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Least Squares Parameter Estimation and the Levenberg-Marquardt Algorithm : Deterministic Analysis, Sensitivities and Numerical Experiments

Frédéric Guyon* Rodolphe Le Riche†

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Abstract

The present paper is a unified presentation of least squares parameter estimation using the Levenberg-Marquardt algorithm. In the first part of the paper, least squares minimization and minimum norm regularizing problems are introduced through their relation to the type of mapping performed by the model. Parameter estimate and model sensitivities are described. The second part of the paper is devoted to the analysis of the Levenberg-Marquardt algorithm. Proof of convergence to the mimimum norm solution of linear least squares is given. The algorithm is interpreted as a semi-implicit method following the steepest slope line. It is proved that the steps taken by the Levenberg-Marquardt algorithm enable measuring parameter sensitivity and model curvatures at no extra cost. Numerical examples are given for linear and nonlinear models, including parameter identification of a material constitutive law.

1 Introduction

Since the original work of Gauss in the 19th century [4], the topic of least squares parameter estimation has received massive attention within both statistical ([3]) and deterministic frameworks ([1], [6]). The concept that the sum of the squares of the differences between the data and the model should be minimal is seen as a maximal likelihood or chi-square fitting principle in statistics or as a projection onto the model space in deterministic mathematics. Applications concern all fields of sciences where the parameters of a model have to be estimated in order to represent, in some sense, observed data ([9] in control, [13] in oceanography and meteorology, [15] in geophysics, [16] in chemistry). Parameter estimation is alternatively called identification or inverse problem. The Levenberg-Marquardt family of algorithms have emerged as robust methods for nonlinear least squares minimizations. Today, they are probably the most often used algorithms for minimizing least squares.

Because of the numerous, specialized and scattered publications dealing with the subject, the authors felt it was useful to draw a complete picture of least squares

*Infobiogen, 7 rue Guy Moquet, 94801 Villejuif, France (guyon@infobiogen.fr).

†Lab. de Mécanique de Rouen, Av. de l'Université, Le Madrillet, 76800 Saint Etienne du Rouvray, France (Rodolphe.Leriche@insa-rouen.fr).

parameter estimation and link them to the Levenberg-Marquardt algorithm. Only the deterministic point of view is covered.

The norms that shall be minimized to ensure parameter identifiability are progressively introduced for injective, surjective, and general linear models. Optimality conditions are given and interpreted as projections. Nonlinear models are then studied. Next, various measures of sensitivities to parameter or data changes are proposed.

The second part of the paper analyzes convergence of Levenberg-Marquardt algorithms. For linear models, it is shown that Levenberg-Marquardt finds the smallest norm least squares parameter estimate. General characteristics of the trajectory taken by the optimizer are given. They shed some light on the robustness of the Levenberg-Marquardt method. It is proved that the trajectory followed by the algorithm permits calculating parameter sensitivity and model curvature free of any extra calculations. Finally, numerical examples on linear and nonlinear models, which include material constitutive laws, are given. Appendices of mathematical review are added that make the presentation self-contained.

2 Least squares Parameter Estimation

2.1 Terminology and Issues

Parameter estimation is the process of fitting a mathematical model to experimental data to determine unknown parameters of the model. The parameters are chosen so that the output of the model match, in some sense, observed experiments. The most general criterion to assess the worth of a set of parameters is the square of the Euclidean distance between the model and the experimental data. There is, for example, strong statistical evidence in favor of least squares estimate for linear models, $f(x) = Ax + e$, where x is the parameters vector and e are unobservable Gaussian random errors ($e \approx N(0, \sigma^2 I)$): the least squares estimate of x is, in that case, the best linear unbiased estimate, the maximum likelihood estimate, and the minimum variance unbiased estimate ([2]).

We shall consider the parameters x to be in a n-dimensional closed and bounded hypercube, $S \subset \mathbb{R}^n$. Experimental data are written as a vector $z \in \mathbb{R}^m$. The model $f(x)$ defines a mapping $f : \mathbb{R}^n \longrightarrow \mathbb{R}^m$. f is assumed to be twice continuously differentiable. (Output) Least squares parameter estimates are solutions of the unconstrained optimization problem,

$$\begin{aligned} \min_{x\in S} \ J(x) \ &= \ \frac{1}{2}\sum_{i=1}^{m} w_i (f_i(x) - z_i)^2 \ = \\ \frac{1}{2}(f(x)-z)^T W (f(x)-z) \ &= \ \frac{1}{2}||C(f(x)-z)||^2. \end{aligned} \tag{1}$$

where the subscript $_i$ denotes components of a vector, $W = C^T C$ is a $m \times m$ positive definite diagonal matrix of weights and $|| \, . \, ||$ is an L2-norm. As other types of least squares problems will soon be described, we sometimes refer to (1) as an output least squares minimization. The weighting term C is deleted by performing the implicit change of variables $Cf(x) \rightarrow f(x)$ and $Cz \rightarrow z$. We have assumed that the minimization (1) is performed using a continuous function f on a closed and bounded set S, therefore conditions of the Weierstrass theorem (Appendix B,[11]) are met, and problem (1) has at least one solution. The set of solutions of (1) is $\mathcal{X} = \arg\min \frac{1}{2}||C(f(x)-z)||^2$. When solving the least squares problem (1), two key issues need to be adressed:

- *Identifiability*; is the solution to (1) unique ?

- *Sensitivity / Stability*; by how much will the parameter estimate change as a result of a perturbation in the data or the model ? Stability adresses the question of the continuity of the solution of (1) under continuous variations of the data z.

Problems that are not identifiable or not stable are said to be ill-posed. Against non-uniqueness, a second, regularizing, minimization is used,

$$\min_{x \in \mathcal{X}} \frac{1}{2} ||x||^2 \tag{2}$$

Let x^* denote the solution of (2) (existence and unicity is discussed in sections 2.2 to 2.5). The minimum norm problem (2) introduces a priori knowledge on good parameters, x_d, when the change of variable $x = \hat{x} - x_d$ is performed.

We now discuss problems (1) and (2) for injective, surjective, and general linear and nonlinear functions $f(x)$. Linear models are of the form $f(x) = Ax$, where A is a constant coefficients $m \times n$ matrix of rank r. A is the gradient of f with respect to x. For a linear model, $A = \nabla f$, where $\nabla f^T = [\nabla f_1^T \ldots \nabla f_m^T]$, and $\nabla f_j = [\frac{\partial f_j}{\partial x_1} \ldots \frac{\partial f_j}{\partial x_n}]$.

2.2 Output Least Squares and Linear Injective Model

2.2.1 Optimization problem

Output least squares involve finding the model output , $y = Ax$, the nearest to the data, z (problem (1)), which can be restated as,

$$\begin{cases} \min_{x \in S, y \in \mathbb{R}^m} \frac{1}{2}||y - z||^2, \\ \text{such that } Ax = y . \end{cases} \tag{3}$$

The most often encountered inverse problems are associated to injective mappings (cf. Appendix A.1). Injective mappings typically occur when enough data exist, which, in turn, imply the characteristic features from linear algebra $m \geq n$, and Rank$A = n$. In that case, the inverse mapping from the model output to the parameters is well defined, and solving (3) is the standard strategy for identifying the model parameters. For noninjective mappings however, (3) can be ill-posed.

2.2.2 Optimality conditions

Problem (3) is convex. The Kuhn and Tucker optimality conditions, which are necessary and sufficient here, say that there exists an m-dimensional vector λ such that,

$$\begin{cases} Ax^* - y^* = 0 \\ y^* - \lambda^* - z = 0 \\ A^T \lambda^* = 0 \end{cases} \tag{4}$$

Eliminating λ^* in (4) yields,

$$\begin{cases} Ax^* = y^* \\ A^T(y^* - z) = 0 \end{cases} \tag{5}$$

The "normal equations" are obtained by further simplifying (5),

Proposition 1 (Normal Equations)
For all $A \in \mathbb{R}^{m \times n}$, the normal equations

$$A^T A x^* = A^T z , \tag{6}$$

are necessary and sufficient conditions for x^* to be a solution of (1). There is at least one x^* solution of (6). If A defines an injective mapping, x^* is unique.

proof : The necessary and sufficient conditions are proved by (4). The right hand side of the linear system (6) is orthogonal to $\mathrm{Ker}A^T A$, therefore the system has at least one solution. Finally, if A is injective, $\mathrm{Ker}A = 0$, and $A^T A$ is nonsingular. □

2.2.3 Interpretation as projection

By definition, minimizing (3) defines an orthogonal projection of z onto the image space of the model $\mathrm{Im}A$ ($\mathrm{Im}f$ in general) parallel to $\mathrm{Ker}A^T$. The projector, $P_{\mathrm{Im}f}$ is written P_1 for ease of notation. The set of solutions of (1) is $\mathcal{X} = \{x \in S \mid Ax = P_1 z$. If A defines an injective mapping, $A^T A$ is nonsingular, and P_1 can be explicited from (6) as,

$$y^* = P_1 z = Ax^* = A(A^T A)^{-1} A^T z \ . \tag{7}$$

More generally, for all A, equations (6) show that the residual $r = Ax - z$ is orthogonal to $\mathrm{Im}A$:

Proposition 2 (Normal Equations as projector onto $\mathrm{Im}A$)
For all $A \in \mathbb{R}^{m\times n}$, the minimization (1), or equivalently the normal equations (6), define an orthogonal projection P_1 of the data z onto $\mathrm{Im}A$ parallel to $\mathrm{Ker}A^T$.

2.2.4 Other comments

The solution y^* of (3) is always unique because it is a projection on a linear subspace. For a linear injective mapping, the parameter estimate x^* of the least squares problem (1), or equivalently (6), is unique. If A is noninjective, x^*, a parameter estimate, is defined up to a vector $u \in \mathrm{Ker}A$, $y^* = Ax^* = A(x^* + u)$.

Note that, in practice, one should not attempt to solve any of the above equations, but rather use orthogonal decompositions (QR on A, cf. [6]) or the pseudo-inverse of A (cf. section 2.4).

2.3 Minimum Norm Least Square and Linear Surjective Mapping

2.3.1 Optimization problem

We now consider linear models such that many choices of parameters can yield the "experimental response", z: there is x, non unique, such that $Ax = z$. Linear surjective mappings are an example of such mappings. Surjective mappings might result from a lack of experimental data: A is such that $m \leq n$ and $\mathrm{Rank}A = m$.

For linear surjective models, the solution to problem (1) is not unique, or, (6) is an underdetermined system: In fact, there is an infinite number of parameter sets $x \in \mathcal{X}$ such that $Ax = z$. That is, parameters are not identifiable from output least squares minimization.

Uniqueness is recovered by introducing a priori knowledge on x through problem (2). (1) and (2) can be formulated in the current context as,

$$\begin{cases} \min_{x\in S} \ \frac{1}{2}||x||^2, \\ \text{such that } Ax = z \ . \end{cases} \tag{8}$$

2.3.2 Optimality conditions

This constrained optimization problem is convex. Necessary and sufficient optimality conditions are,

$$\left\{ \begin{array}{rcl} Ax^* & = & z \\ x^* + A^T \lambda^* & = & 0 \end{array} \right. \tag{9}$$

where λ^* is an m-dimensional vector of Kuhn and Tucker multipliers associated to the constraints of (8).

2.3.3 Interpretation as projection

Problem (8) defines a projection of the null vector onto the vector space of solutions of $Ax = z$. Solving problem (2), or (8), can also be interpreted as projecting any x optimum of the least squares problem ($Ax = z$) onto $\mathrm{Im} A^T$ parallel to $\mathrm{Ker} A$. This projector, $P_{\mathrm{Im} A^T}$, that we write P_2, can be explicited for surjective mappings. One multiplies the last equation of (9) by A. Since A is surjective, AA^T is nonsingular, and λ^* is unique,

$$\lambda^* = -(AA^T)^{-1} Ax \ . \tag{10}$$

Substituting back in the last equation of (9), one obtains,

$$x^* = P_2 x = A^T (AA^T)^{-1} Ax \Rightarrow P_2 = A^T (AA^T)^{-1} A \ . \tag{11}$$

2.3.4 Other comments

If the model is surjective, solving (2) (equivalently (8) or (11)) provides the unique minimum norm solution to the least squares problem. Note that in practice, use of an orthogonal decomposition of A^T (QR method, see [6]) or of the pseudo-inverse (cf. next section) is prefered.

2.4 General Linear Mapping

2.4.1 Optimization problem

In the general case, the mapping performed by A is neither injective nor surjective. There might not be a parameter set such that $Ax = z$, so one resorts to the least squares formulation (1). On the other hand, many parameters $x \in \mathcal{X}$ might solve (1), making the minimum norm problem (2) useful for identifiability. The most general strategy is a composition of output and minimal norm least squares:

$$\left\{ \begin{array}{l} \min_{x \in S} \ \frac{1}{2} ||x||^2, \\ \text{such that } Ax = P_1 z \ . \end{array} \right. \tag{12}$$

One seeks the minimum norm parameter that satisfies the normal equations (expressed as a projection), i.e., that is an optimum of the least squares minimization. Problem (12) is the same as problem (2), with $\mathcal{X}$ defined as a projection.

Proposition 3
The solution x^* of (12) exists and is unique.

proof : The optimization problem (12) is strictly convex, and $\mathcal{X}$ is not empty, from Proposition 1. □

Definition 1
The pseudo-inverse of A, $A^\dagger$, is the matrix such that $x^* = A^\dagger z$, where x^* is the minimal norm least squares solution of (12).

2.4.2 Optimality conditions

The necessary and sufficient optimality conditions of the constrained problem (12) are,

$$\left\{ \begin{array}{rcl} Ax^* & = & P_1 z \\ x^* + A^T \lambda^* & = & 0 \end{array} \right. \tag{13}$$

where λ is an m-dimensional vector of Kuhn and Tucker multipliers associated to the constraints. Equations (13) uniquely define x^*. Note that λ^* is not uniquely defined if $\mathrm{Ker}A^T \neq \{0\}$, which is equivalent to having gradients of the constraints in (12) linearly dependent. The optimality system can be further expanded using the definition of the projector P_1 from (5) and (7),

$$\left\{ \begin{array}{rcl} P_1 z & = & y^* \\ A^T(P_1 z - z) & = & 0 \end{array} \right. \tag{14}$$

to yield,

$$\left\{ \begin{array}{rcl} Ax^* & = & y^* \\ A^T(y^* - z) & = & 0 \\ x^* + A^T \lambda^* & = & 0 \end{array} \right. \tag{15}$$

2.4.3 Interpretation as projection

Problem (12) (or (2)) defines two successive orthogonal projections,

1. P_1 of z onto $\mathrm{Im}A$
2. P_2 of any $x \in \mathcal{X}$ (i.e., $Ax = P_1 z$) onto $\mathrm{Im}A^T$.

Features of the projections P_1 and P_2 described for injective and surjective models, respectively, carry on to the general case. The difference is that $A^T A$ and AA^T may be singular, so the projections cannot be written as (11) and (7).

