

## OPTIMIZATION METHODOLOGY WITH PRINCIPAL COMPONENT ANALYSIS APPLIED IN PORTFOLIO: SIMULATED RESULTS IN GREEN COMPANIES

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### ABSTRACT

This research objectives to develop mathematical models for risk-return that consider simultaneously the linear and non-linear effects of the invested proportions and features of green companies based on their balance sheets/annual reports indicators. The mixture design of experiments is combined with Ward clustered PCA process variables for selecting the most promising companies through generated financial indicators (General Multivariate Indicators method) from the green companies. The green companies are the object of study for this empirical research, they were gathered from Newsweek magazine rank. The proposed Clustered Multilevel Optimization method has showed to be more robust and efficient than the all-other tested methods in this research. That means greater security and less risk to the investor.

### KEYWORDS:

principal components analysis,  
financial indicators,  
DOE,  
green companies,  
portfolio optimization,  
financial ratios,  
balance sheets.

### INTRODUCTION

The consideration of financial indicators acquired from balance sheets of several green companies is an extension studied in this article, since it is possible to encounter several works on portfolio analysis in literature. The study of financial indicators is a very broad topic with an open gap: the company selection method and the use of other data sources besides the stock market history in order to optimize the risk-return function. Investors can benefit from this methodology when selecting the companies that compose their portfolios, adding a numerical analysis to their know-how. The investigation is performed incorporating the financial indicators as a process variable in the mixture design of experiments generated through Principal Component Analysis and Clusters. The green companies classified on Newsweek Magazine were selected as investigation objects. Firstly, an original classification was recreated using the general multivariate index. In the second phase, the balance sheet indicators were calculated and added to the model for cluster division. A risk-return analysis was made for comparison with a portfolio selection method using a mixture design of experiments (de Oliveira et al., 2011) that considers all the selected companies and is based on the portfolio selection proposed by (Markowitz, 1952). The conclusion shows better stability and profitability of the portfolios on a 5-year period and also verify that the proposed methodology is more consistent for company selection.

The balance sheets are a variable that influence portfolio composition and should be taken into consideration. Experimental arrangements were used to analyze portfolio formation using clusters. The investment simulation was used to benchmark the 5 portfolio methods analyzed:

1. CMO (Clustered Multilevel Optimization) – proposed method;
2. CM-DOE (Crossed Mixture Design of Experiment) – proposed by (Piepel, 1999);

3. Markowitz method (Markowitz, 1952);
4. EC-CMO (Excluded Companies from Clustered Multilevel Optimization) – since the CMO classifies the best companies for the investment, this method basically uses the excluded ones to compare results;
5. Equal Investment – this method basically sets the same investment in all companies.

The balance sheets are an important source of financial information and open capital companies are obliged by law to publicly release this data. One of the contributions of this study is to include indicators extracted from balance sheets as a process variable based on Design of Experiments (DOE) in portfolio selection models.

Two new methods for grouping companies considering risk-return were introduced in this article: placement on Newsweek magazine green company rank and financial indicators. A combination of PCA and Crossed Mixture Design of Experiment (CM-DOE) (Piepel, 1999) in order to generate optimal portfolios including green companies are also proposed as an opportunity to incorporate new tools into the conventional models of portfolio selection. Several financial risk ratios were used as basis for PCA, where companies were gathered into three clusters. The indicators were screen using the concept of data mining, and the balance sheet of each company was individually analyzed so that all the relevant information was extracted to generate the indicators.

## MATERIALS AND METHODS

### Green companies

Being green is a considerable task. (Saha and Darnton, 2005) listed some prime aspects for any company to be considered green: ecological concerns, conservation of the fauna and flora, corporative social responsibility, humanitarian concerns, fair trade, clean water, animal welfare, quality, and sustainability. Newsweek’s magazine’s Greenest Companies ratings is a ranking composed of energy productivity, carbon productivity, water productivity, waste productivity, and reputation. Those indicators have a range from 0.00% to 100.00% with a higher percentage representing better/greener score. The U.S. Department of Energy gives monetary motivation and awards to companies that help to recover the environment. The Energy Department invested more than US\$31 billion to support a wide range of clean energy projects across the nation according to the Clearinghouse of 2015.

