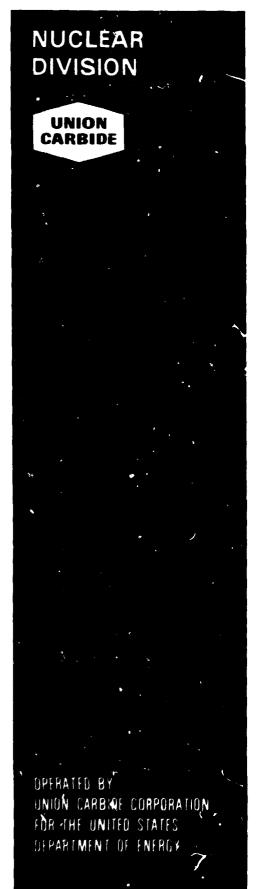
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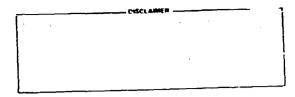
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Research Department
Progress Report

Period Ending June 30, 1981



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MATHEMATICS AND STATISTICS RESEARCH DEPARTMENT PROGRESS REPORT Period Ending June 30, 1981

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UNION CARBIDE CORPORATION—NUCLEAR DIVISION

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ORNL-3264	Period ending January 31, 1962
ORNL-3423	Period ending December 31, 1962
ORNL-3567	Period ending December 31, 1963
ORNL-3766	Period ending December 31, 1964
ORNL-3919	Period ending December 31, 1965
ORNL-4083	Period ending December 31, 1966
ORNL-4236	Period ending December 31, 1967
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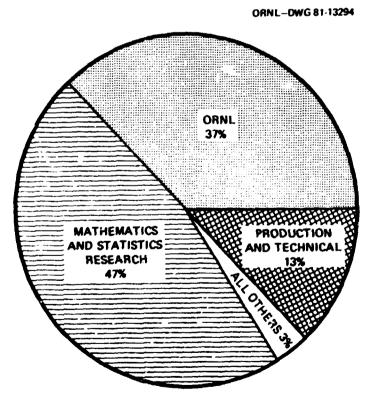
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Preface

OPERATIONS

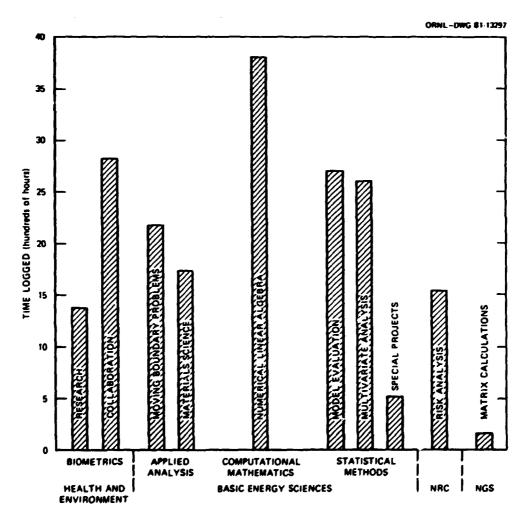
During the 12 months ending 'une 30, 1981, the Mathematics and Statistics Research Department (MSRD) logged 41,745 h of effort in research and service to the components of Union Carbide Corporation—Nuclear Division (UCC-ND). Forty-seven percent of the effort was on projects managed by MSRD, 37% was for consulting and collaboration with ORNL divisions, 13% was for the UCC-ND production and technical staff, and 3% was for all other activities. This distribution of effort is shown in the figure below. The 47%, representing 19,747 h of effort, that was spent on the projects managed by the department was allocated to six projects funded by the U.S. Department of Energy (DOE) Office of Basic Energy Sciences, two funded by the DOE Office of Health and Environmental Powearch, one by the Nuclear



Distribution of Mathematics and Statistics Research Department effort.

Regulatory Commission, and one by the National Geodetic Survey. The figure below shows the distribution of these hours. The progress made in these projects is described in the appropriate chapters of this report.

Mention should be made here of the Special Projects work done by the Statistical Methods staff. Although not as labor intensive as the other projects, it represents important co-potentially important contributions. One result of this effort was the production of the Proceedings of the 1980 DOE Statistical Symposium, which was held in Berkeley, California, in October. Another was the investigation into the feasibility of initiating a research effort in Computational Statistics. A Mini-Workshop on Computational



Distribution of time logged on MSRD-managed projects

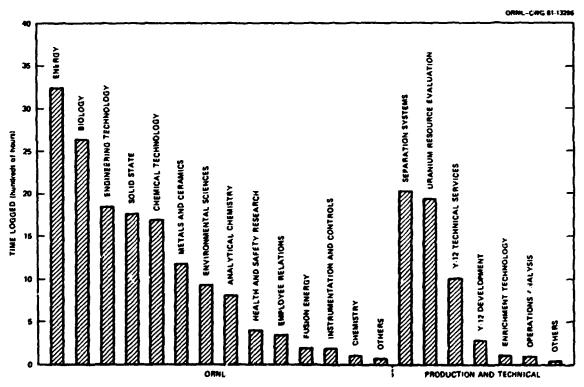
^{1.} T. Truett, D. Margolies, and R. W. Mensing, eds., Proceedings of the 1980 DOE Statistical Symposium, CONF-801045, Oak Ridge National Laboratory (April 1981).

Statistics was held in Oak Ridge in September, a working definition was composed, and plans for proceeding have been formulated.

Fifty percent of the total time logged by the department staff was devoted to assisting scientists and engineers in other units of UCC-ND. The distribution of this effort is shown in the figure below.

CONFERENCES

The department arranged an informal Mini-Workshop or Computational Statistics that was held in the department quarters on September 3 and 4, 1980. The purpose was to investigate the feasibility of organizing a research effort in this area. Seven knowledgeable statisticians and mathematicians from other institutions accepted the invitation to participate. Results of the deliberations were recorded in an informal report.²



Consultation and collaboration with other UCC-ND divisions.

^{2.} R. E. Fundertic et al., "Summary of Discussions, Mini-Workshop on Computational Statistics held on September 3, 4, 1980 in the Mathematics and Statistics Research Department," UCC-ND, January 1981.

PERSONNEL

Several personnel changes took place during the past 12 months. George Cotsonis left MSRD to resume graduate study at Emory University. Pat DiZillo-Benoit accepted an offer from American Cyanamid Company in Connecticut. Alan Zinsmeister took a position with the Mayo Clinic in Minnesota, and Will Lawrence returned to Marquette University at the end of his sabbatical.

New employees are Nancy Price in the Computing Support Section; Tammy Reed in the Secretarial Support Section; Ed Frome, Max Morris, and Rick Schmoyer in Statistics Section A; and John Carpenter in Statistics Section B.

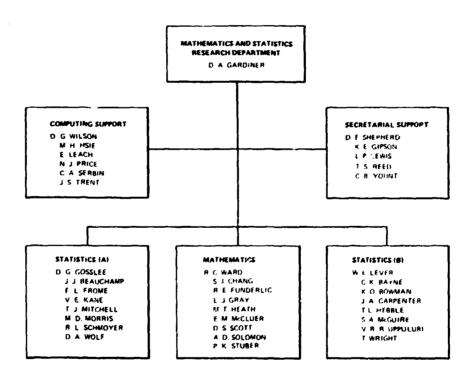
The current organization chart is shown below.

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MATHEMATICS AND STATISTICS RESEARCH DEPARTMENT COMPUTER SCIENCES DIVISION

JUNE 30, 1981



Summary

This report is the twenty-fourth in the series of progress reports of the Mathematics and Statistics Research Department of the Computer Sciences Division, Union Carbide Corporation—Nuclear Division (UCC-ND).

Part A records research progress in biometrics research, materials science applications, model evaluation, moving boundary problems, multivariate analysis, numerical linear algebra, risk analysis, and complementary areas.

Collaboration and consulting with others throughout the UCC-ND complex are recorded in Part B. Included are sections on biology and health wiences, chemistry, energy, engineering, environmental sciences, health and safety research, materials sciences, safeguards, surveys, and uranium resource evaluation.

Part C summarizes the various educational activities in which the staff was engaged. Part D lists the presentations of research results, and Part E records the staff's other professional activities during the report period.

Part A. Mathematical and Statistical Research

1. Biometries Research

D. G. Gosslee T. J. Mitchell M. D. Morris B. W. Turnbull¹ D. A. Wolf

COMPARING TWO METHODS OF MEASUREMENT FOR ACCURACY AND PRECISION

In comparing two measurement techniques, accuracy (degree of systematic error) and precision (degree of random error) are characteristics of interest. These comparisons are not difficult if the true underlying values being measured are known for some set of experimental runs. We have investigated the case in which these values are not known or repeatable and are considered to come from some unspecified distribution. For example, the application that originally motivated this research was the comparison of two devices for measuring blood pressure in nonhuman primates.

Following earlier investigators, we assume a model of the form

$$Y = a + hX + e$$
.

where, for a particular method, λ represents the measurement of λ . The parameters a and b are fixed unknown constants, usually referred to as "fixed" and "proportional" bias, respectively; they determine accuracy. The variable e is a random element with zero expectation; the variance of e determines the precision.

Grubbs introduced a procedure appropriate for comparing precisions of two methods assumed to

We have also noted a similar property for the test of the null hypothesis that pairwise differences of measurements have expertation zero. If proportional biases are assumed to be equal, the null hypothesis tests for equality of fixed biases. If fixed biases are assumed to be equal, it tests for equality of proportional biases.

When more than two methods are compared, statistical procedures exist that can be used to compare fixed bias, proportional bias, and precision. When only two methods are compared, assumptions must be made about at least one pair of parameters to allow inferences about the others. We are currently investigating (1) the joint use of the two tests mentioned above and (2) what conclusions may be drawn depending on each assumption.

ESTIMATION OF TIME TO ONSET AND TIME TO DEATH FOR SPECIFIC DISEASE

One of the main goals in the analysis of survival sacrifice experiments with animals is to estimate the time to onset of a disease and the subsequent time to death from that disease. This is not a straightforward problem because the disease is not generally detectable until death and because of the "censoring" of data from animals that die trom other causes.

We have developed an estimation procedure that can be used to classify each death into one of three

have equal proportional biases. We have noted that the hypothesis and assumption can be reversed. If equal precisions are assumed, Grubbs' procedure tests the null hypothesis that the proportional biases are equal

¹ Cornell University

² F. E. Grubbs, "On Estimating Precision of Measuring Instruments and Product Variability," J. 4m. Stat. Assoc. 43, 243-64 (1948).

types: death caused by the disease, death by competing cause (e.g., sacrifice) with the disease present, or death with the disease absent. Our method uses a two-dimensional EM algorithm to obtain the nonparametric maximum likelihood extimates of the distribution G(t) of the time (Y) to onset of the disease and the distribution F(t) of the time (X) to death from the disease. A slight modification of the algorithm enables the construction of likelihood-based confidence intervals for F(t), G(t), the medians of X and Y, and other functions of interest.

We have tested and demonstrated this method using data on reticulum cell sarcoma from an earlier study' conducted at ORNL with laboratory mice.

CONFIDENCE LIMITS FOR RELATIVE POTENCY IN THE CASE OF ZERO TUMOR RESPONSE

A major objective in the testing of potential skin carcinogens is to determine a meaningful measure of "relative potency" with respect to a standard carcinogen. We have developed a procedure, described elsewhere, for estimating the potency of various test materials relative to beilze[a]pyrene (BaP) in skin-painting experiments; the procedure uses the Weibull distribution as a model for time-to-tumor incidence. When the location parameter wand

Special difficulties occur when none of the animals subjected to the test material develop a tumor. Obviously, the best estimate of relative potency is zero in such cases; the problem is to determine an upper confidence limit.

We have found a relatively simple way of doing this for the case in which the dose-effect function h = f(d) and the shape and location parameters k and w are known for the standard (BaP). (In practice, of course, we do not know these, but estimates of them are reasonally good.) Our method is based on the computation of $L(\rho)$, the probability of observing no tumors if the true relative potency is ρ . This curve decreases from 1 to 0 as ρ increases. The interval $[0, \rho^*]$ can be shown to be a $100(1 - \alpha)^*i$ confidence interval for ρ , where $L(\rho^*) = \alpha$.

A short computer algorithm has been written to find ρ^{\bullet} , given the time on test for each animal in the test group and the required information on the BaP response. As the time on test increases (without tumor occurrence), ρ^{\bullet} decreases. This permits the experimenter to monitor an ongoing experiment in which tumors have not yet appeared, with the prospect of terminating the experiment once ρ^{\bullet} has dropped below a certain level. We also hope to use this computation as an aid in choosing in advance a sample size sufficient to yield a reasonable probability of terminating the experiment in this way if a given number of days elapse without tumor occurrence.

shape parameter k for the Weibull are assumed to be the same for both the standard and the test material, the median time to tumor is directly related to the scale parameter b. The relative potency of the test material at dose d is d⁻¹ times the BaP dose that yields the same value of b found in the test material, where b is estimated under the constraint that k and w are the same for both materials at all dose levels.

^{3.} J. M. Holland, T. J. Mitchell, and H. E. Walburg, "Effects of Prepubertal Ovariectomy on Survival and Specific Diseases in Female RFM Mice Given 300 R of X-Rays," Radiai Res. 69, 317–27 (1977).

^{4.} D. A. Wolf and T. J. Mitchell, "Statistical Analysis of Mortality and Relative Skin Carcinogenicity," appendix to J. M. Holland et al., Chronic Dermal Toxicity of Epoxy Resins, I. Skin Carcinogenic Potency and General Toxicity, ORNI-5762 (March 1981).

S.-J. Chang

S. M. Ohr

1 2

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0.6

0.4

0.2

L. J. Gray

C. A. Serbin

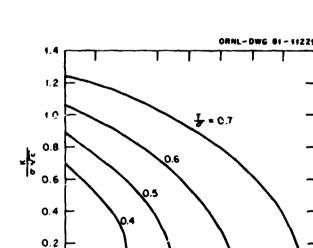
J. A. Horton

T. J. Rudolphi²

T. Kaplani

DISLOCATION-FREE ZONE MODEL OF FRACTURE

Recent observations by electron microscopy have shown that a dislocation-free zone (DFZ) exists between the crack tip and the linear pileup of dislocations in the plastic zone. 32 A singular integral equation is formulated to describe the equilibrium configuration of the dislocations. The distribution function of the dislocations is obtained in terms of elliptic integrals. The condition of compatibility and the elastic stress intensity factor at the crack tip are also derived. At the crack tip, the stress varies as $1 \sqrt{r}$. The stress intensity factor K is found to be primarily a function of the length of the DFZ. whereas the externally applied stress approximately determines the length of the plastic zone (Fig. 1). The magnitude of K is reduced as a result of the emission of dislocations from the crack tip into the plastic zone (Fig. 2). Based on the mechanism of dislocation generation at the crack tip proposed by Rice and Thomson," it is shown that the formation of the DFZ is anticipated when the stress intensity factor K is less than a critical stress intensity factor K_x defined for a spontaneous generation of dislocations. The magnitude of K, relative to the critical stress intensity factor for brittle fracture K. determines the brittle-ductile nature of a material.



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C

.01

.005

0.1

0.6

Fig. 1. Stress intensity factor K vs applied stress T for various sizes of the dislocation-free zone e/c and the plastic zone a/c.

Fig. 2. Decrease of the stress intensity factor K due to the accumulation of the emitted dislocations COP in the plastic zone.

0.8 WA COD 1.0



^{2.} Iowa State University

0

0.2

0.4

^{3.} S. M. Ohi and J. Narrayan, "Flectron Microscope Observation of Shear Cracks in Stainles: Steel Single Crystals," *Philos* Mag. A 41, 82–89 (1980).

S. Kohayashi and S. M. Ohr, "In Situ Fracture Experiments in BCC Metals," Philos. Mag. A 42, 763-72 (1980).

^{5.} S.-J. Chang and S. M. Ohr, "A Model of Shear Cracks with Dislocation-Free Zones," in Acta Scripta Metallurgica International Conf. on Dislocation Modeling of Physical Systems, ed. by C. S. Hartley (forthcoming).

^{6.} J. R. Rice and R. Thomson, "Ductile Versus Brittle Behavior of Crystals," *Philos. Mag.* 29, 73–97 (1974).

CONDITION OF FINITE STRESS IN THE DISLOCATION-FREE ZONE MODEL OF FRACTURE

In our DFZ model of fracture, the elastic stress intensity factor $K/c\sqrt{\pi c}$ for an applied stress T/σ was derived as

$$\frac{K}{\sigma\sqrt{\pi c}} = \frac{2}{\pi} \frac{\sqrt{\alpha^2 - k^2}}{\sigma} F\left(\frac{\pi}{2}, k^2\right) .$$

and the condition of finite stress at the ends of the plastic zone was

$$\frac{\pi}{2} \frac{T}{\sigma} = \frac{\sqrt{\alpha^2 - k^2} \sqrt{1 - \alpha^2}}{\alpha} II\left(\frac{\pi}{2}, \alpha^2, k^2\right).$$

where F and II are the complete elliptic integrals of the first and third kinds respectively. The parameters α^2 and k^2 in the preceding equations denote the relative position between the crack and the plastic zone. The region between them is the DFZ. These two relations link the microscopic parameters of fracture to the fracture parameters of the continuum scale.

The current model is considered an extension of the Bilbry, Cottrell, and Swinden (BCS) theory of fracture. Therefore, as the DFZ vanishes, the function II should be reduced to the inverse cosine function. This relation is not obvious because the function II diverges at $\alpha' = 1$, which corresponds to a vanishing DFZ. The condition of finite stress in its current form is less useful if we want to establish a modified BCS theory. An alternative and more useful form of this condition is derived in terms of the lambda function Λ ,

$$\frac{T}{\sigma} = \sqrt{1 - \alpha^2} \frac{K}{\sigma \sqrt{\pi c}} + \Lambda \left(\cos^{-1} \sqrt{\frac{1 - \alpha^2}{1 - k^2}}, k^2 \right).$$

where Λ can be reduced readily to the inverse cosine function in the BCS case.

BOUNDARY INTEGRAL EQUATION METHOD FOR FRACTURE PROBLEMS WITH MIXED BOUNDARY CONDITIONS

The numerical method for fracture problems, which is based on the boundary integral equation

formulation in elasticity, has been developed. The scheme required the superposition of the analytical solution of a crack problem in an infinite region and an elastic problem not containing the crack but having an outer boundary condition identical to the given problem. This scheme is improved in a new formulation in which the number of unknowns is significantly reduced and the method is capable of solving problems with mixed boundary conditions on the crack surface. The current method is intended to solve the dislocation modeling problems.

