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INTELIGENCIA ARTIFICIAL: MÉTODOS, ALGORITMOS Y APLICACIONES

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16

PSO in Ridge Regression to eliminate multicollinearity in a PTA welding process

JORGE SAÚL RODRÍGUEZ VÁZQUEZ, ROLANDO JAVIER PRAGA ALEJO AND DAVID SALVADOR GONZÁLEZ GONZÁLEZ

PSO in Ridge Regression to eliminate multicollinearity in a PTA welding process.

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Abstract.
Nowadays industrial processes present variability in their processes making their control difficult. Linear regression is a statistical tool that can solve this problem, unfortunately if the process variables are highly related, the model obtained by Ordinary Least Squares (OLS) is not suitable to control or predict. This condition is called multicollinearity. Fortunately, there are statistical metrics capable of detecting linear dependence, such as the variance-covariance matrix, the VIF (Variance Inflation Factors) and the condition number. Ridge Regression (RR) is a method that eliminates the problem of multicollinearity. The basic idea of RR is generate a parameter of bias k that counteracts the dependency between the variables. There are methods that provide the value of bias k but affect model fit. For this reason, other alternatives should be choose. Therefore, in this article, a global optimization was performed applying the PSO metaheuristic on the parameter of bias k, to obtain the value that eliminates multicollinearity without affecting the fit of the model, taking the coefficient of determination R^2 as an objective function. The optimization was applied to a case study, the results were contrasted against the Ridge Regression method, obtaining better results for the Particle Swarm Optimization algorithm proposed in this article.

Keywords: PSO, OLS, Ridge Regression, Multicollinearity, VIF, Optimization.

1 Introduction

Regression remains a widely used statistical technique to model and predict industrial processes [1, 2]. There are different methods that can be used to obtain the regression model estimators, depending on the characteristics of the process. If the variables do not have collinearity, the method of Ordinary Least Squares (OLS) is used, however in most of the processes the variables have linear dependence and alternative methods have to be chosen [3,4] to generate adequate estimators of the regression model.

Ridge Regression (RR) is a viable option to use to treat multicollinearity, this method proposed by Hoerl et al. [5] has been applied in other investigations to eliminate the linear dependence between the input variables [6,7] by means of a parameter of bias k that eliminates the collinearity problem. This value can be obtained using the technique called Ridge trace or an iterative method proposed by Hoerl et al. [8] Currently, there is recent research that has modified the iterative method to calculate the bias value, obtaining good results to eliminate multicollinearity [9, 10, 11]. However, although the previous articles work on this problem, none of them proposes an alternative to avoid reducing the model fit, which can be measured with R^2 statistic.

In addition, optimization is a tool that has been used in various investigations (see Strömberg [12], Munner et al. [13]) in order to find the values of the input variables that generate the optimal solution for the objective function. However, there are problems for which one cannot guarantee to find an optimal solution in a reasonable time and these are classified (according to the theory of computational complexity) as "difficult". When a difficult problem is addressed, nature-inspired algorithms such as PSO (Particle Swarm Optimization), produce good results (Zadeh et al. [14], BharathiRaja et al. [15], Liu et al. [16]) because they only evaluate a part of the solutions and not the whole set of solutions.

Therefore, ones of the objectives of this work are to optimize the choice of the bias K matrix parameters that eliminate multicollinearity without affecting too much the statistical metric R^2.

2 Methods

2.1 Multiple linear regression models

The multiple linear regression model is used when the response variable y depends on a set of return variables X, by matrix notation the model is expressed as:

$$y = X\beta + \varepsilon \qquad (1)$$

Where y is a vector of nx1 observations, X is a matrix of nxp regressors, β is a vector of px1 regression coefficients, ε is a vector of nx1 random errors that are $NID(0, \sigma^2)$. To solve the regression model using Ordinary Least Squares (OLS) the coefficients of β are obtained with the equation:

$$\hat{\beta}_{MC} = (X'X)^{-1}X'y \qquad (2)$$

If the columns of the matrix X are linearly independent then the inverse matrix $(X'X)^{-1}$ will exist, however when the regressors have a strong linear relationship, the inference of the estimators by OLS is wrong. This matrix problem is also called multicollinearity.

2.2 Multicollinearity

Multicollinearity can be defined in terms of the linear dependence between the columns of the matrix X considering that their column vectors are $[X_1,\ X_2, \dots, X_p]$ so the equation can be established as follows $\sum_{j=1}^{p} t_j X_j \approx 0$. This implies that the matrix $X'X$ will be poorly conditioned because its determinant will be close to zero $|X'X| \approx 0$. Therefore, the method of Ordinary Least Squares will produce poor estimators of the individual parameters of the model. A serious problem involving multicollinearity is reflected in the hypothesis tests of the model, since the Type 1 error (reject H_0 when it should not be made) or the Type 2 error (accept H_0 when it should not be).