In Bansal, Pratima; Roth (2000), a survey conducted among 53 companies showed several motivations for companies to be green; Lyon and Shimshack (2012) studied the impacts of media generated by companies sustainability programs. Using Newsweek’s ratings of the 500 largest U.S. firms they found that the top 100 firms of the ranking have experienced abnormal returns of 0.6% to 1.0% higher than the returns of the bottom 400 on the ranking.

### The financial ratios

Financial ratios are an important quantitative way to measure company performance. Failing enterprises exhibit ratio measurements significantly different than those that are thriving, and these can all be described by five key ratios (Altman, 1968). The business risk is the risk that a company fails and it is divided into internal and external sources. The internal source is the general reflection of the variability of the net operating income or net cash flow. The external source is caused by the market which produces price variability for both outputs and inputs (Gabriel and Baker, 1980). In the United States of America, companies that have assets on the exchange market are regulated by the Securities Exchange Act (1934). Companies need to publish all their financial reports in a complete balance sheet. Most of those ratios are focused on the balance sheet and income statements. Cash flows can offer better insights from the ratio analysis when the period is considered continuously (Barua and Saha, 2015). The considered ratios for this study are listed in Table 1, adapted from (Barua and Saha, 2015). These indicators demonstrate the company's financial health.

Tab. 1: Considered ratios

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Analysis of debt usage

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$$1 \quad \text{debt to total capital} = \frac{\text{total debt}}{\text{total capital}}$$

$$2 \quad \text{debt to equity} = \frac{\text{total debt}}{\text{total equity}}$$


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Analysis of Interest Coverage Ratio

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$$3 \quad \text{times interest earned tax} = \frac{\text{earnings before interest and tax}}{\text{interest expense}}$$

$$4 \quad \text{fixed charge coverage} = \frac{\text{earnings before charges and taxes}}{\text{fixed charges}}$$

$$5 \quad \text{times interest earned cash} = \frac{\text{adjusted operating cash flow}}{\text{interest expense}}$$

$$6 \quad \text{fixed charge coverage ratio} = \frac{\text{adjusted operating flow}}{\text{fixed charges}}$$

$$7 \quad \text{capital expenditure ratio} = \frac{\text{cash flow from operations}}{\text{capital expenditures}}$$

$$8 \quad \text{cash from operations to debt} = \frac{\text{cash flow from operations}}{\text{total debt}}$$


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### Principal Component Analysis (PCA)

PCA is probably the best and most aged technique used to analyze multivariate problems (Jolliffe, 2002). (Hotelling, 1933) introduced the PCA method as a technique of the multivariate statistics. It is used to make inferences about the variance-covariance structure in a data set. This concept uses linear combinations of the original variables. There are two main objectives of PCA: Shrink the dimensionality of the dataset and provide interpretation of the data. The relationship between the components is revealed and is often an intermediary step within a broader data group (Johnson, 2002; Puntanen, 2013).

### The mixture and crossed mixture design of experiments

The experiment is the most efficient method of discovery. It is one of several major research strategies (Montgomery, 2012) and can provide a mechanism of action for a particular phenomenon. An alternative to experimentation is passive observation, where a scientist will observe a process in anticipation of an interesting change. This method can often lead to a large amount of data, where identification of relevant information may be difficult. Experimentation, on other hand, can require less effort and generate less non-relevant data (Andersson, 2012). The main difference is that a passive observer just monitors a pre-existing process while the experimenter changes the state and investigates the results of these changes.

Mixture designs are experimental designs where the factors of the design are components or ingredients (Draper and Pukelsheim, 1998) of a mixture (Gozálvez-Zafrilla et al., 2013), i.e., different proportions of any component can change the overall result. Experiments with mixtures are those in which the property studied depends of the proportion of the components, but not on the amount of the mixture (Scheffé, 1963). The proportions are more important than the final quantity of the object of study.

