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ORTHOGONAL LINEAR REGRESSION ALGORITHM BASED ON AUGMENTED MATRIX FORMULATION

ANDRZEJ BARGIELA† and JOANNA K. HARTLEY‡
Department of Computing, The Nottingham Trent University, Burton Street, Nottingham NG1 4BU, England

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Scope and Purpose—In this paper, a new technique for solving the orthogonal least absolute values (ORLAV) regression problem is proposed. While the orthogonal regression is a natural choice in all cases where the regression variables are independent of each other, the fact that it minimises the orthogonal distances from each data point to the regression hyperplane, which is not known in advance, makes it a significantly more difficult problem compared with ordinary linear regression. An important consideration is the way the distances to the regression hyperplane are measured. The selection of L_1 norm (absolute value of orthogonal distances) has a consequence of spanning the regression hyperplane on the number of measurements equal to the number of regression variables and rejecting the remaining measurements. As a result, the least absolute values regression offers a degree of immunity to gross measurement errors which, redundancy permitting, will be found among the rejected measurements. There is only one other algorithm for the solution of the ORLAV regression problem known to the authors (see Ref. [1]). However, it is our contention, that the algorithm proposed here offers a numerically more robust solution since the augmented matrix formulation preserves the condition number of the constraints matrix, while the algorithm based on the linear programming technique [1], inherently relies on pivoting operations. A further noteworthy feature of our algorithm is that it simultaneously provides solutions to the primal and dual regression problem.

Abstract—The problem of n-dimensional orthogonal linear regression is a problem of finding an n-dimensional hyperplane minimising the sum of Euclidean distances between this hyperplane and a given set of m points, where $m \geqslant n$. This nonlinear programming problem has been re-cast in an augmented matrix form and solved as a sequence of iteratively re-weighted least square problems. The proposed algorithm is seen as an alternative to the recently published algorithm by Cavalier and Melloy [1].

1. INTRODUCTION

The results of many scientific investigations are sets of measurement data points which are then used to establish mathematical models (hyperplanes) of physical systems or phenomena. In situations where, for each data point in a set, one of the variables is a function of the remaining variables, a convenient way of calculating the relevant hyperplane is by means of ordinary least squares regression (OLS). These calculations minimise the sum of squares of distances to the hyperplane measured along the direction of the dependent variable [Figs. 1(a) and 1(b)]. However, if there is no obvious functional relationship between variables, it is more appropriate to minimise the sum of squares of Euclidean distances to the hyperplane measured along the normal to the hyperplane, as illustrated in Fig. 1(c). Such regression is referred to as orthogonal least squares (ORLS). Mathematically the ORLS regression is a significantly more difficult problem since the normal direction to the hyperplane is not known in advance, thus giving rise to inherent nonlinearity of the problem.

Both OLS and ORLS can be shown to provide optimal unbiased regression hyperplanes, if the measurement data is affected by the Gaussian measurement noise only. However, they are less well suited to deal with data containing gross measurement errors. Since the objective function in OLS and ORLS evaluates squares of distances to the hyperplane, the outlying measurements are unduly heavily weighted. Consequently, in situations where gross measurement errors do occur, a sum of absolute values of distances is taken in preference to the sum of squares [2]. The analogs of OLS and ORLS regressions derived by substituting the L_2 with the L_1 norm are referred to as ordinary least absolute values (OLAV) and orthogonal least absolute values (ORLAV) regressions.