2.4.4 Other comments

So far, principles of least squares minimization have been presented. In practice, algorithms do not attempt to solve directly the normal equations (6) which are not stable with respect to numerical errors. State-of-the-art solving of least squares problems is based on the pseudo-inverse of A, $A^\dagger$. Let A have r strictly positive singular values, $s_1 \geq s_2 \geq \ldots \geq s_r > 0$ ($\mathrm{Rank}A^T A = r$). The pseudo-inverse of A of Definition (1) is expressed as,

$$A^\dagger = V \begin{bmatrix} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{bmatrix} U^T , \tag{16}$$

where Σ_r^{-1} is a $r \times r$ diagonal matrix composed of s_i^{-1} terms. U and V are $m \times m$ and $n \times n$ orthogonal matrices, respectively. The columns u_i and v_i of U and V are the left and right singular vectors, respectively, associated to singular values of A, s_i, $i = 1, r$. The singular vectors v_i associated to null singular values define a parameter subspace with the same model output, i.e., $\{v_{r+1}, \ldots, v_n\} = \mathrm{Ker}A$. Details on orthogonal decompositions of A, through which $A^\dagger$ is calculated, can be found in [1] and [6]. Once $A^\dagger$ is calculated, for any A, the minimal norm solution of (1) is readily obtained,

$$x^* = A^\dagger z . \tag{17}$$

(see [1] for a proof). It is important to realize that there is no need to perform a singular value decomposition of A to obtain $A^\dagger$. Only two QR decompositions are needed, which is numerically more efficient than a singular value decomposition ([6]).

2.5 Nonlinear Model

Let $f(x)$ be a nonlinear, nonconvex model. Optimality conditions exposed earlier for linear models carry on by replacing A by ∇f. However, because the convexity argument may be lost, optimality conditions are necessary, but no longer sufficient. They characterize candidate optimal parameters. First order optimality conditions associated to the output least squares problem (3) yield,

$$\forall x^* \in \mathcal{X}\ , \quad \left\{ \begin{array}{rcl} f(x^*) & = & y^*, \\ \nabla f(x^*)^T (y^* - z) & = & 0 \ , \end{array} \right. \tag{18}$$

which shows that the residual at $x^* \in \mathcal{X}$, $r = y^* - z$, is orthogonal to $\mathrm{Im}\nabla f(x^*)$. (18) are the nonlinear normal equations. x^* really is a local minimum if $\nabla^2 J(x^*)$ (given in Equation (47)) is positive definite. A geometrical interpretation of the positive definitness of $\nabla^2 J(x)$ is given later (section 3.2.1).

Optimality conditions for a minimal norm least squares problem of the type (8) become, for a nonlinear model,

$$\left\{ \begin{array}{rcl} f(x^*) & = & z, \\ x^* + \nabla f(x^*)^T \lambda^* & = & 0 \ , \end{array} \right. \tag{19}$$

Finally, for a general nonlinear model, necessary optimality conditions of (12) are,

$$\left\{ \begin{array}{rcl} f(x^*) & = & y, \\ \nabla f(x^*)^T (y^* - z) & = & 0 \ , \\ x^* + \nabla f(x^*)^T \lambda^* & = & 0 \ . \end{array} \right. \tag{20}$$

Note that $x^* \in \mathrm{Im}\nabla f(x^*)^T$. A robust numerical method for solving least squares problems should tackle the system of equations (20). One shall see later in the text that Levenberg-Marquardt is such a procedure.

3 Sensitivity of Least Squares Estimates

Calculations are corrupted by experimental and numerical errors, inducing model and data changes. The generic term "sensitivity" designates measures of the influence of the errors on the identified model. Sensitivities concern either a change of least squares norm or a change of parameter estimate.

Sensitivities are calculated, first of all, in order to have a level of confidence in an identified model. But high sensitivities are also hints that numerical difficulties might occur during identification. It is therefore common practice to select experimental data as to minimize sensitivities.

In this section, different viewpoints are taken to describe sensitivities: parameters sensitivity, bounds for linear models, sensitivities in the model space (model curvatures). Relations between parameter and model sensitivities are presented.

3.1 Sensitivity of linear(ized) models to parameters

Singular values of $\nabla f(x)$ (equivalently, the square roots of the eigenvalues of $\nabla f(x)^T \nabla f(x)$) carry important and accessible information on the sensitivities. They fully describe sensitivities of linear models to parameter changes and provide valuable information when identifying moderatly nonlinear models (cf. discussion in section 4.4.1 on assessing model nonlinearities). Calculation of the singular values of $\nabla f(x)$ involves *i)* first order derivation of f, *ii)* either singular value decomposition of an $m \times n$ matrix, ∇f, or the method exposed in section 4.4.2. These steps have a low computational cost compared to sensitivities based on second order derivatives or statistical sampling of models.

3.1.1 Sensitivity of the model response to parameter changes along singular vectors

Let $(s_i\ ,\ v_i)$ be n pairs of singular values and singular vectors of $\nabla f(x)$. First order approximation of f is used,

$$f(x+\Delta x) \;=\; f(x) + \nabla f(x)\Delta x + \mathcal{O}(||\Delta x||^2)\ . \tag{21}$$

If the parameter perturbation is taken along one of the eigenvectors, $\Delta x \;=\; \alpha v_i$, $0 \;<\; \alpha \ll 1$, one has,

$$\frac{||f(x+\alpha v_i) - f(x)||^2}{||v_i||^2} \;=\; \alpha^2 s_i^2\ + \mathcal{O}(||\Delta x||^3)\ . \tag{22}$$

Singular vectors associated to null singular values show directions in the parameter space where, locally, the response of the model does not change. On the contrary, singular vectors associated to large singular values designate directions where the model is particularly sensitive to parameters changes.

For any parameter change, dx, the model sensitivity to parameters at x in the direction dx, $\mathcal{S}_x(dx)$, is defined as,

$$\mathcal{S}_x(dx) \;=\; \frac{dx^T \nabla f(x)^T \nabla f(x) dx}{dx^T dx} \;=\; \frac{\sum_{i=1}^n dx_i^2 s_i^2}{\sum_{i=1}^n dx_i^2}\ , \tag{23}$$

where dx_i is the ith component of dx in the (v_i) basis.

3.1.2 Acceptance region of parameter estimates

Let x^* be a parameter estimate obtained by minimizing the least squares norm J. Perturbed models $f(x^* + \delta x)$ are acceptable providing the error in terms of the norm J is below a certain threshold, the level of significance of the model, q,

$$J(x^* + \delta x) - J(x^*) \;\leq\; q\ . \tag{24}$$

Using a linear approximation of f in J, Equation (24) becomes,

$$\frac{1}{2}\delta x \nabla f(x^*)^T \nabla f(x^*) \delta x \;\leq\; q\ . \tag{25}$$

Parameters satisfying (25) describe an n dimensional ellipsoid whose surface S is,

$$S \;=\; const \left(\frac{q^n}{\det(\nabla f(x^*)^T \nabla f(x^*))} \right)^{1/2} \;=\; const \left(\frac{q^n}{\Pi_{i=1}^n s_i^2} \right)^{1/2} . \tag{26}$$

The product of the singular values of ∇f characterizes the surface of acceptable parameters for a linear or linearized model.

3.1.3 Sensitivity bounds based on perturbation theory

We review in this section bounds on parameter and residual norms found in [5] and [17]. They are based on perturbation theory of linear models. Results apply to all methods for solving minimum norm least squares (including Levenberg-Marquardt).

The condition number of A is $cond(A) \;=\; ||A||\,||A^\dagger|| \;=\; s_1/s_r$.

Under the assumptions that $\eta \;=\; cond(A)||E||/||A|| \;<\; 1$, Rank$(A + E) \;=\;$ Rank$A$, and the perturbed problem is,

$$(x + \Delta x) \;=\; (A+E)^\dagger (z + \Delta z)\ , \tag{27}$$

the following bounds are given in [1],

$$
\begin{aligned}
\frac{||\Delta x||}{||x||} &\leq \frac{cond(A)}{1-\eta}\left(\frac{||E||}{||A||}+\frac{||\Delta z||}{||A||\,||x||}+cond(A)\frac{||E||\,||r||}{||A||^2||x||}\right)+ \\
&\quad cond(A)\frac{||E||}{||A||}\,, &(28)\\
\frac{||\Delta r||}{||z||} &\leq \frac{||E||\,||x||}{||z||}+\frac{||\Delta z||}{||z||}+cond(A)\frac{||E||}{||A||\,||z||}\,, &(29)
\end{aligned}
$$

where Δr is the change in residual between the perturbed and the orignal problem. A term in $cond(A)^2$ occurs in Equation (28), indicating a potentially high sensitivity to errors for large condition numbers. It is however multiplied by $||E||\,||r||$ which often reduces its influence. If the mapping associated to A is surjective ($||r|| = 0$), the term in $cond(A)^2$ cancels out.

The sensitivity of normal equations to round off errors motivates the use of pseudo-inverse for solving (1) and (2), $x = A^{\dagger}z$. Indeed, numerical errors occuring in the product A^TA are proportionnal to s_1^2. One can then show ([5]) that $\frac{||\Delta x||}{||x||}$ is bounded by $cond^2(A)$ without the damping effect of the product with the residual.

3.2 Sensitivities of nonlinear models

3.2.1 Sensitivities to data changes

Proposition 4
Let x^* be a least squares parameter estimate associated to data z. A small perturbation of the data, δz, induces a change of parameter estimate δx^* such that,

$$\nabla^2 J(x^*)\delta x^* = \nabla f(x^*)^T \delta z\ . \tag{30}$$

Let the residual be denoted r, $r = f(x^*) - z$. σ_i and h_i, $i = 1,\ldots,n$, denote the principal curvatures and curvature directions of the model f, a normal to the model surface being $n_{x^*} = -r/||r||$ (cf. Appendix C). δz is decomposed into its parts in $\mathrm{Im}\nabla f(x^*)$ and $\mathrm{Ker}\nabla f(x^*)^T$, $\delta z = \nabla f(x^*)\delta z^0 + \delta z^1$, $\nabla f(x^*)^T\delta z^1 = 0$. Then, the components of δx^* and δz^0 in the (h_i) basis are related through,

$$\delta x_i^* = \frac{1}{1-||r||\sigma_i}\delta z_i^0\ . \tag{31}$$

<u>*proof :*</u> For ease of notation, we temporarily write x for x^*. Normal equations for the initial and perturbed problem are,

$$
\begin{aligned}
\nabla f(x)^T(f(x)-z) &= 0 &(32)\\
\nabla f(x+\delta x)^T(f(x+\delta x)-z-\delta z) &= 0 &(33)
\end{aligned}
$$

The equations are substracted,

$$
\begin{aligned}
&[\nabla f(x+\delta x)^T - \nabla f(x)^T]f(x+\delta x) + \nabla f(x)^T[f(x+\delta x)-f(x)] - \\
&\qquad [\nabla f(x+\delta x)^T - \nabla f(x)^T](z+\delta z) - \nabla f(x)^T\delta z = 0\ .
\end{aligned} \tag{34}
$$

We take the limit of (34) as δx tends to 0, neglecting second order terms and using finite difference formula. For example, the limit of the first term is,

$$
\begin{aligned}
&\lim_{\delta x\to 0}[\nabla f(x+\delta x)^T - \nabla f(x)^T]f(x+\delta x) = \\
&\lim_{\delta x\to 0}[\sum_{i=1}^m f_i(x+\delta x)(\nabla f_i(x+\delta x)^T - \nabla f_i(x)^T)] = \sum_{i=1}^m f_i(x)\nabla^2 f_i(x)\delta x\ .
\end{aligned} \tag{35}
$$

The limit of (34) is,

$$\sum_{i=1}^{m}(f_i(x)-z_i)\nabla^2 f_i(x)\delta x + \nabla f(x)^T \nabla f(x)\delta x \;=\; \nabla f(x)^T \delta z \;, \tag{36}$$

which proves (30).

The second part of the proposition is obtained by decomposing δx and δz in the (h_i) basis,

$$\delta x \;=\; \sum_{i=1}^{m} \delta x_i h_i \quad , \quad \delta z \;=\; \nabla f(x) \sum_{i=1}^{m} \delta z_i^0 h_i + \delta z^1 \;. \tag{37}$$

Reinjecting into (30), simplifying through by $\nabla f(x)^T \nabla f(x)$ and expressing component by component proves (31).

□

Graphical interpretations of Equations (30) and (31) are shown in Figure 3.2.1 when $m = 2$, $n = 1$ (since there is only one curvature, σ_1 is written σ). One readily sees that if the data change is perpendicular to the model tangent, i.e., in $\mathrm{Ker}\nabla f(x^*)^T$, the parameter estimate is unchanged. A case that exhibits an infinite number of solutions, $1/\sigma = ||r||$, is shown on the second plot. The third plot is an example where the normal equations are satisfied, but x^* is really a local maximum of the least squares norm. The fourth plot illustrates linear models. The more favorable case where $\sigma < 0$ is depicted on the fifth plot: x^* is unconditionnally a local minimum of the least squares distance and the parameter estimates are more stable than for positive curvatures since $0 < 1/(1-\sigma||r||) < 1$ in Equation (31).

The discussion on local minima / maxima of the least squares norm is now generalized to any n by means of the positive definiteness of $\nabla^2 J(x^*)$. The generalized curvature equation at x^* is (cf. Appendix C),

$$[\sum_{i=1}^{m} n_{x^*,i}\nabla^2 f_i(x^*)]h_j \;=\; G h_j \;=\; \sigma_j \nabla f(x^*)^T \nabla f(x^*) h_j \quad , \quad j=1,\ldots,n \;, \tag{38}$$

where $n_{x^*} = -r/||r||$ and (h_i) is the basis of the model principal directions. The Hessian of the least squares norm can be related to the principal curvatures,

$$\begin{aligned} h_i^T \nabla^2 J(x^*) h_i \;&=\; h_i^T(-||r||G + \nabla f(x^*)^T \nabla f(x^*)) h_i \;= \\ (1-||r||\sigma_j) h_i^T \nabla f(x^*)^T \nabla f(x^*)) h_i \;. \end{aligned} \tag{39}$$

$\nabla^2 J(x^*)$ is positive definite, i.e., x^* is a local minimum of $J(x)$, if,

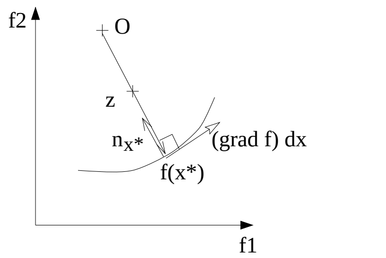
$$1-||r||\sigma_j \;>\; 0 \;,\; \forall\, j=1,\ldots,n \;\Leftrightarrow\; \max_{j=1,n} \sigma_j \;<\; 1/||r|| \;. \tag{40}$$

The curvature should be smaller than $1/||r||$ for x^* to be a minimum of $J(x)$. In particular, this is always true for negative curvatures.