SELF-CONSISTENT CLUSTER THEORY FOR RANDOM ALLOYS WITH SHORT-RANGE ORDER

A self-consistent cluster theory for random alloys was previously announced. This theory had the advantage of being applicable to general Hamiltonians (i.e., with off-diagonal and environmental disorder), and it was demonstrated that the self-consistent equations had a unique analytic solution. The only restriction on this method was that the random variables that describe the occupation of the sites of the alloy had to be independent. We have now shown that short-range order (dependent random variables) can be naturally and simply included in this theory.

The key idea is to view the random variables (stochastic process) as a measure on the space of all possible configurations of the solid. The dependent variables can then be (approximately) related to the simpler independent variables by means of the Radon-Nikodym theorem of measure theory. As a consequence, averaging over the dependent variables can be transformed into an independent average at the cost of multiplying by the Radon-Nikodym derivative. When this is combined with the Augmented Space approach for independent variables, the short-range-order Green's function is expressed as a linear combination of quantities calculated by this method. The coefficients in this

^{7.} B. A. Bilhy, A. H. Cottrell, and K. H. Swinden, "The Spread of Plastic Yield from a Notch," *Proc. R. Soc. Landon, Ser. A* 272, 364–14 (1963).

^{8.} S.-J. Chang and R. B. Morgan, A Boundary Integral Equation Method for Fracture Problems with Mixed Mode Deformations, ORNL CSD-57 (June 1980).

^{9. &}quot;Self-Consistent Cluster Theory for Random Alloys," Mathematics and Statistics Research Department Progress Report, Period Ending June 30, 1980, ORNL CSD-61 (September 1980), pp. 3, 4.

^{10.} T. Kaplan, P. L. Leath, L. J. Gray, and H. W. Diehl, "Self-Consistent Cluster Theory for Systems with Off-Diagonal Disorder," *Phys. Rev. B* 21, 4230-46 (1980).

linear combination are determined by the Radon-Nikodym derivative. Thus, a shori-range-order computation requires little more than does an independent one. Furthermore, this theory produces

analytic approximations because its analytic behavior is determined by the independent-variables theory.

3. Model Evaluation

K. O. Bowman

N. R. Draper¹

T. J. Mitchell

M. D. Morris

D. S. Scott

L. R. Shenton²

M. Sobel³

SCREENING DESIGNS FOR RESPONSE SURFACE EXPERIMENTS

In the early stages of an experimental program, a primary goal is to identify factors (variables) that are important or influential in the process under investigation. Preliminary experiments designed to identify such variables are commonly referred to as screening experiments.

Cotter⁴ introduced a class of designs called systematic fractional replicates, which are useful as screening designs in two-level factorial settings. These experiments consist of 2k + 2 runs, where k is the number of potential independent variables; they yield information on which of the variables may be involved in odd- or even-ordered terms in the model.

When response surface models (polynomials) are used, separating the even and odd powers of each variable is also desirable. This is not a problem in the two-level factorial model because, in each term, a particular variable is present (raised to power I) or absent (raised to power 0). Using a systematic fractional replicate design, odd and even powers of each variable can be separated. Nonzero even powers of a particular variable, however, cannot be separated from zero powers; for example, information about interactions involving the square of a particular variable cannot be separated from information about terms in which that variable is absent.

We have investigated a natural extension of the systematic fractional replicate designs for use when the underlying model is a response surface model. These experiments consist of 4k + 2 runs and allow the separation, for each variable, of odd and nonzero even powers that may appear in terms of odd or even 'overall') order.

ESTIMATION PROBLEMS ASSOCIATED WITH THE WEIBULL DISTRIBUTION

Series in descending powers of the sample size are developed for the moments of the coefficient of variation v^* for the Weibull distribution $F(t) = 1 - \exp[-(t/b)^c]$. A similar series for the moments of the estimator c^* of the shape parameter c is derived from these. Comparisons are made between classical normal assumptions and the newly developed assumptions for the means and variances.

From the first four moments, approximations are given to the distribution of v^* and c^* . In addition, we give an almost unbiased estimator \bar{c} of c when a sample is provided with the value of v^* . We also comment on the validity of the asymptotically normal assessments of the distributions.

Special attention has been given to the validity of the moment series, especially for the mean and variance, when the sample size is small. This has been carried out by the comparison of several algorithms and by simulation studies. In addition, in a few cases, the low-order moments of the coefficient of variation have been approximated by quadrature formulas in two, three, and four dimensions.

Examples of the comparisons are shown in Table 1, and they illustrate the excellent agreement between the algorithms.

Because the Weibull model occurs frequently in practice, the study has wide applicability. The results of this study have been applied to stress/rupture data from strands of a Kevlar yarn.

GROUP-TESTING PROCEDURES

In the group-testing problem, we consider a population of n objects, d of which are "defective." In the i^{th} experimental trial, n_i ($\leq n$) objects are tested simultaneously. Two kinds of outcomes are possible: negative, indicating that none of the n_i items tested are defective, or positive, indicating that at least one of the items is defective. The objective of a group-testing experiment is to classify correctly all n objects as defective or not in as few experimental trials as possible.

L. University of Wisconsin.

^{2.} University of Georgia.

^{3.} University of California, Santa Barbara.

^{4.} S. C. Cotter, "A Screening Design for Factorial Experiments with Interactions," *Biometrika* 66, 317-20 (1979).

Table 1. Comparison of algorithms to evaluate sample coefficient of variation va

C	n = 2	n 3	n = 4	n = 5	n 10
	the second of th		μί (ν°)		
1.5	182657 T	0.488905 1	0.538535 T	0.57333 S	0,624492 S
	0.381964 1	0.488857 L.	0.538555 1	0.56739 1 ::	0.623496 Lie
				0.56794 2cB	0.623529 2cB
2.0	0.306853 T	0.388807 T	0.425863 T	0.44702 S	0.486299 S
	0.306971 L	0.388759 Leg	0.425847 [0.44687 Lag	0.486303 L ₁₂
				0.44691 2cB	0.486309 2cH
2.5	0.254794 []	0.321713 F	0.351650 T	0.34857 S	0.399732 S
	0.251590 L.	0.321278 1.5	0.351575 1 .	0.368438 Lv	0.399732 1 .
	0.259754 Las	0.321980 Las	0.351670 L ₃ .	0.36850 i ;;	0.399732 1.13
3.0	0.217203 T	0.273919 T	0.299245 1	0.31330 S	0.339829 S
	0.217386 L.	0.274103 1.	0.299321 1.5	0.31351 L.	0.339829 1.5
			(00 var(v*)		
0.1	8.3333 T	7.6694 T	7.1345 T		
	8.3984 2cB	7.6170 2cB	7 1128 - 2cB	6.6725, 2cB	5.0100 2cB
	8.0546 L.:	7.6065	7.1216 1	6.6792 1	5,0106 1
1.5	6.3600 T	5.2842 T	4.4154	5.0978 S	2.3325 S
	6.2758 L ₃	5.3024 1	4.2033	3.7838 Las	2.20097 Lis
	6.3686 2cB	5.2338 2cB	4.3925 2cB	3,7740, 2cB	2,20682, 2cB
2.0	4.7434 T	3.7399 T	2 97×5	2.4408 S	1,3030 S
	4.7562 I	3.7496 Lu	2.9815 I is	2,4596 1 55	1,3020 Lin
	5.1878 2cB	3.8169 2cB	2.9975 2cB	2 4645 2cB	1,3021 2/B
2.5	3.5842 T	2.7578 E	2.1538 1	1.7464 S	0.89439 S
	4.0323 La	2.8445 L	2.1779 1.5	1.7603 1.	0.89461 1 .
	4.5132 L	2.8464 1	2 1690 1 ;	1.75. 1.1	0.89444 L.,
3.0	2.7667 T	2.1085 T	1.6362 1	13364 S	0.668256 S
	3.2971 1	2.1751 1.	1.6491 1.	1,3278 1.	0.6682444

T. true; S. direct sum; 2cB. Borel-Padé; and I., Levor's S. term approximate.

Our concern with this problem was motivated by our interest in experimental design strategies to identify the influential parameters and variables in a giren computer model (particularly large, complex energy models). In this context, an "object" is a model variable or parameter; it is "defective" if the model output is highly sensitive to changes in its value. An experimental trial consists of shifting each value of the n, variables by a unit amount from its nominal value in a direction assumed to give a positive change in output. If no appreciable change in output occurs, these variables are all declared to be of negligible influence and are not considered further. Otherwise, we know only that at least one of the tested variables is influential.

We have recently written and documented an interactive computer algorithm to implement a group-testing procedure based on an "information

criterion." The procedure begins with an assignment of prior probabilities p_1, p_2, \ldots, p_r , where p_r is the probability that the f^h object is defective. After each experimental trial, these probabilities are modified and a near-optimal subset of objects is chosen for the next test. This continues until all objects are correctly classified.

We have evaluated this procedure by two simulation studies to compare it with existing alternative methods and to assess the effect of poor guesses in the assignment of prior probabilities.

In the first study, four cases were considered: (1) n = 10, d = 2; (2) n = 10, d = 4; (3) n = 100, d = 2;

^{5. &}quot;Screening Designs for Studying Large Models," Mathematics and Statistics Research Department Progress Report, Period Ending June 30, 1979, ORNI CSD-40 (September 1979), pp. 7-8.

and (4) n = 100, d = 4. In each case, ten different samples were generated by randomly labeling d of the objects as defective. Each p_i was specified to be 0.05 or 0.2; nine types of configurations of p_i were used to represent various mixes of "good" and "bad" guesses. In addition to four variations of our information procedure, three standard methods were also considered: the bisection method, Sobel and Groll's R_i method with p = 0.05, and the R_i method with p = 0.2.

As might be expected, good prior guesses result in large payoffs. Even when the prior guesses are not correlated with reality, the performance of the information procedure appears to be essentially the same as that of the standard R_1 procedure, which is based on a constant p.

A second study was undertaken to evaluate the performance of the information procedure when the prior probabilities p_i are all set equal to a constant p and the defectives follow a binomial distribution with parameters (n, p^*) . For n = 10 and n = 100, 101 simulations were made for each combination of p and p^* in the set (0.025, 0.05, 0.10, 0.20, 0.25). The overall conclusion was that, when in doubt, it is better to guess high: low values of p result in large payoffs when p^* is low, but large penalties result when p^* is high. At high values of p, the results are less sensitive to p^* .

LIKELIHOOD-BASED CHOICE OF k IN RIDGE REGRESSION

A useful way to incorporate external or prior information into the estimation of the vector of coefficients $\boldsymbol{\beta}$ in a linear regression model is by "dummy" data \mathbf{X}_0 (a matrix of regressors) and \mathbf{y}_0 (a response vector), where $\mathbf{y}_0 = \mathbf{X}_0 \boldsymbol{\beta}_0$ is assumed to be normally distributed with mean $\mathbf{X}_0 \boldsymbol{\beta}_0$ and variance-covariance matrix $\sigma_0^2 \mathbf{V}_0$. When these data are combined with the

experimental data (X, y), the least-squares estimate of β is

$$\widetilde{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X} + k\mathbf{T})^{-1}(\mathbf{X}'\mathbf{y} + k\mathbf{T}\boldsymbol{\beta}_0), \qquad (1)$$

where $T = X_0'V_0'X_0$ and $k = \sigma^2/\sigma_0^2$; σ^2 is the error variance for the experimental data. Theil and Goldberger⁷ introduced this approach, which was developed further by Theil.⁸

When V_0 is specified and k is allowed to vary over (0, ∞), Eq. (1) becomes a more general form of the Hoerl-Kennard' family of ridge estimators. Scores of papers representing many different points of view have been written about the choice of k in ridge regression. We have remarkly attacked this problem by considering the akelihood function, where likelihood is based on both experimental and dummy data and where k is regarded as an unknown parameter. Unfortunately, this likelihood is not easy to work with. The main difficulty is that the dummy data, by themselves, fit the model perfectly (namely. when $B = B_0$), so the likelihood function increases without bound when $\beta = \beta_0$ and k approaches infinity. Moreover, several stationary points may exist; so even if the singularity is ignored, the usual likelihood inference techniques will not work.

These difficulties can sometimes be avoided in practice by restricting attention to those values of k for which the experimental data and the dummy data are compatible, according to Theil's test. In examples we have considered the log likelihood L to be unimodal and approximately quadratic in this range. This yields a natural choice for k, at the mode. After maximizing L over k and σ^2 , a quadratic approximation to the resulting function of β produces a likelihood-based confidence region for β that is not a function of k and σ^2 but that takes into account the uncertainties in estimating these parameters.

^{6.} M. Sobel and P. A. Groll, "Group Testing to Eliminate Efficiently All Defectives in a Binomial Sample," *Bell Syst. Tech. J.* 38, 1179–252 (1959).

^{7.} H. Theil and A. S. Goldberger, "On Pure and Mixed Statistical Estimation in Economics," Int. Econ. Rev. 2, 65-78 (1961).

^{8.} H. Theil, "On the Use of Incomplete Prior Information in Regression Analysis," J. Am. Stat. Assoc. 58, 401-14 (1963).

^{9.} A. E. Hoerl and R. W. Kennard, "Ridge Regression: Biased Estimation for Nonorthogonal Problems," *Technometrics* 12, 55 67 (1970).

4. Moving-Boundary Problems

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A. Lacey²

D. G. Wilson

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During the reporting period, research on moving-boundary problems has continued in three directions: analysis of Stefan-type problems, analytical approximations and bounds, and modeling of phase-change processes.

ANALYSIS OF STEFAN-TYPE PROBLEMS

A Stefan-type problem³⁻⁶ of major practical interest is the problem of melting a semi-infinite slab of material that is initially solid and that is at its melt temperature T_{cr} via convective heat transfer from a heat transfer fluid to its surface. The governing parameter for this transfer is the heat transfer coefficient h (kJ/m²-s-o^cC). If the ambient temperature of the transfer fluid is $T_L > T_{cr}$ and the surface temperature is T_{stec} , the heat flux to the surface is $h[T_L - T_{stec}]$. Because no explicit expression is known for the temperature distribution and melting history of this process, we were forced to use either numerical or analytical approximation techniques for its resolution. We have obtained three results that are pertinent to this problem.

1. The Case of Large h

By mathematical analysis we have proved that as h approaches infinity, the surface temperature approaches the ambient fluid temperature while the temperature distribution and melting front approach known functions. Rates of this convergence have been obtained.

- 1. University of Tennessee.
- 2. Victoria University of Wellington, New Zealand.
- 3. A. D. Solomon, V. Alexiades, and D. G. Wilson, "The Stefan Problem with a Convective Boundary Condition," submitted to Q. Appl. Math.
- 4. A. D. Solomon, D. G. Wilson, and V. Alexiades, "The Quasi-Stationary Approximation for the Stefan Problem with a Convective Boundary Condition," to be submitted for publication.
- 5. A. D. Solomon, "On the Limitations of Analytical Approximations for Phase Change Problems with Large Biot Number." submitted to Lett. Heat Mass Transfer.
- 6. D. G. Wilson. "One-Dimensional Multi-Phase Moving Boundary Problems with Phases of Different Densities." submitted to SIAM J. Appl. Math.

2. The Case of Low Specific Heat

We have proved that if the specific heat approaches zero, the temperature distribution and ment front approach functions that are easily found explicitly.

3. Accuracy of Analytical Approximations for High Heat Transfer Coefficient

With the aid of the first two results, we derived a simple criterion for the accuracy of standard analytical approximation techniques for our problem. We have shown that these approximations can be replaced by simple, more accurate expressions when h is large.

ANALYTICAL APPROXIMATIONS AND BOUNDS

Analytical approximations and bounds^{1,3} have been derived for a number of phase-change problems. Two results of interest are:

1. Approximations for an Array of Cylinders of a Phase-Changing Material

A line of N cylinders containing a phase-changing material" is subjected to the flow of a heat transfer fluid. If the material in the cylinders is initially liquid and at melting temperature T_{σ} and if the ambient fluid temperature before encountering the first cylinder is $T < T_{\sigma}$, a freezing process begins in the cylinders, while the air is heated. We wanted to predict the outlet transfer fluid temperature, the total energy stored in the system, and the melting times of the cylinders. Through a variety of techniques, we

^{7.} A. D. Solomon, Simulation of a PCM Storage Subsystem for Air Conditioning Assist, ORNL/CSD-77 (1981).

^{8.} A. D. Solomon, "Some Approximations of Use in Predicting the Behavior of a PCM Cylinder Array," *Lett. Heat Mass Transfer* 8, 237-46 (1981).

derived simple expressions for these quantities, which, when compared with numerical simulations, appear to be extremely accurate. Table 2 shows an example of the accuracy observed for a simulation of 24 cylinders of a Glaubers-sak-based material, where air is the transfer fluid.

Table 2. Comparison of computed and approximate outlet air temperatures

Time (h)	Air temperature (°C)		
	Approximate	Computed	
	12.76	12.76	
2	12.76	12.76	
3	12.76	12.76	
4	12.76	12.75	
5	12.75	12.74	
6	12.74	!2.72	
7	12.72	12.71	
8	12.70	12.67	
9	12.68	12.64	
10	12.65	12.59	
11	12.56	12,52	
12	12.50	12,42	
13	12.42	12.28	
i 4	12.42	12.11	
15	12.17	11.86	
16	11.75	11.52	
17	11.44	11.07	
18	11.04	10.49	
19	10.17	9.67	
20	8.97	8.59	
21	7.24	7.33	
22	6.36	5.85	
23	4.44	4.59	

Source: A. D. Solomon, Simulation of a PCM Storage Subsystem for Air Conditioning Assist, ORNL CSD-77 (1981).

2. A Lower Bound for the Total Energy in a Phase-Changing Material

An effective lower bound for the total stored energy in a phase-changing material has been derived by analysis of the model. The expression complements previously derived upper bounds and estimates. The lower bound and computed values for a case of melting of N-octadecane paraffin wax over a period of 30 h are compared in Table 3.

Table 3. A lower bound on total system energy for an N-octadecane wax-melting process

Time	Computed energy	Lower bound
(b)	(kJ·m²)	(U m²)
0	0	
2	4,687	4,253
4	7,292	6,499
6	9,331	8,237
8	11,064	9,708
l0	12,598	11,007
12	13,988	12,183
14	15,269	13,266
16	16,463	14,274
18	17,586	15,222
30	18,650	15,118
22	19,662	6.971
24	20,630	17,787
26	2i,559	18,569
28	22,452	19.322
30	23,314	20,049

MODELING OF PHASE-CHANGE PROCESSES

Recent work on modeling phase-change processes in materials has been directed mainly toward alloy solidification and mushy zone modeling. 9-12

1. Alloy Solidification

A weak-solution model has been formulated for the solidification of an alloy, including effects of hear conduction and material diffusion. The model includes variability of the freezing front "melt" temperature in accordance with an equilibrium phase diagram. Preliminary computations indicate the physical correctness of the model.