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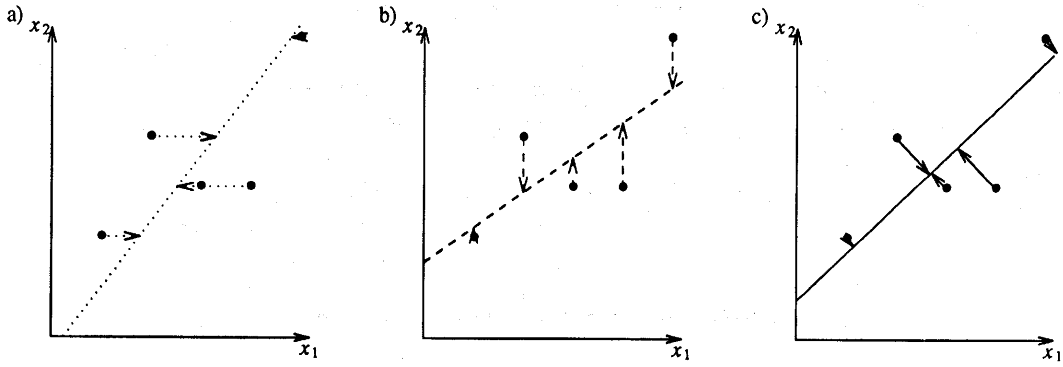
† Dr Andrzej Bargiela is a Reader in Real Time Systems at The Nottingham Trent University. His research interests include applied optimization, parallel and distributed programming and neural computing.
‡ Miss Joanna Hartley is a Research Assistant at The Nottingham Trent University. She is registered on a Ph.D. degree project, researching into parallel algorithms for simulation of network systems.

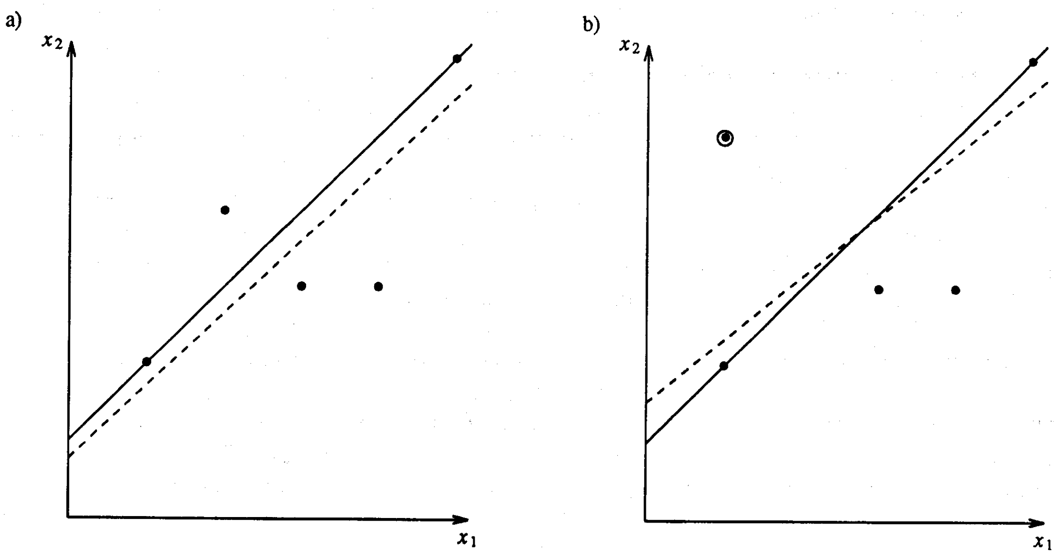


a) $\cdots$, *Least-squares regression with* x_1 *dependent (OLS);*
b) - -, *Least-squares regression with* x_2 *dependent (OLS);*
c) —, *Least-squares regression with* x_1, x_2 *independent (ORLS).*

Fig. 1. Distances measured to appropriate regression line.

An illustration of the error rejection capability of ORLAV regression compared to ORLS regression is given in Fig. 2. The L_1 norm in the ORLAV regression ensures that, in n-dimensional Euclidean space, there are exactly n data points which are taken to span the hyperplane and the remaining $(m - n)$ points are rejected. Therefore the outlier measurements find themselves among the rejected data points, thus having no effect on the calculated hyperplane. By contrast, the ORLS regression takes notice of the erroneous measurements, and the resulting hyperplane in Fig. 2(b) is different to the original one.

This paper is focussed on the orthogonal least absolute values (ORLAV) regression in n-dimensional Euclidean space. Our original contribution is the re-casting of this nonlinear programming problem into an augmented matrix form and solving it as a sequence of iteratively re-weighted least squares problems. The proposed algorithm is seen as an alternative to the algorithm recently proposed by Cavalier and Melloy [1].



