for the identification of anomalous uranium regions? Second, is the measurement of elements, in addition to uranium, beneficial? The traditional approach is uniform, close-spaced (4 to 6 sq miles) sampling with only the measurement of uranium concentrations.

The above two problems are interrelated in that the multivariate data, opposed to the univariate uranium data, should aid in the formulation of a more precise geochemical model. The data, x_{ij} for $i = 1, \ldots, N$ and for $j = 1, \ldots, p$, for the wide-spaced sampling consist of N samples with p measurements per sample. The basic problem is to identify sampling locations that are similar in uranium-related measurements. The relationship among groups of elements can be assessed by simple, partial, multiple, and canonical correlations as well as by R-mode factor analysis. The final geochemical model would combine the derived station associations with the geologic formations. A result of this type of analysis appears in Fig. 7, where the station associations were obtained from a cluster analysis. In the figure, stations whose locations are plotted with the same symbol have similar multi-element concentrations. The shaded areas represent those that are thought to be geologically similar. Other association methods include Q-mode factor analysis, pattern recognition techniques, multidimensional scaling, and discriminant analysis. Similar techniques are used to interpret the combined wide- and close-spaced samples. In the analysis of all the element concentrations, the presence of censored data, which arises when the concentration is known only to be below the laboratory detection limit, presents a problem.

Statistical analysis is also used in the evaluation of field procedures such as total and M-alkalinity comparisons as well as in laboratory studies. Laboratory problems include the design of water sample stability studies to determine whether element concentrations are altered by storage. Experimental design techniques were used to compare water sample treatment methods and to compare different uranium measurement methods.

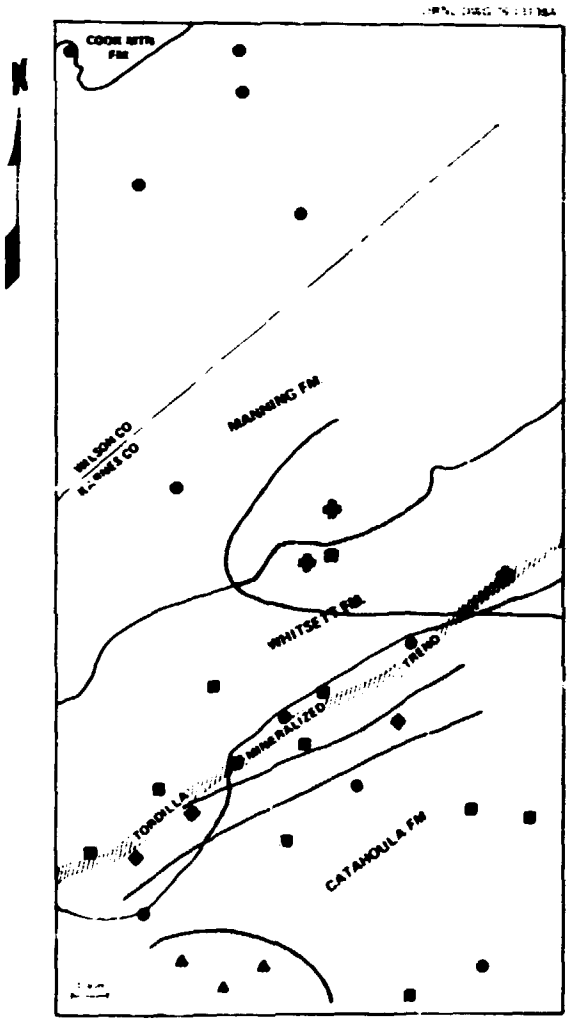

Fig. 7. Cluster analysis of well water in Karnes and Wilson Counties, Texas.

Part C. Educational Activities

The Mathematics and Statistics Research Department participates in numerous educational activities both academic and professional. This year the department has been host to a sequence of distinguished researchers in mathematics and statistics who have made short visits to Oak Ridge. In addition the department has been a cosponsor, with the mathematics department of the University of Tennessee, of a continuing series of colloquia. Members of the department have organized seminars at Oak Ridge and have both organized and spoken at symposia and colloquia at Oak Ridge, at Los Alamos, at the University of Tennessee, and at other colleges and universities through the Oak Ridge Associated Universities (ORAU) Traveling Lecture Program. Department members have also served as part-time university lecturers, thesis advisors for doctoral candidates, and supervisors for students in the ORAU Summer Student Program and other similar programs. Several department members maintain a continuing relationship with the University of Tennessee Oak Ridge Graduate School of Biomedical Sciences. Finally, the department hosts academicians on sabbatical leave.

FIRST ERDA STATISTICAL SYMPOSIUM

The First ERDA Statistical Symposium, organized by Donald A. Gardiner of the Mathematics and Statistics Research Department, Ronald K. Lohrding of the Los Alamos Scientific Laboratory, and Wesley L. Nicholson of Pacific Northwest Laboratories, was held at Los Alamos on Nov. 3–5, 1975. The symposium was attended by 99 statisticians and other scientists representing ERDA, NRC, and 10 ERDA laboratories, 6 universities, and 11 other contractors.