^{9.} V. Alexiades, A. D. Solomon, and D. G. Wilson, An Observation on the Total Energy of a System with Phase Changes, ORNL, CSD-72 (1981).

^{10.} V. Alexiades, A. D. Solomon, and D. G. Wilson, Modelling of Phase Change Processes with Time-Varying Critical Temperature, ORNL, CSD TM-145 (1981).

^{11.} A. D. Solomon, D. G. Wilson, and V. Alexiades, On Two Kinds of Mushy Zones in Solidification (in preparation).

^{12.} D. G. Wilson, A. Lacey, and A. D. Solomor. Composition of Solidified Binary Alloy from a Simple Solidification Model, ORNL CSD-66 (1981).

2. Mushy Zone Modeling

A simple mathematical model has been developed for the appearance of a "mushy" zone (i.e., a zone of finite width in which solid and liquid coexist) in a freezing material. The model arises from energy

conservation considerations and is consistent with experimental observations of paraffin wax solidification. For paraffin wax, a mushy zone width of about 0.5% of the solidified material is typical.

5. Multivariate Analysis

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V. E. Kane

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ROBUSTNESS OF THREE POWER TRANSFORMATION PROCEDURES

Earlier reports²⁻⁴ have described investigations that considered problems associated with the estimation of parameters in the power-shift family of transformations: $Y = \{(X + c)^p - 1\}/p \text{ for } p \neq 0 \text{ and }$ $Y = \ln(X + c)$ for p = 0. During this period, a robustness study was completed that determined how well p was estimated with c = 0 if p exists such that Y is symmetric after transforming X by the power transformation. Three estimation procedures were considered: maximum likelihood; weightedorder statistic, given in Beauchamp, Kane, and Serbin; and Hinkley's percentile, which is based on making selected order statistics of Y symmetric. The comparative robustness of each estimation procedure was evaluated when the transformed data could be made symmetric but not necessarily normal. Seven types of symmetric distributions as well as four contaminated normal distributions were considered over a range of six p values for samples of size n, where n = 25, 50, and 100.

The three procedures were applied to 50,000/n simulations for each value of n and p and for each distributional form. The results indicated that the maximum likelihood estimator was slightly better than the weighted-order-statistic estimator, but both were greatly superior to Hinkley's percentile

estimator. In general, the procedures were robust to symmetric departures from normality, and increasing kurtosis (β_2) caused increasing variation in the estimated p values, as is exhibited in Fig. 3. Single-tailed outliers, however, were found to cause highly biased estimates and increased variation.

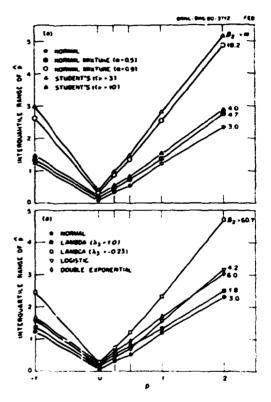


Fig. 3. Interquartile range of maximum likelihood estimate of p for samples of size n = 100.

1. Purdue University. 2. "Transformations to Normality," Mathematics and Statistics Research Department Progress Report, Period Ending June 30, 1978, ORNL/CSD-34 (September 1978), p. 4.

3. "Limiting Values of Various Functions To Be Optimized in Achieving Normality," Mathematics and Statistics Research Department Progress Report, Period Ending June 30, 1979, ORNL/CSD-40 (September 1979), pp. 12-13.

4. "An Evaluation of the Power-Shift Family of Transformations," Mathematics and Statistics Research Department Progress Report, Period Ending June 30, 1980, ORNL CSD-61 (September 1980), p. 10.

CALCULATING MISCLASSIFICATION PROBABILITIES

Misclassification probabilities are an important measure for comparing Fisher's linear and quadratic discriminant functions with alternative methods of discrimination. Theoretical misclassification probabilities for a general discrimination rule and general population structure cannot always be calculated. A method has been devised, however, to calculate misclassification probabilities for discriminating between two bivariate populations when Fisher's

^{5.} J. J. Beauchamp, V. E. Kane, and C. A. Scrbin, Application of the Power-Shift Transformation with Computing Procedures, ORNL/CSD/TM-142 (March 1981).

D. V. Hinkley, "On Power Transformations to Symmetry." Biometrika 62, 101~11 (1975).

linear and quadratic rules and the logistic linear and quadratic rules are used.

The general form of the discriminant rules is

$$Q(X_1, X_2) = b_0 + b_1 X_1 + b_2 X_2$$

$$+b_3X_1X_2+b_4X_1^2+b_5X_2^2$$
.

where $Q(X_1, X_2) < (>) 0$ assigns a sample to population 0 (1) in the bivariate two-population problem. The coefficients b_0 to b_3 are determined by the particular discriminant rule applied and the randor: variables (X_1, X_2) , which may be distributed as a bivariate normal, a bivariate Bernoulli, or a raixture of normal and Bernoulli data. For example, to determine the misclassification probability of classifying an observation from population 0 into population I, it is necessary to integrate over all values of the bivariate density function for population 0, where $Q(X_1, X_2) \le 0$. The misclassification probability reduces to a double summation over all possible values of (X_1, X_2) for bivariate Bernoulli populations and simplifies to a single summation that is a function of the standard normal cumulative distribution function for a mixture of a Bernoulli and a normal population. For the linear discriminant methods, the coefficients b_3 , b_4 , and b_5 are zero, and the evaluation reduces to either summations or to functions of the standard normal cumulative distribution function.

The most difficult case is using the quadratic discriminant function to discriminate between two bivariate normal populations with unequal covariance matrices. This case is simplified by reducing the double integral to a single integral by replacing the bivariate density function with the product of the marginal density of X_2 and the conditional density of X_1 given X_2 . The conditional density can be integrated by means of a standard normal density function, and the marginal density is numerically integrated over the range of X_1 . The range of X_1 is infinite, so approximate limits must be used. By examining the sign and value of the b_0 to b_3 coefficients, the limits of integration can be

determined so that the approximation error can be bounded. Calculating the misclassification probabilities for classifying an observation in population I into population 0 is performed in a similar manner.

These computational procedures can be used to calculate theoretical misclassification probabilities for any procedure that gives estimates of the discriminant coefficients b_0 to b_5 . In particular, these methods are useful in simulation studies because a "double simulation" is not necessary for both the sampled population and misclassification error of $Q(X_1, X_2)$.

COMPARISON OF DISCRIMINATION MODELS

Incorrect specification of the discrimination model may result in unnecessarily high misclassification error rates. A study was initiated to compare misclassification rates from the standard Fisher linear or quadratic classification precedures with rates from corresponding logistic discrimination methods. Also, maximum likelihood error rates were computed for nonnormal data. The robustness of the various classification methods to various departures from the assumed data structure is being examined to assess the application of discrimination methods to general data.

The data structures of primary interest in this study are the traditional normal distribution and Bernoulli (0, 1) data. Standard approaches treat each data type separately, so one area of interest is the mixture of normal and Bernoulli data. Also, the linear or quadratic nature of the discriminant function $Q(X_1, X_2)$ is of interest. Thus, the study considers four types of bivariate data from two populations using classification methods based on bivariate normal data with equal covariance matrices, bivariate normal data with unequal covariance matrices, normal-Bernoulli data, and bivariate Bernoulli data. The theoretical misclassification probabilities of the sample discriminant function are calculated directly, as previously indicated, and provide the basis for comparing the classification methods.

6. Numerical Linear Algebra

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M. T. Heath

R. J. Plemmons?

D. S. Scott

R. C. Ward

LU DECOMPOSITION OF M-MATRICES

We have shown that if A or -A is a singular M-matrix satisfying the generalized diagonal dominance condition $y^TA \ge 0$ for some vector $y \ge 0$, then A (or any symmetric permutation of A) can be factored into A = LU by a certain elimination algorithm, where L is a lower triangular M-matrix with unit diagonal and U is an upper triangular M-matrix.³ The already known existence of LU decompositions for irreducible M-matrices and symmetric M-matrices follow as corollaries. Varga and Cai⁴ followed with a graph-theoretic proof of a converse of the main result above, and we followed that with a short nongraph proof of the converse.

Much of this work was morivated by applications to the solution of homogeneous systems of linear equations $Ax \approx 0$, where A or -A is an M-matrix. These applications arise, for example, in the analysis of Markov chains, network analysis, and inputoutput economic models. Some of this work generalizes compartmental analysis work reported in refs. 5 and 6. Extensions related to stability, updating, and $\partial y(\infty) \partial a_{ij}$ have been obtained.

SPARSE LEAST SQUARES PROBLEMS

The basic algorithm of George and Heath for sparse linear least squares problems has been extended to include rank-deficient problems, linear equality constraints, and updating of solutions. These extensions have been combined to provide a new method for solving sparse square nonsymmetric linear systems, including systems having a few dense rows. All of these algorithms have then implemented in computer software and tested extensively. The version of the code that uses auxiliary storage? has been used to solve problems involving as many as 42,938 equations in 16,756 unknowns.

NONFACTORIZATION ALGORITHMS FOR SYMMETRIC QUADRATIC λ-MATRICES

Quadratic λ -matrix problems consist of determining scalars λ , called eigenvalues, and corresponding $n \times 1$ nonzero vectors \mathbf{x} , called eigenvectors, such that the equation

$$(\mathbf{M}\lambda^2 + \mathbf{C}\lambda + \mathbf{K})\mathbf{x} = \mathbf{0} \tag{1}$$

is satisfied, where M, C, and K are given $n \times n$ matrices. In addition, we assume that M, C, and K are symmetric or Hermitian, that M is definite (either positive or negative), and that the eigenvalues of Eq. (1) are real and can be divided into two disjoint sets P and S with the following properties:

P1: If $\lambda_i \in P$ and $\lambda_j \in S$, then $\lambda_i > \lambda_j$.

P2: If $\lambda_i \in P(S)$ and \mathbf{x}_i is its associated eigenvector, then λ_i is the larger (smaller) root of the quadratic equation $(\mathbf{x}_i^T \mathbf{M} \mathbf{x}_i) \lambda^2 + (\mathbf{x}_i^T \mathbf{C} \mathbf{x}_i) \lambda + (\mathbf{x}_i^T \mathbf{K} \mathbf{x}_i) = 0$.

Based on these assumptions, one can easily verify that theory analogous to the symmetric standard eigenvalue problem holds and that the eigenvalues and eigenvectors of Eq. (1) obey the orthogonality condition

$$(\mathbf{x}_i^T \mathbf{K} \mathbf{x}_i) = \lambda \cdot \lambda (\mathbf{x}_i^T \mathbf{M} \mathbf{x}_i) = 0$$
 for $i \neq j$.

^{1.} University of Waterloo

^{2.} University of Tempessee

^{3.} R. F. Fu iderlic and R. J. Plemmons, LU Decomposition of M-matrices by Elimination Without Prooting, ORNI CSD-71 (January 1981) and Linear Algebra Appl. (torthcoming)

^{4.} R. S. Varga and Da-Yong Cai, "On the LU Decomposition of M-matrices by Gaussian Flimmation Without Pivoting "submitted to Numer, Math.

^{5.} Mathematics and Statistics Research Department Progress Report, Period Ending June 30, 1980, ORNI CSD-61 (September 1980), p. 12.

^{6.} R. F. Funderlic and 3. B. Mankin, "Solution of Homogeneous Systems of Linear Equations Arising from Compartmental Lindels," SIAM J. Sci. Star. Comput. (forthcoming)

^{7.} A. George and M. T. Heath, "Solution of Sparse I incar Least Squares Problems Using Givens Rotations," Linear Algebra Appl. 34, 69-83 (1980).

⁸ M. I. Heath, Some Extensions of an Algorithm for Sparse Emear Least Sanares Problems, ORNI CSD-80 (May 1981). 9 A. George, M. I. Heath, and R. J. Plemmons, "Solution of Large-Scale, Sparse Least Squares Problems Using Auxiliary Storage," 514M J. Sci. Stat. Comput. (forthcoming).

We have developed and analyzed algorithms for computing a few of the eigenpairs of Eq. (1) when M, C, and K are also large and sparse and when factorization of M, C, K, or any linear combination of them is either impossible or undesirable. The algorithms can compute eigenpairs for either the largest or smallest eigenvalues in either P or S For example, in the following algorithm the sequence (σ_i, y_i) converges to eigenpairs (λ_i, x_i) corresponding to the m smallest eigenvalues in P, where the matrix $W(\sigma) \equiv M\sigma^2 + C\sigma + K$:

- 1. Set the vector y_1 to random numbers.
- 2. For k = 1, 2, ..., m, do a and b.

Æ,

- a. Set the r^{th} column of the $n \times k$ matrix X_0 to y, from step 1 if k = 1 or from step 2.b(2) otherwise.
- b. For i = 1, 2, ... until convergence, do (1) and (2).
 - (1) Set $\sigma_i = \theta_k$ where $\theta_{-k} \leq \theta_{-k+1} \leq \cdots \leq \theta_{-1} < \theta_1 \leq \cdots \leq \theta_{k-1}$ are the eigenvalues of

$$\begin{bmatrix} \mathbf{X}_{r1} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_{r1} \end{bmatrix} \left\{ \begin{bmatrix} \mathbf{0} & \mathbf{K} \\ \mathbf{K} & \mathbf{C} \end{bmatrix} - \theta \begin{bmatrix} \mathbf{K} & \mathbf{0} \\ \mathbf{0} & -\mathbf{M} \end{bmatrix} \right\} \begin{bmatrix} \mathbf{X}_{r1} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_{r1} \end{bmatrix}$$

(2) Set the r^{th} column of X_i to y_r , where (μ_j, y_j) are the eigenpairs of $W(\sigma_i)$ with $\mu_1 \le \mu_2 \le \cdots \le \mu_n$ and the y_j are unit length.

We have shown that the sequence $\{\sigma_i\}$ converges monotonically downward and that the convergence is asymptotically quadratic. Similar properties can be shown for the algorithms converging to the m largest eigenvalues in P and to the m smallest and largest eigenvalues in S.

COMPUTING A FEW EIGENPAIRS OF A SYMMETRIC BAND MATRIX

As an intermediate task is running a block Lanczos algorithm, it is necessary to compute a few eigenvalues and eigenvectors of a symmetric band matrix. The algorithms available in EISPACK are not well suited to this problem, so a new algorithm has been developed that incorporates an idea of Gupta's and is more efficient than the EISPACK codes.

NONFACTORIZATION SOFTWARE FOR SYMMETRIC DEFINITE LINEAR AND OUADRATIC EIGENVALUE PROBLEMS

Over the last two years we have developed algorithms that do not require the factorization of any matrix for computing a few eigenvalues and eigenvectors of symmetric definite linear and quadratic eigenvalue problems. The similarity of these algorithms allowed us to implement both of them in a single software package. The subroutines are written in portable FORTRAN and access the matrices involved only through the formation of matrix-vector products, which allows the user to take full advantage of any special structure (sparsity) in his matrices.

SHIFT AND INVERT LANCZOS ALGORITHM

We have continued to develop the shift and invert Lanczos algorithm for computing eigenpairs of a symmetric standard or generalized eigenvalue problem. We have incorporated a preliminary version into a structural analysis package for the Tennessee Valley Authority (see part B for more details). The algorithm appears to be the optimal way of computing eigenvalues when it is possible to factor the appropriate matrix. Further work is needed to optimize the automated decisions of when and where to shift. Implementation of the algorithm will include a reduction scheme developed recently (see the following article) for solving symmetric definite quadratic eigenvalue problems.

SOLVING SYMMETRIC DEFINITE QUADRATIC EIGENVALUE PROBLEMS WITH FACTORIZATION

A quadratic eigenvalue problem

$$(\mathbf{M}\lambda^2 + \mathbf{C}\lambda + \mathbf{K})\mathbf{x} = \mathbf{0}$$

can always be solved via the linearization

$$\begin{bmatrix} 0 & K \\ K & C \end{bmatrix} - \lambda \begin{bmatrix} K & 0 \\ 0 & -M \end{bmatrix} \begin{bmatrix} x \\ \lambda x \end{bmatrix} = 0.$$

which we denote as $(\mathbf{A} - \lambda \mathbf{B})\mathbf{z} = 0$. The best solution techniques for sparse linear problems require the

^{10.} D. S. Scott and R. C. Waru, Solving Quadratic λ-Matrix Problems Without Factorization, ORNI CSD-76 (March 1981).

¹¹ K. K. Gupta, "Eigenproblem Solution by a Combined Sturm Sequence and Inverse Iteration fechniques," *Inter. J. Numer. Methods Eng.* 4, 379-404 (1972).

operator $(A - \sigma B)^{-1}B$ for some choice of σ . In the quadratic context this appears to require the factorization of a $2n \times 2n$ matrix. In ref. 12 we show

12. D. S. Scott, Solving Sparse Quadratic λ-Matrix Problems, ORNL/CSD-79 (November 1980).

that the operator $(A - \sigma B)^{-1}B$ can be implemented by factoring only an $n \times n$ matrix. Furthermore, if M, C, and K are symmetric and satisfy certain definiteness conditions, the Lanczos algorithm can be used as a solution technique.

7. Risk Analysis

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A RANKING METHOD BASED ON STOCHASTIC PAIRED COMPARISONS

Suppose we want to rank k objects according to a characteristic of performance, where the only data we have is based on stochastic paired comparisons. Let θ_{ij} denote the probability that the i^{th} object is "better" than the j^{th} object relative to the characteristic under consideration. This implies that $\theta_{ji} = 1 - \theta_{ij}$ for $1 \le i, j \le k$.

In a previous report,² we considered a modifica-ion suggested by Saaty³ to help rationalize the socalled Arrow's Paradox or the Paradox of Voting. Here, we suggest exponentiating the probabilities θ_{ij} and obtaining $a_n = \exp(2\theta_n - 1)$, so that $(a_n, 1 \le i$, $j \leq k$) will become a reciprocal matrix of the form considered by Saaty. Then the normalized eigenvector corresponding to the largest eigenvalue of this reciprocal matrix yields a ranking of the k objects under consideration. When we have stochastic paired comparison data on k objects by several judges, we suggest using the geometric mean of the exponentiated probabilities to obtain an "average" reciprocal matrix. From this reciprocal matrix, one can obtain the normalized eigenvector associated with the largest eigenvalue and obtain the ranking of the kobjects.

WAITING TIMES AND GENERALIZED FIBONACCI SEQUENCES

Suppose we have a multinomial distribution with k possible outcomes denoted by E_1, E_2, \ldots, E_k and associated probabilities $\pi_1, \pi_2, \ldots, \pi_k$ such that $\pi_i \ge 0$ and $\pi_1 + \pi_2 + \cdots + \pi_k = 1$. At each trial, one of the outcomes is observed. After n independent trials, we are interested in finding the probability of the first occurrence of r specified outcomes in succession. Let E_r denote this event and W_r denote the

waiting time for the first occurrence of E_r . We are interested in the distributional properties of W_r .

