REGRE: A COMBINED METHOD FOR THE COMPUTER SOLUTION OF OPTIMIZATION PROBLEMS WITH CONSTRAINS

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RESUMEN

Se presenta un nuevo método para la resolución de problemas de optimización de funciones objetivos no lineales con restricciones lineales o no lineales. Este método se basa en la combinación de un método derivativo y otro de búsqueda directa. La selección de los algoritmos se realizó teniendo en cuenta la velocidad de convergencia y la precisión en la resolución de problemas de este tipo.

Se concluye que este método es muy eficiente debido a que es capaz de llegar a la solución aún en aquellos casos en que otros algoritmos iterativos pueden diverger. Se presentan en tablas los resultados numéricos alcanzados y las comparaciones con otros métodos.

ABSTRACT

A new method for the solution of optimization problems of non - linear objetive functions with linear or non-linear constraints is shown. The new method is based on a combination of a derivative method and a direct search method. The choice of algorithms was made taking into account the convergence rate and precision in the solution of this type of problems.

To sum up, this method is very efficient since it can arrive at the solution even in cases where other iterative algorithms diverge. The numerical results achieved and their comparisons with the results obtained by other methods are given in different tables.

SCOPE

The determination of the optimum of an objetive non-linear function subjected to linear or non-linear restrictions is a problem which very frecuently occurs in the different stages of the technological and scientific knowledge development. Thus, in Chemical Engineering we have problems such as:

- Parameter estimation
- Sequential experimental design for discrimination among rival models.
- Sequential experimental design for precise parameter estimation
- Solution of algebraic and trascendent equations.
- Optimun design and operation of industrial equipment and processes.

These problems are generally solved as optimization problems by means of the appropiate numerical method.

There is a large bibliography about algorithms to be used in the solution of optimization problems. Each algorithm can be used to solve rapidly and precisely a given type of optimization problem.

However, these algorithms may fail when used in the solution of other problems in which the objetive function is of the same type for which the algorithms have been developed. The failure of the algorithm can be detected in some cases when the optimun value of the objetive function is previously known.

There are, however, many problems where this value is unknown, for example in non-linear regressions where neither the model nor the variance of the experimental error is accurately known.

According to the authors' experience and the work of Spang (1962) Rosembrock & Storey (1966), Berveridge & Schechter (1970) and Buzzi & Casapollo (1972a);these difficulties can be convenienty overcome applying a new method based on a combination of algorithms.

A combination between a derivative and a direct search method is developed in this paper in order to solve optimization problems of non linear objective functions subjected to linear or non-linear constraints. The algorithms were chosen considering the convergence rate and the precision achieved in solving optimization problems of different types.

OPTIMIZATION PROBLEMS AND FORMULATION OF THE OBJECTIVE FUNCTIONS

1. Algebraic and Transcendental Equation System (Buzzi & Casapollo, 1972a)

An algebraic or transcendental system of p equations with the same number of unknowns is written as:

$$\underline{f}\ (\underline{b}) = \underline{0} \qquad (1)$$

In the non-linear systems, the determination of vector $\underline{b}$ values in eqn. (1) is generally subjected to "r" linear or non-linear constraints.

$$\underline{R}_1 (\underline{b}) \leq \underline{Q} (\underline{b}) \leq \underline{R}_2 (\underline{b}) \tag{2}$$

In expressing equation (1) as an optimization problem, the following objective function is obtained:

$$F = \min_{\{\underline{b}\}} \left[\sum_{i=1}^{p} f_i^2 \right] \tag{3}$$

This function is subjected to constraints imposed by equation(2).

2. Parameter Estimation (Draper & Smith (1966),Kitrell (1966), Beck & Arnold (1977), Froment & Hosten (1981), Quiroga & Gottifredi (1982).

The most general case of parameter estimation belongs to the multiple response models with interdependent experimental errors and covariance matrix of unknown experimental errors.

