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**ON THE UNIQUENESS
OF LOCAL MINIMA
FOR GENERAL ABSTRACT
NON-LINEAR
LEAST SQUARE PROBLEMS**

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ON THE UNIQUENESS OF LOCAL MINIMA FOR GENERAL
ABSTRACT NON-LINEAR LEAST SQUARE PROBLEMS

Guy CHAVENT

Abstract : Effectiveness of the inversion of a mapping ϕ defined on a set C by non linear least square techniques rely, among other, on the uniqueness of local minima of the least square criterion, which ensure that numerical optimization algorithm will, (if they do), converge toward the global minimum of the least square functional. We define a number γ depending only on C and ϕ which, if the size of $\phi(C)$ is not too large with respect to its curvature, will be strictly positive, thus yielding uniqueness of all local minima having a value smaller than γ . The condition $\gamma > 0$ will require neither convexity of C nor any monotony property of ϕ , but involves the computation of an infimum over $\partial C \times \partial C$ of first and second derivatives of ϕ . Numerical application to the estimation of two parameters in a parabolic equation will be given.

SUR L'UNICITE DE MINIMA LOCAUX POUR LES PROBLEMES
DE MOINDRES CARRES NON-LINEAIRES.

Résumé : L'inversion d'une application ϕ définie sur C par la méthode des moindres carrés non linéaires se ramène à la résolution d'un problème d'optimisation. La possibilité de trouver effectivement le minimum global dépend de l'existence de minimum locaux. Nous définissons un nombre γ dépendant seulement de C et ϕ qui, lorsque la taille de $\phi(C)$ n'est pas trop grande par rapport à sa courbure, sera strictement positif, assurant ainsi l'unicité des minima locaux ayant une valeur inférieure à γ . La condition $\gamma > 0$ ne requiert ni la convexité de C ni une quelconque propriété de monotonie de ϕ , mais suppose le calcul d'un infimum, sur $\partial C \times \partial C$, contenant les dérivées premières et secondes de ϕ . Une application numérique à l'estimation de deux paramètres dans une équation parabolique est présentée.

Key Words

Inverse problems - non linear least squares -
identification - parameter estimation

Mots Clefs

Problèmes inverses - moindres carrés non linéaires -
identification - estimation de paramètres

1 . INTRODUCTION

Consider :

- $E =$ normed vector space (norm $\| \cdot \|_E$)
 $F =$ prehilbert space (scalar product $\langle \cdot, \cdot \rangle_F$)
 $C =$ closed, C^2 -path-connected subset of E
 $\phi =$ C^2 -mapping of C into F
 $z \in F$ a given point

and the optimization problem :

(I-1) find $\hat{x} \in C$ such that $J(\hat{x}) \leq J(x) \forall x \in C$ where

(I-2) $\forall x \in C, J(x) = \| \phi(x) - z \|_F^2$.

Problem (I-1) is the general least-square setting of the problem :

(I-3) find $\hat{x} \in C$ such that $\phi(\hat{x}) = z$.

when the right-hand side z does not necessarily belong to the image set $\phi(C)$.

Our goal is to find conditions on C and ϕ such that :

(I-4) problem (I-1) cannot admit two distinct local minima (and hence has almost one solution), provided that the distance of z to $\phi(C)$ is taken smaller than certain number $\gamma > 0$.

In this paper, we will be able to ensure uniqueness only of the local minima of J having a value smaller than γ (propositions 3 and 4). We pursue further study to find conditions ensuring uniqueness of all local minima.

Let us now explain our motivations.

The first question is : what kind of applications have motivated the author to undertake this study ? The answer is : parameter estimation problems. In this application, x is the parameter, C is the set of admissible parameter, z is the observed data, and ϕ is the parameter \rightarrow output mapping resulting from the resolution of the model state equations and the observation operator. Our concern is primarily with

overspecified inverse problems, where $\dim F \geq \dim E$, so that we can expect that the derivative $\phi'(x)$ be more or less injective from E into F . In order to be more specific, we can give an example :

Example 1 : we consider the 1-D parabolic equation :

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial}{\partial z} \left(a \frac{\partial u}{\partial z} \right) + bu &= f & \forall z \in [0,1[, \forall t \in [0,T[\\ \text{(I-5)} \quad u(0,t) = u(1,t) &= 0 & \forall t > 0 \\ u(z,0) &= u_0(z) & \forall z \in [0,1] \end{aligned}$$

when the parameters $a \in \mathbb{R}^{+*}$ and $b \in \mathbb{R}^+$ have to be estimated from the measurement $z \in L^2(0,T)$ of the solution u at point $z = \frac{1}{2}$ against time. Here we have $x = (a,b) \in \mathbb{R}^2 = E$, C is a given closed subset of $\mathbb{R}^{+*} \times \mathbb{R}^+$, which represents the a-priori knowledge of the experimenter about the parameter $x=(a,b)$, and ϕ is the mapping which, to a given $x=(a,b) \in C$ makes correspond the $t \rightarrow u(\frac{1}{2},t)$ function of $L^2(0,T) = F$. In this example, the evaluation of $\phi(x)$ involves the resolution of the parabolic equation (I-5); the problem is obviously overspecified as $\dim F = +\infty > \dim E = 2$!

The second question is : why do we address the problem of uniqueness of local minima ? The only way of actually solving the above described parameter estimation problems is to undertake the minimization of J over C on a computer. However, optimization algorithms are only able to find local minima over closed set. Hence the least square problem (I-1) will be practically solvable by an optimization algorithm as soon as C is closed and J has at most one local minimum over C .

This will ensure that the optimization algorithm, once converged, will give the sought global minimum of J . One can also remark that the uniqueness of local minima implies (but is not equivalent to) the uniqueness of the solution \hat{x} of problem (I-1), or in terms of parameter estimation problems, the identifiability of \hat{x} from the knowledge of z and C . Of course, one other extremely important practical problem is that of the stability of the solution \hat{x} of (I-1) with respect to perturbations on the data z ; this problem will not be addressed as such in this paper, but one can remark that, when C is compact, the above uniqueness property will ensure the existence of a unique \hat{x} depending

continuously on z as long as the distance of z to $\phi(C)$ is taken small enough.

The third (and last) question is : what kind of conditions on C and ϕ are we looking for ? The first idea is that we want data-independent conditions : for a given set C and mapping ϕ , we want to be able to decide whether property (I-4) holds or not. If it holds we will get as a by product the upper limit $\gamma > 0$ to the distance of z to $\phi(C)$ for which the uniqueness property of local minima holds. If it does not hold the experimenter will then have to acquire more data (i.e. change the mapping ϕ) and/or augment the a priori available information (i.e. diminish the size of C) before checking again for property (I-4). The second idea is that such conditions will by no way be cheap ! As in view of the applications, no hypothesis will be made on the shape of C and ϕ (no convexity, no monotonicity), the conditions will necessarily involve exploration all over C - which of course will become extremely computer-time consuming as soon as the dimensions of C , i.e. the number of unknown parameters, increases.