—, *ORLAV regression line;*
- - -, *ORLS regression line;*
◉, *the outlier.*

Fig. 2. Comparison of sensitivity to an outlier, of ORLAV and ORLS regression lines.

2. THE ORLAV REGRESSION

Consider the hyperplane $\mathbf{p}^t\mathbf{x} = \alpha$ along with $\mathbf{x}_i$, $i = 1,\ldots, m$, being the given set of points in E_n, Euclidean n-space (with $m \geqslant n$). The normal Euclidean distance from a point $\mathbf{x}_i$ to the hyperplane $\mathbf{p}^t\mathbf{x} = \alpha$ is given by

$$s_i = |\mathbf{p}^t\mathbf{x}_i - \alpha|/\|\mathbf{p}\|. \tag{1}$$

So, the required hyperplane can be found by solving the task:

(P)

$$\text{minimise} \quad \sum_{i=1}^{m} |\mathbf{p}^t\mathbf{x}_i - \alpha|/\|\mathbf{p}\| \tag{2}$$

$$\mathbf{p}, \alpha \quad \text{unrestricted.} \tag{3}$$

Assuming that the normal vector to the hyperplane is of unit length, the above can be written as

(P1)

$$\text{minimise} \quad \sum_{i=1}^{m} |\mathbf{p}^t\mathbf{x}_i - \alpha| \tag{4}$$

$$\text{subject to} \quad \|\mathbf{p}\| = 1 \tag{5}$$

$$\mathbf{p}, \alpha \quad \text{unrestricted.} \tag{6}$$

The nonlinearity in the objective function, due to the absolute values operator, can be dealt with by two simple alterations: Let $d_i = \mathbf{p}^t\mathbf{x}_i - \alpha$, so the objective function becomes

$$\sum_{i=1}^{m} |d_i|$$

which is equivalent to

$$\sum_{i=1}^{m} d_i^2/|d_i|.$$

Now let W be the $m \times m$ diagonal matrix with entires $1/|d_i|$, $i = 1,\ldots, m$.

Also, let A be an $m \times n$ matrix which consists of rows of $\mathbf{x}_i$'s, and let $\mathbf{e} = (1, 1,\ldots, 1)^t \in E_m$. Now (P1) can be rewritten as:

(P2)

$$\text{minimise} \quad \mathbf{d}^t W\mathbf{d} \tag{7}$$

$$\text{subject to} \quad A\mathbf{p} - \mathbf{e}\alpha - \mathbf{d} = \mathbf{O} \tag{8}$$

$$\|\mathbf{p}\| = 1 \tag{9}$$

$$\mathbf{p}, \alpha, \mathbf{d} \quad \text{unrestricted.} \tag{10}$$

As $\|\mathbf{p}\| = 1$ in (9), then $\mathbf{p}^t\mathbf{p} = \|\mathbf{p}\|^2 = 1$ also holds. So (9) can be exchanged for $\mathbf{p}^t\mathbf{p} = 1$, to give

(P3)

$$\text{minimise} \quad \mathbf{d}^t W\mathbf{d} \tag{11}$$

$$\text{subject to} \quad A\mathbf{p} - \mathbf{e}\alpha - \mathbf{d} = \mathbf{O} \tag{12}$$

$$\mathbf{p}^t\mathbf{p} = 1 \tag{13}$$

$$\mathbf{p}, \alpha, \mathbf{d} \quad \text{unrestricted.} \tag{14}$$

Equation (13) is the only non-linear constraint. In order to linearise this constraint, we will introduce additional variable $\mathbf{q}$ which will be iteratively updated and will represent our estimate of $\mathbf{p}$.

