NON-LINEAR REGRESSION WITH MINIMAL ASSUMPTIONS

BY
HARVEY M. WAGNER

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INSTITUTE FOR MATHEMATICAL STUDIES IN THE SOCIAL SCIENCES
Applied Mathematics and Statistics Laboratories
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A curvilinear regression model is treated by linear programming methods, so as to require only mild restrictions on the nature of the non-linearities.

1. Introduction

Consider the regression model

$$y = \sum_{j=1}^{p} f_j(x_j) + \text{error} \tag{1}$$

where y is the dependent variable, and x_j , $j = 1,2,\ldots,p$, are the independent variables. Assume there are available k sets of observations on the variables, viz., y_i and x_{ij} , $i = 1,2,\ldots,k$, and that we wish to estimate the functions $f_j(x_j)$ from these data.* We do not impose the restriction that every $f_j(x_j)$ must be linear, and thus our model may be categorized as curvilinear regression. The usual statistical technique for such models is to specify a mathematical form for each of the functions $f_j(x_j)$, such as $ax_j + bx_j^2$ or $a\log x_j$, and

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* One of the x_j may represent a dummy variable, $x_{ij'} \equiv 1$, $i = 1,2,\ldots,k$.

then to estimate the parameters in the specified forms according to a least squares criterion. An alternative approach, given in [4], employs criteria that permit the use of linear programming models for obtaining the estimated parameter values. In this paper we do not go so far as specifying a mathematical form for the $f_j(x_j)$; rather we impose only mild restrictions on the behavior of the functions; for example, a given $f_j(x_j)$ must be monotonically increasing. Utilizing a linear programming approach, we are able to estimate the functions $f_j(x_j)$ given only the minimal assumptions as to the required shape. In Section 2 we adopt "minimal sum of absolute deviations" as the criterion of best fit; in Section 5 we review alternative criteria.

2. Basic Formulation

To begin, suppose that for each j the values of x_{ij} are distinct, $x_{ij} \neq x_{kj}$ if $i \neq k$. Let $f_j(x_{ij}) \equiv f_{ij}$. Our procedure is to find values for the f_{ij}.

For each observation y_i, we have an Error Constraint,

$$(2) \qquad \sum_{j=1}^{p} f_{ij} + \epsilon_{1i} - \epsilon_{2i} = y_i \quad , i = 1,2,\ldots,k \quad ,$$

$$\epsilon_{1i} \geqq 0 \quad , \epsilon_{2i} \geqq 0 \quad .$$

As is explained in detail in [4], ϵ_{1i} and ϵ_{2i} are interpreted as vertical deviations "above" and "below" the fitted regression function for the i-th set of observations; i.e., the sum $\epsilon_{1i} + \epsilon_{2i}$ represents the absolute deviation between the estimated fit for $\sum_{j=1}^{p} f_j(x_{ij})$ and y_i. Our criterion of best fit is a minimal sum of the absolute deviations.

Next we impose Weak Curvature Constraints on the f_{ij} . To illustrate, we suppose for $j = 1$, $x_{11} < x_{21} < x_{31} < \ldots < x_{k1}$, and we postulate that $f_1(x_1)$ is a monotonic increasing function. Then the Weak Curvature Constraints for the set of f_{i1} are

(3a) $$f_{i1} \leqq f_{i+1,1} \quad , \qquad i = 1,2,\ldots,k-1 \; .$$

In other words, we impose by (3a) a complete ordering on the f_{ij} . By reversing the inequality in (3a), we thereby would impose the restriction that $f_1(x_1)$ be monotonically decreasing. If instead we hypothesize that $f_1(x_1)$ is unimodal, the peak occurring, for example, at a value of x between x_{31} and x_{41} , the Weak Curvature Constraints for the set of f_{i1} are

(3b) $$f_{i1} \leqq f_{i+1,1} \; , \; i = 1,2; \quad f_{i1} \geqq f_{i+1,1} \; , \; i = 4,5,\ldots,k-1.$$

Notice that (3b) depends on being able to specify that the modal value occurs for an x between two given values of x_{i1} . The estimation of f_{i1} does not yield the modal value unless x equals one of the given x_{i1} .