Nevertheless, we believe that such condition will be practically useful for the problems with few unknown parameters, and that they at least will help to understand what happens in non linear least square problems. As test for the forthcoming sufficient condition for (I-4) to hold, we will add to example 1 an extremely simple example :

Example 2 Determine a real number x from the measurement (z_1, z_2) of its cosine and sine. Then we have :

$$(I-6) \quad E = \mathbb{R}, F = \mathbb{R}^2, \phi(x) = (\cos x, \sin x)$$

Of course, one has to restrict a priori the search for x to an interval of length smaller than 2π if we want the problem to have a chance of being well posed ! So suppose we take for example :

$$(I-7) \quad C = [0, X] \quad \text{with} \quad X \text{ given, } X < 2\pi.$$

Then obviously problem (I-1) has a unique global minimum as soon as $d(z, \phi(C)) < \gamma = \sin(X/2)$ as one can see on top of figure I-1 for different data z .

However one sees also on the same figure that there may exist, beside the global minimum, a distinct local minimum, (with value larger than γ !) so that the solution of (I-1) by an optimization algorithm may fail, as condition (I-4) is not satisfied !

In order to satisfy condition (I-4), it is sufficient to replace condition (I-7) by the stronger condition :

$$(I-8) \quad C = [0, X] \quad \text{with} \quad 0 < X < \pi.$$

Then, as one sees on the bottom of figure I-1, condition I-4 holds when

$$(I-9) \quad d(z, \phi(C)) < \sin X.$$

Conditions (I-8) plus (I-9) are clearly equivalent to (I-4), and will be used as bench mark to see how precise the condition which we will derive is.

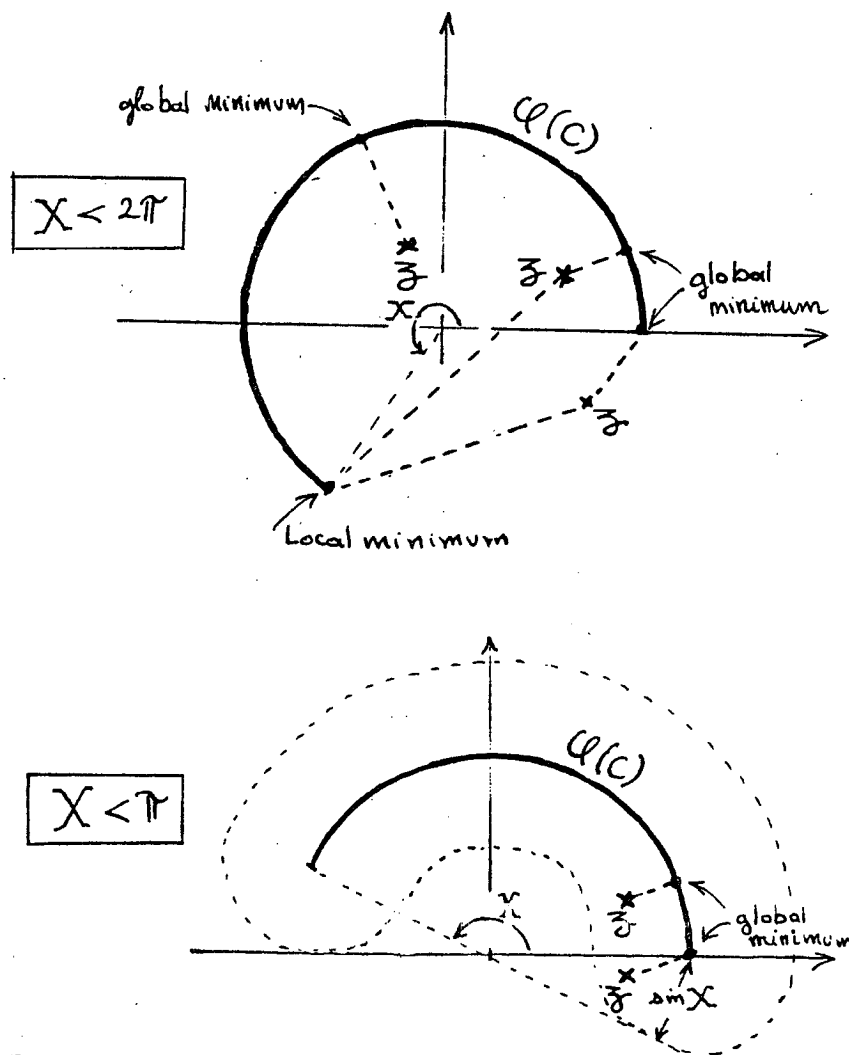


Figure I-1 : determination of $x \in [0, X]$ from the measurement z of $(\cos x, \sin x)$

To conclude this introduction, we will recall a previous result of J. Spiess (1969), who considered exactly the same problem, namely the uniqueness of local minima of problem (I-1), but set on an open and convex set C. In fact he gave data-dependant sufficient conditions, i.e. conditions, which, for a given data z and a given local minimum \hat{x} , imply that \hat{x} is a global minimum. These conditions, when translated into data-independent conditions, read as follows :

Spiess Condition : If

C is an open convex subset of E

ϕ is injective and ϕ^2 over C

$$(I-10) \gamma = \inf_{x,y \in C} \inf_{z \in [xy]} \frac{\|\phi'(z)(y-x)\|^2}{\|\phi''(z)(y-x, y-x)\|^2} \times \frac{\|\phi(x) - \phi(y)\|}{\|\phi(x) - \phi(z)\| + \|\phi(z) - \phi(y)\|} > 0$$

Then

J has at most one local minimum over the open set C as soon as $d(z, \phi(C)) < \gamma$.

If we apply this condition to the simple example 2, where we take now for convenience

$$(I-II) \quad C =]\epsilon, 2\pi - \epsilon[\quad , \quad \epsilon > 0 \text{ given}$$

one checks very easily that :

$$\frac{\|\phi'(z)(y-x)\|^2}{\|\phi''(z)(y-x, y-x)\|^2} = 1 \quad \text{for any } x, y, z$$

and that

$$\frac{\|\phi(x) - \phi(y)\|}{\|\phi(x) - \phi(z)\| + \|\phi(z) - \phi(y)\|} \text{ is minimum for } x, y, z \text{ as in figure I-2.}$$

Hence we get :

$$(I-12) \quad \gamma = \frac{\sin \epsilon}{\sqrt{2(1+\cos \epsilon)}} \sim \frac{1}{2} \sin \epsilon \text{ for small } \epsilon$$

So γ is strictly positive, and the sufficient condition is satisfied, in this example, for all $\epsilon > 0$.

Of course, as C is taken open, Spiess condition does not eliminate the local minima which may arise on $\phi(\partial C)$ (as on figure I-1 top), so that this condition does not answer to our second question. However, it may give a reasonable idea of the kind of condition we are going to derive in the next paragraphs, as they share the property of containing an infimum over couple of points (x,y) of C and over a path (here the $[x,y]$ interval) connecting them.

Let us now be more technical and turn to the derivation of our sufficient condition. The hypothesis and notations given at the beginning of the introduction will hold throughout the remaining of the paper and will not be repeated.