The purpose of the symposium was to bring together those statisticians who comprise the ERDA statistical community so that they might meet one another, present results of their research, and discuss their problems. An important feature of the program was the description of several unsolved, real-life problems which were later discussed at length in sessions planned for that purpose. The proceedings of the symposium, including the discussions, were published in March 1976.[1]

Four papers were presented by the staff of the Mathematics and Statistics Research Department. Charles K. Bayne spoke on "Design Problems for the HTGCR"; K. O. Bowman described "Studies on the Distribution of $\sqrt{b_1}$, b_2 in Normal and Nonnormal Sampling"; Forest L. Miller, Jr., presented "Dielectric Breakdown in Liquid Helium"; and V. R. R. Uppuluri spoke on "Random Matrices and Random Difference Equations." John J. Beauchamp, D. A. Gardiner, David G. Gosslee, and W. E. Lever of the Mathematics and Statistics Research Department (MSRD) served as moderators.

The Second ERDA Statistical Symposium will be held at Oak Ridge National Laboratory on Oct. 25–27, 1976.

DEPARTMENTAL SEMINAR SERIES

C. K. Bayne, J. J. Beauchamp, D. G. Gosslee, V. E. Kane, and D. S. Robson organized a weekly seminar on pattern recognition. There were two participants from outside the department. A review of the literature on the mathematical and statistical aspects of pattern recognition was conducted with each participant preparing and making one or more presentations. This seminar began in January 1976 and ran through May 1976.

1. *Proc. First ERDA Stat. Symp.*, BNWL-1986 (March 1976).

L. J. Gray and F. L. Miller, Jr., organized a weekly seminar on stochastic processes. The material studied came from *A First Course in Stochastic Processes*, by S. Karlin and H. M. Taylor. Participants were mainly from our own department but also included one from the Reactor Division and one from the Environmental Sciences Division of ORNL. This seminar also began in January and ran through May.

Eugene L. Wachspress, during a one-week visit from Knolls Atomic Power Laboratory, gave a four-session seminar based on his book *A Rational Finite Element Basis*. This seminar took place the first week of April 1976.

R. C. Ward presented a five-session seminar titled "Solving Least Squares Problems." The seminar was based on a numerical analysis approach to the problem. Computational errors and stable algorithms were the principal topics discussed. Numerical examples were presented to illustrate specific points. This seminar started June 13, 1976, and met for five weeks.

The department also sponsored a number of presentations given by both department members and visitors. These speakers' names and the topics of their talks are listed at the end of this section.

SPEAKER PROGRAMS JOINTLY SPONSORED WITH THE UNIVERSITY OF TENNESSEE MATHEMATICS DEPARTMENT

V. R. R. Uppuluri of MSRD and Larry Husch of the Mathematics Department at the University of Tennessee arranged a joint colloquium program during the 1975–76 academic year. The colloquium schedule was coordinated with the department's program of visiting mathematicians and statisticians so that each visitor was a colloquium speaker. The list of speakers and the topics of their talks appear at the end of this section.

R. C. Ward of MSRD, with A. Berman and R. J. Plemmons of the Computer Sciences Department of the University of Tennessee, coordinated a weekly series of talks on numerical linear algebra during the winter and spring of this year. The speakers' names and the topics of their talks are listed at the end of this section.

VISITING UNIVERSITY FACULTY

A. Berman of the Mathematics Department of the Technion in Haifa, Israel, after having been a visiting associate professor in the departments of mathematics and computer sciences at the University of Tennessee, is spending the summer with the department. He is working with R. C. Ward on matrix theory problems.

S. F. Ebey of the Mathematics Department of the University of the South, Sewanee, Tennessee, has been a guest of the department while on sabbatical leave during the 1975–76 academic year. During the fall he worked with D. G. Gosslee on several consulting assignments from the ORNL Biology Division, and also with V. R. R. Uppuluri on a project with Loren Fuller of the ORNL Chemistry Division. Since January, Dr. Ebey has served as director of the Southern College University Union (SCUU) Oak Ridge Science Semester, a training program for undergraduate science and mathematics students from participating schools. In this capacity he organized and supervised a seminar series for SCUU students and also taught an evening course on "Scientific Inference and Statistical Methods."

J. W. Heidel of the Mathematics Department of the University of Tennessee, Knoxville, spent a sabbatical year in the department from July 1974 until September 1975. He worked mainly with researchers from the ORNL Biology Division.

D. S. Robson of the Biometrics Unit of Cornell University, Ithaca, New York, spent a six-month sabbatical leave with the department, from January through June, as a statistical consultant to the ORNL Biology Division.

C. P. Quesenberry of the Statistics Department of North Carolina State University, Raleigh, spent the month of June 1976 visiting the department. He worked with F. L. Miller, Jr., on goodness-of-fit problems.

SUPERVISION OF STUDENTS

Max D. Morris, a Ph.D. candidate in statistics at Virginia Polytechnic Institute and State University, worked on factorial designs for the detection of model inadequacies under the direction of T. J. Mitchell and C. K. Bayne. This work is discussed in detail in Part A of this report and will not be summarized here.

ORAU SUMMER STUDENT RESEARCH TRAINEES

Keaven Anderson, Iowa State University, Ames, worked with V. R. R. Uppuluri on computing moments and distributions of waiting times for quota fulfillment sampling. Populations with k classes of objects, n_i objects in the

ith class, $i = 1, 2, \ldots, k$, were investigated, and a "quota," d_i, was assigned to each class. Quotas were filled by sampling from the entire population one object at a time. The random variable of interest was the number of objects sampled from the entire population the first time all class quotas were filled.