(P4)

$$\text{minimise} \quad \mathbf{d}^t W\mathbf{d} \tag{15}$$

$$\text{subject to} \quad A\mathbf{p} - \mathbf{e}\alpha - \mathbf{d} = \mathbf{O} \tag{16}$$

$$\mathbf{q}^t\mathbf{p} = 1 \tag{17}$$

$$\mathbf{p}, \alpha, \mathbf{d} \quad \text{unrestricted.} \tag{18}$$

These constraints can be written in matrix form:

$$\begin{bmatrix} A & -\mathbf{e} \\ \mathbf{q}^t & 0 \end{bmatrix}\begin{bmatrix} \mathbf{p} \\ \alpha \end{bmatrix} = \begin{bmatrix} \mathbf{d} \\ 1 \end{bmatrix},$$

$$\text{let matrix} \quad F = \begin{bmatrix} A & -\mathbf{e} \\ \mathbf{q}^t & 0 \end{bmatrix}, \underline{\theta} = (\mathbf{p}^t, \alpha)^t, \underline{\psi} = (\mathbf{d}^t, 1)^t,$$

$$\text{resulting in} \quad F\underline{\theta} = \underline{\psi}. \tag{19}$$

Equation (19), which represents constraints (16) and (17), introduces the variable $\underline{\theta}$; alongside this the weight matrix W in (15) needs to be modified to give

$$G = \begin{bmatrix} W & \mathbf{O} \\ \mathbf{O}^t & \frac{1}{\varepsilon} \end{bmatrix}$$

($1/\varepsilon$ is the reciprocal of the computational accuracy ε). This results in assigning a large weight to equation (17), which needs to be satisfied to preserve the integrity of the Euclidean distances measurements. So (P4) can be rewritten as:

(P5)

$$\text{minimise} \quad \underline{\psi}^t G \underline{\psi} \tag{20}$$

$$\text{subject to} \quad F\underline{\theta} - \underline{\psi} = \mathbf{O} \tag{21}$$

$$\underline{\theta}, \underline{\psi} \quad \text{unrestricted.} \tag{22}$$

Now, to find the minimum of $\underline{\psi}^t G \underline{\psi}$, substitute $F\underline{\theta}$ for $\underline{\psi}$ and then differentiate with respect to $\underline{\theta}$ and set the result equal to zero:

$$\text{Let} \quad \mathbf{J} = \underline{\psi}^t G \underline{\psi} \tag{23}$$

$$= \underline{\theta}^t F^t G F \underline{\theta}, \tag{24}$$

$$\frac{d\mathbf{J}}{d\underline{\theta}} = 2F^t G F \underline{\theta} = \mathbf{O}. \tag{25}$$

Introducing temporary variables $\underline{\psi}$ and $\underline{\phi}$, representing the partial vector–matrix products in (25), this minimality condition can be written as a set of simultaneous matrix equations

$$F\underline{\theta} = \underline{\psi} \tag{26}$$

$$G\underline{\psi} = \underline{\phi} \tag{27}$$

$$F^t\underline{\phi} = \mathbf{O} \tag{28}$$

or using the augmented matrix formulation:

$$\begin{bmatrix} 0 & -I & F \\ -I & G & 0 \\ F^t & 0 & 0 \end{bmatrix}\begin{bmatrix} \underline{\phi} \\ \underline{\psi} \\ \underline{\theta} \end{bmatrix} = \begin{bmatrix} \mathbf{O} \\ \mathbf{O} \\ \mathbf{O} \end{bmatrix}. \tag{29}$$

If $\mathbf{q}$ is calculated to be, within a given computational accuracy, equal to $\mathbf{p}$ then the problems (P3) and (P4) are identical. The initial vector for $\mathbf{q}$ can be selected quite arbitrarily but, to enhance computational efficiency, it is a good idea to evaluate it by calculating an OLS (ordinary least squares) equation, $\mathbf{q}^t\mathbf{x} = \beta$, where one of the x_j is (arbitrarily) chosen as the dependent variable.

$$\text{Let } \mathbf{q}^t = (\hat{\mathbf{q}}^t, 1) \text{ and } \mathbf{x}^t = (\hat{\mathbf{x}}^t, x_j),$$

$$\text{so } \mathbf{q}^t\mathbf{x} = \beta \text{ can also be written as } \hat{\mathbf{q}}^t\hat{\mathbf{x}} - \beta = -x_j.$$

The algorithm can thus be summarised as follows:

1. Calculate $\hat{\mathbf{q}}$ of $\hat{\mathbf{q}}^t\hat{\mathbf{x}} - \beta = -x_j$, for a given set of points $x_i \in E_n$, $i = 1, \ldots, m$. Normalise $\mathbf{q}$, and continue to 2.