2.3 Multicollinearity detection

There are several techniques to detect multicollinearity, Variance Inflation Factors and the analysis of the eigensystem are the best diagnoses available today because they are easy to calculate, direct interpretation and useful to investigate the specific nature of multicollinearity [17].

1. Variance Inflation Factors: For each term of the model the VIFs measure the combined effect that the dependencies have between the regressors on the variance of each term, the Variance Inflation Factors are defined as:

$$VIF_j = \frac{1}{(1 - R_j^2)} \tag{3}$$

   R_j^2 is the coefficient of determination obtained when the regression is made x_j compared to other $p - 1$ regressors. If the VIF obtained are higher than 10 there is multicollinearity.

2. Condition Number: If one or more eigenvalues are very small, it implies that there is almost linear dependence between the columns of the matrix. The condition number that is defined as:

$$\eta = \frac{\lambda_{max}}{\lambda_{min}} \tag{4}$$

   Where λ_{max} is the maximum eigenvalue and λ_{min} is the minimum eigenvalue of the $X'X$ matrix. If $\eta > 1000$ it indicates strong multicollinearity.

2.4 Ridge Regression.

A review of the literature indicates that there is a wide range of research related to Regression Ridge (see [18,19]), this method proposed Hoerl and Kennard in 1970 suggests adding a parameter bias $k > 0$ in the diagonal of the matrix $X'X$ to eliminate multicollinearity coefficients β of Ridge Regression are obtained by solving:

$$\hat{\beta}_R = (X'X + kI)^{-1}X'y \tag{5}$$

The parameter of bias k can be obtained by means of the Ridge trace, this technique is subjective because a value must be chosen large enough to stabilize the coefficients of the model, but not unnecessarily large so as not to introduce too much bias affecting the Mean Square Error (MSE) obtained by the following equation:

$$MSE(\hat{\beta}_R) = \sigma^2 \sum_{j=1}^{p} \frac{\lambda_j}{(\lambda_j + k)^2} + k^2\beta'(X'X + kI)^{-2}\beta \tag{6}$$

Where λ_j are the eigenvalues of the matrix $X'X$, the first term of the equation is the sum of the variances of the parameters in $\hat{\beta}_R$ and the second term is the square of the bias, from Eq. (7) it is observed that if $k > 0$ the bias in $\hat{\beta}_R$ increases, however the variance decreases. The covariance matrix of $\hat{\beta}_R$ is:

$$Var(\hat{\beta}_R) = \sigma^2(X'X + kI)^{-1}X'X(X'X + kI)^{-1} \tag{7}$$

Because Ridge Regression focuses on the choice of the bias parameter and since the Ridge trace procedure is considered subjective (because criteria are required for its choice), one analytical method that determines the k-value for the Ridge Regression is proposed in [8] as follows:

$$k = \frac{p\hat{\sigma}^2}{\hat{\beta}'\hat{\beta}} \tag{8}$$

From Eq. (8) $\hat{\beta}$ and $\hat{\sigma}^2$ are determined from the Ordinary Least Squares solution. In a later publication [20] proposed an iterative procedure based on Eq. (8) the algorithm stops when $(k_{j+1} - k_j)/k_j \leq 20T^{-1.3}$ where $T = Tr(X'X)^{-1}/p$, at the end of the procedure the bias parameter k_j is used for the Ridge Regression. This procedure has been modified by other authors such as [21] where they compared 26 alterations made to the analytical method by various researchers in recent years.

2.5 Particle Swarm Optimization (PSO).

The Particle Swarm Optimization algorithm was proposed by James Kennedy and Russell Eberhart in 1995, the PSO algorithm is an algorithm in the area of artificial intelligence classified as swarm intelligence, the algorithm is stochastic and inspired by behavior social of some animals [22]. The algorithm allows the solution space to be explored in multiple directions, simultaneously, avoiding local minima.

The algorithm starts with a group of random particles (solutions) and then searches for optimal solutions by updating the generations. In each iteration, each particle is updated with two "best" values. The first value called pbest is the best solution you have achieved so far. The other "best" value called gbest is the best overall in the entire swarm. After finding the best two values, the particles update their velocity and positions applying equations (9) and (10).

$$v_i^{k+1} = w * v_i^k + c1 * rand1 * \left(pbest_i^k - x_i^k\right) + c2 * rand2 * \left(gbest_i^k - x_i^k\right) \tag{9}$$

$$x_i^{k+1} = x_i^k + v_i^{k+1} \tag{10}$$

Where v_i^{k+1}, v_i^k are the velocity of the particle in iteration $k+1$ and k respectively. Also x_i^{k+1}, x_i^k are the position of the particle in iteration $k+1$ and k respectively. Furthermore $rand1$, $rand2$ are random numbers evenly distributed between (0,1). The coefficients $c1$ and $c2$ indicate the degree of confidence in the best position found by the individual particle (cognitive parameter) and that of the entire swarm (social parameter), respectively, w is the weight of inertia used to achieve a balance in The exploration and exploitation of the search space and plays a very important role in the convergence behavior of PSO. The inertia weight is dynamically reduced from 1 to about 0 in each generation according to (11):

$$w_i = w_{max} - \frac{w_{max} - w_{min}}{iter_{max}} * iter \tag{11}$$

Where $iter_{max}$ is the maximum number of iterations and $iter$ is the current number of iterations, w_{max} and w_{min} are the maximum and minimum inertia weight values. The position of each particle is updated using its velocity vector as shown in Eq. (10).