Chris Waguespack, Nicholls State University, Thibodaux, Louisiana wrote a Monte Carlo program to approximate the distributions. An algorithm which reduced the amount of computation necessary for computing the distributions was developed.

Tables of distributions and moments were made for the special case in which $n_i = n$ and $d_i = d$, $i = 1, 2, \ldots, k$. R. R. Coveyou helped to derive a formula for the mean waiting time in this special case.

Keaven Anderson also worked with F. L. Miller, Jr., consulting with the Health Physics Division on finding confidence intervals for the difference of two independent, weighted Poisson random variables. A method for finding intervals without approximating the Poisson distribution was outlined. This method involved finding the shortest acceptance region for any given pair of Poisson parameters.

Carol Horowitz, Carleton College, Northfield, Minnesota, worked with F. L. Miller, Jr., on statistics for testing uniformity in the unit interval. Computer programs were written and used to evaluate the performance of eight different test statistics with 21 alternative distributions. Power tests were performed with sample sizes ranging from 2 to 50.

Chris Waguespack, Nicholls State University, and Beth Wilkinson, Georgia Institute of Technology, Atlanta, working with R. C. Ward, developed two computer programs to test algorithms for solving the algebraic eigenvalue problem $Ax = \lambda x$. One program was designed to test algorithms for A real and symmetric, and the other program was designed to test algorithms for A real and unsymmetric. In addition to generating test cases of differing degrees of numerical difficulty, the programs were designed to help evaluate algorithms by printing the results of various accuracy tests performed on the computed eigenvalues and eigenvectors.

SCUU–OAK RIDGE SCIENCE SEMESTER STUDENT PARTICIPANT

Helen Mary McClellan, University of the South, Sewanee, Tennessee, worked with R. C. Ward on a method for determining experimental designs which are optimal with respect to computational precision. The optimality criterion minimized was the condition number of the least squares matrix determined by the design points and the mathematical model. A computer program was written to implement a Newton-type iterative scheme to converge to the set of optimal design points in a specified region. This work is described in more detail in Part A of this report.

ORAU TRAVELING LECTURERS

Three department members participated in the ORAU Traveling Lecture Program this last year. They were D. G. Gosslee, V. R. R. Uppuluri, and R. C. Ward. The titles of their talks and the locations where the lectures were given are listed at the end of this section.

S-CONTRACT PROGRAM

Professor S. A. Patil, Mathematics Department, Tennessee Technological University, Cookeville, worked with the department under an S contract with the Oak Ridge Associated Universities. In association with V. R. R. Uppuluri and Paul Rubel of ORNL, he is working in the area of Nuclear Safety. A report on inferences about rare events was prepared.

CONSULTANTS

P. M. Anselone, Oregon State University.
E. H. Lee, Stanford University.
C. P. Quesenberry, North Carolina State University.
L. R. Shenton, University of Georgia.
M. Sobel, University of California, Santa Barbara.
D. L. Solomon, Cornell University.

MATHEMATICS AND STATISTICS RESEARCH DEPARTMENT SEMINARS

R. S. Varga, Kent State University, "Iterative Methods for Solving Multi-dimensional Finite Element Problems," Aug. 6, 1975

F. R. Jones, ORAU Graduate Fellow, "Response Surface Designs for the Detection of Model Inadequacy," Aug. 15, 1975

M. L. Moeschberger, University of Missouri, "Some Aspects of Competing Risk Theory," Aug. 19, 1975

K. Anderson, C. Waguespack, and F. Wilkinson, ORAU Summer Student Program, "Discussion of Summer Activities," Aug. 20, 1975

F. L. Frome, University of Texas, "Fitting Equations to Data Using Iterative Weighted Least Squares," Aug. 20, 1975

D. Lurie, Medical College of South Carolina, "Anatomy of Analysis of Variance," Aug. 21, 1975

S. Geisser, University of Minnesota, "Forecasting Survival by Sample Reuse," Aug. 29, 1975

A. Solomon, University of the Negev, "Numerical Approaches to Solution of the Plateau Problem," Aug. 29, 1975

D. Rose, Boeing Computer Services, "Dependent Competing Risks," Dec. 11, 1975

D. Bross, Johns Hopkins University, "Survival Analysis in the Presence of Mixed Distributions," Dec. 15, 1975

B. A. Chartres, University of Virginia, "The Effective Order of Convergence of Numerical Methods for Ordinary Differential Equations," Jan. 6, 1976

D. S. Robson, Cornell University, "Optimal Design for Measuring Simple Exponential Decay with Poisson Sampling Error," Feb. 4, 1976

E. H. Lee, Stanford University (sponsored jointly by Reactor Division), "Elastic-Plastic Theory and Stress Analysis for Finite Strain," Mar. 8, 1976

D. S. Robson, Cornell University, "Identifiable Reparameterization of an Over-Parameterized Likelihood Function," Apr. 2, 1976

M. A. Kastenbaum, Tobacco Institute, "Introduction to Life Tables," Apr. 12, 1976

G. A. Baker, Los Alamos Scientific Laboratory, "Some Mathematical Properties of the Padé Approximation with Applications to Physics," Apr. 15, 1976

