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Progress Report

Period Ending June 30, 1977

OAK RIDGE NATIONAL LABORATORY

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MATHEMATICS AND STATISTICS RESEARCH DEPARTMENT PROGRESS REPORT

for Period Ending June 30, 1977

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Preface

The 1976-77 year was a year of adjustment for the Mathematics and Statistics Research Department. Budgetary restrictions necessitated the discontinuing of the excellent visitors program we had initiated the year before, as well as the joint colloquium series with the University of Tennessee. Also, it was necessary to put more emphasis on reimbursable consulting and collaboration with correspondingly less emphasis on self-generated research. Nonetheless, the staff responded admirably and enjoyed a fruitful year of contributions to the nation's energy efforts.

A scientific highlight was the Second ERDA Statistical Symposium held at the Oak Ridge National Laboratory site and attended by almost 70 statisticians from the ERDA statistical community. Another was the Third Union Carbide Corporation Applied Mathematics Symposium, attended by about 35 Union Carbide mathematicians and statisticians and held at the Oak Ridge Associated Universities Campus.

The department was pleased to welcome Professor Alan D. Solomon, who is on leave from the Ben Gurion University of the Negev, Israel. Dr. Solomon is doing research in moving boundary problems and collaborating with engineers in the Thermal Energy Storage Program.

Robert R. Coveyou retired from the corporation after a third of a century of company service. V. R. R. Uppuluri took a leave of absence to be with the University of California at Santa Barbara, and Kimiko Bowman accepted a temporary assignment to visit universities and industries in Japan for the U.S. Office of Naval Research.

The past year was an exceptional year for awards and honors. Kimiko O. Bowman and David G. Gosslee were elected Fellows of the American Statistical Association by virtue of their signal contributions to the field of statistics. Four statisticians of the department now are Fellows of the ASA. Donald A. Gardiner was elected an Ordinary Member of the International Statistical Institute and became the department's second member to receive this honor. David G. Gosslee was elected a Fellow of the American Association for the Advancement of Science; the department now has three Fellows of the AAAS. The entire department was honored when our last annual report, *Progress Report for the Period Ending June 30, 1976*, ORNL CSD-13, received the Award of Excellence in the category of annual reports from the East Tennessee Chapter of the Society for Technical Communication.

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Part A. Mathematical and Statistical Research

1. Moving Boundary Problems

A. D. Solomon D. G. Wilson

THE APPROXIMATE SOLUTION OF FREE BOUNDARY PROBLEMS BY ANALYTICAL TECHNIQUES

Many physical mechanisms consist of a transfer process, such as diffusion, in a region which is determined by the transfer process and auxiliary initial and boundary conditions. The solution of problems concerned with such mechanisms involves the specification of the so-called "free boundary" of the region and the function defining the transfer process.

As an example of such a mechanism, we can point to the solidification of a semi-infinite slab of material occupying the region $x \geq 0$ and having melt temperature T_{cr}, thermal conductivity K, density ρ, thermal diffusivity α, and latent heat H. Let $T(x, t)$ denote the temperature of the material at point x and time t. Let us assume that at the onset of the solidification process the material is solely liquid at the melt temperature:

$$T(x, 0) = T_{cr}, \quad x > 0. \tag{1}$$

Let the boundary temperature at $x = 0$ be set at a constant value below T_{cr}:

$$T(0, t) = T_0 < T_{cr}, \quad t > 0. \tag{2}$$

Then solidification will take place in an ever-extending region emanating from the cold boundary $x = 0$ and extending to a point $x = X(t)$ that varies with time. The function $X(t)$ defines the "free boundary" of the process. At any time t the intervals $0 < x \leq X(t)$ and $X(t) < x$ consist of solid and liquid material respectively. Moreover, the heat transfer process is governed by the relations

$$T_t = \alpha T_{xx}, \quad 0 < x \leq X(t), \tag{3}$$

$$T(x, t) = T_{cr}, \quad x > X(t), \tag{4}$$

while the free boundary $X(t)$ satisfies the relations

$$\rho H X'(t) = K T_x [X^-(t), t], \tag{5}$$

$$T[X(t), t] = T_{cr}, \tag{6}$$

where $X^-(t)$ denotes the limiting value from the left.

This example admits of a similarity solution,[1] but slight (and realistic) modifications of it result in problems that cannot be solved explicitly. For example, the boundary condition, Eq. (1), may be of the form

$$K T_x(0, t) = h[T(x, 0) - f(t)],$$

where h is a suitable constant and $f(t)$ is, perhaps, a rapidly varying function. Similarly, Eq. (6) may be modified by the fact that T_{cr} might itself be a function of t and even $X(t)$:

$$T[X(t), t] = T_{cr}[X(t), t];$$

clearly, Eqs. (3) and (5) may also admit of modifications in their structure.

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1. H. Carslaw and J. Jaeger, *Conduction of Heat in Solids*, 2d ed., Oxford University Press, London, 1959.

Megerlin[2] introduced an approximation procedure for the solution of such free boundary problems. This method consists of expanding the function $T(x, t)$ in the form

$$T(x, t) = T_{cr} + \sum_{j=1}^{\infty} a_j(t)(x - X)^j$$

and obtaining the $a_j(t)$'s from Eqs. (2)–(6). Due to the complicated structure of the resulting relations, the expansion was not used for $j > 2$. However, even in this limited context the method has good accuracy and is widely used in heat transfer problems. We have broadened both the method and its applicability in a number of ways.

An extension of Megerlin's method has been developed by subdividing the interval $0 < x < X(t)$ into N subregions,

$$[0, X/N] , [X/N, 2X/N] , \ldots , \left[\frac{N-1}{N}X, X\right] ,$$

for N a natural number. Then in the jth region ($j = 1, 2, \ldots$)

$$\frac{j-1}{N}X < x < \frac{j}{N}X .$$

substitute

$$T = \gamma_j + A_j\left(x - \frac{jX}{N}\right) + B_j\left(x - \frac{jX}{N}\right)^2$$

into the equations of the problem applicable to it. This yields a system of ordinary differential equations in γ_j and X which is linear in γ_j and which, for large N, may be solved by standard methods (e.g., Runge-Kutta); for small N the system admits of analytical approximate solutions. We have shown that, for the problem given by our earlier example, this procedure yields approximate solutions $X(t)$ and $T(x, t)$, which as $N \to \infty$ converge to the exact solution. Moreover, the convergence is at least $O(1/N)$.

The Megerlin procedure and its extension have been applied to the following types of problems:

1. rapidly varying boundary conditions,
2. two-phase problems,

2. F. Megerlin, "Geometrisch Eindimensionale Warmeleitung Bein Schmelzen und Erstarren," *Forsch. Ingenieurwes.* 34, 40–46 (1968).

3. time-dependent melting temperature, and
4. parabolic equations with heat source terms.

In all cases the method yields closed-form approximations exhibiting the qualitative dependence of the solution on the parameters of the problem.

Alternative methods based on finite differences[3] and moments[4] have been compared with the Megerlin approach and its extension for small N. Degrees of discrepancy not exceeding 15%, but in most cases below 10%, were obtained.

EXISTENCE AND UNIQUENESS FOR SIMILARITY SOLUTIONS OF ONE-DIMENSIONAL MULTIPHASE STEFAN PROBLEMS

Stefan problems consist of the diffusion or heat equation in regions separated by moving boundaries whose locations must be determined as part of the problem. Problems of this type arise in many phase-change processes and in problems associated with alloys. Stefan[5] published the solution of a special phase-change problem in one Cartesian coordinate in a study of the thickness of polar ice. In this case the solution depended only on the similarity variable $x/\sqrt{t}$, and the location of the single free boundary was proportional to $\sqrt{t}$. Solutions of this form are called similarity solutions.

Similarity solutions for free boundary problems antedate Stefan's published result. Carslaw and Jaeger[1] assert that "the more general result known as Neumann's solution was given by Franz Neumann in his lectures in the 1860s." Similarity solutions are among the few explicit solutions obtainable for Stefan problems and interest in them persists. Numerous authors have given similarity solutions for Stefan problems in various geometries.

These similarity solutions give rise to a system of nonlinear equations for the coefficients of $\sqrt{t}$ which determine the speeds of the internal boundaries. For the simplest Stefan problem, the equation is $x \exp(x^2) \times \operatorname{erf}(x) = \lambda$, where λ is determined by various constants of the problem. Since $x \exp(x^2) \operatorname{erf}(x)$ is monotone increasing, the existence and uniqueness of a solution is obvious.

3. A. Solomon, "Some Remarks on the Stefan Problem," *Math. Comp.* 20, 347–60 (1966).

4. J. Szekely and N. Themelis, *Rate Phenomena in Process Metallurgy*, Wiley, New York, 1971.

5. J. Stefan, "Über die Theorie der Eisbildung, Insbesondere über die Eisbildung im Polarmeere," *Ann. Phys. Chem.* 42, 269–86 (1891).

Although most authors assume that the more complicated nonlinear systems which arise do have unique solutions, few such systems have been analyzed in detail. We have investigated one-dimensional multiphase Stefan problems and established the existence and uniqueness of a solution to the nonlinear equations generated by the similarity solution. A verbal description of a "one-dimensional multiphase Stefan problem" is as follows: a semi-infinite volume of material is initially at a constant temperature, the surface is maintained at a different constant temperature, temperature changes proceed by conduction, and the material may change phase *n* times as it changes from its initial to its final temperature. Our result is that the solution exists and is unique if the temperatures of the intermediate phases are monotonically distributed between the initial and final temperatures. Fortunately, this is exactly what we would expect physically.

2. Numerical Analysis

K. O. Bowman J. E. Cope[1] B. W. Rust[1] L. R. Shenton[2] R. C. Ward

ANALYSIS OF DIVERGENT SERIES

Preliminary work on algorithms for summing divergent series and approximating singularities has been described in a previous report.[3] For mildly divergent series in powers of n^{-1} (the sth coefficient being less than $s!$ in magnitude), Padé approximants may lead to a sequence of apparently converging approximants. Alternative approximants[4] can be derived using

$$F_r(n) = n\bar{\Psi}_{r-1}(n) + \Psi_r(n) \int_a^b \frac{d\sigma(t)}{t+n}, \quad b > a. \quad (1)$$

where $\bar{\Psi}_{r-1}(\cdot)$ and $\Psi_r(\cdot)$ are real polynomials of degrees $r - 1$ and r respectively, $\sigma(t)$ is a nondecreasing function with infinitely many points of increase, and $F_r(n)$ is asymptotically equivalent (to a certain degree) to the given series. The choice of $\sigma(t)$ and the corresponding integral transform can be related to arbitrary Stieltjes (convergent) continued fractions. Asymptotic convergence of this algorithm seems to depend on matching the rate of increase of terms in the power series with those in the series development of the continued fraction.

For strongly divergent series a two-component version of Eq. (1) has been developed.[5] The simplest choice of $\sigma(t)$ is now $1 - e^{-t}$. The determination of the unknowns in the generalization of Eq. (1) can be achieved by simple recursions, avoiding any matrix inversion.

Summation algorithms must be tested against known divergent series (e.g., ref. 6, pp. 121–32), and trivial structures are almost useless. As a starting point, the mean value of the sample standard deviation in exponential sampling was chosen along with Student's one-sample t.[7] It transpires that for the latter, the first four central moments have Stieltjes continued fraction developments leading to monotonic enveloping bounds. This unexpected result suggests the possibility of the relation, for samples of n,

$$\int_{-\infty}^{\infty} x\, d\phi(x) = -1 \Big/ \left| n - 3 + \int_0^{\infty} (x+n)^{-1}\, d\sigma(x) \right| ,$$

where $\phi(\cdot)$ is the distribution function of t (under gamma sampling) and $\sigma(\cdot)$ is a nondecreasing (Stieltjes) weight function.

BOUNDS ON SOLUTIONS OF LINEAR SYSTEMS WITH INACCURATE COEFFICIENTS AND RIGHT-HAND SIDES

Oettli, Prager, and Wilkinson[8,9,10] have dealt with the problem of finding the solution set of a system of M equations in N unknowns,

$$A\mathbf{x} = \mathbf{b},$$

where A and $\mathbf{b}$ are known only to some limited tolerance, $A^\circ - \Delta A \leq A \leq A^\circ + \Delta A$ and $\mathbf{b}^\circ - \Delta\mathbf{b} \leq \mathbf{b} \leq \mathbf{b}^\circ + \Delta\mathbf{b}$, with ΔA and $\Delta\mathbf{b}$ being arrays consisting of positive elements. Given an n-vector $\mathbf{x}$, necessary and sufficient conditions have been established by Oettli et al.[10] for $\mathbf{x}$ to be an exact solution for some system $A\mathbf{x} = \mathbf{b}$, where $A^\circ - \Delta A \leq A \leq A^\circ + \Delta A$ and $\mathbf{b}^\circ - \Delta\mathbf{b} \leq \mathbf{b}$

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1. Computing Applications Department.

2. University of Georgia.

3. "Algorithms for Summing Divergent Series with Particular Reference to Statistical Sampling Moments," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1976*, ORNL/CSD-13, p. 21 (October 1976).

4. L. R. Shenton and K. O. Bowman, "A New Algorithm for Summing Divergent Series, Part 1," *J. Compt. Appl. Math.* **2**, 151–67 (1976).

5. K. O. Bowman and L. R. Shenton, "A New Algorithm for Summing Divergent Series, Part 2," *J. Comput. Appl. Math.* **2**, 259–66 (1976).

6. G. A. Baker, Jr., *Essentials of Padé Approximants*, Academic Press, New York, 1975.

7. L. R. Shenton and K. O. Bowman, "A New Algorithm for Summing Divergent Series, Part 3," *J. Comput. Appl. Math.* **3** (1977).

8. W. Oettli, "On the Solution Set of a Linear System with Inaccurate Coefficients," *SIAM J. Numer. Anal., Ser. B* **2**, 115–18 (1965).

9. W. Oettli and W. Prager, "Compatibility of Approximate Solution of Linear Equations with Given Error Bounds for Coefficients and Right-Hand Sides," *Numer. Math.* **6**, 405–9 (1964).

10. W. Oettli, W. Prager, and J. H. Wilkinson, "Admissible Solutions of Linear Systems with Not Sharply Defined Coefficients," *SIAM J. Numer. Anal., Ser. B* **2**, 291–99 (1965).

$\leq \mathbf{b}^{\circ} + \Delta\mathbf{b}$. We have extended these results and changed their emphasis. If, from some a priori consideration, the orthant in which the true solution vector $\mathbf{x}$ lies is known, and if A and $\mathbf{b}$ are as above, it is possible to compute bounds for $\mathbf{x}$ by linear programming. The tableau for the problem has been developed. Results have been extended to finding confidence intervals for $\mathbf{x}$ in the case where A and $\mathbf{b}$ are random samples from distributions with known variances.

PROBABILISTIC ERROR ANALYSIS OF A PADÉ ALGORITHM FOR COMPUTING THE MATRIX EXPONENTIAL

In a survey paper by Moler and Van Loan,[11] several methods for computing the matrix exponential are discussed and analyzed. For each of these methods, there exist classes of matrices for which inaccurate approximations may result. It is not always known whether such failures result from the inherent sensitivity of the problem or from the instability of the algorithm. In either case, it is desirable for the algorithm to indicate this failure to the user. Ward[12] describes and analyzes an algorithm to compute the matrix exponential based on diagonal Padé approximations. He computes an a posteriori bound on the size of the final error, including the effects of both truncation and roundoff, and returns to the user the minimum number of digits accurate in the norm of the computed exponential matrix. Thus, users can frequently determine that the algorithm has approximated the matrix exponential to their desired accuracy. However, users may be falsely notified of a failure because the error bound may be, and usually is, a severe overestimate of the actual error.

In this study we have performed a probabilistic error analysis of Ward's algorithm and have produced an a posteriori estimate for the expectation and variance of the final error. From the central limit theorem in probability theory, we expect the 95% confidence bound to be a considerable reduction from the strict error bound, thus partially eliminating overly pessimistic results.

11. C. B. Moler and C. F. Van Loan, "Nineteen Ways to Compute the Exponential of a Matrix," *SIAM Rev.*, to be published.

12. R. C. Ward, "Numerical Computation of the Matrix Exponential with Accuracy Estimate," *SIAM J. Numer. Anal.*, to be published.

The algorithm to be analyzed for computing e^A can be briefly stated as follows:

a. balance A; that is, $A' = D^{-1}AD$, where D is a diagonal matrix,
b. scale A; that is, $B = A'2^{-m}$ such that $\|B\|_1 \leq 1$,
c. compute e^B by diagonal Padé approximation,
d. compute $e^{A'} = (e^B)^{2^m}$, and
e. compute $e^A = De^{A'}D^{-1}$.

The following assumptions, which are analyzed by Ward,[13] form the basis for this study:

1. roundoff errors are independent random variables,
2. mantissas of floating-point numbers in a computer are logarithmically distributed,
3. columns of the matrix B are independent and uniformly distributed over the subset of real-column n-vectors $\mathcal{R}^n$ given by

$$\left\{ x \in \mathcal{R}^n \;\middle|\; \sum_{i=1}^{n} |x_i| \leq 1 \right\} .$$

4. columns of the matrix $(e^B)^{2^r}$ for $0 \leq r \leq m$ are independent and uniformly distributed over the subset

$$\left\{ x \in \mathcal{R}^n \;\middle|\; \sum_{i=1}^{n} |x_i| \leq \|(e^B)^{2^r}\|_1 \right\} .$$

Our study shows that the expectation of the error in the computed e^B matrix is the Padé truncation error matrix T_e plus terms of order b^{-2t}, where b is the base of the computer and t is the number of digits used to represent the mantissa of a floating-point number. This is precisely what one would expect. The variance of this error is given by $f(i, j, n)\,\mathrm{Var}[\epsilon] + O(b^{-4t})$, where the maximum of $f(i, j, n)$ for $1 \leq i$ and $j \leq n$ is $12n$ and $\mathrm{Var}[\epsilon]$ is the variance of the basic roundoff error.

Denoting the error in the computed $(e^B)^{2^r}$ matrix by θ^r, the expectation of θ^r, $E[\theta^r]$, for $r = 1$, is given by $2T_e + O(b^{-4t})$. For $r \geq 2$, $E[\theta^r]$ involves only terms of

13. R. C. Ward, "Statistical Roundoff Error Analysis of a Padé Algorithm for Computing the Matrix Exponential," *Proceedings of the Conference on Padé and Rational Approximation*, ed. by E. B. Saff and R. S. Varga, Academic Press, New York, to be published.

order b^{-2t}. The expression for the variance of θ^r can be simplified to the recurrence relation

$$\mathrm{Var}[\theta^r] = \frac{4}{n} \left\| (e^B)^{2^{r-1}} \right\|_1^2 \mathrm{Var}[\theta^{r-1}] + \frac{2}{n^3} \left\| (e^B)^{2^{r-1}} \right\|_1^4 \mathrm{Var}[\epsilon] + O(b^{-4t}) .$$

Finally, the expectation of the error in the norm of the computed e^A matrix is given by

$$\left\{ \left(\sum_{i=1}^{n} d_i \right) E[\theta^m] \Big/ d_J \right\} + O(b^{-2t}) .$$

where J is determined by the column norms of e^A and $\mathrm{Var}[\theta^m]$ and the d_i's are the diagonal elements of the diagonal matrix D determined in step (a) of the algorithm. The simplified expression for the variance of this total error is given by

$$\left\{ \mathrm{Var}[\theta^m] + \frac{8}{n} \| e^A \|^2 \mathrm{Var}[\epsilon] \right\} \left(\sum_{i=1}^{n} d_i^2 \right) \Big/ d_J^2 .$$

Using these results the algorithm PADE8 of Ward has been modified to output the number of digits accurate in the norm of the computed exponential matrix at the 95% confidence level. Thus two integers are now returned to the user, with one integer based on strict error bounds and one based on the probabilistic error analysis.

The few test cases which have been run to date have indicated that the probabilistic error gives a very close estimate to the actual error in the computed exponential matrix.

3. Continuum Mechanics

S. J. Chang   S. M. Ohr[1]   D. N. Robinson[2]   T. C. T. Ting[3]

BOUNDARY REFLECTION OF DIFFRACTED WAVES

Dynamic problems of wave diffraction from a semi-infinite, as well as finite, crack have been studied recently by a number of researchers.[4,5] Current interest in problems of crack arrest requires some understanding of the effect of boundary reflection of the diffracted waves. In the present study we analyzed this effect when a straight boundary is located at an angle α to the direction of a semi-infinite crack. Using Cartesian coordinates (x, y) in the two-dimensional problem, the semi-infinite crack is located on the entire positive x axis. The distance between the straight boundary and the origin is denoted by V. Stress waves are generated from the semi-infinite crack by a suddenly applied normal traction of constant magnitude on the surfaces of the crack. The reflected waves from the boundary will induce additional stress intensities which are of concern in crack arrest problems. The angle α and the distance V can be varied in the problem. When $\alpha = 0$, for example, it corresponds to a beam of finite depth.

Closed-form solution for the transient diffraction problem of a semi-infinite crack is readily obtained by the Wiener-Hopf method supplemented by the Cagniard technique. The effect of reflection from the straight boundary is calculated by the method of wave front analysis.[6] The transport equation is used to calculate the change of the intensity of the wave along the bicharacteristic or ray. The result from the transport equation is only valid close to the wave front.

Several interesting features are incorporated in the present solution scheme. Since the intensity of the diffracted wave is continuous across the wave front whereas the slope is infinite, special treatment[7] must be given to this part of the solution of the transient diffraction problem. After the shear wave reaches the boundary, the method can be continued without difficulty until the critical angle is reached. Then a head wave, which is also calculated, is generated along the boundary.

The solution of the diffraction problem is expressed about the wave front. The longitudinal component of the diffracted waves at $\theta = \pi/2$, for example, in terms of the polar coordinates has the following stress components:

$$\frac{\partial \sigma_x}{\partial t} = -\frac{1}{\pi}\,\frac{1}{2(s_T^2 - s_L^2)}\,\frac{s_T^4 \sqrt{s_L}\, L}{K_+(0)s_R^2}$$

$$\times \left(s_R B - 1 + \frac{s_R}{s_L} \right) \frac{H(t - s_L r)}{\sqrt{t^2 - s_L^2 r^2}}$$

$$= \text{constant} \times \frac{H(t - s_L r)}{\sqrt{t^2 - s_L^2 r^2}} .$$

$$\frac{\partial \sigma_y}{\partial t} = \frac{1}{\pi}\,\frac{1}{2(s_T^2 - s_L^2)}\,\frac{s_T^2(s_T^2 - 2s_L^2)\sqrt{s_L}\, L}{K_+(0)s_R^2}$$

$$\times \left(s_R B - 1 + \frac{s_R}{s_L} \right) \frac{H(t - s_L r)}{\sqrt{t^2 - s_L^2 r^2}} .$$

$$\frac{\partial \sigma_{xy}}{\partial t} = \frac{1}{\pi}\,\frac{1}{2(s_T^2 - s_L^2)}\,\frac{2s_T^2 s_L \sqrt{s_L}}{K_+(0)s_R}\,\frac{H(t - s_L r)}{\sqrt{t^2 - s_L^2 r^2}} .$$

where s_L, s_T, and s_R are the slowness of the longitudinal, transverse, and surface wave speeds respectively. The transverse component at $\theta = \pi/2$ has the following stress components:

$$\frac{\partial \sigma_x}{\partial t} = -\frac{\partial \sigma_y}{\partial t} = \frac{1}{\pi}\,\frac{1}{2(s_T^2 - s_L^2)}\,\frac{s_T^2 \sqrt{s_L}\, L}{r^2 K_+(0)s_R^2}$$

$$\times \left(4 - 4s_R B - \frac{2s_R}{s_L} \right) \sqrt{t^2 - s_T^2 r^2} .$$

$$\frac{\partial \sigma_{xy}}{\partial t} = \frac{1}{\pi}\,\frac{1}{2(s_T^2 - s_L^2)}\,\frac{2s_T s_L^2 \sqrt{s_L}\, L}{K_+(0)s_R}\,\frac{H(t - s_T r)}{\sqrt{t^2 - s_T^2 r^2}}$$

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1. Solid State Division.
2. Engineering Technology Division.
3. University of Illinois at Chicago Circle.

4. L. B. Freund, "Crack Propagation in an Elastic Solid," *J. Mech. Phys. Solids* 20, 129–40 (1972).
5. S.-J. Chang, "Diffraction of Plane Dilatational Waves by a Finite Crack," *Quar. J. Mech. Appl. Math.* 24, 423–43 (1971).
6. T. C. T. Ting and I. H. Lee, "Wave Front Analysis in Composite Materials," *J. Appl. Mech.* 91, 497–504 (1969).
7. R. Courant and D. Hilbert, *Methods of Mathematical Physics*, vol. 2, Interscience, New York, 1962.

The general version of the above equations, which includes the angular variation, is used in the wave-front expansion. The magnitude of the stress after the reflection from the boundary is calculated from the transport equation close to the wave front. The pattern of the reflected wave fronts as well as the induced stress intensity factors from the different components are computed.

CONSTITUTIVE EQUATION FOR ELASTIC-PLASTIC MEDIUM

For practical purposes, a unified constitutive equation is established to describe both creep and plastic deformations for metals at an extended range of temperatures. At room temperature, it can be reduced to the time-independent theory. The formulation is based on the state variable theory of Fardshisheh and Onat[8] in terms of Rice's flow potential representation[9] for the inelastic strain.

The center of the yield surface α in the kinematic hardening model is used as the set of state variables. The growth law, which is the governing equation for α, assumes the following form:

$$\dot{\alpha} = h(\alpha)\dot{\epsilon}^p - r(\alpha)\alpha ,$$

where a dot is used to denote the time derivative of the variable, ϵ^p is the inelastic strain, and the scalar functions $h(\alpha)$ and $r(\alpha)$ denote the effects of the strain hardening and the strain recovery respectively. This expression for $\dot{\alpha}$ is more general than the potential representation of Ponter and Leckie[10] given by

$$\dot{\alpha} = -h(\alpha)\frac{\partial\Omega}{\partial\alpha} .$$

It can be shown that α is a deviatoric tensor and both $h(\alpha)$ and $r(\alpha)$ are functions of the second and third invariants of α, denoted by $J_2(\alpha)$ and $J_3(\alpha)$ respectively. The above growth relation can be interpreted as a kinematic hardening condition in a more general form.

The equation for plastic flow as expressed by the potential of Rice is

$$\dot{\epsilon}^p = \frac{\partial\Omega(f,\alpha)}{\partial f}\frac{\partial f}{\partial\sigma} ,$$

where f is a loading function and Ω is the flow potential. A convenient form of f is

$$f = J_2(\sigma' - \alpha) ,$$

where σ' is the deviatoric component of σ. The elimination of $\dot{\epsilon}^p$ from the growth law and the flow law leads to

$$\frac{\partial\Omega}{\partial f}|\nabla f| = F(\alpha, \dot{\alpha}) ,$$

where ∇f is the gradient of f in the stress space and F is a function of α and $\dot{\alpha}$. The loading function f is solved from the above equation to obtain the yield condition

$$f(\sigma, \alpha) = K(\alpha, \dot{\alpha}) .$$

From the results of uniaxial tests, we expect K to exhibit the property that it tends to the yield constant when the temperature decreases to the room temperature range.