Considering each proportion of the mixture as a weight  $w_i$  of  $q$  components yields the equation (1), which is related to the portfolio constraint of (Markowitz, 1952).

$$\sum_{i=1}^q w_i = 1.0 \quad (1a)$$

$$w_i \geq 0, \quad i = 1, 2, \dots, q \quad (1b)$$

Some of MDE applications can be listed starting with (Misturas, 2008), and (Scheffé, 1963) using the centroid or central point. (Brandvik and Daling, 1998) provided an optimization in product development. (Måge and Næs, 2005) used MDE with process variables or fractional design. There also several works using the original concept of MDE, i.e., using MDE to analyze and optimize the proportions of ingredients of products (Lonni et al., 2012; Ngun et al., 2014; Nikzade et al., 2012) with and without constraints.

MDE supports individual and global constraints. Considering the resolution of the mixture as  $V$ , with  $\eta$  being any integer natural number,  $\Psi$  the maximum value of the mixture and  $n$  the number of assets of the clusters or portfolios in the global mixture shown at the equation (2). When  $V$  decreases, the number of runs in the experiment increases.

$$V = \eta_i \therefore \Pi_{\eta_1} * V = \Psi \text{ and } \Pi_{\eta_2} * V = n \quad (2)$$

The crossed mixture design (CM-DOE) was introduced by combining two different mixtures to create a region of interest as a third mixture (Cornell, 1971), and after that as a two-stage mixture experiment (Cornell and Ramsey, 1997). It is also known as mixture of mixture design (MoM) (Borges et al., 2007; Di Zio et al., 2007; Kang et al., 2011; Piepel, 1999). There is one model of DOE that combines mixture with process variables. (Cornell, 1971) described that kind of model as a design of simplex-lattices and factorial arrangements. This case involved a mixture experiment with  $q$  components plus  $n$  process variables, where  $n$  can be any positive integer.

The optimal characteristic of a product can be found from one model that combines both process variables and component's proportions in the MDE. (Montgomery, 2012) has described the process component as new variables  $z$  considered in this case as the MGI (Multivariate General Index) variable. The terms that involve only the process variables are not included in the model. Both mixture of mixture and mixture with process variable methods were used to perform the analysis.

### Portfolio selection

Harry Markowitz introduced the portfolio selection model (Markowitz, 1952). The portfolio selection is an econometric tool designed to help the investor to decide how much of his wealth should be applied towards each investment. In the case approached by this study, the investments are assets of the stock exchange. However, this can also be applied in different types of investments. (Trippi, 1989) used it for real estate investment; (Better and Glover, 2006) used portfolio in selection of projects; (Delarue et al., 2011) applied it to the electric sector. (Byers et al., 2015) also discussed the application of portfolio theory in a broader sense, including intellectual capital and resources of enterprises.

The risk of the investment using portfolio theory can be higher by only selecting one investment as proven by (Markowitz, 1952), who states that if an investor diversifies between two portfolios, the risk of the compound investment will be smaller than the risk of either single investment. There are many options to solve the portfolio optimization problem, e.g., isomean line (Markowitz, 1952), mean-Gini (Shalit and Yitzhaki, 1984), analytical method (Li and Ng, 2000), min-max rule (Yu et al., 2005), desirability function (de Oliveira et al., 2011), hybrid intelligent algorithm (Zhang et al., 2012) and so on. The choice of the optimization method depends on the analyst, but in all the cases, the goal is the same: a maximum return with the lowest possible risk. The objective in portfolio selection is to make tradeoff between return and risk.

### METHOD

The Newsweek's magazine has a rank formed by 500 companies as Greenest Companies. The rank is composed of five indicators: energy productivity, carbon productivity, water productivity, waste productivity, and reputation, which are updated annually. The steps of the method are numerated to highlight the process.

