Mixed Linear-Nonlinear Least Squares Regression

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Abstract. The problem of fitting experimental data to a given model function $f(t; p_1, p_2, \ldots, p_N)$ is conventionally solved numerically by methods such as that of Levenberg-Marquardt, which are based on approximating the $\chi^2$ measure of discrepancy by a quadratic function. Such nonlinear iterative methods are usually necessary unless the function $f$ to be fitted is itself a linear function of the parameters $p_n$, in which case an elementary linear Least Squares regression is immediately available. When linearity is present in some, but not all, of the parameters, we show how to streamline the optimization method by reducing the “nonlinear activity” to the nonlinear parameters only. Numerical examples are given to demonstrate the effectiveness of this approach. The main idea is to replace entries corresponding to the linear terms in the numerical difference quotients with an optimal value easily obtained by linear regression. More generally, the idea applies to minimization problems which are quadratic in some of the parameters. We show that the covariance matrix of $\chi^2$ remains the same even though the derivatives are calculated in a different way. For this reason, the standard non-linear optimization methods can be fully applied.

Keywords: optimization, nonlinear curve fitting, Levenberg-Marquardt method, numerical derivative, Hessian matrix, Least squares approximation, shortcut derivative, covariance matrix

MSC2010 Classification: 65K10 (49M15, 65H10, 90C53, 90C55, 93E24)
1 Introduction

Linear least squares regression provides a global, fast, and absolute minimum of Chi-squared when the function to be fitted depends linearly on all its parameters. However, when the dependence on even a single parameter fails to be linear, linear regression can no longer be applied, and the solution must be successively approximated. The classical approach, which is widely employed, is to use non-linear least squares regression, which is a procedure treating all the variables as non-linear. In this paper we show how to take advantage of linear regression when the dependence on some of the parameters is linear. The benefits of the method here described are many; in particular it is more robust and frequently faster than the classical approach. In addition, all the benefits of the non-linear methods employing gradients and their covariance matrix still apply.

The techniques which have been developed since the time of I. Newton for calculating local minima of a smooth function $F(p_1, p_2, \ldots, p_N)$ of several real variables form a fundamental part of numerical analysis and have been refined to improve performance as much as possible. They derive from the well known fact that the solution of the minimization problem for a quadratic function of the parameters $p_1, p_2, \ldots, p_N$, say,

$$
\sum_{n,n'} A_{n,n'} p_n p_{n'} + \sum_n b_n p_n + C,
$$

reduces to finding vector quantity $\frac{1}{2} A^{-1} \vec{b}$, i.e., to simply solving a system of linear equations, to determine the point at which the gradient of the function vanishes. In real life, $F$ is usually not of such a particularly simple form, and one must turn to nonlinear methods \[1, 3, 13\]; these are commonly based on approximating $F$ by a a quadratic function near a supposed minimum $\vec{p}$, and improving it via estimations of the gradient $\vec{b}$ and the Hessian matrix $A$ of $F$ at $\vec{p}$.

We are particularly interested in the case when the function $F$ to be optimized (e.g., $\chi^2$ in the case of fitting experimental data with a model $f$) is expressible as a quadratic polynomial in some, but not all, of the variables (for example if we add a single transcendental term to the formula above). Then the optimization problem must be considered as essentially nonlinear. The purpose of this article is to show how to take advantage of as much of the quadratic structure of $F$ as may be present, in order to significantly improve the optimization procedure in many cases.

An important application of optimization principles is to the theory of fitting formulas to data. Given a model function $f_{p_1, p_2, \ldots, p_N}(t)$ of a variable $t$, and a set of experimental data values $(t_1, y_1), (t_2, y_2), \ldots$, one seeks the combination $\vec{p}$ of the parameters $p_n$ for which $f_{\vec{p}}(t_j)$ is most nearly equal to $y_j$. The $\chi^2$ measure of the discrepancy from an exact fit, seen as a function of the $p_n$, indeed becomes a quadratic polynomial when $f_{\vec{p}}(t)$ is linear in all these parameters (see section 3). Linear models occur in many situations, such as polynomial or Fourier approximations, and have the pleasant characteristic of reducing to least squares problems which can be solved by very fast algorithms \[2\].

As an example, an approximation widely used, both in experimental sciences and in theo-
retical mathematical studies, is the exponential fitting

\[ f_{p_1, p_2, \ldots, p_N}(t) = \sum_{n} p_{3n} e^{-\left(\frac{p_{3n-1}}{p_{3n-2}}-t\right)^2}. \]

This is linear in those \( p_n \) for which the index \( n \) is a multiple of 3. By reducing the number of parameters treated nonlinearly by one third, not only do we obtain a reduction in computation time in many cases, but the numerical stability of the fitting problem can also be greatly improved. The same holds for models with alternatives to the classical exponential peaks.

The method given here was first applied to fit infrared \([9]\) and photoemission \([8]\) spectra, and was implemented in the software \(AAnalyzer\) \([6]\) in 1998. More information about this software can be found elsewhere \([7]\). Although the fundamental idea of our method is extremely simple, it has not been analyzed mathematically until now; to our knowledge, all other commercially available software treats fitting problems as totally nonlinear when so much as one nonlinear term is present.

In Section 2 we introduce the notion of “shortcut derivative” of a differentiable function and explain its use for accelerating optimization methods. In Section 3 we apply this concept for acceleration of virtually any standard fitting algorithm. A theoretical result justifying the use of this technique is proved in Section 4, and some numerical examples are given in Section 5. In the final discussion section we compare the efficiency of our method with standard methods.