2. Find the L_1 solution to (P5) by iteratively modifying the weight matrix, G, as follows:

   2.1 Solve the matrix equation (29) which gives the L_2 solution for $\underline{\theta}$, $\underline{\psi}$.

   2.2 Using the calculated discrepancies ψ_i's, modify the corresponding $\overline{G}_{ii}$'s, with $G_{ii} = 1/\psi_i$.

   2.3 If at least n of the original equations are satisfied (corresponding $\psi_i = 0$), continue to 3.
   Otherwise repeat from 2.1.

3. If $\|\tilde{\mathbf{p}}\| = 1$ and $\tilde{\mathbf{p}} = \mathbf{q}$ stop, with $\tilde{\mathbf{p}}$, $\tilde{\alpha}$ as the optimal solution to problem (P). Otherwise, go to 4.

4. Replace $\mathbf{q}$ by $\tilde{\mathbf{p}}/\|\tilde{\mathbf{p}}\|$ and reset the weights to 1; then return to 2.

The algorithm proved to be very robust, and with sets of randomly generated data, with up to $n = 5$ and $m = 100$, the algorithm was found to need a maximum of 10 iterations; with a typical convergence achieved in 2 iterations. The maximum time needed for convergence was 10.3 seconds on the SUN Sparc SLC workstation.

3. THE DUAL

The dual of problem (P5) is derived using the Lagrangian:

$$L(\underline{\psi}, \underline{\theta}; \underline{\eta}) = \underline{\psi}^t G \underline{\psi} + \underline{\eta}^t (F\underline{\theta} - \underline{\psi}) \tag{30}$$

$$\frac{\partial L}{\partial \underline{\psi}} = 2\underline{\psi}^t G - \underline{\eta}^t, \qquad \frac{\partial L}{\partial \underline{\theta}} = \underline{\eta}^t F \tag{31}$$

$$\frac{\partial L}{\partial \underline{\psi}} = \frac{\partial L}{\partial \underline{\theta}} = \mathbf{O}^t \Rightarrow G\underline{\psi} = \tfrac{1}{2}\underline{\eta} \tag{32}$$

$$F^t \underline{\eta} = \mathbf{O} \tag{33}$$

along with the constraint

$$F\underline{\theta} = \underline{\psi}. \tag{34}$$

$$\frac{\partial^2 L}{\partial \underline{\psi}\, \partial \underline{\theta}} = H(\underline{\theta}, \underline{\psi}) = \begin{bmatrix} 2G & 0 \\ 0 & 0 \end{bmatrix} \tag{35}$$

So, owing to the structure of $\underline{\psi}$, H is always positive definite; therefore there will be a minimum at any stationary point.

Let $\underline{\eta} = 2\underline{\phi}$.

So the dual of (P5) can be written as:

(D5)

$$\text{maximise} \quad \underline{\phi} \tag{36}$$

$$\text{subject to} \quad F\underline{\theta} = \underline{\psi} \tag{37}$$

$$F^t \underline{\phi} = \mathbf{O} \tag{38}$$

$$G\underline{\psi} = \underline{\phi} \tag{39}$$

$$\underline{\theta}, \underline{\psi} \quad \text{unrestricted.} \tag{40}$$

The solution of the dual problem (D5) involves, therefore, solving the same set of equations as (P5), with the variable $\underline{\phi}$ being the dual variable. Consequently our algorithm gives simultaneous solution to the primal and dual problem.

4. EXAMPLES

Example 1

Using the same example as Cavalier and Melloy [1] seems appropriate for this paper.

