9. *References:* R. A. Pfeiffer and W. W. Stone, TRAM for the Philco-2000. KAPL-M-RPC-1 (March 24, 1961).

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LOS ALAMOS LEAST SQUARES

1. Name of code: Los Alamos Least Squares
2. Computer for which code is designed: IBM 704
   Programming system: FORTRAN II
3. Nature of problem solved: Least squares fitting of linear or nonlinear functions in several independent variables. Thus, the program determines an estimate of A in the function $y = f(X; A)$ by means of minimizing the sum of squares. In the function, X is a vector of observed variables and A is a vector of parameters to be determined. In this context, a linear function is one whose partial derivatives with respect to the elements of A are all independent of A; a nonlinear function has at least one of the elements of A appearing in at least one of these partial derivatives. An example of a linear function is the usual linear regression model $y = XA = a_1x_1 + a_2x_2 + \cdots + a_kx_k$. A nonlinear function is the sum of exponentials model $y = a_1e^{a_2x} + a_3e^{a_4x} + \cdots + a_{k-1}e^{a_kx}$.
4. Method of solution: The iterative method of Gauss (sometimes called the Gauss-Seidel method) is used. The function is expanded with respect to A in a first-order Taylor's series about some point A_0. A vector of "corrections," say D, is obtained by multiple regression methods and a new estimate $A_1 = A_0 + D$ is obtained. The process is repeated until the vector D is "sufficiently small." The function and its derivatives with respect to the parameters are supplied to the program by the user by means of a subroutine.
5. Restrictions on complexity of problem: As originally conceived, the program was written for a 32K memory and would handle up to 500 data points, up to 5 independent variables, and up to 20 parameters. Different versions of the code are written for various memory sizes; 8K is usually sufficient, but it can be scaled to 4K. No restrictions have so far been encountered as to the nature or complexity of the function as long as no discontinuities exist in the function or its derivatives over the range of usefulness; i.e., the data must be physically significant, "well-behaved," and reasonably describe the function to be fitted. The Los Alamos 704 underflow is automatically set to zero, and the code does not check UV-OV conditions. Program and data are read on-line, with output going to BCD Tape 9.
6. Running time: Varies widely depending upon number of data points, parameters and independent variables; from 5 sec to 5 min. From 5 to 15 iterations are usually sufficient.
7. Unusual features: A damping factor is introduced to help control nonconvergent oscillations. Estimates of the standard deviation of all parameters are included with the solutions. Any (or all) parameters may be held at constant values. Arbitrary weighting of the observations y is permitted. The program package is "subroutine-ized" so that its various parts are easily modified or incorporated into other programs.
8. Present status: Several programs developed during the evolution of the present general code are currently operating at various Laboratories under such names as FRENIC, PEERLESS, and EXPO. 7090 Monitor versions are now being developed.
9. *Reference:* R. H. Moore and R. K. Ziegler, The solution of the general least squares problem with special reference to high-speed computers. Los Alamos Scientific Laboratory Report LA-2367 (October 15, 1959). This report contains a more complete set of references.

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9-RENUPAK (UNC-90-1)

1. Code designation: 9-RENUPAK (UNC-90-1)
2. Computer and programming system: Program is written in [F.A.P.] for the IBM-7090. A 32K core and ten tape units are required.
3. Problem solved: 9-RENUPAK treats the penetration of an infinite, homogeneous medium by neutrons from a point or plane isotropic source. The energy spectrum of the source must be continuous so that, for example, strictly monoenergetic source problems are excluded. The code output gives the neutron flux and current for both point and plane isotropic sources, as well as an integral over energy of the flux times an arbitrary response function, i.e., dose, activation, etc.
4. Method of solution: Computation is based on the moments method (*1–5*). After the moments are computed they are used to reconstruct the flux and current. The flux is assumed to consist of a linear combination of functions of given form, and constants in the expansion are adjusted so that the moments of the linear combination are the same as the computed moments of the flux.
5. Physics approximations: In the elastic slowing down treatment the neutron energy-angle relationship is taken into account properly. The code treats both elastic and inelastic scattering of neutrons. The inelastic scattering of neutrons is assumed to be isotropic in the laboratory system with a choice of several nuclear models in computing its energy dependence. In particular, the code allows for both discrete energy levels (when the levels are well separated) as well as a continuum of energy levels when the levels are very close. For heavy materials a statistical model is available.
6. Restrictions on complexity of problem: Maximum number of groups $\leqq 400$, isotopes $\leqq 5$, response functions $\leqq 16$. Only Gaussian and exponential fits available at present.
7. Typical running time: A typical calculation with 200 energy steps and 8 response functions, yielding both Gaussian and exponential fits for both point and plane source, takes about 12 min on the IBM-7090.