D. S. Robson, Cornell University, "Marginal Size of the One-Sided Fisher Exact Test," May 12, 1976

K. Frankowski, University of Minnesota, "Accuracy of Numerical Calculations," May 13, 1976

L. J. Gray, "Averaging Functions or Augmented Space Revisited," June 9, 1976

UT-MSRD JOINT COLLOQUIA

K. Hoffman, Tulane University, "Categorical Methods in Topological Algebra," Oct. 21, 1975; "Topological Semigroups: Applications, Theory, and History," Oct. 22, 1975; "Recent Developments in the Theory of Compact Lawson Semi-lattices," Oct. 23, 1975

R. Gentry, University of Guelph, "Mathematical Models of Blood Coagulation," Oct. 29, 1975

H. Shugart, ORNL, "Modelling Forest Succession," Nov. 5, 1975

R. J. Rowlett, University of Tennessee, "Classifying Free Actions on Smooth Manifolds," Nov. 19, 1975

B. W. Rust, CSD, UCCND, "Numerical Aspects of Fredholm Integral Equations of the First Kind," Nov. 12, 1975

W. B. Gragg, NASA Langley Research Center, "Derivative Free Algorithms for Nonlinear Least Squares Problems," Jan. 30, 1976

S. M. Ulam, University of Florida, "Some Problems in Combinatorics and Mathematical Biology," Feb. 17, 1976

A. Hatcher, Princeton University, "Simple Homotopy Theory and Homemorphisms of Manifolds," Feb. 18, 1976

R. Barlow, Florida State University, "Techniques for Analyzing Multivariate Failure Data," Feb. 25, 1976

W. Gautschi, Purdue University, "Pitfalls in Computation," Mar. 3, 1976

G. W. Stewart, University of Maryland, "Detecting and Correcting Rank Deficiency," Mar. 10, 1976

R. S. Varga, Kent State University, "Iterative Methods for Multi dimensional Finite Element Problems," Mar. 17, 1976

P. R. Halmos, Indiana University, "Bounded Matrices," Mar. 24, 1976

M. Cohen, Cornell University, "Contracting and Collapsing Topological Spaces," Mar. 31, 1976; "Whitehead Torsion, Group Extensions, and Zeeman's Conjectures in High Dimensions," Apr. 1, 1976

E. Wachspress, Knolls Atomic Power Laboratory, "The Eternal Triangle," Apr. 5, 1976

J. M. Ortega, NASA Langley Research Center, "The Many Facets of Scientific Computing," Apr. 14, 1976

D. R. McMillan, Jr., University of Wisconsin at Madison, "Simple Connectivity of Quotient Spaces," Apr. 21, 1976

J. Stampfli, Indiana University, "A New Look at Fugledes Theorem," Apr. 28, 1976

G. Kallianpur, University of Minnesota, "Energy Inequality for Gaussian Processes," May 5, 1976

C. R. Rao, Indian Statistical Institute, "Some Thoughts on Regression and Prediction," May 24, 1976; "A Review of Characterization of Probability Distributions," May 25, 1976

W. N. Everitt, University of Dundee, "On the Inequality of Laudau $\|f'\|^2 \leq 4\|f\|\|f''\|$," May 26, 1976

R. Fletcher, University of Dundee, "A Review of Methods for Minimization with Nonlinear Constraints," June 11, 1976

UT-ORNL NUMERICAL LINEAR ALGEBRA SEMINARS

S. M. Serbin, "Solution of Matrix Pencil Systems," Jan. 16, 1976

W. P. Gragg, "Derivative Free Algorithms for Nonlinear Least Squares Problems," Jan. 30, 1976

R. C. Ward, "Numerical Computation of the Matrix Exponential," Feb. 6, 1976

L. J. Gray, "Computation of Eigenvalue Distributions for Random Matrices," Feb. 13, 1976

D. G. Wilson, "Construction of a Jacobi Matrix from Spectral Data," Feb. 20, 1976

K. Fox, "Cholesky Decomposition of Symmetric Idempotent Matrices," Feb. 27, 1976

B. W. Rust, "Suboptimal Constrained Interval Estimation by Linear Programming," Mar. 5, 1976

V. Wallare, "Markov Processes in Queuing Theory," Mar. 12, 1976

A. Berman, "Matrix Consistency and Splittings," Apr. 9, 1976

R. J. Plemmons, "Characterizations and Applications of M-Matrices," Apr. 23, 1976

C. P. Huang, "The Jacobi Method for Computing Eigenvalues," Apr. 30, 1976

ORAU TRAVELING LECTURE PRESENTATIONS

D. G. Gosslee, "Training Statistical Consultants," University of Kentucky, Lexington, Oct. 1, 1975; Virginia Commonwealth University, Richmond, Oct. 3, 1975; Southern Methodist University, Dallas, Tex., Feb. 25, 1976; Texas A&M, College Station, Feb. 26, 1976; Louisiana State University, Baton Rouge, Mar. 11, 1976

V. R. R. Uppuluri, "Random Matrices and Random Difference Equations," Mathematics Department, University of California at Santa Barbara, Nov. 6, 1975; Mathematics Department, Memphis State University, Memphis, Tenn., Dec. 1, 1975

R. C. Ward, "Numerical Algorithms for the Generalized Eigenvalue Problem," University of Kentucky, Lexington, Nov. 11, 1975; Thomas More College, Ft. Mitchell, Ky., Nov. 12, 1975

Part D. Presentations of Research Results

Publications

BOOKS AND PROCEEDINGS

K. O. Bowman and W. E. Dusenberry.[1] "Transformation of the Pearson System with Special Reference to Type IV," pp. 381–90 in *A Modern Course on Statistical Distributions on Scientific Work*, vol. 1, ed. G. P. Patil, S. Kotz, and J. K. Ord, D. Reidel, Boston, 1975.