Let's find the hyperplane $\mathbf{p}^t\mathbf{x} = p_1x_1 + p_2x_2 = \alpha$, which minimises the sum of the normal

Euclidean distances to the points $\mathbf{x}_1 = (1, 2)^t$, $\mathbf{x}_2 = (2, 4)^t$, $\mathbf{x}_3 = (3, 3)^t$, $\mathbf{x}_4 = (4, 3)^t$, $\mathbf{x}_5 = (5, 6)^t$. The problem (P5) is written as:

$$\text{minimise} \quad \sum_{i=1}^{5} d_i^2/|d_i| \tag{41}$$

$$\text{subject to} \quad p_1 + 2p_2 - \alpha - d_1 = 0 \tag{42}$$

$$2p_1 + 4p_2 - \alpha - d_2 = 0 \tag{43}$$

$$3p_1 + 3p_2 - \alpha - d_3 = 0 \tag{44}$$

$$4p_1 + 3p_2 - \alpha - d_4 = 0 \tag{45}$$

$$5p_1 + 6p_2 - \alpha - d_5 = 0 \tag{46}$$

$$q_1 p_1 + q_2 p_2 = 1 \tag{47}$$

$$\mathbf{p}, \alpha, \mathbf{d} \quad \text{unrestricted.} \tag{48}$$

Choosing x_1 as the dependent variable, then calculating the OLS equation results in the line $x_1 - 0.76x_2 = 0.26$; a choice of x_2 as the dependent variable, gives $-0.7x_1 + x_2 = 1.5$. This system is solved using equation (29):

$$\text{with} \quad \mathbf{q} = \begin{bmatrix} -0.7 \\ 1 \end{bmatrix} \quad \text{being used as the initial vector,}$$

$$\text{which normalises to} \quad \mathbf{q} = \begin{bmatrix} -0.573 \\ 0.819 \end{bmatrix}$$

$$\text{and} \quad F = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 4 & -1 \\ 3 & 3 & -1 \\ 4 & 3 & -1 \\ 5 & 6 & -1 \\ -0.573 & 0.819 & 0.0 \end{bmatrix} \quad \underline{\theta} = \begin{bmatrix} p_1 \\ p_2 \\ \alpha \end{bmatrix} \quad \underline{\psi} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \\ 1 \end{bmatrix}$$

The outcome is:

$$\underline{\theta} = \begin{bmatrix} 0.7071 \\ -0.7071 \\ -0.7071 \end{bmatrix}, \quad \underline{\phi} = \begin{bmatrix} -0.5 \\ -1.0 \\ 1.0 \\ 1.0 \\ -0.5 \\ -2.8284 \end{bmatrix} \quad \text{and} \quad \underline{\psi} = \begin{bmatrix} 0.0 \\ 0.707 \\ -0.707 \\ -1.414 \\ 0.0 \\ 1.0 \end{bmatrix}$$

With either $\mathbf{q} = (1, -0.76)^t$ or $\mathbf{q} = (-0.7, 1)^t$ as the initial vector in (47), the algorithm generates the ORLAV regression line, $0.7071x_1 - 0.7071x_2 = -0.7071$. Alongside this result, the algorithm determines the dual vector ϕ which can be interpreted as: the weights associated with each of the data points $\underline{\pi} = (-0.5, -1.0, 1.0, 1.0, -0.5)^t$ and the sum of the normal Euclidean distances, $\lambda = 2.8284$. So, the results confirm those of Cavalier and Melloy [1]. The algorithm took 2 iterations to achieve the solution.

