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Improving Partial Least Squares regression based on meta-heuristic optimization algorithms

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Abstract A popular method that combines and generalizes features from multiple regression and principal component analysis is called partial least squares regression (PLS). When we need to predict a collection of dependent variables from a very big number of independent factors, PLS is especially helpful. However, the performance of PLS depends on the number of components. Meta-heuristic algorithm implementation has grown in popularity among researchers. In this study, a Meta-heuristic algorithm is proposed to determine the number of components. The suggested approach will effectively assist in identifying the appropriate number of components with a strong forecast. The proposed approach is contrasted with two well-known approaches. The experimental results provide a thorough demonstration of the suggested method's superiority in prediction ability.

Keywords Meta-heuristic algorithm, Partial least squares regression.

AMS 2010 subject classifications 93E24, 46N10

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1. Introduction

Since statistical modeling explains the relationship between several explanatory variables and the response variable of interest, it is significant in many scientific research fields. The linear regression model makes the assumption that the explanatory variables do not correlate. However, this assumption may not hold in many real-world situations. Consequently, applying a linear regression model might not be suitable [1, 20, 21].
By identifying a set of latent factors, partial least square (PLS) regression, a multivariate technique that generalizes and integrates principal components analysis and the multiple linear models, aims to maximize the covariance between the response and covariates. As a result, PLS regression narrows the set of uncorrelated PLS components to a smaller number of explanatory variables [2, 3, 22, 23, 24, 25, 26].

However, the appropriate selection of latent components to be employed is one of the PLS most important decisions. "The cross-validation technique, the information criteria, the coefficient of determination, and the PRESS statistic, which is based on the leave-one-out technique, are the most popular methods used in determining the best latent components [3, 27, 28, 29, 30, 31].
Determining the best latent components in PLS can be considered as an optimization problem. Because the search space grows exponentially with increasing problem dimension, exact algorithms are unable to tackle complex problems in an acceptable amount of time. In addressing these issues, meta-heuristic algorithms which fall under

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the domain of approximation algorithms perform well [4, 5, 6, 7, 8, 32, 33, 34, 35, 36, 37, **?**]. Equilibrium optimization is a well-known example of a metaheuristic method.
To select the optimal latent components in PLS, an equilibrium optimization approach is provided in this study. The suggested approach will effectively assist in determining the suggested method's superiority in many simulated examples and a real data application with a high prediction.

2. Material and Methods

2.1. Partial least squares (PLS) regression

When there is a high degree of correlation between the explanatory components and when there are more explanatory variables than observations, the PLS is a tool for the linear regression approach that was created to connect many regressions for one or more of the response variables via latent variables [7, 38, 39, 40]. Using a set of latent variables or PLS factors that maximize the explained covariance between a response vector (y) and a data matrix (X), PLS seeks to model their relationship.
Let $\mathbf{Y}_{n\times q} = \left(\mathbf{y_1}, \mathbf{y_2}, \ldots, \mathbf{y_q}\right)$ and $\mathbf{X}_{n\times p} = \left(\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_p}\right)$. "Assuming that $\mathrm{y}_1, \mathrm{y}_2, \cdots, \mathrm{y}_q$ are mean-centered, and $\mathrm{x}_1, \mathrm{x}_2, \cdots, \mathrm{x}_p$ are mean-centered and scaled to unit variance. In the PLS algorithm, latent components $\mathbf{T}_{n\times H} = (\mathbf{t_1}, \mathbf{t_2}, \ldots, \mathbf{t_H})$ are computed from successive optimization problems. In the first iteration the loadings on $\mathbf{X}$and $\mathbf{Y}$ (denoted as $\mathbf{w_1}, \mathbf{c_1}$) satisfies both maximum variances of $\mathbf{t_1} = \mathbf{X w_1}$ and $\mathbf{u_1} = \mathbf{Y c_1}$, as well as correlation between $\mathbf{t_1}$ and $\mathbf{u_1}$, which can be obtained by:

$$(1)\ \arg\max_{w_1, c_1} \left[corr\left(\mathbf{Y c_1}, \mathbf{X w_1}\right) \sqrt{var\left(\mathbf{X w_1}\right) var\left(\mathbf{Y c_1}\right)} \right]$$

$$\text{s.t. } \mathbf{w_{12}} = 1,\ \mathbf{c_{12}} = 1$$

where the $\| \bullet \|_2$ is the l_2-norm. The solution of the direction vector (loading) $\mathbf{w_1}$is the $\mathbf{X^T Y Y^T X}$ eigenvector of corresponding to the largest eigenvalue λ_1, i.e.