K. O. Bowman and M. A. Kastenbaum,[2] "Sample Size Requirement: Single and Double Classification Experiment," pp. 111–232 in *Selected Tables in Mathematical Statistics*, ed. D. B. Owen and H. L. Harter, American Mathematical Society and Institute of Mathematical Statistics, New York, 1975.

S. J. Chang, "Energy Release Integral for Dissipative Materials," *Proceedings 5th Canadian Congress of Applied Mechanics*, University of New Brunswick, Fredericton, N.B., Canada, 1975.

S. J. Chang and L. J. Zappas,[3] "Several Relations for Comparison of a General Rate Fluid and the BKZ Fluid," *Proceedings 7th International Congress on Rheology*, Chalmers University of Technology, Gothenburg, Sweden, to appear.

W. M. Generoso,[4] Katherine T. Cain,[4] Sandra W. Huff,[4] and D. G. Gosslee, "Inducibility by Chemical Mutagens of Heritable Translocations in Male and Female Germ Cells of Mice," chapter in *Advances in Modern Technology*, vol. 1, ed. W. G. Flamm and M. A. Mehlman, Hemisphere Publishing Corp., Washington, D.C., to appear.

L. R. Shenton[5] and K. O. Bowman, *Maximum Likelihood Estimation in Small Samples*, Charles Griffin and Company, England, in press.

L. R. Shenton[5] and K. O. Bowman, "Comments on the Distribution of the Variance in Sampling from the Logistic Distribution," *40th Session of the International Statistical Institute*, International Statistical Institute, Warsaw, 1975.

JOURNAL ARTICLES

T. N. Bhargava[6] and V. R. R. Uppuluri, "Sampling Distribution of Gini's Index of Diversity," *J. Appl. Math. Comput.*, to appear.

T. N. Bhargava[6] and V. R. R. Uppuluri, "Population Disagreement and Gini's Index of Diversity," *Gen. Syst.*, submitted.

K. O. Bowman and J. J. Beauchamp, "Pitfalls with Some Gamma Variate Simulation Routines," *J. Stat. Comput. Simulation* **4**, 141–54 (1975).

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1. Eli Lilly and Company.
2. Tobacco Institute.
3. National Bureau of Standards.
4. Biology Division, ORNL.
5. University of Georgia.
6. Kent State University.

K. O. Bowman and L. R. Shenton,[5] "'Omnibus' Test Contours for Departures from Normality Based on $\sqrt{b_1}$ and b_2," *Biometrika* 62, 243–50 (1975).

K. O. Bowman and L. R. Shenton,[5] "A New Algorithm for Summing Divergent Series, Part II: Two-Component Borel Summability Model," *J. Comput. Appl. Math.*, submitted.

C. R. Brinkman,[7] R. K. Williams,[7] R. L. Klueh,[7] and T. L. Hebble, "Mechanical and Physical Properties of 2¼ Cr–1 Mo Steel in Support of Clinch River Breeder Reactor Plant Steam Generator Design," *Nucl. Tech.* 28, 490–505 (March 1976).

C. Brownie[8] and D. S. Robson, "Models Allowing for Age-Dependent Survival in Band Return Data," *Biometrics*, to appear.

R. E. Cline[9] and R. E. Funderlic,[10] "A Theorem on the Rank of a Difference of Matrices," *Bull. AMS* 82, 48 (1976).

S. F. Ebey and J. J. Beauchamp, "Larval Fish, Power Plants, and Buffon's Needle Problem," *Am. Math. Mon.*, submitted.

J. W. Elwood,[11] S. G. Hildebrand,[11] and J. J. Beauchamp, "Contribution of Gut Contents to the Concentration and Body Burden of Elements in *Tipula* sp. from a Spring-fed Stream," *J. Fish. Res. Board Can.*, to appear.

L. D. Eyman,[11] C. W. Gehrs,[11] and J. J. Beauchamp, "Sublethal Effect of 5-Chlorouracil on Carp (*Cyprinus carpio*) Larvae," *J. Fish. Res. Board Can.* 32, 2227–29 (1975).

L. J. Gray, "Products of Hermitian Operators," *Proc. AMS*, to appear.

L. J. Gray and D. G. Wilson, "Construction of a Jabobi Matrix from Spectral Data," *J. Linear Algebra Its Appl.*, to appear.

L. J. Gray, "Jordan Representation for a Class of Nilpotent Operators," *Indiana Univ. Math. J.*, to appear.

L. J. Gray and T. Kaplan,[12] "Distribution of Vibrational Modes in an Amorphous Linear Chain," *Physica*, to appear.

L. J. Gray, "On Bi-quasitriangular Operators," *Proc. AMS*, to appear.

L. J. Gray and T. Kaplan,[12] "Off Diagonal Disorder in Random Substitutional Alloys," *J. Phys., C*, to appear.

L. J. Gray and T. Kaplan,[12] "Elementary Excitations in Random Substitutional Alloys," *Phys. Rev.*, submitted.

S. E. Herbes[11] and J. J. Beauchamp, "Toxic Interaction of Mixtures of Resorcinol and 6-Methylquinoline to *Daphnia magna*," *Bull. Env. Contam. Toxicol.*, submitted.