Suppose $E_r = \{E_1, E_1, \dots, E_l\}$, which corresponds to the occurrence of the same outcome (E_l) r times in a row. Then we have the following.

Proposition: The probability distribution of the discrete random variable W, is given by

$$P[W_r = n + r] = \pi_1^r \sum_{j=0}^r (-1)^j \binom{n - jr}{j} [(1 - \pi_1)\pi_1^r]^j$$
$$- \pi_1^{r+1} \sum_{j=0}^r (-1)^j \binom{n - 1 - jr}{j} [(1 - \pi_1)\pi_1^r]^j,$$
$$n = 0, 1, 2, \dots. (1)$$

When we have a binomial distribution, that is, k = 2, and $\pi_1 = \pi_2 = 1/2$, we have

$$\beta_{n,r} = 2^{n+r} P(W_r = n + r) = A_{n,r} - A_{n-1,r}, \qquad (2)$$

where

$$A_{n,r} = 2^n \sum_{j \in \mathbb{N}} (-1)^j \binom{n-jr}{r} (1/2)^{(r+1)j}, \qquad (3)$$

with

$$A_{i,r} = 2^j$$
, for $0 \le i \le r$.

We note that the sequences $\{\beta_{n,r}\}$ are generalized Fibonacci sequences. Specifically, for r = 2, $\{\beta_{n,r}\}$ is the Fibonacci sequence, given by 1, 1, 2, 3, 5, 8, 13, For r = 3, we have the so-called Tribonacci sequence, given by 1, 1, 2, 4, 7, 13, 24, 44, For r = 4, one can verify that

$$\beta_{m+4,A} = \beta_{m+3,A} + \beta_{m+2,A} + \beta_{m+3,A} + \beta_{n,A} . \tag{4}$$

and the sequence $\{\beta_{n,4}\}$ is given by 1, 1, 2, 4, 8, 15, For general r, one can verify that

$$\beta_{mr,s} = \beta_{mr-1,s} + \beta_{mr-2,s} + \cdots + \beta_{n,s} \,. \tag{5}$$

where $\beta_{0,r} = 1$, which is an r step generalization of Fibonacci sequence.

The special case of the multinomial distribution with $\pi_1 = \pi_2 = \cdots = \pi_k = 1/k$ gives another aspect

^{1.} Tennessee Technological University.

^{2.} V. R. R. Uppuluri, "Consensus and Ranking Based on Paired Comparisons," Mathematics and Statistics Research Department Progress Report, Period Ending June 30, 1980, ORNL-CSD-61 (September 1980), p. 15.

^{3.} T. L. Saaty, "A Scaling Method for Priorities in Hierarchical Structures," J. Math. Psych. 15, 234-81 (1977).

of the generalization of Fibonacci sequences. The probability distribution of W, given in the preceding proposition yields

$$\gamma_{n,r}^{(k)} = k^{n+r} P[W_r = n + r] = B_{n,r}^{(k)} - B_{n-1,r}^{(k)}, \quad (6)$$

where

$$B_{n,r}^{(k)} = k^n \sum_{j=0}^{n} (-1)^j \binom{n-jr}{j} \left[\frac{(k-1)}{(k^{r+1})} \right]^j . \tag{7}$$

Now, one can verify that

$$\gamma_{n+r,r}^{(k)} = (k-1)[\gamma_{n+r-1,r}^{(k)} + \gamma_{n+r-2,r}^{(k)} + \cdots + \gamma_{n,r}^{(k)}].$$

with

$$\gamma_{r,r}^{(k)} = 1 \text{ and } \gamma_{s,r}^{(k)} = 0 \text{ for } s < r.$$
 (8)

which for the special case k=2 gives the recursion satisfied by the r step generalization of the Fibonacci sequence given in Eq. (5). For r=2 and k=3, the sequence $\{\gamma_{n,2}^{(1)}\}$ is given by 1, 2, 6, 16, 44, 120, For r=3 and k=3, the sequence $\{\gamma_{n,3}^{(3)}\}$ is given by 1, 2, 6, 18, 52, 152, 444, Thus the special cases derived from the proposition contain several generalizations of the Fibonacci-type sequences. The prob-

ability-generating function of the random variable W, succinctly expresses these sequences. During this study the following alternative expressions were obtained for the Tribonacci numbers:

$$\beta_{n,3} = \frac{1}{(c-1)(c+3)}$$

$$\times \left\{ c^{n/2+1} \left[\frac{\sin(n+1)\theta}{\sin \theta} - \frac{c^{3/2}\sin n\theta}{\sin \theta} - \frac{1}{c^{n-1}} \right] \right\}$$
for $n = 2, 3, ...$

where

$$c = \frac{1}{3} \left[(\sqrt{297} + 17)^{1/3} - (\sqrt{297} - 17)^{1/3} - 1 \right].$$

$$\theta = \pi - \arcsin\left(\frac{\sqrt{3-c^2}}{2}\right),\,$$

and $\beta_{0,3}$ and $\beta_{1,3}$ are defined to be equal to 1.

These expressions for Tribonacci numbers seem to be new, and they correspond to the Golden number representations of the Fibonacci numbers.

8. Complementary Areas

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THE CELL MEANS MODEL AND ANALYSIS OF VARIANCE PARAMETERS

It is frequently more natural for scientists and statisticians to interpret estimable functions in terms of cell means rather than the "usual" analysis of variance parameters. Explicit expressions that establish a one-to-one correspondence between the cell means and the usual form of estimable functions have been derived. Computer packages (e.g., SAS) that output the usual form of estimable functions are already available. These expressions are needed to augment such packages to output the cell means form as well.

ROBUST SHRINKING ESTIMATORS

Let the model $Y = X\beta + e$ denote a multiple regression model for which the distribution of the error vector e belongs to a class C. Conditions are given under which shrinking estimators for β exist that improve on a given robust estimator for all β and all error distribution in C. Explicit expressions for robust shrinking estimators have been developed through an asymptotic analysis.

A simulation study was performed to assess the improvement of one such estimator. For error distributions with heavy tails, the improvement caused by shrinking was remarkable.

A GENERALIZATION OF THE EHRENFEST URN MODEL

The Ehrenfest Urn Model² has been applied to heat-exchange problems between two isolated bodies. The basic model can be described as an urn containing w_0 white and b_0 black balls. A ball is drawn at random from the urn and is replaced by a ball of opposite color. The interest is in $E(W_n)$, the expected number of white balls in the urn after n drawings with replacement. Several modifications

and generalizations of the model are known.

A new sampling scheme for the establishment of goals, which is a generalization of the Ehrenfest Model, is introduced. Briefly, we assume an urn with w_0 white balls and b_0 black balls. The total number of balls in the urn is held constant at N, where $N = w_0 + b_0$ initially. The object is to change the number of white balls in the urn through independent random trials. On the n^{th} trial, select a ball at random and replace it in the following manner:

If it is white, $\{a \text{ black ball with probability } \alpha_1, \text{ replace it by: } \{a \text{ white ball with probability } 1 - \alpha_1.$

If it is black, $\{a \text{ white ball with probability } \alpha_2.$ replace it by: $\{a \text{ black ball with probability } 1 - \alpha_2.$

The following theorem results.

Theorem: Based on this sampling scheme,

$$E(W_n) = \frac{1}{1-\lambda} \left[\{ (1-\lambda^n)a - (1-\lambda^{n-1})\lambda \} w_0 + \{ (1-\lambda^n)b \} b_0 \right],$$

where $a = 1 - \alpha_1/N$, $b = \alpha_2/N$, and $\lambda = 1 - (\alpha_1 + \alpha_2)/N$, where λ is an eigenvalue of the matrix

$$\begin{bmatrix} 1 - \alpha_1/N & \alpha_2/N \\ \alpha_1/N & 1 - \alpha_2/N \end{bmatrix}$$

In practice, to establish the stated goal of $E(W_n)$, for given N, w_n , and n, the experimenter chooses α_1 and α_2 that will satisfy the result given in the theorem.

Thus the sampling scheme is a tool for the attainment of certain goals that one may want to accomplish over time. The scheme is appealing because it leaves the choice of replacement at each trial to chance while at the same time it achieves a predetermined goal concerning the desired proportion of whe shalls.

Numerical examples are given and possible applications have been suggested; various simulation studies are planned. For further details, see ref. 3.

^{1.} Computing Applications Department.

^{2.} P. Ehrenfest and T. Ehrenfest, "Uber zwei bekannte Einwände gegen das Boltzmannsche H-Theorem," Phys. Z. 8, 311-14 (1907).

CONFIDENCE ELLIPSE FOR A BIVARIATE CALIBRATION PROBLEM

Suppose that a bivariate measurement vector y is related to stresses R_1 and R_2 by the relationship

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} B_{11} + B_{21}R_1 + B_{31}R_2 \\ B_{12} + B_{22}R_1 + B_{32}R_2 \end{bmatrix} + \begin{bmatrix} ERROR_1 \\ ERROR_2 \end{bmatrix}.$$

where the error vector is distributed as a bivariate normal distribution with mean 0 and covariance matrix Σ . Suppose further that, from a planned calibration experiment, independent data pairs (y_a, R_a) , $R_a^T = (1, R_{1a}R_{2a})$, $\alpha = 1, \ldots, N$, are obtained, and the estimates **b** of **B** and **S** of Σ are computed as proscribed by Anderson.⁴

If one observes an additional vector y_0 without observing its stress vector R_0 , the $100(1 - \gamma)$ confidence ellipse for the unknown stresses R_{10} and R_{20} is given by:

$$R_0^T \{b^{*T}S^{-1}b^{*} - A^{*}\}R_0 \leq 0$$
,

where

$$\mathbf{A}^{\bullet} = \left(\sum_{\alpha=1}^{N} \mathbf{R}_{\alpha} \mathbf{R}_{\alpha}^{T}\right) \bullet Q_{\gamma} + Q_{\gamma} .$$

$$\mathbf{b}^{\bullet} = \left\{ \begin{array}{l} y_{10} - b_{11}, -b_{21}, -b_{31} \\ y_{20} - b_{12}, -b_{22}, -b_{32} \end{array} \right\} \ .$$

and

$$Q_7 = [(N-3)(2)F_{2,N-4,1-7}]/(N-4)$$
.

CONFIDENCE CONTOUR ELLIPSES FOR BIVARIATE POPULATIONS

In many experiments more than one response variable is being monitored. Therefore, it is desirable to make use of any correlation structure existing among the response variables in deriving confidence statements or in making inferences. For response variables from a bivariate normal distribution, a computer program has been written to construct a joint confidence region on their mean and a joint prediction region for a future observation. The output of the program includes summary statistics for each of the variables and a plot of the resulting confidence region. Options are available in the program to vary the confidence level, to input multiple data sets, to construct a prediction region for a future observation vector, and to construct the joint confidence region on the slope and intercept of a linear regression line.

^{3.} V. R. R. Uppuluri and T. Wright, "A Note on a Further Generalization of the Ehrenfest Urn Model" (in preparation).

^{4.} T. W. Anderson, An Introduction to Multivariate Statistical Analysis, Wiley, New York, 1958.

Part B. Statistical and Mathematical Collaboration

9. Biology and Health Sciences

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BIOASSAY OF METAL IONS

Metal ion toxicities for 13 metals were investigated in Drosophila melanogaster. Thirty flies were exposed at each of three to six dose levels; ten flies per replicate vial were used. To linearize the log doseresponse curve, the proportion of flies affected by each dose was transformed by the probit transformation.3 Maximum likelihood estimates of median effective concentration (LC₅₀), the slope (b) of the line, and their standard errors were computed using the SAS PROBIT procedure. The spacing of doses was designed to minimize the standard errors of the estimates of the LC₅₀, primarily, and of the slope, secondarily. Interpretation of slopes for different metal ions was facilitated by estimating the concentrations, which include 95% of the tolerance distribution. These concentrations, (LC_{27.5}, LC_{2.5}), their difference, and the log of their ratio $[\log(LC_{2.5}/LC_{2.5}) = 3.92 (1/b)]$ were used to characterize the biochemical properties of each metal and to compare the toxicities of these metals at low doses. The standard deviation of the distribution of log tolerances, 1/b, and the standard error of 1/b were also computed by the SAS PROBIT procedure.

Statistical tests of significance were made to determine the variations in estimated medians and estimated slopes for experiments performed at different times. These statistical analyses provide a basis for the characterization of strains of flies for use in genetic and biochemical experiments examining the action of metal ions.

EFFECT OF A GROWTH-INHIBITING AGENT ON EPITHELIAL CELL GROWTH

Total cell growth by density wa, reparated into growth because of attached cells and growth because of exfoliated cells. A growth-inhibited model was fit and estimates of the growth potential and the decrease in growth potential parameters were obtained. Using total growth as the dependent variable, it was determined that sufficient growth time was not granted for reliable estimates of the above parameters (i.e., growth had not leveled off to the extent necessary to reliably estimate the decrease in growth potential).

EFFECT OF EXPLANT NUMBERS AND GROWTH TIME IN PRODUCING UNIFORM GROWTH CULTURE DISHES

Overall growth curves were produced by using secondary explant growth data for culture dishes containing 2, 3, 4, 5, and 6 explants per dish. The

I. Biology Division.

^{2.} University of Tennessee.

^{3.} D. J. Finney, Statistical Method in Biological Assay, 26 ed., Griffin, London, 1971.

desire was to establish which combination of explants per dish and number of weeks of growth is optimum for producing the highest uniform density of culture growth. Results were inconclusive and the experiment will be replicated.

COMPARISON OF CELL GROWTH AND SURVIVAL BETWEEN CONTROLS AND CELLS TREATED WITH BENZO[A]PYRENE (Bap)

Tracheal explants were placed in organ cuiture in 60-mm tissue culture dishes with 2.0 mL of Wihc medium. Three days after the explants had been in organ culture, they were exposed to the carcinogen BaP (control explants were exposed to 0.2% DMSO). The explants were exposed for 3 d and then remained in organ culture for 25 d. Twenty-eight days after exposure, the explants were placed in primary culture with WRIHc medium, and every 7 d the explants were removed from the dish and replanted. An outgrowth was considered a primary culture if, after 3 weeks from removal of the explant, the outgrowth remained viable. The explants were replanted 12 times.

When primary cultures of a particular planting reached 1.0 to 2.0 cm² in area, all primary cultures were exposed to the selection medium (SM) for 28 d. When 8 or more control and BaP primary cultures were available, one-half were immediately exposed to the SM, and the rest were exposed 28 d later. The early and late groups were paired on area. After 28 d, cultures showing epithelial degeneration and sloughing were discarded. Cultures surviving SM were placed in WR1hc medium until subculture.

When primary cultures reached $i0^5$ cells or slow growing cultures aged 240 to 260 d, they were dissociated in 0.2% trypsin and 0.07% EDTA for no more than 10 min. Cells not remaining in the dish were seeded at 4×10^5 per 60-mm dish, or when cell yields were low, in 35- or 16-mm dishes. These secondary or dissociated cultures were subcultured at confluence for 5 cycles before being collected and stored at -70° C.

The growth of the primary cultures was assessed by calculating the total cell number per primary culture from area and cell density measurements. Cell numbers were calculated at the start of SM, at the termination of SM exposure, 30 d after termination of exposure, and at subculture. The growth of secondary cultures was calculated from the number of population doublings by using the number of cells

counted at dissociation and the original seeding density. The number of multinucleated cells was scored per 1000 cells counted in duplicate dishes.

EFFECT OF 6-MERCAPTOPURINE ON THE MOUSE REPRODUCTIVE PROCESS

The material 6-mercapt opurine is useful in treating leukemia, but, unfortunately, it has an adverse side effect—alteration of the reproductive process. To investigate the nature of the effect (i.e., how spermatogenesis was altered, a number of experiments were performed on mice. Early experiments determined that the proportion of spermatids at the various stages of sperm development was essentially unaltered by treatment, but the progression through the stages was altered for cells at a particular level of development when exposure occurred.

In later experiments, we investigated the possibility of genetic breakdown caused by 6mercaptopurine, the result of which would be a greater proportion of dead implants. Treated males were mated with females about one menth after treatment. Two females were kept with each male for 10 d; the females were replaced as they became pregnant. Late in the term of pregnancy, the female was opened and the proportion of dead implants determined. The experimental factors to be investigated were treatment with 6-mercaptopurine, the effect of 150 rads of radiation, the length of time between treatment and implantation, and a blocking factor (replication of the experiment). A mixedmodel analysis of variance was performed on the transformed proportion of dead implants. Results indicated an additive effect due to radiation treatment. The effectiveness of 6-mercaptopurine denended on time between treatment and implantation. with an increase to an observed maximum at about 33 d, followed by a gradual decrease back to normal.

ENZYME ACTIVITY

Samples of the enzyme HGPRT taken from various cell lines were labeled and heated for varying times. From each cell type, time-heated combination samples were taken at four time points and counted. The enzyme activity is defined as the slope in the linear relationship between counts per minute and sampling time. The purpose of this experiment was to quantify the effects of cell line and time heated on enzyme activity.

A linear relationship between the natural logarithm of enzyme activity and time heated was fit for

each cell line by using weighted least squares. The weights used were the inverses of the approximate variances for log-enzyme activity. When possible, parallel lines were fit for the cell lines. Half activity and its approximate standard error were calculated from these fits.

CHRONIC DERMAL TOXICITY OF PARAHO SHALE OIL AND DISTILLATES

Preliminary analyses of the skin oncogenic effect of the Paraho process shale oil and related distillates were carried out. This work is a result of a needed effort to assess environmental and health effects as an integral part of synfuck technology development. A complete description of these preliminary findings can be found elsewhere. The statistical methods used are similar to those described in other portions of this section.

CHRONIC DERMAL TOXICITY OF EPOXY RESINS

Experiments were recently completed in which the effects of epoxy resins on dermal toxicity, skin carcinogenicity, and synergistic carcinogenic interaction were studied. This work was a continuation of a program sponsored by the U.S. Department of Energy (DOE) to evaluate epoxy resins for potential occupational health risks.

Groups of inbred male and female C3H mice were exposed to doses of commercially available epoxy resins for a period of 24 months, beginning when the animals were 10 weeks old. The material was applied to their shaved backs three times a week. Time until first tumor and time until death were recorded.

The primary goal of this study was to determine the carcinogenic potency of the resins relative to a known efficient skin carcinogen, benzo(a)pyrene (BaP).