The flow rule for the inelastic strain can be derived by the usual procedure in plasticity. This yields a slightly more general form than usual due to the recovery mechanism. As expected, the presence of the strain recovery destroys the linearity between the rate of stress and the rate of strain. From the growth equation and the flow equation, we obtain

$$\mathrm{tr}\left(\frac{\partial f}{\partial\sigma}\dot{\alpha}\right) = h(\alpha)\frac{\partial\Omega}{\partial f}|\nabla f|^2 - r(\alpha)\,\mathrm{tr}\left(\alpha\frac{\partial f}{\partial\sigma}\right) ,$$

where tr denotes the trace function. Substituting it into the potential representation of the inelastic strain, one obtains the flow rule

$$\dot{\epsilon}^p = \frac{\partial f/\partial\sigma}{h(\alpha)|\nabla f|^2}\left[\mathrm{tr}\left(\frac{\partial f}{\partial\sigma}\dot{\alpha}\right) + r(\alpha)\,\mathrm{tr}\left(\frac{\partial f}{\partial\sigma}\alpha\right)\right] .$$

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8. F. Fardshisheh and E. T. Onat, "Representation of Elastic-Plastic Behavior by Means of State Variables," pp. 89–115 in *Problems of Plasticity, Symposium on Foundations of Plasticity, Warsaw*, Noordhoff, Leyden, 1973.

9. J. R. Rice, "On the Structure of Stress-Strain Relations for Time-Dependent Plastic Deformation in Metals," *J. Appl. Mech.* 37, 728–37 (1970).

10. A. R. S. Ponter and F. A. Leckie, "Constitutive Relationships for the Time-Dependent Deformation of Metals," *J. Eng. Mater. Technol.* 98, 147–51 (1976).

or, by using the yield condition, one obtains

$$\dot{\underset{\sim}{\epsilon}}^{p} = \frac{\partial f/\partial \underset{\sim}{\sigma}}{h(\underset{\sim}{\sigma})|\nabla f|^{2}} \left(\mathrm{tr} \left[\frac{\partial f}{\partial \underset{\sim}{\sigma}} \left[\dot{\underset{\sim}{\sigma}} + r(\underset{\sim}{\sigma}) \underset{\sim}{\sigma} \right] \right] - \frac{dK}{dt} \right) .$$

This equation provides a basic time-dependent structure for the inelastic solid. It is obvious that with vanishing $r(\underset{\sim}{\sigma})$ and dK/dt it reduces to the well-known flow rule in time-independent plasticity.

EFFECT OF SURFACE INHOMOGENEITY ON ELASTIC WAVE PROPAGATION

This investigation is concerned with the effect of surface mass on elastic wave propagation in two-dimensional half-space due to a suddenly applied force on the surface. This is an extension of the well-known "Lamb's problem," which ignores the surface mass. A discussion of this surface mass wave propagation problem has been given by Strick,[11] and the method of integral transform has been used to obtain its solution. One significant phenomenon of this problem is its absence of Rayleigh surface wave in contrast to the Lamb problem. Due to the surface mass, the inverse transform of the problem has been made through the computation of residues, whereas for Lamb's problem the Cagniard technique has been used. It is interesting to observe that by using an asymptotic theorem of integral transform, we can derive the solution of the Lamb problem by passing to the limit as the surface mass tends to zero.

Cartesian coordinates (x, y) are used to describe the two-dimensional elastic medium. With the half-space defined by $y \leq 0$ and $-\infty < x < \infty$, 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

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

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11. E. Strick, "Propagation of Elastic Wave Motion Along a Fluid/Solid Interface," *Philos. Trans. R. Soc. London Ser. A* 251, 455–523 (1959).

The transformed governing equations of motion are

$$c_2^2 u^*_{,yy} + p^2 (c_1^2 \eta^2 - 1) u^* + p\eta (c_1^2 - c_2^2) v^*_{,y} = 0 ,$$

$$c_1^2 v^*_{,yy} + p^2 (c_2^2 \eta^2 - 1) v^* + p\eta (c_1^2 - c_2^2) u^*_{,y} = 0 ,$$

with the boundary condition along $y = 0$ given by

$$PH(t)\delta(x) + \sigma_{xy} = m\ddot{u} ,$$

$$QH(t)\delta(x) + \sigma_y = m\ddot{v} .$$

where P and Q are surface forces, m' is the surface mass, the σ's are stress components, and (u, v) is the displacement vector.

Stress components have been determined from the above expression; for example, the vertical component σ_y is

$$\sigma_y = (I_{1p} P + I_{1q} Q) + (I_{2p} P + I_{2q} Q) .$$

where I_{im} for $i = 1, 2$ and $m = p, q$ denotes the wave component with speed c_i due to the surface force m. For brevity, we only compute I_{1p} to illustrate its consistency with the solution of Lamb's problem. Using the inverse Laplace transform $\mathcal{L}^{-1}$, we have

$$\mathcal{L}^{-1}(I_{1p}) = \frac{c_1^2}{c_2^2 \pi} \, \mathrm{Im} \int_{r/c_1}^{\infty} \mathcal{L}^{-1}$$

$$\times \left[\left(\frac{\gamma_1^2}{\eta^2} + 1 - \frac{2c_2^2}{c_1^2} \right) \frac{\eta^3 \left(2\gamma_2 + \frac{m'}{\mu} p \right)}{R'} \right]_{\eta = \eta_{L+}}$$

$$\times \; e^{-pt'} \frac{\partial \eta_{L+}}{\partial t'} \, dt' ,$$

where

$L+$ is the Cagniard contour;

$$\gamma_i = (c_i^{-2} - \eta^2)^{1/2} , \quad \mathrm{Re}(\gamma_i) \geq 0 , \quad \text{for } i = 1, 2 ;$$

$$R' = (\gamma_1 \gamma_2 + \eta^2) \frac{m'}{\mu} p + \frac{1}{c_2^2} (\gamma_1 + \gamma_2) \frac{m'}{\mu} p + R ;$$

and R denotes the characteristic equation of the Rayleigh wave. The Laplace inversion of the integrand, denoted by $\mathcal{L}^{-1}(F)$, is given by

$$\mathcal{L}^{-1}(F)=\left(\frac{\gamma_1}{\eta^2}+1-\frac{2c_2^2}{c_1^2}\right)$$

$$\times\ \frac{\eta^3}{(\gamma_1\gamma_2+\eta^2)\left(\frac{m'}{\mu}\right)^2(p_+-p_-)}$$

$$\times\left|\left(2\gamma_2+\frac{m'}{\mu}p_+\right)e^{p_+(t-r)}-\left(2\gamma_2+\frac{m'}{\mu}p_-\right)e^{p_-(t-r)}\right| .$$

Thus, for $m'\to 0$ we can show from Watson's Lemma that I_{1p} reduces to one component of Lamb's solution. Other components can be treated in a similar manner.

FORCES ON DEFECTS IN LINEAR ELASTICITY

The energy momentum tensor in elasticity has been introduced by Eshelby[12] to calculate the change of energy for an elastic medium containing defects. The crack extension force is defined as the change of energy per unit extension of the crack. Therefore, the energy momentum tensor can be used to represent the crack extension force. A tensor quality Π, which is slightly different from that of Eshelby when considering the effect of body forces, has been derived.[13] Since plastic deformations, or distribution of dislocations, can be represented by the equivalent body forces, we may use this tensor quality Π to calculate the effect of the distribution of dislocations to the crack extension force.

Let $\mathfrak{E}$ be the energy density of the elastic body; that is,

$$\mathfrak{E}=\tfrac{1}{2}c_{ikmn}\frac{\partial u_i}{\partial x_k}\frac{\partial u_m}{\partial x_n}-u_i f_i ,$$

where f_i is the body force, u_i is the displacement vector, and c_{ikmn} is an elastic constant. Obviously,

$$\frac{\partial\mathfrak{E}(u_i,u_{i,k},x_i)}{\partial x_m}=\frac{\partial\mathfrak{E}}{\partial u_i}\frac{\partial u_i}{\partial x_m}+\frac{\partial\mathfrak{E}}{\partial u_{i,k}}\frac{\partial u_{i,k}}{\partial x_m}+\frac{\partial\dot{\mathfrak{E}}}{\partial x_m} ,$$

where

$$u_{i,k}=\frac{\partial u_i}{\partial x_k}$$

and $\partial\dot{\mathfrak{E}}/\partial x_m$ is the explicit derivative of $\mathfrak{E}$; in our case,

$$\frac{\partial\dot{\mathfrak{E}}}{\partial x_m}=-u_i\frac{\partial f_i}{\partial x_m} .$$

It can be shown that

$$\frac{\partial\dot{\mathfrak{E}}}{\partial x_m}=\frac{\partial\Pi_{mk}}{\partial x_k}=-u_i\frac{\partial f_i}{\partial x_m} ,$$

where, with σ_{ik} as the stress tensor,

$$\Pi_{mk}=\mathfrak{E}\delta_{mk}-\sigma_{ik}u_{i,m} .$$

The tensor of Eshelby is

$$c_{mk}=e\delta_{mk}-\sigma_{ik}u_{i,m} ,$$

where e is the strain energy density; the crack extension force can be shown to be

$$F_m=\int_V\frac{\partial\Pi_{mk}}{\partial x_k}\,dv .$$

where V is a volume enclosing the crack edge.

Suppose that internal stresses are present in the elastic body due to, for example, the presence of defects. Let $\epsilon_{ij}^s(x_j)$ be the self-strain which is considered as the source of the internal stress. The total strain

$$\epsilon_{ij}^T=\epsilon_{ij}^s+\epsilon_{ij}$$

is defined to be the sum of the self-strain and the elastic strain. It is easy to show that a fictitious body force

$$f_i=-\frac{\partial}{\partial x_j}(c_{ijmn}\epsilon_{mn}^s)$$

can be used to replace the effect of the internal stress. This method is generally attributed to Duhamel and Neumann, who treated the special case of thermal stresses. This body force will be substituted into the tensor Π to calculate the effect due to the presence of defects.

12. J. D. Eshelby, "Energy Relations and the Energy-Momentum Tensor in Continuum Mechanics," pp. 77–115 in *Inelastic Behavior of Solids*, ed. by M. Kanninen et al., McGraw-Hill, New York, 1970.

13. G. Liebfried, Technische Hochschule, Aachen, Germany, private communication.

4. Matrices and Other Operators

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T. Kaplan[3] R. S. Varga[4] R. C. Ward

STABILITY AND SEMIPOSITIVITY OF MATRICES

The purpose of this study was to characterize and interrelate various degrees of stability and semipositivity for real square matrices. The standard conditions for three major classes of matrices were made both stronger and weaker, and the resulting classes were examined. These major classes were diagonally stable, stable, and semipositive matrices denoted by $\mathcal{A}$, $\mathcal{L}$, and $\mathcal{S}$ respectively. Their relationship to the classes of matrices whose principal minors are positive, denoted by $\mathcal{P}$, and nonnegative, denoted by $\mathcal{P}_0$, was also examined.

The matrix A is in $\mathcal{L}$ if the real parts of its eigenvalue are positive. By a well-known theorem of Liapunov,[5] A is stable if and only if there exists a positive definite matrix X such that $AX + XA^T$ is positive definite. The matrix A is in $\mathcal{A}$ if the X above may be taken to be diagonal (cf. Barker, Berman, and Plemmons[6]). The matrix A is in $\mathcal{S}$ if $Ax > 0$ for some $x > 0$ (cf. Fiedler and Pták[7]).

With each of the classes $\mathcal{A}$, $\mathcal{L}$, and $\mathcal{S}$ we associate two superclasses, denoted by $\mathcal{W}\mathcal{A}$, $\mathcal{W}\mathcal{L}$, $\mathcal{W}\mathcal{S}$ and $\mathcal{N}\mathcal{W}\mathcal{A}$, $\mathcal{N}\mathcal{W}\mathcal{L}$, $\mathcal{N}\mathcal{W}\mathcal{S}$ defined as follows:

1. $A \in \mathcal{W}\mathcal{A}$ ($\mathcal{N}\mathcal{W}\mathcal{A}$) if there exists a positive (nonzero, nonnegative) diagonal matrix D such that $AD + DA^T$ is positive semidefinite.

2. $A \in \mathcal{W}\mathcal{L}$ ($\mathcal{N}\mathcal{W}\mathcal{L}$) if there exists a positive definite (nonzero, positive semidefinite) matrix X such that $AX + XA^T$ is positive semidefinite.

3. $A \in \mathcal{W}\mathcal{S}$ ($\mathcal{N}\mathcal{W}\mathcal{S}$) if $Ax \geq 0$ for some $x > 0$ ($x \geq 0$).

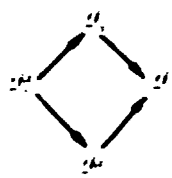
Let $\mathcal{G}$ denote any of these nine classes. With each $\mathcal{G}$, we associate subclasses using the following notation:

$A \in \mathcal{G}^D$ if DA is in $\mathcal{G}$ for every positive diagonal matrix D.

$A \in \mathcal{G}_P$ if every principal submatrix of A is in $\mathcal{G}$, and

$A \in \mathcal{G}_P^D$ if every principal submatrix of A is in $\mathcal{G}^D$.

We can immediately verify the following inclusion tree:



In addition to the 38 classes defined above, we also consider the class $\mathcal{P}_0^+$ defined by Johnson[8] to consist of matrices in $\mathcal{P}_0$ which have at least one positive minor of each order.

Our results are summarized in Fig. 1 as a directed graph having classes as vertices in which there is a sequence of directed edges from vertex $\mathcal{X}$ to vertex $\mathcal{Y}$ if and only if $\mathcal{X}$ is contained in $\mathcal{Y}$. Equivalent classes are represented by their most inclusive class; that is, $\mathcal{N}\mathcal{W}\mathcal{L}_P$ represents the equivalent classes $\mathcal{N}\mathcal{W}\mathcal{L}_P$ and $\mathcal{N}\mathcal{W}\mathcal{L}_P^D$ and $\mathcal{A}$ represents the equivalent classes $\mathcal{A}$, $\mathcal{A}_P$, $\mathcal{A}^D$, and $\mathcal{A}_P^D$.

STABILITY AND SEMIPOSITIVITY OF MATRICES WITH NONPOSITIVE OFF-DIAGONAL ENTRIES

The four classes of matrices $\mathcal{A}$, $\mathcal{L}$, $\mathcal{P}$, and $\mathcal{S}$ defined in the preceding article of this report are in general different. However, restricted to the class of n-by-n real

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1. University of Tennessee.
2. Computing Applications Department.
3. Solid State Division.
4. Kent State University.
5. A. M. Liapunov, "Problème Général de la Stabilité du Mouvement," a translation from the Russian, republished in *Annals of Mathematics*, No. 17, Princeton Press, Princeton, 1947.
6. G. P. Barker, A. Berman, and R. J. Plemmons, *Positive Diagonal Solutions to the Lyapunov Equations*, Mathematics Research Center Report 76-087, University of Wisconsin, Madison, 1976.
7. M. Fiedler and V. Pták, "Some Generalizations of Positive Definiteness and Monotonicity," *Numer. Math.* 9, 163–72 (1966).
8. C. R. Johnson, "Second, Third, and Fourth Order D-Stability," *J. Res. Natl. Bur. Stand.* 78B, 11–13 (1974).

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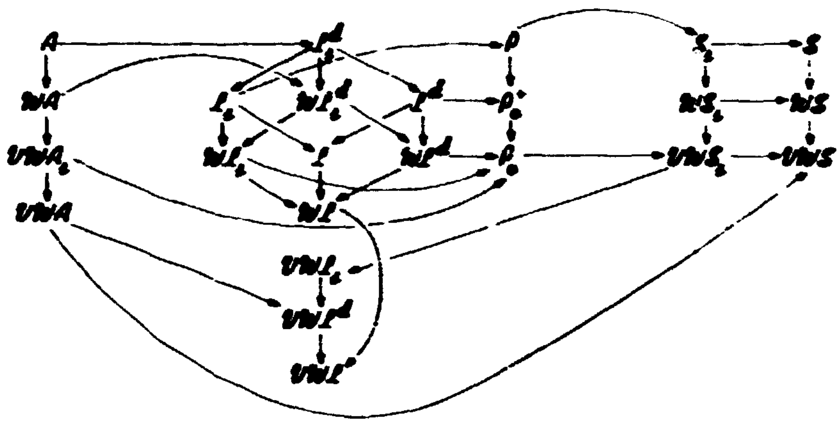

Fig. 1. Inclusion tree for major classes of matrices.

matrices with nonpositive off-diagonal entries, they all become the class of nonsingular M-matrices (cf. Plemmons[9]). Variants of these four classes with this restriction have been characterized and interrelated.

To present the results of this study, we use the concept of reduced normal form (cf. Varga[10]). If a real n-by-n matrix A is reducible, there is a permutation matrix P for which PAP^T is in reduced normal form:

$$PAP^T = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1k} \\ & A_{22} & \cdots & A_{2k} \\ & & \ddots & \vdots \\ \text{C} & & & A_{kk} \end{bmatrix}$$

where each A_{ii}, $1 \leq i \leq k$, is either square and irreducible, or a 1-by-1 null matrix. For our purposes here, it is convenient to define a 1-by-1 null matrix to be irreducible. We also use the notation of the preceding article and denote the class of zero matrices by $\mathcal{O}$.

The results of our study yield the following characterizations for classes of matrices with nonpositive off-diagonal entries:

1. The classes $\mathcal{A}$, $\mathcal{L}_1^d$, $\mathcal{L}_1$, $\mathcal{L}^d$, $\mathcal{L}$, $\mathcal{P}$, $\mathcal{P}_*$, $\mathcal{S}_1$, and $\mathcal{S}$ are all equivalent to the class of nonsingular M-matrices.
2. The class $\mathcal{W}\mathcal{A}$ is equivalent to the class of irreducible M-matrices.
3. The classes $\mathcal{W}\mathcal{L}$, $\mathcal{W}\mathcal{L}^d$, $\mathcal{W}\mathcal{L}_1$, and $\mathcal{W}\mathcal{L}_1^d$ are all equivalent to the class of M-matrices with "property C." [The M-matrix $A = \rho I - B$ has "property C" if and only if $\lim_{k \to \infty} (\rho^{-1} B)^k$ exists.]
4. The classes $\mathcal{V}\mathcal{W}\mathcal{A}_2$, $\mathcal{P}_2$, and $\mathcal{V}\mathcal{W}\mathcal{S}_1$ are all equivalent to the class of M-matrices.
5. Let $A \in \mathcal{P}_2$. Then, using the notation of the reduced normal form,
   (i) $A \in \mathcal{W}\mathcal{A}$ iff A_{ii} singular implies $A_{ij}^T = A_{ji} \in \mathcal{O}$ for all $j \neq i$;
   (ii) $A \in \mathcal{W}\mathcal{S}$ iff A_{ii} singular implies $A_{ij} \in \mathcal{O}$ for all $j \neq i$;
   (iii) $A \in \mathcal{W}\mathcal{L}$ iff A_{ii} and A_{jj} singular, $j > i$, imply $A_{ij} \in \mathcal{O}$.
6. The class $\mathcal{W}\mathcal{S}_1$ is equivalent to the class $\mathcal{W}\mathcal{S}$.
7. Let A be irreducible. Then, $A \in \mathcal{V}\mathcal{W}\mathcal{S}$ iff $A \in \mathcal{P}_2$.
8. The class $\mathcal{V}\mathcal{W}\mathcal{A}$ is equivalent to the class $\mathcal{V}\mathcal{W}\mathcal{S}$.

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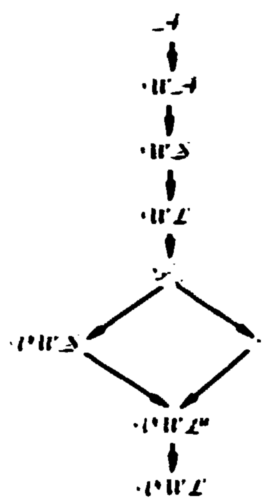
9. R. J. Plemmons, "A Survey on the Theory and Applications of M-Matrices," *J. Lin. Alg. Appl.*, to be published.
10. R. S. Varga, *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, N.J., 1962.

9. Using the notation of the reduced normal form, we have

   (i) $A \in$ [illegible] iff there is an r such that $A_{rr} \in$ [illegible] with $A_{ir} \in$ [illegible] for all $i \neq r$;

   (ii) $A \in$ [illegible] iff A has an eigenvalue λ with Re $\lambda \geq 0$.

Denoting the classes of M-matrices given in 1, 3, and 4 above by [illegible] and [illegible] respectively, our results are summarized by the following directed graph:



THE RANK OF A DIFFERENCE OF MATRICES AND ASSOCIATED GENERALIZED INVERSES

Our work on this topic, which has been partially described in a previous report,[11] has been concluded. Various representations have been obtained for characterizing the rank of $A - S$ in terms of rank (A) + k where A and S are arbitrary complex matrices and k is a function of A and S. It has been shown that if $S = AMA$ for some matrix M and if G is any matrix satisfying $A = AGA$, then

$$\text{rank}\,(A - S) = \text{rank}\,(A) - \text{nullity}\,(I - SG)\ .$$

Several alternative forms of this result have been established, as have many equivalent conditions to have

$$\text{rank}\,(A - S) = \text{rank}\,(A) - \text{rank}\,(S)\ .$$

Denoting the Moore-Penrose inverse of the matrix B by B^+, it has been shown that

$$(A - S)^+ = (I - A^+S)^+(A^+ - A^+SA^+)(I - SA^+)^+$$

if and only if $AA^+S = S = SA^+A$. Other interesting forms for $(A - S)^+$, some of which have been previously known, have been derived from the above relation.

OPERATORS COMMUTING WITH A COMPACT QUASI-AFFINITY

Lomonosov's Theorem states that any operator which commutes with a compact has an invariant subspace. It is, therefore, of interest to determine which operators can commute with a compact quasi-affinity. In a recent paper, Foias, Pearcy, and Voiculescu[12] show that a nonbiquasitriangular operator which commutes with a compact quasi-affinity must have infinite index at the semi-Fredholm points in its spectrum. They also present an example to show that this phenomenon can occur; however, this example is wrong. We modify their example, and thus demonstrate that it is possible for a nonbiquasitriangular operator to commute with a compact quasi-affinity.

COMPUTATION OF WIENER-FEYNMAN INTEGRALS

The solution to many problems in mathematics and physics can be expressed as a Wiener-Feynman (path) integral. However, for computational purposes, the path integral is difficult to handle. Most previous methods eventually rely upon computing a multi-dimensional integral of large dimension. Using a method borrowed from disordered systems,[13] we have expressed the path integral as a matrix element of an operator. Thus, we have replaced the difficult numerical integration by a (hopefully) tractable linear algebra problem.

We have completed calculations using our method for the harmonic oscillator, which is a simple problem whose exact solution is known. Our computed answer was in good agreement with the solution. Work is now in progress on the anharmonic oscillator.

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11. "Rank and Decomposition of the Difference of Matrices and Generalized Inverses," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1976*, ORNL/CSD-13, p. 20 (October 1976).

12. C. Foias, C. Pearcy, and I. Voiculescu, "On the Staircase Representation of Biquasitriangular Operators," *Mich. Math. J.* **22**, 343–52 (1975).

13. T. Kaplan and L. J. Gray, "Elementary Excitations in Random Substitutional Alloys," *Phys. Rev. B* **14**, 3462–70 (1976).

5. Experimental Design

C. K. Bayne E. R. Jones[1] T. J. Mitchell M. D. Morris[2]

D-OPTIMAL THREE-LEVEL FACTORIAL DESIGNS

The least-squares estimator of the $m \times 1$ vector of unknown coefficients β in the linear model

$$E[\mathbf{y}] = X\beta$$

is a function of the $n \times 1$ vector of observations $\mathbf{y}$ and the $n \times m$ "expanded design matrix" X. The least-squares estimator $\hat{\beta} = (X'X)^{-1}X'\mathbf{y}$ has variance-covariance matrix given by $(X'X)^{-1}\sigma^2$, where σ^2 is the variance associated with the experimental error. Since X depends only on the model and the experimental design, the experimenter can choose a design for a model that will yield a variance-covariance matrix that is "optimal" in some sense. One such design criterion, which minimizes the volume of the joint confidence region for the least-squares estimators of the β's, is the criterion of "*D*-optimality." Specifically, a *D*-optimal design maximizes the determinant of $X'X$.

In a previous report,[3] the construction of *D*-optimal fractions of three-level factorial designs with p factors has been described for factorial effects models ($2 \leq p \leq 4$) and quadratic response surface models ($2 \leq p \leq 5$). These designs have been generated using Mitchell's DETMAX[4] algorithm and an algorithm that produces *D*-optimal balanced-array designs. The best *D*-optimal designs and their properties have been cataloged[5] and compared to designs now in the literature. Although the designs have been constructed to maximize the determinant of $X'X$, other properties such as the average and maximum variance of the fitted values over the 3^p possible factor combinations have been calculated to assist experimenters in choosing a design. In addition, the "*D*-efficiency," which is a measure of the determinant of each design and is independent of the parameterization of the model, has also been given.

For those designs that can be run sequentially, a diagram has been drawn indicating how, starting with a *D*-optimal design, a new *D*-optimal design can be constructed by adding only one design point or a group of design points.

DESIGN OF EXPERIMENTS TO DETECT MODEL INADEQUACY

In the planning of experiments, it is often helpful to tentatively postulate a model relating the response to the experimental variables and then to determine those combinations of levels of the experimental variables that should be run to estimate most precisely the parameters of that model. It is important, however, not to ignore the possibility that the proposed model may be underspecified, in that some terms have been omitted. We shall denote the assumed model by

$$\eta_1(\mathbf{x}) = \mathbf{f}_1'(\mathbf{x})\theta_1 \qquad (1)$$

and the true response by

$$\eta(\mathbf{x}) = \mathbf{f}_1'(\mathbf{x})\beta_1 + \mathbf{f}_2'(\mathbf{x})\beta_2 \quad ,$$

where $\mathbf{x}$ is a point in the "region of interest" $\mathcal{X}$ in the space of the experimental variables and $\mathbf{f}_1(\mathbf{x})$ and $\mathbf{f}_2(\mathbf{x})$ are vector functions of $\mathbf{x}$ specified by the model and the true response. For example, one might propose to fit a first-order model in two dimensions:

$$\eta_1(x_1, x_2) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 \quad , \qquad (2)$$

while the true response may be quadratic:

$$\eta(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 \quad . \qquad (3)$$

In this case

$$\mathbf{f}_1'(\mathbf{x}) = [1, x_1, x_2] \text{ and } \mathbf{f}_2'(\mathbf{x}) = [x_1^2, x_2^2, x_1 x_2] \quad .$$

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1. Texas A&M University.

2. ORAU Laboratory Graduate Participation Fellow, Virginia Polytechnic Institute and State University.

3. "*D*-Optimal Three-Level Factorial Designs," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCCND/CSD-18, pp. 8–9 (October 1975).

4. T. J. Mitchell, "Computer Construction of *D*-Optimal First-Order Designs," *Technometrics* **16**, 211–20 (1974).

5. T. J. Mitchell and C. K. Bayne, *D-Optimal Fractions of Three-Level Factorial Designs*, ORNL/CSD-19 (January 1977).

The problem we consider here is the design of experiments to detect the presence of nonzero β_2. In a previous report,[6] we proposed several criteria for doing this and applied them to the computerized construction of a large number of designs with a specified number n of observations. Here we shall avoid the combinatorial difficulties that are involved with constructing designs for fixed n and consider an experimental design to be a measure ξ on $\mathcal{X}$. This tactic, which is often used in optimal design theory, results in designs that stipulate the *proportion* of the available experimental runs to be placed at various "points of support" in $\mathcal{X}$. Such a design is called "approximate" since it will not be exactly attainable unless $\xi(\mathbf{x})$ is a multiple of n^{-1} at each point of support.