Abraham Hsie,[4] Patricia A. Brimer,[4] Toby J. Mitchell and D. G. Gosslee, "The Dose-Response Relationship for Ethyl Methanesulfonate-Induced Mutations at the Hypoxanthine-Guanine Phosphoribosyl Transferase Locus in Chinese Hamster Ovary Cells," *Somatic Cell Genet.* 1, 247–61 (1975).

A. W. Hsie,[4] P. A. Brimer,[4] Toby J. Mitchell, and D. G. Gosslee, "The Dose-Response Relationship for Ultraviolet Light-Induced Mutations at the Hypoxanthine-Guanine Phosphoribosyl Transferase Locus in Chinese Hamster Ovary Cells," *Somatic Cell Genet.* 1, 383–89 (1975).

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7. Metals and Ceramics Division, ORNL.
8. Cornell University
9. University of Tennessee.
10. Computing Applications Department.
11. Environmental Sciences Division, ORNL.
12. Solid State Division, ORNL.
13. Comparative Animal Research Laboratory.
14. The University, Southampton, England.

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C. P. Quesenberry[18] and F. L. Miller, Jr., "Power Studies of Some Tests for Uniformity," *J. Stat. Comput. Simulation*, to appear.

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T. Yamada,[21] M. E. Roesel,[4] and J. J. Beauchamp, "The Cell Cycle Parameters in Dedifferentiating Iris Epithelial Cells," *J. Embryol. Exp. Morphol.* 34, 497–510 (1975).

W. D. Youngs[8] and D. S. Robson, "Estimating Survival Rate from Tag Returns: Model Tests and Sample Size Determination," *J. Fish. Res. Board Can.* 32, 2365–71 (1975).

REPORTS

C. K. Bayne, "Experimental Design for HTGR Fuel Rods," *Proc. First ERDA Stat. Symp.*, BNWL-1986 (March 1976).

C. K. Bayne and D. R. Johnson,[7] *Relationship Between Length Variations of HTGR Fuel Rod Stack Lengths and Individual Rod Lengths*, ORNL/TM-5544, to be published.

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15. Texas A & M University.
16. University College, London.
17. Boston University.
18. North Carolina State University.
19. University of California at Santa Barbara.
20. University of Minnesota.
21. Institut Suisse de Recherches Experimentales sur le Cancer, Lausanne, Switzerland.

J. J. Beauchamp, K. O. Bowman, and F. L. Miller, Jr., *Statistical Analysis of Environmental Data*, UCCND-CSD-INF-64 (October 1975).

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V. R. R. Uppuluri and S. A. Patil,[23] *Inferences about Rare Events*, ORNL/CSD-12 (June 1976).

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R. C. Ward and L. J. Gray, *Eigensystem Computation for Skew-Symmetric Matrices and a Class of Symmetric Matrices*, ORNL/CSD-9 (May 1976).

Oral Presentations

(At Meetings of Professional Societies, Conferences, etc.)

C. K. Bayne, "Experimental Design for HTGR Fuel Rods," presented at the First ERDA Statistical Symposium, Los Alamos Scientific Laboratory, N.M., Nov. 3–5, 1975.

C. K. Bayne, "Choosing the Number of Observations in an Experimental Design," presented at the Second Union Carbide Corporation Applied Mathematics Symposium, Tarrytown, N.Y., Feb. 24, 1976.

K. O. Bowman and J. J. Beauchamp, "Effect of Nonnormality on the t-Statistic," presented at the spring meeting of the Institute of Mathematical Statistics, College Station, Tex., Mar. 8–10, 1976.

K. O. Bowman, "Test of Departure from Normality," presented at the Second Union Carbide Corporation Applied Mathematics Symposium, Tarrytown, N.Y., Feb. 24, 1976.

K. O. Bowman and L. R. Shenton,[5] "Studies on the Distributions of $\sqrt{b_1}, b_2$ in Normal and Non-normal Sampling," presented at the First ERDA Statistical Symposium, Los Alamos Scientific Laboratory, Los Alamos, N.M., Nov. 3–5, 1975.

K. O. Bowman and L. R. Shenton,[5] " 'Omnibus' Test Contours for Departures from Normality Based on $\sqrt{b_1}, b_2$," presented at the Joint Meeting of the American Statistical Association, The Biometric Society, and the Institute of Mathematical Statistics, Atlanta, Ga., Aug. 25–28, 1975.

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22. Jozef Stefan Institute, Yugoslavia.
23. Tennessee Technological University.

C. R. Brinkman,[7] R. K. Williams,[7] R. L. Klueh,[7] and T. L. Hebble, "Mechanical and Physical Properties of 2¼ Cr–1 Mo Steel in Support of Clinch River Breeder Reactor Plant Steam Generator Design," presented at the International Conference on Materials for Nuclear Steam Generators, Gatlinburg, Tenn., Sept. 9–12, 1975.

S. J. Chang and L. J. Zapas,[3] "Several Relations for Comparison of a General Rate Fluid and the BKZ Fluid," presented at the 7th International Congress on Rheology, Chalmers University of Technology, Gothenburg, Sweden, Aug. 23–27, 1976.

R. E. Cline[9] and R. E. Funderlic,[10] "What Makes the Rank of a Matrix Change?" presented at the SIAM Fall National Meeting, San Francisco, Calif., Dec. 3–5, 1975.