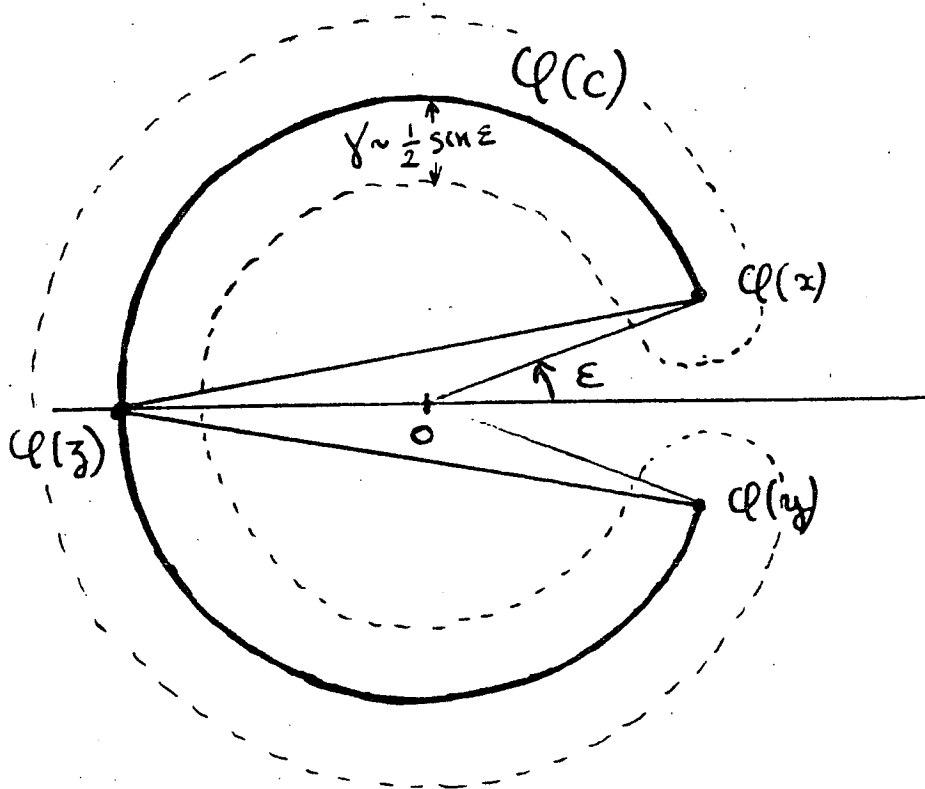


Figure I-2 : Application of the Spiess condition to example 2.

1 - HOW TO RECOGNIZE THE EXISTENCE OF TWO DISTINCT LOCAL MINIMA ?

Let $x, y \in C$, $x \neq y$, be two such local minima (see figure 1.1). Using the hypothesis that C is \mathcal{C}^2 -path-connected, we may choose one \mathcal{C}^2 -path going from x to y , i.e one \mathcal{C}^2 mapping $s : \theta \rightarrow s(\theta)$ from some $[\theta_0, \theta_1]$ interval of \mathbb{R} in E , satisfying

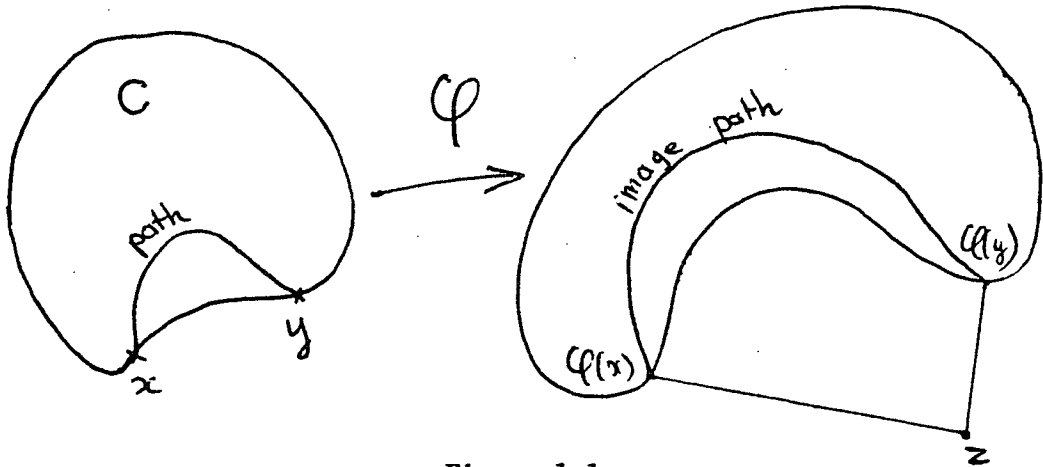


Figure 1.1

$$(1.1) \quad \begin{cases} s(\theta_0) = x, & s(\theta_1) = y \\ s(\theta) \in C & \forall \theta \in [\theta_0, \theta_1] \end{cases}$$

We consider now the function $f : [\theta_0, \theta_1] \rightarrow \mathbb{R}$ defined by :

$$(1.2) \quad f(\theta) = \| \phi(s(\theta)) - z \|^2 \quad \forall \theta \in [\theta_0, \theta_1]$$

which we have depicted on figure 1.2, in the case where $f(\theta_0) = \| \phi(x) - z \|^2 \geq f(\theta_1) = \| \phi(y) - z \|^2$

From the properties of x and y , it is clear that one can find θ_1' such that :

$$(1.3) \quad \begin{cases} \theta_0 < \theta_1' \leq \theta_1 \\ f(\theta) \geq f(\theta_0) = \| \phi(x) - z \|^2 & \forall \theta \in [\theta_0, \theta_1'] \\ f(\theta_1') = f(\theta_0) = \| \phi(x) - z \|^2 \end{cases}$$

From here two cases may occur :

$$i) f(\theta) \equiv f(\theta_0) \quad \forall \theta \in [\theta_0, \theta_1]$$

then of course $f''(\theta) = 0 \implies f''(\theta) \leq 0$

ii) $f(\theta) > f(\theta_0)$ for some subinterval of $[\theta_0, \theta_1]$, so that there exists some $\bar{\theta}$ in this interval such that $f''(\bar{\theta}) \leq 0$;

So if we set

$$(1.4) \quad y' = s(\theta_1)$$

we obtain the :

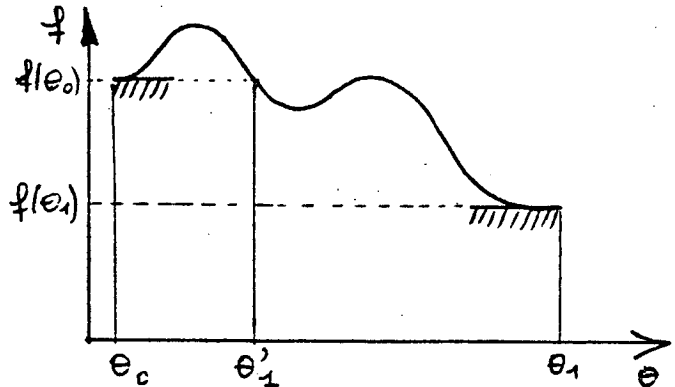


Figure 1.2.