Our main approach to designing experiments to detect model inadequacy has been to maximize in some sense the noncentrality $\lambda = \beta_2' L(\xi)\beta_2$, where the lack of fit matrix $L(\xi)$ is given by

$$L(\xi) = M_{22}(\xi) - M_{21}(\xi)M_{11}^{-1}(\xi)M_{12}(\xi)$$

and

$$M_{ij}(\xi) = \int_{\mathcal{X}} \mathbf{f}_i(\mathbf{x})\mathbf{f}_j'(\mathbf{x})\xi(d\mathbf{x}) \quad , \qquad i, j = 1, 2 \quad .$$

This criterion, which was introduced by Atkinson and Fedorov[7] and called "*T*-optimality," is motivated by the fact that both the expectation of the residual sum of squares under the assumed model and the power of the normal-theory lack-of-fit test are monotonically increasing functions of λ. A principal impediment to the application of this criterion is that β_2 is unknown. To circumvent this difficulty, we introduced[6] a measure of model inadequacy τ,

$$\tau = \min_{\theta_1} \int_{\mathcal{X}} |\eta(\mathbf{x}) - \mathbf{f}_1'(\mathbf{x})\theta_1|^2 \, d\mathbf{x} \quad .$$

This measure, which represents the degree of departure of the true response $\eta(\mathbf{x})$ from the class of assumed models given by Eq. (1), turns out to be, like λ, a quadratic function in β_2:

$$\tau = \beta_2' T\beta_2 \quad ,$$

where

$$T = \mu_{22} - \mu_{21}\mu_{11}^{-1}\mu_{12}$$

and the $\{\mu_{ij}\}$ are the region moment matrices:

$$\mu_{ij} = \int_{\mathcal{X}} \mathbf{f}_i(\mathbf{x})\mathbf{f}_j'(\mathbf{x})\,d\mathbf{x} \Big/ \int_{\mathcal{X}} d\mathbf{x} \quad .$$

The choice of a design to maximize (1) the minimum value of λ or (2) the average value of λ on contours of constant τ leads, respectively, to the following criteria:

1. Λ_1-optimality: maximize the minimum eigenvalue of $T^{-1}L$, and
2. Λ_2-optimality: maximize the trace of $T^{-1}L$.

We have recently proved two theorems that are useful in verifying the optimality of a proposed design. Both of them utilize the vector $\mathbf{g}(\mathbf{x}, \xi)$, which is defined as follows for M_{11} nonsingular:

$$\mathbf{g}(\mathbf{x}, \xi) = \mathbf{f}_2(\mathbf{x}) - M_{21}(\xi)M_{11}^{-1}(\xi)\mathbf{f}_1(\mathbf{x}) \quad .$$

Theorem 1. The following three conditions are equivalent, where H is a specified positive semidefinite matrix:

1. ξ^* maximizes $\mathrm{tr}[HL(\xi)]$.
2. $\sup_{\mathbf{x} \in \mathcal{X}} \mathbf{g}'(\mathbf{x}, \xi^*)H\mathbf{g}(\mathbf{x}, \xi^*) = \mathrm{tr}[HL(\xi^*)]$, and
3. $\mathbf{g}'(\mathbf{x}, \xi^*)H\mathbf{g}(\mathbf{x}, \xi^*)$ attains its maximum at the points of support of ξ^*.

For Λ_2-optimality, take $H = T^{-1}$ in Theorem 1.

Theorem 2. The following two conditions are sufficient for ξ^* to be Λ_1-optimal:

1. $L(\xi^*) = hT$ for some constant h, and
2. there exists a positive semidefinite matrix H such that $\mathrm{tr}[TH] = 1$ and

$$\xi^* \text{ maximizes } \mathrm{tr}[HL(\xi)] \quad . \tag{4}$$

In applications it is more useful to replace Eq. (4) by conditions (2) or (3) of Theorem 1, with $\mathrm{tr}[HL(\xi^*)] = h$.

These theorems have been applied to find Λ_1-optimal and Λ_2-optimal designs for detecting the presence of

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6. F. R. Jones and T. J. Mitchell, *Response Surface Designs for the Detection of Model Inadequacy*, UCCND-CSD-21 (November 1975).

7. A. C. Atkinson and V. V. Fedorov, "The Design of Experiments for Discriminating Between Two Rival Models," *Biometrika* 62, 57–69 (1975).

second-order polynomial terms when the assumed model is first order and the region of interest is cubic (see, for example, Eqs. (2) and (3) above). Λ_1-optimal designs in k variables have been found for $k \leq 4$, and Λ_2-optimal designs have been found for all k. These designs, which are not necessarily unique, are supported on points of the 3^k lattice (i.e., each $x_i = -1, 0$ or 1) on spheres of radius 0, 1, $\sqrt{k-1}$, and $\sqrt{k}$. When $k = 2$, for example, the Λ_1-optimal design specifies that approximately 8% of the experimental runs should be at each corner of $\mathcal{X}$ (which is the square: $-1 \leq x_i \leq 1$, $i = 1, 2$), 12% should be at the midpoint of each edge, and the remaining 20% should be at the center.

DESIGNS TO DETECT THE PRESENCE OF INTERACTIONS IN FACTORIAL EXPERIMENTS

In a previous report,[8] we described the initial results of an investigation whose purpose was to construct designs for detecting the presence of two-factor interactions in factorial experiments. The criterion used was the maximization of the trace of the lack-of-fit matrix L, which is equivalent in this setting to Λ_2-optimality as defined by Jones and Mitchell.*

As a result of this previous work, we have conjectured that in the 2^k case, where each of the k factors can take only two levels, the optimal design in the class of *foldover* designs is tr(L)-optimal. We have now obtained general rules for constructing optimal foldover designs in 4, 6, or 8 runs to augment our previous computer work, which constructed optimal foldovers in up to 16 runs for $k \leq 8$. To investigate the power of these designs under the χ^2 lack-of-fit test, a simulation study was conducted and the results tabulated. Even the smaller designs were surprisingly powerful for detecting the presence of interactions of moderate size.

Further evidence in support of our conjecture that tr(L)-optimal foldovers are globally optimal was obtained by means of a comparison with tr(L)-optimal designs from the class of balanced arrays of strength 3 and from the class of "near-foldovers," which become foldovers if a single run is changed. However, we have been unable to prove the conjecture in general.

For designs of size $N < 2k$, the tr(L)-optimal foldovers have the practical disadvantage that neither the main effects nor the two-factor interactions are individually estimable. However, these designs are easily augmented with a few additional runs to permit estimation of the main effects. We have constructed tables of such "compromise" designs. We have also demonstrated by means of an example the potential utility of the tr(L)-optimal foldovers in the first stage of a two-stage experiment in which one first tests the hypothesis that there are no two-factor interactions. The results of this test then influence the choice of the runs to be made in the second stage, which is primarily for the purpose of parameter estimation.

In the 3^k case, where each factor can take on any of three levels, we were unable to find an optimal design class comparable to the foldovers in the 2^k case. We have obtained some limited results, however, based on computer searches.

A complete search was made of designs for 3^2 experiments which have two or fewer runs at each lattice point. The form of each design and its corresponding value of tr(L) were tabulated.

Designs for 3^3 and 3^4 experiments were constructed using balanced arrays and two different sequential optimization procedures. It was apparent that tr(L)-optimal designs in 4, 6, 8, or 9 runs are found by totally confounding additional factors with factors in optimal 3^2 designs. This was not true for larger designs.

As with designs for 2^k experiments, a simulation study was performed in order to investigate the power of the χ^2 test for lack of fit when small tr(L)-optimal designs are used.

Since small tr(L)-optimal designs for 3^3 and 3^4 experiments do not provide estimability of *all* main effects, we attempted to construct designs for which main effects are estimable and values of tr(L) are relatively high. For design sizes of 18 or less, it appeared that these designs were not substantially better [in the tr(L) sense] than comparable D-optimal designs.

Designs were also developed for sequential experimentation, as in the 2^k case. These were found by augmenting (D-optimally) small Λ_2-optimal designs.

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8. "Factorial Designs for Detection of Model Inadequacies," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1976*, ORNL/CSD-13, pp. 8–9 (October 1976).

6. Statistical Testing

J. J. Beauchamp K. O. Bowman F. L. Miller, Jr. C. P. Quesenberry[1]
L. R. Shenton[2] V. R. R. Uppuluri

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

During this reporting period the work on this project has been in the area of determining the actual level of significance expected when tabled *t* values are used on samples from nonnormal distributions. Since it has not been possible to evaluate the general expression for this probability, except for a very few cases, we must rely on Monte Carlo procedures and approximations to the distribution of the *t* statistic when the parent distribution is nonnormal. (See Shenton et al.[3] and Geary[4] for two approximation methods investigated.) Corrections and extension to terms of order n^{-3} of Geary's procedure were used in the evaluation. Certain Padé approximations were also used to evaluate needed summations. As a result of this research we have found that the probabilities calculated from the approximations to the *t* distribution reasonably agree with the Monte Carlo results for sample sizes greater than or equal to 25 for $0 < \sqrt{\beta_1} < 1.5$ and $2.0 < \beta_2 < 4.5$. If the values of $\sqrt{\beta_1} > 1.0$ are omitted, the approximations give good results for sample sizes down to approximately 10. The results of this research will be summarized in an article to be published in the open literature.

TESTS FOR UNIFORMITY

The power study of tests of uniformity described in previous reports[5,6] has been extended to include four Neyman Smoothness tests, the Kuiper test, the Pearson Probability Product test, the Sherman statistic, and the Sukhatme test. In addition, most powerful test (MPT) statistics have been evaluated for three of the four families of alternative distributions[5,6] to construct power envelopes against which to compare the performance of the competing statistics. Figure 2 displays the performance of several test statistics against a symmetric triangular alternative distribution. In Fig. 2 the power of the Kolmogorov-Smirnov statistic *D*, the Cramér–von Mises statistic W^2, Pearson's χ^2 statistic with ten equal-sized subintervals χ^2_{10}, the Neyman

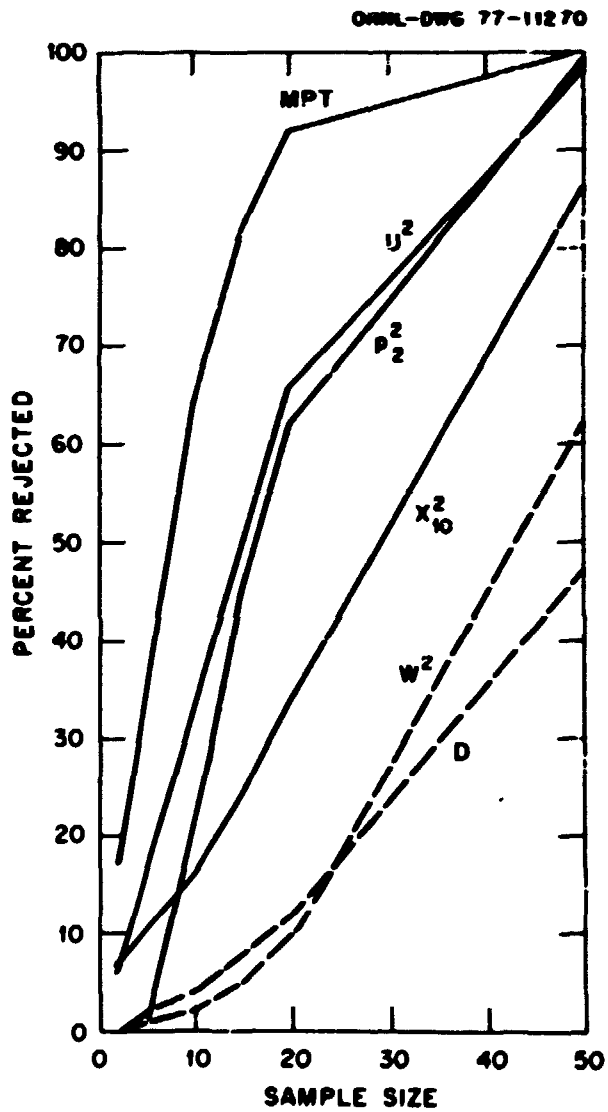

Fig. 2. Relative power of tests of uniformity for a triangular density.

1. North Carolina State University.
2. University of Georgia.
3. L. R. Shenton, K. O. Bowman, and D. Sheehan, "Sampling Moments of Moments Associated with Univariate Distributions," *J. R. Stat. Soc. B* 33, 444–57 (1971).
4. R. C. Geary, "Testing for Normality," *Biometrika* 34, 209–42 (1947).
5. C. P. Quesenberry and F. L. Miller, Jr., "Power Studies of Some Tests for Uniformity," *J. Stat. Comput. Simulation* 5, 169–91 (1977).
6. "Power Studies for Tests of Uniformity," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1974*, ORNL-4989, pp. 3–5.

Smoothness test $p_2^{\,2}$, and Watson's U^2 are compared to the power of the MPT.

LOG-LAPLACE DISTRIBUTION

A random variable $-\infty < Y < \infty$ is said to have a double exponential or a Laplace distribution if the probability density function $g_\lambda(y)$ is given by

$$g_\lambda(y) = \frac{\lambda}{2}\exp(-\lambda|y|)\,, \quad -\infty < y < \infty\,.$$

In analogy with the lognormal distribution, we let $X = \exp(Y)$ and say that X has a log-Laplace distribution. The cumulative distribution function $F_\lambda(x)$ of X is given by

$$F_\lambda(x) = \begin{cases} x^\lambda/2 & \text{for } 0 < x \leq 1\,, \\ 1-(1/2x^\lambda) & \text{for } 1 \leq x\,. \end{cases}$$

The probability density function $f_\lambda(x)$ of X is given by

$$f_\lambda(x) = \begin{cases} \lambda x^{\lambda-1}/2 & \text{for } 0 \leq x \leq 1\,, \\ \lambda/2x^{\lambda+1} & \text{for } 1 \leq x\,. \end{cases}$$

A sketch of the family of log-Laplace distribution functions shows that this family will be useful for several applications. For example, the biologists and health physicists who are concerned about the low-level effects of radiation doses are interested in the slope of the cumulative distribution function at the origin. This family for $\lambda = 1$ has a linear growth and for $\lambda = 2$ has a quadratic rise at the origin. If one has data for certain values of the dose $x_1, x_2, \ldots, x_n$ (away from the zero dose), one can use the standard statistical methodology for inference about the shape parameter λ.

The reciprocal of a log-Laplace random variable also has the same distribution. This can be seen from the probability statements

$$\begin{aligned} \text{Prob}[Z \equiv (1/X) \leq z] &= \text{Prob}[X \geq 1/z] \\ &= 1 - \text{Prob}[X \leq 1/z]\,. \end{aligned}$$

The likelihood ratio criterion of a simple hypothesis vs a simple alternative about the parameter λ depends on the product of independent identically distributed log-Laplace random variables. This can be deduced from the distribution of the sum of independent identically distributed Laplace random variables.

Proposition: The probability density function of $Y = Y_1 + \ldots + Y_n$ where each Y_i has a Laplace distribution is given by

$$\sum_{k=0}^{n-1} \binom{n+k-1}{k} \frac{1}{2^{n+k}} \frac{\lambda^{n-k}}{(n-k-1)!} e^{-\lambda|y|}|y|^{n-k-1}\,.$$

We note that this result is more general than the problem posed by Feller.[7]

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7. W. Feller, *An Introduction to Probability Theory and Its Applications*, vol. 2, p. 64, Wiley, New York, 1966.

7. Multivariate, Multipopulation Classification

M. Sobel[1] V. R. R. Uppuluri

MULTIVARIATE HYPERGEOMETRIC DISTRIBUTIONS: EXTREMAL FREQUENCIES

Suppose we have a finite population of N objects classified into $b + 1$ categories. Let each of the b categories have M objects, and the $(b + 1)$st category have $N - bM$ objects. Suppose we sample without replacement. Then after n objects are selected without replacement, we are interested in the distributional properties of the maximum (minimum) of the observed frequencies.

We study this "without replacement" problem in parallel to the "with replacement" problem. The latter problem corresponds to the distributional properties of the maximum (minimum) frequency of a sample from a multinomial distribution studied by Sobel, Uppuluri, and Frankowski.[2]

After n objects are selected without replacement, let $H^{(b)}_{M,N}(r, n)$ denote the probability that each of the b categories appears at least r times. Then we have

Proposition 1:

$$H^{(b)}_{M,N}(r, n) = H^{(b)}_{M,N}(r, n - 1) + \frac{\binom{M-1}{r-1}\binom{N-M}{n-r}}{\binom{N-1}{n-1}} H^{(b-1)}_{M,N-M}(r, n - r).$$

More generally, after n objects are selected without replacement, let $H^{(b,j)}_{M,N}(r, n)$ denote the probability that j specified categories appear r times each, and $b - j$ categories appear at least r times. Then we have the basic recursion given by

Proposition 2:

$$H^{(b,j)}_{M,N}(r, n) = \frac{n}{n - jr}\left[1 - \frac{j(M - r)}{N - n + 1}\right] H^{(b,j)}_{M,N}(r, n - 1) + \frac{(b - j)r}{n - jr} H^{(b,j+1)}_{M,N}(r, n).$$

We have the following boundary conditions:

$$H^{(b,j)}_{M,N}(r, br) = \left\{\binom{M}{r}\right\}^{b} \Big/ \binom{N}{br} \quad \text{for all } j;$$

$$H^{(b,b)}_{M,N}(r, n) = \left\{\binom{M}{r}\right\}^{b} \binom{N - bM}{n - br} \Big/ \binom{N}{n} \quad \text{for all } n.$$

These recursions and boundary conditions are useful to compute $H^{(b)}_{M,N}(r, n)$ very fast and with high accuracy. We hope to exploit the basic recursion not only for computational purposes but also to study the properties of the associated waiting-time random variables.

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1. University of California at Santa Barbara.
2. M. Sobel, V. R. R. Uppuluri, and K. Frankowski, "Dirichlet Distribution — Type 1," *Selected Tables in Mathematical Statistics, Vol. IV, IMS*, American Mathematical Society, Providence, R. I., 1977.

8. Statistical Estimation

N. R. Draper[1] T. J. Mitchell

RIDGE REGRESSION AS A MEANS OF UTILIZING "PRIOR" INFORMATION

The linear model:

$$y_i = \beta_0 + \beta_1 X_{1i} + \ldots + \beta_p X_{pi} + \epsilon_i\,, \quad i = 1, 2, \ldots, n\,, \quad (1)$$

is frequently used to "correlate" n observations of a response y with a set of p "predictors" $X_1, X_2, \ldots, X_p$ where the β's are unknown coefficients and ϵ_i is a random error. If the predictors are "scaled and centered" via the transformation

$$Z_{ji} = (X_{ji} - \bar{X}_j)/S_j^{1/2}\,,$$

where

$$\bar{X}_j = \left(\sum_{i=1}^{n} X_{ji}\right)\Big/ n \text{ and } S_j = \sum_{i=1}^{n} (X_{ji} - \bar{X}_j)^2\,,$$

then the model, Eq. (1), may be written

$$y_i = \beta_0{}' + \theta_1 Z_{1i} + \ldots + \theta_p Z_{pi} + \epsilon_i\,, \quad i = 1, 2, \ldots, n\,, \quad (2)$$

where

$$\theta_j = S_j^{1/2}\beta_j\,.$$

In practice, this transformation is a recommended first step as a technique for removing nonessential ill-conditioning.

The least-squares estimators of the unknown parameters in Eq. (2) are

$$\beta_0{}' = \bar{y} = \left(\sum_{i=1}^{n} y_i\right)\Big/ n$$

and

$$\hat{\theta} = (Z'Z)^{-1}Z'\mathbf{y}\,, \quad (3)$$

where $\mathbf{y}$ is the $n \times 1$ vector of observed responses, Z is the $n \times p$ matrix whose (i, j) element is Z_{ji}, and $\hat{\theta}$ is the $p \times 1$ vector of least-squares estimates of the θ's.

When $Z'Z$ is "ill-conditioned," that is, the ratio of its largest to its smallest eigenvalue is large, $\hat{\theta}$ can be unsatisfactory in that its elements may be much too large in magnitude or incorrect in sign. This situation frequently occurs when the data have been collected routinely from an undesigned experiment, in which the predictors are heavily correlated with one another. Hoerl and Kennard[2] proposed instead of the least-squares estimator a family of *ridge estimators* of the form

$$\hat{\theta}_k = (Z'Z + kI)^{-1}Z'\mathbf{y}\,, \quad (4)$$

where I is the $p \times p$ identity matrix and the ridge parameter k indexes the members of the family. (The estimator of $\beta_0{}'$ is $\bar{y}$ no matter what the value of k is.)

For small values of k the ridge estimator, Eq. (4), will have a lower mean-square error than the least-squares estimator, Eq. (3) (which corresponds to $k = 0$). Hoerl and Kennard recommended that the choice of k be made by examining the ridge trace, that is, the plot of the elements of $\hat{\theta}_k$ as a function of k. As k increases from 0, the estimated θ's change rapidly initially and then slowly approach 0. The lowest value of k at which the $\hat{\theta}$'s seem to stabilize at "sensible" values is the one chosen.

The Hoerl-Kennard approach, which we shall refer to as "standard" ridge regression, obviously has features that are arbitrary [the form of Eq.(4)] and subjective (the choice of k). The problem of making the ridge regression procedure more objective and more rigorous has recently attracted the attention of many researchers.

Our research in this area was motivated by (a) an uneasy feeling that the "standard" method is often inappropriate and (b) a desire to make sense out of the overwhelming array of suggestions for applying ridge regression which have recently been published.

Our basic viewpoint is that ridge regression is essentially a method by which external or prior information about the β's or about the response itself is incorporated into the basic regression setup. We consider

1. University of Wisconsin.

2. A. E. Hoerl and R. W. Kennard, "Ridge Regression: Biased Estimation for Non-orthogonal Problems," *Technometrics* 12, 55–67 (1970).

several ways of expressing these feelings, all of which lead to a general form of ridge estimator.

Conventional Bayesian approach

In this approach, which has been described by Lindley and Smith,[3] a prior distribution is placed upon the β's and the mode of the posterior distribution is taken as the estimate of β.

Restriction of β to a specified ellipsoidal region

This is essentially the approach of Hoerl and Kennard,[2] where the ellipsoidal region has the form

$$\sum_{j=1}^{p} S_{jj}\beta_j^2 < c ,$$

and the constant c depends on k. This yields the standard ridge estimator, Eq. (4). A more general approach is to consider regions of the form $(\beta - \beta^*)'T(\beta - \beta^*) < c$, where T is nonnegative definite. This generalization involves choosing T and β^* as well as k.

Formally expressing a preference for a "stable" response

Suppose R is a specified "region of interest" in the space of the original variables $\xi_1, \xi_2, \ldots, \xi_r$. [The p predictors in the model, Eq. (1), are functions of the ξ's.] We shall define the *instability* of the true response function $\eta(\xi)$ over R, assuming Eq. (1) is correct, to be the variance of $\eta(\xi)$ induced by a uniform distribution over R. (More generally, other distributions over R could be used to give different emphasis to different parts of R.) The instability is easily shown to be the quadratic form $\beta'U\beta$, where the elements of U are known. Our viewpoint is that, of all the possible values of β that are equally "good" as far as the data are concerned (i.e., that have the same residual sum of squares), we shall prefer the one that gives the most stable response over R. This leads to the estimator

$$\hat{\beta}_k = (X'X + kU)^{-1} X'y .$$

This approach also provides a natural way to extend ridge regression to models in which the predictors are nonlinear functions of the ξ's.

Augmenting the observed data with "dummy" observations

A very useful and flexible way of bringing prior feelings formally into the estimation procedure is to estimate the response, subjectively, at points that were not observed in the experiment. By including the "dummy" observations together with the actual observations in the regression equations, a ridge-type estimator is obtained. The most extensive development of this approach was given by Theil,[4] even before the first Hoerl-Kennard paper on ridge regression appeared.

All of the above approaches lead to a general ridge estimator of the form

$$\hat{\beta}_k = (X'X + kT)^{-1}(X'y + kT\beta^*) ,$$

where T is a nonnegative definite matrix and β^* is a $p \times 1$ vector. The choice of k, T, and β^* depends on the particular approach being used as well as on the nature of the prior information.

3. D. V. Lindley and A. F. M. Smith, "Bayes Estimates for the Linear Model," *J. R. Stat. Soc. B* 34, 1–41 (1972).

4. H. Theil, "On the Use of Incomplete Prior Information in Regression Analysis," *J. Am. Stat. Assoc.* 58, 401–14 (1963).

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Part B. Statistical and Mathematical Collaboration

The Mathematics and Statistics Research Department collaborates with many divisions of Oak Ridge National Laboratory and other UCC-ND and ERDA installations. Each quarter the individual statisticians and mathematicians report and document major collaborations, which are listed in Table 1 by division for fiscal year 1977. Some of these activities are summarized in this part of the report.

Table 1. Tabulation of collaborations by statisticians and mathematicians during fiscal year 1977

Division	Number
Biology, ORNL	34
Metals and Ceramics, ORNL	29
Environmental Sciences, ORNL	15
Y-12 Plant	12
Engineering Technology, ORNL	11
Analytical Chemistry, ORNL	9
Uranium Resources Evaluation Project	8
Energy, ORNL	8
Solid State, ORNL	7
Oak Ridge Gaseous Diffusion Plant	6
Health Physics, ORNL	4
Chemistry, ORNL	4
Nuclear Regulatory Commission	4
Institute for Energy Analysis	3
Computer Sciences Division	2
Comparative Animal Research Laboratory	2
Chemical Technology, ORNL	1

9. Analytical Chemistry

C. K. Bayne M. R. Guerin[1] R. W. Holmberg[1]

PREDICTION OF HISTOPATHOLOGICAL PROBABILITIES

An analysis of the series I, II, and III data from the Less Hazardous Cigarette Program was made to find sources which cause variation in the histopathological probabilities of a mouse being tumor free when smoke condensate was skin painted on the mouse. The sources of variation were limited to five chemical measurements of smoke condensate – nicotine, pH, phenols, colorimetric phenol, and benzo[a]pyrene – and the concentrations at which the smoke condensate was applied to the mice. Nine mathematical models of different combinations of these six variables were investigated to find the "best" predictor variables for the histopathological probabilities. Although the scope of this study was limited to six variables, it does show that the concentration of the skin painting condensate (C), the amount of nicotine (N), and the condensate pH make a major contribution to the variation of the histopathological probabilities.

The best prediction model had a multiple correlation coefficient of 64.1%, and the coefficients with their associated standard deviation in parentheses are

$$\hat{P} = 2.371 - 3.624 \times 10^{-2} C + 4.665 \times 10^{-4} C^2$$
$$(0.161)\ (0.388 \times 10^{-2})\ \ (0.566 \times 10^{-4})$$
$$8.846 \times 10^{-3} N \quad 1.948 \times 10^{-1} \mathrm{pH}$$
$$(1.464 \times 10^{-3})\ \ (0.233 \times 10^{-1})$$
$$+ 1.182 \times 10^{-3} N \cdot \mathrm{pH} \,. \quad (1)$$
$$(0.254 \times 10^{-3})$$

In Fig. 3, the observed values are plotted against the predicted values of the "best" model. If there were perfect agreement, the observed values would fall on the prediction line drawn from the lower left-hand corner to the upper right-hand corner. One standard deviation (S) from the predicted line is S = 0.099; the number of points that are one, two, and three standard deviations from the prediction line are given in Table 2.