R. E. Cline[9] and R. E. Funderlic,[10] "Decompositions of Differences of Matrices and Generalized Inverses," presented at the SIAM National Meeting, Chicago, June 1976.

L. J. Gray, "Construction of a Jacobi Matrix from Spectral Data," presented at the American Mathematical Society Meeting, San Antonio, Tex., Jan. 25, 1976.

L. J. Gray, "Calculation of Eigenvalue Distributions of Random Matrices," presented at the Numerical Linear Algebra Seminar, University of Tennessee, Feb. 13, 1976.

D. G. Gosslee, "The Statistician in General Practice," presented at the North Texas Chapter of the American Statistical Association, Dallas, Tex., Feb. 25, 1976.

T. L. Hebble, "On the Use of Historic Data to Establish Standards of Materials Behavior for the Nuclear Systems Materials Handbook," presented for the Nuclear Regulatory Commission, Washington, D.C., May 17, 1976.

B. S. Lugue,[10] B. W. Rust,[10] and W. Van Winkle,[11] "The Problem of Determining the Length of the Prediction Error Filter in Maximum Entropy Spectral Analysis," presented at the SIAM-SIGNUM 1975 Fall Meeting, San Francisco, Calif., Dec. 3–5, 1975.

F. L. Miller, Jr., "Dielectric Breakdown in Liquid Helium," presented at the First ERDA Statistical Symposium, Los Alamos Scientific Laboratory, Los Alamos, N.M., Nov. 3–5, 1975.

J. Rant[22] and B. W. Rust,[10] "Constrained Interval Estimation by Linear Programming," presented at the SIAM 1975 National Meeting, Troy, N.Y., June 9–11, 1975.

B. W. Rust,[10] "Mathematical Foundations Underlying the Burrus Techniques of Spectral Unfolding," invited address, Radiation Shielding Information Center Seminar-Workshop on Radiation Energy Spectra Unfolding, Oak Ridge National Laboratory, Apr. 12–13, 1976.

B. W. Rust,[10] "Numerical Aspects of Fredholm Integral Equations of the First Kind," Weekly Colloquium, University of Virginia, Department of Applied Mathematics, Sept. 18, 1975; Weekly Colloquium, University of Tennessee, Department of Mathematics, Nov. 12, 1975.

B. W. Rust,[10] "Constrained Interval Estimation for Ill-Posed Problems," invited address, SIAM-SIGNUM 1975 Fall Meeting, San Francisco, Calif., Dec. 3–5, 1975.

L. R. Shenton[5] and K. O. Bowman, "Comments on the Distribution of the Variance in Sampling from the Logistic Distribution," presented at the 40th Session of the International Statistical Institute, Warsaw, Poland, September 1975.

M. Sobel,[19] V. R. R. Uppuluri, and K. Frankowski,[20] "Applications of Dirichlet Distributions," invited paper, 151st Meeting of the Institute of Mathematical Statistics, Santa Barbara, Calif., Mar. 26, 1976.

V. R. R. Uppuluri, M. Sobel,[19] and K. Frankowski,[20] "Waiting Times and Dirichlet Distributions," invited paper, 151st Meeting of the Institute of Mathematical Statistics, Santa Barbara, Calif., Mar. 26, 1976.

V. R. R. Uppuluri, "Mathematical Models for Physical and Natural Phenomena," presented for the Mathematics Department, Centre College, Danville, Ky., Mar. 30, 1976.

R. C. Ward, "Numerical Computation of the Matrix Exponential," presented at the SIAM-SIGNUM 1975 Fall Meeting, San Francisco, Calif., Dec. 3–5, 1975; Numerical Linear Algebra Seminar, University of Tennessee, Knoxville, Feb. 6, 1976.

D. G. Wilson. "Stefan Problems," presented for the Nuclear Regulatory Commission, Washington, D.C., Apr. 15, 1976.

D. G. Wilson. "Construction of a Jacobi Matrix from Spectral Data," presented for the Numerical Linear Algebra Seminar, University of Tennessee, Knoxville, Feb. 20, 1976.

Seminars

The Department sponsors a seminar program that covers a wide variety of mathematical and statistical interests. The formal seminars held during the period of this report are listed below.

K. Anderson, C. Waguespack, and E. Wilkinson, ORAU Summer Student Program, "Discussion of Summer Activities," Aug. 20, 1975.

G. A. Baker, Los Alamos Scientific Laboratory, "Some Mathematical Properties of the Padé Approximation with Applications to Physics," Apr. 15, 1976.

A. P. Basu, University of Missouri, "Estimates of Reliability of Complex Systems," June 21, 1976.

D. Bross, Johns Hopkins University, "Survival Analysis in the Presence of Mixed Distributions," Dec. 15, 1975.

B. A. Chartres, University of Virginia, "The Effective Order of Convergence of Numerical Methods for Ordinary Differential Equations," Jan. 6, 1976.

K. Frankowski, University of Minnesota, "Accuracy of Numerical Calculations," May 13, 1976.

E. L. Frome, University of Texas, "Fitting Equations to Data Using Iterative Weighted Least Squares," Aug. 20, 1975.

S. Geisser, University of Minnesota, "Forecasting Survival by Sample Reuse," Aug. 29, 1975.

W. B. Gragg, NASA Langley Research Center, "Derivative Free Algorithms for Nonlinear Least Squares Problems," Jan. 30, 1976.