## 2 Shortcut derivatives

We present here the concept of “shortcut derivative” in a fairly general context, to be specialized later, and explain its relevance to optimization problems.

### 2.1 Optimization relative to a subset of parameters

Consider a smooth real-valued function \( F(\vec{p}, \vec{q}) \) to be optimized, where we have arbitrarily separated the variables into a length-\( M \) vector \( \vec{p} = (p_1, p_2, \ldots, p_M) \) of real numbers varying in some region \( \Omega_1 \) of Euclidean space \( \mathbb{R}^M \) and an \( N \)-vector \( \vec{q} = (q_1, q_2, \ldots, q_N) \) in \( \Omega_2 \subseteq \mathbb{R}^N \). Let \( 1 \leq m \leq M \). For \( \delta > 0 \), we modify the classical difference quotient

\[ D_F(\delta, m) = \frac{1}{2\delta} \left( F(\vec{p} + \delta e_m, \vec{q}) - F(\vec{p} - \delta e_m, \vec{q}) \right), \]  

which is the standard numerical approximation for the partial derivative \( \partial F(\vec{p}, \vec{q}) / \partial p_m \), as follows. Here we have written \( \vec{e}_m = (0, 0, \ldots, 1, 0, \ldots, 0) \) for the \( m \)-th canonical basis vector of \( \mathbb{R}^M \), i.e., \( \vec{p} + \delta e_m = (p_1, p_2, \ldots, p_{m-1}, p_m + \delta, p_{m+1}, \ldots, p_M) \).

**Definition 1** For each fixed \( \vec{p} \) define \( \vec{q}^*(\vec{p}) \in \mathbb{R}^N \) as the value of \( \vec{q} \) minimizing \( F(\vec{p}, \vec{q}) \), that is, satisfying

\[ F(\vec{p}, \vec{q}^*(\vec{p})) = \min_{\vec{q} \in \Omega_2} f(\vec{p}, \vec{q}). \]  

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Then the shortc

t derivative of $F(p, \vec{q})$ with respect to the single parameter $p_m$, and relative to the parameter subset $\vec{q}$, is the limit of

$$D^*_F(\delta, m) = \lim_{\delta \to 0} \frac{1}{2\delta} (F(\vec{p} + \delta \vec{e}_m, \vec{q}^*(\vec{p} + \delta \vec{e}_m)) - F(\vec{p} - \delta \vec{e}_m, \vec{q}^*(\vec{p} - \delta \vec{e}_m)))$$

(3)

as $\delta \to 0$. Similarly we have the second shortcut derivative as the limit of

$$D^{*2}_F(\delta, m, m') = \lim_{\delta \to 0} \frac{1}{4\delta^2} \left( F(p + \delta \vec{e}_m + \delta \vec{e}_{m'}, \vec{q}^*(p + \delta \vec{e}_m + \delta \vec{e}_{m'})) - F(p - \delta \vec{e}_m + \delta \vec{e}_{m'}, \vec{q}^*(p - \delta \vec{e}_m + \delta \vec{e}_{m'})) 
- F(p + \delta \vec{e}_m - \delta \vec{e}_{m'}, \vec{q}^*(p + \delta \vec{e}_m - \delta \vec{e}_{m'})) + F(p - \delta \vec{e}_m - \delta \vec{e}_{m'}, \vec{q}^*(p - \delta \vec{e}_m - \delta \vec{e}_{m'})) \right)$$

(4)

When discussing shortcut derivatives, we will assume, as is common in studies of numerical techniques, that the minimizer $\vec{q}^*(\vec{p})$ is unique. This may often be achieved by working locally, i.e., by reducing $\Omega_1$ to a region of interest. The existence of the limits (3), (4), will be established in the following discussion.

The gradient derivative of $F$ separates naturally into two parts,

$$\nabla F = (\nabla_p F, \nabla_q F),$$

(5)

where $\nabla_p = (\partial / \partial p_1, \ldots, \partial / \partial p_M)$ and $\nabla_q = (\partial / \partial q_1, \ldots, \partial / \partial q_N)$. Thus for fixed $\vec{p}$, the vector $\vec{q}^*(\vec{p})$ can be characterized by the property

$$\nabla_q F|_{\vec{q}^*(\vec{p})} = 0.$$

(6)

It follows from the Implicit Function Theorem that $\vec{q}^*: \Omega_1 \to \mathbb{R}^N$ is then a smooth function, assuming that the Jacobian matrix of the correspondence $\vec{q} \mapsto \nabla_q F|_{(\vec{p}, \vec{q})}$ is nonsingular.

The notion of shortcut derivative is intimately connected with the “reduced function” $F^*: \Omega_1 \to \mathbb{R}$, which we define by

$$F^*(\vec{p}) = F(\vec{p}, \vec{q}^*(\vec{p})).$$

(7)

Applying the Chain Rule for derivatives to (7) yields

$$\frac{\partial F^*}{\partial p_m} = \frac{\partial F}{\partial p_m} + \sum_{n=1}^{N} \frac{\partial F}{\partial q^*_n} \frac{\partial q^*_n}{\partial p_m},$$

(8)

where the right-hand side is evaluated at $(\vec{p}, \vec{q}^*(\vec{p}))$, and $q^*_n: \Omega_1 \to \mathbb{R}$ are the coordinate functions of $\vec{q}^*$,

$$\vec{q}^*(\vec{p}) = (q^*_1(\vec{p}), \ldots, q^*_N(\vec{p})).$$

As an immediate consequence of (6) and (8), we have

**Proposition 2** $\nabla F^*|_{\vec{p}} = \nabla_p F|_{(\vec{p}, \vec{q}^*(\vec{p}))}$. 

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Further, by placing $F^*$ in place of $F$ in (1) one immediately sees the following.