$$\mathbf{X^T Y Y^T X w_1} = \lambda_1 \mathbf{w_1} \tag{1}$$

Then the score $\mathbf{t_1}$ which is the projection of $\mathbf{X}$on the direction $\mathbf{w_1}$ can be obtained by:

$$\mathbf{t_1} = \mathbf{X w_1} \tag{2}$$

Then, ordinary least squares regression is conducted on $\mathbf{X}$using $\mathbf{t_1}$, and the residual of $\mathbf{X}$can then be calculated with Eq. (3):

$$\mathbf{E_1} = \mathbf{X} - \mathbf{t_1 p_1^T} \tag{3}$$

Where $\mathbf{p_1}$is the loading and can be expressed as $\mathbf{p_1} = \frac{\mathbf{X^T t_1}}{\|\mathbf{t_1}\|^2}$. By replacing $\mathbf{X}$with$E_1$and $\mathbf{Y} = \mathbf{Y} - \mathbf{t_1 q_1^T}$in Eq.(1), the coefficient $\mathbf{w_1}$ and score $\mathbf{t_2}$of second PLS components can be calculated. After $h$iteration, scores matrix $\mathbf{T}$with $h$latent components can be obtained.

For the PLS algorithm, the columns of matrix $\mathbf{T}$are orthogonal to each other. In addition, columns of matrix $\mathbf{W}$are also orthogonal to each other. If $\mathbf{Y}$is univariate and $\mathbf{X}$ and $\mathbf{Y}$have the relationship $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, where the $\boldsymbol{\varepsilon}$ is a random vector of normal distribution with the variance $\boldsymbol{\sigma^2}$, then the estimation of $\boldsymbol{\beta}$ using the PLS method can be expressed as:

$$\hat{\boldsymbol{\beta}}^{\mathbf{PLS}} = \mathbf{W(W^T X^T X W)^{-1} W^T X^T Y} \tag{4}$$

Another desirable property of the PLS algorithm is its consistency. For univariate $\mathbf{Y}$ it has been previously shown that under some moderate regularity conditions, $\left\| \hat{\boldsymbol{\beta}}^{PLS} - \boldsymbol{\beta} \right\| \to 0$ if $p/n \to 0$in probability, and $\left\| \hat{\boldsymbol{\beta}}^{PLS} - \boldsymbol{\beta} \right\| > 0$ if $p/n \to k_0 > 0$ in probability [9-14]".

2.2. *Equilibrium optimization algorithm*

The Equilibrium optimizer algorithm (EOA) is investigated as a new meta-heuristic with fewer parameters and easy to understand. It is inspired by the nature of chemical equilibrium principles. It is observed that the molecules of a system interact with each other with certain characteristics. For example, molecules in a higher energy state tend to move to a state with lower energy, while molecules in a lower state move to a higher one. This is a direct translation of the hill climbing algorithms present in SAs and local searches. However, moving directly to a higher or lower state can trap the system in a local minimum or maximum. This situation is typical in nature where the energy level of a system is insufficient to reach a stable state. This problem is also present in current optimization algorithms [15, 41, 42]:

$$V\frac{dC}{dt} = QC_{eq} - QC + G \tag{6}$$

where C, V, Q, $_{V\frac{dC}{dt}}$, G, and $_{C_{eq}}$ are defined as in the original source. Eq. (5) can also be changed [16, 17, 18, 19]:

$$\frac{dC}{\lambda C_{eq} - \lambda C + \frac{G}{V}} = dt \tag{5}$$

Eq. (6) shows how Eq. (5) integrates over time:

$$\int_{c_0}^{c} \frac{dC}{\lambda C_{eq} - \lambda C + \frac{G}{V}} = \int_{t_0}^{t} dt \tag{6}$$