Each relative potency calculation used only data from a single test material (at several doses) and from the BaP dose groups. Males and females were considered separately because of the noticeably greater tumor incidence in males tested using the logrank test. The median time to tumor (T_{50}) was estimated from the three-parameter Weibull distribution fit to each group. An equation expressing the logarithm of T_{50} less the Weibull location parameter as a linear function of the logarithm of dose was fit for the BaP and the test material. Relative potency was calculated in terms of the relative BaP dose required to elicit the equivalent effect at each test dose. Confidence limits on relative potency were obtained by using Fieller's theorem. Complete details on the statistical methodology can be found in ref. 5.

PREDICTING MOLECULAR WEIGHTS OF DNA GENOMES BY SLAB-GEL ELECTROPHORESIS

Slab-gel electrophoresis can be used to estimate the molecular weight of DNA. The procedure involves first denaturing DNA strands to eliminate their secondary molecular structure, then subjecting the strands to an electrophoretic current, which causes them to slowly migrate across a viscous gel. When strands of unknown molecular weights are run in conjunction with known standards, regressing the molecular weights of the standards on the distance migrated (mobility) gives an equation for predicting the molecular weights of the unknowns. The prediction equation currently used incorporates a constant as well as terms in mobility and log mobility and results in high R^2 values if the range of mobilities is not too large. However, increasing the range for prediction would be useful because known standards. are rare and expensive to obtain. A method for doing this is being studied. Some known standards can be cut with enzymes into pieces that satisfy known relationships. By running cuts of these standards, we hope to use constrained regression to improve the accuracy of prediction.

SISTER CHROMATID EXCHANGES IN MELANOMA AND COLON TUMORS

The rate of sister chromatid exchanges (SCE) is accepted as an index of potency of chemical carcinogens. In the current study, SCE are counted in (human) normal, melanoma, and colon tumor cell lines at four dose levels of Mitomycin C, including zero-dose controls. At each tissue-dose combination,

^{4.} J. M. Holland, L. C. Gipson, M.2. Whitaker, L. J. Stephens, G. M. Clemmer, and D. A. Wolf, "Chronic Dermal Toxicity of Paraho Shale Oil and Distillates," in *Health Effects Investigation of Oil Shale Development*, ed. by W. H. Griest, M. R. Guerin, and D. L. Colfin, Ann Arbor Science Publishers, Ann Arbor, Mich., 1981.

^{5.} D. A. Wolf and T. J. Mitchell, "Statistical Analysis of Mortality and Relative Skin Carcinogenicity," appendix in Chronic Dermal Toxicity of Epoxy Resins in Skin Car mogenic Potency and General Toxicity, ORNI - IM-5762 (March 1981)

^{6.} J. M. Holland, L. C. Gipson, M. J. Whitaker, B. M. Eisenhower, and T. J. Stephens, Chronic Dermat Toxicity of Epoxy Resins in Skin Carcinogenic Potency and General Loxicity, ORNI, TM-5762 (March 1981).

20 cells in metaphase are analyzed for number of chromosomes and number of SCE. The entire experiment is replicated.

In addition to the dose response for the three tissue types, the relationship of SCE frequency to number of chromosomes in each cell is also of interest. Karyotypic instability, the tendency of mutant cells to have abnormal numbers of chromosomes, was found to be unrelated to SCE-chromosome rates for cells in any given dose-tissue group. Dose responses for the different tissues differed significantly. Colon tumor cells showed a threshold effect not seen in the normal tissue; melanoma showed yet another response.

DIESEL FUEL AEROSOLS

A study supported by the U.S. Army is under way to investigate the effects of diesel fuel smoke screens on rats. Phase I of the study consisted of acute exposures to determine a region of maximum effect with minimum mortality. Various models, including the PROBIT model, were used to derive a 97.5% lower confidence limit for the LD₀₁. This dose and one-third of it are tentatively proposed as dose levels (in addition to controls) for phase II, a multiple exposure study.

Phase II will consist of 12 treatment groups defined by dose, time of exposure, and number of exposures per week. These groups must be blocked into sets of 4 because of the logistics of rat shipments as well as manpower. The confounding of certain effects with blocks is unavoidable, but all but a few can be estimated without bias. The purposes of phase II are range finding, refinement of assay techniques, and gaining general information for a final and more elaborate phase III.

RELATIONSHIPS BETWEEN CARDIOVASCULAR DISEASE AND TRACE ELEMENTS IN DRINKING WATER

During the past 20 years, epidemiological studies have led to conflicting conclusions about the relationship of cardiovascular disease to the hardness of water (i.e., amount of calcium it contains). It has been speculated that these contradictions are due to confounding factors, namely, the presence or absence of trace elements such as cadmium or lead. A study is under way to assess the effects of these two elements as well as calcium and magnesium on cardiovascular disease in white Carneau pigeons. Along with a dirtary factor (fat), these elements are combined in treatment groups to produce a 2⁵-factorial experiment. Six-month increments in exposure time make a sixth factor.

Data from the first five exposure periods are being analyzed. Analysis of variance is revealing the effects of the elements on end points such as blood pressure and arterial plaque size and numbers. Of particular interest is the apparent ability of calcium to suppress cadmium-induced increases in these end points and, in the absence of cadmium, to cause a slight increase itself. This, of course, is exactly the sort of confounding that was speculated.

10. Chemistry

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MODELING THE ACTIVITY COEFFICIENT OF NITRIC ACID

The Wilson equations⁵ for a two-component system are being modified to predict activity coefficients in the three-component system of nitric acid, magnesium nitrate, and water. Currently, four unknown coefficients are estimated from three sets of equilibrium data. If a suitable model can be found, the results will be compared with recent nonequilibrium data.

EQUILIBRIUM CONCENTRATIONS IN FUEL REPROCESSING

Calculation of equilibrium concentrations in a nuclear fuel reprocessing model requires the solution of a large system of nonlinear algebraic equations. A natural and straightforward linear iterative method for solving this system yields rapid, early improvement of an initial estimate for the solution, but ultimately fails to converge. More powerful nonlinear techniques are locally convergent, but they require a relatively good starting point. The behavior of these methods was studied and explained both theoretically and numerically, which led to a very robust hybrid approach to such problems that has been implemented through computer software.

MULTIPHOTON DISSOCIATION OF MOLECULES

It has been observed empirically that some molecules may be dissociated when sufficiently energized by a laser. Such processes have been simulated theoretically by using both semiclassical and quantum mechanical models and by solving numerically the resulting ordinary and partial differential equations. Of particular interest is the onset of chaotic (stochastic, ergodic, and turbulent) behavior of the solutions. In addition to providing a better understanding of underlying physical mechanisms, such as nonlinear resonance phenomena, this work has potential applications in such areas as laser isotope separation.

X-RAY FLUORESCENCE ANALYSIS OF URANIUM AND PLUTONIUM

A statistically designed experiment was performed to examine the precision of measuring uranium and plutonium concentrations in an aqueous solution (nitric acid) and in organic solutions [triethylhexanonic phosphoric acid (TEHP)] by x-ray fluorescence. The experimental design examined solutions with five concentrations of uranium in the range of 1 to 20 mg/mL in the presence or absence of 10% plutonium concentrations. The nitric acid concentrations in the aqueous solution were at 1, 3, and 6 M, and the TEHP levels were 8, 16, and 32% of the volume in the organic solutions.

X-ray fluorescence analysis is based on the number of characteristic x rays from uranium and plutonium atoms that have been energized by the x rays. Calibration curves for uranium and plutonium concentrations are derived from the number of counts from solutions of known concentrations of the two elements. Past experience indicated that the number of counts of characteristic x rays behaved quadratically and complicated the analysis of unknown solutions. To overcome this problem, the aqueous and organic solutions were spiked with yttrium and thorium, respectively.

Calibration curves were based on the ratio of the number of counts for uranium and plutonium to the number of counts for yttrium and thorium. Using the ratio of counts, the calibration curves are linear in the aqueous solution, but there is an effect caused by nitric acid. This effect was traced to the decrease in the yttrium counts when nitric acid concentrations were increased. In addition, the calibration curve for

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^{5.} G. M. Wilson, "Vapor-Liquid Equilibrium; A New Expression for the Excess Free Energy of Mixing," J. Am. Chem. Soc. 86, 127 (1964).

^{6.} R. M. Counce, The Scrubbing of Gaseous Nitrogen Oxides in Packed Towers, ORNL-5676 (November 1980).

the plutonium count ratio depends on the presence or absence of uranium in the aqueous solution. Calibration curves for the two count ratios in the organic solution were not affected by the different TEHP concentrations, but the curves did show significant quadratic behavior. The quadratic coefficient of the uranium calibration curve is affected by the presence of plutonium, and both the linear and quadratic coefficients of the plutonium calibration curve are affected by the presence of uranium.

DEHYDRATION AND DENITRATION OF URANYL NITRATE HEXAHYDRATE

Uranium from spent reactor fuel is separated and recycled by a process in which it is converted to uranyl nitrate hexahydrate [UO₂(NO₃)₂-6H₂)], which thermally decomposes to uranium trioxide. The kinetics of this decomposition were studied by the thermal analysis method of differential scanning calorimetry (DSC). This method measures the change in enthalpy with respect to time when a sample of the material is heated at a constant rate.

The DSC data were analyzed using the Sestak-Berggren equation, which represents different controlling mechanisms for solid-phase reactions by different values of the equation's parameter. Parameters for the Sestak-Berggren equation were estimated by the method of least squares. The estimated models fitted the DSC data with multiple correlation coefficients greater than 99%. However, estimated models that represent the nucleation process and the diffusion process can represent the DSC data with equal precision. These models also give estimated activation energy values that appear to be underestimated, and in some cases, at the 5% level, these values are not significantly different from zero. Therefore, the best prediction models for the DSC data lead simultaneously to several reaction mechanisms and to ambiguous estimated activation energies. Because temperature and time are linearly related in the DSC thermal analysis method, the DSC data cannot be represented by a model that is an independent product of both a temperature function and a time function. To determine the reaction mechanisms and the activation energies, an additional analytical method is necessary to verify the DSC thermal analysis data.

11. Energy

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A THOMPSON SCATTERING DIAGNOSTIC FOR A LOW-DENSITY, HIGH-TEMPERATURE, STEADY-STATE PLASMA

The modeling of photon count data from what is assumed to be a Maxwellian (Gaussian) distribution was attempted with the goal of estimating the density and temperature of a plasma within the ELMO Bumpy Torus. Because of physical constraints, only the right half of the distribution was observable, and these data were recorded as counts in one of five mutually exclusive and exhaustive intervals. Using natural logarithms of the total count in each interval, the model $\ln(\operatorname{count})_i = \beta_0 + \beta_1 X^2 + \epsilon_i$ was fit, where X_i is the distance from μ to the midpoint of the interval. Defining X_i thusly sets $\mu = 0$, and the first-order term for X_i and the cross-product term both vanish. The estimation of the parameters was hampered by low frequencies in some of the extreme intervals.

ANALYSIS OF EUS FIELD TEST DATA

The Energy Utilization Systems (EUS) field test data concerning the performance of heat-pump-hot-water heaters were analyzed by using both a model currently in use and a proposed model. The proposed model resulted in a tenfold increase in \mathbb{R}^2 . Further improvement is hampered by the lack of control over installation procedures, placement of the unit, and placement or reading of measuring devices used to collect the data. Further modeling of laboratory data is expected in the near future.

SUMMARY STATISTICS ON THE 1977 FPC FORM 4 DATA BASE

ORNL was involved with the validation of the Federal Power Commission (FPC) Form 4 data base for the Office of Energy Information Validation (OEIV). Part of this project was the task of preparing summary statistics for the file. Requests centered around two main subject areas: (1) dividing the range of generation capacities into mutually exclusive and exhaustive categories and determining the number of companies and plants within each category and (2) determining the number of companies generating electricity.

Coding inconsistencies inherent in the data files and misspellings of company or plant names hampered the completion of these tasks. Each request was completed by sending listings to OEIV for comments and then adjusting the approach used to accommodate new ideas or corrections.

ANALYSIS AND COMPARISON OF DATA FILES

The Office of Oil and Gas Information System (OGIS) supplied ORNL with data tapes for the 1977 American Petroleum Institute (API), American Gas Association (AGA), and EIA-23 (Energy Information Administration) data bases. The project consisted of three main efforts: (1) editing the API/AGA files and schedules 1 to 3 of the EIA-23 file; (2) obtaining aggregate totals for specified variables at national, state, subdivision, and field levels; and (3) determining whether the EIA-23 file could be modeled from the API/AGA file with reasonable accuracy.

Unanticipated organizational problems built into the files by OGIS caused extreme problems in reading the files accurately. The most severe problems were in three areas: inconsistent spellings of field and reservoir names, numeric values written as packed decimals that could not be read correctly by SAS or FORTRAN programs, and a file structure not consistently in any logical sequence. These

I. Fusion Energy Division.

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^{5.} Energy Division.

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problems and suggested solutions were reported to OGIS.

Requests for specific listings were received from OGIS throughout the life of the project; thus, task 2 was an ongoing one. These listings permitted comparisons of totals, supposedly representing the same quantity, between the API/AGA and EIA-23 files. The impact of frame discrepancies between the different collecting agencies and sample coverage differences made comparisons of volumes between the API/AGA and EIA-23 files difficult to interpret.

Task 3 was contracted to George A. Milliken, Professor of Statistics at Kansas State University. In Dr. Milliken's final report, evidence was presented in support of the feasibility of predicting EIA-23 values from pre-1977 API/AGA data files. If OGIS completes 1978 and 1979 data files for the API/AGA data base, the quality of the predicted values will warrant completion of this task.

MODIFICATIONS TO THE ERATO CODE

The ERATO code is used by the ORNL Fusion Energy Division to determine the stability of an equilibrium of the linear ideal magnetohydrodynamic equations for a plasma in a tokamak reactor. Modification of the code to take advantage of the sparsity of the matrices involved began last year. More changes were incorporated this year to further reduce the CPU time, memory, and I/O required by the code.

ON THE ACCURACY OF PUBLISHED ESTIMATES OF ENERGY-RELATED PARAMETERS

In addition to the ongoing validation surveys of energy-related data collection systems, efforts began this year to provide statements of accuracy for data published by the EIA. The general approach was to compare published EIA estimates with comparable estimates from other sources.

Two simple tools were suggested that can be used in the comparison of several comparable estimates of

the same parameter. One, the tolerance coefficient, makes a statement about the accuracy of the estimates versus the target parameter; the other, the maximum ratio, gives a measure of the closeness among the estimates.

A useful result is presented or determining when at least one of the estimates in the collection will be more than $100\alpha\%$ away from the true parameter where $0 < \alpha < 1$.

MEASURING EFFECTIVENESS OF ATTIC INSULATION

Quantitative estimates of the effectiveness of attic insulation are typically based on a system component approach [i.e., summation of R or U values (from tables) for the individual components of the house structure]. This approach neglects degradation of insulation effectiveness caused by the effects of air infiltration, convection heat loss, insulation aging, insulation moisture content, or any other factors normally present in the attic insulation's environment. Consequently, valid questions can be raised about the true effectiveness of attic insulation; these questions can only be resolved by analyzing field data.

Actual energy consumption and weather data for approximately 35 single-family residences in the Knoxville. Tennessee, area were examined to determine the effectiveness of attic insulation. For each residence, linear regression techniques were used to determine the average winter energy consumption rate (kJ/degree-day) for two years before and three years after the attic insulation was installed. Comparison of energy consumption rates before and after installation showed a decrease in 85% of the residences. Seasonal variation and balance-point changes were also investigated for each residence.

^{7.} H. Tsao and T. Wright. Tolerance Coefficient and Maximum Ratio: A Note on Two Simple Tools for the Comparison of Several Estimates of the Same Parameter in preparation).

12. Engineering

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CENTRIFUGE FORCED RESPONSE, MODE SHAPES, BALANCING

CLYINDER, a rotor dynamics computer program, was introduced in a previous report." This program has been documented. From CLYINDER a new program, SYMCYL, is evolving: SYMCYL is being used to simulate rotor imperfections and to provide deflections to test the seasibility of a new balancing technique. This technique, implemented in an evolving program, INCYL, had required least squares software for stacked, banded matrices; that is, the least squares matrix is of the form $(B_1^r, \ldots,$ $B_N^{T_i}$, where each B_i is of order 400 and 5 and width 8. A reformulation of the problem has and to a large band matrix bordered down one side. Appropriate software is being developed, investigation of the condition of the B_i matrices is being pursued, and extensive simulation studies are being planned.

Development of the computer program MODE SHAPE, which calculates the natural frequencies and mode shapes of a rotor, was discussed in a previous report. The original MODE SHAPE has been superseded by MODE SHAPE II. Recent modifications to MODE SHAPE II include a more flexible input and an output more readily plotted by the software.

Computer-produced movies to depict the centerline of a spinning rotor were introduced in a previous report. The latest movie, MOVIE II, depicts actual centrifuge data at operating speed and build data. Components of the build function from MODE SHAPE II (fit by the least squares method) are successively and additively subtracted from the build curve to depict their contribution. A report describing the programming of such a movie has been published. The report assumes the input is discrete output from a machine or output from CYLINDER. In the report, which documents the computer program REVOLV, a makeshift example models a hypothetical steel rotor. Related three-dimensional Calcomp plots have been useful in depicting actual centrifuge deflections, MODE SHAPE II, and CYLINDER deflections. Also, plotting software is available to assess how closely curves from different rotor models resemble each other. One curve is held fixed, while the second is rotated and scaled to match the first by using the least squares method. The residual is plotted in three dimensions.

ELECTROCHEMICAL MACHINING

A project on the modeling of the electrochemical machining (ECM) process has been started. The first goal of the project is to produce a computer code that will predict optimum working parameters for an arbitrary tool shape. Optimum in this case means minimizing machining error (i.e., the geometrical difference between the machined part and the tool). The method to be used is that of Kozak. Eventually, it is hoped that this will lead to a code that will predict the tool shape, given the desired geometry of the machined part.

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^{8.} R. E. Funderlic, "Mode Shape Analysis and Centrifuge Rotor Response to Balance Weights," Mathematics and Statistics Research Department Progress Report, Period Ending June 30, 1980, ORNL CSD-61 (September 1980), p. 29.

^{9.} S. A. Haw and R. E. Fundersic, Implementation of a Computer-Produced Movie, ORNL CSD TM-130 (November 1980).

^{10.} J. Kozak, "Ontimization of the Electrochemical Machining Process from the Point of View of Geometrical Accuracy," Arch. Budowy Masz. 22, 387-98 (1975).

LATENT-HEAT THERMAL ENERGY STORAGE

Collaboration in latent-heat thermal energy storage (TES) via a phase-change material (PCM) has centered on the use of analytical and computational methods for analyzing and predicting the behavior of various (TES) systems. The following are some of the significant achievements of this effort, which were obtained during the reporting period.