**Proposition 3** The shortcut derivative of $F(p, q)$ with respect to $p_m$, relative to the variables of $q^*$, is equal to $\partial F^*(p)/\partial p_m$.

**Remark 4** Obviously, when $(p^{\text{opt}}, q^{\text{opt}})$ is a minimum point for $F$, necessarily $q^{\text{opt}}(p^{\text{opt}})$, and $p^{\text{opt}}$ is a minimum point for $F^*$. Conversely, a minimum point $p^{\text{opt}}$ for $F^*$ generates a minimum point $(p^{\text{opt}}, q^{\text{opt}})$ for $F$ via $q^*$. This fact is relevant under the assumption that minimum points of $q^*$ may be obtained at low computational cost. In general, this will hold when the first and second partial derivatives of $F$ with respect to the variables $q_n$ may be calculated at low computational cost. In particular this holds when $F$ is a quadratic polynomial in $q_1, \ldots, q_n$ for every fixed $p$.

### 2.2 Shortcut acceleration of optimization methods

With the above ingredients we can already outline the the shortcut algorithm. It is simply the minimization of $F^*$ of equation (7).

Specifically, consider any of the well-known methods of optimization which require calculation or estimation of the gradient vector $\nabla$ and the Hessian matrix $H$ of the function $F$ to be optimized. Assume that it is feasible to calculate the function $q^*$ defined implicitly by (2). Begin with an initial guess $p^{\text{init}}$, for the parameters $p_1, \ldots, p_M$, and evaluate $q^*(p^{\text{init}} \pm \delta_m e_m)$ (9) for $1 \leq m \leq M$. The offsets $\delta_m$ may be chosen according to the sensitivity of $F$ in each variable. The values (9) are applied in (3) and (4) to approximate the shortcut partial derivatives of $F$ with respect to $p_m$, which are used in place of the usual numerical approximations of the derivatives to form the shortcut gradient $\nabla F^*$ and the shortcut Hessian matrix $H^*$, which are then used in place of the true gradient and Hessian in the chosen algorithm—this will be justified in Section 4. The algorithm produces an improved value for the minimizer $\hat{p}$, which then as usual takes the place of $p^{\text{init}}$ in the following iteration. When sufficient accuracy is obtained, a final application of $q^*$ to the resulting $\hat{p}$ completes the desired optimal parameter $(\hat{p}, q^*(\hat{p}))$ as explained in Remark 4.

### 3 Fitting of mixed linear-nonlinear models

We apply the above considerations to explain how to manage the problem of fitting experimental data to a model function which is linear in some variables $q_1, \ldots, q_N$ and (possibly) nonlinear in the remaining variables $p_1, \ldots, p_M$. Such a function can be expressed in the general form

$$f(t) = f_{\bar{p}, \bar{q}}(t) = \sum_{n=1}^{N} q_n \varphi_{n, \bar{p}}(t) + \psi_{p}(t).$$

(10)
for some functions \( \varphi_{n,p} \) \((n = 1, \ldots, N)\) and \( \psi_p \) which do not depend on \( \vec{q} \). (The term \( \psi_p \) rarely appears in physical applications, and the reader may wish to ignore it in what follows.) One wishes to choose \( \vec{p}, \vec{q} \) so as to minimize (perhaps locally) the Chi-squared quantity \( \chi^2 \)

\[
\chi^2 = \chi^2(\vec{p}, \vec{q}) = \sum_t (f_{\vec{p},\vec{q}}(t) - y_t)^2 w_t
\]

This sum is taken over a finite collection of sample values of the independent variable \( t = t_1, t_2, \ldots \), to which there are associated measurements \( y_t \), and respective weights \( w_t > 0 \). It is common to take \( w_t = y_t^{-1} \) as the inverse of the covariance of \( y_t \), but the particular choice of \( w_t \) will not be relevant to our considerations.

We now consider the minimization of \( F = \chi^2 \) in the context of the previous section. The first and second partial derivatives of (11) with respect to \( p_m \) are

\[
\frac{\partial (\chi^2 y)}{\partial p_m} = -2 \sum_t (f(t) - y_t) \frac{\partial f(t)}{\partial p_m} w_t,
\]

\[
\frac{\partial^2 \chi^2}{\partial p_m \partial p_m'} = 2 \sum_t \left( \frac{\partial f(t)}{\partial p_m} \frac{\partial f(t)}{\partial p_m'} - (f(t) - y_t) \frac{\partial^2 f(t)}{\partial p_m \partial p_m'} \right) w_t.
\]

As discussed in [13], the second terms of the summands in (13) are generally discarded in numerical work not only because the factors \( f(t) - y_t \) tend to be small, but because greater numerical stability is achieved this way. Thus for fitting problems we will make no use of (4).