This results in

$$C = C_{eq} + (C_0 - C_{eq})F + \frac{G}{\lambda V}(1 - F) \tag{7}$$

In the equation (7), F is calculated as follows:

$$F = \exp[-\lambda(t - t_0)] \tag{8}$$

To determine the concentration in the control volume with a known turnover rate, use Eq. (9). Using uniform random initialization, the search space is evenly initialized, and the starting concentrations are built based on the particle count and dimension:

$$C_i^{initial} = C_{\min} + rand_i(C_{\max} - C_{\min}) \qquad i = 1, 2, ..., n \tag{9}$$

$_{C_{\min}}$ and $_{C_{\max}}$ stand for the min and max values for the dimensions, n is the total number of particles in the population, and Randi is a random vector in the interval [0, 1].
Each agent in this system has the ability to change its position to another point within its search space by considering its neighborhood. This ability is different for each agent, an agent that has higher energy tends to stay away from its threshold because it doesn't want to spend much effort to change its state, and on the contrary, an agent that has lower energy tends to seek its refinement because it has an eagerness to change its state to get a better condition. This condition can be represented by the minima and maxima value of a function. The equilibrium pool is constructed using these five particles, which are proposed as equilibrium candidates:

$$\vec{C_{eq,pool}} = \{\vec{C_{eq(1)}}, \vec{C_{eq(2)}}, \vec{C_{eq(3)}}, \vec{C_{eq(4)}}, \vec{C_{eq(ave)}}\} \tag{10}$$

Every iteration, each particle modifies its concentration using a random selection procedure from candidates chosen with an equal chance. Given that a real control volume's turnover rate can change over time, it is assumed that $_{\lambda}$ is a random vector with a range of [0, 1]. $_{\vec{F}=e^{-\vec{\lambda}(t-t_0)}}$ (13)
Time, t, decreases with the number of iterations since it is a function of iteration (Iter): $_{t=(1-\frac{Iter}{Max_iter})^{(a_2\frac{Iter}{Max_iter})}}$

In this case, the maximum and current iterations are represented by max_iter and Iter, respectively, whereas the constant a2 governs the capacity for exploitation. To guarantee convergence, the search speed should be slowed

down while simultaneously improving the algorithm's exploration and exploitation capabilities:

$$\overrightarrow{t_0} = \frac{1}{\overrightarrow{\lambda}}(-a_1 sign(\overrightarrow{r} - 0.5)[1 - e^{-\overrightarrow{\lambda} t}]) + t \tag{11}$$

where the fixed value a1 controls the exploring capacity. Higher exploring capabilities are correlated with larger a1 and worse exploitation performance.

Equation (16) represents the updated version of equation (13) after equation (15) was substituted:

$$\overrightarrow{F} = a_1 sign(\overrightarrow{r} - 0.5)[e^{-\overrightarrow{\lambda} t} - 1] \tag{12}$$

The generation rates are described as a first order exponential decay process in the typical model that follows: $\overrightarrow{G}=\overrightarrow{G_0}e^{-\overrightarrow{k}(t-t_0)}$

where k represents the decay constant and G0 represents the initial position. The last set of generation rate formulas are as follows:

$$\overrightarrow{G} = \overrightarrow{G_0}e^{-\overrightarrow{\lambda}(t-t_0)} = \overrightarrow{G_0}\overrightarrow{F} \tag{13}$$

Where:

$$\overrightarrow{G_0} = \overrightarrow{GCP}(\overrightarrow{C_{eq}} - \overrightarrow{\lambda}\overrightarrow{C}) \tag{14}$$

$$\overrightarrow{GCP} = \begin{cases} 0.5r_1 & r_2 \geq GP \\ 0 & r_2 < GP \end{cases} \tag{15}$$

where the GCP vector is created by repeating the value that is derived from Eq (20) and the random integers r1 and r2 are in the range [0, 1]. The GCP is uses to account for the generation term's possible contribution to the updating process. The mechanism underlying this contribution is found in Eqs.(19) and eq.(20). Eq.(20) has an effect on every particle. The following is the final guideline for updating the EO:

$$= \overrightarrow{C}_{eq} + (\overrightarrow{C} - \overrightarrow{C}_{eq}).\overrightarrow{F} + \frac{\overrightarrow{G}}{\overrightarrow{\lambda} V}(1 - \overrightarrow{F}) \tag{16}$$