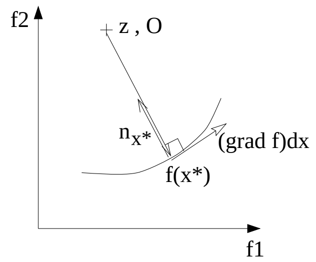
3.2.2 Parameters and model sensitivities

At a parameter estimate x^*, $\nabla J(x^*) = 0$. A relative change in J is dominated by second order terms,

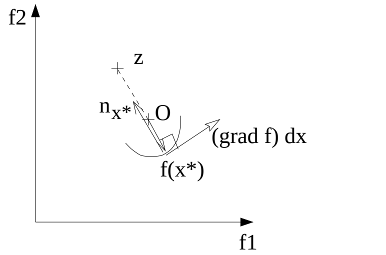
$$\begin{aligned} \frac{x^T \nabla^2 J(x^*) x}{x^T x} \;&=\; \left(1-||r||\frac{x^T G x}{x^T \nabla f(x^*)^T \nabla f(x^*) x}\right) \frac{x^T \nabla f(x^*)^T \nabla f(x^*) x}{x^T x} + \mathcal{O}(x) \\ &=\; [1-||r||\mathcal{C}_{x^*}(x)]\,\mathcal{S}_{x^*}(x) + \mathcal{O}(x) \;, \end{aligned} \tag{41}$$



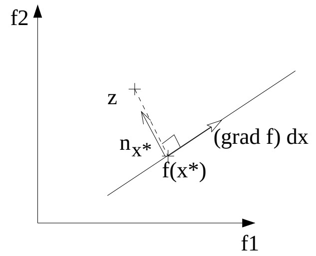
Local minimum, $\sigma > 0$, $1/\sigma > ||r||$, amplified perturbations since $1 < 1/(1-\sigma||r||) < \infty$.



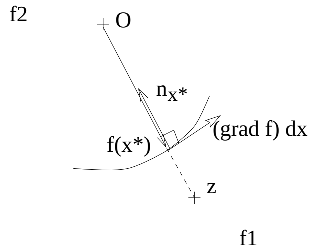
Infinity of solutions, $\sigma > 0$, $\sigma||r|| = 1$.



Local maximum, $\sigma > 0$, $1/\sigma < ||r||$.



Linear model, $\sigma = 0$, $\delta x^* = \nabla f(x^*)^\dagger \delta z$.



Local minimum, $\sigma < 0$, $1-\sigma||r|| > 1$, damped perturbations since $0 < 1/(1-\sigma||r||) < 1$.

Figure 1: Examples of model curvatures, $m = 2$, $n = 1$. O is the center of curvature.

where $\mathcal{S}_{x^*}(x)$ is the parameter sensitivity introduced in (23) and $\mathcal{C}_{x^*}(x)$ is a model normalized curvature (cf. (157) in Appendix C). (41) can be rewritten in the (v_i) and (h_i) bases using,

$$x = \sum_{i=1}^{n} x_{v,i} v_i \quad , \quad x = \sum_{i=1}^{n} x_{h,i} h_i \ , \tag{42}$$

$$\frac{x^T \nabla^2 J(x^*) x}{x^T x} = \left(1 - ||r|| \frac{\sum_{i=1}^n \sigma_i x_{h,i}^2}{\sum_{i=1}^n x_{h,i}^2}\right) \frac{\sum_{i=1}^n s_i^2 x_{v,i}^2}{\sum_{i=1}^n x_{v,i}^2} \ . \tag{43}$$

The first term of the right hand side of Equation (41) or (43) involves only model curvatures, σ_i, and is independent of a parameter change (for example, $x = D\bar{x}$ in scaling). It is a model sensitivity. The second term is independent of model curvatures but depends on the parameters choice through the s_i's. It is a parameter sensitivity. The overall sensitivity of the least squares norm at the optimum is the product of model and parameter sensitivities.

4 Levenberg-Marquardt algorithms

A general deterministic view of least squares problems has been presented. It now serves as framework for analyzing well-known, robust identification methods, Levenberg-Marquardt algorithms. Original techniques for deriving sensitivities based on Levenberg-Marquardt trajectory are proposed.

4.1 Principles of Levenberg-Marquardt algorithms

Levenberg-Marquardt methods are classically derived by sequentially linearizing $f(x)$ in problem (1). In order to maintain validity of the linearization, move limits on the variable x are added. At iteration k, the following subproblem is solved,

$$\left\{ \begin{array}{l} \min_{x \in S} J_L(x) \ = \ \frac{1}{2} ||(f(x_k) + \nabla f(x_k)(x - x_k) - z)||^2 \\ \text{such that } g(x) \ = \ \frac{1}{2}||x - x_k||^2 \ - \ \delta_k \ < \ 0 \end{array} \right. \tag{44}$$

First order necessary and sufficient conditions of optimality for (44) are the basis for the Levenberg-Marquardt algorithms,

$$(\nabla f(x_k)^T \nabla f(x_k) + \lambda_k I)(x - x_k) \ = \ - \nabla f(x_k)^T (f(x_k) - z) \ . \tag{45}$$

λ_k is the Lagrange multiplier associated to the constraint of (44). Different implementations of the Levenberg-Marquardt algorithm vary *i)* in the way λ_k (equivalently δ_k) is adjusted at each iteration, *ii)* in the way the linear system (45) is solved, *iii)* in the way relation (45) is scaled. Implementations based on QR decomposition are usually preferred because they are less sensitive to round-off errors (cf. [12], [5]).

Levenberg-Marquardt iterations can be interpreted also with respect to the gradient and Hessian of the least squares norm $J(x)$,

$$\nabla J(x)^T \ = \ \nabla f(x)^T (f(x) - z) \ , \tag{46}$$

$$\nabla^2 J(x) \ = \ \nabla f(x)^T \nabla f(x) \ + \ \sum_{i=1}^{m} \nabla^2 f_i(x)(f_i(x) - z_i) \ . \tag{47}$$

If the rightmost term of Equation (47) can be neglected (which occurs when the residual $(f_i(x) - z_i)$ is small with respect to $\nabla^2 f_i(x)$), and if λ_k is small, Levenberg-Marquardt resembles a quasi-Newton method. If λ_k is large, Levenberg-Marquardt tends to a steepest descent method,

$$\lim_{\lambda_k \to \infty} (x - x_k) \;=\; -\frac{\nabla J(x_k)^T}{\lambda_k} \;. \tag{48}$$

We now study convergence using (1) and (2), first for linear models, and next in general.

4.2 Convergence in the linear case

We study Levenberg-Marquardt algorithms when identifying the parameters x of a linear model $f(x) \;=\; Ax$.

4.2.1 A smallest norm least squares minimizer

Proposition 5 (Convergence of Levenberg-Marquardt, linear model) *Suppose the Levenberg-Marquardt process converges to x^*. Then $x^* \;=\; A^\dagger z$, i.e., it is solution of smallest norm least squares problems (1) and (2).*

<u>*proof :*</u> Convergence of x to x^* in Equation (45) yields,

$$(\nabla f(x^*)^T \nabla f(x^*) + \lambda_k I)(x^* - x^*) \;=\; 0 \;=\; -\nabla f(x^*)^T (f(x^*) - z) \;, \tag{49}$$

which are the normal equations, $A^T A x^* \;=\; A^T z$, necessary and sufficient conditions for x^* to be solution of (1).

The second part of the proof is carried out by reccurence. The algorithm is started at $x_0 \;=\; 0$. Then,

$$\begin{aligned} x_1 &= (A^T A + \lambda_0 I)^{-1} A^T z \\ &= A^T (A A^T + \lambda_0 I)^{-1} z \;, \end{aligned} \tag{50}$$

where use was made of the fact that $(A^T A + \lambda I)^{-1} A^T \;=\; A^T (A A^T + \lambda I)^{-1}$, which can be easily seen by multiplying on the left by $(A^T A + \lambda I)$ and on the right by $(A A^T + \lambda I)$. Equation (50) shows that $x_1 \;\in\; \mathrm{Im} A^T$. Suppose now that $x_k \;\in\; \mathrm{Im} A^T$. Then,

$$\begin{aligned} x_{k+1} &= x_k - (A^T A + \lambda_k I)^{-1} A^T (A x_k - z) \\ &= x_k - A^T (A A^T + \lambda_k I)^{-1} (A x_k - z) \;, \end{aligned} \tag{51}$$

so that $x_{k+1} \;\in\; \mathrm{Im} A^T$. At convergence, $x^* \;\in\; \mathrm{Im} A^T$, and since the normal equations are also satisfied by x^*, the necessary and sufficient conditions for x^* to solve problem (2), equations (15), are satisfied. □

In the linear case, Levenberg-Marquardt algorithms performs the two fundamental projections that guarantee a unique parameter estimate.

4.3 Convergence in the nonlinear case

For general nonlinear models, one cannot expect finding better than local minima of the least squares norm using a gradient based search procedure such as Levenberg-Marquardt. It is easy to think of nonlinear functions with misleading slope lines near x_0 that take the search to a local optimum, away from the global optimum.

In terms of local optimum determination for continuously differentiable models f, we shall see next that Levenberg-Marquardt defines a a robust minimization process.

4.3.1 A Robust Minimization Scheme

Propositions 6 and 7 prove that Levenberg-Marquardt will not fail finding a descent direction, unless x is a local optimum.

Proposition 6
$\forall\lambda > 0$, $\nabla f^T \nabla f + \lambda I$ is positive definite.

proof : $x^T(\nabla f^T \nabla f + \lambda I)x \;=\; x^T \nabla f^T \nabla f x + \lambda x^T x \;=\; ||\nabla f x||^2 + ||x||^2 \;>\; 0 \quad \forall\, x \neq 0.$
□
Proposition 6 guarantees that (45) can be solved since $(\nabla f(x_k)^T \nabla f(x_k) + \lambda_k I)$ is non singular.

Proposition 7
For any continuous bounded function f, Equation (45) defines a descent direction.

proof : $\nabla J(x_k)^T(x - x_k) \;=\; -\nabla J(x_k)^T(\nabla f(x_k)^T \nabla f(x_k) + \lambda_k I)^{-1}\nabla J(x_k) \;<\; 0$ because $(\nabla f(x_k)^T \nabla f(x_k) + \lambda_k I)$, hence its inverse, is positive definite. □
As λ_k increases, the size of the step $||x - x_k||^2$ decreases. At each iteration, because the Levenberg-Marquardt direction is a descent direction, there exists a λ_k such that $J(x) \;<\; J(x_k)$, unless x_k is a stationary point, $\nabla J(x_k) \;=\; 0$.

On a theoretical point of view, global convergence results of the Levenberg-Marquardt method have been established ([12],[14]). For example in [12], it is proved that, if f is continuously differentiable, $J(x_k)$ is bounded, and ∇f is uniformly continuous, the Levenberg-Marquardt method converges to a stationary point,

$$\lim_{k \to \infty} ||\nabla J(x_k)||^2 \;=\; 0 \;. \tag{52}$$

The normal equations are therefore satisfied at convergence,

$$\nabla f(x^*)^T(f(x^*) - z) \;=\; 0 \;. \tag{53}$$

It can also be obtained by substituting x^* into Equation (45). However, in general, a minimum norm solution is not reached.

4.3.2 Interpretation of Levenberg-Marquardt as a linearization and regularization scheme

Further insight into the convergence of Levenberg-Marquardt algorithm is obtained by interpreting each iteration (45) of the process in terms of linearized and regularized subproblems.

Proposition 8
Each iteration of the Levenberg-Marquardt algorithm is equivalent to solving a linearized constrained optimization problem. It is also equivalent to a linearized and regularized optimization problem.

proof : The first part of the proof is the way Levenberg-Marquardt was introduced in (44) and (45). Optimality conditions of the problem,

$$\min_{x \,\in\, S} \frac{1}{2}||(f(x_k) + \nabla f(x_k)(x - x_k) - z)||^2 \;+\; \lambda_k \frac{1}{2}||x - x_k||^2 \;, \tag{54}$$

are given by Equation (45), which proves the second statement. λ_k is the regularization factor. □

Proposition 9
At each iteration of the Levenberg-Marquardt algorithm, the linearized problem on a sphere of radius $||x_{k+1} - x_k||$ is solved:

$$\left\{ \begin{array}{l} \min_{x \in S} \frac{1}{2}||(f(x_k) + \nabla f(x_k)(x - x_k) - z)||^2 \\ \textit{such that } \frac{1}{2}||x - x_k||^2 \ < \ \frac{1}{2}||x_{k+1} - x_k||^2 \end{array} \right. \tag{55}$$

<u>*proof :*</u> Proposition 9 was originally given in [10]. Levenberg-Marquardt algorithm solves the necessary and sufficient optimality conditions at each iteration and the Hessian matrix, $(\nabla f(x_k)^T \nabla f(x_k) + \lambda_k I)$ is positive definite. □

Let x_L^* denote the optimum of the linearized output least squares at iteration k:

$$x_L^* \ = \ \arg \min_{x \ \in \ S} J_L(x) \ = \ \arg \min_{x \ \in \ S} ||(f(x_k) + \nabla f(x_k)(x - x_k) - z)||^2 \ . \tag{56}$$

The algorithm does not "overshoot" x_L^*:

Proposition 10
Convergence to the optimum of the linearized problem is performed from within the sphere centered on x_k and of radius $||x_L^* - x_k||$,

$$||x_{k+1} - x_k|| \ \leq \ ||x_L^* - x_k|| \ . \tag{57}$$

<u>*proof :*</u> x_L^* is solution of the linearized output least squares, therefore,

$$J_L(x_L^*) + \frac{\lambda_k}{2}||x_{k+1} - x_k|| \ \leq \ J_L(x_{k+1}) + \frac{\lambda_k}{2}||x_{k+1} - x_k|| \ . \tag{58}$$

x_{k+1} is solution of the linearized regularized problem,

$$J_L(x_{k+1}) + \frac{\lambda_k}{2}||x_{k+1} - x_k|| \ \leq \ J_L(x_{x_L^*}) + \frac{\lambda_k}{2}||x_L^* - x_k|| \ . \tag{59}$$

Equations (58) and (59) together prove (57). □

4.3.3 Levenberg-Marquardt's trajectory

The trajectory followed by the Levenberg-Marquardt algorithm approximates the steepest slope line $s(t)$, solution of,

$$\left\{ \begin{array}{lcl} \frac{ds}{dt} & = & - \nabla J(s)^T \ , \\ s(0) & = & x_0 \ , \end{array} \right. \tag{60}$$

where t is the independent variable. In fact, Levenberg-Marquardt performs a semi-implicit numerical integration of the ordinary differential equations (60).
<u>*proof :*</u> Implicit Euler integration applied to Equation (60) yields,

$$s_{t+1} - s_t \ = \ - \Delta t \ \nabla J(s_{t+1})^T \ . \tag{61}$$

We now approximate $\nabla J(s_{t+1})^T$ as in (47), neglecting second order term ($\sum_{i=1}^m \nabla^2 f_i(x)(f_i(x) - z_i)$ is small),

$$\frac{1}{\Delta t}(s_{t+1} - s_t) \ = \ - \nabla J(s_t)^T - \nabla f(s_t)^T \nabla f(s_t)(s_{t+1} - s_t) \ , \tag{62}$$

or,

$$(\nabla f(s_t)^T \nabla f(s_t) + \frac{1}{\Delta t})(s_{t+1} - s_t) \;=\; -\nabla J(s_t)^T \;, \tag{63}$$

which is equivalent to Equation (45) with $\lambda_k = 1/\Delta t$. $\square$
Semi-implicit integration procedures are usually stable. Therefore, Levenberg-Marquardt will most often follow the steepest descent line on J. An example of the trajectory followed by Levenberg-Marquardt is given in Figure 7. One sees that contour lines are cut perpendicularly, especially for large λ's.