1. The principal component analysis (PCA) is applied to the original indicators creating a new classification by the multivariate general index (MGI): the PCA was performed considering all the original indicators with three components

to compute and to evaluate the correlation matrix. The MGI is then calculated using equation (4). A new ranking came up assuming the highest values for MGI and their corresponding companies (Papandrea et al., 2016). This phase changes the original order of the ranking, considering just the indicators that most impacts the PCA scores. The companies are now selected according to the MGI based on their sustainability indicators.

$$MGI = \sum W_{PC_{ij}} * Eigenvalue_{PC_i} \quad (4)$$

2. Obtain the historical data of stock prices from the NASDAQ databank. The considered data comprehends the past 5 years of the selected companies. After downloading the data, each company had their monthly closing prices segregated for the risk calculations and the individual returns (Papandrea and Paiva, 2016a).
3. Download of Balance Sheets of the Annual Report: The same 20 companies have had their financial balance sheets downloaded from their official websites or from NASDAQ's webpage. These sheets had to be analyzed individually in order to extract the information needed to calculate the financial ratios based on balance sheets: the necessary data for the calculation of each of the indicators, described in Tab. 1, were recorded and calculated using those sheets (Papandrea Pedro and Anderson, 2016).
4. Risk ( $\sigma$ ) and return ( $\mu_i$ ) calculation with replication: the risk and return of each company was calculated using the average and standard deviation of the standardized values from the equation (5). The same calculation was made to the original values and to the replicated values (Papandrea Pedro and Anderson, 2016). The monthly closing values of each asset of each company were replicated using the ARMA-GARCH model, with  $lag = 1$  (Papandrea and Paiva, 2016b).

$$r_i = \frac{\log(P_i)}{\log(P_{i-1})} \quad (5)$$

5. Generation of clusters based on indicators calculated to create smaller mixes: the ratios debt to total capital, debt to equity, times interest earned, fixed-charge coverage, times interest earned - cash basis, fixed charge coverage ratio - cash basis, capital expenditure ratio and CFO to debt were grouped by Ward linkage method (Ward, 1963), Euclidean distance measure and related in three clusters (Papandrea and Paiva, 2016c).
6. PCA applied to financial indicators in order to define the process variables (-1) and (+1): the process from the PCA of item 1 was now done using the variables of the financial ratios from item 3, the MGI was also calculated in the same way.

The steps mentioned above describe the method for creation and selection of process control variables using balance sheet indexes. The consideration of these indexes is made possible on the portfolio indicator analysis through the usage of DOE and mixture process variables.

## RESULTS AND DISCUSSIONS

PCA was applied on the Newsweek's Greenest Companies ratings; this is shown in Fig. 1 and detailed in Tab. 2. That ranking is based upon the following criteria in percent scale: energy productivity, carbon productivity, water productivity, waste productivity, reputation. From here, three groups were formed. The three scores of the PCs calculated and grouped by the MGI (20) lead to a new ranking. The (Papandrea et al., 2016) shows the Newsweek ranking versus the MGI ranking. Forty four companies were considered because they possess all the necessary data for analysis and for not having undergone mergers or closure in considered periods. The top twenty companies were extracted which are detailed in (Papandrea and Paiva, 2016c) with their NASDAQ codes. Fig. 1 shows also the principal components of: 1-Reputation, 2-Energy productivity, 3-Carbon

productivity, 4-Water productivity, 5-Waste productivity. The five indicators were gathered in three groups. Of those groups, the twenty highest PCA scores were added to our selection, considering the numerical signal. The second stage was to research and calculate the financial ratios shown in Tab. 1.