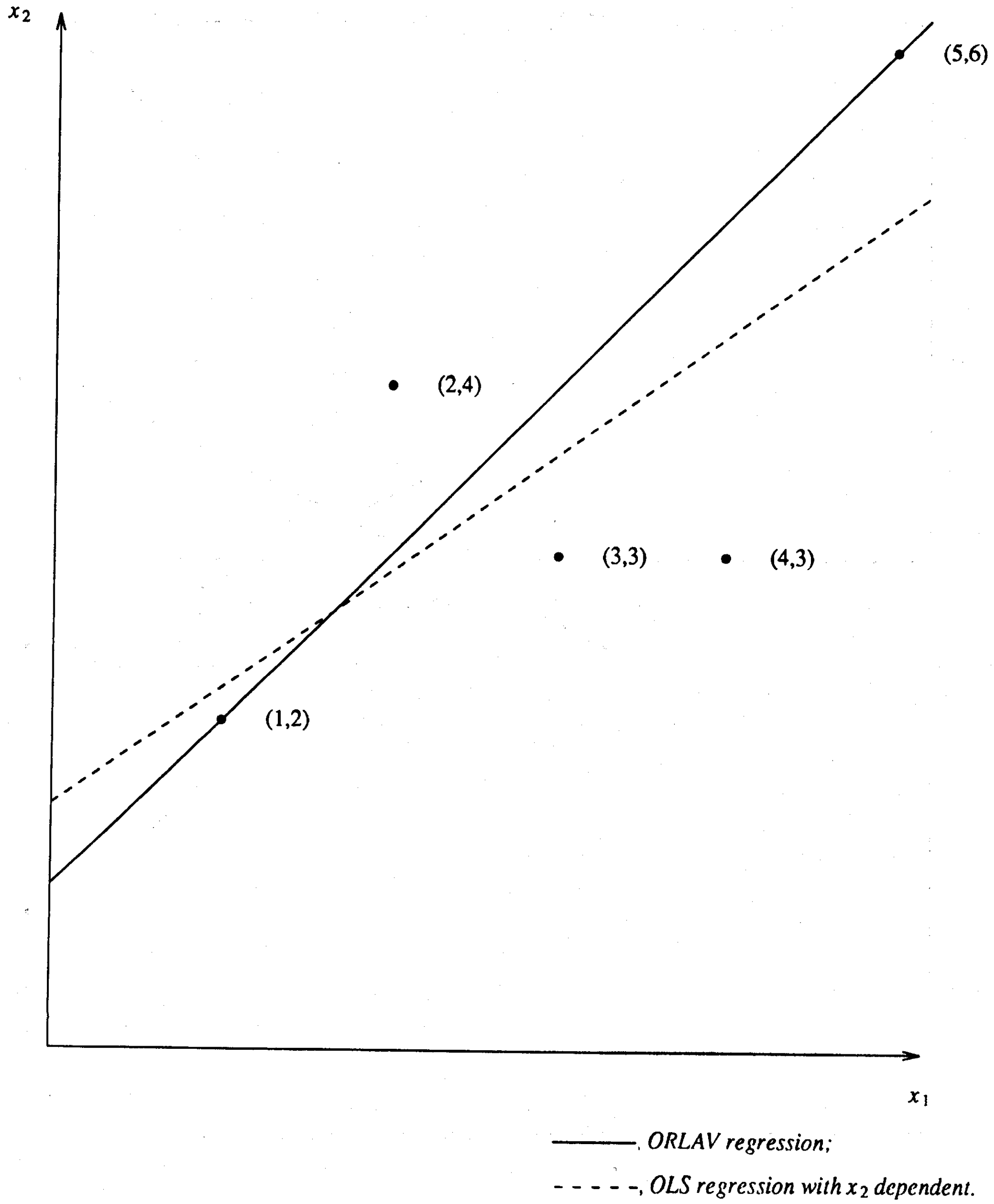


Fig. 3. Lines described in Example 1.

Example 2

To illustrate the robustness of the algorithm, the starting solution was chosen to be the vector *normal* to the final solution vector. The solution was found in 5 iterations:

Figure 4 illustrates the progression of the solution hyperplane from 1. through to 5. and emphasises the robustness of the algorithm.

The 1st. iteration determines the initial line through (2,4) and (3,3).
The 2nd. iteration is a rotation of the hyperplane around (2,4) and passing through (4,3).
The 3rd. iteration is a rotation of the hyperplane around (4,3) and passing through (3,3).
The 4th. iteration is a rotation of the hyperplane around (3,3) and passing through (1,2).
The 5th. iteration is a rotation of the hyperplane around (1,2) and passing through (5,6).