Proposition 1 :

If :

$$z \in F$$

x, y = local minima of J over C , $x \neq y$ ($\| \phi(x) - z \|^2 \geq \| \phi(y) - z \|^2$)

$s : [\theta_0, \theta_1] \rightarrow C$ - path from x to y

Then :

there exists $\theta_1' \in]\theta_0, \theta_1]$ such that $f(\theta_1') = f(\theta_0) = \| \phi(x) - z \|^2$ and there exists $\bar{\theta} \in]\theta_0, \theta_1[$ such that $f''(\bar{\theta}) \leq 0$

2 . GIVEN $z \in F$, $x, y' \in C$ SUCH THAT $\| \phi(z) - z \| = \| \phi(y') - z \| = 0$ AND A PATH s FROM x TO y' , WHAT DOES $f''(\bar{\theta}) < 0$ IMPLY ?

Let us first introduce some quantities related to the image-path $\{ \phi(s(\theta)), \theta \in [\theta_0, \theta_1] \}$ in F :

$$(2.7) \quad \begin{cases} v(\theta) = \phi'(s(\theta)) \cdot s'(\theta) & \text{- velocity,} \\ a(\theta) = [\phi'(s(\theta)) \cdot s'(\theta)]' & \text{- acceleration.} \end{cases}$$

Then the first and second derivatives of $f(\theta)$ can be expressed

as :

$$(2.2) \quad f'(\theta) = 2 \langle \phi(s(\theta)) - z, v(\theta) \rangle$$

$$(2.8) \quad f''(\theta) = 2 \|v(\theta)\|^2 + 2 \langle \phi(s(\theta)) - z, a(\theta) \rangle$$

From (8) we get :

$$(2.4) \quad |f'(\theta)| \leq 2 f(\theta)^{\frac{1}{2}} \|v(\theta)\|$$

which together with (2.3) and the Cauchy-Schwarz inequality yield :

$$(2.5) \quad f''(\theta) \geq \frac{f'(\theta)^2}{2f(\theta)} - 2 f(\theta)^{\frac{1}{2}} \|a(\theta)\|$$

We define now a function $g : [\theta_0, \theta_1] \rightarrow \mathbb{R}$ by the following 1-D elliptic problem :

$$(2.6) \quad \begin{aligned} -g''(\theta) &= \|a(\theta)\| & \forall \theta \in [\theta_0, \theta_1] \\ g(\theta_0) &= g(\theta_1) = 0 \end{aligned}$$

We may remark that this function g is independant of z (whereas f was not!), and that it is a positive concave function.

Plugging (2.6) into (2.5) yields then :

$$\text{i.e.} \quad \frac{f''(\theta)}{2f(\theta)^{\frac{1}{2}}} - \frac{f'(\theta)^2}{4f(\theta)^{\frac{3}{2}}} - g''(\theta) \geq 0$$

$$(2.7) \quad \frac{d^2}{d\theta^2} [f(\theta)^{\frac{1}{2}} - g(\theta)] \geq 0$$

which proves that the function $\theta \rightarrow f(\theta)^{\frac{1}{2}} - g(\theta)$ is convex, and hence, as $f(\theta_0) = f(\theta_1) = d$ (where d is the common value of $\|\phi(x) - z\|$ and $\|\phi(y') - z\|$) :

$$(2.8) \quad f(\theta)^{\frac{1}{2}} \leq g(\theta) + d \quad \forall \theta \in [\theta_0, \theta_1]$$

But on the other hand, from $f''(\bar{\theta}) \leq 0$ we get, using (2.3) and the Cauchy-Schwartz inequality :

$$0 \geq f''(\bar{\theta}) \geq 2 \|v(\bar{\theta})\|^2 - 2 f(\bar{\theta})^{\frac{1}{2}} \|a(\bar{\theta})\|$$

and hence :

$$(2.9) \quad f(\bar{\theta})^{\frac{1}{2}} \geq \frac{\|v(\bar{\theta})\|^2}{\|a(\bar{\theta})\|}$$

From (2.8) and (2.9) we get then :

$$(2.10) \quad d \geq \frac{\|v(\bar{\theta})\|^2}{\|a(\bar{\theta})\|} - g(\bar{\theta})$$

So we have proven the

Proposition 2 :

If

$z \in F$

$x, y' \in C$ such that $\|\phi(x) - z\| = \|\phi(y') - z\| = d$

$s : [\theta_0, \theta_1] \rightarrow C$ a path from x to y'

then

$\bar{\theta} \in [\theta_0, \theta_1]$

$f''(\bar{\theta}) \leq 0$

$$\implies d \geq \frac{\|v(\bar{\theta})\|^2}{\|a(\bar{\theta})\|} - g(\bar{\theta})$$

3 - A FAMILY OF SUFFICIENT CONDITION FOR THE UNIQUENESS OF CERTAIN LOCAL MINIMA OF PROBLEM (I-1)

Suppose we have chosen a strategy S in order to associate to every couple (x, y) of points of C a C^2 -path s from x to y :

$$S : (x, y) \in C \times C \quad s = S(x, y) : [\theta_0, \theta_1] \rightarrow C \text{ st } \begin{cases} s(\theta_0) = x \\ s(\theta_1) = y \\ s \text{ is } C^2 \end{cases}$$

Then from propositions 1 and 2 we get immediately the following sufficient condition :

Proposition 3 (sufficient condition associated to the strategy S) :

Suppose that

$$(3.1) \quad \gamma = \inf_{x, y \in C} \inf_{\substack{s=S(x, y) \\ \theta \in [\theta_0, \theta_1]}} \left\{ \frac{\|v(\theta)\|^2}{\|a(\theta)\|^2} - g(\theta) \right\} > 0$$

Then the problem (I-1) has at most one local minimum with value smaller than γ as soon as $d(z, \phi(C)) < \gamma$.

This condition does not look very handy. But before simplifying it somewhat and indicating which strategy S to choose, let us explicit on a simpler case its meaning.

Example 3 Suppose that

C is convex (and hence C^2 -path-connected !)

ϕ is such that numbers $\alpha > 0$, $\beta > 0$ exist with

$$(3.2) \quad \begin{cases} \|\phi'(x) \cdot y\| \geq \alpha \|y\| \\ \|\phi'(x)(y, y)\| \leq \beta \|y\|^2 \end{cases} \quad \forall x \in C, \quad \forall y \in E$$

$$(3.3) \quad S(x, y) = s \quad \text{defined by} \quad \begin{aligned} \theta_0 &= 0, \quad \theta_1 = 1 \\ s(\theta) &= x + \theta(y-x) \end{aligned}$$

Then

$$\begin{aligned} \|v(\theta)\| &\geq \alpha \|y-x\| \\ \|a(\theta)\| &\leq \beta \|y-x\|^2 \end{aligned}$$

and hence, from the maximum principle :

$$g(\theta) \leq \frac{\beta}{2} \|y-x\|^2 \theta(1-\theta) \leq \frac{\beta}{8} \|y-x\|^2$$

and :

and :

$$\frac{\|v(\theta)\|^2}{\|a(\theta)\|^2} - g(\theta) \geq \frac{\alpha^2}{\beta} - \frac{\beta}{8} \|y-x\|^2$$

Then from proposition 3 we get the (weaker) sufficient condition :

Proposition 4

Suppose that (3.2) holds and that :

$$(3.4) \quad \gamma = \inf_{(x,y) \in C} \left\{ \frac{\alpha^2}{\beta} - \frac{\beta}{8} \|y-x\|^2 \right\} > 0$$

or equivalently

$$\beta \text{ diam } C < 2\sqrt{2} \alpha \quad \text{and} \quad \gamma = \frac{\alpha^2}{\beta} - \frac{\beta}{8} (\text{diam } C)^2$$

Then the problem I-1 has at most one local minimum with value smaller than γ as soon as $d(z, \phi(C)) < \gamma$.