The form (10) for \( f \) leads to the expansion

\[
\chi^2(\vec{p}, \vec{q}) = \sum_n \sum_{n'} \left( \sum_t \varphi_n \varphi_{n'} w_t \right) q_n q_{n'} + \sum_n \left( \sum_t 2(\psi - y_t) \varphi_n w_t \right) q_n + \sum_t (\psi - y_t)^2 w_t,
\]

which is quadratic in \( q_1, \ldots, q_N \) for fixed \( \vec{p} \). With this, the partial derivatives of \( \chi^2 \) with respect to the linear parameters \( q_n \) are easily obtained in terms of

\[
\frac{\partial f(t)}{\partial q_n} = \varphi_n(\vec{p}, t).
\]

Namely, one finds that (12) becomes

\[
\frac{\partial (\chi^2 y)}{\partial q_n} = 2 \sum_{n'} \left( \sum_t \varphi_n \varphi_{n'} w_t \right) q_{n'} + 2 \sum_t (\psi - y_t) \varphi_n w_t
\]

which conveniently represents the gradient of \( \chi^2 \) in the form \( \nabla \chi^2 = A \vec{q} + \vec{b} \). Thus for fixed \( \vec{p} \), the (absolute) minimum of \( \chi^2 \) is attained when \( A \vec{q} + \vec{b} = 0 \). Typically there are more data points \( t \) than the number \( N \) of parameters and this is an overdetermined linear system, so there does not exist an exact solution to this system, but the residual \( A \vec{q} + \vec{b} \) is minimized in terms of the \( L_2 \) norm by the linear least squares regression [13] which is available as a standard function of many
numerical software packages. In this sense, by Definition 1, this linear least squares solution is the best approximation for \( \tilde{\mathbf{q}}^*(\tilde{\mathbf{p}}) \). In contrast to the \( p_m \)-derivatives, the quantities involved in setting up this linear system for the \( q_n \)-derivatives require no special numerical derivation, since they are already calculated whenever \( f_{\tilde{\mathbf{p}}, \tilde{\mathbf{q}}}(t) \) itself is evaluated.

4 Reduced covariance matrix

The Hessian matrix \( H \) appearing in a nonlinear optimization procedure is associated with the correlations of the fitted model with the original data; we will study it here and comment more fully in Section 6 below.

We return to the generality of a function \( F_{\tilde{\mathbf{p}}, \tilde{\mathbf{q}}} \) to be minimized as in Section 2. Let \( H^*_{\delta} \) denote the approximation of the shortcut Hessian matrix corresponding to a parameter displacement \( \delta > 0 \). (More precisely, \( \delta = \delta_m \) refers to a displacement in a single direction \( \mathbf{e}_m \) for notational simplicity; our statements will be valid as well for a vector of displacements \( (\delta_1 \ldots \delta_M) \).) The true Hessian matrix \( H \) of \( F \) admits a natural block decomposition

\[
H = \begin{pmatrix}
H_{pp} & H_{pq} \\
H_{qp} & H_{qq}
\end{pmatrix} \in \mathbb{R}^{M+N,M+N}
\]

with \( H_{pp} \in \mathbb{R}^{M,M} \), \( H_{pq} \in \mathbb{R}^{M,N} \), \( H_{qp} \in \mathbb{R}^{N,M} \), and \( H_{qq} \in \mathbb{R}^{N,N} \). The symmetries \( H_{pp} = (H_{pp})^T \), \( H_{qp} = (H_{pq})^T \), \( H_{qq} = (H_{q})^T \) are a consequence of the fact that the order of differentiation is irrelevant. Consider the inverse matrices

\[
\eta(\delta) = \left( \eta_{jj}(\delta) \right) = (H^*(\delta))^{-1},
\]

\[
\eta = (H_{pp})^{-1},
\]

and denote

\[
H^*(0) = \lim_{\delta \to 0} H^*(\delta).
\]

It is well known that the matrix entries of \( H^{-1} \) represent the covariances of the full set of fitted parameters \( p_1, \ldots, p_M, q_1, \ldots, q_N \), and the diagonal elements, the variances, are of particular importance (see for example [13, Sect. 15.4, 15.6], especially equation (15.4.15)). Similarly, the entries of \( \eta \) are the covariances of the parameters \( p_1, \ldots, p_M \) for the fitting corresponding to the minimization of \( F \). The following result was discovered empirically.

**Theorem 5** Suppose that the Hessian matrix \( H \) is invertible. Then \( H^*(\delta) \) is also invertible for each \( \delta > 0 \), and

\[
\eta_{m,m'}^*(\delta) \to \eta_{m,m'} \text{ as } \delta \to 0
\]

for \( 1 \leq m \leq M, 1 \leq m' \leq M \). In other words, \( H^*(\delta)^{-1} \to H_{pp}^{-1}(p,q)^* \) as \( \delta \to 0 \).

We devote the rest of this section to the proof of this result, which depends on two lemmas. Note that we do not claim that \( H^*(\delta) \) approximates \( H \) in any way.
Lemma 6 The Jacobian matrix of the function $\vec{q}^*$,

$$J\vec{q}^* = \left( \frac{\partial q^*_{mn}}{\partial p_m} \right)_{1 \leq n \leq N, 1 \leq m \leq M} \in \mathbb{R}^{N \times M} $$

is given by the formula

$$J\vec{q}^* = -H_{qq}^{-1}H_{qp}.$$  \hspace{1cm} (18)

Proof. From (6) and the Chain Rule,

$$0 = \frac{\partial^2 F}{\partial q_n \partial p} (\vec{p}, \vec{q}^*(\vec{p})) = \frac{\partial F}{\partial q_n} + \sum_{n'=1}^{N} \frac{\partial^2 F}{\partial q_n \partial q_{n'}} \frac{\partial q^*_{n'}}{\partial p_m} \bigg|_{\vec{q} = \vec{q}^*(\vec{p})}$$

for $1 \leq m \leq M, 1 \leq n \leq N$. In matrix form this is $0 = H_{qp} + H_{qq}(J\vec{q}^*)$. The invertibility of $H$ implies the invertibility of $H_{qq}$, from which the result follows. \hfill \square

Lemma 7 $H^*(0) = H_{pp} - H_{pq} H_{qq}^{-1} H_{qp}$.