The following objetive function is obtained from the maximum likelihood principle:

$$F = \min_{\{\underline{b}\}} \left[\det (\Psi) \right] \tag{4}$$

However,if the covariance matrix of experimental errors is known the objetive function is:

$$F = \min_{\{\underline{b}\}} \left[\sum_{i=1}^{v} \sum_{k=1}^{v} W_{ik} \sum_{j=1}^{n} (Y_{ji} - \eta_{ji})(Y_{ik} - \eta_{jk}) \right] \tag{5}$$

From a mathematical point of view, equation (5) can be adapted to different statistical considerations used in parameter estimation.

3. Sequential Experimental Design for Discrimination among Rival Models. (Box & Hill (1967)).

For the discrimination among rival models Box and Hill deduced the following expression from the information theory:

$$F = \max_{\{X_{=n+1}\}} \left[\sum_{i=1}^{m-1} \sum_{j=1+1}^{m} \pi_{i,n} \pi_{j,n} \left\{ \frac{\sigma_i^2 - \sigma_j^2}{(\sigma^2 + \sigma_i^2)(\sigma^2 + \sigma_j^2)} + \right. \right. \tag{6}$$

$$\left. \left. + (\hat{Y}_n^i - \hat{Y}_n^j)^2 \left(\frac{1}{\sigma^2 + \sigma_i^2} + \frac{1}{\sigma^2 + \sigma_j^2} \right) \right\} \right].$$

4. Sequential Experimental Design for Precise Parameter Estimation. (Hunter et al (1969), Kittrel et al. (1968), Buzzi & Donatti (1970), Hosten (1974), Hosten & Emig (1975), Froment & Hosten (1981)).

The following equation represents a criterion for an experimental sequential design for a precise parameter estimation, given by Box and Lucas (1959).

$$F = \underset{\{\underset{=}{X}_{n+1}\}}{\text{Max}} \left\{ \det \left| \sum_{i=1}^{v} \sum_{j=1}^{n} \sigma^{ij} \; \underset{=}{X}_i^T \; \underset{=}{X}_j \right| \right\} \qquad (7)$$

These are only some of optimization problems that very frequently occur in Chemical Engineering and related subjects. They require the use of numerical methods for their solution.

Equations (4) & (7) define several types of objetive functions, therefore a general optimization program must take these observations into account.

Algorithm Choice

Buzzi and Casapollo's detailed analysis on the most important algorithms, and their respective modifications (1972 a,b) have been suggested as the numerical techniques to solve optimization problems. Their analysis emphasizes algorithm classification, its advantages and disadvantages, and the criteria which have been suggested to overcome the critical situations.

Buzzi and Casapollo used their analysis to make a program to solve problems similar to those represented in equations (1) and (2). They selected the Newton-Raphson method and the Nelder & Mead method as basic algorithms.

The authors of this paper have studied the behaviour of the Nelder & Mead method in the resolution of problems similar to those shown in equation (5) by means of a simulation technique of generated data through a numerical integration system. It was noticed, even in the simplest case of a single response, that the method could not solve the problem with precision.

The following conclusions are the result of the previously metioned Study:

a) To increase the method efficiency it is necessary to optimize the magnitude of the distance between the simplex vertexes.

This may be done at the beginning or during the reconstitution of the simplex figures.

b) The method stops at points quite far from the optimum and any attempt to automatize the method to bring it closer to the optimun requires a very long computing time.

For these reasons the authors rejected this algorithm as the

direct search method and based on their experience they chose Buzzi's OPTNOV method (1967 a,b). The main advantages of this method are:

- It is safely convergent
- The optimum is determined with acceptable precision.
- It has given good results in the solution of problems similar to those shown in equation (5), with experimental data coming from differential integral reactions.
- It allows optimization problem solutions with non-linear constraints.

The main disadvantage noticed is its slow convergence rate which is very notarious when the method is compared to other algorithms which have demonstrated to be efficient in the solution of quadratic functions similar to those shown in equation (1). This disadvantage can be conveniently overcome combining the OPTNOV method with some derivative method.

The Marquardt method (1963) is one of the most important derivative methods. It is widely used as an optimization method due to the advantages that it offers (convergence rate and stability) in the solution of problems similar to those shown in equation (1). However, it has been noticed that the Marquardt method does not have good convergence stability when solving parameter estimation problems. This disadvantage can be overcome by using the OPTNOV method which has good convergence stability and the OPTNOV method disadvantage can be overcome by using the Marquardt method which has good convergence rate.

