CC/NUMBER 18
MAY 5, 1986

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Dye J L & Nicely V A. A general purpose curvefitting program for class and research use. *J. Chem. Educ.* 48:443-8, 1971.
[Michigan State University, East Lansing, MI]

A general-purpose nonlinear regression program is described. The program was designed to operate on various computers with minimum further programming. It regresses user-defined equations onto data to estimate parameters in the equations. The program was designed to fit kinetic data but is easily used for a variety of spectroscopic, electrochemical, or other data types. Examples of applications are given. [The *Science Citation Index*® (*SCI*®) indicates that this paper has been cited in over 170 publications.]

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January 16, 1986

In early 1966 Dye's research group was studying the chemistry of solvated electrons and solutions of alkali metals in ammonia and amines. V.A. Nicely had just begun investigation of the magnetic properties of such solutions and collected literature on curvefitting for application to electron spin resonance (ESR) spectra. John Bartelt, in another research group, had been evaluating curvefitting procedures, and we shared information and evaluations. We found published procedures for nonlinear least squares regression that provided good convergence under a variety of conditions, as well as publications with approximations to statistical quantities for nonlinear regression parameters.

During this period, Dye had been upgrading manual data analysis to provide punched-card input for computer analysis of stopped-flow kinetics data. Nonlinear least squares procedures applied to several trial data sets gave encouraging results, but integrating the differential equations and writing special computer programs for each proposed mechanism took too much time.

To minimize the labor and provide a uniform approach to curvefitting, we decided to let the computer integrate differential equations and also to approximate derivatives numerically. Then we wrote a program suitable for a large variety of problems with minimal reprogramming and usable without repeated concern for the details of computation. Indeed, this is the key to the popularity of the program—a flexible and easy-to-use subroutine is all that the user must consider. Comments from the research group led to program improvements. Furthermore, when switching the code to run on a newly installed computer (CDC 6500), we learned the value of standardized code. During his sabbatical year at Ohio State University in 1968, Dye installed the program on IBM equipment and further improved the standardization and generality of the code.

By 1970 the program had been used successfully by a number of colleagues for a variety of purposes. Then Dye decided to introduce the program's use as a part of the graduate chemical kinetics class. Favorable response from students and colleagues prompted us to publish a description of the program and to make it available through the MSU Computer Center.

Since the original publication, we have used the program with minor modifications on a number of computers to analyze a variety of kinetic, spectroscopic, and electrochemical data. Special versions of the program have incorporated a generalization to fit multiple data sets. While the published program was oriented to card format and batch processing, newer versions use interactive input with the bulk of the program stored on tape or in virtual memory. In the years since this paper appeared, the program has been distributed to hundreds of institutions in this country and abroad. The availability, generality, and ease of application are the main reasons for frequent citation of this article.

The literature in this area is vast and many computer programs have been developed. We call attention to an annotated bibliography of related computer programs,[1] to work on statistical significance of parameters,[2] and to a recent comparison of convergence speeds.[3]

1. **Hogg J L.** Computer programs for chemical kinetics: an annotated bibliography. *J. Chem. Educ.* 51:109-12, 1974.
2. **Pattengill M D & Sands D E.** Statistical significance of linear least-squares parameters. *J. Chem. Educ.* 56:244-7, 1979.
3. **Hovanec J W & Ward J R.** Nonlinear least-squares fitting of first-order rate coefficients. (Comparison between the Gauss-Seidel method and Swain's KORE program.) *Comput. Chem.* 9:23-5, 1985.

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