Title
A METHOD FOR MINIMIZING A FUNCTION OF n VARIABLES

Author
Nierenberg, William A.

Publication Date
1959-08-01

UCRL 3816 Rev

UNIVERSITY OF
CALIFORNIA
Ernest O. Lawrence
Radiation
Laboratory

A METHOD FOR MINIMIZING A FUNCTION OF n VARIABLES

BERKELEY, CALIFORNIA

DISCLAIMER

UCRL-3816 Rev
Physics and Mathematics

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

A METHOD FOR MINIMIZING A FUNCTION OF n VARIABLES

William A. Nierenberg

August 1959

Printed for the U. S. Atomic Energy Commission

A METHOD FOR MINIMIZING A FUNCTION OF n VARIABLES

William A. Nierenberg

Lawrence Radiation Laboratory
and
Department of Physics
University of California
Berkeley, California

August 1959

ABSTRACT

This is a method for finding the minimum of a function of an arbitrary number of variables by a series of successive approximations using a paraboloidal fit. The method is particularly suited for computer programming if a matrix inverting routine is available.

A METHOD FOR MINIMIZING A FUNCTION OF n VARIABLES

William A. Nierenberg

Lawrence Radiation Laboratory
and
Department of Physics
University of California
Berkeley, California

August 1959

I. INTRODUCTION

A method is described that is useful in finding the minimum of a function of n variables by a series of trial attempts of rapid convergence. For machine computation it has the virtue of a very simple program independent of the number of variables. It has become common to test such methods by observing the number of formal steps required to find the minimum of a quadratic form. This method does this in one step.

The actual procedure involved is the following. A function of n variables $f(x_i)$ is to be minimized. If the x_i are trial values, then the next trial values are $x_i - dx_i$, where the dx_i are the solutions of the linear equations

$$\sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i \partial x_j} \, dx_i = \frac{\partial f}{\partial x_j} \quad . \tag{1}$$

Since most computer libraries are equipped with matrix-solving routines, the problem of coding and finding the successive trial values is simple. The derivatives, of course, are evaluated at the trial points successively. The matrix $\partial^2 f / \partial x_i \partial x_j$ is positive definite if the minimum is absolute and the corresponding determinant is greater than zero. (By "positive definite" is meant that the curvature at the minimum measured in any normal plane is greater than zero.) If the curvature vanishes in any direction, the determinant is zero and the minimum is not absolute. If the minimum is not absolutely definite but the determinant of the system is not zero, the method still converges to the minimum.

II. PROOF

The condition for a minimum of the function $f(x_i)$ is that for some point x_i^o we have

$$\partial f/\partial x_i = 0. \tag{2}$$

If this derivative is expanded about x_i^o, we get

$$\frac{\partial f(\vec{x})}{\partial x_i} = \frac{\partial f(\vec{x}^o)}{\partial x_i} + \sum_j \frac{\partial^2 f(\vec{x}^o)}{\partial x_i \partial x_j} dx_j + 0(dx_j dx_k). \tag{3}$$

By virtue of Eq. (2), the first term on the right-hand side vanishes. By neglecting terms of the third or higher order we reach Eq. (1). Since we have $dx_i = x_i - x_i^o$, the next approximation to x_i^o is given by

$$x_i' = x_i - dx_i. \tag{4}$$

If $f(x_i)$ is quadratic, then the third and higher orders vanish identically. In this case the solutions represented by x_i' are exact in one trial.

III. GEOMETRICAL

A picture is available that can help interpret the method in special cases. In one dimension the method is illustrated in Fig. 1. In the diagram x represents a trial point to the minimum of f(x), the solid curve. The present method determines the best-fitting (osculating) parabola to that point and the minimum of the parabola determines the position of the next trial point. Clearly the fit is perfect if f(x) is a parabola itself. If the point is a maximum for the function, the method works equally well. In a two-dimensional problem where the minimum is absolute, a paraboloid of one sheet with an elliptic cross section is fitted to the trial point. If the minimum is not absolute, a saddle-point paraboloid is fitted to the trial point and the method still converges. In n dimensions, the topology is more complicated. The sign of the determinant $G = ||\partial^2 f/\partial x_i \partial x_j||$ does not give unique information on the curvature of the point. The eigenvalues of the matrix give a measure of the curvature at the minimum. If they are all positive the minimum is absolute, if any are negative, it is not. The routine as described works equally well in all cases provided that none of these eigenvalues vanish.