3 Application.

A PTA (Plasma Transfer Arc) welding process is modeled where 4 input variables are involved and the relationship against an output variable is studied. Table 1 shows the 33 observations of the process:

Table 1. Observations of the welding process PTA.

x_1 Powder feed rate [%]	x_2 Powder feed rate [g / min]	x_3 Process speed [cm / min]	x_4 Welding Current [Amps]	y Area HAZ[mm^2]
70	26	80	60	4.908
60	21	100	60	5.184
50	18	80	80	4.859
60	21	100	80	3.693
60	21	100	70	3.623
70	26	100	70	3.504
70	26	120	80	3.711
60	21	100	70	3.737
70	26	120	60	3.371
50	18	100	70	3.345
60	21	100	70	3.541
60	21	100	70	4.092
50	18	80	60	4.674
60	21	100	70	4.023
60	21	100	70	3.47
60	21	100	70	3.478
50	18	120	80	3.202
50	18	120	60	3.081
60	21	100	70	3.447
60	21	100	70	4.016
60	21	120	70	2.719
60	21	100	70	3.526
70	26	80	80	4.584
60	21	80	70	4.662
60	21	100	50	3.498
60	21	80	50	4.449
60	21	120	50	3.197
50	18	120	50	2.985
60	21	120	50	3.028
70	26	120	50	2.099
70	26	160	50	1.813
70	26	140	50	2.406
70	26	180	50	1.945

Whit process data of Table 1 the bias is calculated to eliminate multicollinearity. Table 2 shows and compare the results of the bias k_i parameters obtained by the three techniques OLS, RR and PSO.

Table 2. Values k_j bias obtained with the three techniques.

OLS	Iterative Method [20]	PSO
$k = 0$	$k = 0.998$	$k = \begin{bmatrix} 0.5459 \\ 0.0708 \\ 0.0100 \\ 0.1522 \end{bmatrix}$

Table 3 shows the results of the Variance Inflation Factors to determine the elimination of multicollinearity. If any VIF value exceeds 10 then the linear dependency is still present among the regressors.

Table 3. VIF obtained based on the values k_j

Element	OLS	RR	PSO
VIF_1	33.77	0.11979	0.0842
VIF_2	34.86	0.11571	0.8571
VIF_3	1.48	0.22863	1.2786
VIF_4	1.27	0.23546	0.8888

Table 4 shows the coefficient of determination R^2 for OLS, RR and PSO. This statistical metric indicates the proportion of variance explained by the model. A value for R^2 close to 1 implies that most of the variability of prediction y is explained by the regression model.

Table 4. Adjusting the model based values k_j

	OLS	RR	PSO
Metric R^2	0.7451	0.4070	0.7367

4 Conclusions.

As shown in Table 2, there is more than one way to obtain the bias parameters that eliminate multicollinearity, so it is necessary to include other metrics that determine which of the techniques is better. Furthermore, considering that by means of the PSO metaheuristic a bias vector is obtained and not just a parameter as in Ridge Regression, it is necessary to indicate what effect it has on the regression.

A first metric considered was the Variance Inflation Factors since they indicate the degree of multicollinearity presented by input variables, as observed in Table 3 when applying Ordinary Least Squares the VIF_1 and VIF_2 have value of 33.77 and 34.86 respectively, this indicates that the data present collinearity problems because the

values should not be exceed than 10. When applying Ridge Regression the four VIF values were less than 10, thus indicating that the bias value k = 0.99812 obtained by the method [20] eliminates multicollinearity between variables. The same occurs with the bias vector generated by PSO, the four VIF are less than 10.
Table 4 shows the results where the coefficient of determination R^2 is considered as a metric. For OLS an R^2 of 74.51% is obtained, the result could be considered adequate, however, in the presence of multicollinearity, the model generated unstable regression estimators. In RR an R^2 of 40.70% is obtained, the percentage is far from 1 for the model to be considered representative of the process, even when multicollinearity has been eliminated. With the PSO method an R^2 of 73.67% is obtained, it is considered a better result than the previous two, because collinearity is eliminated and the model fit is not affected too much.
In conclusion, applying PSO to obtain the parameters of bias k is better than OLS and RR because PSO in addition to eliminating multicollinearity and having a model fit close to 1, more stable regression estimators will be obtained.

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