1. Analytical Chemistry Division.

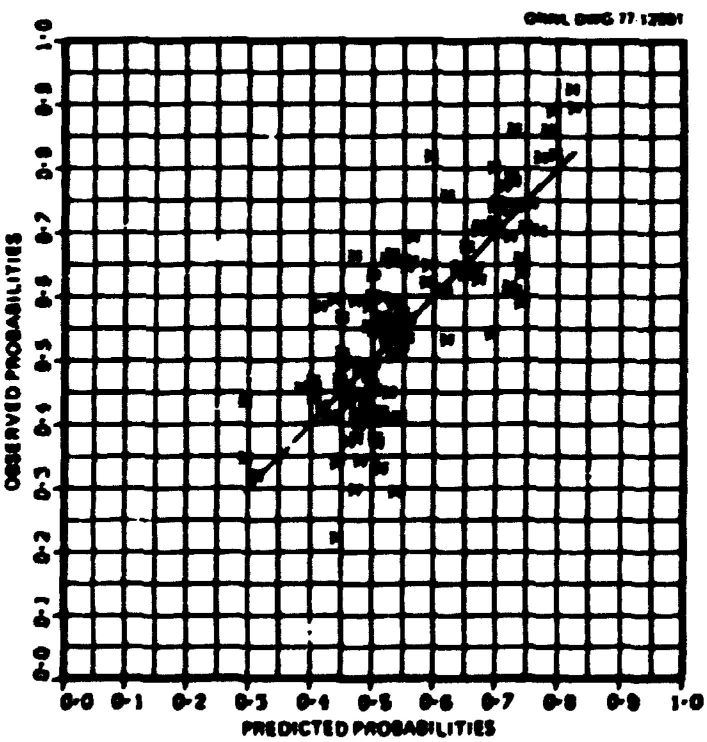

Fig. 3. Observed histopathological probabilities (*) vs predicted histopathological probabilities (line).

Table 2. Number of points one, two, and three standard deviations ($S = 0.089$) from the prediction line

Distance from the prediction line (standard deviations)	Number of points	Percent
0–1	88	67.7
1–2	36	27.7
2–3	6	4.6

CIGARETTE SMOKE PARTICLE DISTRIBUTION

The distribution of the size of cigarette smoke particles is an important factor that determines where cigarette smoke is deposited in the lungs of test animals during cigarette smoke inhalation studies. These studies are used to determine the effects of cigarette smoke on different tissues of test animals. The diameter of cigarette smoke particles can be measured from photographs of smoke particles deposited on a filter pad.

The hypothesis that the logarithms of the smoke particle diameters, $\ln(d)$, have a normal distribution can be tested by the Bowman-Shenton test,[2] which is based on the statistics $\sqrt{b_1}$ and b_2 that estimate skewness ($\sqrt{\beta_1}$) and kurtosis (β_2) respectively. Skewness is a measure of symmetry about the mean, and kurtosis is a measure of the flatness of the distribution. At the 5% significance level, the Bowman-Shenton test indicates that most of the smoke particle diameter data sets do not have a significant departure from the lognormal distribution. That is, the logarithm of the diameters can be assumed to have an approximate normal distribution.

However, for several data sets, the transformation $\ln(d)$ does have a significant departure from normality. A more general transformation, $\ln(d - \xi)$, where ξ is a constant to be determined, was formed to give nonsignificant departures from normality for all cases examined. For example, Table 3 displays the statistics of smoke particle diameters taken from eight photographs ranging from the center of a filter pad (set 1) to the outer edge (set 8). The sets are ranked from the lowest value to the highest value of the $\sqrt{b_1}$ statistic for the smoke particle diameters. The expected values of $\sqrt{b_1}$ and b_2 for data from a normal distribution are $E(\sqrt{b_1}) = 0$ and $E(b_2) = 3(n - 1)/(n + 1)$ for a sample size of n.

The logarithm of the diameters for sets 6, 8, 2, and 1 show a significant departure from a normal distribution. If the alternate transformation $\ln(d - \xi)$ is used, none of the data sets show a significant departure from normality. The scaling parameters ξ were estimated[3] from the data quantities q_α where $\text{Prob}[d \geq q_\alpha] = \alpha$, the data means, and the standard deviations. The estimates of the scaling parameter adjust each of the data sets so that the fits to the "tails" of the normal distribution were improved.

2. 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).

3. J. Aitchison and J. A. C. Brown, *The Lognormal Distribution*, Cambridge Univ. Press, New York, 1957.

Table 3. Skewness and kurtosis statistics for diameter (d), $\ln(d)$, and $\ln(d - \hat{\xi})$

Set	Sample size	Diameter (d), (μm)		$\ln(d)$		$\ln(d - \hat{\xi})$		$\hat{\xi}$
		$\sqrt{b_1}$	b_2	$\sqrt{b_1}$	b_2	$\sqrt{b_1}$	b_2	
6	194	0.38	2.84	0.60	3.40[a]	0.04	2.67	−0.53
8	181	0.55	3.21	0.62	3.23[a]	0.07	2.75	0.83
2	122	0.55	3.41	0.51	3.27[b]	0.19	2.91	0.83
1	102	0.56	3.58	0.55	3.30[b]	0.23	2.97	1.02
7	195	0.89	4.56	0.28	3.31	0.03	3.09	0.17
5	156	0.91	3.89	0.12	3.15	0.03	3.20	0.07
4	154	0.94	4.14	0.20	3.02	0.05	2.85	0.11
3	167	1.73	8.80	0.22	3.11	0.01	3.02	0.07
Total	1271	0.86	4.71	0.35	3.23[a]	0.07	2.98	−0.25

[a]Significant at the 5% significance level.
[b]Significant at the 10% significance level.

10. Biological Research

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PROTEIN BREAKDOWN IN A CELL

A mathematical model of the process of protein breakdown in a cell was constructed to test the hypothesis that the rates of breakdown in cell cyto-plasm and cell nucleus are significantly different.

It was assumed that the nucleus and cytoplasm exchange protein at competing rates and that the protein in each decays at a specific rate. The resulting initial value problem:

$$\dot{C}_c = -k_1 C_c + k_2 C_n - \gamma_1 C_c\,, \quad C_c(0) = C_0\,,$$

$$\dot{C}_n = -k_2 C_n + k_1 C_c - \gamma_2 C_n\,, \quad C_n(0) = 0\,,$$

where k_1 and k_2 are the exchange rates and γ_1 and γ_2 are the decay rates, was solved explicitly using the 2×2 matrix exponential. The solution is

$$C_c(t) = [C_0/(\lambda_1 - \lambda_2)][A \exp(\lambda_1 t) - B \exp(\lambda_2 t)]\,,$$

$$C_n(t) = [C_0/(\lambda_1 - \lambda_2)]\{(AB/k_2)[\exp(\lambda_1 t) - \exp(\lambda_2 t)]\}\,,$$

where $A = \lambda_1 + k_2 + \gamma_2$; $B = \lambda_2 + k_2 + \gamma_2$; and λ_1, λ_2 are the real, distinct, negative eigenvalues of the coefficient matrix:

$$\begin{pmatrix} -k_1 - \gamma_1 & k_2 \\ k_1 & -k_2 - \gamma_2 \end{pmatrix}$$

with $\lambda_1 > \lambda_2$.

As expected, the model gave the protein concentration in both nucleus and cytoplasm as a sum of decaying exponentials. However, the experimentally observed quantity, total protein concentration, appeared to be adequately represented by a single decaying exponential. The expression for total protein concentration given by our model was

$$C_T(t) = \alpha[\beta \exp(\lambda_1 t) - \delta \exp(\lambda_2 t)]\,,$$

where $\alpha = C_0/[(\lambda_1 - \lambda_2)k_2]$, $\beta = A(B - k_2)$, and $\delta = (A - k_2)B$. The possibilities which permit C_T to be representable as a single decaying exponential are (1) $\gamma_1 = \gamma_2$, that is, the decay in nucleus and cytoplasm is at the same rate (in this case $A = k_2$ and $\delta = 0$); and (2) the time over which experimental data were taken was too short to observe the second exponential. There appears to be no fortuitous combination of parameters which result in $C_T \sim e^{-\lambda t}$ (except the trivial case $k_1 = 0$ in which no exchange occurs).

RADIATION-INDUCED CHROMOSOME ABERRATIONS

Statistical methods were used to analyze the frequency of chromosome aberrations in mouse oocytes exposed to acute or chronic radiation.[4] A model was developed to account for the fewer aberrations resulting from exposure to fractionated doses of acute radiation relative to the corresponding total dose in a single exposure. The method of Birnbaum[5] was used and extended to perform statistical tests of significance. Linear and quadratic approximations to models derived from one- and two-hit target theory associated with chronic and acute exposures, respectively, were used. Linear and quadratic terms were fitted simultaneously to the frequency of aberrations by the method of weighted least squares. That is, the intercept and the coefficient of the dose variable were estimated by utilizing the chronic and the single acute data, while the coefficient of the dose-squared variable was estimated from the acute data only, by minimizing the weighted

1. Biology Division.
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4. "Fractionation Effects on X-Ray Induced Chromosome Aberrations in Mouse Oocytes," *Biol Div. Ann. Prog. Rep. June 30, 1976* ORNL-5195, pp. 57–58 (November 1976).

5. A. Birnbaum, "Statistical Methods for Poisson Processes and Exponential Populations," *J. Am. Stat. Assoc.* 49, 254–66 (1954).

sum of squares of deviations from the model for all observed aberration frequencies.

For the fractionated acute doses the following equation is proposed.

$$Y = N[a + bD + c(d_1^2 + d_2^2) + 2c[1 - f(t)]d_1d_2] + e\ ,$$

where Y is the number of aberrations observed in N cells, d_1 and d_2 are the fractionated doses totaling D, e is the observational error, t is the time between exposures, and $f(t)$ is a function of time such that $f(0) = 0$ and $f(\infty) = 1$. When $f(t)$ is defined to be zero or one, for all t, two models termed interactive and additive, respectively, are obtained. The equation for the interactive model is

$$Y = N(a + bD + cD^2) + e$$

and for the additive model is

$$Y = N[a + bD + c(d_1^2 + d_2^2)] + e\ .$$

Since $c > 0$ and $D^2 > d_1^2 + d_2^2$, the additive model produces fewer aberrations.

Tests of significance comparing the two models, for four values of t, using Birnbaum's method, have been made on data from experiments in the Biology Division, ORNL. These statistical tests were made by substituting observed aberration frequencies for expected frequencies at single acute doses. To use Birnbaum's method, the proportion of aberrations in the fractionated dose group,

$$p = Y_f/(Y_f + Y_s)\ ,$$

is compared with the expected proportion, π, under each model, where Y_f and Y_s are the observed number of aberrations in the fractionated and single dose groups respectively.

The expected proportion for the interactive model is

$$\pi = N_f/(N_f + N_s)\ .$$

The test is accomplished by computing the probability of obtaining a value of p, or one more extreme, in random sampling from a binomial probability distribution with parameters π and $N = N_f + N_s$.

The expected proportion for the additive model when $d_1 = d_2$ is

$$\pi = 2N_f/(2N_f + N_s)\ .$$

When $d_1 \neq d_2$, in the additive model,

$$p = Y_f/(Y_f + Y_{s1} + Y_{s2})\ ,$$

where Y_{s1} and Y_{s2} are the number of aberrations observed in N_{s1} and N_{s2} cells in single acute dose groups corresponding to the fractionated doses d_1 and d_2 respectively. In this case, π is a function of N_f, N_{s1}, N_{s2} and the expected values of Y_f, Y_{s1}, and Y_{s2}. Since the expected values are unknown, we propose an approximation for π using N_f and the harmonic mean H, of N_{s1} and N_{s2}, namely $\pi \cong N_f/(N_f + H)$. Further development of the model using exponential terms in the function $f(t)$ is in progress.

RADIATION-INDUCED MUTATIONS AS A FUNCTION OF DOSE AND DOSE RATE

Two models have been proposed to relate the specific locus mutation frequency in irradiated mice to dose (D) and dose rate (λ). In both models, the initial lesion is caused by a single ionization track and may be repaired before it is manifested as a mutation. The models are described as follows:

Model I

This model takes the form

$$y = k_1D(1 - p_1p_2) + p_0\ , \qquad (1)$$

where

y = mutation frequency at dose D,

k_1 = lesions per unit dose,

p_1 = maximum probability of repair, $0 \leq p_1 \leq 1$,

p_2 = efficiency of repair, $0 \leq p_2 \leq 1$,

p_0 = mutation frequency for the controls.

When the efficiency of repair $p_2 = 1$, the function becomes

$$y = k_1D(1 - p_1) + p_0\ ; \qquad (2)$$

that is, it is a straight line with slope $k_1(1 - p_1)$. When $p_2 = 0$, we have

$$y = k_1D + p_0\ . \qquad (3)$$

The effect of dose and dose rate on the repair system expresses itself through the parameter p_2. Specifically, we assume that p_2 is given by the logistic function

$$p_2(D, \lambda) = [1 + \exp(a + b \ln D + c \ln \lambda)]^{-1} . \qquad (4)$$

There are no biological grounds for this choice: it is simply a flexible curve that for $b > 0$ and $c > 0$, decreases from 1 to 0 as the dose or dose-rate increases. This equation may conveniently be modified if the dose has been administered in F equal fractions. In this case, it can be shown that one needs only to add the term $-b \ln F$ to the argument of the exponential function in Eq. (4).

At a given dose rate the mutation frequency y as given by Eqs. (1) and (4) is tangent to Eq. (2) at $D = 0$. Its slope increases initially with D and then decreases as y approaches Eq. (3) asymptotically. Within the experimental range of doses and dose rates, y is closely approximated by the straight line, Eq. (3), at high doses and dose rates and by the straight line, Eq. (2), at low dose rates.

Model II

Lesions are assumed to occur randomly, with the rate proportional to λ. That is, in a given interval of time Δt, the expected number of lesions is $k_1 \lambda \Delta t$. If the repair system is functioning, some proportion p_1 of these lesions is repaired, so the expected number of unrepaired lesions in the interval Δt is $(1 - p_1)k_1 \lambda \Delta t$. We further assume that the repair system can fail and that its time until failure has an exponential distribution with mean μ, which may depend on the conditions of the irradiation, particularly dose rate. After the repair system has failed, all lesions in its jurisdiction go unrepaired and become mutations. Under the above assumptions, the expected mutation frequency is given by

$$y = p_0 + k_1 D - \frac{k_1 \lambda p_1}{\mu} (1 - e^{-\mu D/\lambda}) , \qquad (5)$$

where p_0 is the expected mutation frequency in the controls. In fitting the model to data, we have assumed further that

$$\mu = k_2 \lambda^{\alpha} ; \qquad (6)$$

that is, the hazard for the repair system is proportional to some power of the dose rate.

Both Model I and Model II have been fitted to Russell's data[6,7] on mouse spermatozonia (14 - 17 data points) and oocytes (9 data points). Fitting was done by weighted least squares, where the weights are based on the assumption that the number of mutations at each dose and dose rate has a Poisson distribution. Both models fit well, particularly to the oocyte data.

Another model, based on the assumption that at high doses and dose rates the lesions are primarily two-track events, has been proposed by Abrahamson and Wolff.[8] The goodness of fit of their model, which is applicable to high and low (but not intermediate) dose rates was used by them to argue for the validity of their assumptions. Since Models I and II fit the data even better, the two-track hypothesis is not necessary to explain the behavior of the observed mutation frequencies as a function of dose and dose rate.

LENS OPACITY STUDIES

During this period our effort has been directed toward the application of the dose-response relationship to estimate the Relative Biological Effectiveness (RBE), summarized in earlier reports.[9] Using the estimated dose-response relationship, specific comparisons were made among different types of radiation (e.g., neutron, gamma, and x-ray) and between the two methods of delivering this radiation (acute and chronic). The following are the comparisons made from these data: (1) acute and chronic gamma radiation results; (2) acute and chronic neutron radiation results; and (3) x-ray and acute gamma radiation results. The acute radiation was found to be more effective than the chronic radiation with the differences decreasing with increasing dose. Estimations of the RBE of fission neutrons with respect to gamma rays were obtained for both acute and chronic radiation. While for the acute radiation, we found the RBE to be a decreasing function of dose, the chronic radiation data resulted in an increasing RBE as a function of dose. However, the estimated variance of the RBE values were larger than the RBE values over much of the dose range of interest because of the small

6. W. L. Russell, "Studies in Mammalian Radiation Genetics," *Nucleonics* 23, 53 - 56, 62 (1965).

7. W. L. Russell, personal communication.

8. S. Abrahamson and S. Wolff, "Re-analysis of Radiation-Induced Specific Locus Mutations in the Mouse," *Nature* 264, 715 - 19 (1976).

9. "Lens Opacity Study," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCCND/CSD-18, p. 32 (October 1975); and *Math. Stat. Res. Dep. Prog. Rep. June 30, 1976*, ORNL/CSD-13, p. 28 (October 1976).

sample size in the chronic gamma treatment group. Therefore, the practical significance of this result is doubtful. Additional work is in progress to find an explanation of this anomaly. In addition, we have been able to demonstrate a significant age-response relationship in the control animals which does not appear to exist among the treated animals, especially at the high doses.

An additional experiment, which was carried out in the same manner as the above experiment, has been conducted to examine the dosimetric characteristics of a partial-body neutron shield for mouse irradiations. The present types of dosimeters available for neutron measurements are generally too large for use in many experiments. Therefore, the mouse lens has been examined as a potential biological dosimeter both to substantiate present information and to check smaller areas where bulky dosimeters were ineffective, for example, an area 0.5 cm from the edge of the exposure port. In this experiment, only neutron radiation was used, but the mice were placed at different distances above and below the edges of the exposure port in order to determine if these changes in position were significant. Two different runs were made for the irradiated animals, so it was possible to test for a significant run effect.

There was interest in potential future comparisons of the results of this experiment with the experiment discussed previously in this article. Therefore, the same expression was used to describe the time percent-lens-opacity or time-response relation for each cage of animals. No significant difference could be detected in the results from one run to another. The response for the irradiated animals was significantly greater than that for the control group of animals. In addition, when two groups of animals were irradiated at 19.3 and 26.3 rads, respectively, at the same position from the edge of the exposure port, a significant dose effect was observed. The question of a significant position effect has not been conclusive because of the confounding of the dose and position factors. Additional analysis will be needed to unravel this question.

DESIGN OF A SERIAL SACRIFICE EXPERIMENT

Statistical methods were used to plan a long-term experiment on factors causing cardiovascular disease. The determination of the number of animals, the choice of experimental design for the combinations of factors, and the determination of the number of additional animals required to ensure that a given number would be available for each period of a serial sacrifice schedule were important to the plan of the experiment.

Observational and epidemiological studies have indicated that the level of lipids and the level of several elements in the diet are associated with cardiovascular disease. A controlled experiment on the effect of lipid level and the effects of four elements singly and in combination will be performed using pigeons, because their metabolism closely resembles that of humans.

The number of pigeons required to have a reasonable chance of detecting real differences in the incidence of cardiovascular disease due to different levels of the factors was determined by standard statistical methods. That number plus the additional number of animals needed to allow for natural mortality through the several years period was required before the breeding program could be initiated.

Some animals will be killed and examined pathologically during each period to investigate basic mechanisms of the development of the disease. The following formula was derived to estimate the number (N) of pigeons needed at the beginning of the experiment in order to have K animals available for sacrifice in each of I periods.

$$N = \frac{K\sum_{i=1}^{I}\left(\prod_{j=0}^{i} q_j\right)}{\prod_{i=1}^{I} q_i} .$$

where $q_0 = 1$ and q_i, for $i > 1$, is the probability that a pigeon alive at the beginning of the ith period will survive to the end of that period. Information from previous experiments on the mortality frequency distributions, for high and low lipid levels, was used to estimate the q's.

The five factors, each at two levels, result in 32 diet combinations. Since K must be less than 32, the sacrifice schedule was designed using experimental designs to minimize the confounding of the factor effects with time effects, such as aging. Fractional factorial designs which do not confound time effects with individual factor effects, two-factor interactions, nor other important interactions were proposed. With these designs it is also possible to perform tentative statistical analyses as the experiment progresses.

SEQUENTIAL TESTS FOR MUTAGENICITY OF CHEMICALS

The development of efficient experimental procedures to detect mutagenic chemicals by testing for heritable translocations is continuing.[10] In order to test chemicals for mutagenicity they are subjected to a subset of a battery of tests. One such test is the heritable translocation test, which is based, in part, on the fertility of the offspring of treated animals. Statistical methods are being used to improve a sequential test to minimize the errors of misclassification of chemicals and the costs of testing. These tests are particularly expensive, because a large number of treated animals are required for the detection of the relatively small increases in mutation rates caused by chemicals which must be used in concentrations below their toxic levels.

The two errors to be minimized are the probabilities of classifying an animal with reduced fertility as a fertile animal and of classifying a fertile animal as one with reduced fertility. Our currently recommended procedures are based on both empirical distributions and the binomial distribution. The binomial distribution fits experimental data well for normal animals but does not fit well for animals with reduced fertility. The latter distributions exhibit extra-binomial variation, and better approximating distributions will be used, possibly compound distributions.

Another statistical problem is the determination of the number of animals needed in treated and control groups, each of which is to be tested by the sequential procedure, to screen each chemical. The spontaneous mutation rate is approximately 0.001, and it is necessary to have experiments which are sensitive enough to have a high probability (≥ 0.95) of detecting induced mutation rates in the range 0.002 to 0.1, with greatest interest in the range 0.002 to 0.01.

INHALATION CARCINOGENESIS

A large study of the combined effects of two carcinogens (BaP and BaP + Fe_2O_3) and three gases (HCHO, C_3H_4O, and NO_2) on mortality and disease incidence in hamsters has been completed. The treatment groups are shown in Table 4. When there are several groups in a particular "cell" in the table, each represents a different dose or mode of treatment, except for the BaP controls (1B1, 1B4, 1B5) and room controls (101, 102, 103).

Table 4. Classification of experimental groups according to carcinogen and gas

Each group represents a chamber of 88 animals, except for those marked with an asterisk, in which there were 44 animals

Carcinogen	Gas: None	HCHO	C_3H_4O	NO_2
None	101*	1H1		1N1
	102*	1H9		
	103*			
BaP	1B1*	1H7	1A3	1N2
	1B4*	1H8		1N3
	1B5*	1F1		1N4
		1F2		1N7
BaP and Fe_2O_3	2B1	2H1	2A1	2N1
		2H2		
		2H3		

This was a survival experiment in which the animals were examined at death for the presence of various diseases, particularly tumors of the respiratory tract. A comprehensive statistical analysis of these data has begun, based on the following outline.

I. Survival Analysis
   A. Plots of Survival Curves
   B. Mean Age at Death
   C. Median Age at Death
II. Analysis of Tumor Frequencies
   A. Number of Tumors per Animal
   B. Number of Animals with Tumor(s)
III. Cross-Classification Tables

In addition to presenting the summary statistics (means and standard errors) associated with each end point or response of interest, we have made comparisons, using Student's *t*-test, of the various treated groups with the appropriate controls. We were presented with some difficulty in these comparisons by the extra variation among cages and among chambers. We partially avoided this difficulty by taking the experimental unit to be the cage, where each cage housed four hamsters. For example, the average number of tumors per animal within a given cage was defined as a response for that cage. The same approach was used in the analysis of the number of tumor-bearing animals. However, we have not been entirely successful in

10. "Sequential Tests for Mutagenic Effects," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCCND/CSD-18, p. 30 (October 1975).

dealing with the extra variation among chambers, primarily because there was hardly any true replication with respect to chambers. We are now in the process of determining the extent to which the variation among chambers affects the statistical significance of our results.

Separate analyses are being made for tumors at four sites of interest within the respiratory tract as well as the entire respiratory tract. Four different types of respiratory tract tumors (carcinoma, papilloma, adenoma, and sarcoma) are also being analyzed separately.

So far, the analysis for tumor rates has involved no correction for differences in mortality patterns among the groups. These corrections will be made using methods described in previous reports.[11,12]

The cross-classification tables that have been compiled are mainly for purposes of reference. Some of them tabulate the association between tumor response and group and between tumor response and age at death, for various definitions of tumor response. Others show the association between pairs of sites with respect to tumor response, and also the association between pairs of tumor types, for example, carcinoma and adenoma.

DECONVOLUTION OF FLUORESCENCE DECAY DATA

The convolution integral, Eq. (1), arises naturally whenever one studies the time-dependent response of a linear system,

$$\begin{aligned} p(t) &= \int_0^t dt'\, q(t')f(t - t') \\ &= \int_0^t dt'\, q(t - t')f(t') . \end{aligned} \quad (1)$$

In Eq. (1) the function $p(t)$ is the actual response of the system to the input $q(t)$. The function $f(t)$ is the "delta function response" of the system, that is, it is the response of the system to an input equal to a Dirac delta function occurring at time zero. The function $f(t)$ contains all the interesting physics of the system without any distortion due to details of the input function.

The usual problem in practice is to make use of Eq. (1) and measurements of the functions $p(t)$ and $q(t)$ to determine essential physical properties of a linear system. Here we are concerned with the fluorescent decay of molecular systems, where $p(t)$ and $q(t)$ have been measured using single photon counting methods. Thus the data from measurements of these functions will be assumed to be in the form of a series of positive integers $\{p_i\}$ and $\{q_i\}$, $i = 1, 2, ..., n$, representing numbers of photons in sequential time intervals (channels).

Previously,[13] we reported a method for deconvoluting fluorescence decay data by expressing Eq. (1) in terms of the discrete approximation

$$P_i = \sum_{j=1}^{i} F_j q_{i-j+1} , \quad i = 1, 2, ..., n , \quad (2)$$

and minimizing the weighted residual sum of squares,

$$S(\mathbf{F}) = \sum_{i=1}^{n} \frac{1}{p_i} (p_i - P_i)^2 , \quad (3)$$

subject to linear constraints on the solution $\mathbf{F} = (F_1, F_2, ..., F_n)$. A fast quadratic programming algorithm was written to solve for $\mathbf{F}$.

We have now incorporated into our program a method for constructing a *likelihood interval* for each F_i. The right and left end points, r_i and l_i, of this interval are solutions to

$$S_i(x) - S(\hat{\mathbf{F}}) = 3.84 , \quad (4)$$

where $S_i(x)$ is the minimum of $S(\mathbf{F})$ subject to $F_i = x$ and the given linear constraints on $\mathbf{F}$ and where $\hat{\mathbf{F}}$ is the solution to the minimization problem, Eq. (3). Both r_i and l_i indicate how far F_i can be moved from its optimum ($\hat{F}_i$) before the residual sum of squares is increased by the amount 3.84. An increase of this magnitude represents approximately a 47-fold *decrease* in likelihood. The reason for the choice of 3.84 is that in the unconstrained least-squares problem, the likelihood interval gives exactly the 95% confidence limits for F_i. For the constrained problem that we are dealing with here, the probability that this likelihood interval covers the true value of F_i is not known; however, some

11. "Cocarcinogenic Effects of Smog and Iron Oxide," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1974*, ORNL-4989, p. 22 (December 1974).

12. "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).

13. "Deconvolution of Fluorescence Decay Data," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1974*, ORNL-4989, pp. 8–9 (December 1974).

simulations we have done indicate that its interpretation as a 95% confidence interval is not misleading.

