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This Week's Citation Classic

Marquardt D W. An algorithm for least-squares estimation of nonlinear parameters. *J. Soc. Indust. Appl. Math.* **11**:431-41, 1963.
[Engineering Department, E.I. DuPont, Wilmington, DE]

Computing procedures for estimating from data the best parameter values in a nonlinear model had generally been variations of the Taylor series or gradient methods. These frequently failed, but for different reasons. This paper explains why, and presents a new method that proved to be widely successful. The paper develops a firm theoretical basis for the algorithm, showing why it should inherit the best features of both predecessors while avoiding their serious limitations. [The *SCI*® indicates that this paper has been cited over 995 times in the period 1963-1977.]

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"My work on nonlinear estimation began in the early 1950s, motivated by problems from chemical engineering and physics. I worked with some of the first digital computers in industry. This provided early feedback on the numerical behavior of classical textbook methods, when their trial-and-error procedures were carried beyond the few iterations previously feasible.

"This paper was my third in this field.[1,2] The first two employed variants of the classical gradient and Taylor-series methods to solve specific problems. Continuing research led to the new algorithm, which was successfully applied on many problems before its theoretical basis was completed. It was clear from the beginning that this was a real breakthrough. At first by plotting and later by algebraic calculation, I had observed that the gradient and Taylor-series methods invariably give correction vectors whose included angle γ is nearly a right angle. Recognition of the orientation of these vectors in the sum-of-squares contours explained for the first time the apparently anomalous behaviors ot the previous methods.

"This paper was devoted entirely to the mathematics and numerical analysis of the new method. A key theorem shows that a controlled parameter λ of the new algorithm causes the direction of the correction vector to vary monotonically, having the two earlier methods as undesirable extremes. Hence it may be viewed as an optimum interpolation between them.

"An interesting sidelight: A small but very critical part of the algorithm involving a logical test on the angle γ is described in a footnote. This γ-test is included in our NLIN2 computer program, which has been supplied to many requestors since its publication in 1966.[3] Many others have programmed the algorithm on their own, but a number of such users have not included the γ-test, and have not achieved nearly as good results. I've eschewed footnotes ever since!

"The practical reliability of the method —its ability to converge promptly from a wider range of initial guesses than other typical methods — is a factor in its continued popularity. The growing use of nonlinear models in both the sciences and the social sciences also must be a factor in the citation history of this paper.

"The consolidation of prior technologies into a common conceptual framework, here geometric and algebraic, can sometimes be a turning point of technical progress, hence such papers may be often-cited. Indeed, a later paper[4] consolidated the theoretical concepts of this paper with those of two other lines of research, biased linear estimation and generalized inverses of matrices. Having spent twenty-five years in industrial consulting and research, I continue to be enthused by the abundance of good research topics and good guidance on fruitful research paths that come from the continual feedback from real problems with all of their practical complications, and their time pressures for useful answers."

1. **Marquardt D W.** Solution of non-linear chemical engineering models. *Chem. Eng. Prog.* **55**:65-70, 1959.
2. **Marquardt D W, Bennett R G & Burrell E J.** Least squares analysis of electron paramagnetic resonance spectra. *J.MoI. Spectrosec.* **7**:269-79, 1961.
3. **Marquardl D W.** Leasl squares estimation of nun linear parameters (NLIN 2). Program available from author. Augusl 1966.
4. **Marquardl D W.** Generalized inverses, ridge regression, biased linear estimation, and nonlinear estimation. *Technometrics* **12**:591-612. 1970.