The Marquardt method characteristics important in the development of an optimization program are:

1. In each interaction the method predicts the step and direction in which the optimum value is located. Both are calculated by means of the following equation:

$$(\underline{\underline{G}}^T \underline{\underline{G}} + \lambda \underline{\underline{I}}) (\underline{b}^{q+1} - \underline{b}^q) = - \underline{\underline{G}}^T \underline{f} \qquad (8)$$

Lagrange's multiplier, λ, behaves as an empiric parameter whose value shows the direction in which the optimun value must be looked for. This direction is the resultant between the direction expressed by the hill-climbing method and that expressed by the methods based on Taylor's series. It is easy to see that for $\lambda \to 0$, the solution of equation (8) expresses, the same step and direction as the Newton-Gauss method does.

On the other hand, for $\lambda \to \infty$, $b^{q+1} \to b^q$ are noticed. They are very close together and in the direction given by the hill climbing method.

Marquardt's criterion to calculate the λ parameter values has been modified by the authors of this paper. The flow diagram of the modified Marquardt method is shown in Fig. 1.

According to equation (8), knowledge of the Jacobian Matrix $\underline{\underline{G}}$ is required. Its elements are $\{g_{ij}\} = \{\partial f_j / \partial b_i\}$; they can be calculated knowing the analitical or numerical derivatives. These alternatives have been considered in the development of the program. The numerical analysis

of the elements $\{g_{ij}\}$ was done according to the followin equations:

$$g_{ij} = \frac{f_j(b_1, \ldots, b_i + \delta_i, \ldots, b_p) - f_j(b_1, \ldots, b_i, \ldots, b_p)}{\delta_i}$$

with i = 1, ..., p, j = 1,..., n. The diferential elment δ_i is calculated as $|b_i| 10^{-4}$. If the resul is $\delta_i \leq 10^{-7}$ it will be considered $\delta_i = 10^{-7}$.

The method cannot be easily adapted to solve optimization problems with constrains.

It is required the use of a triangularization or matrix inversión numerical method to solve equation (8). The behaviour of Choleski's method has been studied with this objective in mind (Ralston & Wilf (1966), Pipes (1963), Golub (1965), Scarborough (1966), Salvadori & Baron (1969), Peters & Wilkimason (1970)).

The main observations are:

a) It allows the solution of equation (8) through triangularization saving computing time.
b) It allows the calculus of the determinant of a "p" order matrix. (4) and (7).
c) It can be used to estimate the inverse of a matrix. This allows the solution of the most general case shown in equation (5).
d) It is not advisable to use the method if simple precision is required, because the errors between $\underline{C}$ and $\underline{b}$ or the resulting matrix $(\underline{C}^T \underline{C})$ $(\underline{C}^T \underline{C})^{-1}$ errors are big and become bigger as "p" increases.
e) It is noticed that the relative error belongs to the 10^{-10} order or lower when working with double precision and with the 20^{th} order matrixes.

For these reasons Choleski's method has been chosen and implemented in such a way so as to allow the first row to be interchanged with the largest absolute value element row of the first column.

Golub's criterion (1965) was rejected because it is more accurate but it needs more computing time.

OPTNOV - MARQUARDT Combined Program

This program based on the direct search OPTNOV method and the derivative Marquardt method is called REGRE.

In this program some of the followimg alternatives can be chosen to solve optimization problems:

i. The use of the OPTNOV method only (KD = 0).
ii. The use of the methods combined with $\{g_{ij}\}$ numerical calculus (KD = 1).
iii. The use of the combined methods with $\{g_{ij}\}$ analytical calculus (KD = 2).

These are expresed by the user in its external subroutine. Internal and external subroutine interactions are shown in Fig.2. The REGRE

subroutine leads all operations and takes the decisions.The main characteristics of each subroutine are:

REGRE: It is Buzzi's OPTNOV modified subroutine (1968 b).
AUREA: It is Buzzi's PASSOI and AURNOV combined subroutines.
FUNLIM: It is Buzzi's FUNNOV modified subroutine.
ROTAR: It is Buzzi's ROTAR modified subroutine.
The main modifications concern the redefinition of the OPTNOV method original variables just to reduce the program requirements.
MEDE: It is the development of Marquardt's method shown in Fig.1.
CHOLES: It is the development of Choleski' method.
IMPRI: It is a subroutine through which initial, intermediate and final values from optimization variables and finals of some statistical variables are printed.

