A NOTE ON A THEOREM USED IN NON LINEAR LEAST SQUARES

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F.S.U. Statistics Report M 64

The Florida State University
Tallahassee, Florida
January, 1965

Financial assistance was given by the Office of Naval Research, The Wisconsin Alumni Research Foundation and the National Science Foundation.
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The non-linear least squares problem may be defined as the estimation of parameters in a model by least squares when the parameters enter into the model non-linearly. Given the model

\[ f = f(\theta, \xi), \]

where \( \theta \) is the \( p \times 1 \) vector parameters and \( \xi \) is a vector of independent variables, and an \( n \times 1 \) vector of observations \( y \), the computational part of the estimation problem is to find values of \( \theta \) for which

\[ S(\theta) = \sum_{u=1}^{n} [y_u - f(\theta, \xi_u)]^2 \]

is a minimum, where \( y_u \) was observed when \( \xi = \xi_u \).

An algorithm developed by Marquardt [1] combines some of the best features of two commonly used methods, that of Gauss and the method of steepest descent. (See Marquardt for references.) Consider the truncated Taylor series expansion about the current iterate, denoted by \( \theta^o \):

\[ f(\theta, \xi) = f(\theta^o, \xi_u) + \sum_{j=1}^{p} \left( \theta - \theta^o \right)_j \frac{\partial f(\theta, \xi_u)}{\partial \theta_j} \bigg|_{\theta^o}. \]

Let \( X \) be the \( n \times p \) matrix \( \left\{ \frac{\partial f(\theta, \xi)}{\partial \theta_j} \bigg|_{\theta^o} \right\} \), and \( r \) the \( n \times 1 \) vector of "current" residuals, i.e., \( r = y - f(\theta^o, \xi_u) \). If the function \( f(\theta, \xi) \) entering into \( S(\theta) \) is replaced by its linear approximation, we have an approximation to \( S(\theta) \), namely
\[
\hat{S}(\theta) = \sum_{u=1}^{n} \left[ y_u - f^{o}(\theta^o, \xi_u) + \sum_{j=1}^{p} (\theta_j - \theta_j^o) \frac{\partial f(\theta, \xi_u)}{\partial \theta_j} \right] \theta^o \]
\[
= (r - X\hat{\theta})' (r - X\hat{\theta}),
\]

where \( \hat{\theta} \) is the \( p \times 1 \) vector \( \theta - \theta^o \).

The algorithm of Marquardt uses the system of linear equations
\[
(X'X + \lambda I)\hat{\theta} = X'r, \quad (1)
\]
where \( \lambda \) is a scalar \( \geq 0 \), and the solution \( \hat{\theta} \) gives the required step to the next iterate. We observe that when \( \lambda = 0 \),

(1) is identical to the Gauss method and yields the exact minimum of the approximate sum of squares \( \hat{S}(\theta) \), while as \( \lambda \to \infty \), \( \hat{\theta} \) becomes more nearly proportional to \( X'r \), which, apart from a positive constant, is the negative gradient or vector of steepest descent at \( \theta^o \). Marquardt's paper includes three theorems, the first two of which are due to Morrison [2]. We state the first theorem:

Theorem 1. Let \( \lambda \geq 0 \) be arbitrary and let \( \hat{\theta}^o \) satisfy (1). Then \( \hat{\theta}^o \) minimizes \( \hat{S}(\theta) \) on the sphere centered at \( \theta^o \) whose squared radius is \( \hat{\theta}^o'r\hat{\theta}^o \).

The purpose of this note is to offer a stronger version of Theorem 1. Although this result does not affect Marquardt's algorithm, the mode of proof is essentially a geometric argument and quite different from the proofs of Morrison and Marquardt.

Theorem 1a. Let \( \lambda \geq 0 \) be arbitrary and let \( \hat{\theta}^o \) satisfy (1). Then \( \hat{\theta}^o \) minimizes \( \hat{S}(\theta) \) everywhere except within the ellipse \( \Omega \) consisting of all points \( \theta \) such that \( \hat{S}(\theta) = \hat{S}(\theta^o + \hat{\theta}^o) \). In particular, \( \hat{\theta}^o \) determines the unique minimum of \( \hat{S}(\theta) \) on and
within the sphere \( \psi \) centered at \( \vartheta^* \) whose squared radius is \( \delta^* \).  

Proof. Since \( \dot{S}(\vartheta) \) is a linear model sum of squares, we know that the contours in \( p \)-dimensional \( \vartheta \)-space which generate constant levels of \( \dot{S}(\vartheta) \) are concentric ellipsoids such that if \( \vartheta^a, \vartheta^b \) and \( \vartheta^c \) are points that are outside, on, and within a given ellipsoid, respectively, then \( \dot{S}(\vartheta^a) > \dot{S}(\vartheta^b) > \dot{S}(\vartheta^c) \).

This remark proves the first assertion of the theorem, since all points on the surface of \( \Omega \), in particular the point \( \vartheta^* + \delta^* \), minimize \( \dot{S}(\vartheta) \) outside of the interior of \( \Omega \).

To prove that the sphere \( \psi \) is included within the region minimized by \( \delta^* \), we show that \( \psi \) is externally tangent to the ellipsoid \( \Omega \), as in Figure 1. The gradient of \( \dot{S}(\vartheta) \) is given by

\[
\frac{\partial \dot{S}(\vartheta)}{\partial \vartheta} = \frac{3}{2} (r - X\delta)'(r - X\delta) = -2\lambda'(r - X\delta),
\]

which, at \( \vartheta = \vartheta^* + \delta^* \), i.e., at \( \delta = \delta^* \), is

\[
-2(\lambda_1 r - X_1 X_1^\delta^*).
\]

But a rearrangement of (1) gives

\[
X_1^\delta^* = X_1 r - \lambda I \delta^*,
\]

which, when substituted into (2) yields that the gradient of \( S(\vartheta) \) at \( \vartheta^* + \delta^* \) is

\[
-2\lambda \delta^*,
\]

which, for \( \lambda > 0 \), is a vector collinear with \( \delta^* \), but with opposite direction.\(^*\)

\(^*\) When \( \lambda = 0 \), \( \delta^* \) yields the minimum of \( \dot{S}(\vartheta) \), and \( \Omega \) is the point \( \vartheta^* + \delta^* \).
Figure 1. The sphere $\Psi$ and the ellipse $\Omega$ of Theorem 1a.

The concentric ellipses are contours of constant $\dot{S}(\theta)$.

The solutions of (1) when $\lambda = 0$ and $\lambda \to \infty$ are also illustrated, respectively, as $\hat{\delta}$ and $\delta_g$. 
5.

But the gradient of $\dot{S}(\theta)$ is perpendicular to the plane tangent to $\Omega$ at $\theta^0 + \delta^0$, and pointing out from $\Omega$, whereas $\delta^0$ is a vector originating at the center of $\psi$ and terminating on the surface of $\Omega$, at $\theta^0 + \delta^0$. Hence $\psi$ and $\Omega$ are externally tangent at $\theta^0 + \delta^0$. Finally, $\delta^0$ determines the unique minimum of $\dot{S}(\theta)$ on and within $\psi$ because $\psi$ and $\Omega$ can be tangent at only one point.
REFERENCES