Proof. Again by the Chain Rule,

$$\frac{\partial F^*}{\partial p_m} (\vec{p}) = \frac{\partial F}{\partial p_m} (\vec{p}, \vec{q}^*(\vec{p})) + \sum_{n=1}^{N} \frac{\partial F}{\partial q_n} (\vec{p}, \vec{q}^*(\vec{p})) \frac{\partial q^*_{n}}{\partial p_m}$$

for $1 \leq m \leq M$. Now differentiate with respect to $p_{m'}$,

$$\frac{\partial^2 F (\vec{p}, \vec{q}^*(\vec{p}))}{\partial p_m \partial p_{m'}} = \left( \frac{\partial F}{\partial p_m} + \sum_{n=1}^{N} \frac{\partial^2 F}{\partial p_m \partial q_n} \frac{\partial q^*_{n}}{\partial p_{m'}} \right) + \sum_{n=1}^{N} \left( \frac{\partial^2 F}{\partial q_n \partial p_{m'}} \frac{\partial q^*_{n}}{\partial p_m} + \frac{\partial^2 F}{\partial p_{m'} \partial q_n} \frac{\partial q^*_{n}}{\partial p_m} \right)$$

for $1 \leq m' \leq M$. By (9), the last sum vanishes, and upon substituting the definitions of the entries of $H_{pp}$, $H_{pq}$, $H_{qq}$, we find

$$h^*_{mn}(0) = h_{m,m'} + \sum_{n=1}^{N} \left( h_{mn'} \frac{\partial q^*_{n}}{\partial p_{m'}} + \frac{\partial q^*_{n}}{\partial p_m} h_{mn} \right) + \sum_{n=1}^{N} \sum_{n'=1}^{N} \frac{\partial q^*_{n}}{\partial p_m} h_{nn'} \frac{\partial q^*_{n'}}{\partial p_{m'}}.$$

In matrix notation this is

$$H^*(0) = H_{pp} + H_{pq} J\vec{q}^* + (J\vec{q}^*)^T H_{qp} + (J\vec{q}^*)^T H_{qq} J\vec{q}^*.$$
so upon substituting the formula of Lemma 6 and canceling, we arrive at the result.

**Proof of Theorem 5.** By Cramer’s rule, we want to compare the matrix entries

\[
\eta_{m,m'} = \frac{\det \text{Sub}_{m,m'} H}{\det H},
\]

\[
\eta_{m,m'}^*(0) = \frac{\det \text{Sub}_{m,m'} H^*(0)}{\det H^*(0)},
\]

where we write \( \text{Sub}_{m,m'} A \) for the submatrix of \( A \) obtained by removing the \( m \)-th row and \( m' \)-th column. It will suffice to show

\[
\det H^*(0) = \frac{1}{\det H_{qq}} \det H,
\]

\[
\det \text{Sub}_{m,m'} H^*(0) = \frac{1}{\det H_{qq}} \det \text{Sub}_{m,m'} H,
\]

since upon dividing these two formulas we obtain \( \eta_{m,m'}^*(0) = \eta_{m,m'} \).

We deduce (19) from Lemma 7 and the formula for the determinant of a block matrix

\[
\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det D \det (A - BD^{-1}C),
\]

valid when \( A \) and \( D \) are square submatrices and \( D \) is invertible. Indeed,

\[
\det H = \det H_{qq} \det (H_{pp} - H_{pq} H_{qq}^{-1} H_{qp}) = \det H_{qq} \det H^*(0).
\]

To verify (20) we apply \( \text{Sub}_{m,m'} \) to both sides of the formula of Lemma 7

\[
\text{Sub}_{m,m'} H^*(0) = \text{Sub}_{m,m'} H_{pp} - \text{Sub}_{m,m'} [H_{pq} H_{qq}^{-1} H_{qp}].
\]

Applying the general rule \( \text{Sub}_{m,m'} (ABC) = (\text{Sub}_{m,0} A) B (\text{Sub}_{0,m'} C) \), we find the block structure

\[
\text{Sub}_{m,m'} H = \begin{pmatrix} \text{Sub}_{m,m'} H_{pp} & \text{Sub}_{m,0} H_{pq} \\ \text{Sub}_{0,m'} H_{qp} & H_{qq} \end{pmatrix}
\]

and invoking Lemma 7 again, the block determinant is

\[
\det \text{Sub}_{m,m'} H = \det H_{qq} \det \left( \text{Sub}_{m,m'} H_{pp} - (\text{Sub}_{m,0} H_{pq})(H_{qq}^{-1})(\text{Sub}_{0,m'} H_{qp}) \right)
\]

\[
= \det H_{qq} \det \left( \text{Sub}_{m,m'} H_{pp} - \text{Sub}_{m,m'} [H_{pq} H_{qq}^{-1} H_{qp}] \right)
\]

\[
= \det H_{qq} \det \text{Sub}_{m,m'} H^*(0),
\]

which is (20). This completes the proof. \( \square \)
5 Numerical examples

We compare the results of solving fitting problems in a model which is linear in the variables $q_1, \ldots, q_N$ by the method of shortcut derivatives and by the classical approach, which treats all variables equally, i.e., using a parameter set

$$p_1, \ldots, p_M, p_{M+1}, \ldots, p_{M+N}$$

where we denote $p_{M+n} = q_n$ for $1 \leq n \leq N$. The conversion to the classical formulation is easily programmable in terms of the expression (10) simply by incorporating the $\varphi_n$ terms into the function $\psi$ and reindexing the variables.