The external subroutines that must be implemented by the user are:

MAIN: It is the main program through which the control parameter values of the REGRE and the initial values of the optimization independent variables as well as any other related information are introduced.
FUNCIO: It is the subroutine where the objetive function calculus form is expressed.
LIMITE: It is the subroutine where the restriction calculus form is expressed.
DERANA: It is an optional subroutine where the terms of the Jacobian matrix are expressed. If anyone chooses KD = 0 or KD = 1,this subroutine must be annulled.

The subprogram operative control is given by the REGRE subroutine. The calculus operations start with the memorization of the optimization variables and the constrains control. If one of the constrains is violated, the subprogram notices this anomaly and the control is immediately transferred to the MAIN. Otherwise F(memorized as F°) is calculated. This criterion was chosen taking into account the fact that many times the constrains are imposed to prevent the internal function calculus whose arguments exceed the higher accepted values.Once F° is calculated MEDE, subroutine takes the operation control and the calculations go on as shown in Fig. 1. According to the reasons why MEDE operations end, the REGRE decisions are:

1a. If the best absolute value of the objetive function found at the moment, "F_{opt}", is lower than a certain value, for example 10^{-8},or if the number of interactions planned by the user are achieved,the operation control returns to MAIN.
2a. If the constraint control over $\underline{b}^{q+1}$ shows that they violate the constraints the $\underline{b}$ value corresponding to "F_{opt}" is retaken and the operation sequencies related to the initial OPTNOV cycle continue.
3a. If an unstable convergence region is detected ($j \geq 10+ p$), if it belongs to a $\underline{b}$ variable insensitive region or if λ value is too high (e.q. $\lambda > 10^8$), the $\underline{b}$ values corresponding to F_{opt} are retaken and the OPTNOV "antricrisis" cycle continues.

Once the OPTNOV initial cycle is completed in the REGRE according to option 2, the operation control returns to MEDE, because the critical region was left behind and the Marquard's method can continue with rapid convergence.

After the cycle is completed, the completion causes are analized in the REGRE and the following decision are taken.

1b. If no improvements is noticed in F_{opt}, the operation continues according to what was first planned in the OPTNOV.

2b. On the other hand, if a better F value in "F_{opt}" is obtained, decisions 1a, 2a or 3a are taken.

The constraint controls and decision criteria are the same as Buzzi's (1969 a,b).

The REGRE memory requirements thought to solve optimization problems given by equations (1) to (7) are of the following order:

$$17\ p + p^2 + n(2v + u + pv) + 3\ r$$

Use of the OPTNOV - Marquardt combined method in the solution of problems.

Classical examples were chosen to compare the combined method to other algorithms. The program is developed in FORTRAN IV computer language with simple and double precision called REGRE and REGRED respectively.

In the final result tables, NI expresses how many times the objective function was evaluated. The best objective function value obtained in the NI interactions is shown in column F. The NI value agrees with the number of the final interaction.

Conclusions and significance

The method, called REGRE, was applied to different examples chosen for their comparison with other algorithms.

The method has shown excellent convergence velocity even for problems due to bad conditional of the variables as the example suggested by Powell (1964) or as the highly unbalanced functions referred to by Buzzi (1968) and Tabato e Ito (1973). Because the REGRE method is a combination of the OPTNOV direct search method and the Marquardt derivative method, it has more acuracy and reliability than each of the two mentioned before. The REGRE method has also shown an excellent behavior in the resolution of problems of parameter estimation in systems with complex chemical reactions.

The results obtained by the application of the REGRE method to different examples are given in Tables.

Example 1

$$f_1 = 10^4\ b_1\ b_2 - 1 \qquad f_2 = e^{-b1} + e^{-b2} - 1.0001$$

$$F = f_1^2 + f_2^2$$

This example is cited by Buzzi & Cassapollo (1972b). Originally it was proposed by Powell (1964) as a complex particular case due to a bad conditioning of the two variables. Table I shows REGRED program and other authors' results.