Momentary reflection is sufficient to demonstrate that the foregoing analysis is modified in a straightforward manner if, for a given j , the x_{ij} values are not ordered monotonically. For example, if ordering the x_{i1} yields $x_{31} < x_{11} < x_{81} < x_{91} < x_{21} \cdots$, and we postulate that $f_1(x_1)$ is a monotonically increasing function, then instead of the Weak Curvature Constraints (3a), we have

$$f_{31} \leqq f_{11} \leqq f_{81} \leqq f_{91} \leqq f_{21} \cdots \; .$$

Similarly, it is possible by a set of inequality constraints to impose partial orderings on the f_{ij} to produce bimodal functions, functions having both a single relative minimum and a single relative maximum, etc.

Up to this point, we have assumed that for each j the values of the x_{ij} are distinct. If, for a particular j, two or more values of x_{ij} are identical, then the corresponding f_{ij} must be equal. Consequently for each j it is only necessary to define a variable f_{ij} in (2) wherever identical values for x_{ij} occur. Likewise in (3) it is only necessary to define inequalities for the distinct f_{ij}.

The basic linear programming model may now be stated as finding values for the f_{ij} which

(4) $$\text{minimize } [\sum_{i=1}^{k} \epsilon_{1i} + \sum_{i=1}^{k} \epsilon_{2i}],$$

subject to the linear constraints (2) and (3).

We complete our discussion of the basic formulation by determining the number of restrictive relations and variables that comprise the model. For the sake of definiteness, suppose that all the functions $f_j(x_j)$ are postulated to be monotonic. Let N be the total number of distinct f_{ij} to be included in the constraints.* Then (2) and (3) imply

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* Specifically, for each j, let n_j be the total number of distinct values of x_{ij}; then $N = \sum_{j=1}^{p} n_j$.

Number of Equalities = k (Error Constraints)

Number of Inequalities = $N-p$ (Weak Curvature Constraints)

Number of Variables = $N + 2k$ (f_{ij}, ϵ_{1i}, and ϵ_{2i}).

If slack variables are added to the Weak Curvature Constraints to convert them to equalities, we have

$$\text{Number of Equalities} = k + N - p$$

$$\text{Number of Variables} = 2(N + k) - p\,.$$

Although in some real regression applications these numbers need not be negligible, the method remains feasible since current linear programming computer codes are capable of solving several hundred equations in many hundreds of unknowns.

In our discussion so far we have restricted only ϵ_{1i} and ϵ_{2i} to be non-negative. In the next section we discuss placing analogous restrictions on the f_{ij}, but here we mention that if an f_{ij} is unrestricted in sign, then a common way of treating it within the usual format of a linear programming model having all non-negative variables is to let $f_{ij} \equiv f^{+}_{ij} - f^{-}_{ij}$, $f^{+}_{ij} \geq 0$, $f^{-}_{ij} \geq 0$, i.e., to substitute into the model restrictions in place of f_{ij} , the difference between two non-negative variables. This device increases the number of variables but has no effect on the number of constraints. We return to the question of model size in Section 4, where we discuss the dual formulation.

3. Additional Constraints

We may, if we wish, impose stronger properties on the estimated values for the $f_j(x_j)$ functions. We illustrate several such possibilities. We may add Positioning Constraints such as, for each j , some or all of the f_{ij} must be non-negative, the smallest f_{ij} must be no smaller than L_j , and the largest f_{ij} must be no larger than U_j . These restrictions are all representable as linear inequalities.

We may apply Strong Curvature Constraints instead of, or in addition to, (3). For example, if the estimate for $f_1(x_1)$ is to be strictly monotonically increasing and the minimal allowable difference between two adjacent values of f_{i1} is to be δ_{i1}, then (3a) would be modified to the linear relation

(3c) $$f_{i1} + \delta_{i1} \leqq f_{i+1,1} \quad .$$

Similarly, if there is to be a maximal allowable difference η_{i1} between two subsequent values of f_{i1}, then we would add the linear constraints

(3d) $$f_{i1} + \eta_{i1} \geqq f_{i+1,1} \quad .$$

The relations (3c) and (3d) imply absolute differences between adjacent values for f_{i1}. It is also possible to impose constraints on the relative differences between values for f_{i1}; to illustrate, we may require

(3e) $$(f_{21} - f_{11}) \leqq \alpha(f_{31} - f_{21})$$ $$(f_{21} - f_{11}) \geqq \beta(f_{31} - f_{21})$$

where α and β are given positive constants.

Finally, it is possible to specify an exact mathematical form for any particular $f_j(x_j)$. For example, if we postulate that $f_1(x_1) = ax_1^2$, then we modify (2) to

(5) $$ax_{i1}^2 + \sum_{j=2}^{p} f_{ij} + \epsilon_{1i} - \epsilon_{2i} = y_i \quad , \ i = 1,2,\ldots,k \quad ,$$

and eliminate the Curvature Constraints for x_1; the linear programming model treats a as a variable in the optimization process.