This result was already given in [1] together with a lipschitz continuity result of the $z \rightarrow \hat{x}$ mapping and, in the case where E is a Banach space, an existence result for \hat{x} .

However, the estimation (3.4), which involves upper and lower bounds, over all $x \in C$ and for all directions y , are very rough, and may yield too restrictive conditions on the size of C for practical use.

So we come back to the less constraining estimation (3.1) of proposition 3.

4 - CHOICE OF A STRATEGY S

The problem is now to choose the strategy S, which associates to any couple $(x,y) \in C \times C$ a C^2 -path s from x to y , in such a way that the number γ defined by (3.1) is the largest possible (and hence the "size" condition on C the least restrictive possible).

For given $x,y \in C$, the choice of a path going from x to y can be conceptually split into two steps :

- choose the geometry of the path,
- choose the time-law, i.e. the parametrization of the path.

We will choose these two items separately.

4.1 - For given $x, y \in C$ and a given geometry of a path from x to y , how to choose the time-law ?

We consider first a particular parametrization $\hat{s}(\hat{\theta})$ of the path from x to y where $\hat{\theta}$ is the curvilinear abscissa on the image path $\phi \circ \hat{s}(\theta)$.

Such a parametrization satisfies, by definition :

$$(4.1) \quad \|\dot{\hat{\theta}}\| = \|\phi'(\hat{\theta}) \cdot \dot{\hat{\theta}}\| = 1$$

and will exist as soon as $\phi'(x)$ is injective everywhere over C . At points where $\phi'(x)$ is not injective, $\dot{\hat{\theta}}$ may still exist, but $\dot{\hat{\theta}}$ will have to be infinite.

By deriving (4.1) we get, as usual, that, on the image path, the velocity $\dot{\hat{\theta}}$ and the acceleration $\hat{a}(\hat{\theta})$ are orthogonal :

$$(4.2) \quad \hat{a}(\hat{\theta}) = [\phi'(\hat{s}) \cdot \hat{s}']' \perp \dot{\hat{\theta}} = \phi'(\hat{s}) \cdot \hat{s}'$$

We consider then any other parametrization $s(\theta)$ of the same geometric path, which is necessarily of the form :

$$(4.3) \quad \begin{aligned} s(\theta) &= \hat{s}(\chi(\theta)) \\ \text{where } \chi &: [\theta_0, \theta_1] \rightarrow [\hat{\theta}_0, \hat{\theta}_1] \end{aligned}$$

One checks then easily that :

$$(4.4) \quad \begin{aligned} v(\theta) &= \chi'(\theta) \dot{\hat{\theta}} \\ a(\theta) &= \chi'(\theta)^2 \hat{a}(\hat{\theta}) + \dot{\hat{\theta}} \chi''(\theta) \end{aligned}$$

But as $\hat{a}(\hat{\theta})$ and $\hat{v}(\hat{\theta})$ are orthogonal we get

$$(4.5) \quad \|a(\theta)\| = \left\{ \chi'(\theta)^4 \|\hat{a}(\hat{\theta})\|^2 + \chi''(\theta)^2 \|\hat{v}(\hat{\theta})\|^2 \right\}^{1/2}$$

and hence

$$(4.6) \quad \|a(\theta)\| \geq \chi'(\theta)^2 \|\hat{a}(\hat{\theta})\|$$

In order to compare the numbers $\hat{\gamma}$ and γ associated by (3.1) to the two parametrizations $\hat{s}(\hat{\theta})$ and $s(\theta)$ of the same geometrical path, we compare the arguments of the inf in (3.1) :

i) Obviously one gets from (4.4) and (4.6)

$$\frac{\|v(\theta)\|^2}{\|a(\theta)\|} \leq \frac{\chi'(\theta)^2 \|\hat{v}(\hat{\theta})\|}{\chi'(\theta)^2 \|\hat{a}(\hat{\theta})\|} = \frac{\|\hat{v}(\hat{\theta})\|^2}{\|\hat{a}(\hat{\theta})\|}$$

ii) In order to compare $g(\theta)$ and $\hat{g}(\hat{\theta})$, we set

$$(4.8) \quad \tilde{g}(\theta) = \hat{g}(\chi(\theta))$$

and will compare $g(\theta)$ and $\tilde{g}(\theta)$. One first checks easily that $\tilde{g}(\theta)$ satisfies the following equation :

$$(4.9) \quad \begin{cases} -\tilde{g}''(\theta) = \chi'(\theta)^2 \|\hat{a}(\chi(\theta))\| & \forall \theta \in [\theta_0, \theta_1] \\ \tilde{g}(\theta_0) = \tilde{g}(\theta_1) = 0 \end{cases}$$

Comparing with the equation defining $g(\theta)$

$$(4.10) \quad \begin{cases} -g''(\theta) = \|a(\theta)\| & \forall \theta \in [\theta_0, \theta_1] \\ g(\theta_0) = g(\theta_1) = 0 \end{cases}$$

we get, using (4.6) and the maximum principle :

$$g(\theta) \geq \tilde{g}(\theta) \quad \forall \theta \in [\theta_0, \theta_1]$$

and hence

$$(4.11) \quad g(\theta) \geq \hat{g}(\hat{\theta})$$

Summarizing the results (4.7) and (4.11) we get :

$$\frac{\|v(\hat{\theta})\|^2}{\|a(\hat{\theta})\|} - g(\hat{\theta}) \geq \frac{\|v(\theta)\|^2}{\|a(\theta)\|} - g(\theta)$$

which proves that

$$(4.12) \quad \hat{\gamma} \geq \gamma$$

CONCLUSION : For a given geometric path going from x to y , the best parametrization is obtained when θ is the curvilinear abscissa on the image-path.

In the sequel, we will omit the hat on s , θ , etc... and θ will always denote the curvilinear abscissa on the image path.