A slab, cylinder, or sphere of PCM, initially at its melting temperature and in solid state, is subjected to convective heat transfer from a warm transfer fluid of temperature T_m at its surface. If its radius is L and its thermal diffusivity is α , then its melting time is given by

$$\frac{L^2}{\alpha \text{St}(1+\beta)} \left[0.5 + \frac{1}{\text{Bi}} + 0.5(0.25 + 0.17\beta^{-}) \text{St} \right],$$

where $\beta = 0$, 1, 2 as the body is a slab, cylinder, or sphere and as Bi and St are the Biot and Stefan numbers, respectively. The Biot number is the ratio of convective heat transfer to the body over conductive heat transfer in it. The Stefan number represents the ratio of sensible heat drop (between $T_{\rm in}$ and the melting temperature) to the latent heat and is the key parameter in phase-change models. This relation is accurate to within a 10% relative error over the range $0 \le St \le 4$ and $0.1 \le Bi$.

A PCM rectangle of side lengths a and b is initially in its solid state at the melting temperature and is subjected to a constant, uniform boundary temperature above its melting point. The melting time of the rectangle is then given by

$$\frac{a^2}{8\alpha \text{St}}$$
 (1 + 0.25St), for $\frac{a}{b} \le \frac{2(1 + 0.42\text{St})}{\pi(1 + 0.25\text{St})}$

and

$$\frac{ab}{4\pi\alpha \text{St}} (1 + 0.42\text{St})$$
, for $\frac{a}{b} > \frac{2(1 + 0.42\text{St})}{\pi(1 + 0.25\text{St})}$.

Here a is assumed to be the chorter side, $a \le b$. This relation has been found to be accurate to within a

10% relative error for $St \le 4$. Other similar results have been obtained for a variety of problems. 14-16

In support of the study of the crawl-space-heatpump augmentation concept. 'a simulation program was prepared for a 3-m-deep (10-ft), 12-m-long (40ft) rectangular region in the ground below a tunnel that is thermally insulated from the house above. The simulation includes air that is being pumped through the tunnel from the (cold) ambient air and predicts the temperature of the air at points including its outlet; the simulation also predicts the air temperature in the earth at various depths. The program includes the effects of possible surface freezing of ground moisture. Using the program, comparisons between observed temperature values and computer predictions were made during February 1980 for a tunnel beneath a test house. The computer model was found to accurately predict temperature trends and to differ by only a few degrees at most from the recorded data. A typical result is that obtained for 12:00 noon on February 12:

Temperature (°F)

Thermocouple	Observed	Predicte	
1	31	32	
2	39	35	
3	39	37	
4	37	34	
5	41	37	
6	44	39	
7	37	36	
8 -	40	38	
9	42	,39	
10	23	20	
11	29	27	
12	33	31	

Here, thermocouples 1 through 9 are located at various positions and depths in the earth, and thermocouples 10 through 12 give the air duct

^{11.} A. D. Solomon, "A Note on the Stelan Number in Slab Melting and Solidification," Lett. Heat Mass Transfer (1981) (forthcoming).

^{12.} A. D. Solomon, "On the Melting Time of a Sample Body with a Convection Boundary Condition," Lett. Hear Ways Transfer 7, 183–88 (1980).

^{13.} A. D. Solomon, "An Expression for the Melting Time of a Rectangular Body," Icir. Hear Mass. Transfer 7, 379-84 (1980).

^[14] A. D. Solomon, "On Moving Boundary Problems and Fatent Heat Thermal Energy Storage, Part I," Israel Chem. Eng., 11, 17–19 (1980).

^{15.} A. D. Solomon, "On Moving Boundary Problems and Latent Heat Thermal Energy Storage, Part II," *Israel Chem. Eng.* (1981) (forthcoming).

^{16.} A. D. Solomon, "Some Useful Relations for Phase Change Heat Transfer Problems," *Indus. Math.* (forthcoming).

^{17.} M. Ternes, "Crawl-Space-Assisted Heat Pump," Proceedings of Thermal Energy Storage, Fourth Annual Review Meeting, DOE Publication CONF-791232, December 1979, pp. 272-76.

temperatures. In particular, thermocouple 12 gives the air duct outlet temperature, reflecting the warming effect of the ground.

There is currently a lot of interest in examining the potential use of the University of Delaware PCM Chubs for various TES purposes. One such purpose is in storage-assisted air conditioning, which involves the use of Chub arrays in parallel with a lower-power air conditioning system in a home. The study of this system requires a simulation tool that will (1) accurately model the temperature distribution and phase-change process within the Chub and, at the same time, (2) take into account the fact that an array of Chubs at lower temperature may dehumidify the warmer, humid air flowing over them. With this in mind, we have extended the TES program¹¹ to model arrays of PCM cylinders with an air transfer fluid undergoing possible dehumidification. We assume convective heat transfer at each cylinder surface and make use of a package simulating the psychrometric table for humid air. The program is now running and will be compared with data obtained from tests currently being carried out. 18,19 Additional simulation efforts have been applied to a variety of questions. 20

DYNAMIC ANALYSIS OF PIPING SYSTEMS

Dynamic analysis of piping systems is a required part of the design of a nuclear reactor. The major mathematical task involved in dynamic analysis is the calculation of 10 to 100 eigenvalues and eigenvectors of a generalized eigenvalue problem. The Tennessee Valley Authority uses the software package TPIPE to solve dynamic analysis problems. The eigensolver in TPIPE was replaced by a shift and invert Lanczos algorithm, which resulted in a factor of 3 reduction in computing time required for a problem with 3600 degrees of freedom. The modified code is currently being certified for production use.

^{18.} A. D. Solomon, Simulation of a PCM Storage Subsystem for Air Conditioning Assist, ORNL CSD-77 (forthcoming).

^{19.} J. Rizzato, F. Arvil, M. Lang, and A. Tortora, "Storage-Assisted Air Condition," presented at U.S. DOE Thermal Energy Storage Contractors' Meeting, Demer, Colo., May 14-15, 1980.

20. A. D. Solomon, "On Surface Effects in Heat Transfer Calculations," Comput. Chem. Eng. 5, 1-5 (1981).

13. Environmental Sciences

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PHOSPHOROUS DYNAMICS IN STREAMS

A compartmental mode! of phosphorous dynamics in a stream ecosystem leads to an initial boundary value problem for a system of three ordinary and two partial differential equations. This system includes both convection and diffusion terms and is, therefore, of mixed type. The system was solved numerically using the method of lines with spatial discretization by cubic spline interpolation. The purpose of this project is to gain insight into the phenomenon of nutrient spiraling in stream ecosystems.

COMPARISON OF PHOSPHORUS ELIMINATION RATES

A study was conducted to evaluate the effect of microconsumers (protozoans) on phosphorus turnover using ¹²P as a tracer. The first phase of the experiment involved collecting random samples of stream sediment and allocating them to the following treatment groups: (1) sterile (no living microorganisms present), (2) live (natural living microorganisms), (3) pasteurized (same as live without the microconsumers), and (4) pasteurized-reinoculated (same as pasteurized, but with microconsumers reinoculated). These treatments make it possible to evaluate the effect of removing all microorganisms, as well as the effect of the process of removing the microconsumers (pasteurization) on the PO₄-P sorption and turnover by the stream sediments.

To measure the sorption of ³²PO₄ from the stream water, the replicate containers in each treatment group were first exposed to equal concentrations of ³²PO₄ until this concentration reached equilibrium. Turnover of ³²P associated with the sediments in each treatment was measured by placing the containers in artificial streambeds and periodically collecting sediment samples from each replicate for two weeks. The ³²P concentrations were recorded for

each sample and used to evaluate the 32P turnover for each treatment group. The double exponential relation $y(t) = a_1e^{-b_1t} + a_2e^{-b_2t}$ was found to adequately describe the concentration y(t) as a function of time since the sediments from each treatment were placed in the streambed t. Nonlinear least squares estimation procedures were used to determine the parameters a and b from the observations on each replicate. The multivariate statistical technique, canonical analysis, was used to evaluate significant treatment group differences by using the vector of estimated parameters from each replicate. The results of this analysis showed that significant treatment differences do exist, primarily from the differences in the estimated a coefficients. Because these coefficients can be associated with the equilibrium level of 32P achieved during the uptake (sorption) portion of this experiment, the results of this study support the conclusions of earlier studies, which were that sterilization and pasteurization affect uptake of PO4 by stream sediments. The absence of significant differences in the b coefficients indicates a need to modify the experimental technique to reduce the possibility of contamination in some of the treatment groups during the turnover phase of the experiment.

EFFECTS OF TEMPERATURE ON PREDICTING IMPINGEMENT

A model to describe changes in fish impingement as a function of water temperature and change in water temperature was described in an earlier report.³ The predictive model, which incorporates the moving average and lagged effects of temperature and change in temperature, has been evaluated using impingement data for two fish species most often impinged at the Tennessee Valley Authority's Kingston Steam Plant. Formulation of the temperature model

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^{3. &}quot;Impingement at the Tennessee Valley Authority Kingston Steam Plant." Mathematics and Statistics Research Department Progress Report. Period Ending June 30, 1980, OP.NI, CSD-61 (September 1980), pp. 32-33.

allowed testing of meaningful hypotheses about effects of water temperature and rate of change of water temperature on the magnitude of impingement. A comparison of the derived model with another model that ignored effects of temperature by assuming no change in impingement over short periods of time (\$\leq 3\$ d) showed that adjustment for temperature effects increased the accuracy of the predicted impingement for both species. Effects of hydrology on the distribation of fish on different intake screens were inferred from hydrological mapping near the intake area. The modeling approach and conclusions about hydrological effects may be applied to other systems in which cold-stressed schooling fish are impinged.

COMPARISON OF TWO METHODS OF "Sr DETERMINATIONS

Water samples collected from monitoring wells located within and near the ORNL burial grounds have been routinely analyzed for radioactivity. The established methodology for 50 Sr determination in aqueous samples involves chemical separation. A comparison between the standard chemical separation method and that of the more rapid Cerenkov radiation counting method was made on samples from waste disposal areas. For each sample, a **Sr determination was recorded for each of the two methods. The first step in the statistical analysis was to examine probability plots of the distribution of the ⁹⁰Sr determination values for each method, this distribution was found to be reasonably approximated by a log normal distribution. The paired transformation observations were evaluated to determine if a significant difference existed between the two methods. The results of this analysis indicated a high correlation (r = 0.99) and no significant difference (P > 0.40) between the two methods. The results of this analysis have given additional evidence that the Cerenkov radiation counting method reduces both cost and sample processing time when screening samples with low 90 Sr concentrations.

QUADRATIC CALIBRATION OF TRACE METAL CONCENTRATION

Atomic absorption spectrophotometry is used to determine the concentration of trace metals in seawater. Analysis of seawater samples has shown the "signal" (y) from the spectrophotometer to be related to the trace metal concentration (x_1) and salinity (x_2) through the polynomial approximation y

= $b_0 + b_1x_1 + b_2x_2 + b_3x_1x_2 + b_6x_1^2$. A calibration curve has been determined from an analysis of samples with known x_1 , x_2 values by using this relation. In addition to providing estimates of the b coefficients, the calibration data provided an estimated covariance matrix. Samples with unknown x_1 concentration and independently determined x_2 concentration by an alternative method were analyzed. Because the determination of x_2 is known to be very accurate, it was assumed that $var(x_2) = 0$. With this information, a confidence interval on x_1 was obtained for a given signal (y) and fixed salinity (x_2) by using the results of Ferris. This analysis will be quite helpful in obtaining interval estimates of trace metal concentration from unknown samples.

ACUTE TOXICITY OF ACRIDINE TO A CALANOID COPEPOD

A laboratory study was performed using a calanoid copepod (Diaptomus calvipes) as a test animal to investigate the acute toxicity of acridine, an azaarene found in some coal conversion effluents. Separate groups of animals were raised at 3 temperatures (16, 21, and 26°C); random samples of animals were then subjected to 3 feeding regimes ranging from starved to well fed for 5 d before testing. The purpose of incorporating the different feeding regimes into the experimental design was to investigate the effect of nutritional state on mortality from exposure. Groups of 60 animals, in a 1:1 sex ratio. were exposed at each of 6 concentrations of acridine from 2.4 to 10.0 mg/L. In addition, control groups (no acridine) were incorporated in the experimental design to monitor the experimental technique. For each combination of experimental factors (temperature, feeding regime, sex, and acridine concentration), the animals were observed at 24-h intervals for 96 h, and the number of dead animals was noted.

The following logistic model has been proposed to describe the survival time T of the animals in a treatment group defined by a combination of experimental factors:

$$P(T < t) = 1/\{1 + \exp((\mu - \ln t) / \delta\}\}.$$

where t is the observation time (24, 48, 72, 96 h), μ is the location parameter, and δ is the scale parameter.

^{4.} Y. M. Ferris, Propagation of Error Procedure for General Quadratic Calibration Curves, TID-4500-R60, Dow Chemical USA, Golden, Colo. (September 1974).

Maximum likelihood procedures were used to obtain the parameter estimates for each treatment group. Preliminary analysis of the data indicates that the logistic model is doing an adequate job of describing the survival data for each treatment group. Additional analyses will be performed to determine if a toxic threshold model describes the change in the estimated half-life, $\exp(\mu)$, as a function of acridine concentration. The estimated parameters in the threshold model can then be used to examine the effects of the other experimental factors of water temperature, sex, and feeding regime on survival.

DIGESTION RATES OF FRESHWATER PREDATORS

Laboratory experiments have been performed to determine the time required by predators (large-mouth bass) to digest prey (minnows or shad) at various temperatures. This information is critical in developing a methodology for determining field consumption (daily ration) of predators. Knowledge of field consumption is important for evaluating the effects of prey availability on growth and mortality and for estimating the impact of predators on their

food supply. The experimental design involved holding individual bass in cages at fixed water temperature and feeding them a known weight of prey. Predator stomachs were pumped at various intervals following feeding to remove the partially digested prey. Six different water temperatures from 14 to 28°C were examined, and a sufficient number of predators were initially fed at each temperature so that four individual fish could be randomly selected at each of the predetermined observation times. The measured response for each fish was the percentage of the known initial food that was digested in each sample interval. A linear log-log regression function was found to do an adequate job in describing the time versus percentage digestion data for each temperature group. A comparison of the different water temperature groups was made in terms of the estimated parameters and also in terms of the estimated times to 95% digestion. Inverse regression was used to obtain confidence limits on the time to 95% digestion. Results of the statistical analysis have been helpful in quantifying the impact of predators on their food supply and in evaluating the effects of prey availability on predator growth and mortality.

14. Health and Safety Research

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CALIBRATION OF THERMOLUMINESCENT DOSIMETER METER BADGES

The new thermoluminescent dosimeter (TLD) badges have been studied extensively in an attempt to .termine how to estimate an employee's radiation exposure from the energy trapped in the TLD's two lithium fluoride (LiF) chips.

These studies included both short- and long-term studies that were designed to establish a relationship between the exposure and the TLD's response and to determine how well the LiF chips held their responses over time.

RADIATION MONITORS, THRESHOLD DETERMINATION

The goal was to establish alarm thresholds for the detection of varying amounts of ²³⁵U using walk-through detectors. The detection technique consisted of two components. The first component checks for possible metal serving as a shield to the uranium, and the second component is a ²³⁵U detector. Limits were to be set to satisfy DOE requirements. It was desired to set alarm thresholds so that the chances of incorrect detection were small. Data were collected to verify underlying model assumptions that were necessary for the establishment of realistic alarm thresholds.

SAMPLING PLAN FOR INDUSTRIAL HYGIENE MONITORING OF THE H-COAL PILOT PLANT

Coal liquefaction products are expected to have major use as boiler fuels, fuel oil, and chemical feedstocks, and the projected energy production is several quads in the next two decades. The H-Coal process is one of several methods under intensive technological study, and operation of a pilot plant will provide engineering data for scale-up. The objective of the H-Coal Environmental and Health Program is to provide data and information to support analyses and assessments of coal liquefaction technology.

A sampling plan for monitoring plant areas and personnel at the H-Coal pilot plant size was developed and reviewed. The focus of the plan is the identification of potential exposure to contaminants currently unregulated. The goal is to achieve an integrated industrial hygiene activity that will provide the necessary information for subsequent commercialization of the H-Coal process.

Consideration is currently being given to the analysis of some of the data being reported.

MONITORING FOR COMPLIANCE WITH DECOMMISSIONING CRITERIA

The use of stratified samp!ing was explored in a report⁷ designed as a general-purpose guide for those with concern for the final steps needed to ensure that a former radiological site has been cleared up to the point that it is safe to release that site for unrestricted public use. The guide is aimed at two parties: (1) the licensee who wants to dispose of the site and (2) the regulatory agency inspector who wants to be sure that the site is (or is not) safe to release.

The purpose of this report is to give guidance and direction on how the licensee shall carry out his final survey, such that its design, procedures, results, and interpretations can be compared with existing standards.

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^{7.} C. F. Holoway, J. P. Witherspoon, H. W. Dickson, P. M. Lantz, and T. Wright, Monitoring for Compliance with Decommissioning Termination Survey Criteria, NUREG CR-2082, ORNL: HASRD-95 (June 1981).

15. Material Sciences

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R. L. Hustand¹
H. Inouye¹

W. E. Lever

C. T. Liu¹ D. W. Post²

A. C. Schaffhauser¹

IRIDIUM PROGRAM

Statistical analyses of iridium sheet chemistry and impact data were conducted in support of an iridium task force created to identify sources of problems in producing flight-quality hardware for the Iridium Base Technology Program. The major problem is the tendency of iridium cups to crack when fabricated from particular batches of raw material. These cups are to contain the power sources for future space flights and must withstand minimum impact standards. No major problem source could be identified. Varying methods in reporting data over several iridium batches made it difficult to reach valid conclusions. Also, chemistries were usually reported

as a range of values or as an upper or lower limit. The greatest value in the analysis is in learning when and what new data need to be collected; the analysis focuses on what you have and where you ought to be going.

KEVLAR YARN

The study of the properties of Kevlar yarn has continued. Based on the results of studies reported previously, sampling plans are being prepared to allow for the evaluation of a new lot of material. The review of proof testing methodologies for products using Kevlar yarn has continued on a reduced level.

^{1.} Metals and Ceramics Division.

^{2.} Y-12 Development Division.

^{3. &}quot;Kevlar Yarn," Mathematics and Statistics Research Department Progress Report, Period Ending, June 30, 1980, ORNL/CSD-61 (September 1980), p. 36.

16. Safeguards

E. E. Johnson¹

W. E. Lever

VARIANCE FORMULAS FOR INVENTORY DIFFERENCES

The error propagation variance formulas developed for the Y-12 Plant material balance area (MBA-

72) feasibility study² have been augmented to account for process correlations that were previously omitted.