4.4 Sensitivities estimation using Levenberg-Marquardt

Sensitivity analysis of least squares problems has been related earlier in this text to 2 fundamental quantities, the model curvatures (σ_i or $\mathcal{G}_x(dx)$, cf. Appendix C) and parameter sensitivities (s_i^2 or $\mathcal{S}_x(dx)$). We shall see how Levenberg-Marquardt's iterates give access, under certain conditions, to elements of those sensitivities.

4.4.1 Model curvatures, λ_k variations and sensitivity analysis

A relation between λ_k, the Lagrange multiplier of the Levenberg-Marquardt method, the model curvatures and singular values of ∇f is exhibited.

Proposition 11 (λ_k lower bound)
In a neighbourhood of x^*, a Levenberg-Marquardt iteration reduces the least squares norm if,

$$\lambda_k \;>\; -\frac{1}{2} s_1^2 (1 + ||r|| \min_i(\sigma_i)) \;. \tag{64}$$

In particular, if,

$$-\frac{1}{||r||} \;<\; \min_i(\sigma_i) \qquad \textit{and} \qquad \max_i(\sigma_i) \;<\; \frac{1}{||r||} \;, \tag{65}$$

Levenberg-Marquardt converges to a local minimum with

$$\lim_{k \to \infty} \lambda_k \;=\; 0 \;. \tag{66}$$

<u>*proof :*</u> An iteration of Levenberg-Marquardt is described by,

$$(x_{k+1} - x_k) \;=\; -[\nabla f(x_k)^T \nabla f(x_k) + \lambda_k I]^{-1} \nabla f(x_k)^T (f(x_k) - z) \;. \tag{67}$$

Second order Taylor expansion of $J(x_{k+1})$ is used,

$$\begin{aligned} J(x_{k+1}) - J(x_k) \;=\;& \nabla J(x_k)(x_{k+1} - x_k) + \frac{1}{2}(x_{k+1} - x_k)^T \nabla^2 J(x_k)(x_{k+1} - x_k) \\ & + ||x_{k+1} - x_k||^2 \mathcal{O}(x_{k+1} - x_k) \;. \end{aligned} \tag{68}$$

Expanding terms,

$$\begin{aligned} J(x_{k+1}) - J(x_k) \;=\;& (f(x_k) - z)^T \nabla f(x_k)(x_{k+1} - x_k) + \\ & \frac{1}{2}(x_{k+1} - x_k)^T [\nabla f(x_k)^T \nabla f(x_k) - ||r|| \sum_{i=1}^{m} \frac{-r_i}{||r||} \nabla^2 f_i(x_k)](x_{k+1} - x_k) \\ & + ||x_{k+1} - x_k||^2 \mathcal{O}(x_{k+1} - x_k) \;. \end{aligned} \tag{69}$$

(67) in (69) yields,

$$
\begin{aligned}
J(x_{k+1}) - J(x_k) \ = \ & -(x_{k+1}-x_k)^T[\nabla f(x_k)^T \nabla f(x_k) + \lambda_k I](x_{k+1}-x_k) \\
& + \frac{1}{2}(x_{k+1}-x_k)^T[\nabla f(x_k)^T \nabla f(x_k) - ||r|| \sum_{i=1}^{m} \frac{-r_i}{||r||} \nabla^2 f_i(x_k)](x_{k+1}-x_k) \\
& + ||x_{k+1}-x_k||^2 \mathcal{O}(x_{k+1}-x_k) \ .
\end{aligned}
\tag{70}
$$

This Equation and the descent condition $J(x_{k+1}) < J(x_k)$ provide a lower bound on λ_k,

$$
\begin{aligned}
\lambda_k \ > \ & -\frac{1}{2}\frac{(x_{k+1}-x_k)^T \nabla f(x_k)^T \nabla f(x_k)(x_{k+1}-x_k)}{(x_{k+1}-x_k)^T(x_{k+1}-x_k)} \\
& \left(1 + ||r|| \frac{(x_{k+1}-x_k)^T(\sum_{i=1}^{m} -r_i/||r|| \nabla^2 f_i(x_k))(x_{k+1}-x_k)}{(x_{k+1}-x_k)^T \nabla f(x_k)^T \nabla f(x_k)(x_{k+1}-x_k)}\right) \\
& + \mathcal{O}(x_{k+1}-x_k) \ .
\end{aligned}
\tag{71}
$$

Near x^*, $-r_i/||r|| \approx n_{x,i}$. Introducing model parameter sensitivity $\mathcal{S}_{x^*}(x_{k+1}-x_k)$ (23) and model normalized curvature $\mathcal{C}_{x^*}(x_{k+1}-x_k)$ (cf. (41) or (157)), the descent condition is,

$$
\lambda_k \ > \ -\frac{1}{2}\mathcal{S}_{x^*}(x_{k+1}-x_k)[1 + ||r||\mathcal{C}_{x^*}(x_{k+1}-x_k)] \ . \tag{72}
$$

By definition, $\mathcal{S}_{x^*} \ > \ 0$. If $\mathcal{C}_{x^*}(x_{k+1}-x_k) \ > \ -1/||r||$, any choice of $\lambda_k \ \geq \ 0$ is suitable. The most critical case of (72) is (64). Equations (40) and (72) prove the end of the proposition. □

Condition (65) is satisfied by linear models which converge to x^* with vanishing λ_k. There is another interpretation of vanishing λ_k's with linear models: λ_k is the Lagrange multiplier of the optimization problem (44). Its value is the ratio,

$$
\lambda_k \ = \ \lim_{\Delta\delta_k \ \to \ 0} -\frac{\Delta J_L(x)}{\Delta \delta_k} \ . \tag{73}
$$

There are two ways Levenberg-Marquardt converges : either the move limits given by $g(x)$ stop being active, $\Delta J_L(x)$, thus λ_k, tend to 0, or the model is nonlinear at x^* and the move limits remain active at the optimum. For a linear model, the move limit is useless, and the adaptation of λ_k (cf. algorithm in section 5) make it vanish.

Since Levenberg-Marquardt attempts to reduce λ_k as long as condition (71) is satisfied and λ_k is positive, λ_k can be approximated by λ_k^e,

$$
\lambda_k^e \ = \ \max(0, \lambda_k^s) \ , \tag{74}
$$

with,

$$
\begin{aligned}
\lambda_k^s \ = \ & -\frac{1}{2}\frac{(x_{k+1}-x_k)^T \nabla f(x_k)^T \nabla f(x_k)(x_{k+1}-x_k)}{(x_{k+1}-x_k)^T(x_{k+1}-x_k)} \\
& \left(1 + ||r|| \frac{(x_{k+1}-x_k)^T(\sum_{i=1}^{m} -r_i/||r|| \nabla^2 f_i(x_k))(x_{k+1}-x_k)}{(x_{k+1}-x_k)^T \nabla f(x_k)^T \nabla f(x_k)(x_{k+1}-x_k)}\right) \ .
\end{aligned}
\tag{75}
$$

Conversly, taking λ_k as an approximation to λ_k^e, providing $\lambda_k^e \ > \ 0$, is a way to estimate a measure of the model's curvature, $\mathcal{C}_{x^*}(x_{k+1}-x_k)$, free of any extra computation,

$$
\mathcal{C}_{x^*}(x_{k+1}-x_k) \ = \ \lim_{k \to \infty} \frac{-(\mathcal{S}_{x^*}(x_{k+1}-x_k) + 2\lambda_k)}{||r||\mathcal{S}_{x^*}(x_{k+1}-x_k)} \ . \tag{76}
$$

If λ_k^s is negative, for example when model curvatures are positive, it is not possible to estimate model curvatures using (76) because $\lambda_k^e = 0$.

4.4.2 Parameter sensitivity estimation

For a linear model, Levenberg-Marquardt iterates provide all necessary information for calculating singular values and vectors of A, s_i^2 and v_i. Parameter sensitivities such as described in section 3.1 can then be computed.

Proposition 12 (Singular Value Analysis by Levenberg-Marquardt)
For a linear model, $y = Ax$, fitted to z by means of the Levenberg-Marquardt algorithm, the smallest nonzero singular value of A, s_r, and the associated right singular vector, v_r, are given by the limits,

$$\lim_{k\to\infty} \frac{[x_{k+1} - x_k]}{||x_{k+1} - x_k||} = v_r \ , \tag{77}$$

$$\lim_{k\to\infty} \frac{||A(x_{k+1} - x_k)||^2}{||x_{k+1} - x_k||^2} = s_r^2 \ . \tag{78}$$

<u>*proof :*</u> Recall the convention of Equation (16), $s_1 \geq s_2 \geq \dots \geq s_r > 0$, $s_{r+1} = \dots = s_n = 0$ and $\{v_{r+1}, \dots, v_n\} = \mathrm{Ker}A$. The fundamental relation (45) is written for 2 consecutive iterations,

$$x_{k+1} = x_k - (A^TA + \lambda_k I)^{-1}A^T(Ax_k - z) \ , \tag{79}$$

$$x_k = x_{k-1} - (A^TA + \lambda_{k-1} I)^{-1}A^T(Ax_{k-1} - z) \ . \tag{80}$$

Substracting yields,

$$(A^TA + \lambda_k)d_{k+1} - \lambda_{k-1}d_k = 0 \ , \tag{81}$$

where $d_k = x_k - x_{k-1}$. We project d_k in the right singular vectors basis,

$$d_k = \sum_{i=1}^{n} d_{i,k} v_i \ . \tag{82}$$

Equation (81), when written for each component in the singular vectors basis, can be solved for $d_{i,k+1}$,

$$d_{i,k+1} = \left(\frac{\lambda_{k-1}}{s_i^2 + \lambda_k}\right) d_{i,k} \ . \tag{83}$$

Let us first consider null singular values, $s_{r+1} = \dots = s_n = 0$. It has been shown in Equation (51) that $x_k \in \mathrm{Im}A^T \Rightarrow d_k \perp \mathrm{Ker}A \Rightarrow d_{i,k} = 0 \ , \ k = r+1, \dots, n$. The steps taken by the Levenberg-Marquardt method do not have any component in $\mathrm{Ker}A$. Ratio (77) will not have any component along v_i, $i = r+1, \dots, n$. Equation (83) shows that the larger s_i^2, the faster $d_{i,k}$ tends to 0. The last steps taken by Levenberg-Marquardt are dominated by $d_{r,k}$, for all histories of λ_k's. This is proved by studying the ratio,

$$R_{i,k} = \frac{d_{i,k}}{d_{r,k}} = \frac{s_r^2 + \lambda_{k-1}}{s_i^2 + \lambda_{k-1}} \frac{d_{i,k-1}}{d_{r,k-1}} \quad , \quad i = 1, \dots, r \ . \tag{84}$$

Since the smallest nonzero singular value is s_r, $\frac{s_r^2+\lambda_{k-1}}{s_i^2+\lambda_{k-1}} < 1$, $i < r$, and,

$$\lim_{k\to\infty} R_{i,k} = 0 \ , \ i < r \ . \tag{85}$$

One can use $d_k/||d_k||$ as an improving approximation to v_r. Note that it is necessary also for d_0 to have a component along v_r. Otherwise, $d_k/||d_k||$ tends to $v_{r'}$ such that $s_{r'}$ is the smallest nonzero singular value of A and d_0 has a component along $v_{r'}$.

We express the ratio of the limit (78) in the (v_i) basis,

$$\frac{||A(x_k - x_{k-1})||^2}{||x_k - x_{k-1}||^2} \;=\; \frac{d_k^T A^T A d_k}{d_k^T d_k} \;=\; \frac{\sum_{i=1}^r s_i^2 d_{i,k}^2}{\sum_{i=1}^r d_{i,k}^2} \; . \tag{86}$$

Dividing the numerator and the denominator by $d_{r,k}^2$, and applying (85),

$$\lim_{k\to\infty} \frac{||A(x_k - x_{k-1})||^2}{||x_k - x_{k-1}||^2} \;=\; \lim_{k\to\infty} \frac{\sum_{i=1}^r s_i^2 R_{i,k}^2}{\sum_{i=1}^r R_{i,k}^2} \;=\; s_r^2 \; . \tag{87}$$

□

From the d_k's, it is possible to estimate values of other singular values and associated singular vectors by removing the influence of already determined (s_i, v_i)'s. For example, to determine the second nonzero smallest singular value and associated singular vector, one forms,

$$d'_k \;=\; d_k - (d_k^T v_r) d_k \; , \tag{88}$$

which tends to v_{r-1}. The ratio of (78) can then be used with d' instead of d to estimate s_{r-1}^2. The procedure can be repeated to obtain further singular values and vectors. Note that such backtracking process is particularly sensitive to round off errors at the end of the search where the contributions of large magnitude singular modes have almost entirely vanished from the d_k's. However, plots of the results will typically exhibit stable regions which can be taken as reasonable estimations of the (s_i, v_i)'s. The stability regions occur at times ordered according the magnitude of the singular values. The time of convergence that should be used to assess s_1 comes before stability of the ratios characterizing s_2, etc.