With this parametrization, the formula (3.1) simplifies somewhat, and moreover gains a geometrical interpretation : now the radius of curvature $\rho(\theta)$ of the image path at point $\phi \circ s(\theta)$ is given, as $\|v(\theta)\| = 1$ and $v(\theta) \perp a(\theta)$, by :

$$(4.13) \quad \rho(\theta) = \frac{1}{\|a(\theta)\|}.$$

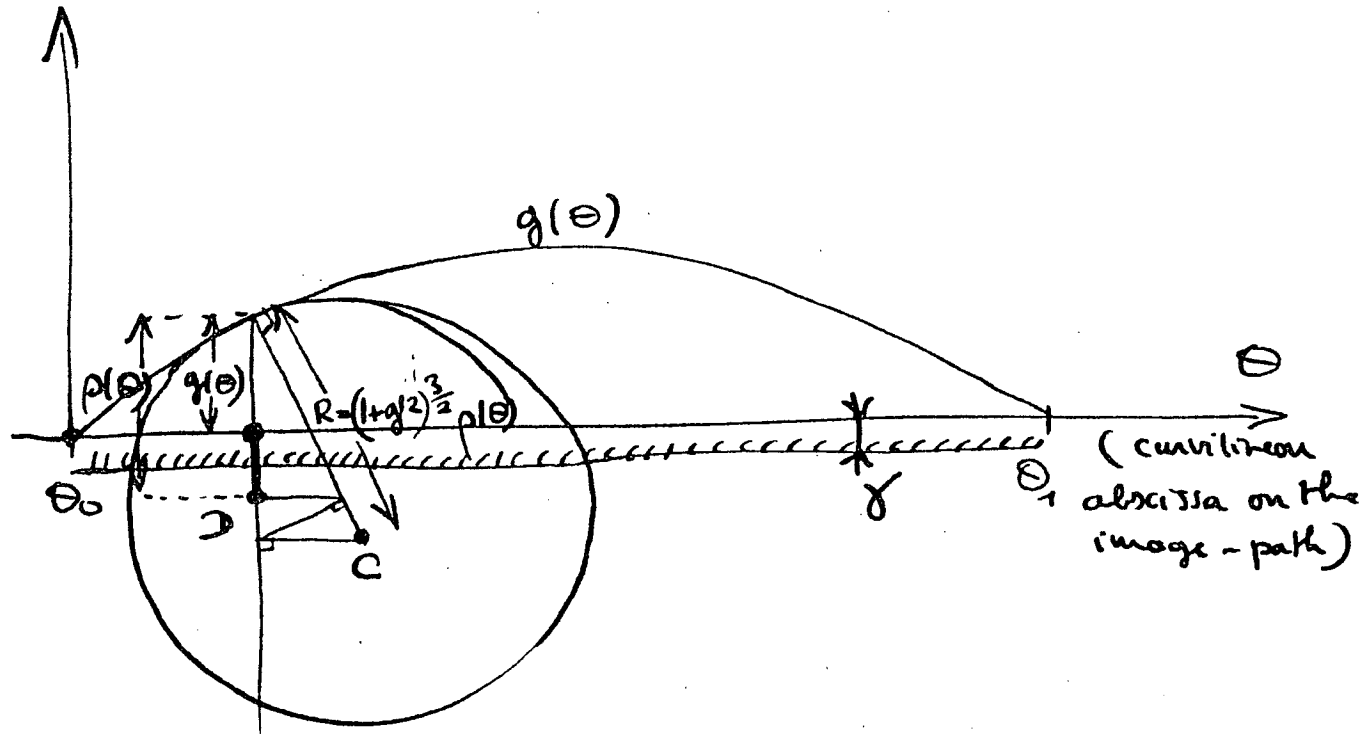
Hence, when the parameter θ is chosen to be the curvilinear abscissa along the image path, (3.1) reduces to :

$$(4.14) \quad \gamma = \inf_{x,y \in C} \inf_{\substack{s=S(x,y) \\ \theta \in [\theta_0, \theta_1]}} \{ \rho(\theta) - g(\theta) \} > 0$$

where $g(\theta)$ is defined by :

$$(4.15) \quad \begin{cases} -g''(\theta) = \frac{1}{\rho(\theta)} \\ g(\theta_0) = g(\theta_1) = 0 \end{cases} \quad \text{for } \theta_0 \leq \theta \leq \theta_1$$

Figure 4.1 :



We have illustrated on figure 4.1 a geometrical construction of γ from the data of the $\theta \rightarrow g(\theta)$ function : the point D should never get above the horizontal hatched line.

4.2 . GIVEN $x, y \in C$, GIVEN A PATH s FROM x TO y , AND GIVEN TWO POINTS x', y' BELONGING TO THAT PATH s , HOW DO γ (ASSOCIATED TO x, y) AND γ' (ASSOCIATED TO x', y') COMPARE ?

If x' and y' correspond to the parameters θ'_0 and θ'_1 of the $[\theta_0, \theta_1]$ interval, it is clear from figure 4.2 and from the maximum principle for elliptic equations that :

(4.16) $\gamma' \geq \gamma$

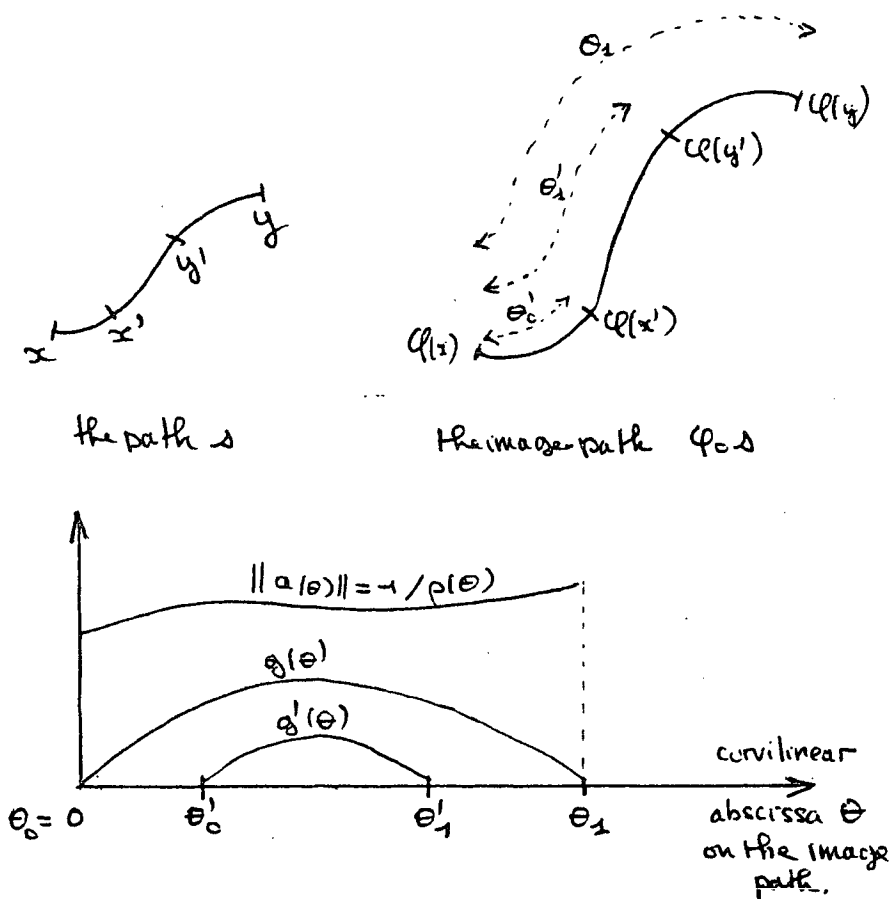


Figure 4.2

CONCLUSION : As soon as the strategy S chosen is stable with respect to restriction (i.e. if $S(x',y') = S(x,y) |_{[\theta_0',\theta_1']}$), it is sufficient, in order to calculate γ , to consider only couples of the boundary ∂C of C

Hence (3.1) or (4.14) reduce to :

$$(4.16) \quad \gamma = \inf_{x,y \in \partial C} \inf_{\substack{s=S(x,y) \\ \theta \in [\theta_0, \theta_1]}} \left\{ \rho(\theta) - g(\theta) \right\} > 0$$

where

θ is the curvilinear abscissa along the image path

and where $g(\theta)$ is defined by

$$(4.15) \quad \begin{aligned} -g''(\theta) &= \frac{1}{\rho(\theta)} && \text{for } \theta_0 \leq \theta \leq \theta_1 \\ g(\theta_0) &= g(\theta_1) = 0 \end{aligned}$$

4.3 - HOW TO CHOOSE THE GEOMETRICAL PATH FROM x TO y ?