The error propagation approach of determining the reliability of the uranium inventory differences is one of several possible approaches to the problem now being considered by management.

I. Y-12 Quality Division.

^{2. &}quot;Variance Formula for Inventory Differences," Mathematics and Statistics Research Department Progress Report. Period Ending, June 30, 1980, ORNL CSD-61 (September 1980), p. 39.

17. Surveys

G. M. Adamson¹
H. Broadbent²
E. Leach
J. S. Trent
G. M. Goodwin¹
H. Reesor¹
J. Graham²
C. A. Serbin
T. Wright

AMERICAN WELDING SOCIETY STUDENT MEMBERSHIP SURVEY

A census survey of student membership in the American Welding Society (AWS) was conducted to better understand student member makeup and to find ways of encouraging greater participation in the society by both members and nonmembers. Of the 3054 questionnaires sent to students, 1551 were completed and returned—a response rate of 50.8%. This compares favorably with the 51.3% response rate for student members in the general membership survey conducted in 1977.³

Results confirmed the widely held view that the instructor in the vocational or trade school and in the university plays a significant role in building student membership. Nearly two-thirds of the respondents listed "encouragement by an instructor" as a reason for joining; "encouragement by other students" accounted for 10% of the responses; and "encouragement by AWS members" accounted for 5%. The instructor also played an equally important role in first introducing AWS to students. Those students encouraged to join by instructors or other students tended to be less active in local AWS meetings. The student members who joined for social reasons,

technical development, or industry contacts tended to participate more actively in local activities.

The survey also confirmed the existence of two strong groups within the student membership (as there were similar groups within the overall organization). One group has a strong scientific, engineering background; the other group has a strong vocational or trade background. This dichotomy permeated the entire structure and was seen clearly in the responses to questions.

WORD PROCESSER USAGE

Word processor usage (percentage of time in actual use) in the Metals and Ceramics Division was determined by estimating the parameter in the binomial distribution from data taken over a period of 25 d. Daily inspections were started at randomly selected times, once each morning and once each afternoon. A shortened work day was defined as 8:30 to 11:00 AM and 1:30 to 3:15 PM to minimize the effect of absences caused by varying work schedules. The overall mean was 46.9%, with a confidence level of 95% for the mean falling within the interval of 43.9% to 49.9%; the median was 50.0%. Downtime as a result of machines being repaired or waiting for repair was not included in the results; such downtime was negligible.

As a group, the eight secretaries averaged 51.5%, whereas the six machines in the Reports Office and the two machines used by part-time employees averaged 44% and 37%, respectively. If the two secretaries on leaves of absence during the experiment were omitted from the calculation, the remaining six secretaries were using their machines nearly two-thirds (64%) of the time.

I. Metals and Ceramics Division.

^{2.} American Welding Society.

^{3. &}quot;Mail Survey of American Welding Society Membership." Mathematics and Statistics Research Department Progress Report, Period Ending, June 30, 1978, ORNL CSD-34 (September 1978), pp. 42-44.

18. Uranium Resource Evaluation

C. S. Bard^t

C. L. Begovich² T. R. Butz¹

J. G. Grimes¹

V. E. Kane

E. Leach

D. E. Myers'

D. A. Wolf

URANIUM RESOURCE EVALUATION PROGRAM

The Mathematics and Statistics Research Department (MSRD) has supported the Union Carbide Corporation Nuclear Division's (UCC-ND) involvement in the Uranium Resource Evaluation (URE) Program since 1976. Early efforts were directed at data collection procedures and automation of many statistical analyses. Research, reported previously, was also conducted on multivariate methods that enhance low-level uranium anomalies and enable the identification of possible new sources of mineralization. Currently, work is being completed in enhancement methods, and general assistance is being provided for the historical archiving of about I million samples in Oak Ridge.

The reconnaissance portion of the URE program is complete: more than 700,000 total samples were collected in various parts of the United States. The current UCC-ND effort is directed toward the chemical analysis and reporting of over 125,000 samples from Los Alamos National Laboratory and Savannah River Laboratory. About 150 data reports will be completed during FY 1981. Also, a national URE historical archive for sediment and selected water samples has been established in Oak Ridge. The data processing required for this effort is being provided by the Computer Sciences Division.

OPTIMAL INTERPOLATION PARAMETERS

Interpolation methods are often used before contouring geochemical data because most contouring procedures require values on a regularly spaced grid. Most interpolation procedures require specification of several parameters, and it is well known that the appearance of the resulting contours can change appreciably, depending on the choice of parameters. The estimation of the value of a geochemical measurement, z(x, y), at the location x, y often

involves inverse distance weighting (IDW). Consider n sample values z_1, \ldots, z_n , where $z_i = z(x_i, y_i)$; then, the IDW procedure estimates unknown values by computing

$$z(x,y)=\sum_{i=1}^n w_i z_i / \sum_{j=1}^n w_j.$$

where

$$w_i = \begin{cases} 0 & \text{if } r_i > c \\ r_i^{-p} & \text{if } r_i \leq c \end{cases}$$

and r_i is the distance from x, y to x_i, y_i . A least squares procedure was developed to estimate the parameters p and c.

Geochemical data sets are often large, and it is possible to omit n' samples (say, n' = n/4) from the least squares estimation of p and c and compute

$$S(p) = \frac{\sum_{i=1}^{n'} [z_i - \hat{z}_i(p)]^2}{\sum_{i=1}^{n'} (z_i - \hat{z})^2}.$$

where $\hat{z}(p)$ is estimated from the n - n' samples. A value of S(p) > 1 implies estimation is worse than using the mean value as an estimator. Figure 4 gives examples of S(p) curves (c fixed) that provide geologists with comparative element information as well as possible variability of the final estimate of p.

VARIOGRAM MODELS AND KRIGING

A study was conducted to assess the potential application of Kriging to geochemical data. Kriging

L. Uranium Resource Evaluation Project

^{2.} Computing Applications Department.

^{3.} Department of Mathematics, University of Arizona

⁴ D. F. Myers, C. I., Begovich, I. R., Butz, and V. F. Kane, Application of Kriging to Hydrogeochemical Data from the National Frantim Resource Evaluation Program, Vianium Resource Evaluation Project Report K. J. R-44 (December 1980)

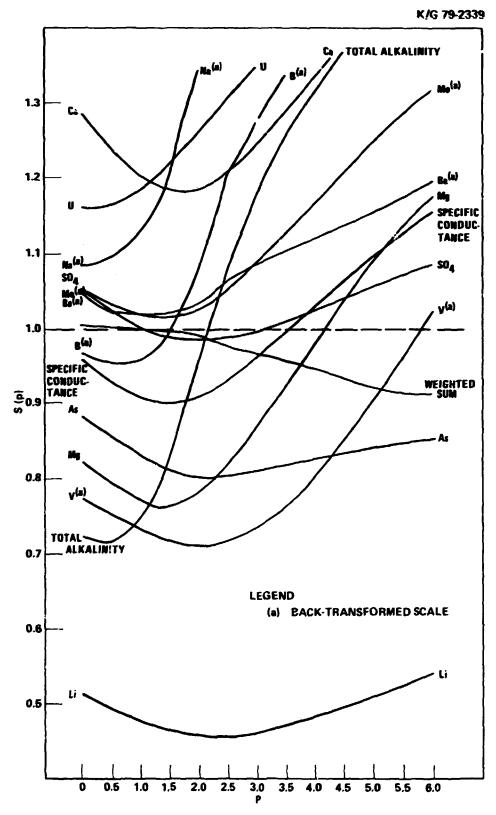


Fig. 4. S(p) vs p for the Ogaliala Formation.

has traditionally been applied to mining problems; thus, application to geochemical data presented several difficulties. It was necessary to construct variogram models for each element and geologic formation considered. Four general types of models (linear, constant-linear, concave, and convex) were found appropriate for all cases considered. A procedure was developed for estimating the variogram in both isotropic and anisotropic cases. The variogram analysis enabled assessment of the assumption of statistical independence of regional samples, which is commonly used in standard analyses. Finally, the estimated variograms were used in computing Kriged estimates used in contouring applications.

IDENTIFYING POTENTIAL URANIUM MINERALIZATIONS

A common geological exploration method used to identify mineral potential in an unknown area is to make analogies with known areas. Several of the URE Special Study Project areas included known uranium deposits that were sampled to characterize a mining region. The remaining samples from the project area were grouped according to geologic unit. Standard quadratic discriminant analysis techniques were used to derive classification criteria, which were then used to classify the samples into the mine group or one of the geologic unit groups. Contour plots of the samples' posterior probabilities, assuming the samples were from the mine group, were useful in outlining areas thought to have uranium potential.

An extension of the technique described by Beauchamp et al. was also implemented to identify

potential uranium mineralization. Unknown areas with uranium potential are expected to have interelement relationships similar to those in the mine, but the intensity of the signal expressed as the concentration levels of the various elements might be different. Instead of using an anomalous population and a single background population as described by Beauchamp et al., multiple background populations were considered.^{6,7}

GEOCHEMICAL SAMPLE ARCHIVE

Samples collected in the URE Program are being placed in archival storage in Oak Ridge. This archive is to serve as a long-term historical record for the URE samples. The MSRD developed an automated system that enables entry and retrieval of selected sample information. It is possible to enter a geographic region and identify the URE samples within the region along with the archival storage location.

^{5.} J. J. Beauchamp, C. L. Begovich, V. E. Kane, and D. A. Wolf, "Application of Discriminant Analysis and Generalized Distance Measures to Uranium Exploration," *Math. Geol.* 12, 539-58 (1980).

^{6.} T. R. Butz, N. E. Dean, C. S. Bard, R. N. Helgerson, J. G. Grimes, P. M. Pritz, and D. A. Wolf, "Hydrogeochemical and Stream Sediment Detailed Geochemical Survey for Edgemont, South Dakota; Wyoming," Uranium Resource Evaluation Project Report K. UR-38, supplement I (forthcoming).

^{7.} T. R. Butz, D. J. Tieman, J. G. Grimes, C. S. Bard, R. N. Helgerson, P. M. Pritz, and D. A. Wolf, Stream Sediment Detailed Geochemical Survey for Data Creek Basin, Arizona, Uranium Resource Evaluation Project Report K. UR-34, supplement 1 (forthcoming).

47.

Part C. Educational Activities

The Mathematics and Statistics Research Department (MSRD) is active in a number of educational areas of a professional and academic nature. This year the department was responsible for organizing a mini-workshop on computational statistics. Department members also organized and participated in various seminar series and were involved with several courses presented in the in-hours training program. In addition, several members served as visiting lecturers to sponsoring colleges for an Oak Ridge Associated Universities (ORAU) program, supervised students, and engaged in university teaching. Finally, interaction with university personnel on consulting and research activities is encouraged through short- and long-term visits and the general use of consultants.

WORKSHOP ON COMPUTATIONAL STATISTICS

The department organized a mini-workshop on computational statistics, which was held in Oak Ridge. Tennessee, on September 3-4, 1980. Seven statisticians and mathematicians from other institutions participated: R. L. Anderson (University of Kentucky), B. W. Brown (M. D. Anderson Hospital, Houston), R. E. Cline (University of Tennessee), E. L. Frome (ORAU), J. E. Gentle (International Mathematical and Statistical Libraries, Inc., Houston), M. D. McKay (Los Alamos National Laboratory), and G. W. Stewart (University of Maryland). Including MSRD members, approximately 20 people participated in the program.

The purpose of the workshop was to learn more about computational statistics and its potential importance to the Department of Energy's Applied Mathematical Sciences program. Topical areas of discussion included possible definitions of computational statistics, current research programs in computational statistics, new research areas where work was needed, the number and qualifications of people necessary to conduct a research program, and the organization of such a research program.

IN-HOUSE EDUCATION PROGRAMS

The department served as host on June 22-23 for a "dry run" of an American Statistical Association (ASA) short course to be offered at the 1981 national meeting of ASA in Detroit. The course was based on the second edition of the text *Practical Nonparametric Statistics* (Wiley, New York, 1980). The author of the text, W. J. Conover from Texas Tech University, and R. L. Iman from Sai dia National Laboratory presented the course to over 30 statisticians from the Oak Ridge area.

C. K. Bayne and T. J. Mitchell taught the Practical Statistics II course during the spring quarter as part of the Oak Ridge National Laboratory (ORNL) In-Hours Continuing Education Program for Scientific and Technical Personnel. This course, a continuation of the Practical Statistics I course, covered (1) analysis of variance, (2) regression analysis, and (3) design of experiments.

- M. T. Heath taught a course entitled Computer Methods for Mathematical Computations during the winter 1981 term to 25 students in the ORNL in-hours continuing education program. The emphasis of this course was on the use of high-quality numerical software to solve mathematical problems such as system of linear or nonlinear algebraic equations, interpolation, integration, differential equations, optimization, least squares, and eigenvalue problems.
- W. E. Lever acted as class monitor for one presentation of the J. Stuart Hunter film course on experimental design topics, which was jointly sponsored by the Y-12 Training Department and Quality Division. Offered to Y-12 and K-25 employees, about 22 employees regularly attended the classes. The course consisted of 33 video cassette presentations, which are being leased by the Union Carbide Corporation for a ten-year period.

SEMINAR SERIES

The department conducts a biweekly seminar series dealing with the research and consulting activities of the staff. Outside speakers are also invited to give other presentations. The names of the speakers, their affiliations, if not with MSRD, and the titles of their talks are listed at the end of this section. The seminar series is coordinated by D. G. Wilson.

- R. C. Ward of MSRD and R. J. Plemmons of the Departments of Mathematics and Computer Science. University of Tennessee, organized a weekly seminar series on matrix methods in numerical analysis. The series, held at the University of Tennessee this year, began in January and continued into March. This is the sixth consecutive year for the series organized by MSRD and the University of Tennessee. The speakers' names, their affiliations, if not with MSRD, and the titles of their talks are given at the end of this section.
- V. E. Kane and S. A. McGuire organized a weekly study group based on a short course given at the 1980 annual ASA national meeting in Houston, Texas. The text, Regression Diagnostics, by D. A. Belsley, E. Kuh, and R. E. Welsch (Wiley, New York, 1980) was the basis for both the short course and seminar series. The intent of this short course was to acquaint staff members with approaches to identifying influential observations and sources of collinearity while simultaneously introducing computer software that facilitates implementation of the techniques. The course was conducted from April through August; 12 MSRD staff members participated.
- M. D. Morris helped organize a study group to examine statistical methods used in epidemiologic studies. Meetings are held monthly and are attended by statisticians and epidemiologists from ORNL and the Tennessee Valley Authority office in Chattanooga. Topics of interest include statistical treatment of epidemiologic confounders and the use of cluster analysis and tests of aggregation in epidemiologic studies. The series started in March and will continue through the fall.

ORAU TRAVELING LECTURERS

Various department members participate in a Traveling Lecture Program administered by ORAU. During the report period, six department members were involved in the program: L. J. Gray, V. E. Kane, D. S. Scott, A. D. Solomon, V. R. R. Uppuluri, and T. Wright. Typically, lecturers visit the sponsoring universities and consult with their mathematicians and statisticians. A lecture for the undergraduate and graduate students is always presented. Titles of these lectures are given at the end of this section.

SUPERVISION OF STUDENTS

Students regularly work with MSRD members under the sponsorship of the Great Lakes Colleges Association and ORAU Student Research Participation programs as ORAU Graduate Fellows and as summer employees. Also, several students participate in co-op programs in which time is spent at MSRD.

- E. M. McCluer, a co-op student from Tennessee Technological University, spent June 1980 through May 1981 working with R. E. Funderlic on computational problems in rotor dynamics for the Separation Systems Division. This work will continue during the summer of 1981 along with work, supervised by J. W. Wachter from the Consolidated Fuel Reprocessing Program, on computational problems associated with the application of microscopic process monitoring to safeguards problems. Another co-op student from Tennessee Tech, P. K. Stuber, will continue this work on rotor dynamics starting in June. Their work is described in Part B of this report.
- S. A. Haw, a former ORAU student research participant from Nicholls State University, did support programming with E. M. McCluer on Separation Systems Division work during the summer of 1980.
- W. Harper and A. Prasad participated in the Summer Research Apprenticeship Program for High School Students sponsored by ORAU, Knoxville College, and ORNL. The work on problems in Boolean algebra and associated applications was supervised by T. Wright.

UNIVERSITY TEACHING ACTIVITIES

- J. J. Beauchamp taught a course entitled Statistics for Biologists for the University of Tennessee Oak Ridge School of Biomedical Sciences during the summer of 1980.
- D. A. Gardiner taught a three-quarter sequence entitled Introduction to Mathematical Statistics for the University of Tennessee Department of Mathematics starting in the fall of 1980.
- L. J. Gray taught three courses, Partial Differential Equations, Complex Variables, and Vector Analysis, for the University of Tennessee Department of Mathematics during the 1980-1981 school year.
- T. J. Mitchell was an instructor in the short course Statistical Design and Analysis of Engineering Experiments, which was sponsored by the University of Wisconsin Engineering Extension Department, May 11-15, 1980, at Madison, Wisconsin.
- D. S. Scott taught two courses, FORTRAN Programming, and Data Structures and Non-Numerical Programming, for the University of Tennessee Computer Sciences Department during the fall and spring quarters of the 1980-1981 school year.
- T. Wright gave several lectures on A Finite Population Approach to the Concepts of Probability and Statistics at Atlanta University on April 1, 1981, as part of a Graduate Seminar Series for students in industrial chemical engineering. The talks were sponsored by Union Carbide Corporation's University Relations Program.

SHORT-TERM VISITING RESEARCHERS

A number of researchers visited MSRD for several days to consult with department members on research or consulting problems.

Professor Å. Björck, Department of Mathematics, Linköping University, visited on February 12-13, 1981, consulting with R. E. Funderlic, M. T. Heath, D. S. Scott, and R. C. Ward on numerical linear algebra problems.

Professor S. Breuer of Tel Aviv University in Israel visited on July 28-August 1, 1980, to discuss research on moving boundary problems and in materials science with S.-J. Chang and A. D. Solomon.

Professor J. A. George, dean of the Faculty of Mathematics, University of Waterloo, visited on November 3-5, 1980, and on May 11-15, 1981, consulting with M. T. Heath on large, sparse systems of linear equations and least squares problems.

Professor G. H. Golub, chairman of the Computer Science Department, Stanford University, visited on November 3-5, 1980, consulting with members of the Numerical Linear Algebra Research Project.

Dr. S. Marks and Mr. M. Lang of the Institute for Energy Conversion and Professor C. Lozano of the Mathematics Department, University of Delaware, visited on July 21-23, 1989, to consult with A. D. Solomon and D. G. Wilson on various aspects of research in moving boundaries and thermal energy storage.