L. J. Gray, "Averaging Functions or Augmented Space Revisited," June 8, 1976.

E. R. Jones, ORAU Graduate Fellow, "Response Surface Designs for the Detection of Model Inadequacy," Aug. 15, 1975.

M. A. Kastenbaum, Tobacco Institute, "Introduction to Life Tables," Apr. 12, 1976.

E. H. Lee, Stanford University (sponsored jointly by Reactor Division), "Elastic-Plastic Theory and Stress Analysis for Finite Strain," Mar. 8, 1976.

D. Lurie, Medical College of South Carolina, "Anatomy of Analysis of Variance," Aug. 21, 1975.

M. L. Moeschberger, University of Missouri, "Some Aspects of Competing Risk Theory," Aug. 19, 1975.

D. S. Robson, Cornell University, "Optimal Design for Measuring Simple Exponential Decay with Poisson Sampling Error," Feb. 4, 1976; "Identifiable Reparameterization of an Over-Parameterized Likelihood Function," Apr. 2, 1976; "Marginal Size of the One-Sided Fisher Exact Test," May 12, 1976.

D. Rose, Boeing Computer Services, "Dependent Competing Risks," Dec. 11, 1975.

A. Solomon, University of the Negev, "Numerical Approaches to Solution of the Plateau Problem," Aug. 29, 1975.

R. S. Varga, Kent State University, "Iterative Methods for Solving Multi-Dimensional Finite Element Problems," Aug. 6, 1975.

ARTICLES REVIEWED OR REFEREED FOR PERIODICALS

Reviewer or referee	Number of articles reviewed or refereed for indicated periodical																							
	Ann. Stat.	*Appl. Math.*	*Biometrics*	*Commun. Stat.*	*Comput. Rev.*	*Health Phys.*	*J. Am. Stat. Assoc.*	*J. Appl. Probab.*	*J. Fish Res. Board Can.*	*J. Molecular Biol.*	*J. Stat. Comput. Simulation*	*J. Theor. Biol.*	*J. Wildlife Mgmt.*	*Math. Comput.*	*Math. Rev.*	*Nucl. Sci. Eng.*	*SIAM J. Appl. Math.*	*SIAM Rev.*	*Technometrics*	*Trans. Amer. Fish Soc.*	Proposals	Total
Bayne, C. K.																			1			1
Beauchamp, J. J.			1			1													1			3
Bowman, K. O.				1			2												1		18	22
Chang, S. J.		5																				5
Coveyou, R. R.														1	7	1					1	10
Gardiner, D. A.																					2	2
Lever, W. F.																					1	1
Miller, F. L., Jr.						1				1	1											3
Mitchell, T. J.																			5			5
Robson, D. S.			4				1		2			1	2							2		12
Rust, B. W.*																		1				1
Uppuluri, V. R. R.	1						5	1							6						2	13
Ward, R. C.																1						1
Wilson, D. G.					2																	2
Total	1	5	5	1	2	2	6	1	2	1	1	1	2	1	13	1	1	1	8	2	24	81

*Computing Applications Department.

Part E. Professional Activities

Members of the Mathematics and Statistics Research Department participate in the activities of several professional and academic institutions. Some of their contributions are outlined below.

C. K. Bayne	
Member:	*Technometrics* Prize Committee
J. J. Beauchamp	
Instructor:	Division of Mathematics and Science, Roane State Community College
Representative:	ORNL In-House Training Program
Moderator:	Research Paper Session, First ERDA Statistical Symposium
K. O. Bowman	
Panelist:	Women in Science Program, National Science Foundation
S. J. Chang	
Visiting Associate Professor:	Department of Materials Engineering, University of Iowa
D. A. Gardiner	
President-Elect:	Oak Ridge Chapter of Sigma Xi
Professor:	Department of Mathematics, University of Tennessee
Chairman:	Committee on Membership, Dues, and Publications, American Statistical Association
Member:	Board of Directors of the American Statistical Association Executive Committee of Section on Physical and Engineering Sciences, American Statistical Association Committee on Statistics of the Southern Regional Educational Board Mathematics and Statistics Committee, University of Tennessee International Editorial Board, *Communications in Statistics* Editorial Advisory Board, *Journal of Statistical Computation and Simulation*
D. G. Gosslee	
Lecturer:	Oak Ridge Graduate School of Biomedical Sciences, University of Tennessee
Member:	Finance Committee for the 1976 International Biometrics Conference
Moderator:	Research Paper Session, First ERDA Statistical Symposium
L. J. Gray	
Member:	ORNL Ph.D. Recruitment Program
W. F. Lever	
Member:	*Technometrics* Prize Committee

F. L. Miller, Jr.
Lecturer: Traveling Lecture Program, Oak Ridge Associated Universities

V. R. R. Uppuluri
Chairman: Mathematics Section, Tennessee Academy of Sciences

Lecturer: Traveling Lecture Program, Oak Ridge Associated Universities
Institute of Mathematical Statistics and the American Statistical Association
Oak Ridge Graduate School of Biomedical Sciences, University of Tennessee

R. C. Ward
Lecturer: Traveling Lecture Program, Oak Ridge Associated Universities

D. G. Wilson
Lecturer: Department of Mathematics, University of Tennessee