IV. SPECIAL CASES

The most important special case is where $||\partial^2 f/\partial x_i \partial x_j||$ vanishes at a trial point. This implies that at least one of the eigenvalues of the matrix $G_{ij} = \partial^2 f/\partial x_i \partial x_j$ vanishes at that point. This means that at x_i on the surface $f(\vec{x}) = C$, there is a direction where the variation of $f(\vec{x})$ is linear to terms of order dx^3 in that neighborhood. The correct formal procedure is as follows.

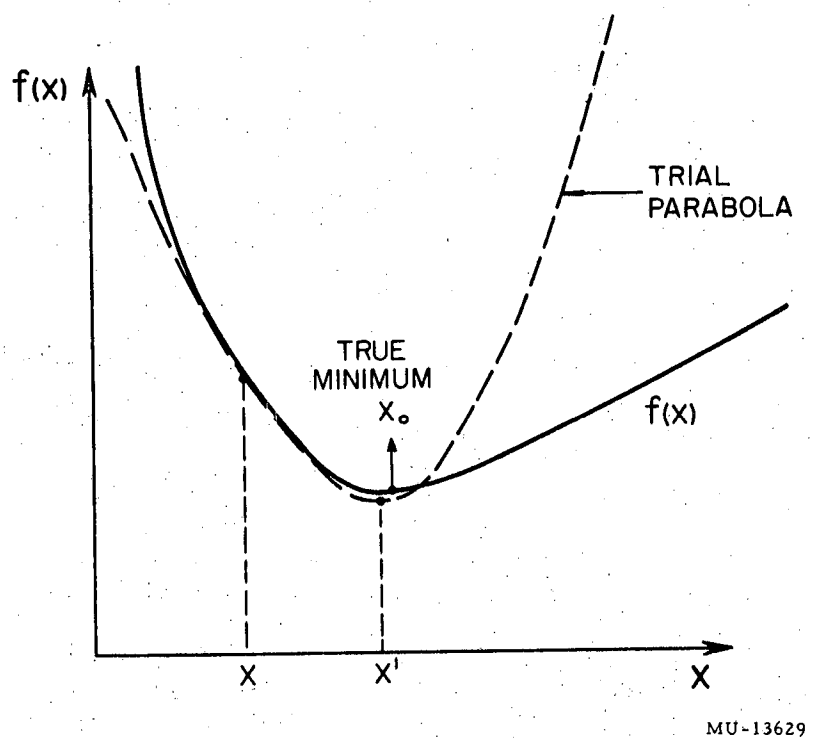

Fig. 1. Example of a trial fit by the parabolic method. The solid curve is the true function. The dotted curve is the trial parabola to the point x. x' is the minimum of the trial parabola and is the new trial point.

Choose any of the n equations of the set of Eq. (1)--say, for example, that belonging to i = 1; replace each element G_{ij} ($G_{ij} = \partial^2 f/\partial x_i \partial x_j$) in that equation by its signed minor Δ_{ij} with respect to G. Replace the right-hand member of the equation, i = 1, by zero. (That is, replace $\partial f/\partial x_1$ by 0.) Solve the resultant set of equations for the dx_i. Then proceed as before. Analytically the equations to be solved are

$$\Delta_{11}dx_1 + \Delta_{12}dx_2 + \ldots + \Delta_{1n}dx_n = 0,$$

$$\frac{\partial^2 f}{\partial x_2 \partial x_1}\, dx_1 + \frac{\partial^2 f}{\partial x_2^2}\, dx_2 + \ldots + \frac{\partial^2 f}{\partial x_2 \partial x_n}\, dx_n = \frac{\partial f}{\partial x_2},$$

$$\ldots\ldots\ldots\ldots, \qquad (5)$$

$$\frac{\partial^2 f}{\partial x_n \partial x_1}\, dx_1 + \frac{\partial^2 f}{\partial x_n \partial x_2}\, dx_2 + \ldots + \frac{\partial^2 f}{\partial x_n^2}\, dx_n = \frac{\partial f}{\partial x_n}.$$

It does not matter which one of the equations is replaced; the dx_i that result are the same. This procedure is the best procedure to follow if det G = 0.