For linear models, another ratio characterises the smallest non-zero singular value of A. To derive it, we first multiply Equation (45) by d_k^T and solve for λ_k:

$$\lambda_k \;=\; -\frac{d_k^T \nabla f(x_k)^T \nabla f(x_k) d_k}{d_k^T d_k} \;-\; \frac{d_k^T \nabla f(x_k)^T (f(x_k) - z)}{d_k^T d_k} \; . \tag{89}$$

As discussed in section 4.4.1, λ_k vanishes when identifying a linear model. In Equation (89), one knows from Proposition 12 that the first part of the right hand side tends to $-s_r^2$. When λ_k tends to 0, the second term in (89) converges to s_r^2,

$$\lim_{k\,\to\,\infty} -\frac{d_k^T \nabla f(x_k)^T (f(x_k) - z)}{d_k^T d_k} \;=\; s_r^2 \; . \tag{90}$$

Practically, it is advised to use ratio (78) rather than ratio (90) to estimate s_r because it converges faster (it does not depend on λ_k's convergence).

There is a special case that is worth being mentionned where estimation of the largest singular value s_1^2 is considerably simplified: $s_1^2 \;>>\; s_i^2 \;,\; i \;>\; 1$. We write $z \;=\; Ax^* + z_1,\; z_1 \;\in\; \mathrm{Ker}A^T$.

$$(A^T A + \lambda_0 I) d_1 \;=\; -A^T(Ax_0 - z) \;=\; A^T A(x^* - x_0) \; . \tag{91}$$

Solving for the components of d_1, the first step, in the basis of the singular vectors (v_i), gives,

$$d_{1,i} \;=\; \frac{s_i^2}{s_i^2 + \lambda_0}(x^* - x_0)_i \; . \tag{92}$$

$d_{1,i}$ is an increasing function of s_i^2. If $s_1^2 >> s_i^2$, $i \neq 1$, ratios (77) and (78) are approximations to v_1 and s_1^2, respectively.

Proposition 12 for estimating singular values of ∇f, i.e., characterizing parameter sensitivities, is rigourous for linear models. It also applies to moderatly nonlinear models (cf. experiments given in sections 5.2 and 5.3.4). Near x^*, a model is said to be moderatly nonlinear if it satisfies conditions (65).

In practice, variations of λ_k reveal if the model is sufficiently linear to use Equations (77) and (78). If the linear approximation to the model of problem (44) is close to the model, Levenberg-Marquardt steps, such as given by Equation (45), are successful (i.e., reduce the least squares norm J), which causes λ_k to diminish (cf. algorithm in section 5). A monotonous decrease of λ_k is thus an indication of model linearity, and vice versa, a sudden increase in λ_k reveals a local nonlinearity of the model.

Ratios (77) and (78) apply after several (of the order of 10) consecutive steps with a decrease in λ_k. On the opposite, after an increase in λ_k, the first step is mainly along v_1, the singular vector associated to the largest singular value (as shown in (92), considering the first step of the search as the first step after an increase in λ_k).

4.5 Scaling

The issue of scaling is critical for problems where model parameters have different values. We describe here the main relations underlying scaling and reinterprete singular value analysis when scaling is performed.

Scaled variables $\bar{x}$ are written for each iteration k,

$$D(k)\bar{x} = x \, , \tag{93}$$

where $D(k)$ is a positive definite diagonal matrix. Elements of $D(k)$ are taken as one of the two choices:

1. When we have some insight into typical values of the parameters, $x_{r,i}$,

$$D(k)_i = x_{r,i} \, . \tag{94}$$

2. When too little is known about the problem to infer a typical value for x_i, scaling is performed according to the scheme proposed in [12] where the coefficients $D_i(k)^{-1}$ of $D(k)^{-1}$ are updated norms of the sensitivities,

$$\begin{aligned} D_i(0)^{-1} &= ||(\nabla f(x_0))_i|| \\ D_i(k)^{-1} &= \max\{||(\nabla f(x_k))_i||, D_i(k-1)\} \end{aligned} \tag{95}$$

   The maximum value is used because derivatives tending to 0 make the steps unreliable.

Default derivation is with respect to x. From (93), derivatives in scaled and unscaled variables are related by,

$$\nabla_{\bar{x}} f_j = \nabla f_j D(k) \qquad , \qquad \nabla_{\bar{x}} f = \nabla f D(k) \, . \tag{96}$$

Assuming (94) is the scaling scheme,

$$||(\nabla f(x_k))_i||^2 = \sum_{j=1}^{m} \left(\frac{\partial f_j(x_k)}{\partial x_i} \right)^2 = \frac{1}{x_i^2} \sum_{j=1}^{m} \left(\frac{\partial f_j(x_k)}{\partial \bar{x}_i} \right)^2 \, . \tag{97}$$

This shows that if $||(\nabla_{\bar{x}} f(x_k))_i|| \approx 1$, scaling strategies (94) and (95) are equivalent.

Scaled version of Levenberg-Marquardt is obtained by rewriting the move limit of Equation (44) in terms of scaled variables,

$$\left\{ \begin{array}{lcl} \min_{x \in S} J_L(x) & = & \frac{1}{2}||(f(x_k) + \nabla f(x_k)(x - x_k) - z)||^2 \\ \text{such that } \bar{g}(\bar{x}) & = & \frac{1}{2}||\bar{x} - \bar{x}_k||^2 - \delta_k < 0 \end{array} \right. \tag{98}$$

Necessary and sufficient optimality conditions for (98) yield,

$$(\nabla_{\bar{x}} f^T \nabla_{\bar{x}} f + \lambda_k I)(\bar{x} - \bar{x}_k) = -\nabla_{\bar{x}} f^T (f(D(k)\bar{x}_k) - z) . \tag{99}$$

We write the derivatives with respect to the unscaled x variables,

$$[(D(k)^T \nabla f^T \nabla f D(k)) + \lambda_k I](\bar{x} - \bar{x}_k) = -D(k)^T \nabla f^T (f(D(k)\bar{x}_k) - z) . \tag{100}$$

Multiplying by $(D(k)^T)^{-1} = D(k)^{-T}$ and expressing in terms of x's, we obtain a scaled version of Levenberg-Marquardt,

$$(\nabla f^T \nabla f + \lambda_k D(k)^{-T} D(k)^{-1})(x - x_k) = -\nabla f^T (f(x_k) - z) . \tag{101}$$

Iterates of the scaled Levenberg-Marquardt enable singular value analysis, although Proposition 12 no longer applies. Generalized singular vectors and values $\bar{v}_i$ and $\bar{s}_i$, which characterize $AD(k)$, are obtained,

$$\lim_{k \to \infty} \frac{D(k)^{-1}[x_{k+1} - x_k]}{||D(k)^{-1}(x_{k+1} - x_k)||} = \bar{v}_r , \tag{102}$$

$$\lim_{k \to \infty} \frac{||A(x_{k+1} - x_k)||^2}{||D(k)^{-1}(x_{k+1} - x_k)||^2} = \bar{s}_r^2 . \tag{103}$$

$$\tag{104}$$

The proof is the same as in Proposition 12, but using Equation (100) instead of (45). Similarly, all comments made in section 4.4.2 carry on here, but in the scaled space of $\bar{x}$.

4.6 Handling boundary constraints

In most practical cases, upper and lower bounds are put on the parameters to be identified. Those bounding constraints have a specially simple structure : they are linear, when a lower bound is active the corresponding upper bound is inactive, and constraints are compatible providing the upper bound is larger than the lower bound. This makes efficient handling schemes possible.

Note that strategies based on projecting onto the bounding hypercube the step $(x_{k+1} - x_k)$ (calculated in (45)) may cause loss of the descent direction. Schemes based on reducing the step length (even through an increase in λ_k) cause the algorithm to stall, trying to follow constraint boundaries with vanishing step sizes.

Variable bounds should be handled by checking the Kuhn and Tucker conditions of the constrained problem,

$$\left\{ \begin{array}{l} \min_{d \in S} J_L(x) = \frac{1}{2}||(f(x_k) + \nabla f(x_k)d - z)||^2 \\ \text{such that } \frac{1}{2}||d||^2 - \delta_k \leq 0 \\ x_k + d - x_{max} \leq 0 \\ -x_k - d + x_{min} \leq 0 \end{array} \right. \tag{105}$$

where $d = x - x_k$.

The move limit constraint is considered to be active (like in deriving the Levenberg-Marquardt algorithm). Let $\mu \in \mathbb{R}^n$ and $\gamma \in \mathbb{R}^n$ denote Lagrange multipliers associated to upper and lower bounds, respectively. The Kuhn and Tucker conditions for problem (105) are,

$$\begin{aligned}
(\nabla f(x_k)^T \nabla f(x_k) + \lambda_k I)d + \mu - \gamma &= -\nabla f^T (f(x_k) - z) && (106)\\
\mu_i(x_{k,i} + d_i - x_{max,i}) &= 0 && (107)\\
\gamma_i(-x_{k,i} - d_i + x_{min,i}) &= 0 && (108)\\
\mu &\geq 0 && (109)\\
\gamma &\geq 0 && (110)\\
x_k + d - x_{max} &\leq 0 && (111)\\
-x_k - d + x_{min} &\leq 0 && (112)\\
& && (113)
\end{aligned}$$

Satisfying the Kuhn and Tucker conditions is decomposed in 2 subproblems (active set method). First, a decision is made on which constraint is active. Next, equations (106) to (108) are solved. Equations (109) to (112) are checked a posteriori. If any of them is violated, a new decision is made on which constraint is active and the process is repeated.

Once a choice has been made about active constraints, equations (107) and (108) imply,

$$\begin{aligned}
\text{if } \mu_i \neq 0 \quad &\Rightarrow \quad \gamma_i = 0 \ , \ d_i = x_{max,i} - x_{k,i} && (114)\\
\text{else if } \gamma_i \neq 0 \quad &\Rightarrow \quad \mu_i = 0 \ , \ d_i = x_{min,i} - x_{k,i} && (115)\\
\text{else } \mu_i = 0 \ , \ \gamma_i = 0 \quad &\Rightarrow \quad d_i \text{ unknown.} && (116)\\
& && (117)
\end{aligned}$$

Of the $3n$ unknowns (n parameters and $2n$ multipliers), n are left which are obtained from Equation (106).

The rule for adding or deleting constraints from the active set is:

- If there are violated constraints add the most cirtical to the active set,
- Else if there are negative μ_i's or γ_i's, delete, at random, one of the associated constraint from the active set,
- Else stop (the Kuhn and Tucker conditions are satisfied).

5 Numerical Experiments

A simple implementation of the Levenberg-Marquardt algorithm is used. Updating of λ_k is performed by multiplying or dividing by a factor ν. λ_k is decreased if progress is noticeable with respect to an expected progress L, and λ_k is not below machine accuracy `acc`.

The algorithm is,

1. $k = 0$, $\lambda = \lambda_0$, $x_k = x_0$.
2. Solve (106) to (112) for $x = x_{k+1}$.
3. If $||x_{k+1} - x_k|| < xtol * x_k$ or $J(x_{k+1}) < J_{min}$ or number of J evaluations $>$ max. evaluations or $\lambda_k > \lambda_{max}$, stop.

4. λ_k update:

$$L = ||f(x_k) - z||^2 - ||f(x_k) + \nabla f(x_k)(x_{K+1} - x_k)||^2$$

(a) If $(J(x_k) - J(x_{k+1}) > 0.75 * L)$ and $(\lambda_k > acc)$, $\lambda_k = \lambda_k / \nu$,

(b) If $J(x_k) - J(x_{k+1}) < 0.25 * L$, $\lambda_k = \lambda_k * \nu$,

5. If $J(x_{k+1}) < J(x_k)$, $k = k + 1$

6. goto 2.

$xtol$ is set equal to 1.e-8 in the experiments reported here.

5.1 A Linear Example

We consider a set of m experiments described by the vector z of components,

$$z_i = 2i^2 + 3i + 4 \ , \ i = 1, m \ , \tag{118}$$

and a model $f(x)$,

$$f_i(x) = x_1 i^2 + x_2 i + x_3 \ , \ , \ i = 1, m \ , \tag{119}$$

where x_j, $j = 1, 3$ are three parameters to be determined. By definition, the optimal set of parameters is $x^* = (2., \ 3., \ 4.)^T$. For $m \geq 3$, there is one and only one set of parameters such that the model represents exactly the experiments. The problem is well posed, or ∇f defines a bijective mapping. Any output least squares method, such as the Levenberg Marquardt algorithm, will find the optimal set of parameters. For $m = 2$, there are an infinite number of models that will match the experiments. This is the case discussed in Section 2.2.4 for surjective models and we will dwell on it. We consider,

$$\nabla f(x) = A = \begin{bmatrix} 1. & 1. & 1. \\ 4. & 2. & 1. \end{bmatrix} \qquad \text{and} \qquad z = (9., 18.)^T \ . \tag{120}$$

Rank$A$ = 2. Starting the Levenberg Marquardt algorithm from $x_0 = (-5., 9., -10.)^T$, $\lambda_0 = 1$, $\nu = 2$, convergence occurs at $x^* = (-1.7857, 14.3571, -3.5714)^T$. One checks that this x^* is the solution the nearest to the starting point, as described in Proposition 5, by performing the change of variable $\hat{x} = x - x_0$:

$$\left\{ \begin{array}{l} \min_x \frac{1}{2}||x - x_0||^2 \\ \text{such that } Ax = z \end{array} \right. \Leftrightarrow \left\{ \begin{array}{l} \min_{\hat{x}} \frac{1}{2}||\hat{x}||^2 \\ \text{such that } A\hat{x} = z - Ax_0 \end{array} \right. , \tag{121}$$

The smallest distance property is verified by comparing x^* determined by Levenberg-Marquardt to the pseudo-inverse solution:

$$x^* = A^\dagger (z - Ax_0) + x_0 \ , \text{ where } A^\dagger = \begin{bmatrix} -0.5000 & 0.3571 \\ 0.5000 & -0.0714 \\ 1.0000 & -0.2857 \end{bmatrix} . \tag{122}$$

Convergence of the normalized output least squares norm is shown in Figure 2 using Levenberg-Marquardt without scaling. Square of singular values and singular vectors of A are,

i	s_i^2	v_i
1	23.40175	$[8.4920e-01, 4.5814e-01, 2.6262e-01]^T$
2	$5.9825e-01$	$[-4.5545e-01, 3.8373e-01, 8.0332e-01]^T$
3	0.	$[2.6726e-01, -8.0178e-01, 5.3452e-01]^T$

Estimates of the singular values and vectors derived from the Levenberg-Marquardt convergence are compared to their actual values in Figures 3 and 4, respectively. For the largest singular value and its singular vector, s_1 and v_1, accurate estimates are obtained from iteration 1 to iteration 7. For s_2 and v_2, iterations 4 to 11 provide accurate estimates. Note in Figure 3 that estimating s_2 using (90) is not as precise as using (78).