For a given $x, y \in \partial C$, we are now looking for a path s from x to y , which will be parametrized by the curvilinear abscissa θ along the image path $\phi \circ s$, such that the quantity

$$(4.17) \quad \inf_{\theta \in [\theta_0, \theta_1]} \left\{ \rho(\theta) - g(\theta) \right\}$$

appearing in (3.1) or (4.14) is maximum.

The first remark is that the quantity (4.17) depends only on the geometrical properties of the image path $\phi \circ s$ going from $\phi(x)$ to $\phi(y)$:

θ is the curvilinear abscissa along this path
 $\rho(\theta)$ is the radius of curvature of this path
 $g(\theta)$ is defined from θ_0 , θ_1 and $\rho(\theta)$

So we can replace ⁽¹⁾ the task of choosing a path s from x to y in C by that of choosing a path S from $\phi(x)$ to $\phi(y)$ in $\phi(C)$ in such a way that the quantity (4.17) is maximized.

In this new setting the mapping ϕ is used only, together with the set C , for the definition of the set $\phi(C)$ in which the sought path S has to stay.

The second remark is that, whenever the segment $[\phi(x), \phi(y)]$ is fully included in $\phi(C)$ then one can choose $S = [\phi(x), \phi(y)]$, which yields $\rho(\theta) = +\infty$ and $g(\theta) = 0$, hence $\gamma = +\infty$ so that S is obviously the sought optimal solution !

The third remark is that, if one chooses a path S from $\phi(x)$ to $\phi(y)$ with both large radii of curvature and a large length $\theta_1 - \theta_0$, as the one depicted in figure 4.3, for which we have :

$$\left\{ \begin{array}{l} \rho(\theta) = R > 0 \\ \theta_0 = 0, \theta_1 = 2\pi R \end{array} \right. \quad \forall \theta \in [\theta_0, \theta_1]$$

Then the function g is of the form

$$g(\theta) = \frac{1}{2R} (\theta - \theta_0)(\theta_1 - \theta) \quad \forall \theta \in [\theta_0, \theta_1]$$

and is maximum at the point $\theta = \frac{\theta_0 + \theta_1}{2} = \pi R$

$$g(\pi R) = \frac{\pi^2}{2} R$$

so that

$$\rho(\pi R) - g(\pi R) = \left(1 - \frac{\pi^2}{2}\right) R \geq 0 .$$

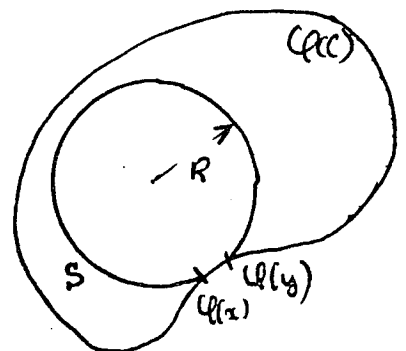


Figure 4.3

(1) at least conceptually !

So we see that paths S with both large ρ and large length are not optimal.

From the two last remarks, we may conjecture that the optimal S is the minimum-length path going from $\phi(x)$ to $\phi(y)$ in $\phi(C)$ - But this still remains to be proved.

So we can propose two strategies for the choice of the path s from x to y :

Strategy 1 determine a path s from x to y in such a way that $S = \phi \circ s$ is the minimum-length path going in $\phi(C)$ from $\phi(x)$ to $\phi(y)$. This procedure may (if our conjecture is true !) yield the optimal number γ , and hence the less constraining condition on the size of C .

However, from the practical point of view, such strategy seems very difficult to implement, as one would have to solve, for each couple $x, y \in C$, a complicated optimization problem in a high dimensional space.

Strategy 2 choose s as the minimum length path going in C from x to y . This procedure is surely non-optimal, but will guarantee that the corresponding image path $S = \phi \circ s$ will not have a too great length, as soon as upper bounds on $\|\phi'(x)\|$ are available. Moreover, as the set C is defined by explicit constraints, and is usually of non-void interior, the minimum length path in C from x to y can be determined relatively easily (in many cases it will be the $[x, y]$ interval).

To conclude this paragraph, let us see, on the very simple example 2 of the introduction, how close our final condition (4.14) (4.15) with strategy 1 or 2 comes to the solution of this example.

We have seen in the introduction (see figure I-1 and formula (I-8)) that the least square functional for the search of a real number x from measurements of its cosine and sine had a unique local minimum with value smaller than $\gamma = \sin \frac{X}{2}$ (which of course is the global minimum) as soon as we search for x in the $[0, X]$ interval with $X < 2\pi$.

If we now apply condition (4.16) (4.15) to this problem, we have to compute the argument of the infimum in (4.16) only for a path going from 0 to X . Obviously, the path

$$(4.18) \quad s(\theta) = \theta, \quad 0 \leq \theta \leq X$$

has all the desired properties :

θ is the curvilinear abscissa are the one of circle which is the image of the $[0,x]$ interval by the ϕ function defined in (I-6).

s yields the minimal length path as well in the image set as in the parameter set so strategies 1 and 2 are equivalent here.

Along this path, one has :

$$\rho(\theta) = 1 \quad (\text{radius of curvature of image circle})$$

and hence

$$g(\theta) = \frac{1}{2} \theta(X-\theta)$$

which is maximum at $\theta = \frac{X}{2}$:

$$g(\theta) \leq g\left(\frac{X}{2}\right) = \frac{X^2}{8}$$

Hence we get from (4.16) the condition

$$\gamma = 1 - \frac{X^2}{8} > 0$$

or :

$$X < 2\sqrt{2} = 2,828$$

which is to be compared to the best possible condition $\chi < 2\pi$ exhibited for this example in the introduction. We see that the result is not too bad, but as $2\sqrt{2} < 2\pi$ we cannot conclude whether the condition (4.16) (4.15) with strategy 1 is optimal or not. But one may remark that $2\sqrt{2} < \pi$, which proves that, on this example, our condition $\gamma > 0$ yields in fact uniqueness of all local minima.

5 . NUMERICAL APPLICATION

For historical reasons, the numerical application we are going to present was not made using (4.14) with the curvilinear abscissa in the data-space parametrization, but using a weaker version of (3.1) with constant-velocity-in-the-parameter-space time law. The geometry of the path going from x to y was given by strategy S_2 of paragraph 4.3 (minimum length in the parameter space), and C was taken convex.