To solve Eq. (4) requires the approximation of the function $S_i(x)$, which does not have a known closed-form solution. We have used a quartic spline interpolation for this purpose.

This procedure is now incorporated into our deconvolution program and has been applied in several test cases using real data.

SURVIVAL ANALYSIS OF MICE TREATED WITH X RAYS AND MMS

A 2 X 3 factorial experiment was conducted to examine the effects on mice of x rays and the chemical methyl methanesulfonate (MMS) (administered in drinking water). The experimental groups are shown in Table 5, with the median age at death for each group shown in parentheses. These data include the results of two separate experiments; hence the presence of two groups in some of the treatment "cells." The first was a survival study in which the mice were left until death, and the second was a serial sacrifice study in which a predetermined number of mice were killed at regular intervals and examined for the presence of various diseases.

Table 5. Experimental groups

Each group includes 100–150 mice. Corrected median ages at death are given in parentheses.

Age at which MMS treatment began[a] (weeks)	X ray	
	0 R	300 R[b]
0	2B(825)	2A(700)
	2D(803)	2C(712)
4	1A(826)	1B(730)
	1F(804)	1E(766)
12	1C(870)	1D(708)

[a]MMS was given at 20 mg kg^{-1} day^{-1} in the drinking water.

[b]X-ray exposure was at six weeks.

The medians shown in Table 5 were each obtained from a Kaplan-Meier plot,[14] which corrects the empirical time-to-death distribution for accidental deaths and deaths due to extraneous causes, such as the outbreak of pneumonia which affected several of the groups.

Comparisons among the corrected survival curves were made using the odds-ratio analysis described in a previous report,[12] where the "disease of interest" is defined to be death from all causes other than accident, sacrifice, or pneumonia. The initial phase of the analysis compared the survival curve of each member of a pair (e.g., 2B and 2D) within a treatment cell. There were no significant differences, with the possible exception of Groups 1B and 1E, where the odds-ratio appeared to change significantly with time, so the decision was made to pool each such pair of groups.

The next phase of the analysis consisted of comparing each MMS treatment with the appropriate control to evaluate the effect of MMS. All four of these comparisons indicated that the risk of mortality (in terms of the odds-ratio) associated with each MMS group was greater than that of its control. In three cases, however, there was notable variation in the relative risk with time. This means that the effect of MMS may not be so simple as to be conveniently expressed in terms of a single relative risk statistic. We are currently investigating this point.

We have also begun an examination of the interaction between x ray and MMS as it affects survival, again using the odds-ratio method of assessing relative risks. We will then apply essentially the same techniques to other end points, such as the prevalence of specific diseases.

14. E. L. Kaplan and P. Meier, "Nonparametric Estimation from Incomplete Observations," *J. Am. Stat. Assoc.* 53, 457–81 (1958).

11. Chemistry and Physics Research

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CALCULATION OF THE DENSITY OF STATES OF ALLOYS

A basic step in the calculation of the density of states of an alloy is the computation of the following quantity:

$$\mathrm{Im}[(zI - A)^{-1}_{rs}] \ . \qquad (1)$$

where Im denotes the imaginary part of a complex number, z is a complex number equal to $\sigma + i\epsilon$ for arbitrary real numbers σ and ϵ, A is an $n \times n$ large, sparse, symmetric matrix, and $1 \leq r, s \leq n$. An algorithm, coded as subroutine ITLANC, has been developed to compute this quantity for an arbitrary number of values of σ.

The basis of this algorithm is the method of Lanczos. Defining $v_0 \equiv 0$ and given v_1, Lanczos' iterative method[2] can be described by

$$\beta_{j+1} v_{j+1} = A v_j - \alpha_j v_j - \beta_j v_{j-1}$$

with $\alpha_j = v_j^T A v_j$ and $\beta_{j+1} \geq 0$ chosen so that $\|v_{j+1}\| = 1$. After k iterations, we have

$$A V_k = V_k T_k + \beta_{k+1} v_{k+1} e_k^T \ . \qquad (2)$$

where V_k is an $n \times k$ matrix whose jth column is v_j, T_k is a $k \times k$ symmetric tridiagonal matrix whose (j, j) element is α_j and $(j, j+1)$ element is β_{j+1}, and e_k is the kth column of the $k \times k$ identity matrix. If we subtract σV_k from both sides of Eq. (2), we have

$$(A - \sigma I) V_k = V_k (T_k - \sigma I) + \beta_{k+1} v_{k+1} e_k^T \ .$$

Thus, performing the Lanczos iteration on a matrix obtained by subtracting an arbitrary scalar σ from the diagonals of A produces the same identical v_j's and β_j's with the α_j's shifted by the quantity σ.

Let $v_1 = e_s$, the sth column of the $n \times n$ identity matrix; partition V_k as follows:

$$V_k = \begin{bmatrix} \bar{U}_k \\ u_k^T \\ U_k \end{bmatrix}$$

where $\bar{U}_k$ is the indicated $(r-1) \times k$ submatrix, u_k^T is the rth row, and U_k is the indicated $(n-r) \times k$ submatrix; and let y_k be the solution to

$$(T_k - \sigma I) y_k = \bar{e}_1 \ ;$$

then, $u_k^T y_k \to e_r^T (A - \sigma I)^{-1} e_s$ as $k \to \infty$. The quantity $e_r^T (A - \sigma I)^{-1} e_s$ is the (r, s) element of the inverse of $A - \sigma I$.

Subroutine ITLANC has the capability of performing additional Lanczos iterations to obtain the desired accuracy of Eq. (1) as σ, the real part of z, varies over the values of interest. ITLANC also may detect convergence before all the available iterations have been used.

DISORDERED SYSTEMS WITH SHORT-RANGE ORDER

In previous work,[3] we have detailed a method for treating disordered systems described by independent random variables. However, many physical systems, including alloys and amorphous solids, possess short-range order, and therefore, their mathematical description requires dependent random variables. We have shown how to extend our previous work to this more general situation. In essence, given any collection of discrete random variables, we can construct an equivalent operator-valued weak distribution. Thus in order to compute configuration averages, we can define an appropriate nonrandom Hamiltonian defined on a larger space and use conventional approximation techniques.

Model calculations are shown in Fig. 4 for a one-dimensional binary alloy, whose configurations are

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1. Solid State Division.

2. C. C. Paige and M. A. Saunders, "Solution of Sparse Indefinite Systems of Linear Equations," *SIAM J. Numer. Anal.* 12, 617–29 (1975).

3. T. Kaplan and L. J. Gray, "Elementary Excitations in Random Substitutional Alloys," *Phys. Rev. B* 14(8), 3462–70 (1976).

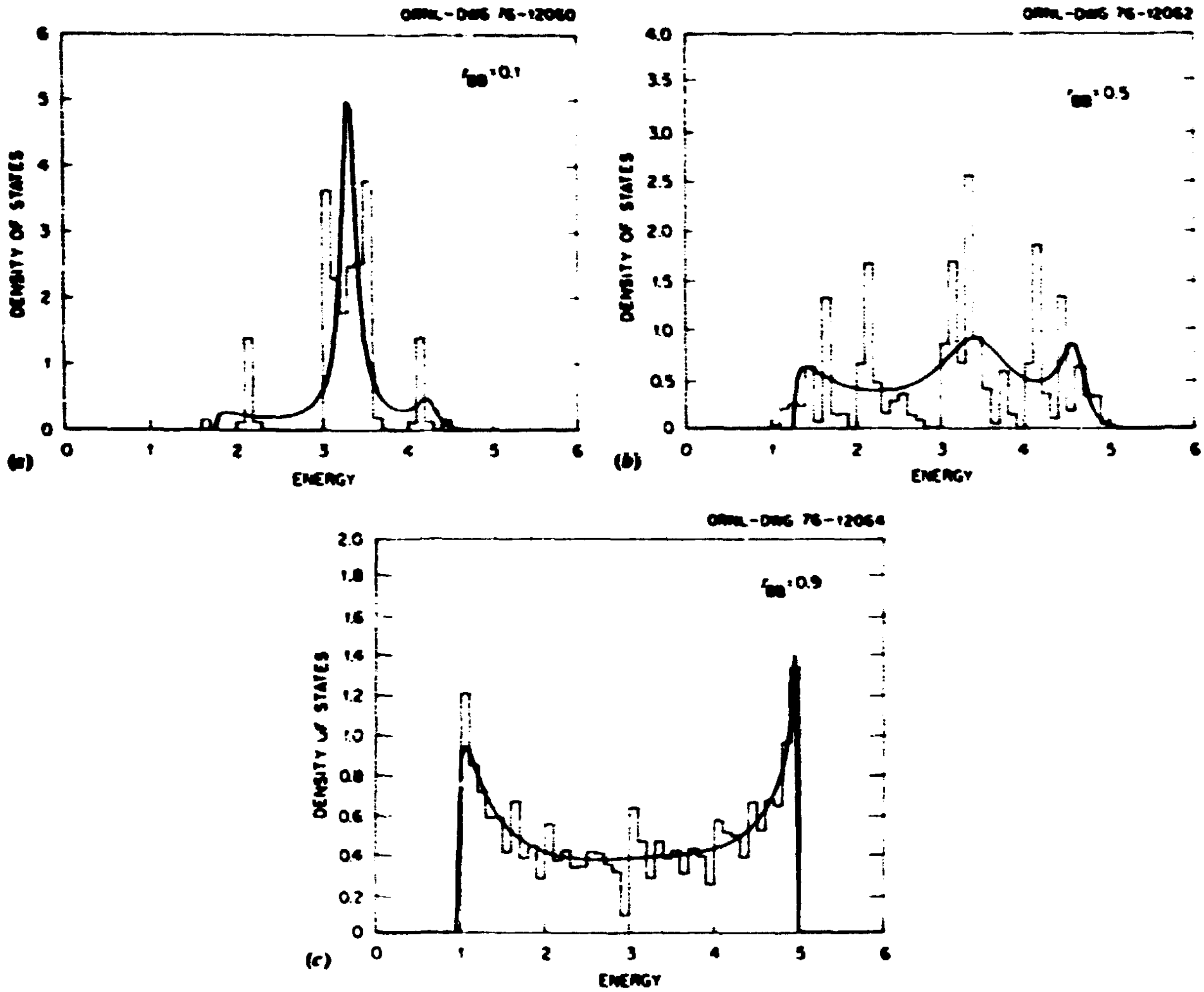

Fig. 4. Comparison of the density of states calculated in the ASF with a recursion level of 8 (smooth curve) with the corresponding exact calculation (histogram) for a 100,000 atom chain. (*a*) f_{BB} = 0.1; (*b*) f_{BB} = 0.5; (*c*) f_{BB} = 0.9.

determined by a Markov process. The parameter f_{BB} is the probability of finding a B atom at a site given that there is a B atom immediately to the left.

SPECTRAL DENSITIES OF DISORDERED SYSTEMS

In many experiments on disordered solids it is the spectral densities which must be calculated in order to properly understand the result. For example, in neutron scattering experiments the inelastic cross section is related to the spectral density of a displacement-displacement Green's function.

Using the Augmented Space Formalism (ASF),[3,4] we can express the spectral density of a disordered system as a matrix element of a new nonrandom operator. The ASF is particularly well suited for this purpose, since it automatically includes the translational invariance which results from averaging over all configurations of the disordered system. Standard numerical approximation techniques can be used to calculate the matrix elements.

Model calculations have been completed for the spectral density of a one-particle propagator of a three-dimensional simple cubic A-B alloy. Calculations for an actual physical system are in progress.

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4. T. Kaplan and L. J. Gray, "Elementary Excitations in Disordered Systems with Short Range Order," *Phys. Rev. B* 15(6), 3260 66 (1976).

12. Energy Research

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SENSITIVITY OF THE ECONOMY TO ENERGY DECISIONS

In a previous report,[3] a relationship between the economy and energy decisions was described by the sensitivity of an eigenvalue in a generalized eigenvalue problem. The first-order perturbation of the eigenvalue was given in terms of its left and right eigenvectors and the eigenvalue itself. This project has been completed by the development of algorithms for determining these parameters.

The combination shift QZ algorithm[4] should be used to determine the eigenvalue of the relevant generalized eigenvalue problem. Then, an inverse iteration algorithm should be used to determine the left and right eigenvectors for the eigenvalue of interest. The inverse iteration algorithm used for this project, coded as subroutine GINVIT, can compute either the left or right eigenvector using the eigenvalue and the input matrices; GINVIT returns the factorization and pivot information for possible later use. Also, GINVIT can compute either the left or right eigenvector from this returned information in an extremely efficient manner.

FIELD DEMONSTRATION OF COMMUNICATION SYSTEMS FOR DISTRIBUTION AUTOMATION

The Electric Power Research Institute (EPRI) and ERDA have jointly planned to conduct a field demonstration of communication systems for distribution automation. The purpose of the demonstration is to illustrate the feasibility of various communication methods to remotely control and monitor aspects of an electric utility under operating conditions.

Some of the advantages to be derived from an automated distribution system are (1) load management, (2) time-of-day metering, (3) status monitoring, (4) fault detection and isolation, (5) distribution network switching, (6) equipment control, (7) remote meter reading, and (8) data for load research.

Four manufacturer/utility teams are participating in the demonstration; the teams are as follows: American Science and Engineering/San Diego Gas and Electric, Compu-Guard/Carolina Power and Light, Westinghouse/Detroit Edison, and Darco/Omaha Public Power District. Each team will install equipment at approximately 750 customer sites to demonstrate various aspects of their communication systems. The sites will be distributed among residential, multifamily, commercial, and industrial customers and between underground and overhead circuits for both urban and suburban areas. The demonstration is planned to continue for at least one year.

The role of the Mathematics and Statistics Research Department (MSRD) in the demonstration was to (1) review the manufacturer's proposals in terms of site selection, experimental design, and data analysis; (2) devise a form to indicate the type of experimental variables and test results that should be reported; and (3) suggest methods of analyzing the data to detect factors that influence the error rates in the communication system or the reliability of the equipment.

The review of the manufacturer's proposals indicated that three areas were not adequately addressed by the terms: (1) the method of selecting the customers for the demonstration, (2) the criteria that would be used to judge a successful demonstration, and (3) the statistical methodology to be used to analyze the data generated by the demonstration.

Since little attention had been paid to the manner in which the data should be collected, a list of experimental parameters was compiled as a general guide for the teams to use to gather information for the data analyses. This list was partitioned into five parts: (1) sample point history; (2) error rate in general; (3) error rate per customer; (4) meter reading data; and (5) equipment reliability data.

To avoid the pitfall of not answering the original objectives of the project, the teams were encouraged to set up similar objectives and data collection and analysis plans as soon as possible. To initiate this planning, a data analysis methodology was suggested which could be used by the teams as a common basis for their analyses of the data arising from the field demonstration.

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1. Energy Division.
2. Institute for Energy Analysis, ORAU.
3. "Effect of Energy Decisions on the Economy," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1976*, ORNL/CSD-13, p. 32 (October 1976).
4. R. C. Ward, "The Combination Shift QZ Algorithm," *SIAM J. Numer. Anal.* **12**, 835–53 (1975).

13. Engineering Technology Research

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RESEARCH ON LATENT HEAT, THERMAL ENERGY STORAGE SUBSYSTEMS

One of the key elements of a successful program of solar energy utilization is the method to be used for thermal energy storage (TES). In an effort to reduce the size and complexity of thermal energy storage systems, most of which currently rely on using large masses of rock for sensible heat storage, a significant research program is under way with the aim of developing methods for storage of thermal energy as latent heat in so-called phase-change materials (pcm), which will melt or solidify according to whether heat is stored or released. The goal of the analytical modeling part of this program is the development of analytical and computer models which will accurately predict the performance of latent heat, thermal energy storage subsystems.

In the work performed up to the present time, two kinds of activities have been carried out. The first is the attainment of qualitative information about the behavior of pcm subject to a variety of external temperature condition, in slab, cylinder, and spherical geometries. The second has been the development of more accurate mathematical methods for use in the analytical and computer models. More specifically, the following results have been obtained.

1. *Approximation of the temperature distribution.* Polynomial and broken-line approximations for the temperature distribution in a wall were derived for a variety of boundary conditions. These approximations will be employed as possible alternatives to infinite series expansions for the temperature[3] and finite difference approximations.[4]

2. *Approximate solutions of moving boundary problems.* A comparison was made between several approximation methods for the solution of a moving boundary problem in the slab geometry. The methods studied included those of Goodman[5] and Megerlin.[6] In addition, the Megerlin method was extended to an approximation scheme based on subdivision of the pcm region which, for a large family of problems, was shown to yield a sequence of temperature and phase-boundary approximations converging to their exact values.

3. *Simulation of a latent heat storage mechanism for a slab.* A mathematical simulation was derived for the latent heat storage mechanism in a slab of pcm separated by a wall from a channel in which hot (or cold) fluid is flowing. The simulation was based upon the use of the Megerlin method in the pcm and a straight-line temperature distribution in the wall. Results were obtained for the pcm Penzoil (112/118) White Scale Paraffin Wax and walls composed of copper and methylmethacrylate, for a variety of fluid temperatures and flow rates. It was found that the heat storage process was initially strongly dominated by the wall, whereas for larger times the wall properties had an insignificant effect.

4. *The effect of augmenting the pcm with a good conducting filler material.* In the wish to estimate the effect on the heat storage rate and boundary history of a TES system of the addition of good conducting fillers to a poor conducting pcm, a one-dimensional slab model was examined for a variety of pcm's and fillers. A typical result obtained was the prediction that by adding 1.5 vol % of aluminum filler to the Penzoil (112/118) White Scale Paraffin Wax, the latent heat storage rate will be enhanced by a factor of 3.55. Generally speaking, the enhancement effect appears to be highly significant.

5. *The effect of a sinusoidal input temperature.* Analytical predictions were derived for the free boundary history and the rate of latent heat storage for the slab geometry when the boundary temperature is sinusoidal. As in 3 (above), the effect of the wall and channel flow diminish rapidly, and the TES process is dominated by the pcm properties.

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2. Engineering Technology Division.
3. H. Carslaw and J. Jaeger, *Conduction of Heat in Solids*, 2d ed., Oxford Univ. Press, London, 1959.
4. G. Smith, *Numerical Solution of Partial Differential Equations*, Oxford Univ. Press, London, 1965.
5. T. Goodman and J. Shea, "The Melting of Finite Slabs," *J. Appl. Mech.* 32, 16–24 (1960).
6. F. Megerlin, "Geometrisch Eindimensional Warmeleitung Beim Schmelzen and Erstarren," *Forsch. Ingenieurwes.* 34, 40–46 (1968).

6. *The effect of uncertainty of physical properties.* The fact that many pcm's exhibit additional solid-solid transitions, supercooling, and other "uncertainties" requires that we have an understanding of the sensitivity of the predicted estimates of, for example, heat storage rates and boundary history to this possible variability or uncertainty. Assuming randomness of such properties as the latent heat, thermal conductivity, and others, expected values and probability distributions were derived for the rate of heat storage and free boundary in the slab case. These relations will be incorporated into the testing procedure for the computer simulation program.

POWER PLANT PERFORMANCE

The statistical analyses underlying a report of the Council on Economic Priorities on power plant performance have been evaluated.[7] The Council report compared coal and nuclear electrical generation plants by regressing capacity factor (a measure of electricity generated to electricity which could be generated) on factors such as age, size, coal quality, and type of generating unit. None of the report's principal regression equations explained more than 41% of the variability in the data. For instance, boiling water reactors (BWR) were treated as functions of unit size. This explains 11% of the variation of individual BWR capacity factors about the mean value. Given the large amount of residual variability, the resulting uncertainties of predicted capacity factors are so large that the predications are of little use in comparing generating facility types.

DYNAMIC FAR-FIELD STRESSES GENERATED BY A SUDDENLY APPEARING CRACK

As reported previously,[8] Smith estimated the dynamic stress-intensity factor for a longitudinal crack located on a cylindrical shell in conjunction with the planning of crack-arrest experiments in intermediate-vessel-size geometries. The crack was opened by the internal pressure of the cylinder. He used Freund's[9] solution for an approximate calculation. Freund's solution is mainly concerned with obtaining the dynamic stress-intensity factor for a semi-infinite crack on an infinite flat plate. In his solution, the effect of the edge reflection has been neglected and the solution far from the crack has not been discussed in detail. In view of the finite radius of the cylindrical surface in the problem as considered by Smith, the stress waves generated by the opening of the crack will travel around the cylindrical surface and contribute to the stress intensity. The purpose of this study was to assess the significance of the returning waves by use of a solution of the related dynamic problem of a flat plate with a suddenly appearing crack.

From the principle of superposition, the problem of the crack opened by the internal pressure is equivalent to that of a stationary crack with suddenly applied traction on the surface of the crack. In the following discussion only the latter problem is considered. The method of analysis in this study[10] is based on that used by Freund but with more calculations for the dynamic stress distribution away from the crack. The result shows that a plane wave propagates outward in the direction perpendicular to the surface of the crack. It has a magnitude equal to the applied surface traction and a bandwidth equal to the length of the crack. In addition, two cylindrical waves are generated from the tip of the crack. One propagates with the longitudinal wave speed and the other with the transverse wave speed. Close to the wave fronts, the vertical stress components are proportional to $\sqrt{t - s_L r}$ and $(t - s_T r)^{3/2}$, respectively, where s_L and s_T are the slowness (i.e., the inverse of the longitudinal and transverse wave speeds respectively), r is the distance to the crack tip, and t is time. Clearly, the intensities close to both of the cylindrical wave fronts are negligible as compared with the major plane wave. Therefore, in the short period of time after the longitudinal wave has traveled a complete round of the cylinder, the major plane wave can be used to approximate the stress-intensity factor for the crack on the cylindrical surface. In addition to these components, a head wave is generated from the surface of the crack for $s_L r < t < s_T r$. Its existence compensates the surface traction induced by the longitudinal component of the cylindrical waves before the arrival of the transverse component.

7. R. L. Simard, *A Critique of the Council on Economic Priorities Text, Power Plant Performance — Nuclear and Coal Capacity Factors and Economics*, ORNL/TM-5846 (1977).

8. G. C. Smith, "A Simple Method for Analyzing the Dynamic Propagation and Arrest of Axial Through-Thickness Cracks in Cylinders," *Q. Prog. Rep. Heavy-Section Steel Tech. Program Oct.–Dec. 1975*, ORNL/NUREG/TM-3, pp. 66–84.

9. L. B. Freund, "Crack Propagation in an Elastic Solid Subjected to General Loading," *J. Mech. Phys. Solids* **20**, 129–40 (1972).

10. S.-J. Chang, "An Analytical Solution for the Dynamic Far-Field Stresses Generated by a Suddenly Appearing Crack," *Q. Prog. Rep. Heavy-Section Steel Tech. Program July–Sept. 1976*, ORNL/NUREG/TM-64, pp. 55–68.

14. Environmental Sciences Research

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EVALUATION OF POLYCYCLIC AROMATIC HYDROCARBONS AND ARYL AMINES

Polycyclic aromatic hydrocarbons (PAH) and aryl amines (AA) are commonly found in the environment as a result of the combustion of fossil fuels. Because many of these substances have known carcinogenic properties, a study was done to examine the effect of different PAH and AA in aquatic environments. The experiment evaluated the extent and rate at which PAH and AA are removed from solution and accumulated by *Daphnia*, an important component of aquatic food webs. *Daphnia* were placed in water containing a known concentration of a dissolved PAH or AA, and over an experimental period of 24 to 48 hr, samples of animals were taken and the PAH or AA concentration observed. The PAH or AA concentration in the water was also monitored.

A model has been proposed to describe the dynamics of the PAH or AA concentration in the water as well as in the *Daphnia*. The model is flexible enough to be useful in describing the dynamics of the PAH or AA concentration in the animals when the PAH or AA concentration in water is constant as well as decreasing over the experimental period. A two-stage iterative nonlinear estimation procedure has also been used to obtain estimates of the uptake and depletion parameters. From the fitted concentration curves, we have also been able to estimate the curve of the concentration factor (concentration in animals/concentration in water) for more than a dozen PAH and AA compounds. Comparisons among the different PAH and AA have been very helpful using the estimated uptake and depletion parameters. In addition, estimated LD_{50} values from the mortality data of this study have been quite helpful.

1. Graduate research participant, University of Tennessee, Knoxville.

2. Environmental Sciences Division.

3. Great Lakes Colleges Association student, DePauw University.

POPULATION GROWTH OF THE CALANOID COPEPOD

During the course of an investigation studying the effects of various environmental factors on the population growth in copepods, it became necessary to sample laboratory cultures that were kept in 30-liter aquaria. It soon became evident as the experiment continued that the animals were not distributed evenly throughout the tank. The sides and corners contained the highest density of animals with a marked decrease in density as one moved toward the center. A stratified sampling procedure was initiated in the following areas of each aquarium: (1) exterior, which included the volume of water along the sides of the aquarium within a band width of approximately 55 mm, and (2) interior, which included the remaining volume of the aquarium.

The nonparametric median test was used to detect significant differences in the observed density levels between the exterior and interior areas. A significant difference ($P < 0.01$) was found between the two areas. Although there was not sufficient data available, there was an indication that the corners contained higher density levels than the remaining exterior area. The results from the stratified sampling scheme were then used to obtain an estimate of the total population size in an aquarium, and an approximation was also found to the variance of this estimate.

EFFECT OF DENSITY AND FOOD LEVEL ON THE CALANOID COPEPOD

Data are being analyzed from a study to determine the effects of varying density and food supply level on the reproduction of the calanoid copepod, *Diaptomus clavipes*. There were 18 containers subjected to a fixed feeding regime, and each container had a fixed density level of animals (twelve containers each with one pair of animals, four containers each with three pairs of animals, and two containers each with six pairs of animals). Over the experimental period of 21 days, all females with clutches were collected from the containers, and the following observations were recorded to determine if feeding or density had an effect on reproduction: (1) number of eggs per clutch, (2) total volume of clutch, and (3) egg size. After removing the clutches, the females were returned to the same containers.

The first stage of the data analysis employed linear regression models to examine the effect of density level and feeding regime on the observed number of eggs per clutch. In addition, partial correlation coefficients have been calculated to consider the joint variation between pairs of variables after fixing other variables. These analyses will prove to be quite helpful in clarifying the effects of population density and food level.

METHYLATION OF INORGANIC MERCURY

An experiment has been conducted to examine the presence or absence of an in vivo mercury methylating process in brook trout. In particular, the interest was in the potential conversion of inorganic mercury to methyl mercury within the fish. Seven tanks, with 50 fish per tank, were used for this experiment with (1) four of the tanks receiving equivalent amounts of inorganic mercury and (2) three of the tanks serving as controls. All of the fish were of the same size and age and were randomly allocated to the tanks. Fish were collected from the tanks during the experimental period of approximately 50 weeks and analyzed for total mercury and methyl mercury concentration.

The data consisted of the measured mercury concentrations in each sampled fish for the different tissues analyzed (muscle, liver, intestine, and skin) at the various sampling times during the experimental period. The goal of the analyses of these data was to determine if the concentrations for the fish from the test and control tanks differed significantly. Since concentration varies with growth rate, the statistical analyses were done on both the organ burden and the body burden of mercury. A semilog linear regression model was found to be adequate for describing the total organ burden of mercury and methyl mercury as a function of time since the start of the experiment. A weighted regression was recommended because of the change in variance of the observed burdens as a function of time. The weighted slope estimates of the regression lines were more precise than those found using the unweighted regression estimates. As a result of these regression analyses, we were able (1) to indicate those organs that had a significant change in their organ burdens and (2) to determine whether or not the control and test groups differed. In addition, these statistical analyses supported the contention that the food chain can be an important uptake route for methyl mercury.