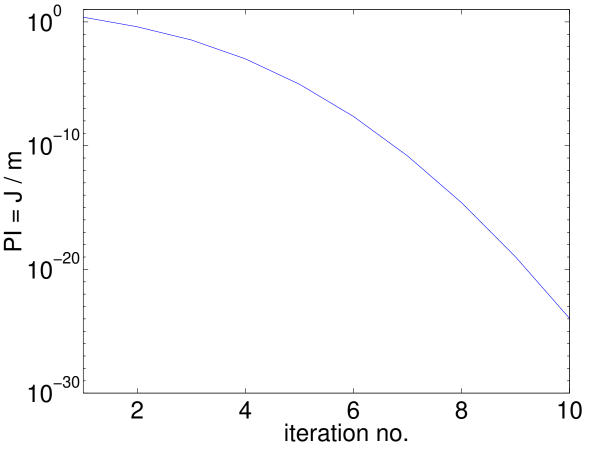


Figure 2: Normalized Output LS, $||f - z||^2/(2m)$, vs. iterations, no scaling

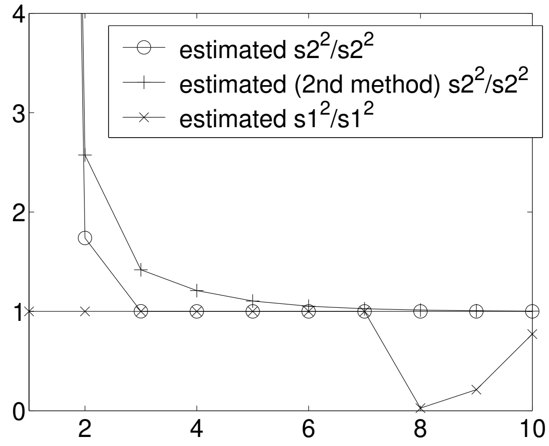


Figure 3: Ratio of estimated singular value to its actual value, vs. iteration number. The default method refers to Equation (78) while the 2nd method refers to Equation (90). No scaling.

Figures 5 and 6 present singular value analysis from the Levenberg-Marquardt iterates with scaling (95) applied. Singular values and vectors of $AD(k)^T$ are,

i	$\bar{s}_i^2$	$\bar{v}_i$
1	2.85582	$[5.7317e-01, 5.9143e-01, 5.6717e-01]^T$
2	$1.4418e-01$	$[6.5469e-01, 8.574e-02, -7.5102e-01]^T$
3	$0.$	$[4.9281e-01, -8.0178e-01, 3.3806e-01]^T$

The same comments as in the unscaled run stand.

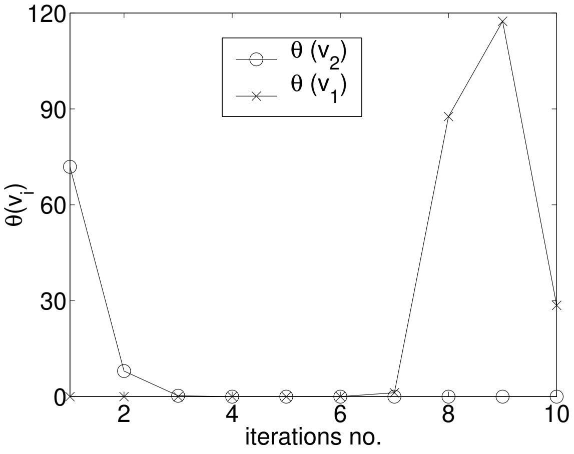


Figure 4: Angle between right singular vectors and their estimate, $\theta(v_i)$ (in ^{o}), vs. iteration number. No scaling.

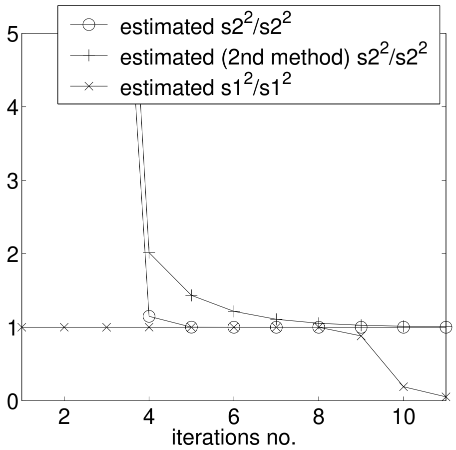


Figure 5: Ratio of estimated singular value to its actual value, vs. iteration number. The default method refers to Equation (104) while the 2nd method refers to Equation (90) for scaled variables. Scaling (95).

5.2 Wide Valley Function

For the purpose of visualizing Levenberg-Marquardt 's trajectory, we consider the "wide valley function" $f(x)$,

$$\begin{cases} r = \frac{\sqrt{2}}{2}(x_1 - x_2) \quad , \quad d = \frac{\sqrt{2}}{2}(x_1 + x_2) \\ \text{if } r < -a \text{ , } J(x) = (r+a)^2[\cos(\alpha d) + 1.1] \text{ ,} \\ \text{if } -a \le r \le a \text{ , } J(x) = 0 \text{ ,} \\ \text{if } r > a \text{ , } J(x) = (r-a)^2[\cos(\alpha d) + 1.1] \text{ ,} \\ \text{ with } \alpha = 0.5 \text{ , } a = 1. \end{cases} \tag{123}$$

Minimization is carried out on $J(x) = \frac{1}{2}f(x)^T f(x)$, the "data" being $z = 0$. There is 1 observation, $m = 1$, and two parameters, $n = 2$. Contour lines of

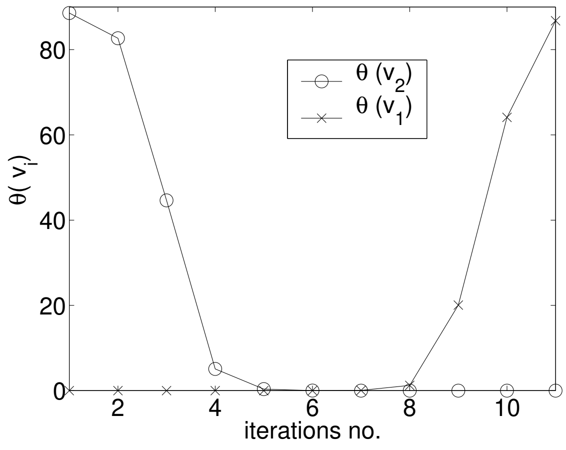


Figure 6: Angle between right singular vectors and their estimate, $\theta(v_i)$ (in ^{o}), vs. iteration number. Scaling (95).

J are shown in Figure 7. It is a continuously differentiable nonlinear function of 2 variables. The function has a set of minima with a nonempty interior, a valley of width $2a$ centered around the line $x_1 = x_2$, $J = 0$. An example of convergence of the method started at $x_0 = (5., -7.6)^T$ is shown in Figure 7. One can see that the method converges to the edge of the global optima set but, contrarily to the linear case, it no longer converges to the point the nearest to x_0 (indicated as the projection in Figure 7). Figure 7 further illustrates the effect of the λ_k history on the trajectory : trajectory 1 has smaller λ's than trajectory 2. ν is chosen near 1 on purpose, so that λ's adapt slowly. As a result, on this example, the first run takes larger steps (at least at the beginning of the optimization). In both cases, the average path followed by the search is the steepest slope line (as is shown in Section 4.3.3). The Levenberg Marquardt algorithm oscillates around this line with an amplitude inversely proportional to λ, but, in all cases, the oscillations remain stable.

The properties of the algorithm regarding singular value analysis (Proposition 12) are trivially satisfied on this example since there is only one nonzero singular value. Figure 8 shows the perfect match between the exact s_1 and its estimation. The same applies to the singular vector v_1.

5.3 Identification of the parameters of material constitutive laws

We now turn to the identification of the parameters governing a material model. For demonstrative purposes, we first consider a simple problem, the Maxwell rheological model. It is simple enough to calculate second order derivatives and illustrate λ_k convergence (see section 4.4.1). We next study the so-called elasto-visco-plastic model [7], or *EVP*, which is implemented in many structural calculation softwares for simulating nonlinear metal behaviour.

Constitutive laws relate two basic ingredients of the response of a solid, the strain $\epsilon(t)$ and the stress $\sigma(t)$, which are functions of time t. The strain $\epsilon(t)$ is a normalized elongation or contraction of a material piece. The stress $\sigma(t)$ is the force normalized by material cross-section applied to the material in a certain direction. Describing a material means, in that context, relating strain and stress histories, $\epsilon(t)$ and $\sigma(t)$, respectively. We assume here that the strain history, $\epsilon(t)$, is an imposed

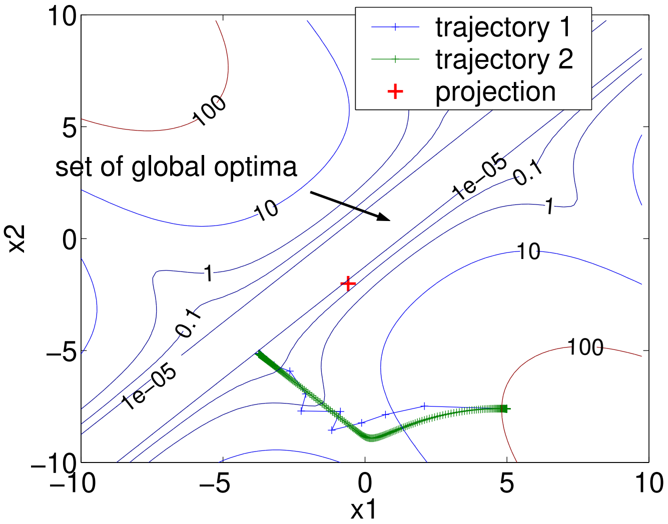


Figure 7: Convergence of Levenberg-Marquardt algorithm on the wide valley function. Trajectories 1 and 2 start from the same point, but have different λ histories: $\lambda_0 = 0.001$, $\nu = 1.1$, for trajectory 1, $\lambda_0 = 10.e+06$, $\nu = 1.1$ for trajectory 2. No scaling.

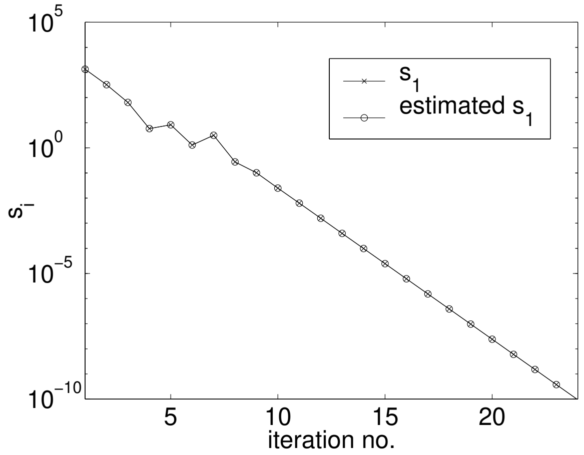


Figure 8: Exact and estimated s_1 for the Wide Valley function at each iteration. Estimation is based on formula (78). $x_0 = (5., 2., 0.)^T$, $\lambda_0 = 1.$, $\nu = 10.$. No scaling.

input. The response of the model is the stress, $\sigma(t)$. Measurements of strains and stresses are performed at discrete times, t_i, $i = 1, \ldots, m$. Refering back to earlier terminology, $f_i \equiv \sigma(t_i)$ and $z = (\sigma_e(t_1) \ \ldots \ \sigma_e(t_m))^T$, where $\sigma_e(t)$ is the measured experimental stress at time t.

5.3.1 Maxwell Rheological Model

The Maxwell model is unidimensionnal, composed of a spring and a damper in series (cf. Figure 9). The strain is kept constant here, $\epsilon(t) = \epsilon$. The stress "relaxation" is observed. An analytical expression for the stress is easily obtained by integrating the relations,

$$\sigma = E\epsilon_e \ , \tag{124}$$
$$\sigma = K\dot{\epsilon}_i \ , \tag{125}$$

which gives,

$$\sigma(t) = E\epsilon \exp(-\frac{E}{K}t) \ . \tag{126}$$

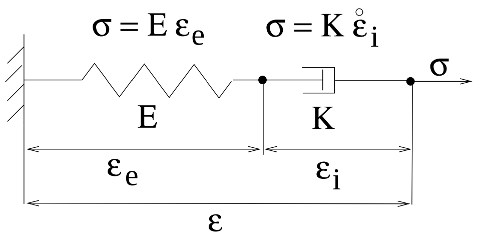


Figure 9: Maxwell model.

The goal of the identification is to determine the parameter K based on 2 stress measures, $\sigma(t_1)$ and $\sigma(t_2)$. Results are given for $t_1 = 0.01$, $t_2 = 2$, $E = 2000\ MPa$. Three data sets are considered, $z = (100.8 - 7.5)^T$, $z = (14.8 - 0.85)^T$, and $z = (3.8 - 0.01)^T$, respectively. The first data set, along with model response for different K values is shown in Figure 10. The parameter estimate for all data sets is near $K = 1460$, which is purposedly taken in the high negative curvature region (otherwise λ_k tends to 0). Figure 11 gives

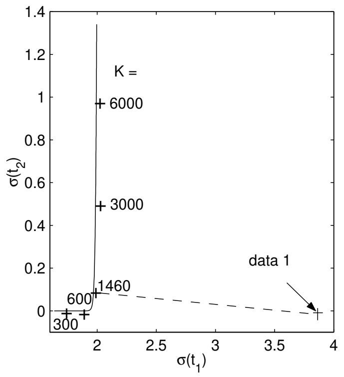


Figure 10: Model response for varying K values and first data set, model space.