TABLE I. $f_1 = 10^4 b_1 b_2 - 1$; $f_2 = e^{-b1} + e^{-b2} - 1.0001$; $F = f_1^2 + f_2^2$
initial value point $\underline{b}$ (0;1): F=1.13; Results:$\underline{b}$(1.098 E-5;9.106)
F = 0.

METHOD OR AUTHOR	F	b_1 x 10^5	b_2	NI
REGRED: KD = 0	1.10778 E - 4	2.2	4.543162	223
REGRED: KD = 1	3.6281 E -20	1.097	9.1136253	37
REGRED: KD = 2	1.3221 E -19	1.09725	9.1136252	13
Buzzi Ferraris & Cassapollo(1972b) Ref. (2)	1.4338 E -13	1.098159	9.1061461	26
Ref. (3)	7.3881 E - 9	1.1064	9.0380	223
	5.2812 E - 8	1.2524	7.9841	202
Morales & Quiroga (1980)(Newton-Raphson method)	2.3 E -22	1.098	9.10614	12

Example 2. Non - linear regression.

$$F = \sum_{i=1}^{N} W_i (Y_i - \eta_i)^2$$

$$\eta = \beta_1 + (0.49 - \beta_1) \exp \left\{ -\beta_2 (X - 8) \right\}$$

The problem reported by Draper & Smith (1966) was solved using the REGRED program in order to study its behaviour in the solution of non-linear regression problems.

The final results for the two initial values of $\underline{b}$ are shown in table II.

TABLE II $F=\sum_{i=1}^{N} (Y_i - \eta_i)^2 p_i$; $\eta = \beta_1 + (.49 - \beta_1) \exp \left\{ -\beta_2 (x - 8) \right\}$

Initial value point: $\underline{\beta}$ (0.389; 0.1); F = 0.5145

METHOD	F	b_1	b_2	NI
REGRED : KD = 0	0.4976	0.38757	9.1513 E-2	300
REGRED : KD = 1	0.4976	0.38754	9.141 E-2	215
REGRED : KD = 2	0.4976	0.38754	9.142 E-2	244

Example 3. Parameter estimation in multiresponde models.

$$\eta_1 = \beta_1 \frac{X}{2} + \beta_2 \left(\frac{X}{2}\right)^2$$

$$\eta_2 = \beta_1 / X + \beta_2 X$$

$$\eta_3 = \beta_1 + \beta_2 X$$

$$\eta_4 = \beta_1 / 2 + \beta_2 e^{X/3}$$

$$\eta_5 = 10 - 0.32 X (\beta_1 + \beta_2 X)$$

This example was chosen to study the REGRE and REGRED program behaviours in the solution on non-linear regression problems in multiresponse models.

Tables III.A, III.B and III.C shows REGRED program results.

TABLE III.A - Experimental Data of a multiresponse system. Problem 3.

X	Y_1	Y_2	Y_3	Y_4	Y_5
1.	6.88	11.86	11.88	6.97	6.84
2.	9.60	6.19	11.84	7.56	5.03
3.	16.97	3.87	12.80	7.14	3.07
4.	25.57	4.14	14.76	9.38	2.45
5.	30.29	2.63	14,52	10.05	2.13
6.	38.39	2.08	15,64	11.75	2.26
7.	47.45	2.41	17.08	15.28	3.31
8.	56.21	2.28	18.09	19.53	4.96
9.	65.01	1.79	18.84	24.70	7.02
10.	75.69	2,22	20.32	33.22	10.07

TABLE III.B - Covariance Matrix $\mathbf{C}$, Problem 3 (σ_{ij})

J \ I	1	2	3	4	5
1	1.	0,364	0,482	0.245	- 0.036
2	0.364	0.25	0.195	0.206	0.0042
3	0,482	0.195	0.25	0.14	- 0.016
4	0.245	0.206	0.14	0.25	0.0227
5	- 0.036	0.0042	- 0.016	0.0227	0.0225

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TABLE III.C - Results Related to Parameter Estimation Problem 3.