THERMOREGULATION IN FISH

A study has been done to test for evidence of predictive thermoregulation in mosquito fish. From this type of thermoregulation a fish will tend to move to the top if the water temperature is below the acclimation temperature or to the bottom if the water temperature is above the acclimation temperature. The procedure used in this study involved fish in a tank with the water temperature greater than, less than, or equal to one of the acclimation temperatures of interest. For each experimental run, 12 fish from each acclimation group were used. Therefore, a total of 36 fish were used for each run, and a run was made at each acclimation temperature. Three fish of the same acclimation temperature were placed in each of four cylinders within a tank, and the average position of the fish in each cylinder was recorded for a period of one hour after the fish became adjusted to the new environment.

The experimental data were examined to determine the effect of test temperature (x_1) and acclimation temperature (x_2) on the depth preference (r), as measured by the average depth over a fixed period of time of the fish within a particular cylinder. The following model was used to describe the data:

$$E(r) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 \ .$$

The results of the regression analysis showed no significant effect ($P > 0.10$) from x_1, x_2, or $x_1 x_2$. Since multiple observations were available at each combination of (x_1, x_2), a lack-of-fit test was also performed to determine the adequacy of the model and was not found to be significant ($P > 0.10$). Although the results of these statistical analyses have been inconclusive as far as the proposed thermoregulation hypothesis, valuable information has been obtained that will be useful in the planning of additional experiments and possibly in a modification of a new thermoregulation hypothesis.

INFLUENCE OF ADULT DENSITY ON A CALANOID COPEPOD ZOOPLANKTER

Preliminary results from the data analysis of a study on population dynamics of a zooplankter have been previously summarized.[4] Starting with a second-order regression model in terms of variables related to female

4. "Influence of Adult Density on a Calanoid Copepod Zooplankter," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1976*, ORNL/CSD-13, p. 33 (October 1976).

size, adult density, and water temperature, the observed clutch size had been reasonably explained by a linear model containing 13 terms after applying a statistical variable selection procedure. Since the previous analysis did not take into account that the observed number of eggs per clutch might be a Poisson random variable, a test was performed to test this hypothesis. Except for a few cases that could be attributed to outlier observations, the Poisson assumption was reasonable. Therefore, the regression analysis was done on the reduced second-order model using weights appropriate for Poisson-distributed data.[5] The results of this analysis made it possible to test for the adequacy of the approximation and the assumed Poisson distribution. Additional analyses of these data have been done by calculating the principal components of the standardized variables related to female size, adult density, and water temperature, and then using these new variables to explain the variation in the observed clutch size. The benefit of this approach is the orthogonality of the new variables. Correlations of these new variables with the original observed variables may be used to make a physical interpretation of the new variables.

USE OF LINEAR LOGISTIC MODEL TO EVALUATE TOXIC SUBSTANCES

During this period the work on the use of the linear logistic model to evaluate the effect of toxic substances has been in the area of the derivation of approximate variance expressions for the estimated concentration levels of the toxic substances necessary to achieve a fixed level of mortality. In particular, in the expression of the probability that an organism will die from a concentration, x_1, of substance one and from a concentration, x_2, of substance two, that is,

$$P = (\exp M)/(1 + \exp M) ,$$

where

$$M = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 ,$$

we have used the maximum likelihood estimates of the β's and their associated covariance matrix to find approximations to the variance of the estimated value of x_1 for fixed values of x_2 and P. This is denoted by $\mathrm{Var}(x_1|x_2)$. A similar expression for $\mathrm{Var}(x_2|x_1)$ for fixed values of x_1 and P has also been derived.

In addition, Fieller's theorem has been applied to obtain approximate confidence regions on x_1, for fixed values of x_2 and P, from the maximum likelihood estimates of the β's with their associated covariance matrix. Similar expressions for approximate confidence regions on x_2 for fixed values of x_1 and P have also been derived using Fieller's theorem. All of these expressions will assist in the planning of future experiments investigating the effect on mortality of the joint application of toxic substances.

5. E. L. Frome, M. H. Kutner, and J. J. Beauchamp, "Regression Analysis of Poisson-Distributed Data," *J. Am. Stat. Assoc.* 68, 935–40 (1973).

15. Health Physics Research

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LEUKEMIA INCIDENCE OF ATOMIC BOMB SURVIVORS

Leukemia data from studies of atomic bomb survivors have been analyzed using calculations of absorbed dose to active bone marrow. Previous analyses have used estimates of tissue kerma in air and neglected the self-shielding of internal organs by the survivor's body. The risk estimates were obtained by fitting a function of the form $Y_e = AD_n + BD_\gamma^2$, where Y_e is the incidence rate in excess of control incidence rate, D_n is the neutron dose, and D_γ is the gamma dose. The control incidence rate was computed from survivors exposed to 0–9 rads. The risk estimates obtained in this analysis are in good agreement with the risk estimates obtained by the BEIR Committee[2] from data on x-ray-treated spondylitis and menorrhagia patients. Previous risk estimates, using dose estimates based on tissue kerma in air, have not been in good agreement.

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1. Health Physics Division.
2. *Report of the Advisory Committee on the Biological Effects of Ionizing Radiations*, NAS-NRC, Washington, D.C., 1972.

16. Materials Research

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PERFORMANCE OF HTGR FUEL PARTICLES DURING CURED-IN-PLACE CARBONIZATION

Fuel rods for the High-Temperature Gas-Cooled Reactor (HTGR) are made by bonding together coated microspheres of fertile particles (thorium) and fissile particles (uranium) in a pitch matrix to form 2-in. fuel rods. The fuel rods are then placed in a prismatic graphite block and cured by driving off the volatile substances from the pitch matrix with heat. Since the coatings on the fuel particles are the primary containers of fissionable material, the effects on the particle coatings of the different factors of the cured-in-place process were examined for fertile particles.

Three different strengths of HTGR fuel particles were used to make fuel rods which are placed in four graphite blocks. Each of these graphite blocks was heated at a different rate to a final processing temperature. An experimental design was constructed to examine the effects of different particle strengths, graphite block holes, and heating rates on the response of coke yield and particle failure fraction in a fuel rod. The coke yield is the percentage of the weight of the carbonized matrix to the weight of the original matrix, and the failure fraction in a fuel rod is measured by the amount of thorium leached (µg) from a fuel rod (using the chlorine leach technique) divided by the total amount of thorium in a fuel rod. A statistical analysis of the results indicates that the variations in coke yields are due to different heating rates, and the variations in failure fraction are due to both different heating rates and different strengths of particles.

The variable levels chosen for the experimental design are shown in Table 6.

The effect of fuel rod location was not measured because there were only 72 available fuel rods and 81 possible combinations of the levels of the four variables. Any effect due to location was confounded with particle strength, so the particle strength effects also include the effects due to location. The fuel rods were randomized in each hole and replicated twice at each position.

The percentage of coke yield was found to depend on the heating rate of the graphite block in a quadratic manner. As the heating rate increased, the coke yield decreased; this relation can be expressed by the equation:

$$\text{coke yield} = 39.131 - 1.539\ \text{heat} + 0.053(\text{heat})^2 \ .$$

The failure fraction depends on both heating rate and particle strength; the worst conditions are at heating rates 1°C/min and 5°C/min with particle strengths of 5.14 lb and 5.78 lb (see Table 7). The lowest failure fractions occur with the 6.85-lb particle strength at all heating rates. The confidence intervals on the failure fractions indicate that only three intervals include the critical value 1×10^{-4} failure fraction. These three intervals occur at the conditions shown in Table 7.

1. Metals and Ceramics Division.
2. Development Division, Y-12.

Table 6. Variable levels of the experimental design

Variable	Level
Heating rate	1°C/min; 5°C/min; 10°C/min; 15°C/min
Particle strength	5.14 lb; 5.78 lb; 6.85 lb
Hole in graphite block	Hole 1; Hole 2; Hole 3
Location of fuel rod in the graphite block hole	Top (+1); middle (0); bottom (−1)

Table 7. Worst conditions for the failure fractions

Heating rate (°C/min)	Particle strength	Mean failure fraction ($\times 10^{-4}$)
1	5.14	1.76
3	5.78	1.64
5	5.14	0.78

DISTRIBUTION OF THE NUMBER OF PRECURSOR ATOMS FORMED DURING IRRADIATION

Consider a container of uranium being irradiated and a particular precursor being formed from fission. This precursor can then decay to a stable element. For this process, the probability distribution of the number of precursor atoms, $M(t)$, at given time, t, can be derived from its probability generating function.

The stochastic model of the probability of m precursors existing in the time interval $(t, t + \Delta t)$ is

$$\begin{aligned} \text{Prob}\{m, t + \Delta t\} = {} & \text{Prob}[m, t]\text{Prob}[\text{no precursors form or decay in } \Delta t] \\ & + \text{Prob}[m - 1, t]\text{Prob}[\text{one precursor forms in } \Delta t] \\ & + \text{Prob}[m + 1, t]\text{Prob}[\text{one precursor decays in } \Delta t] \ . \end{aligned}$$

This stochastic model may be formulated in terms of the probability of fission, P_f, the number of fission neutrons per fission, ν, the number of precursors produced per fission, β, and the decay rate of the precursor, λ. From this formulation, the following differential-difference equation can be derived by letting $\Delta t \to 0$:

$$\begin{aligned} d\,\text{Prob}[m, t]/dt = {} & -(P_f\beta\nu + m\lambda)\text{Prob}[m, t] \\ & + P_f\beta\nu\,\text{Prob}[m - 1, t] + (m + 1)\lambda\,\text{Prob}[m + 1, t] \ . \quad (1) \end{aligned}$$

According to Eq. (1), the probability generating function for $\text{Prob}[m, t]$, given by

$$G(x, t) = \sum_{z=0}^{\infty} x^z\,\text{Prob}[z, t] \ , \quad |x| \leq 1 \ , \quad (2)$$

is a solution to the first-order initial value problem:

$$\begin{aligned} \partial G(x, t)/\partial t = {} & P_f\beta\nu(x - 1)G(x, t) \\ & - \lambda(x - 1)\,\partial G(x, t)/\partial x \ , \quad G(x, 0) = 1 \ . \quad (3) \end{aligned}$$

An explicit solution to Eq. (3) can be found by reducing the problem to an initial value problem for a first-order linear ordinary differential equation. The solution is

$$G(x, t) = \exp\left[\left(\frac{P_f\beta\nu}{\lambda}\right)(x - 1)(1 - e^{-\lambda t})\right] \ . \quad (4)$$

This is the probability generating function of the Poisson distribution with expected value

$$E[M(t)] = \left(\frac{P_f\beta\nu}{\lambda}\right)(1 - e^{-\lambda t}) \ .$$

Since each probability distribution has a unique probability generating function, $M(t)$ has a Poisson probability distribution.

ZWOK RATE CONSTANT PREDICTION EQUATION

A statistical analysis of isothermal Zircaloy-4 water oxidation kinetic (ZWOK) data was made to determine the parameters in the exponential model for rate constants as a function of temperature for the (1) oxide layer, (2) alpha layer, (3) ξ layer (oxide + alpha), and (4) total oxygen consumed.

A specimen of Zircaloy-4 was placed in the Mini-ZWOK steam-oxidation apparatus, and steam was passed over the outer surface of the specimen. This experiment was repeated for various lengths of time under isothermal conditions over a temperature range of 900 to 1500°C (1652 to 2732°F) at 50°C (90°F) intervals with at least ten specimens being oxidized at each temperature.

After each experiment, the oxide layer thickness and alpha layer thickness were measured, with the Xi layer and the total oxygen consumed calculated from these measurements. The rate of reaction for the four measurements was assumed to follow a parabolic kinetics model in time — that is, the square of the measurements was a linear function of time. The slopes of each of the linear functions were estimated using the method of least squares. These slopes represent estimates of the isothermal rate constants. The logarithms of the rate constants were assumed to be related linearly to the reciprocal of temperature or by a simple Arrhenius relationship. The parameter estimates for the linear models are listed in Table 8.

Table 8. Prediction equations for the logarithm of the rate constants

Model	Prediction equation	Applicable range
Oxide	$\hat{\ln}\,\delta_{\phi}^2/2 = -4.48868 - 18060.28(1/T)$	1050–1504°C
Alpha	$\hat{\ln}\,\delta_{\alpha}^2/2 = -0.27230 - 24228.91(1/T)$	905–1504°C
Oxide + alpha	$\hat{\ln}\,\delta_{\xi}^2/2 = -1.07462 - 20988.50(1/T)$	1050–1504°C
Total oxygen	$\hat{\ln}\,\delta_{T}^2/2 =$ −1.7[illegible]986 $- 20097.96(1/T)$	1050–1504°C

To judge the quality of the estimated parameters, individual and joint 90% confidence intervals were calculated for the true values of the parameters and are illustrated in Fig. 5 for the oxide layer. The individual confidence intervals of the true values are appropriate for specifying ranges for the possible value of each individual parameter irrespective of the value of the other parameter. To calculate a region in which both parameters may occur simultaneously, the joint confidence region takes into account the covariance and the relative sizes of the variances of the two corresponding estimators. Each pair of points inside the joint confidence region determines a prediction line contained inside the confidence interval about the estimated prediction line. Those points on the joint confidence region boundary determine prediction lines which are tangent to the confidence interval boundaries on the estimated prediction line.

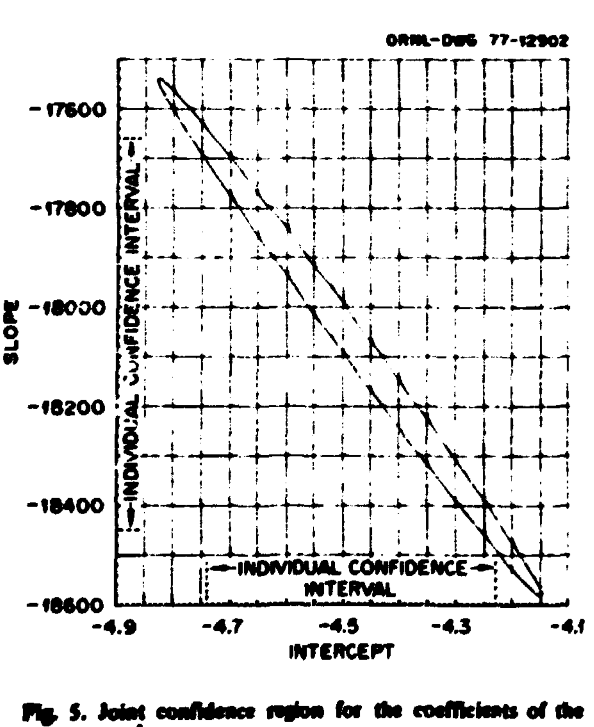

Fig. 5. Joint confidence region for the coefficients of the oxide model: $\hat{\ln}\,\delta_{\phi}^2/2 = -4.48868 - 18060.28(1/T)$.

CREEP-RUPTURE OF ALLOY MATERIALS

In support of the Brayton Power System and HTGR programs, mathematical descriptions of creep-rupture and time to 1% strain are being developed for several alloys including Hastelloy X, Hastelloy S, Alloy 617, Alloy 625, Udimet 700, and Waspaloy. Most of these equations are linear functions of reciprocal temperature, stress, and logarithm of stress. Lower limits of stress to cause rupture and 1% strain are also defined using tolerance limits about the logarithm of time.

For example, the following linear form was found to adequately describe the expected value of both rupture life and time to 1% strain for Hastelloy X sheet:

$$\log_{10} t = b_0 + b_1\left(\frac{1}{T}\right) + b_2(\log_{10}\sigma) + b_3\left(\frac{1}{T}\log_{10}\sigma\right) \ ,$$

where

t = expected value of rupture life or time to 1% strain, in hours,

T = temperature, °C,

σ = stress, MPa.

Least-squares estimates of unknown constants with standard errors are shown in Table 9.

Expected values and lower limits at selected levels of stress and temperature are given in Table 10. These lower limits are based on the lower ($P = 0.90$, $\lambda = 0.95$) tolerance limit about the logarithm of rupture life (or time to 1% strain). Data and expected values are plotted

Table 9. Least-squares estimates

	Rupture life	Time to 1% strain
b_0	-17.3 ± 0.88	-18.6 ± 0.86
b_1	$(2.41 \times 10^4) \pm 980$	$(2.40 \times 10^4) \pm 910$
b_2	2.84 ± 0.35	3.49 ± 0.41
b_3	$(-6.45 \times 10^3) \pm 360$	$(-6.88 \times 10^3) \pm 380$
	Other statistics	
Number of tests	84	124
R^2 (coefficient of determination), %	90	87
Residual mean square	0.634	0.117

Table 10. Hastelloy X sheet expected values and lower limits for rupture life and time to 1% strain

Temperature, °C (°F)	Stress, MPa (ksi)	Rupture life, hours		Time to 1% strain, hours	
		Lower limit	Expected value	Lower limit	Expected value
649 (1200)	138 (20)	7600	49,000	160	1300
	172 (25)	1800	10,000	35	270
	207 (30)	520	2,700	9.5	75
760 (1400)	55 (8)	6600	40,000	260	1800
	69 (10)	2200	11,000	82	530
	103 (15)	270	1,200	9.2	55
871 (1600)	21 (3)	4100	24,000	200	1400
	28 (4)	1300	6,400	61	380
	41 (6)	240	1,000	11	64
982 (1800)	7 (1)	2200	13,000	100	750
	14 (2)	230	1,000	11	66
	21 (3)	55	220	2.6	16

in Figs. 6 and 7 for rupture life and time to 1% strain respectively. Symbols represent tests performed at different temperature levels. Plotting the dependent variable rupture life (or time to 1% strain) on the abscissa conforms to accepted practice in material-properties research. Care should be exercised in interpreting the graphs since variability is in the horizontal direction.

ANALYSIS OF DATA FROM VARISTRAINT TESTS ON INCOLOY 800

Varistraint tests at five levels of strain were performed on seven heats of Incoloy 800. The simple correlations between total crack, a measure of hot cracking, and chemistry were computed for each element and several combinations of elements at each of the five strain levels. These simple correlation coefficients are a normalized measure of the linear dependence between two random variables and were used as a source for the subjective comment to compare current results with an earlier report of York and Flurry.[3]

There appears to be no linear relationship between hot cracking and the elements carbon, aluminum, and

3. J. W. York and R. L. Flurry, *Assessment of Candidate Weld Metals for Joining Alloy 800*, WNET-119, Westinghouse Tampa Div. (February 1976).

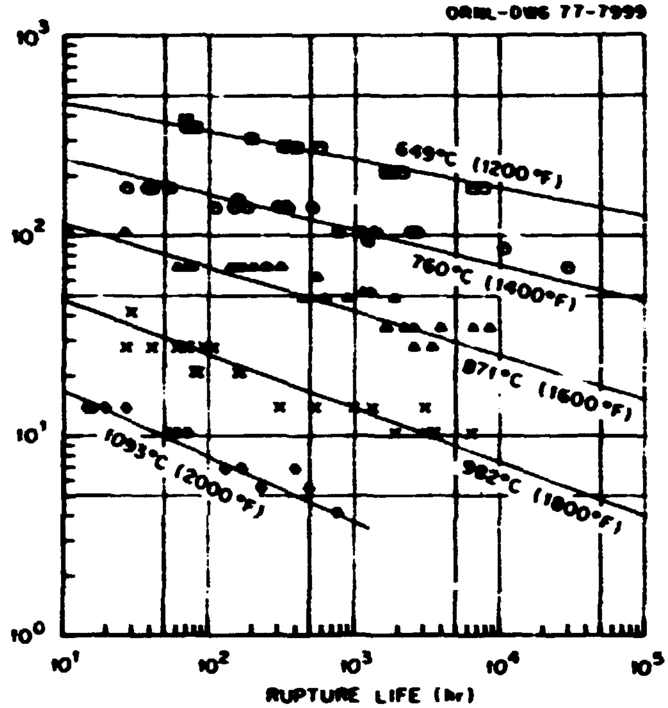

Fig. 6. Hastelloy X sheet expected value of rupture life.

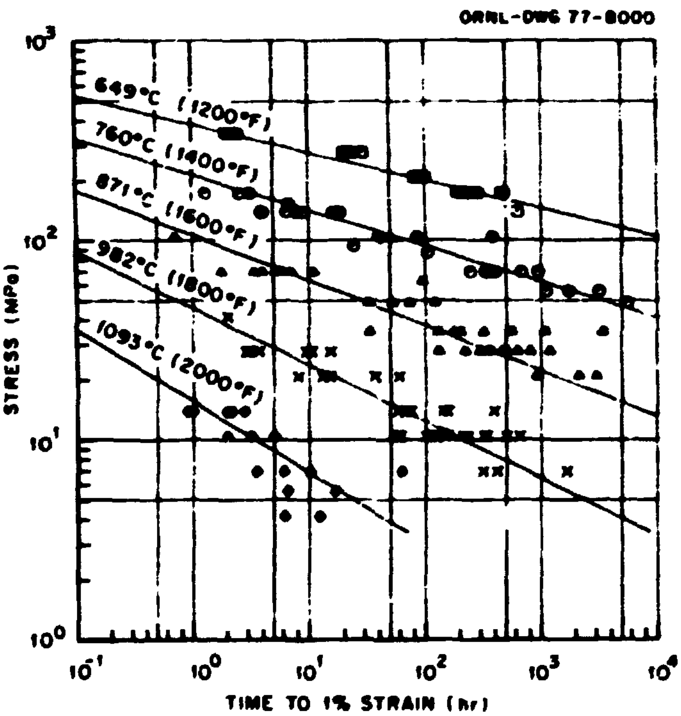

Fig. 7. Hastelloy X sheet expected value of time to 1% strain.

titanium as reported by York and Flurry. Also, the reported (Al + Ti)/(C + Si) ratio was found to be a "reasonable" predicter of hot cracking in Incoloy 800. The simpler forms Ti/(C + Si) and Ti/Si performed better than the reported ratio at the higher strain levels. Numerous other combinations of elements were considered and were found to be equal to or worse than the above ratios. None clearly stood out as being superior.

The correlation between hot cracking and aluminum, titanium, and silicon appears to be an increasing function of varistraint strain level, while the correlation with manganese tends to be a decreasing function of strain level. Although there is insufficient information to determine if these effects are real, future effort should not overlook the possibility of a significant strain effect.

A SUMMARY OF RESULTS FROM PILOT MEMBERSHIP SURVEYS

A mail survey of the American Welding Society (AWS) membership is expected in 1977. The purpose of the survey is to gain better understanding of the makeup of the Society. To prepare for the overall survey, pilot surveys of the Houston and Niagara Frontier sections were conducted in 1976.

The questionnaires of the two sections differed in content and in time of delivery, the second questionnaire hopefully being an improvement over the first. Also, students were excluded in the Niagara Frontier survey but not in the Houston survey. The increased response rate in the Niagara Frontier survey (42.1% vs 18.1% in the Houston survey), attributable to the use of prepaid, self-addressed return envelopes, is still too small to permit valid inferences about the two sections. The conclusions should be verified by an expanded survey. A brief summary of the findings of the pilot study follows:

Typical Member

The average or typical member of the Houston and Niagara Frontier sections has been with AWS for about ten years and is 43 years old with a bachelor's degree in an engineering or scientific field. He is at the management level in the fabricated metal products industry and earns $20,000 to $30,000 a year. He is neither a union member nor a registered professional engineer.

Education

Differences are noted with respect to age. As expected, the younger members have received more formal education. Members of the Houston section with only a high school diploma decrease from 1 in 4 for those at least 50 years of age to fewer than 1 in 10 for the youngest group. A correspondingly larger number of the younger members have attended junior college. Similar but mixed trends are found in the Niagara Frontier section.

Job Function

Of the respondents, 18% indicated first-level management responsibilities ("president, owner, officer"). 20% indicated second-level management responsibilities ("manager, director, superintendent"), and 18% claimed to be welding engineers. "Sales" and "metallurgist" were the job categories next in line. Only 4% of the respondents marked their job function as "welder or cutting operator." One in fifteen (6.8%) belongs to a union, whereas 1 in 4 (23.6%) is a registered professional engineer. The percentages are not additive since multiple responses were permitted.

Compensation

Because Houston has a low cost of living, it may be of interest to look at salaries. The two sections may be compared by deleting the younger age group and all returns that do not specify age. From the remainder, two-thirds (68.1%) of the Houston members earned more than $20,000, while only slightly better than half (56.7%) of the Niagara members were similarly compensated. However, results above $30,000 agree remarkably well. Approximately 1 in 4 received an annual income of $30,000 or more, 1 in 10 received $40,000 or more, and 1 in 20 received $50,000 or more. Note that these figures apply to those respondents known to be at least 30 years of age.

Length of Membership

The distribution of length of membership as adjusted to equal time intervals shows a high proportion of new members in both sections. Better than one-third of the section members responding have been with the Society less than three years. This phenomenon is seen at all age levels. Nearly half (46.2%) of the members over 40 years of age have been with the Society less than ten years, one-fourth less than five years.

Many factors may be contributing to this surge in new members of all ages. These statistics may reflect the results of an active campaign to recruit new members. There may be an increased attraction of the Society brought about by expanded benefits and improved response to membership needs. Also, there may be a significant segment of individuals who for various reasons join for short periods of time. This latter segment includes those who are promoted into and then out of short-term positions that benefit from AWS membership, those who join to receive the wide range of publications free or at reduced prices, and those who join to please their teachers.

Journal Readership

Current applied technology paced by the Feature Articles and New Products sections ranks a strong first in interest among readers of the *Welding Journal* with articles about people and events bringing up the rear. There is substantial interest among younger members in advertisements and in the Practical Welder section. This interest does not seem to be shared by the older members.

A question added to the Niagara Frontier questionnaire asked which Journal section was most important. Feature Articles, New Products, and Practical Welder sections stood out as being most important. Readers under 30 years of age considered the sections on Practical Welder and Tech Topics to be most important. The Research Supplement ranked fourth and fifth except in the 30–39 age group, where it tied with Practical Welder for second in importance to Feature Articles.

Reasons for Membership

The Niagara Frontier survey requested that three answers be ranked in order of importance. Results show that "professional contacts" and "section technical meetings" were strong primary reasons for being a member of AWS. Receipt of the *Welding Journal* and other publications were mentioned as frequently but tended to be of secondary importance.

Overall Survey

A stratified sample survey is being recommended for the overall membership survey to be conducted in the latter part of this year. A sample survey can achieve results equivalent to a census survey but at greatly reduced costs. Stratification according to type of membership, size of local section, and geographical location will be necessary for improving precision of estimates within these subgroups. Follow-up mailings will be necessary to achieve a high rate of return so that nonrespondent bias is minimized.

ANALYSIS OF DRY DENIER VARIABILITY IN KELVAR YARN

The variability patterns of denier in spools of Kelvar yarn have been investigated. The analysis of the denier data indicated that the denier within a spool of yarn was relatively uniform. However, the analysis also indicated that a significance between spool variability existed.

Generally, the results of the analysis of the denier data indicated that one set of use specifications for the whole lot of spools would not be feasible and that each spool in the lot would have to be considered independently. The denier measurements were collected as specified in an experimental design previously reported.[4]

As previously indicated,[4] a subset of the design points were to be used to study the patterns of variability in the chemical structure of the yarn. As was true with the denier analysis, a significance between spool variation was indicated for one of the chemical components of the yarn.