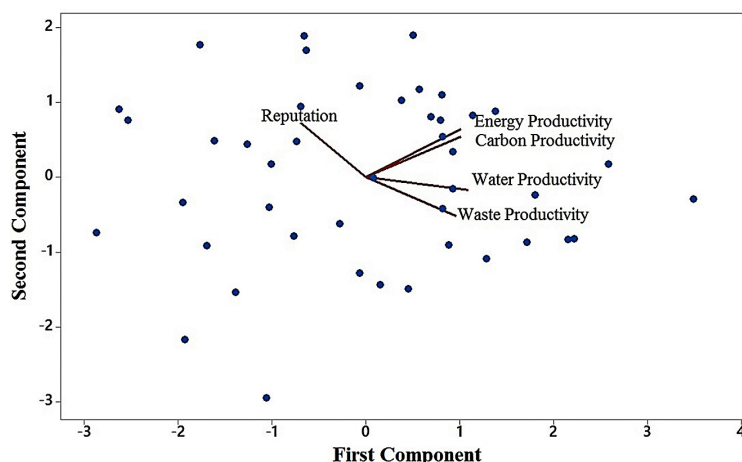


Fig. 1: PCA on *Newsweek* ranking

Tab. 2 Eigen analysis of the *Newsweek* Ranking

Eigen analysis				
Eigenvalue	2.037	0.998	0.621	0.343
Proportion	0.509	0.250	0.155	0.086
Cumulative	0.509	0.759	0.914	1.000
Variable	PC1	PC2	PC3	
Energy Productivity	0.544	-0.463	-0.234	
Carbon Productivity	0.532	-0.415	0.482	
Water Productivity	0.506	0.387	-0.669	
Waste Productivity	0.406	0.681	0.515	
Reputation	-0.321	0.588	-0.572	

The reputation is out of the considerations because it resembled with no indicator, showing a negative PC value.

The analysis of the annual financial report of each company has been considered to calculate the financial ratios described in Tab. 1. After that, a PCA was applied to gather those ratios in four groups (Fig. 7: A-Debt to capital, B-Debt to equity, C-Fixed-charge covered ratio, D-Times interest earned-cash, E-Fixed-charge coverage, F-Times interest earned-tax, G-Capital expenditure ratio, H-Cash from operations to debt). Three main component scores were identified for each company (PCA1, PCA2, and PCA3). Each PCA score also has a related weight. The weightings for PCA1, PCA2, and PCA3 are  $W_{PCA_1} = 0.575$ ,  $W_{PCA_2} = 0.184$ , and  $W_{PCA_3} = 0.137$ . A multivariate global index (MGI) was then calculated using these proportions. The Ward method was applied on the scores to divide the companies into. The MGI was used to classify each cluster in variable (-1), (+1) by the algorithm: if the company's MGI in the cluster is less than the average of the MGI of its cluster, the process variable is -1; otherwise, it is +1. MGI works as process variables in the crossed mixture. The (Papandrea Pedro and Anderson, 2016) have the financial ratios calculated.

The higher the indicators of debt (in millions) the lower will be the MGI while indicators of the interest coverage ratio will increase the MGI. This indicates that the more a company owes, the more opportunity for your MGI be increased. Fig. 2 shows a cluster grouping process by the variable MGI.