The proof is as follows. Since det G vanishes, the eigenvalue equation

$$\sum_j G_{ij}dx_j = \lambda dx_i$$

has as a possible solution $\lambda = 0$. The eigenvector direction in dx_i space corresponding to this root is a direction along which the second derivative of f is zero. It is desirable to proceed in a direction perpendicular to this direction consistent with the spirit of Eq. (1). In effect, there is a superfluous variable in this neighborhood and the n first derivatives of f are no longer linearly independent in this neighborhood.* The unnormalized eigenvector corresponding to $\lambda = 0$ has as components the signed minors of any row. By replacing Eq. (1), i = 1, by

$$\sum_i \Delta_{1j}\, dx_j = 0,$$

we are imposing the condition that the direction of the step be perpendicular to the straight line and therefore leave its region as rapidly as possible.

The geometrical interpretation in two dimensions is clear. The quadric surface that is a best fit is a paraboloid that is formed by parallel straight lines through a given parabola; such a surface has either no

* This is made formally clear by recognizing that the Jacobian of the set of functions $\partial f/\partial x_i$ is det G and that the vanishing of this determinant implies a linear relation among the $\partial f/\partial x_i$.

minimum or no absolute minimum. This step takes the function to the trough of the paraboloid in a direction perpendicular to the ruling lines. If the exact function behaves like this everywhere, there of course is no solution to the minimal problem. This situation is an analytic oddity and is not likely to occur in actual practice, unless a starting point is chosen that is not an approximate solution but rather a "convenient" point suitable for a variety of similar calculations. If the first minors do not all vanish, Eq. (5) has a solution because its determinant has the value

$$\sum_{i=1}^{n} \Delta_{1i}^{2},$$

which is a positive number different from zero.

If the first minors all vanish, there is a degeneracy associated with $\lambda = 0$ and this method can be generalized. However, this is so pathological a case that it would be well to either choose another trial point or re-examine the function f.

V. APPLICATIONS TO LEAST-SQUARES FITTING

In using this method to fit sets of data to n unknowns, the function f has the form

$$f = \sum_{a=1}^{m} \left[M_a - f_a(x_i) \right]^2 \omega_a \tag{6}$$

where ω_a is the statistical weight of the ath measure M_a. By the usual methods it can be shown that the standard deviation of x_i about its minimum value x_i^o is

$$\boxed{\overline{(\Delta x_i)^2} = \Delta_{ii}/\det G,} \tag{7}$$

where Δ_{ij} has the same meaning as before, namely, the signed minor of G_{ij}. The Δ_{ii} (the minors along the diagonal) must all be greater than zero and, since G is the matrix for an absolute minimum, the sign is safe. (Perhaps the quickest way to see that $\Delta_{ii} > 0$ is by the following argument. Construct the matrix G^{-1}, where G_{ij} is replaced by $\Delta_{ji}/(\det G)^n$. This is the reciprocal of G. The eigenvalues of G^{-1} are the reciprocals of those of G, and therefore it follows that G^{-1} is positive definite also. Therefore its diagonal elements Δ_{ii} are also positive.)

It is important to note that this result, Eq. (7), is different from the form usually encountered for the error in that second derivatives of the functions f_i are involved. This may make an appreciable difference in the estimate of the uncertainty in some cases. Finally, the test function

$$p_f^2 = \frac{f(\vec{x}^o)}{m-n} \tag{8}$$

should be constructed. Here p_f^2 is the well-known test for the correctness of the functional dependencies that go into Eq. (6). For $p_f^2 >> 1$, the experimental assumptions are under suspicion. For $p_f^2 << 1$, the agreement can only be considered fortuitous. The rule, therefore, should be to include p_f^2 as a factor in Eq. (7), for $p_f^2 > 1$, and ignore it for $p_f^2 < 1$.

There is a close relationship between this method and Gauss's method as described in most of the standard statistical works. The method of Gauss as usually employed uses linearized functions f_a in the neighborhood of the minimum and an iterative procedure to find this minimum. It can be shown, however, that under some circumstances--depending on the values of $\partial^2 f_a / \partial x_i \partial x_j$ and the quality of the eventual fit--the approximation actually diverges no matter how close the initial point was chosen. If it weren't so, the standard method is much more rapid numerically because it does not require the second partial derivatives. With high-speed computing machines it would appear more desirable to use a method capable of exact convergence over a wide range of parameters than one which offers no a priori guarantee of convergence.

This work was done under the auspices of the U. S. Atomic Energy Commission.