λ_k and its estimate, λ_k^e, as obtained in (75) for all 3 data sets. λ_k^e is always within 10 % of λ_k. Qualitative interpretation of λ_k^e is confirmed by the experiment: one checks that negative curvatures are necessary for λ_k to be substantially beyond 0, and as the residual at the parameter estimate increases, λ_k increases.

5.3.2 Elasto-visco-plastic model

The EVP model is nonlinear and $(n-1)$ times continuously differentiable (see below). There are 4 unknown parameters. The model is evaluated by integrating

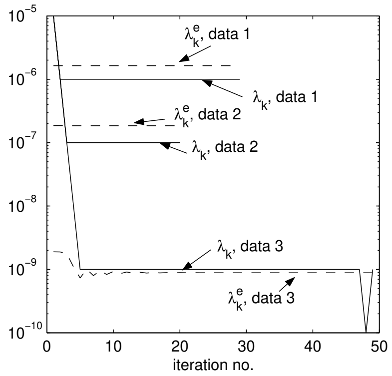


Figure 11: λ_k and its estimate, λ_k^e.

the following set of partial differential equations (a 1-dimensional *EVP* without hardening, [7]):

$$\left\{\begin{array}{rcl} \dot{p} & = & \eta\langle\frac{|\sigma| \;-\; R_i}{K}\rangle^n \\ \dot{\epsilon_i} & = & \eta\dot{p} \\ \dot{\epsilon_e} & = & \dot{\epsilon} - \dot{\epsilon_i} \end{array}\right. \qquad (127)$$
$$\text{and}\ \left\{\begin{array}{rcl} \sigma & = & E\epsilon_e \\ \eta & = & sign(\dot{\epsilon}) \end{array}\right.$$

where, for ease of notation, dependence of the variables p, ϵ, ϵ_i, ϵ_e, σ on t is implicit. Dot denotes differentiation with respect to time, and $\langle x\rangle \;=\; x$ if $x > 0$, else $=\; 0$. The 4 parameters of the model are E, K, n, and R_i.

Gradient of the stress is calculated by differentiating the partial differential equations (127) with respect to the parameters. It produces supplementary partial differential equations to integrate. The left hand side of the sensitivity equations are $\frac{\partial\dot{\sigma}}{\partial E}$, $\frac{\partial\dot{\sigma}}{\partial K}$, $\frac{\partial\dot{\sigma}}{\partial n}$, and $\frac{\partial\dot{\sigma}}{\partial R_i}$.

For example, derivatives with respect to E are obtained by integrating the following equations:

$$\frac{\partial\dot{\sigma}}{\partial E} \;=\; \dot{\epsilon_e} \;+\; E\frac{\partial\dot{\epsilon_e}}{\partial E} \qquad (128)$$
$$\frac{\partial\dot{\epsilon_e}}{\partial E} \;=\; -\frac{\partial\dot{\epsilon_i}}{\partial E} \qquad (129)$$
$$\frac{\partial\dot{\epsilon_i}}{\partial E} \;=\; \eta\frac{\partial\dot{p}}{\partial E} \qquad (130)$$
$$\frac{\partial\dot{p}}{\partial E} \;=\; \frac{n\eta}{K}\dot{p}^{(}(n-1)/n) * (\epsilon_e - E * \frac{\partial\epsilon_i}{\partial E}) \qquad (131)$$

Experimental data, σ_e, have been generated using $E^* \;=\; 200000.MPa$, $K^* \;=\; 1550$, $n^* \;=\; 4$, and $R_i^* \;=\; 10.MPa$. Two experiments are used and compared for the identification process, a cyclic fatigue test at constant strain rate of $\dot{\epsilon} \;=\; 10^{-4}$, and a relaxation test where $\epsilon \;=\; 5.10^{-3}$ is constant (cf. Figures 12 and 13 for strain / stress histories). Both tests have 501 data points equally spaced in time.

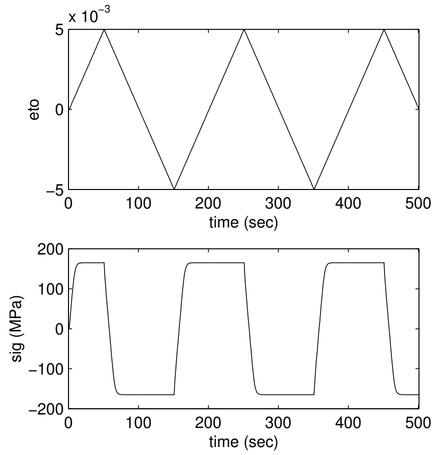


Figure 12: Fatigue test, strain eto and “experimental” stress sig

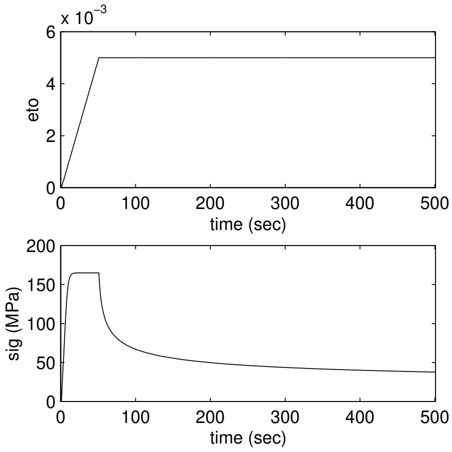


Figure 13: Relaxation test, strain eto and “experimental” stress sig

5.3.3 Relaxation versus Fatigue

Identification is carried out using $\lambda_0 = 1$, $\nu = 4$, and the scaling scheme of Equation (94). Lower and upper bounds on the parameters are, respectively, $E_{min} = 100000\ MPa$, $E_{max} = 400000\ MPa$, $K_{min} = 100$, $K_{max} = 10000$, $n_{min} = 2$, $n_{max} = 10$, and $R_{i,min} = 0.5\ MPa$, $R_{i,max} = 200\ MPa$. In Figure 14, convergence of the algorithm is compared starting from 4 different points using either fatigue or relaxation data. For all starting points, convergence is 2 to 10 times faster using relaxation rather than fatigue information. Accuracy of the results is also better: the average error[1] commited on identified E, K, n and R_i is, for the fatigue test, 0.0058, 3.48, 2.54, and 32.16 %, respectively, against 0.0002, 0.0016, 0.0007, and 0.0028 % for the relaxation. Conditionning of $(D^T \nabla f^T \nabla f D)$ is, as presented in section 3.1.3, a good indication of the sensitivity of the parameter estimates to perturbations in the data or the model. More generally, we see with the current experiment that it is a hint about the difficulty at identifying the parameters

[1]defined as $\sum_{i=1}^{4} \frac{|x_j^i - x_j^*|}{4|x_j^*|} \times 100$, $j = 1, n$, where x_j^i is the jth parameter calculated at the end of the ith identification.

using Levenberg-Marquardt. At x^*, $(\bar{s_1}^2/\bar{s_r}^2) = 6.802e07/4.345e-01 = 1.5653e08$ for the fatigue and $(\bar{s_1}^2/\bar{s_r}^2) = 2.188e07/2.468e02 = 8.8674e04$ for the relaxation. The difference in conditionning is attributed to the smallest singular value which is near 0 for the fatigue test. The associated singular vector is,

$$v_4 \;=\; D\bar{v_4} \;=\; \begin{pmatrix} 2.111393536295494e-01 \\ 9.759855024642624e-01 \\ -1.693933436883089e-03 \\ 5.356867478283022e-02 \end{pmatrix} . \tag{132}$$

Most points used for the identification using the fatigue test are part of an asymptote (Figure 13). The asymptote is described by,

$$\sigma \;=\; const \quad\Rightarrow\quad \dot{\sigma} \;=\; 0 \quad\Rightarrow\quad \dot{\epsilon}_e \;=\; 0 \quad\Rightarrow\quad \dot{\epsilon}_i \;=\; \dot{\epsilon} \; . \tag{133}$$

Equation (127) yields, in traction ($\eta = 1$), at the asymptote,

$$\mathcal{A}(E, K, n, R_i) \;=\; K(\dot{\epsilon})^{1/n} + R_i - const \;=\; 0 \; . \tag{134}$$

$x^* \;=\; (E^*, K^*, n^*, R_i^*)$ satisfy Equation (134) ($\dot{\epsilon} \;=\; 1e{-}4$, $const \;=\; 165$), and so do all parameter sets having the same asymptote. It turns out that the singular vector associated to the smallest singular value, v_4, is tangent to the surface described by $\mathcal{A}$ in (134). Indeed,

$$\nabla\mathcal{A}/||\nabla\mathcal{A}|| \;=\; \begin{pmatrix} 0 \\ (\dot{\epsilon})^{1/n} \\ \frac{-K\ln(\dot{\epsilon})}{n^2}(\dot{\epsilon})^{1/n} \\ 1 \end{pmatrix} /||\nabla\mathcal{A}|| \;=\; \begin{pmatrix} 0 \\ 1.120688866677762e-03 \\ 9.999365728399350e-01 \\ 1.120688866677762e-02 \end{pmatrix} , \tag{135}$$

and,

$$\nabla\mathcal{A}^T v_4 \;\approx\; 0 \; , \tag{136}$$

so that v_4 is perpendicular to $\nabla\mathcal{A}$. Once a parameter set having roughly the right asymptotes has been determined (which occurs rapidly considering the importance of the asymptote on J), the direction of parameter changes such that the asymptote remains in place is v_4, which is a low sensitivity direction. The conditionning problem of the fatigue test is due to parameters satisfying the asymptote equation.

5.3.4 Approximate sensitivity analysis on a nonlinear function

For linear models, ratios (77) and (78), which are expressed only in terms of the steps and the gradient of the model, perform a singular value analysis of the model, which may serve as parameter sensitivity analysis. Generalization of the approximate sensitivity analysis to nonlinear models has been discussed in Section 4.4.1. Figures 15 to 18 illustrate on the EVP example, using fatigue and relaxation data, how the search is mainly along v_4 as λ_k decreases, and is mainly along v_1 after a sudden increase in λ_k. In Figures 15 and 17, the angle between the search direction and the singular vectors of $[D^T \nabla f^T \nabla f D]$ is given as a function of the iteration number. In Figures 16 and 18, ratio (78) is compared to the singular values as a function of the iteration number.

6 Conclusions

Deterministic concepts underlying least squares minimization for parameter estimation have been reviewed. Least squares and minimum norm problems have been

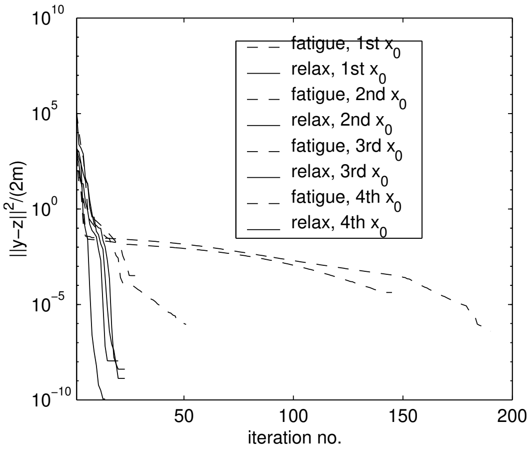


Figure 14: Comparison of identifications in terms of $J/(2m)$ for fatigue and relaxation tests, starting from 4 different x_0's: 1st x_0 $[E; K; n; R_i]$ $= [110000.; 550.; 2.5; 100.]$; 2nd x_0 $[E; K; n; R_i] = [300000.; 550.; 8.; 5.]$; 3rd x_0 $[E; K; n; R_i] = [110000.; 3550.; 8.; 5.]$; 4th x_0 $[E; K; n; R_i] =$ $[300000.; 3550.; 2.5; 100.]$.

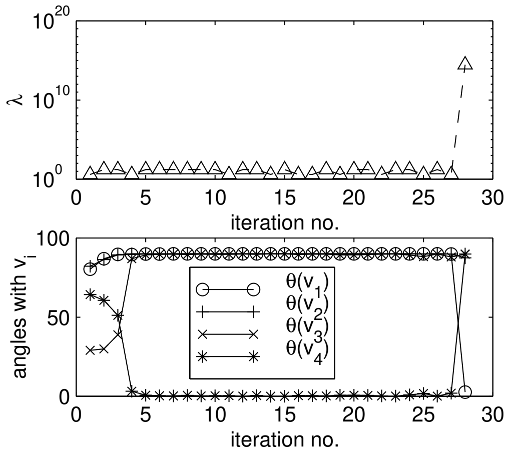


Figure 15: Angles between steps $(\bar{x}_{k+1} - \bar{x}_k)$ and singular vectors of $[D^T \nabla f^T \nabla f D]$, fatigue test, $x_0 = [170000, 550, 6, 30]^T$.

gradually introduced to maintain identifiability of the model parameters, considering linear injective, surjective, and general models. Least squares estimates sensitivities have been discussed through parameter sensitivity and model curvatures. Based on those concepts, a popular method for solving general least squares problems, the Levenberg-Marquardt algorithm, has been analyzed. It has been shown that Levenberg-Marquardt

- converges to the smallest norm least squares solution for linear models,
- follows the steepest slope line of the least squares norm,
- gives relevant information for parameter and model sensitivity analysis.

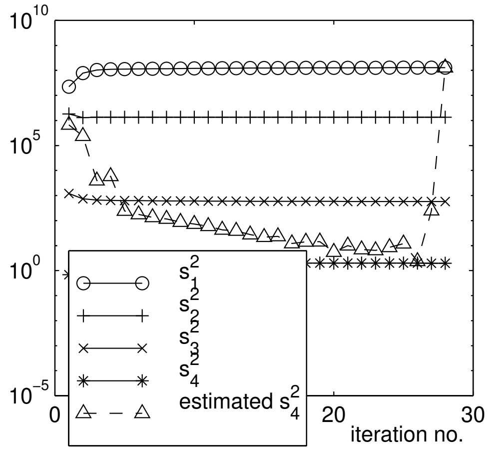


Figure 16: Exact and estimated eigenvalues of $[D^T \nabla f^T \nabla f D]$, fatigue test, $x_0 = [170000, 550, 6, 30]^T$.

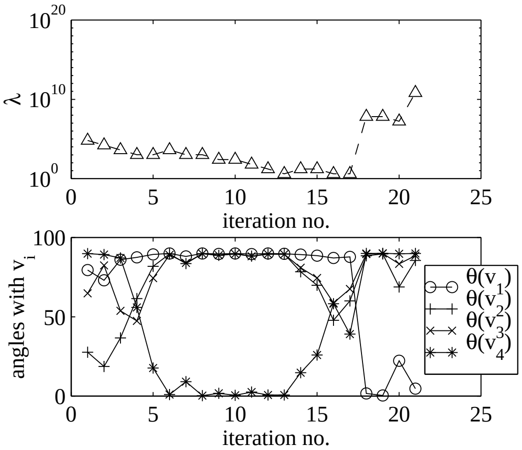


Figure 17: Angles between steps $(\bar{x}_{k+1} - \bar{x}_k)$ and singular vectors of $[D^T \nabla f^T \nabla f D]$, relaxation test, $x_0 = [170000, 550, 6, 30]^T$.