Professor D. S. Robson, Biometrics Unit, Cornell University, visited on February 23-25, 1981, to consult on problems in the Multivariate Analysis, Biometrics, and Model Evaluation Research projects.

Professor W. Y. Tan, Department of Mathematics, Memphis State University, visited on March 18-19, 1981, to consult with D. G. Gosslee and T. J. Mitchell on research in statistical models for mutation assays.

Professor W. A. Thompson of the University of Missouri visited during August 1980 to consult with V. R. R. Uppuluri on mathematical and statistical problems in risk analysis.

Professor B. W. Turnbull, School of Operations Research and Industrial Engineering, Cornell University, visited on October 12-15, 1980, January 6-9, 1981, and June 22-25, 1981, to consult with T. J. Mitchell on research in the design and analysis of survival sacrifice experiments.

LONG-TERM VISITING RESEARCHERS

Several university researchers spent extended periods at MSRD working on both consulting and research problems encountered by the MSRD staff.

Professor V. Alexiades, Department of Mathematics, University of Tennessee, visited with A. D. Solomon and D. G. Wilson for five weeks during the summer of 1980 and for one day each week since the summer. Their work on various moving boundary problems is described in Part A of this report.

Professor G. J. Davis, Department of Mathematics, Georgia State University, visited with V. E. Kane, R. C. Ward, and D. S. Scott periodically from October 1980 through June 1980 on a Faculty Participation Agreement with ORAU. Research projects in computational statistics and large, sparse eigenvalue problems were initiated. He also plans to visit MSRD as an ORAU faculty research participant from mid-June until mid-July 1981 to continue research on these projects.

Professor G. P. McCabe, Department of Statistics, Purdue University, continued the research activities started during his May 12-30, 1980, visit with MSRD. C. K. Bayne, J. J. Beauchamp, and V. E. Kane each spent a week at Purdue University during September 1980 continuing the Multivariate Analysis Research Project work initiated in May.

Professor S. A. Patil, Mathematics Department, Tennessee Technological University, visited V. R. R. Uppuluri periodically from October 1980 through June 1981 on a Faculty Participation Agreement with ORAU. Research was conducted on waiting time problems and empirical Bayesian methods applied to problems in nuclear safety.

Professor R. J. Plemmons, Departments of Mathematics and Computer Science, University of Tennessee, visited with R. E. Funderlic and M. T. Heath for four weeks during the summer of 1980. His research on sparse linear least squares problems and factorization of M-matrices is summarized in Part A of this report.

Professor J. B. Robertson, Mathematics Department, University of California at Santa Barbara, spent four weeks during July-August 1980 working with V. R. R. Uppuluri on the identification of mathematical and statistical problems in risk analysis.

Professor T. J. Rudolphi, Department of Engineering Science and Mechanics, Iowa State University, visited with S.-J. Chang for three weeks in August 1980 and four weeks in June 1981. They worked on boundary integral equation formulations for edge-crack problems related to materials science applications. Their research is summarized in Part A of this report.

Professor L. R. Shenton, Office of Computing and Information Services, University of Georgia, visited K. O. Bowman in September 1980 for two weeks, in December 1980 for one week, and in April 1981 for one week to consult on research problems in the Model Evaluation Project.

LIST OF CONSULTANTS

- V. Alexiades, University of Tennessee
- J. A. George, University of Waterloo
- G. H. Golub, Stanford University
- G. P. McCabe, Purdue University
- R. J. Plemmons, University of Tennessee
- J. Robertson, University of California at Santa Barbara
- D. S. Robson, Cornell University
- T. J. Rudolphi, Iowa State University
- B. W. Turnbull, Cornell University
- W. G. Wolfer, University of Wisconsin

MSRD SEMINARS

- R. E. Funderlic, "Overview of SIAM Summer Research Conference in Numerical and Statistical Analysis," July 1, 1980.
- J. B. Robertson, University of California at Santa Barbara, "Some Perspectives on the Kaplan-Meier Estimator," July 11, 1980.
- R. E. Funderlic, "Solving Homogeneous Linear Systems of Equations Arising from Compartmental Models," July 16, 1980.
- S. Breuer, Tel-Aviv University, "A Lower Bound for the Eigenvalues of the Elliptic Dirichlet Problem for a General Domain in Terms of Its Characteristic Dimension," July 29, 1980.
- S. Breuer, Tel-Aviv University, "Saint Venant's Principle in Linear and Nonlinear Elasticity," July 31, 1980.
- J. Neuberger, North Texas State University, "Steepest Descent Methods for Nonlinear PDE's," July 30, 1980.
- S.-J. Chang, "A Dislocation Model of Fracture," August 20, 1980.
- R. Sposto, University of California at Los Angeles, "Log Odds Ratio Estimation from Data Stratified on a Continuous Covariate," August 28, 1980.
- C. Deans, University of Minnesota, "Developments in Survival Analysis with Applications," September 9, 1980.
- M. J. Stewart, Virginia Polytechnic Institute & State University, "Randomization Analysis of Replicated Randomized Complete Block Designs," September 15, 1980.
- T. Wright, "Multiway-Stratification-A Tool for Controlled Selection," September 24, 1980.
- J. D. Knoke, University of North Carolina, "Discriminant Analysis with Continuous and Discrete Variables," October 6, 1980.
- M. T. Heath, "Sparse Least Squares," October 8, 1980.
- M. D. Morris, "The Comparison of Precisions for Two Methods of Measurements," October 9, 1980.
- G. A. Cotsonis, "Small Tektronics Graphics Programming," October 22, 1980.
- B. Kagstrom, University of Umea, Sweden, "Numerical Computation of the Jordan Normal Form of a Complex Matrix," November 3, 1980.

- T. J. Mitchell, "Supersaturated Designs for Sensitivity Analysis of Computer Models," November 5, 1980.
- R. C. Ward, "Solving Quadratic \(\Lambda \text{Matrix Problems Without Factorization," November 19, 1980.
- D. G. Gosslee, "Some Current Consulting and Collaboration," December 3, 1980.
- D. G. Wilson, "Progress on the Moving Boundary Front," December 17, 196 J.
- L. J. Gray, "Disordered Systems Versus Augmented Space Strikes Back," January 7, 1981.
- A. D. Solomon, "Simple Approximations for Predicting the Behavior of an Array of Phase Change Material Cylinders," January 14, 1981.
- T. L. Hebble, "On Interrogating Systems-Two Problems." January 21, 1981.
- V. E. Kane, "Variable Selection in Multivariate Analysis or Why a Condition Number of 30 Can Be Bad," February 4, 1981.
- C. K. Bayne, "Computing Quadratic Misclassification Probabilities," February 18, 1981.
- J. J. Beauchamp, "Application of the Power-Shift Transformation," March 4, 1981.
- K. O. Bowman, "Moment Estimators for the Weibull Density," March 18, 1981.
- W. E. Lever, "Dose Estimation Problems with the New TLD Meter Badges," April 1, 1981.
- G. E. Dinse, Harvard University, "Non-Parametric Estimation of the Prevalence and Survival Functions from Incomplete Observations," April 6, 1981.
- E. L. Frome, ORAU Medical Division, "The Analysis of Rates Using Poisson Regression Models," April 8, 1981.
- W. H. Olson, Consultant with ORNL Biology Division, "Chemical Dosimetry, Harber's Rule and Linear Systems," April 13, 1981.
- C. A. Serbin, "Survival Tips for the Novice User of the PDP-10," April 15, 1981.
- D. A. Walsh, University of Washington, "Some Methods for the Analysis of Biomedical Time Series with Emphasis on Growth," April 21, 1981.
- E. M. McCluer, "What I Have Learned from MSRD," April 29, 1981.
- V. R. R. Uppuluri, "Waiting Times and Generalized Fibonacci Sequences," May 13, 1981.
- A. D. Solomon, "On the Stefan Problem with a Convective Boundary Condition," May 27, 1981.
- D. S. Scott, "Computing a Few Eigenpairs of a Symmetric Band Matrix and Other Reflections on Three Years in Oak Ridge," June 10, 1981.
- T. J. Rudolphi, Iowa State University, "The Boundary Element Method for Zoned Media with Discontinuous Stresses," June 24, 1981.

SIXTH ANNUAL UNIVERSITY OF TENNESSEE/MSRD-SPONSORED SEMINARS ON MATRIX METHODS IN NUMERICAL ANALYSIS

- T. M. Rao, Computer Science Department, University of Tennessee, "Error-Free Solutions to Matrix Problems," January 16, 1981.
- D. S. Scott, "Advantages of Inverted Operators in Rayleigh-Ritz Approximations," January 23, 1981.
- M. D. Gunzburger, Department of Mathematics, University of Tennessee, "Need for Pivoting in Solving Indefinite Linear Systems," January 30, 1981.

- R. E. Funderlic, "They Always Change the Problem (Updating)," February 6, 1981.
- Å. Björck, Department of Mathematics, Linköping University, Linköping, Sweden, "A Bidiagonalization Algorithm for Solving Large, Sparse Ill-Posed Linear Systems," February 13, 1981.
- M. T. Heath, "Algorithms for Sparse Least Squares Problems," February 20, 1981.
- R. T. Gregory, Computer Science Department, University of Tennessee, "Error-Free Computation with Rational Numbers," March 6, 1981.
- R. C. Ward, "Quadratic λ-Matrix Problems," March 13, 1981.

ORAU TRAVELING LECTURE PRESENTATIONS

- A. D. Solomon, "The Analysis and Solution of Moving Boundary Problems of Stefan Type in Heat-Transfer Process," Auburn University, Auburn, Alabama, October 30, 1980.
- T. Wright, "Who Says That Counting Is As Easy As 1-2-3?" Cameron University, Lawton, Oklahoma, December 2, 1980, and Brescia College, Owensboro, Kentucky, January 27-28, 1981.
- L. J. Gray, "The Mathematics of Disordered Systems," Memphis State University, Memphis, Tennessee, December 4, 1980.
- D. S. Scott, "The Shift and Invert Lanczos Algorithm," North Carolina State University, Raleigh, North Carolina, February 2, 1981.
- V. R. R. Uppuluri, "Sampling Proportional to Random Size," Southern Methodist University, Dallas, Texas, April 9, 1981, and University of Texas at Arlington, Texas, April 10, 1981.
- V. E. Kane, "Applications of the Power-Shift Transformation," Virginia Commonwealth University, Richmond, Virginia, April 15, 1981.

Part D. Presentations of Research Results

Publications

BOOKS AND PROCEEDINGS

- J. J. Beauchamp, C. L. Begovich, V. E. Kane, and D. A. Wolf, "Application of Discriminant Analysis and Generalized Distance Measures to Uranium Exploration," pp. 20-43 in *Proceedings of the 1979 DOE Statistical Symposium*, CONF-791016, Oak Ridge National Laboratory, Oak Pidge, Tenn., September 1980.
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- C. S. Cheng³ and L. J. Gray, "A Characterization of Group Divisible Designs and Some Related Results," pp. 31-39 in *Proceedings of the Conference on Combinatorial Mathematics, Optimal Designs and Their Applications, Annals of Discrete Mathematics*, vol. 6, 1980.
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^{6.} The Chinese University of Hong Kong.

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^{25.} University of Arizona.

^{26.} Technical Services Division, Y-12.

^{27.} University or Missouri Columbia.

^{28.} Energy Division

^{29.} Victoria University of Wellington, New Zealand.

^{30.} Industrial Safety and Applied Health Physics Division.

Oral Presentations

- K.:O. Bowman, "Models for Approximating the Percentage Points of Distributions," presented at the Conference on Applications of Numerical Analysis and Special Functions in Statistics, University of Maryland, College Park, Oct. 2-8, 1980.
- K. O. Bowman, "Almost Unbiased Estimators for the Shape Parameter of the Weibull Distribution," presented at the Sixth Union Carbide Corporation Applied Mathematics Symposium, South Charleston, W.Ya., Oct. 16-17, 1980.
- S.-J. Chang, "Dislocation Pile-Up Problem with Eshelby-Stroh Interaction," presented at the 110th Annual Meeting of the American Institute of Metallurgical Engineers, Chicago, Ill., Feb. 22-26, 1981.
- S.-J. Chang and S. M. Ohr,² "Dislocation-Free Zone at the Crack Tip," presented at the 110th Annual Meeting of the American Institute of Metallurgical Engineers, Chicago, 1ll., Feb. 22-26, 1981.
- R. E. Funderlic and J. B. Mankin, "Homogeneous Linear Systems of Equations Arising from Compartmental Models," presented at the SIAM 1980 Fall Meeting, Houston, Tex., Nov. 7 1980.
- D. A. Gardiner, "Statistical Research and Collaboration in Oak Ridge," presented to the faculty and students of the Department of Statistics, North Carolina State University, Raleigh, Mar. 20, 1981.
- B. G. Cosslee, "Nonparametric Estimates of the Median Effective Dose," presented to the Graduate Toxicology Program, University of Tennessee, Knoxville, May 7, 1981.
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- L. J. Gray and T. Kaplan; A Self-Consistent Cluster Theory for Random Alloys with Short-Range Order, presented at the 1981 March Meeting of the American Physical Society, Phoenix, Ariz., Mar. 16–20, 1981.
- M. T. Heath, "Solution of Sparse Linear Least Squares Problems Using Givens Rotations," presented at the University of Waterloo, Ontario, Canada, July 18, 1980.
- M. T. Heath, "The Role of Applied Mathematicians in Industry," presented at the University of the South, Sewance, Tenn., Apr. 13, 1981.
- M. T. Heath, "Numerical Software for Optimization," presented at the Management Science Seminar, University of Tennessee, Knoxville, May 29, 1981.
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^{31.} University of Wisconsin.

- T. J. Mitchell and M. D. Morris, "Design of Two-Level Multifactor Experiments for Detecting the Presence of Interactions," presented at the 1980 Army Conference on Design of Experiments, Las Cruces, N.M., Oct. 22-24, 1980.
- T. J. Mitchell and B. W. Turnbull,³² "Nonparametric Estimation of the Distributions of Time to Onset and Time to Death for Specific Diseases in Survival/Sacrifice Experiments," presented at the Spring Regional Meetings of the Biometric Society (ENAR) and the American Statistical Association, Richmond, Va., Mar. 22–25, 1981.
- M. D. Morris, "Comparing Two Methods of Measurement for Accuracy and Precision," presented to the Department of Experimental Statistics, Louisiana State University, Baton Rouge, Mar. 9, 1981, and at the Seventh Union Carbide Corporation Applied Mathematics Symposium, Tonawanda, N.Y., May 6-7, 1981.
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- D. S. Scott, "Solving Quadratic λ-Matrix Problems with Factorization," presented at the SIAM 1980 Fall Meeting, Houston, Tex., Nov. 6, 1986
- D. S. Scott, "The Shift and Invert Lanczos Algorithm," presented to the Computer Science Department, University of California at Berkeley, Apr. 27, 1981.
- D. S. Scott, "Nonfactorization Software for Symmetric Linear and Quadratic Eigenvalue Problems," presented at the 1981 DOE NASIG Meeting, Lawrence Berkeley Laboratory, Berkeley, Calif., May 1, 1981.
- C. A. Serbin, "TES-A Program for Simulating Phase Change Processes," presented at the Sixth Union Carbide Corporation Applied Mathematics Symposium, South Charleston, W.Va., Oct. 16, 1980.
- V. R. R. Uppuluri, "Analysis of Paired Comparisons," presented at the 1980 International Conference on Cybernetics and Society (IEEE), Boston, Mass., Oct. 9, 1980.
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- V. R. R. Uppuluri, "Sampling Proportional to Random Size." presented to the Department of Mathematics, University of Tennessee, Knoxville, Feb. 18, 1981.
- V. R. R. Uppuluri, "Ranking Methods Based on Paired Comparison Data," presented as a Management Science Seminar, University of Tennessee, Knoxville, May 8, 1981.

^{32.} Cornell University.

- V. R. R. Uppuluri and S. A. Patil. "Waiting Times and Generalized Fibonacci Sequences," presented at the 90th Meeting of the Tennessee Academy of Sciences, Oak Ridge, Nov. 21, 1980.
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- R. C. Ward and D. S. Scott, "Solving Quadratic λ-Matrix Problems Without Factorization," presented at the SIAM 1980 Fall National Meeting, Houston, Tex., Nov. 6, 1980, and at the 1981 Army Numerical Analysis and Computers Conference, Huntsville, Ala., Feb. 26, 1981.
- D. G. Wilson, "One Dimensional, Multi-Phase Moving Boundary Problems with Phases of Different Densities," presented at the SIAM 1980 Fall National Meeting, Houston, Tex., Nov. 6, 1980.
- D. G. Wilson. "Composition of Solidified Binary Alloy from a Simple Solidification Model," presented at a special session on Free Boundary Problems at the Fall Meeting of the Southeastern Section of the American Mathematical Society, Knoxville, Tenn., Nov. 14, 1980.
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- T. Wright, "A Finite Population Approach to the Concepts of Probability and Statistics," presented at Atlanta University, Atlanta, Ga., Apr. 1, 1981.

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Part E. Professional Activities

Members of the Mathematics and Statistics Research Department participate in several activities in support of their professions. Some of their contributions are listed below.

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Member:

Technometrics Prize Committee

Program Committee, 1980 DOE Statistical Symposium

Instructor:

In-Hours Continuing Education Program

J. J. Beauchamp

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Traveling Lecture Program, Oak Ridge Associated Universities

Graduate School of Biomedical Sciences, University of Tennessee-Oak Ridge

Representative:

Professional Education Resource Committee, ORNL

K. O. Bowman

Member.

International Editorial Board, Communications in Statistics:

Part B. Simulation and Computation

American Statistical Association (ASA) Committee of Representatives to the

American Association for the Advancement of Science (AAAS)

(Representative to Section T)

Associate editor:

Statistical Computation and Simulation

Reviewer:

National Science Foundation

Contributing editor:

Current Index to Statistics

Lecturer:

Visiting Lecture Program, Committee of Presidents of Statistical

Societies (COPSS)

Organizer:

Symposiums, AAAS Annual Meeting, Washington, D.C., 1982:

"If Japan Can, Why Don't We?" and "The Software Explosion"

S.-J. Chang

Reviewer:

Applied Mechanics Review

R. E. Funderlic

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Department of Mathematics, University of Tennessee

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University Relations Program, Oak Ridge Associated Universities

Reviewer:

Mathematical Reviews

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Organization Committee, 1982 Sparse Matrix Symposium

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D. A. Gardiner

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Working Group, DOE Program Directions for Research in Statistical Methods

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Editorial Board, Statistical Computation and Simulation

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T. L. Hebble

Coordinator:

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Associated with Radioactive Waste Disposal

V. E. Kane

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1981 DOE Statistical Symposium Workshop on Computational Statistics

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Committee on Statistics and the Environment, American Statistical

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