Ec.	KD	REGRED					REGRED				
		F	b_1	b_2	S	NI	F	b_1	b_2	S	NI
(16)	Inic.	1.812 E 3	12	0.5	-	1	1.812 E 3	12	0.5	-	1
	0	15.5276	10.017	1.0012	15.5276	107	15.5275	10.017	1.00115	15.527	118
	1	15.5276	10.017	1.0012	15.5276	83	15.5275	10.0176	1.00119	15.527	98
	2	15.5276	10.0171	1.00119	15.5276	77	15.5275	10.0176	1.00119	15.527	97
(14)	Inic.	9.1806E 4	12.	0.5	-	1	9.1806 E 4	12.	0.5	-	1
	0	2.06112E 2	10.0119	1.0023	15.537	160	2.0609 E 2	10.0119	1.00225	15.537	160
	1	2.0615 E 2	10.0169	1.00256	15.539	243	2.0609 E 2	10.0124	1.00227	15.536	300
	2	2.0609 E 2	10.0126	1.0023	15.537	300	2.0609 E 2	10.0132	1.00233	15.536	182
(17)	Inic.	2.5475 E 5	12	0.5	-	1	1.5475 E 3	12.	0.5	-	1
	0	7.1733 E-6	10.00247	1.000484	15.567	187	7.1478 E-6	10.0028	1.00053	15.564	196
	1	1.3451 E-5	10.00823	1.00272	15.549	300	1.2306 E-5	10.0124	1.00118	15.531	300
	2	7.1733 E-6	10.00238	1.000471	15.567	222	7.1455 E-6	10.0022	1.00052	15.567	205