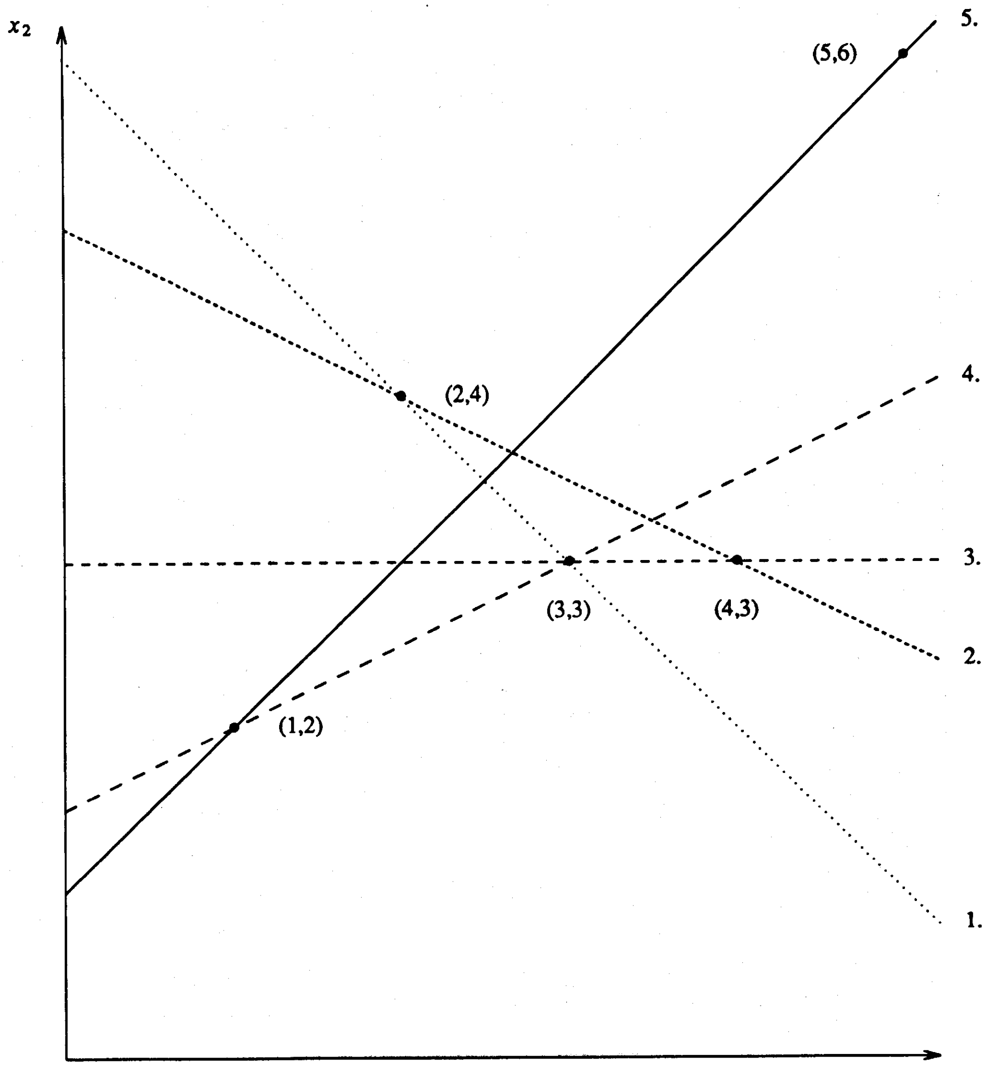


Fig. 4. Demonstrates rotation of the hyperplane until eventual solution is found.

5. CONCLUSIONS

A new technique for solving n-dimensional orthogonal linear regression (ORLAV) has been proposed in this paper. The ORLAV regression is a nonlinear, nonconvex programming problem. It has been re-cast in an augmented matrix form and solved as a sequence of iteratively re-weighted least squares problems. The algorithm is numerically robust (the augmented matrix preserves the condition number of the constraints matrix) and it gives a simultaneous solution to the primal and dual problems.

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