COAL RESEARCH PROGRAM

An experiment design is being prepared to study erosion and corrosion of hard surface materials for handling coal slurries at high temperatures, in support of the coal research program. These experiments are expected to be conducted on site.

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4. "Evaluation of Characteristics of Kelvar Yarn," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1976*, ORNL/CSD-13, p. 45 (October 1976).

17. Sampling Inspection and Quality Control

R. S. Leete[1] W. E. Lever R. C. Meacham G. L. Grametbauer[2]

AN INVESTIGATION OF THE TUBE SHEET INSPECTION PLANS

Tube sheets supplied by a vendor for use on the gaseous diffusion process were subjected to a quality control inspection by both the vendor and the Oak Ridge Gaseous Diffusion Plant (ORGDP). One part of this inspection involved checking for oversize holes in the tube sheets. The procedures used by the vendor and ORGDP appeared to give conflicting results; the vendor's inspection often yielded 30 to 100 oversize holes, while the inspection at the gaseous diffusion plant typically yielded not any or only one oversize hole.

An investigation to resolve the apparent differences between the two plans found them to be generally complementing, rather than contradicting, each other; the two procedures had vastly different properties. The vendor's plan resulted in poorly defined samples which generally yielded a lower-bound estimate of the total number of oversize holes in the sheet. The nature of the plan limited severely the statistical interpretation of the results of the inspection and tended to imply a lower quality than actually existed.

The ORGDP plan was found to have a precisely defined sampling plan, which was based on the proportion of oversize holes in the sheet. Since the plan was precisely defined, it was readily subject to statistical interpretation. However, as a quality control procedure the plan had a very poor manufacturer's risk and, when rigidly enforced, would have led to the rejection of many otherwise acceptable tube sheets.

Because both plans had serious drawbacks, a set of potential alternatives was presented which involved suggested changes in both inspection plans.

INSPECTION PROBABILITIES

The results of the inspection of a unit are dependent on many features, such as the tolerances allowed by the specifications, the patterns of variation present in the unit being inspected, and the variation patterns present in the measurement process. As a planning aide for production and inspection schedulers, values of probabilities associated with the results of inspections were calculated. These probabilities were calculated under the assumption that the true value of the measurement was a random value from a normal distribution and that the error in the measuring device was a random variable from a different normal distribution.

For a series of potential tolerances, unit variations, and measurement error variations, the probabilities of the potential disposition of the measured unit were tabled.[3]

INSPECTION FREQUENCIES FOR ERDA QUALITY AUDIT

By a reinspection of a randomly chosen set of parts previously found acceptable, ERDA continually audits the effectiveness of quality control inspection procedures used in the Y-12 plant.

A new sequential audit procedure has been developed by ERDA which will have parts reinspected at a rate that is a function of the part production levels and the number of reinspected parts which do not meet specifications. Because this procedure has never been used before and has varying inspection levels, the number of additional inspectors required to fulfill this task was not known. To estimate the number of additional inspectors required, a simulation study of the reinspection process was conducted using proposed production levels for the Y-12 plant and historical data on the results of previous reinspections. The study was conducted for each general type of part inspected, and tables of month-by-month projected inspection frequencies were generated.

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1. Technical Division, Y-12.
2. Instrumentation and Quality Assurance Development, ORGDP.

3. W. E. Lever and R. S. Leete, Jr., *A Study of the Relationship of Three Factors on Errors in Inspection*, UCCND/Y-2075 (April 1977).

18. Uranium Resource Evaluation Research

F. L. Miller, Jr. C. E. Nichols[1] V. E. Kane

URANIUM RESOURCE EVALUATION PROGRAM

The National Uranium Resource Evaluation (NURE) Program was established by the Energy Research and Development Administration to evaluate uranium resources and to identify favorable areas for detailed uranium prospecting throughout the United States. The Hydrogeochemical and Stream Sediment Reconnaissance Survey part of the NURE Program is to identify areas in the United States which are favorable for uranium exploration. This is accomplished by a reconnaissance of surface water, groundwater, stream sediment, lake sediment, and plants. Union Carbide Corporation, Nuclear Division, will survey approximately one million square miles over a 12-state area collecting 130,000 samples.

From the initial planning stages, the Union Carbide Uranium Resource Evaluation Project has received statistical support in field data collection, sampling design, interpretative data reports, and special testing studies. This year we have been concerned with the identification of laboratory or data processing errors and finding statistical methods that aid in the identification of promising uranium districts.

Before any data interpretation is performed, it is desirable to correct any errors that may have occurred in the laboratory or the computerization of the data. The large volume of data necessitated that an automated data verification process be developed. Consequently, a principal component analysis procedure was instituted in which outlier samples are easily identified. In the principal component analysis, the unusual nature of the outlier samples is assessed with regard to the multivariate nature of the data. These samples are then reanalyzed in the laboratory, ensuring high quality for the final data.

A typical collection of data would be a survey over 21,000 km^2 (8000 sq miles) with a sample collected about every 26 km^2 (10 sq miles). Each sample has approximately 25 associated measurements. A basic problem is to uncover any geographic patterns in the data which may be related to uranium mineralization. Two mathematical techniques have proven successful. The first is a weighted-sum contour of uranium-related elements. Let X_{ij} denote the ith measurement for the jth sample, $i = 1, \ldots, p$; $j = 1, \ldots, N$; then the quantity

$$Y_j = \sum_{i=1}^{p} w_i X_{ij}$$

is a weighted sum of measurements for the jth sample. The weights, w_i, combine a subjective weighting as well as a scale adjustment for the ith variable. The y's are plotted and contoured, generally showing smoothed variation patterns. Because uranium-related elements are used, regional uranium patterns are more easily identified. This technique differs from most other smoothing methods in that the multielement characteristics of a sample, rather than the mathematical methods, are responsible for the smoothing.

The second method used in assessing geographic patterns is cluster analysis, in which the uranium-related elements are weighted the most heavily. It is desirable to weight an element heavily if it separates the data according to geology and is related to uranium. Geologic variation is assessed by plots such as Fig. 8, in which sulfate separated some of the geologic units. Once weights are determined, plots such as Fig. 9 are constructed by geologists to identify potential uranium districts. Research in various clustering methods is continuing to obtain the best possible interpretation of the data.

BOTANICAL COMPARISONS

During the Llano field trial, the regular samples were supplemented with samples of pairs of tree species at many sample locations. For each of six pairs of tree species (cedar-elm, cedar–live oak, cedar-sycamore, elm–live oak, elm-sycamore, and elm-willow), the concentrations of ten elements (Al, B, Ba, Ca, Fe, Mg, Mn, P, Pb, and U) in one species were regressed on each element concentration in the other species. A difficulty in doing this is that element concentrations are not measured without error. The estimation procedure is unbiased, but significance testing can lead to statistically invalid conclusions. The purpose of the regressions was to see how well one could predict the element content of one tree from that of another, with further goals of using similar techniques to estimate missing values and to construct contours of equal uranium concentration from the botanical data.

1. Uranium Resource Evaluation Project.

ORNL-DWG 77-12865

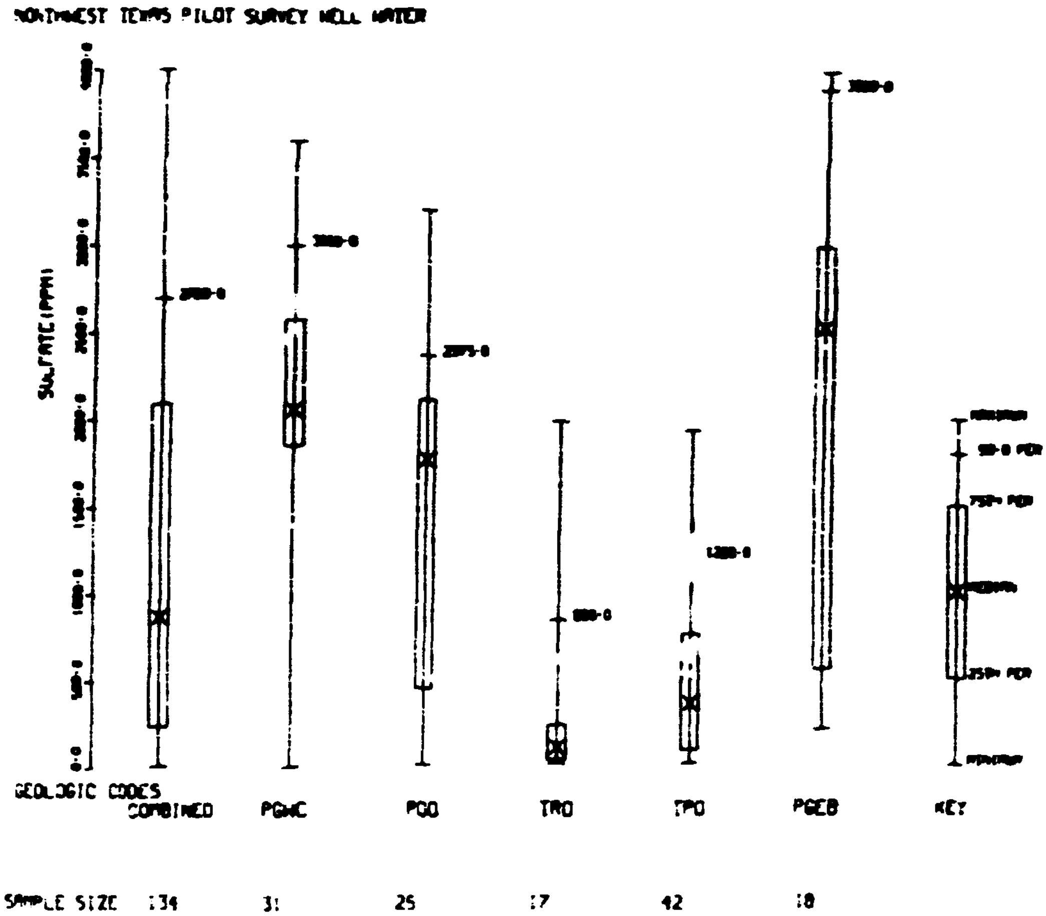

Fig. 8. Plot of percentiles by geologic strata in Northwest Texas.

ORNL-DWG 77-10854

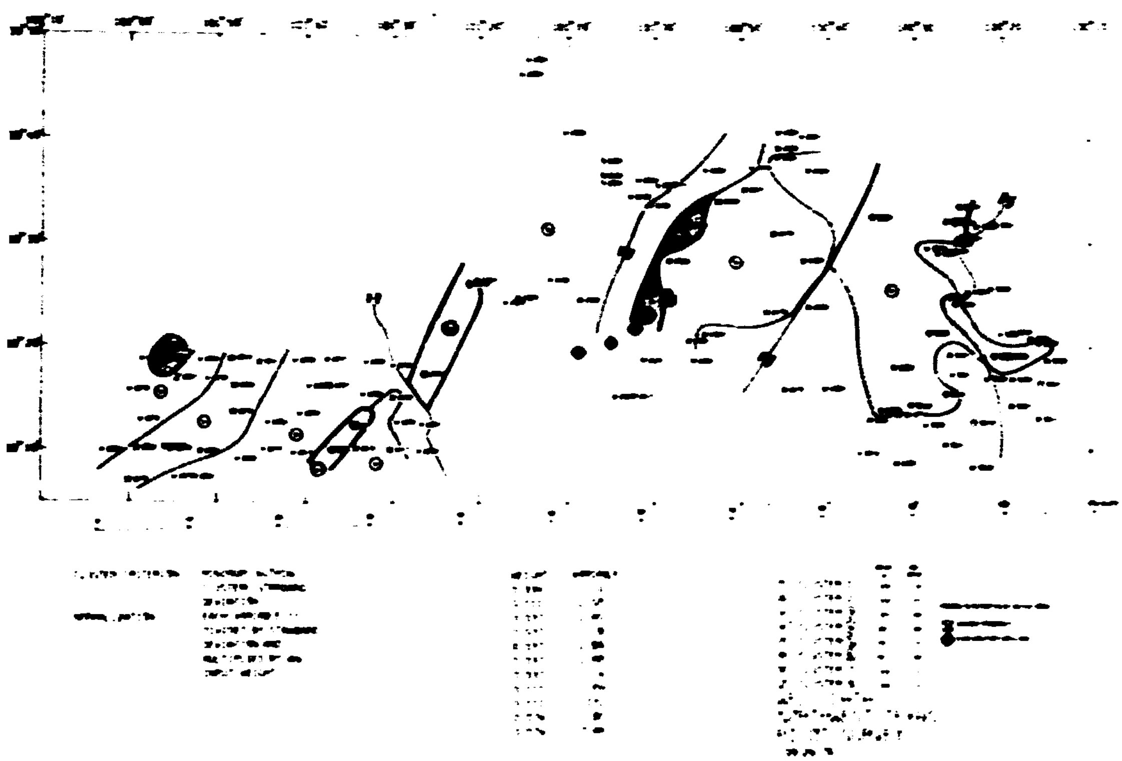

Fig. 9. Interpretative map derived from cluster analysis indicating potential uranium districts.

Part C. Educational Activities

The Mathematics and Statistics Research Department engages in a variety of educational activities both academic and professional. This year the department was host for both the Second ERDA Statistical Symposium and the Union Carbide Corporation Applied Mathematics Symposium. Individual department members have presented short courses at Oak Ridge and at UCLA; organized several seminar series and a workshop; served as part-time university lecturers, thesis advisors for doctoral candidates, and supervisors for students in the Oak Ridge Associated Universities (ORAU) Summer Student Program and other similar programs; given talks under the auspices of the ORAU Traveling Lecture Program; and worked with academicians visiting the department.

SECOND ERDA STATISTICAL SYMPOSIUM

The Second ERDA Statistical Symposium was held October 25-27, 1976, at Oak Ridge National Laboratory. The program was planned by Donald A. Gardiner of MSRD, Ronald K. Lohrding of Los Alamos Scientific Laboratories, Wesley L. Nicholson of Pacific Northwest Laboratories, and George P. Steck of Sandia Laboratories. Organization and local arrangements were handled by Kimiko O. Bowman, Charles K. Bayne, William E. Lever, and Forest L. Miller, Jr., all of MSRD. There were 65 participants representing ERDA, NRC, ERDA laboratories, universities, and contractors in the ERDA statistical community.

The program consisted of three technical sessions at which research papers were presented, three sessions at which problems were presented, and three sessions at which the problems were discussed. Local participants in the program were Roger F. Hibbs of UCC-ND, Alex Zucker of ORNL, and Victor E. Kane and Toby J. Mitchell of MSRD. Also featured on the program were tours of the American Museum of Atomic Energy and the Oak Ridge National Laboratory.

The proceedings of the symposium, including the discussions, were published in April 1977 by Los Alamos Scientific Laboratories.[1]

The Third ERDA Statistical Symposium is planned for October 26-28, 1977, at the Pacific Northwest Laboratories. MSRD will be responsible for the publication of these proceedings.

UNION CARBIDE CORPORATION APPLIED MATHEMATICS SYMPOSIUM

The third Union Carbide Corporation Applied Mathematics Symposium, organized by C. K. Bayne and D. G. Wilson of MSRD, was held April 18-19, 1977, in the ORAU administration building at Oak Ridge. The purpose of the symposium was to bring together practitioners of applied mathematical techniques within Union Carbide. Participants consisted of 36 applied mathematicians, statisticians, engineers, and computer scientists from 11 Union Carbide installations. Nine talks were given in three technical sessions. From MSRD, A. D. Solomon presented a paper titled, "The Response of a Latent Heat Thermal Energy Storage Process to a Sinusiodal Input Temperature," and D. A. Gardiner served as a session chairman.

1. *Proc. Second ERDA Stat. Symp.*, LA-6758-C (April 1977).

SEMINAR SERIES

A. D. Solomon, on sabbatical leave from David Ben Gurion University, organized a colloquium on moving boundary problems. This colloquium began in October 1976 and continued through June 1977. Participants were mainly from MSRD, but there were attendees from the Computing Applications Department and the Chemistry, Metals and Ceramics, and Engineering Technology divisions. The speakers' names and the titles of their talks are given at the end of this section.

R. C. Ward of MSRD and R. J. Plemmons of the mathematics department of the University of Tennessee organized a seminar series on matrix methods in Numerical Analysis. This series started in January and continued into March. The speakers' names and the titles of their talks are given at the end of this section.

F. L. Miller, Jr., coordinated the continuing department seminar series. These seminars are intended to acquaint the MSRD staff with each other's work and to encourage interaction. Occasional outside speakers are also invited to inform us on research in progress at ORNL and at other facilities. The speakers' names and the titles of their talks are listed at the end of this section.

IN-HOUSE CONTINUING EDUCATION PROGRAM

T. L. Hebble and R. C. Ward taught the statistical and numerical linear algebra sections, respectively, of the course entitled "Numerical Analysis—Least Squares" coordinated by R. E. Funderlic of the Computing Applications Department, CSD, UCC-ND. The course consisted of eight 2-hr lectures subdivided as follows: one lecture on applications, three lectures on numerical linear algebra approaches, three lectures on statistical approaches, and one lecture on available software. Fifteen employees enrolled and completed the course during the 1977 winter session.

J. J. Beauchamp and T. J. Mitchell taught a 10-week course entitled Practical Statistics. The purpose of the course was to acquaint the participants with statistical methods applicable to problems of concern to ORNL and the UCC-ND. The course emphasized (1) point and interval estimation, including the calculation of standard errors of functions of measured variables, and statistical inference (e.g., hypothesis testing); (2) regression analysis; and (3) experimental design. The course was given in the fall quarter to 24 students and, because of the overwhelming demand, again in the winter quarter to 22 students.

UCLA SHORT COURSE

T. J. Mitchell of MSRD and Professor Norman Draper of the University of Wisconsin gave a one-week course on "Regression Analysis and Response Surface Applications," April 4–8, 1977, for the University Extension, UCLA.

MOVING BOUNDARY PROBLEMS WORKSHOP

A. D. Solomon organized a one-day workshop on moving boundary problems at which six researchers from five different divisions of ORNL spoke about their problems. The workshop was held in the Environmental Sciences Building at ORNL on May 5, 1977. D. G. Wilson of MSRD served as session chairman.

VISITING UNIVERSITY FACULTY

A. Berman of the Mathematics Department of the Technion in Haifa, Israel, spent the summer of 1976 working with R. C. Ward of MSRD on matrix theory problems. With R. S. Varga of Kent State University they published a report, ORNL CSD-21, on matrices with nonpositive off-diagonal elements.

A. D. Solomon joined the department in September 1976. He is on extended leave from his post as chairman of the mathematics department at the David Ben Gurion University, Beersheva, Israel. He has been working with D. G. Wilson on moving boundary problems and with the Engineering Technology Division of ORNL on problems related to thermal energy storage by a phase-change material.

B. W. Turnbull of Cornell University is working with MSRD staff analyzing biological data. He arrived June 8, 1977, for a stay of approximately three months.

ORAU TRAVELING LECTURERS

Six department members participated in the ORAU Traveling Lecture Program this last year. They were J. J. Beauchamp, T. L. Hebble, F. L. Miller, Jr., T. J. Mitchell, A. D. Solomon, and R. C. Ward. The titles of their talks and the dates and locations where they were given are listed at the end of this section.

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.

John Klein, a Ph.D. candidate in statistics at the University of Missouri, spent June 1977 of this report period (and will spend the summer) working with T. J. Mitchell of MSRD, J. B. Storer of the Biology Division, and B. W. Turnbull, a visiting professor of Operations Research from Cornell, analyzing data from experiments on the effect of low-level radiation on mice.

Two students, Steve Blume from Iowa State University and Dan Callon from Franklin College, worked with department members in the summer of 1976 as ORAU Summer Student Research Trainees. Keaven Anderson, a graduate of Iowa State University now doing graduate work at Stanford, was a summer employee with the department in 1976 and again in 1977. Bob Wolfson and Mike Slocum from Kalamazoo College spent the fall quarter of 1976 with the department under the auspices of the Great Lakes Colleges Association. Roy Tamura from Oberlin College worked with several department members during the month of January.

CONSULTANTS

P. M. Anselone, Oregon State University.
E. H. Lee, Stanford University.
C. S. Lever, Oak Ridge.
D. S. Robson, Cornell University.
L. R. Shenton, University of Georgia.
M. Sobel, University of California, Santa Barbara.
D. L. Solomon, Cornell University.

MSRD MOVING BOUNDARY PROBLEMS COLLOQUIUM SPEAKERS

D. G. Wilson, "A Uniqueness Theorem for the Stefan Problem," October 14, 1976

L. J. Gray, "On W. Kyner's Existence Proof for a Free Boundary Problem of the Heat Equation," October 21, 1976

A. D. Solomon, "On the Asymptotic Behavior of Solutions of Phase Change Problems - a Paper of A. Friedman," October 28, 1976

S.-J. Chang, "Some Exact Solutions for the Moving Boundary Problems of the Heat Equation," November 4, 1976

S.-J. Chang, "On an Exact Similarity Solution to a Multi-Phase Stefan Problem," November 11, 1976

R. C. Ward, "On the Numerical Solution of a Phase Change Problem," November 18, 1976

D. G. Wilson, "A Weak Solution Numerical Method for Phase Change Problems," December 2, 1976

A. D. Solomon, "The Solution of Moving Boundary Problems via a Change of Variable Method," December 9, 1976

A. D. Solomon, "On a Method of Lines Approach to the Numerical Solution of a One-Phase Stefan Problem," December 16, 1976

A. D. Solomon, "An Integro-differential Equation Method for Freezing of a Corner," December 30, 1976

R. C. Ward, "The Use of Tau Methods for Moving Boundary Problems," January 6, 1977

S.-J. Chang, "A Laplace Transform Approach to Moving Boundary Problems," January 13, 1977

D. G. Wilson, "Moment Methods for Moving Boundary Problems," January 20, 1977

L. J. Gray, "A Phase Change Problem for a Wedge," January 27, 1977

R. J. Ribando, Engineering Technology, "Convective Instability in a Melt Layer Being Heated from Below," February 3, 1977

S.-J. Chang, "Boundary Layer Temperature Profiles in Freezing Liquid Metals to Bernard Convection," February 10, 1977

A. D. Solomon, "Freezing of Liquids in Forced Flow Inside Circular Tubes," February 17, 1977

A. D. Solomon, "The Effect of Melting in Heat Transfer to Submerged Bodies," February 24, 1977

R. J. Ribando, Engineering Technology, "The Melting of Ice in a Hot, Humid Stream of Air," March 3, 1977

L. J. Gray, "Solidification of Molten Steel," March 10, 1977

D. G. Wilson, "An Analysis of the Dip Soldering," March 17, 1977

Ilana Siman-Tov, "Heat Transfer in Continuous Casting Machine Molds," March 24, 1977

J. V. Wilson, Engineering Technology, "A Model of Heat Transfer in Fluidized Beds," March 31, 1977

Ilana Siman-Tov, Computer Sciences, "A Coupled Flow and Phase-Change Problem in a Porous Medium," April 14, 1977

A. D. Solomon, "On the Freezing of Sea Water," April 21, 1977

D. G. Wilson, "Unsteady-State Diffusion or Heat-Conduction with Moving Boundary," April 28, 1977

L. J. Gray, "A Moving Boundary Problem Arising in Statistical Decision Theory," May 12, 1977

A. D. Solomon, "A Model of a Cryosurgical Procedure," May 19, 1977

A. D. Solomon, "Solidification of a Semitransparent Material," May 26, 1977

A. D. Solomon, "On Freeze Drying in Food Processing," June 2, 1977

S.-J. Chang, "Moving Boundary Problems in Elastic-Plastic Medium," June 9, 1977

J. V. Wilson, Engineering Technology, "On the Growth of Bubbles," June 16, 1977

UT-MSRD SEMINARS ON MATRIX METHODS IN NUMERICAL ANALYSIS

R. J. Plemmons, University of Tennessee, "Block Iterative Methods for Large Sparse Least Squares Problems," January 7, 1977

J. E. Cope, CSD, UCC-ND, "Bounds on Solutions of Linear Systems with Inexact Data," January 21, 1977

R. T. Gregory, University of Tennessee, "Computing Eigenvalues Using a Norm-Reducing Jacobi-Like Algorithm," January 28, 1977

S. H. Watson, CSD, UCC-ND, "Applying Matrix Techniques to Health Physics Problems," February 4, 1977

C. P. Huang, University of Tennessee, "Global Convergence of the Shifted QR Algorithm for Normal Matrices," February 11, 1977

M. T. Heath, Stanford University, "Partial Hessian Update in Constrained Optimization," February 17, 1977

R. E. Bank, University of Chicago, "Marching Algorithms for Elliptic Boundary Value Problems," February 24, 1977

B. W. Rust, CSD, UCC-ND, "Least-Squares Analysis of Time Series," March 4, 1977

M. D. Gunzburger, University of Tennessee, "Some Open Matrix Problems in Numerical PDE," March 11, 1977

MSRD DEPARTMENT SEMINARS

R. C. Meacham, "Time Sharing and Terminal Usage," July 1, 1976

J. A. John, The University, Southampton, England, "Outliers in Factorial Experiments," August 16, 1976

A. Berman, Israel Institute of Technology, "Diagonal Solutions to the Lyapunov Equation," August 17, 1976

W. S. Chern, Energy Division, "Econometric Techniques in Energy Modeling," August 18, 1976

R. S. Varga, Kent State University, "Zeros and Poles of Padé Approximations to exp(x)," August 31, 1976

T. J. Mitchell, "Ridge Regression," September 1, 1976

R. A. McLean, "Restriction Errors in Experimental Design Models," September 8, 1976

J. R. Van Ryzin, University of Wisconsin, "Nonparametric Bayesian Estimation of Survival Curves," September 16, 1976

G. H. Golub, Stanford University, "Numerical Quadrature and Inverse Eigenvalue Problems," September 22, 1976

T. C. T. Ting, University of Illinois, "Propagation of Discontinuities in Nonlinear Media," September 29, 1976

S.-J. Chang, "A Problem of Elastic Wave Diffraction," October 13, 1976

J. E. Akin, University of Tennessee, "Basic Concepts of Finite Element Analysis," October 6, 1976

James Godbold, ORAU Medical Division, "An Adaptive Approach to Multiple Comparisons," October 20, 1976

Charles Van Loan, Cornell University, "Some Computational Problems in Connection with the Linear Optimal Regulator Problem," October 27, 1976

R. C. Meacham, "Time Sharing and Graphics," November 3, 1976

D. G. Gosslee, "Statistical Aspects of Enzyme Kinetics Experiments," November 10, 1976

A. D. Solomon, "How to Model a Solar Energy Storage Unit," November 17, 1976

S. Serbin, University of Tennessee, "Approximate Methods for Time-Dependent Problems Obtained by Rational Approximation," December 1, 1976

Max Gunzburger, University of Tennessee, "Stability of Finite Element Methods for Hyperbolic Partial Differential Equations," December 8, 1976

S.-J. Chang, "A Discussion of the Lax-Wendroff Method for Conservation Laws," December 15, 1976

D. G. Wilson, "The Moving Boundaries Defined by a Similarity Solution of a Multiphase Stefan Problem," January 5, 1977

R. C. Ward, "The Theory and Application of Statistical Error Analysis," January 12, 1977

T. L. Hebble, "Designing a Membership Survey for the American Welding Society," January 19, 1977

L. J. Gray, "Introduction to Wiener-Feynman Integrals and Their Numerical Approximation," January 26, 1977

G. Novelli, Biology Division, "The Potential Use of Tumor Specific Transfer Factor in Treating Human Cancer," February 2, 1977

C. K. Bayne, "Analysis of Unbalanced Data with SAS.76," February 9, 1977

V. E. Kane, "Robust Estimation with Unusual Estremes in the Data," February 16, 1977

K. O. Bowman, "Certain Aspects of Divergent Series," February 23, 1977

F. L. Miller, Jr., "Leukemia Incidence in Hiroshima and Nagasaki," March 2, 1977

W. E. Lever, "Experiences with ERDA, EPRI, and the Electric Utility Industry," March 9, 1977

J. J. Beauchamp, "A Model to Describe the Change in Concentration of Polycyclic Aromatric Hydrocarbons and Amines in Daphnia," March 16, 1977

J. R. Whiteman, Brunel University, Middlesex, England, "Variational Inequalities with Applications to Moving Boundary Problems," March 23, 1977

A. D. Solomon, "The Effect of Adding a Good Conducting Filler Material to the pcm in a Latent Heat Storage Mechanism," March 30, 1977

S.-J. Chang, "Plastic Deformation of Metals at Finite Strains," April 6, 1977

Denis Newbold, Environmental Sciences, "Problems with a Test for Pollution Effects Based on Ranked Ecological Distances," April 13, 1977

T. J. Mitchell, "Approximate Experimental Designs for Detecting Model Inadequacy," April 27, 1977

D. G. Gosslee, "Statistical Analysis of Mutation Frequencies—Two Examples," May 4, 1977

Wei-O Wong, Comparative Animal Research Laboratory, "Univariate Versus Multivariate Tests in Repeated-Measures Experiments," May 11, 1977

M. D. Morris, "Designs for the Detection of Inadequacy in Factorial Models," May 18, 1977

D. G. Wilson, "Uniqueness and Nonexistence for Similarity Solutions of One-Dimensional Multi-Phase Stefan Problems," June 1, 1977

R. C. Ward, "Lanczos Algorithm and Computing Entries of a Matrix Inverse," June 8, 1977

L. J. Gray, "Optimal Designs, (0,1) Matrices, and a Conjecture of T. J. Mitchell," June 22, 1977

T. L. Hebble, "Potpourri," June 29, 1977

ORAU TRAVELING LECTURE PRESENTATIONS

J. J. Beauchamp, "Larval Fish, Power Plants, and Buffon's Needle Problem," University of Missouri, Columbia, November 29, 1976; Thomas More College, Covington, Kentucky, March 30, 1977

T. L. Hebble, "Developing Mathematical Models in the Physical Sciences," University of Lowell, Lowell, Massachusetts, October 19, 1976; University of Puerto Rico, Ponce Regional College, Ponce, Puerto Rico, April 26, 1977; University of Puerto 'ico, Mayaguez, Puerto Rico, April 27, 1977; University of Puerto Rico, Rio Piedras, Puerto Rico, May 3, 1977

F. L. Miller, Jr., "Data Analysis in the Physical Sciences," Virginia Commonwealth University, Richmond, March 4, 1977

T. J. Mitchell, "Designs for Detecting Model Inadequacy in Factorial Experiments," Texas A&M University, College Station, March 31, 1977

A. D. Solomon, "Thermal Energy Storage Unit," University of Wisconsin, Eau Claire, November 9, 1976

R. C. Ward, "Numerical Algorithms for the Solution of the Generalized Eigenvalue Problem," Memphis State University, Memphis, Tennessee, September 23, 1976; Mississippi State University, Starkville, November 10, 1976; Appalachian State University, Boone, North Carolina, November 15, 1976; University of Tennessee at Chattanooga, March 30, 1977; Cornell University, Ithaca, New York, April 15, 1977

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Part D. Presentation of Research Results

Publications

BOOKS AND PROCEEDINGS

J. W. Arendt,[1] T. R. Butz,[1] G. W. Cagle,[1] V. E. Kane, and C. E. Nichols,[1] "A New Approach for Geochemical Surveys of Large Areas for Uranium Resource Potential," *Proceedings of the International Atomic Energy Agency on Nuclear Power and Its Fuel Cycle*, to be published.