In the following numerical experiments, the method of Levenberg-Marquardt [10, 13] was programmed in Mathematica (Wolfram) and run on an ordinary laptop computer. We avoided fancy variations such as in [18].

Example 1. Consider a model function with four parameters,

$$f_1(t) = q_1 e^{-t/p_1} + q_2 \sin \frac{t}{p_2}, \quad t = 1, 2, \ldots, 100,$$

with the particular values $(p_1, p_2) = (20, 5), (q_1, q_2) = (6, 1)$ as in Figure 1.

The nearby parameter $\vec{p}_{\text{init}} = (19, 4.9)$ is chosen for illustrative purposes. The parameter set is automatically completed with $\vec{q}_{\text{init}} = \vec{q}^* (\vec{p}_{\text{init}}) = (6.19664, 0.947731)$ approximately. We consider the question of minimizing $\chi^2$ as $p_1$ varies while leaving $p_2 = 4.9$ fixed, to see how close we can come back to the true value of $p_1 = 20$. There are two natural ways to do this: (a) to leave the value of $\vec{q}$ fixed, thus considering parameter sets $(p_1, p_2, q_1, q_2)$ in which only $p_1$ varies; (b) to optimize the $q$-values along with $p_1$, thus considering $(p_1, p_2, q_1, q_2^*(p_1, p_2))$.

![Figure 1: Model curve](image-url) for “true” values of its 4 parameters (left). With $p_2$ fixed, plots of $\chi^2$ are given (right) as a function of $p_1$ where the initial optimum value $\vec{q}^\text{init}$ is fixed (solid), and with $\vec{q}$ optimized for each $p_1$ (dashed). The minima of these plots are approximations for the true minimum at $p_1 = 20$. 

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Figure 2: Comparison of shortcut method to classical fitting for Example 1. In the black region, both methods converge to the true value (marked with a white spot). The outer white area is the region of $p_1, p_2$ values for which neither method converges to the correct $f_1(t)$, and in the intermediate gray area only the shortcut method works. The many small black “islands” in the gray area contain values where the classical method may be considered to converge “accidentally”; one could not reliably choose an initial guess near such points.

that case (a) is simply a straight line in the 4-dimensional parameter space, while (b) is a curve in this space specially adapted to our problem.

One sees in Figure 1 that the graph of the values of $\chi^2$ for case (a) lies above the graph of $\chi^2$ for case (b). The minimum value of the former curve is approximately 19.35, whereas the minimum of the latter is approximately 19.85, much closer to the true value $p_1 = 20$. This phenomenon illustrates why the shortcut method tends to require fewer iterations to approximate minima; of course, in general one is locating a minimum on a higher-dimensional hypersurface of which we have been able to illustrate only a 1-dimensional slice here.

For the same model function (21), Figure 2 depicts the region in the $p_1$-$p_2$ plane of initial guesses from which both the shortcut method and the classical method converge to the correct values $p_1 = 20$, $p_2 = 5$, lying properly within the region where only the shortcut method gives the correct solution. In order to make this comparison, the classical method was started with the “guess values” of $q_1, q_2$ given by $\vec{q}^*(p_1, p_2)$. In practice, one would almost surely make a poorer initial guess if $\vec{q}^*$ were not evaluated, and the contrast between the sensitivity of the two methods to the initial guess would be found to be even greater than shown here.

Example 2. For this example we take as model function a variable number of Gaussian peaks,

$$f_2(t) = e^{-(t/p_1)^2} + \sum_{n=1}^{N} q_n e^{-(t-n)^2/5^2}. \quad (22)$$

The peaks centered at the positive integer points $t = 1, 2, \ldots, N$ have fixed widths but variable heights. In contrast, the single peak centered at $t = 0$ has variable width determined by $p_1$, the only nonlinear parameter, sufficient to preclude the sole use of least squares regression.
Figure 3 shows the advantage of the shortcut method for this example. The increasing number of data points (with a spacing $\Delta t = 0.1$ between consecutive points) is an additional factor in requiring more calculation time as the number $N + 1$ of peaks increases. It is seen that the running times are approximated by $0.01 \times N^{2.3}$ and $0.003 \times N^{2.9}$. For the shortcut method, the Levenberg-Marquardt required 2 iterations for the entire range of values of $N$, while the classical method required 3 iterations for $N > 45$. The number of function calls in the classical method grew steadily from 50% greater for low values of $N$ to 35 times greater for $N = 60$, easily offsetting the higher cost of the calculation of $\vec{q}^*$ in each derivative.

Example 3.

A situation which presents a greater opportunity for the shortcut method is the simultaneous fitting of several “files” of data. An application occurs in X-ray photoelectron spectroscopy (XPS) [12], in which the chemical composition of a sample material is to be determined by the energy distribution of the electrons leaving a surface illuminated by X-rays at different angles (one file for each angle). For physical reasons the centers and widths of the peaks are not affected by a change in angle of the incident beam, so these parameters are common to the collection of model functions which must be fit simultaneously (“shared-parameters hypothesis”, as described in [12]).