Hence, for any $x, y \in C$ the path $s(\theta)$ was :

$$(5.1) \quad s(\theta) = x + \theta (y-x) \quad \theta \in [0,1]$$

The sufficient condition for (3.1) was obtained in the following way : using the fact that, for any $v \in H_0(0,1) = \left\{ v \in L^2(0,1) \mid v' \in L^2(0,1), v(0) = v(1) = 0 \right\}$, one has $|v(\theta)| \leq \frac{1}{2} \|v'\|_{L^2(0,1)}$ and $\|v\|_{L^2(0,1)} \leq \frac{1}{\pi} \|v'\|_{L^2(0,1)}$, and that, from its definition (2.6) as the solution of an elliptic boundary value problem, the function g satisfies $\|g'\|_{L^2(0,1)}^2 \leq \|g\|_{L^2(0,1)} \times \|a\|_{L^2(0,1)}$, we get the following majoration for $g(\theta)$:

$$(5.2) \quad |g(\theta)| \leq \frac{1}{2\pi} \|a\|_{L^2(0,1)}$$

Thus a sufficient condition for (3.1) to hold is :

$$(5.3) \quad \gamma = \inf_{x,y \in \partial C} \left\{ \inf_{\theta \in [0,1]} \frac{\|v(\theta)\|^2}{\|a(\theta)\|} - \frac{1}{2\pi} \|a\|_{L^2(0,1)} \right\} > 0$$

We applied the condition (5.3) to example 1 of the introduction. However, rather than checking, for a priori given admissible parameter sets C , if condition (5.3) holds or not, we used an alternative approach : supposing we have been given by engineer some nominal value $\bar{x} = (\bar{a}, \bar{b}) \in \mathbb{R}^{+*} \times \mathbb{R}^+$ of the unknown parameters, we tried to answer the question "how large can the parameter set C be chosen around (\bar{a}, \bar{b}) , still maintaining the uniqueness of local minima of problem I-1 over C ?" This amounts to find, "around" a given \bar{x} , the "largest" set \bar{C} for

which $\gamma=0$ so that any set C strictly included in \bar{C} will yield strictly positive γ . This was done by computing the value of the argument of the infimum in (5.3) for segments on increasing length centered at \bar{x} and lying on a finite number of straight lines going through \bar{x} , until one reaches, in each direction the zero value. At this stage, all couples $[x, 2\bar{x}-x] \in \partial C$ which are symmetrical with respect to \bar{x} have been tested. Then the couples (x,y) with $y \neq x$ one tested, eventually diminishing the length of one $[x, 2\bar{x}-x]$ interval if the argument of (5.3) happens to be negative for the $[x,y]$ segment. Of course, this procedure will produce domains dependant on the order in which the (x,y) segments are tested in the second part of the algorithm.

The numerical results, taken from Charles, are shown on figure 5.1. The interesting thing to be noted is that the size of the "maximal" sets given by condition (5.3) is already not ridiculous from a practical point of view. Using condition (4.16) would yield still larger sets, with no basic increase in computational time. On the other hand, the use of the much more restrictive condition (4.3) would lead, in this examples, to maximal set of the size of a point on the figure 5.1, and is thus inadequate for practical use.

6 . CONCLUSION

We have studied the uniqueness of the local minima of general non-linear least square problems, under the main hypothesis that the mapping to be inverted is regular C^2 and has an injective derivative. We have derived for that a sufficient condition which involves a minimization over all geodesic curves of the image set of a quantity which involves the radius of curvature of the geodesic curve and a function related to the radius of curvature through the resolution of an elliptic problem (see (4.16)). This condition has been optimized among a class of possible sufficient conditions, but it is not known wether or not it is the best possible condition. However, numerical examples have shown that the proposed condition makes it possible obtain practically interesting results for a two parameter estimation problem.

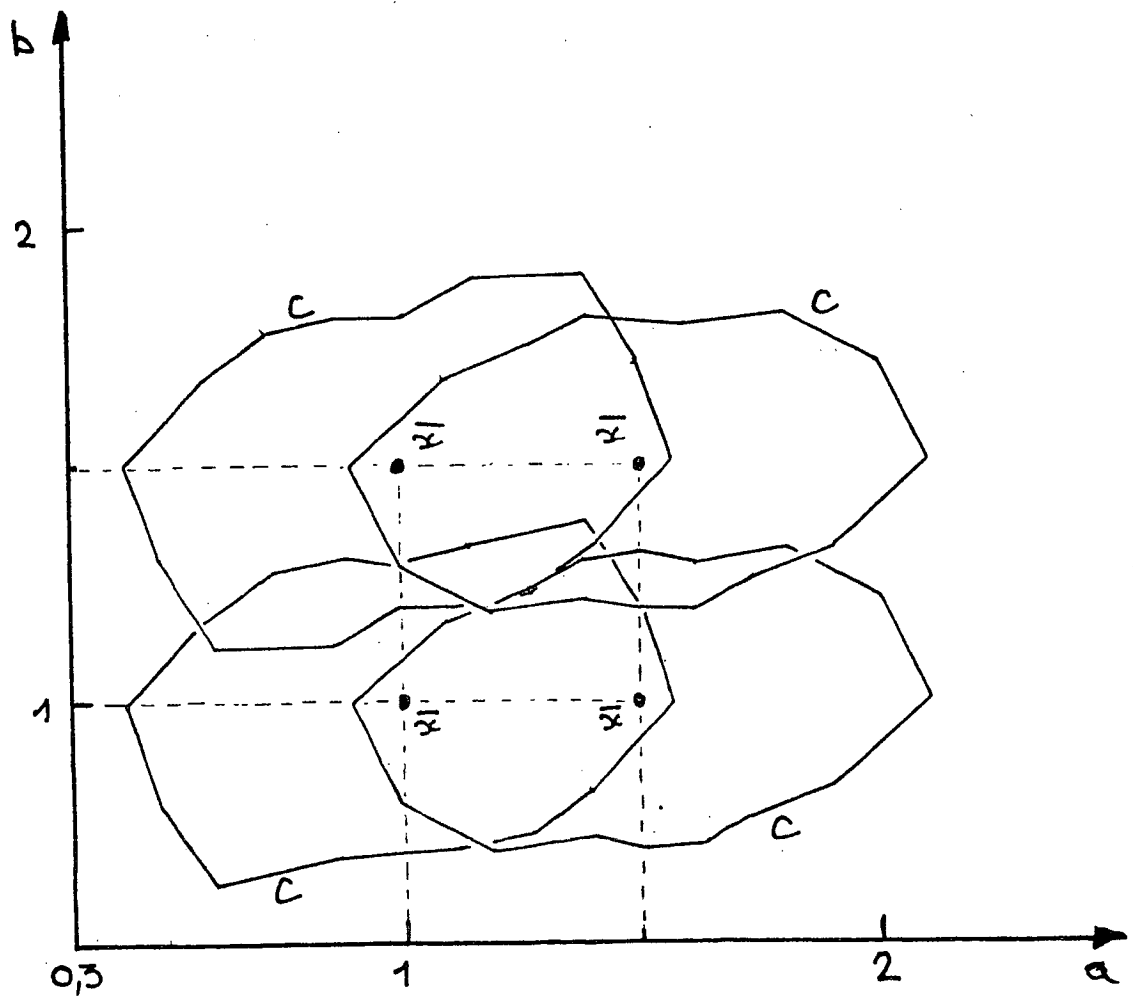


Figure 5.1 : "Maximal" sets C obtained for example 1 around different nominal values $\bar{x} = (\bar{a}, \bar{b})$ of the parameters.

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