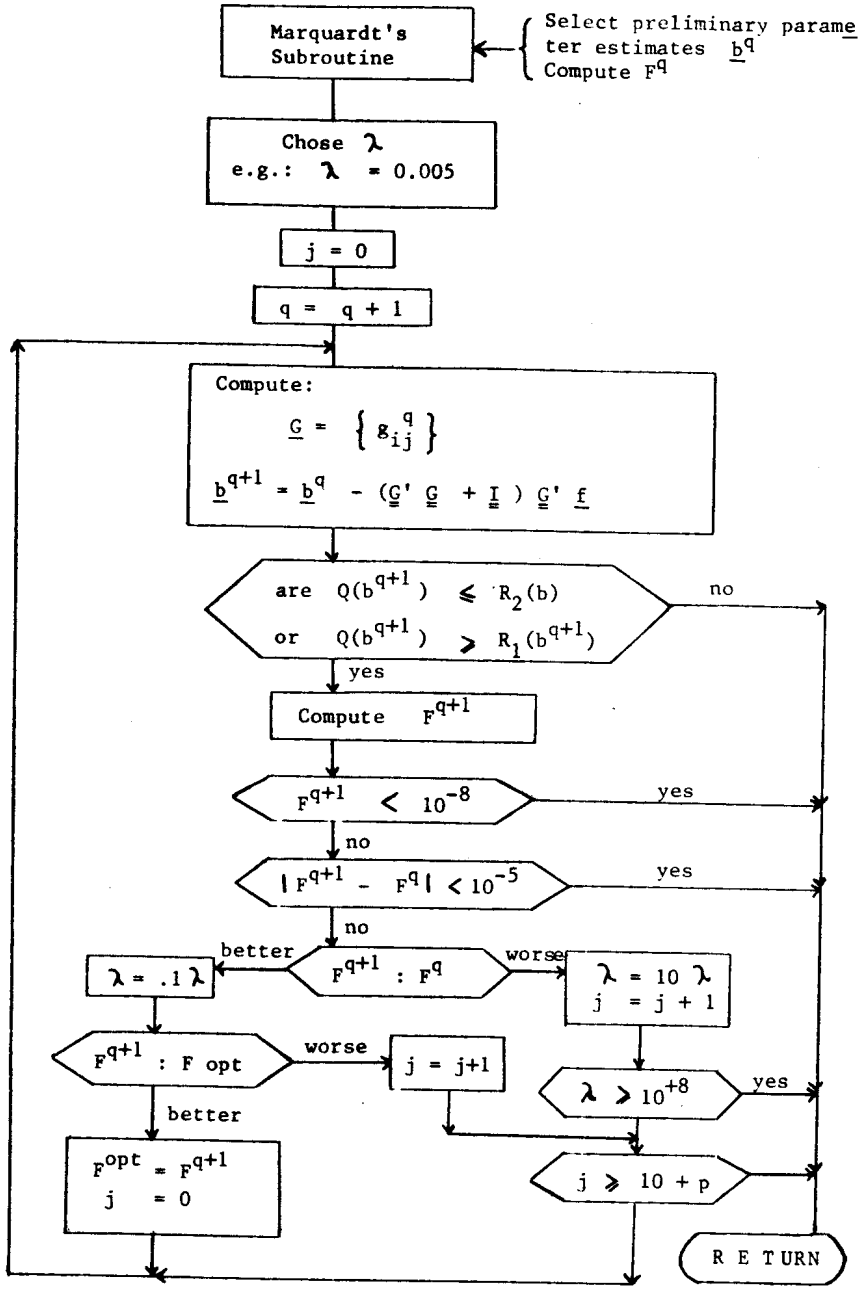

FIGURE 1. Flow diagram of used Marquard's method

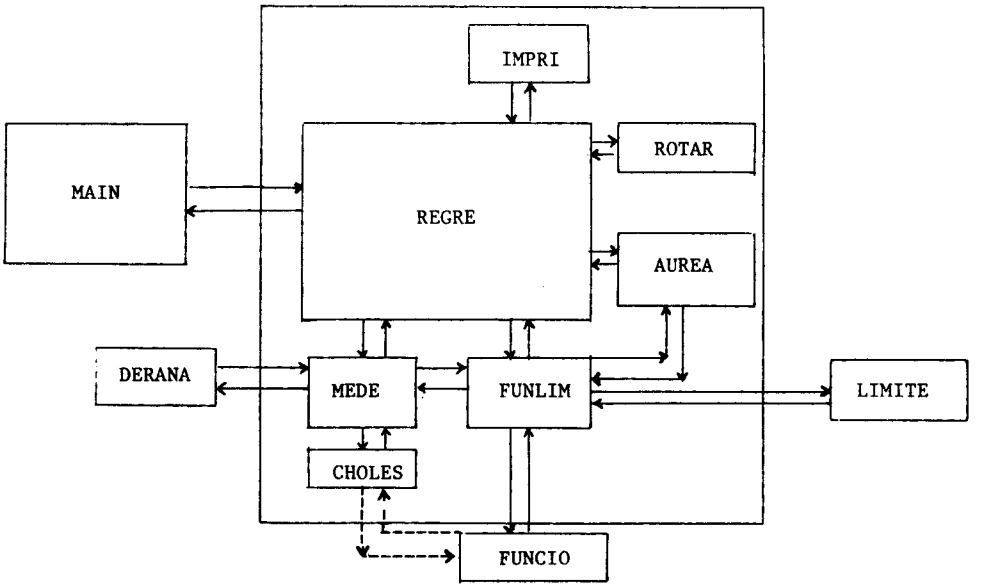

FIG. 2 Interaction between internal and external subroutines.

NOTATION

$\underline{b}$: (p x 1) vector of parameter estimates.

$\underline{f}$: (p x 1) vector of trascendent or algebraic equations.

F : objective function

$\underline{\underline{G}}$: (n x p) jacobian matrix

n : number of observations

p : number of parameter

$\underline{Q}(\underline{b})$: (r x 1) vector of constrained functions

r : number of constraints

$\underline{R}_1(\underline{b})$;$\underline{R}_2(\underline{b})$: (r x 1) vectors of the inferior and superior boundaries respectively.

S^2 : estimate of error variance

$\underline{\underline{X}}$: (n x p) matrix of settings of independent variables.

Y_{ji} : observed value of the i-th response variable during the j-th experiment.

u : number of independent variables

v : number of dependent variables

W : (v x v) weighting matrix

Greek Symbols

δ : infinitesimal element

η_{ji} : true, unknown, value of i-th response variable corresponding to the j-th observation.

λ : Lagragian multipliers.

$\pi_{i,n}$: probability of model i after n experiments.

σ_i^2 : variance of predicted value of dependent variable under model i.

$\underline{\underline{\Psi}}$: (v x v) covariance matrix of experimental errors in the multivariate regression situation.

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