To simulate this phenomenon we use the model function

$$f_3(t) = q_1e^{((t-p_1)/p_4)^2} + q_2e^{((t-p_2)/p_5)^2} + q_3e^{((t-p_3)/p_6)^2} + q_4t + q_5$$

(23)

in which the last two terms represent the “background noise”. (In practice many other models are often used in which the peaks are not Gaussian.) Let us suppose that sample data is given for $k = 1, 2, \ldots, K$ readings, sharing common values of $p_1, \ldots, p_6$ but each with its own set of linear parameters

$$\vec{q}^{(k)} = (q_{k,1}, \ldots, q_{k,5})$$

As illustrated in Figure 4, there is a set of sample data $\vec{y}^{(k)}$ for each $k$, which determines in turn a discrepancy function $\chi^2_k(\vec{p}, \vec{q})$. The closeness of the collective fitting corresponding to
the $5K + 6$ parameters $\vec{p}, \vec{q}^{(1)}, \ldots, \vec{q}^{(K)}$ is measured by the sum
\[ \Phi(\vec{p}, \vec{q}^{(1)}, \vec{q}^{(2)}, \ldots, \vec{q}^{(K)}) = \sum_{k=1}^{K} \chi^2_k(\vec{p}, \vec{q}). \] (24)

It should be noted that the partial derivative of $\Phi$ with respect to $p_m$ is the sum of the corresponding derivatives of $\chi^2_k$, while the partial derivative of $\Phi$ with respect to $q_n$ is given by the partial derivative of the single summand of (24) in which the parameter $q_n$ appears. For this reason it is a straightforward matter to represent the gradient and Hessian of $\Phi$ in terms of the entries of the gradients and Hessians of the various $\chi^2_k$.

Using this information, we calculated the best fit via the Levenberg-Marquardt method for the function $\Phi^*(\vec{p}) = \Phi(\vec{p}, \vec{q}^{*(1)}(\vec{p}), \vec{q}^{*(2)}(\vec{p}), \ldots, \vec{q}^{*(2)}(\vec{p}))$, where $\vec{q}^{*(k)}$ denotes the optimization of the five $q$-values
\[ \vec{q}^{(k)} = (q_1^{(k)}, q_2^{(k)}, \ldots, q_5^{(k)}) \]

*Figure 4: Simulation of five files of data results formed of three slightly overlapping Gaussian peaks, with increasing heights approximately proportional to the noise baseline. Here $0 < t < 4$.*

*Figure 5: Count of function evaluations and computing time for shortcut algorithm (dashed) and traditional Levenberg-Marquardt calculation (solid) for increasing numbers $K$ of simultaneous files of data modeled by (23).*
with respect to the data \( \vec{y}^{(k)} \). For comparison, the classical Levenberg-Marquardt was applied after translating the \( t \)-variable of the model functions in such a way as to form a single function on an interval \( K \) times as long as the original one, and incorporating all the variables in a single \( p \)-list via the relation \( \vec{q}^{(k)} = (p_{5k-4}, p_{5k-3}, \ldots, p_{5k}) \). The \( \chi^2 \) of this auxiliary function is precisely the sum in (24). Thus the resulting minima are identical. As Figure 5 shows, the computational cost is reduced significantly by the use of shortcut derivatives.

6 Comparison of methods

We discuss briefly some of the differences in the results produced by the shortcut method with respect to traditional regression methods.

6.1 Direct advantages of the linear-nonlinear method

1. Robustness of computation. As illustrated by Example 1 and many other examples we have calculated, the linear-nonlinear method tends to offer more flexibility in the choice of initial guess for the optimization procedure.

The robustness of is more strongly manifested when shared parameters are involved such as in Example 3. This phenomenon was previously studied in the case of files of data in [12, Fig. 7], where it was noted that precision of the assessment of the shared-parameters (\( p \)-variables) increases with the number of files. Although this is, in fact, expected because each file adds information, it could be somewhat counterintuitive. A belief holds in parts of the physics community that there is a limit on the number of parameters, holding covariances among each other, that can be simultaneously optimized; limits of 17 to 20 have been suggested. In this example, we have shown that it is possible to optimize a far greater number of parameters simultaneously (e.g., 156 parameters when \( N = 30 \)) even though the covariance between each pair of variables is not zero. In general, the use of the mixed linear-nonlinear method described here tends to increase the robustness of the optimization process since linear regression provides the best possible value of the linear parameters at each step. The method inherits some important characteristics of linear regression since it is also possible to catch the culprit parameters if the minimization has multiple solutions (e.g., too many free parameters or too many peaks).

2. Estimation of uncertainty. As is well known, \( H^{-1} \) evaluated at optimal \((p, q)\) is a very relevant matrix inasmuch as its diagonal elements measure the covariance of the \( p \)-parameters [13]. In the discussion of the particular case study of [12, Fig. 7] it was found numerically that the standard deviation predicted through \( H^{-1} \) is quite similar to the actual standard deviation obtained through many trials. Thus Theorem 5 allows one to use the diagonal elements of \( H^*(\delta)^{-1} \) to report the uncertainty on the \( p \)-parameters even though the derivatives are obtained in a nonstandard way.