4. Dual Formulation

As we have demonstrated earlier [4], there may be computational efficiencies arising from solving the dual linear programming problem [3]; in the process of optimizing the dual problem, an optimum solution to the original regression model is automatically generated [4]. We demonstrate the argument with reference to the example at the end of Section 2, postulating further the restrictions $f_{ij} \geqq 0$. Let w_i denote the dual variables, where, in the primal model, $i = 1,2,\ldots,k$ correspond to the Error Constraints and $i = k+1,k+2,\ldots,k+N-p$ correspond to the Weak Curvature Constraints. Then the dual relations associated with the error variables ϵ_{1i} and ϵ_{2i} are

(6a) $$w_i \leqq 1 \quad , \qquad -w_i \leqq 1 \quad , \qquad i = 1,2,\ldots,k \quad .$$

We make a transformation of variables

(7) $$z_i \equiv w_i + 1 \quad , \qquad i = 1,2,\ldots,k \quad ,$$

and substitute $(z_i - 1)$ for w_i first into the N dual relations associated with the variable f_{ij}, and then into (6a), the latter yielding a set of upper bounds

(6b) $$0 \leqq z_i \leqq 2 \quad , \qquad i = 1,2,\ldots,k \quad .$$

As a result, we have in the dual model

Number of principal inequalities = N (corresponding to the primal f_{ij} variables)

Number of upper bound inequalities = k

Number of variables = k + N - p .

If slack variables are added to the principal inequalities, we have

Number of principal equalities = N

Number of upper bound inequalities = k

Number of variables = 2N + k - p .

Therefore if the dual problem is solved directly instead of the primal model, a reduction of (k-p) equations and k variables occurs at the extra computational expense of handling k bounded variables. There are efficient algorithms for solving bounded variables problems (see [2] and [3]) and a number of computer codes are available. If additional constraints are appended in the primal problem, such as those suggested in Section 3, then utilizing the dual problem becomes a more attractive approach since these relations increase only the number of dual variables and not the number of dual restrictions.

5. Alternative Objective Functions

Instead of employing a minimal sum of absolute deviations as a criterion of best fit, it is possible to use a Chebyshev or a least squares criterion. Under a Chebychev criterion, we seek to find values for the f_{ij} which minimize the maximum absolute error between the fitted relation and y . To accomplish this aim, we have in place of (2) pairs of Error Constraints

$$(8) \qquad \left.\begin{aligned} -\sum_{j=1}^{p} f_{ij} + \epsilon &\geqq -y_i \\ \sum_{j=1}^{p} f_{ij} + \epsilon &\geqq y_i \end{aligned}\right\} \quad i = 1,2,\ldots,k \ , \qquad \epsilon \geqq 0$$

and in place of (4), the objective function

(9) minimize ϵ .

Continuing with our example wherein there are N distinct f_{ij} , and $f_{ij} \geqq 0$, we have in the primal model

Number of inequalities = $2k + N - p$ (Error and Weak Curvature Constraints)

Number of variables = $N + 1$.

In the dual formulation the above values for the number of inequalities and variables are interchanged, leading to the conclusion that the dual is in general computationally more efficient to solve.

Under a least squares criterion, the only change in the basic formulation of Section 2 is the objective function, which is then stated as follows:

$$\text{(10)} \qquad \text{minimize } \left[\sum_{i=1}^{k} \epsilon_{1i}^2 + \sum_{i=1}^{k} \epsilon_{2i}^2 \right] .$$

This problem is a quadratic programming model, and can be solved by a method such as that in [5], for which computer routines are available. It is also possible to employ a linear programming version if the squared functions in (10) are represented in terms of piecewise linear approximations [1].

6. Concluding Remarks

The model in this paper permits a large degree of flexibility in estimating non-linear regression functions.* If the underlying purpose

* We point out that the approach is well suited to situations in which the x_{ij} represent rank order measurements.

for finding the functions is entirely pragmatic, then one may utilize the solution values for the f_{ij} without further consideration. To the extent that the ultimate purpose may be to discover simple "regression laws," then, once the values for the f_{ij} are found and plotted against x_{ij}, one may wish to postulate a particular mathematical form for each $f_j(x_j)$ function, and estimate the parameters in the mathematical forms either by least squares or by linear programming methods.

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