2.3. The proposed approach

The number of latent components that is properly chosen determines how effective PLS is. To identify the latent components in the PLS, an EOA is suggested in this work. The suggested approach will effectively assist in locating the optimal value with strong prediction accuracy. The following are the parameter combinations for our suggested methodology.

1. The initial set of parameters is 25 members and the number of iterations is $\mathrm{t_{max}}= 300$.
2. Every member's position is chosen at random. The latent components are represented by a member's position. The members' starting positions are produced from a uniform distribution in the interval [0,p-1].
3. The definition of the health advantage is

$$\text{fitness} = \min \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2, \tag{17}$$

4. We use Eq. (12) to update the positions.
5. We keep repeating steps 3 and 4 until $t_{\max}$ is reached.

3. Results

To test the performance of our proposed approach, EOA, a Monte Carlo simulation study was carried out. For comparison, the performances of the methods based on the cross-validation (CV) and Akaike information criterion

(AIC) are given as well. The Monte Carlo simulation is based on two cases: In Case 1, there are five variables which are generated from a 5-variate normal distribution with mean vector $\boldsymbol{\mu}$ and covariance matrix Σ. While in Case 2, there are 8 variables which are generated from a 8-variate normal distribution with mean vector. The simulation scenario considers: sample size $n \in \{30, 50, 100, 150\}$, vector of true parameters is25, 40, 10,80, 15, 23, 40, 6 and $\sigma_j^2 = 1$ for $j = 1, \ldots, 8$, values of correlation coefficient 0.85, 0.90 and 0.95, with 1000 Monte Carlo replications for each sample size. With a mean of 0.5 and a standard deviation of 1, a normal distribution yields the response variable y.

Tables 1 and 2 summarize the MSE values for the used methods. It is revealing from Tables 1 and 2 that EOA yielded lower MSE. A comparison with EOA shows that better results were obtained from CV and AIC methods". For example, when n=50 and $\rho = 0.90$, the proposed method achieves the highest performance as its MSE is much lower than that of CV at 15.192 and that of AIC at 13.315.

It is evident from the techniques that the CV attains poor performance in selection the best latent components. For instance, in the case 2 (Table 2), the MSE when n=150 was 15.47, 16.786, and 17.35, respectively which are higher than those of AIC and EOA.

Table 1. The performance of the used methods for case 1

methods				
n=30	CV	12.256	13.572	14.136
	AIC	10.068	11.391	12.259
	EOA	7.371	8.084	8.895
n=50	CV	13.312	14.628	15.192
	AIC	11.124	12.447	13.315
	EOA	8.427	9.14	9.951
n=100	CV	14.887	16.203	16.767
	AIC	12.699	14.022	14.89
	EOA	10.002	10.715	11.526
n=150	CV	15.47	16.786	17.35
	AIC	13.282	14.605	15.473
	EOA	10.585	11.298	12.109

4. Conclusion

The use of meta-heuristic algorithms in research has become more and more common. Finding the ideal number of latent components for partial least squas proposed. According to the simulation results, the suggested strategy, EOA, outperformed other approaches in terms of IMSE.

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Table 2. The performance of the used methods for case 2

methods				
n=30	CV	17.464	18.78	19.344
	AIC	15.276	16.599	17.467
	EOA	12.579	13.292	14.103
n=50	CV	18.52	19.836	20.4
	AIC	16.332	17.655	18.523
	EOA	13.635	14.348	15.159
n=100	CV	20.095	21.411	21.975
	AIC	17.907	19.23	20.098
	EOA	15.21	15.923	16.734
n=150	CV	20.678	21.994	22.558
	AIC	18.49	19.813	20.681
	EOA	15.793	16.506	17.317

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