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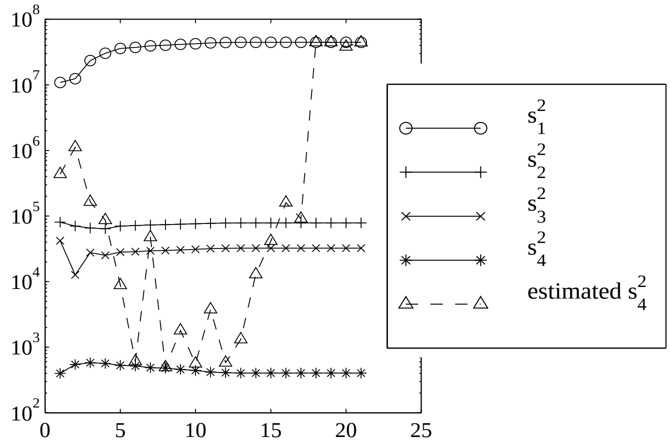

Figure 18: Exact and estimated eigenvalues of $[D^T \nabla f^T \nabla f D]$, relaxation test, x_0 $= [170000, 550, 6, 30]^T$.

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A Some Numerical Analysis Results

Results presented here are an arbitrary selection of what is used in the body of the text and not basic engineer's knowledge. Matrix operations, definitions of dimension of a vector space S, $\dim S$, of the rank of a matrix, Rank$A$, of the image space and the null space ImA and Ker$A$, are assumed to be known. For a more complete presentation, the reader is refered to [5] or [2].

A.1 Linear Algebra

We consider a real coefficients matrix of m rows and n columns, $A \in \mathcal{M}_{mn}(\mathbb{R})$, associated to the linear mapping $A : \mathbb{R}^n \rightarrow \mathbb{R}^m$.

- the rank of a matrix is Rank$A = dim$ImA.
- Ker$A^T = (\text{Im}A)^\perp$.
- A is injective if and only if,

$$\forall x_1, x_2 \in S,\ Ax_1 = Ax_2 \Rightarrow x_1 = x_2 \,. \tag{137}$$

- A is surjective if and only if, $\forall\ z \in \mathbb{R}^m$, $\exists\ x \in \mathbb{R}^n$ (not necessarily unique) $\mid Ax = z$.
- A is bijective if and only if it is injective and surjective.
- A is injective (resp. surjective) if and only A^T is surjective (resp. injective).
- A is injective if and only if RankA $= n$.
- A is surjective if and only if RankA $= m$.
- A is injective if and only if Ker$A = \{0\}$.
- A is injective if and only if $A^T A$ is nonsingular.
- A is surjective if and only if AA^T is nonsingular.
- A is positive definite if and only if A is nonsingular.

A.2 Projections

- We define a projection $\mathcal{P}_V(x)$ of $x \in U$ on the set V as the set of minimum distance points,

$$\mathcal{P}_V(x) = \{y \mid y = \arg\min_{v \in V} ||x - v||^2\} \,. \tag{138}$$

- When $\mathcal{P}_V(x)$ has one element, we define the projector $P_V(x)$ as the mapping that associates to x the element of the projection, $P_V : x \rightarrow \mathcal{P}_V(x)$.
- $P_V(x)$ is an orthogonal projector if and only if $P_V(x)P_V(x) = P_V(x)$ and $(x - P_V(x)) \perp P_V(x)$.
- P is a linear orthogonal projector if and only if $P^2 = P$ and $P^T = P$.

B Optimality Conditions

We very briefly remind the principal optimization arguments used in the body of the article. Readers willing to deepen the topic are refered to [11].

- A set $S \subset \mathbb{R}^n$ is convex if and only if

$$\left.\begin{array}{r} \forall x \in S \\ \forall y \in S \\ \forall \lambda (0 \leq \lambda \leq 1) \end{array}\right\} \Rightarrow \lambda x + (1-\lambda) y \ \in \ S \tag{139}$$

- A function $f \ : \ \mathbb{R}^n \ \rightarrow \ \mathbb{R}$ defined on a convex set S is convex if,

$$\forall x \in S \ , \ \forall y \in S \ , \ \forall \lambda \in [0,1] \ ,$$
$$f(\lambda x + (1-\lambda) y) \ \leq \ \lambda f(x) + (1-\lambda) f(y) \ . \tag{140}$$

  The function is strictly convex if the inequality is strictly satisfied.

- Let f be twice continuously differentiable. f is convex if and only if $\forall x \in S$, the Hessian, $\nabla^2 f(x)$, is positive semi-definite.

- We consider the optimization problem,

$$\left\{\begin{array}{l} \min_{x \in S} f(x) \\ h_i(x) \ = \ 0 \ , \ i = 1,p \end{array}\right. \tag{141}$$

  If S is convex, f is convex and $h_i(x)$ are linear functions, the optimization problem (141) is convex.

- A global optimum is a point $x^* \ \in \ S$ that satisfies the optimization constraints $h_i(x^*) \ = \ 0$, and such that $\forall x \ \in \ S \ , \ f(x^*) \ \leq \ f(x)$.

- x^0 is a local optimum of (141) if and only if there exists a neighbourhood $\mathcal{V}(x^0)$ of x^0 such that x^0 is the global optimum of

$$\left\{\begin{array}{l} \min_{x \in S} f(x) \\ h_i(x) \ = \ 0 \ , \ i = 1,p \\ x \ \in \ \mathcal{V}(x^0) \end{array}\right. \tag{142}$$

- (Weierstrass Theorem) If f is a continuous real valued function defined on $S \ \in \ \mathbb{R}^n$, S closed and bounded, then the optimization problem $\min_{x \in S} f(x)$, has an optimum solution $x^* \ \in \ S$. The optimization problems considered in this paper satisfy the above conditions.

- (Constraints Qualification) Two sufficient conditions for the equality constraints to be "qualified" are:

  - h_i, $i \ = \ 1,p$ are linear functions and there exists a point $\bar{x}$ such that $h_i(\bar{x}) \ = \ 0$, $i = 1,p$.
  - At a candidate optimum x^0, $h_i(x^0) \ = \ 0$ and $\nabla h_i(x^0)$ are linearly independent, $i = 1,p$.

- (First order optimality conditions – Kuhn and Tucker) Let assume that f and h_i, $i = 1,p$ are continuous differentiable functions and the constraints are qualified at x^0. A necessary condition for x^0 to be a local optimum is that there exist λ_i, $i = 1,p$, such that,

$$\left\{\begin{array}{l} \nabla f(x^0) \ + \ \sum_{i=1}^{p} \lambda_i \nabla h_i(x^0) \ = \ 0 \\ h_i(x^0) \ = \ 0 \ , \ i = 1,p \end{array}\right. \tag{143}$$

  The λ_i's can be positive or negative.

- If the optimization problem (141) is convex, the Kuhn and Tucker conditions (143) are necessary and sufficient for x^0 to be a global optimum.

C Generalized Curvatures

Curvatures are classically expressed for space curves or surfaces. A general description of curvatures is introduced here for hypersurfaces $f : \mathbb{R}^n \longrightarrow \mathbb{R}^m$. Generalized curvatures are needed, for example, when estimating sensitivities of an identified model f to parameter and data changes (cf. section 3).

The center of curvature of a parametric hypersurface is located on the intersection of normals at 2 points of f, as those points tend towards each other. This definition excludes cases where normals do not intersect, such as torsional curvatures.

The normal variety at x, n_x, is defined by,

$$\nabla f(x)^T n_x \;=\; 0 \; . \tag{144}$$

At $x + \alpha h$, where α is a scalar and $h \in \mathbb{R}^m$,

$$\nabla f(x+\alpha h)^T n_{x+\alpha h} \;=\; 0 \; . \tag{145}$$

The intersection of the normals is written,

$$f(x) + \rho n_x \;=\; f(x+\alpha h) + \beta n_{x+\alpha h} \; , \tag{146}$$

where ρ and β are scalars. Multiplying (146) by $\nabla f(x+\alpha h)^T$ and dividing by α yields,

$$\rho \frac{\nabla f(x+\alpha h)^T - \nabla f(x)^T}{\alpha} n_x \;=\; \nabla f(x+\alpha h)^T \frac{f(x+\alpha h) - f(x)}{\alpha} \; , \tag{147}$$

where use of (144) has been made. Generalized curvature equations are composed of (147) as α tends to 0, the restriction that n_x is a unit vector, and equation (144):

$$\left\{ \begin{array}{rcl} \sum_{i=1}^m n_{x,i} \nabla^2 f_i(x) h_j & = & \frac{1}{\rho_j} \nabla f(x)^T \nabla f(x) h_j \; , \; j = 1, \ldots, n \\ ||n_x|| & = & 1 \\ \nabla f(x)^T n_x & = & 0 \end{array} \right. \tag{148}$$

This general eigensystem has n eigenvectors, h_j, and eigenvalues, $\sigma_j = 1/\rho_j$ (the proof is provided below for $\nabla f(x)$ injective). σ_i and h_i, $i = 1, \ldots, n$ are the principal curvatures and curvature directions, respectively. Curvatures of $f : \mathbb{R} \longrightarrow \mathbb{R}^2$ are illustrated in Figure 19. The terms $dx^T \nabla f(x)^T \nabla f(x) dx$ and $dx^T (\sum_{i=1}^m n_{x,i} \nabla^2 f(x)) dx$ are given a special meaning as norms of changes projected on the tangent and normal hyperplanes, respectively. This is seen by writing the Taylor series expansion of f,

$$f(x+dx) - f(x) \;=\; \nabla f(x) dx + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial f}{\partial x_i \partial x_j} dx_i dx_j + \mathcal{O}||dx^3|| \; , \tag{149}$$

and performing the scalar products $(f(x+dx) - f(x))^T \nabla f(x) dx$ and $(f(x+dx) - f(x))^T n_x$.

We further study Equation (148) for injective $\nabla f(x)$ (i.e., $m > n$). For ease of writing, we introduce,

$$G \;=\; \sum_{i=1}^m n_{x,i} \nabla^2 f_i(x) \qquad \text{and} \qquad A \;=\; \nabla f(x) \; . \tag{150}$$

A is injective so $(A^TA)^{-1}$ exists and the pseudo-inverse of A is $A^\dagger = (A^TA)^{-1}A^T$. The following statements are equivalent:

$$\begin{aligned}
Gh_j &= \sigma_j A^T A h_j && (151)\\
\Longleftrightarrow (A(A^TA)^{-1}G(A^TA)(A^TA)^{-1}A^T)Ah_j &= \sigma_j A h_j && (152)\\
\Longleftrightarrow (A^\dagger)^T G(A^\dagger) &= \sigma_j A h_j && (153)\\
\Longleftrightarrow K(Ah_j) &= \sigma_j (Ah_j) \ , && (154)
\end{aligned}$$

where $K = (A(A^TA)^{-1}G(A^TA)(A^TA)^{-1}A^T)$ is an $m \times m$ symmetric matrix. The eigensystem,

$$Kw_j = \gamma_j w_j \ , \tag{155}$$

has m real eigenvalues γ_j and the associated eigenvectors w_j , $j = 1, \ldots, m$ form an orthogonal basis of $\mathbb{R}^m$ since K is real and symmetric. We write the w_i's so that $(w_1, \ldots, w_n)$ is an orthogonal basis of $\mathrm{Im}A$ and $(w_{n+1}, \ldots, w_m)$ is an orthogonal basis of $\mathrm{Ker}A^T$ (always possible since $\mathrm{Im}A \oplus \mathrm{Ker}A^T = \mathbb{R}^m$). For $j = n+1, \ldots, m$, $Kw_j = 0 \Rightarrow \gamma_j = 0$. There is at least n h_i's such that $w_i = Ah_i$, $i = 1, \ldots, n$, which are solutions of the general eigenvalue system (148) with $\gamma_i = \sigma_i$. The h_i's, $i = 1, \ldots, n$, are a basis of $\mathbb{R}^n$:

$$\sum_{i=1}^{n} \beta_i h_i = 0 \qquad \Leftrightarrow \qquad \sum_{i=1}^{n} \beta_i A h_i = 0 \qquad \Rightarrow \qquad \beta_i = 0 \ , \ i = 1, \ldots, n \ . \tag{156}$$

Finally, for any $dx \in \mathbb{R}^n$, $dx = \sum_{i=1}^n dx_i h_i$, and Rayleigh's quotient associated to the eigensystem (148) is,

$$\mathcal{C}_x(dx) = \frac{dx^T G dx}{dx^T A^T A dx} = \frac{\sum_{i=1}^n \sigma_i dx_i^2}{\sum_{i=1}^n dx_i^2} \ . \tag{157}$$

We call $\mathcal{C}_x$ the model normalized curvature at x in the direction dx. Extremal values of $\mathcal{C}_x$ are,

$$\begin{aligned}
\max_{dx \in \mathbb{R}^n} \frac{dx^T G dx}{dx^T A^T A dx} &= \max_{i=1,n} \sigma_i && (158)\\
\min_{dx \in \mathbb{R}^n} \frac{dx^T G dx}{dx^T A^T A dx} &= \min_{i=1,n} \sigma_i && (159)\\
& && (160)
\end{aligned}$$

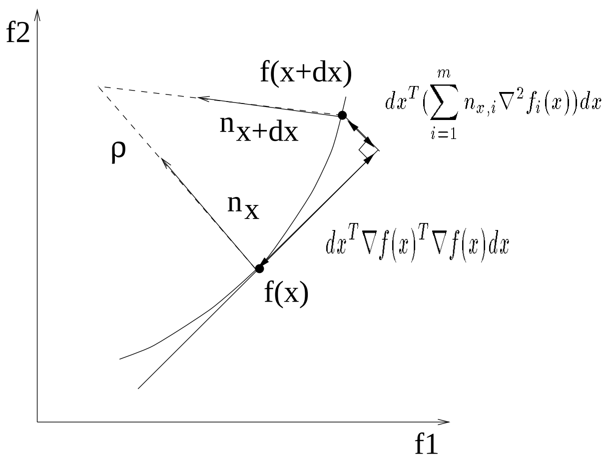

Figure 19: Model Space, $m = 2$