K. O. Bowman and L. R. Shenton,[2] "Summing Asymptotic Moment Series," pp. 121-25 in *Proceedings of the Statistical Computing Section*, American Statistical Association, Washington, D.C., 1976.

S.-J. Chang and L. J. Zapas,[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, 1976.

S.-J. Chang and T. C. T. Ting,[4] "Boundary Reflections of the Diffracted Waves from a Semi-Infinite Crack," *Proceedings, 6th Canadian Congress of Applied Mechanics*, University of British Columbia, Vancouver, B.C., Canada, to be published.

W. M. Generoso,[5] Katherine T. Cain,[5] Sandra W. Huff,[5] and D. G. Gosslee, "Heritable Translocation Test in Mice," chapter in *Chemical Mutagens—Principles and Methods for Their Detection*, vol. V, ed. Alexander Hollaender, Plenum Press, accepted.

W. M. Generoso,[5] Katherine T. Cain,[5] Sandra W. Huff,[5] 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., in press.

V. E. Kane, "Clustering Problems for Geochemical Data," *Proceedings of the Second ERDA Statistical Symposium*, LA-6758-C, Los Alamos Scientific Laboratory, Los Alamos, N.M., April 1977.

V. E. Kane, "Data Verification Procedures," *Proceedings of the Symposium on Hydrogeochemical and Stream Sediment Reconnaissance for Uranium in the United States*, to be published.

V. E. Kane, "Geostatistics," *Proceedings of the Symposium on Hydrogeochemical and Stream Sediment Reconnaissance for Uranium in the United States*, to be published.

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1. Uranium Resource Evaluation Project.
2. University of Georgia.
3. National Bureau of Standards.
4. University of Illinois at Chicago Circle.
5. Biology Division.

G. D. Kerr,[6] T. D. Jones,[6] J. M. L. Hwang,[6] F. L. Miller, Jr., and J. A. Auxier,[6] "Air Analysis of Leukemia Data from Studies of Atomic Bomb Survivors Based on Estimates of Absorbed Dose to Active Bone Marrow," *Proceedings, 4th International Congress of the International Radiation Protection Association*, IRPA, Paris, 1977.

P. Mazur,[5] N. Rigopoulos,[5] F. L. Miller, Jr., and S. S. Stevens,[5] "Computer-Assisted Techniques for the Estimation of Cell Volumes During the Permeation of Glycerol into Multicellular Mouse Embryos," *Proceedings, Society for Cryobiology*, Minneapolis, 1977.

T. J. Mitchell, "Analysis of Disease Incidence Data from Survival Experiments," *Proceedings of the Second ERDA Statistical Symposium*, LA-6758-C, Los Alamos Scientific Laboratory, Los Alamos, N.M., April, 1977.

R. C. Ward, "Statistical Roundoff Error Analysis of a Padé Algorithm for Computing the Matrix Exponential," *Proceedings of the Conference on Padé and Rational Approximation*, ed. E. B. Saff and R. S. Varga, Academic Press, New York, to be published.

JOURNAL ARTICLES

A. Berman[7] and R. C. Ward, "*ALPS*: Classes of Stable and Semipositive Matrices," *J. Linear Algebra Its Appl.*, submitted.

A. Berman,[7] R. S. Varga,[8] and R. C. Ward, "*ALPS*: Matrices with Nonpositive Off-Diagonal Entries," *J. Linear Algebra Its Appl.*, submitted.

A. Berman[7] and R. C. Ward, "Stability and Semipositivity of Re... Matrices," *Bull. AMS* 83, 262-63 (1977).

M. K. Booker,[9] T. L. Hebble, D. O. Hobson,[9] and C. R. Brinkman, "Mechanical Property Correlations for 2¼ Cr-1 Mo Steel in Support of Nuclear Reactor Systems Design," *Int. J. Pressure Vessels Piping*, submitted.

K. O. Bowman and L. R. Shenton,[2] "A New Algorithm for Summing Divergent Series, Part II: Two-Component Borel Summability Model," *J. Comput. Appl. Math.* 2, 259-66 (1976).

K. O. Bowman, "Some Quality Control Activity in Japan," *ONR Tokyo Sci. Bull.* 2 (1977).

K. O. Bowman, "Japanese Government Statistical Activities," *ONR Tokyo Sci. Bull.* 2 (1977).

K. O. Bowman, J. J. Beauchamp, and L. R. Shenton,[2] "The Distribution of the *t*-Statistic under Non-Normality," *Int. Stat. Rev.*, submitted.

K. O. Bowman and L. R. Shenton,[2] "Asymptotic Series and Stieltjes Continued Fractions for a Gamma Function Ratio," *J. Comput. Appl. Math.*, submitted.

R. E. Cline[10] and R. E. Funderlic,[11] "The Rank of a Difference of Matrices and Associated Generalized Inverses," *J. Linear Algebra Its Appl.*, accepted.

E. H. Curtis,[12] J. J. Beauchamp, and B. G. Blaylock,[13] "Application of Various Mathematical Models to Data from the Uptake of Methyl Mercury in Bluegill Sunfish (*Lepomis macrochirus*)," *Ecol. Modelling*, to be published.

6. Health Physics Division.
7. Technion-Israel Institute of Technology, Israel.
8. Kent State University.
9. Metals and Ceramics Division.
10. University of Tennessee.
11. Computing Applications Department.
12. Curtis and Associates, Terre Haute, Indiana.
13. Environmental Sciences Division.

T. A. DeRouen[14] and T. J. Mitchell, "An Application of *G*-Minimax Techniques to the Problem of Fixed Precision Estimation of the Binomial," *J. Stat. Comput. Simulation*, submitted.

W. E. Dusenberry[15] and K. O. Bowman, "The Moment Estimator for the Shape Parameter of the Gamma Distribution," *Commun. Stat., Part B, Simulation Computation*, to be published.

S. F. Ebey[16] and J. J. Beauchamp, "Larval Fish, Power Plants, and Buffon's Needle Problem," *Am. Math. Mon.*, to be published.

J. W. Elwood,[13] S. G. Hildebrand,[13] 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.* 33, 1930-38 (1976).

D. A. Gardiner, V. R. R. Uppuluri, and S. A. Patil,[17] "Inferences About Rare Events," *Technometrics*, submitted.

L. J. Gray, "Jordan Representation for a Class of Nilpotent Operators," *Indiana Univ. Math. J.* 26, 57-64 (1977).

L. J. Gray, "Operators Commuting with a Compact Quasi-Affinity," *Proc. AMS*, to be published.

L. J. Gray, "Perturbation of the Essential Central Spectrum," *Proc. AMS*, submitted.

L. J. Gray, "Products of Hermitian Operators," *Proc. AMS* 59, 123-26 (1976).

L. J. Gray and T. Kaplan,[18] "Disordered Systems with Short-Range Order," *J. Phys. C* 9, L483-87 (1976).

L. J. Gray and T. Kaplan,[18] "Distribution of Vibrational Modes in an Amorphous Linear Chain," *Physica* 83B, 310-13 (1976).

L. J. Gray and T. Kaplan,[18] "Elementary Excitations in Disordered Systems with Short-Range Order," *Phys. Rev.* 15, 3260-66 (1977).

L. J. Gray and T. Kaplan,[18] "Elementary Excitations in Random Substitutional Alloys, *Phys. Rev.* 14, 3462-70 (1976).

L. J. Gray and T. Kaplan,[18] "Off-Diagonal Disorder in Random Substitutional Alloys," *J. Phys. C* 9, L303-7 (1976).

L. J. Gray and D. G. Wilson, "Construction of a Jacobi Matrix from Spectral Data," *J. Linear Algebra Its Appl.* 14, 131-34 (1976).

T. L. Hebble, P. Patriarca,[7] G. M. Goodwin,[7] and R. T. King,[7] "A Summary of Results from Pilot Membership Surveys," *Weld. J. (Miami, Fla.)*, to be published.

S. E. Herbes[11] and J. J. Beauchamp, "Toxic Interaction of Mixtures of Two Coal Conversion Effluent Components (Resorcinol and 6-Methylquinoline) to *Daphnia magna*," *Bull. Env. Contam. Toxicol.* 17, 25-32 (1977).

M. D. Hogan,[19] P. Y. Chi,[19] T. J. Mitchell, and D. G. Hoel,[19] "Association Between Chloroform Levels in Finished Drinking Water Supplies and Various Site-Specific Cancer Mortality Rates," *Am J. Epidemiology*, submitted.

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14. University of Washington.
15. University of Utah Medical Center.
16. University of the South, Sewanee, Tennessee.
17. Tennessee Technological University, Cookeville, Tennessee.
18. Solid State Division
19. National Institute of Environmental Health Sciences, Research Triangle Park, North Carolina.

J. M. Holland,[5] T. J. Mitchell, and H. E. Walburg, Jr.,[20] "Effects of Prepubertal Ovariectomy on Survival and Specific Diseases in Female RFM Mice Given 300R of X Rays," *Radiat. Res.* 69, 317–27 (1977).

J. A. John[21] and T. J. Mitchell, "Optimal Incomplete Block Designs," *J. R. Stat. Soc., Ser. B* 39 (1977), in press.

V. E. Kane, "Statistical Models for X Chromosome Inactivation," *Biometrics*, submitted.

A. P. Li,[22] D. G. Gosslee, D. S. Robson,[23] and A. W. Hsie,[5] "Steady-State Kinetics Studies on the Adenosine 3':5'-Phosphate-dependent Protein Kinase in Chinese Hamster Ovary Cells," *Biophys. Biochem. Acta*, submitted.

S. B. McLaughlin,[13] N. T. Edwards,[13] and J. J. Beauchamp, "Spatial and Temporal Patterns in Transport and Respiratory Allocation of ^{14}C-Sucrose by White Oak (*Quercus alba* L.) Roots," *Can. J. Botany*, submitted.

T. J. Mitchell and C. K. Bayne, "D-Optimal Fractions of Three-Level Factorial Designs," *Technometrics*, submitted.

C. P. Quesenberry[24] and F. L. Miller, Jr., "Power Studies of Some Tests for Uniformity," *J. Stat. Comput. Simulation* 5, 169–91 (1977).

L. R. Shenton[2] and K. O. Bowman, "A New Algorithm for Summing Divergent Series, Part I: Basic Theory and Illustrations," *J. Comput. Appl. Math.* 2, 151–67 (1976).

L. R. Shenton[2] and K. O. Bowman, "A New Algorithm for Summing Divergent Series, Part III: Application," *J. Comput. Appl. Math.* 3, 35–51 (1977).

L. R. Shenton[2] and K. O. Bowman, "A Bivariate Model for the Distribution of $\sqrt{b_1}$ and b_2," *J. Am. Stat. Assoc.* 72, 206–11 (1977).

L. R. Shenton[2] and K. O. Bowman, "Generalized Continued Fractions and Whittaker's Approach," *J. Comput. Appl. Math.*, submitted.

V. K. Sikka,[9] R. W. Swindeman,[9] T. L. Hebble, C. R. Brinkman,[9] and M. K. Booker,[9] "Residual Cold Work and Its Influence on Tensile Properties of Types 304 and 316 Stainless Steels," *Nucl. Tech.* 31, 96–114 (1976).

R. C. Ward, "Numerical Computation of the Matrix Exponential with Accuracy Estimate," *SIAM J. Numer. Anal.*, to be published.

R. C. Ward and L. J. Gray, "Eigensystem Computation for Skew-Symmetric Matrices and a Class of Symmetric Matrices," *ACM Trans. Math. Software*, submitted.

R. C. Ward and L. J. Gray, "The ZD Algorithm to Solve the Eigenvalue Problem for Skew-Symmetric and a Class of Symmetric Matrices," *ACM Trans. Math. Software*, Algorithms Section, submitted.

D. G. Wilson, "Existence and Uniqueness for Similarity Solutions of One-Dimensional Multi-Phase Stefan Problems," *SIAM J. Appl. Math.*, submitted.

D. G. Wilson, "Piecewise Linear Approximations to Tabulated Data," *ACM Trans. Math. Software* 2, 388–91 (1976).

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20. Comparative Animal Research Laboratory.
21. The University of Southampton, England.
22. Cancer Research and Treatment Center, University of New Mexico, Albuquerque, New Mexico.
23. Biometrics Unit, Cornell University, Ithaca, New York.
24. North Carolina State University.

REPORTS

A. Berman[7] and R. C. Ward, *ALPS: Classes of Stable and Semipositive Matrices*, ORNL/CSD-14 (October 1976).

A. Berman,[7] R. S. Varga,[8] and R. C. Ward, *ALPS: Matrices with Nonpositive Off-Diagonal Entries*, ORNL/CSD-21 (March 1977).

A. J. Caputo,[9] D. R. Johnson,[9] and C. K. Bayne, *Argon Permeability of Graphite Fuel Elements for High-Temperature Gas-Cooled Reactors*, ORNL/TM-5816 (May 1977).

S.-J. Chang, "An Analytical Solution for the Dynamic Far-Field Stresses Generated by a Suddenly Appearing Crack," *Heavy-Section Steel Technology Program Quarterly Progress Report for July-September, 1976*, ed. G. D. Whitman, ORNL/NUREG/TM-64 (January 1977).

R. E. Cline[10] and R. E. Funderlic,[11] *The Rank of a Difference of Matrices and Associated Generalized Inverses*, U. Tenn. CS-76/20 (November 1976).

V. E. Kane, T. Baer,[25] and C. L. Begovich,[11] *Principal Component Testing for Outliers*, K/UR-7 (to be published).

V. E. Kane, N. M. Larson,[11] and V. C. Nall,[11] *Computer Program to Generate Pearson, Kendall, and Spearman Correlations*, K/UR-8 (to be published).

W. E. Lever and R. S. Leete, Jr.,[26] *A Study of the Relationship of Three Factors on Errors in Inspection*, UCCND/Y-2075 (April 1977).

T. J. Mitchell and C. K. Bayne, *D-Optimal Fractions of Three-Level Factorial Designs*, ORNL/CSD-19 (January 1977).

M. D. Morris[27] and T. J. Mitchell, *Designs for the Detection of Inadequacy in Factorial Models*, ORNL/CSD/TM-30 (July 1977).

Oral Presentations

J. J. Beauchamp, "Larval Fish, Power Plants, and Buffon's Needle Problem," presented at the Mid-Missouri Chapter of the American Statistical Association, Columbia, Missouri, November 29, 1976.

K. O. Bowman and L. R. Shenton,[2] "Summing Asymptotic Moment Series," presented at the joint meeting of the American Statistical Association and the Biometric Society, Boston, Massachusetts, August 23-26, 1976.

K. O. Bowman, "The Test for Departure from Normality," presented at the Hiroshima University, Hiroshima, Japan, May 10, 1977.

K. O. Bowman, "A Bivariate Model for the Distribution of $\sqrt{b_1}$ and b_2," presented at the Radiation Effects and Research Facilities, Hiroshima, Japan, May 11, 1977.

K. O. Bowman, "Test of Normality and the Japanese-American Statistician," presented at Tokyo University, Tokyo, Japan, May 31, 1977.

K. O. Bowman, "The New Test for Departure from Normality," presented at the Institute of Statistical Mathematics, Tokyo, Japan, June 1, 1977.

25. Technical Services Division, K-25.
26. Technical Division, Y-12.
27. Virginia Polytechnic Institute and State University, ORAU Graduate Fellow.

A. J. Caputo,[9] D. R. Johnson,[9] and C. K. Bayne, "Gas Permeability of Graphite Fuel Elements for the High-Temperature Gas-Cooled Reactor," presented at the American Ceramic Society meeting, Chicago, Illinois, April 23-28, 1977.

A. J. Caputo,[9] D. R. Johnson,[9] and C. K. Bayne, "Process Variables Affecting In-Block Carbonization of HTGR Fuel Elements," presented at the American Ceramic Society meeting, Chicago, Illinois, April 23-28, 1977.

S.-J. Chang and T. C. T. Ting,[4] "Boundary Reflection of the Diffracted Waves from a Semi-Infinite Crack," presented at the 6th Canadian Congress of Applied Mechanics, Vancouver, B.C., Canada, May 30-June 3, 1977.

J. E. Cope[11] and B. W. Rust,[11] "Bounds on Solutions of Linear Systems with Inaccurate Coefficients and Right-Hand Sides," presented at the SIAM Fall Meeting, Atlanta, Georgia, October 19, 1976, and at the Third Union Carbide Corporation Applied Mathematics Symposium, Oak Ridge, April 19, 1977.

D. G. Gosslee, "The Statistical Design and Analysis of Enzyme Kinetic Experiments," presented to the University of Tennessee-Oak Ridge Graduate School of Biomedical Sciences, Oak Ridge, February 7 and 9, 1977.

D. G. Gosslee, "The Statistical Properties of Sequential Chemical Mutagenicity Tests," presented at the Heritable Translocation Workshop, Stanford Research Institute, Menlo Park, California, May 26, 1977.

L. J. Gray, "Approximation of Wiener-Feynman Integrals," presented at the American Mathematical Society meeting, Toronto, Canada, August 25, 1976.

T. L. Hebble, "On the Use of Historic Data to Establish Standards for Elevated Temperature Application," presented at the TMS/AIME Fall Meeting, Niagara Falls, New York, September 20, 1976.

T. L. Hebble, "Estimating Heat-to-Heat Variation in Mechanical Properties from a Statistician's Point of View," presented at the 1976 ASME International Joint Petroleum Mechanical Engineering and Pressure Vessels and Piping Conference, Mexico City, Mexico, September 22, 1976.

T. L. Hebble, "AWS Membership Survey: Analysis of Pilot Surveys of the Houston and Niagara Frontier Sections," presented at the American Welding Society Committee on Long-Range Goals and Objectives, Miami, Florida, November 8, 1976.

V. E. Kane, "Clustering Problems for Geochemical Data," presented at the Second ERDA Statistical Symposium, Oak Ridge, October 25-27, 1976.

V. E. Kane, "Geostatistics," presented at the Symposium on Hydrogeochemical and Stream Sediment Reconnaissance for Uranium in the United States, Grand Junction, Colorado, March 16-17, 1977.

V. E. Kane, "Data Verification Procedures," presented at the Symposium on Hydrogeochemical and Stream Sediment Reconnaissance for Uranium in the United States, Grand Junction, Colorado, March 16-17, 1977.

T. J. Mitchell, "Analysis of Disease Incidence Data from Survival Experiments," presented at the Second ERDA Statistical Symposium, Oak Ridge, October 25-27, 1976.

T. J. Mitchell and M. D. Morris,[27] "Designs for Detecting Model Inadequacy in Factorial Experiments," presented at the Spring Meeting of the Southeast Texas Chapter of the American Statistical Association, College Station, Texas, March 31, 1977.

T. J. Mitchell, E. R. Jones,[28] and M. D. Morris,[27] "Optimal Designs for Detecting Model Inadequacy," presented at Cornell University, Ithaca, New York, May 12, 1977, and at the Joint Meetings of the Institute of Mathematical Statistics (Central Region) and the American Statistical Association, Madison, Wisconsin, May 16-18, 1977.

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28. Institute of Statistics, Texas A&M University.

A. D. Solomon, "The Response of a Latent Heat Thermal Energy Storage Process to a Sinusoidal Input Temperature," Third Union Carbide Corporation Applied Mathematics Symposium, Oak Ridge, April 18, 1977.

R. C. Ward, "Quality Software for Computing the Matrix Exponential," invited paper, Conference on Padé and Rational Approximation, Tampa, Florida, December 15-17, 1977.

ARTICLES REVIEWED OR REFEREED FOR PERIODICALS

Reviewer or referee	Number of articles reviewed or refereed for indicated periodical																
	ACM Trans. Math. Software	*AMS*	*Am. Stat.*	*Ann. Stat.*	*Appl. Mech. Rev.*	*Commun. Stat.*	*Comput. Rev.*	*Health Phys.*	*Int. Stand.*	*J. Appl. Mech.*	*J. R. Stat. Soc., Ser. B*	*J. Stat. Comput. Simulation*	*Math. Rev.*	*Nucl. Sci. Eng.*	*Technometrics*	Proposals	Total
Bayne, C. K.			1												1		2
Beauchamp, J. J.															1		1
Bowman, K. O.						1						1			1	1	4
Chang, S.-J.					4					1							5
Coveyou, R. R.													7	1			8
Gosslee, D. G.															1		1
Gray, L. J.		1															1
Hebble, T. L.															1		1
Lever, W. E.						1			2								3
Miller, F. L., Jr.												1					1
Mitchell, T. J.				1				1			1				2		5
Solomon, A. D.													8	1		1	10
Ward, R. C.	1																1
Wilson, D. G.							1										1
Total	1	1	1	1	4	2	1	1	2	1	1	2	15	2	7	2	44

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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
	Local Arrangements Committee, Second ERDA Statistical Symposium
Chairman:	Third Union Carbide Corporation Applied Mathematics Symposium

J. J. Beauchamp

Instructor:	Division of Mathematics and Science, Roane State Community College
Coordinator and Instructor:	In-Hours Continuing Education Program
Respresentative:	ORNL Professional Education Resource Committee
Lecturer:	Traveling Lecture Program, Oak Ridge Associated Universities

K. O. Bowman

Panelist:	Women in Science Program, National Science Foundation
Member:	Editorial Board, *Communications in Statistics; Part B, Simulation and Computation*
Liaison Scientist:	Office of Naval Research, Department of Navy
Chairman:	Local Arrangements Committee, Second ERDA Statistical Symposium

S.-J. Chang

Reviewer:	*Applied Mechanics Reviews*

R. R. Coveyou

Reviewer:	*Mathematical Reviews*
	Nuclear Science and Engineering

D. A. Gardiner

President:	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, American Statistical Association
	Executive Committee, Section on Physical and Engineering Sciences, American Statistical Association
	International Editorial Board, *Communications in Statistics; Part A, Theory and Methods*
	Editorial Board, *Journal of Statistical Computation and Simulation*

D. G. Gosslee

Lecturer:	Oak Ridge Graduate School of Biomedical Sciences, University of Tennessee

L. J. Gray

Member:	ORNL Ph.D. Recruitment Program
Participant:	NSF Summer Research Institute on Operator Theory, University of New Hampshire

T. L. Hebble

Lecturer:	Traveling Lecture Program, Oak Ridge Associated Universities

V. E. Kane

Assistant Professor:	Department of Mathematics, University of Tennessee

W. E. Lever

Member:	*Technometrics* Prize Committee
	Committee to Review International Standards in Statistics, American Statistical Association
	Local Arrangements Committee, Second ERDA Statistical Symposium

F. L. Miller, Jr.

Lecturer:	Traveling Lecture Program, Oak Ridge Associated Universities
Member:	Local Arrangements Committee, Second ERDA Statistical Symposium

T. J. Mitchell

Lecturer:	Oak Ridge Graduate School of Biomedical Sciences, University of Tennessee
	Traveling Lecture Program, Oak Ridge Associated Universities
Instructor:	In-Hours Continuing Education Program
	Continuing Education in Engineering and Mathematics, University Extension, UCLA
Member:	ORNL Graduate Fellowship Selection Panel

A. D. Solomon

Reviewer:	***Computing Reviews***
	Mathematical Reviews

R. C. Ward

Lecturer:	**Traveling Lecture Program, Oak Ridge Associated Universities**
Member:	**Applied Mathematics Committee, University of Tennessee**
Panelist:	**Panel Discussion on Directions for Research, Conference on Padé and Rational Approximation**
Reviewer:	***Computing Reviews***

D. G. Wilson

Lecturer:	**Department of Mathematics, University of Tennessee**
Reviewer:	***Computing Reviews***
Member:	**Organization Committee, Third Union Carbide Corporation Applied Mathematics Symposium**