The advantage of this is that in the covariance analysis of a fitting problem, the inversion of the smaller matrix \( H^*(\delta) \) for fixed, small \( \delta > 0 \) is less costly than the inversion of the full matrix \( H \).

3. Operation count and computation time. It must be recognized that each iteration of the
shortcut method is computationally more costly than the corresponding classical method, due to the evaluations of $\vec{q}^*$ in each shortcut derivative.

Consider the computing time required for the classical method, i.e., for a sequence of model functions of the form $f(p_1, \ldots, p_M)$ with increasing numbers $M$ of the parameters, the evaluation of which we will assume implies a computational cost proportional to $M$. (This does not hold for Example 2, where the number of data points $t$ also grows with $M$.) The cost of evaluating first and second partial derivatives numerically grows as $O(M)$, which implies that the gradient vector of $f$ costs $O(M^2)$. Forming the Hessian of $\chi^2$ via (13) requires $O(M^2)$ operations once the first partial derivatives are known (since we are assuming the number of $t$ values is fixed). The solution of an $M \times M$ matrix equation by least squares costs $O(M^3)$, which is thus the cost of a single iteration of an $M$-parameter fitting.

Now we consider a model function of the form (10). Each evaluation of $\varphi_1(\vec{p}), \ldots, \varphi_1(\vec{p})$ costs $O(MN)$ since each function individually costs $O(M)$. An evaluation of $f(\vec{p}, \vec{q})$ thus also costs $O(MN)$ (this is independent of whether we are speaking of a single $t$ or the entire fixed set of $t$ values). To evaluate all the partial derivatives $\partial(\chi^2)/\partial q_n$, $1 \leq n \leq N$ by (10) requires $O(N^2)$ multiplications, so the cost of the Hessian of $\chi^2$ with respect to $\vec{q}$ costs whichever is greater of $O(MN)$ and $O(N^2)$. Following Definition 1, we see that an evaluation of $\vec{q}^*(\vec{p})$ is carried out by minimizing with respect to the $N$ variables $q_1, \ldots, q_N$, which means solving an $N \times N$ system. Hence the cost of $\vec{q}^*(\vec{p})$ is $O(MN) + O(N^3)$.

The shortcut derivatives $\partial f/\partial p_m$, $1 \leq m \leq M$ are obtained from (3) with $f$ in place of $F$, with a total cost of $O(M^2N) + O(MN^3)$, which by (13) is the cost of the shortcut Hessian of $\chi^2$, an $M \times M$ matrix. Since the solution of the $N \times N$ system is only $O(N^3)$, the iteration cost for the shortcut method is $O(M^2N) + O(MN^3)$. A more refined analysis, for which the number $T$ of data points is allowed to grow, gives the value $O(M^2NT) + O(MN^3)$.

In comparison, the classical method has a cost of $O((M+N)^3)$. Thus it can be seen that the shortcut method will be more costly in the long run when $M$ is at least of the same proportion as $N$. In Examples 2 and 3, the ratio $M/N$ effectively tends to zero, which accounts for the considerable savings of time with the shortcut method.

In our application of the Levenberg-Marquardt procedure, in many cases we have found sometimes, but not always, that fewer iterations are necessary than with the classical method, but never more. In experiments with model functions such as

$$\sum_n q_n e^{-\left(\frac{p_{2n-1}}{t-p_{2n}}\right)^2},$$

in which the $p$, $q$ variables are in proportion of $2:1$, with the peaks centered at integer points $p_{2n} = 1, 2, \ldots$, the shortcut method greatly reduces the number of iterations required, but the computation time grows faster than in the traditional method, due to the cost of calculating $\vec{q}^*$ in the shortcut derivatives. It would be interesting to look for ways of reducing the cost of $\vec{q}^*$ if possible.
6.2 Other approaches to linear-nonlinear regression problems

We have reviewed the mathematical literature in optimization and regression fairly carefully, as well as descriptions of available software, and to the best of our knowledge, the mixed linear-nonlinear approach does not seem to have been considered previously apart from its use in the software [6], where shortcut derivatives were applied without theoretical justification. Also, Theorem 5 was discovered empirically [12] by noticing that the first M diagonal elements of $H^{-1}$ appeared to be numerically equal (within rounding errors) to the diagonal elements of $H^*(\delta)^{-1}$. The algorithm in [6] calculates the computationally cheaper quantities $H^*(\delta)^{-1}$ as approximations of the covariances of the parameters. The excellent results obtained compared to other similar programs, and the unexplained coincidence of the inverse diagonal elements motivated the present investigation of the mathematical properties of this approach.

In fact, there has been little systematic research into the idea of combining linear and nonlinear aspects of fitting problems. An ad-hoc method for $f(t) = q_1 e^{p_1 t} + q_2 e^{p_2 t}$, suitable for working out by hand calculation, is described in [5]. Exponential regressions of an arbitrary number summands are discussed in [15]. Chapter 9 of [4] gives a detailed discussion of a linear-nonlinear problem, one of the few we have found on this subject: a process of heat produced by cement hardening which is nonlinear in time and linear in some of the other control variables. The approach there alternates linear and nonlinear approximation, but is quite different from the method described here. Fitting of parametrized curves $(y(t), z(t))$ in the plane is discussed in [16], in which linearity also plays an important role.

Many types of industrial problems (see for example [17]), as well as calculations in mathematical biology [11, 14], mathematical finance, and other areas, require fitting of model curves or surfaces to observed data. We believe that many such areas could benefit from the shortcut method of optimization.

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