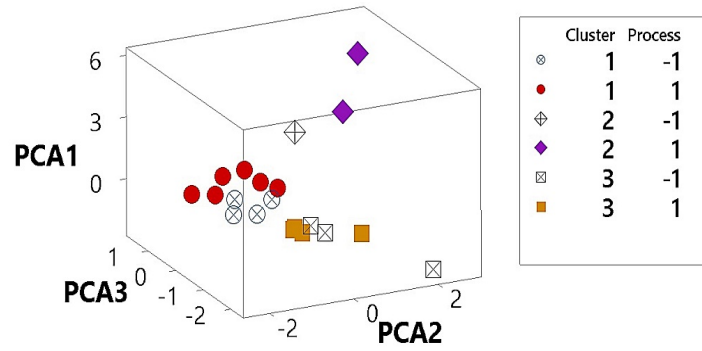


Fig. 2: Clusters and MGI process variables

The return and the risk of the company's asset are considered the average and the standard deviation (volatilities) of the monetary quote value of each closed month. Their values were approximated based on historical spanning 120 months as described in Section 3. The (Papandrea and Paiva, 2016c) shows the allocation of enterprises by cluster and within each cluster divisions. The first cluster indicate the companies that make up the process variables in each cluster by PCA; the second shows the companies that make up the process variables by cluster in the MGI. These divisions are the composition of portfolios. Instead of a random company selection performed by the investor, the cluster process selects which companies will be inside each group and the PCA defines which companies will compose the portfolio. The (Papandrea and Paiva, 2016c) also shows the division of the companies that make up each cluster divided into process variables, it includes the companies that will compose the crossed mixture portfolios with its structure formed by portfolios of clusters, portfolios of companies with process variables. The CMO arrangement does not consider all companies, only those selected by the MGI values. The PCA values that are higher or lower than the average of MGI indicate the companies that will be selected by the process variables (-1) e (+1). The average values for the clusters are: *Cluster 1* =  $-0.10$ , *Cluster 2* =  $2.56$ , and *Cluster 3* =  $-0.96$ . All types of design are described in (Papandrea and Paiva, 2016d).

The optimizations were performed using the desirability method. Firstly, each cluster has been optimized completely, considering all the companies that compose it, divided only by MGI, and considering it as process variables. Note that the cluster 2 with (-1) process variable was not optimized because it is composed of only one company. This is considered for the next optimization. Afterwards, the clusters comprise a new optimized portfolio, and in this, the returns and risks of each cluster previously optimized will be the input values of the next optimization. Next, the optimization of the crossed mixture model with process variables is made considering only a few companies in each cluster, depending on their MGI values. Finally a global optimization using the Markowitz model of portfolio, which consists of all companies in a same set. This optimization does not consider process variables, but the values of return and risk.

The Tab. 3 shows the result of each optimization. The lower is the level of individual clusters the highest will be the compound by the mixture of mixture.

Tab. 3 Results of optimization

Type	Companies/PCA/Cluster/MGI						Results		
Cluster1 -1	AAPL	IHS	SIAL	TAP			RP	SP	Desirability
$\gamma_i^*$	0.6910	0.0000	0.0000	0.3090			0.0194	0.0502	0.8257
Cluster1 +1	ADBE	ADI	BHI	MOS	QCOM	SPRINT	RP	SP	Desirability
$\gamma_i^*$	0.9060	0	0	0.094	0	0	0.0087	0.0632	0.9919
Cluster2 -1	EMC						RP	SP	Desirability
$\gamma_i^*$	1.0000						0.0055	0.0811	-
Cluster2 +1	BIIB	NKE					RP	SP	Desirability
$\gamma_i^*$	0.6010	0.3990					0.0173	0.0665	0.6784

Cluster3 -1	CLX	CMA	WYN					RP	SP	Desirability
$\gamma_i^*$	0.8930	0.0000	0.1070					0.0055	0.0500	0.7917
Cluster3 +1	BLL	CCE	MAS	MET				RP	SP	Desirability
$\gamma_i^*$	0.9930	0.0000	0.0000	0.0070				0.0112	0.0584	0.9938
CMO	Cluster1	Cluster2	Cluster3	MGI				RP	SP	Desirability
$w_i^*$	0.0000	0.7530	0.2470	+1				0.0157	0.0500	0.8690
CM-DOE	PCA1	PCA2	PCA3	Cluster1	Cluster2	Cluster3	MGI	RP	SP	Desirability
$w_i^*$	0.0000	0.8440	0.1560	0.0000	1.0000	0.0000	+1	0.0784	0.1092	0.9281
Markowitz	AAPL	ADBE	ADI	BHI	IHS	MOS	QCOM	RP	SP	Desirability
	0.0260	0.0430	0.0310	0.0000	0.0860	0.0450	0.0490			
	SPRINT	SIAL	TAP	BIIB	EMC	NKE	BLL			
$w_i^*$	0.0000	0.0720	0.0490	0.2090	0.0730	0.0970	0.1680	0.0123	0.0508	0.8305
	CCE	CLX	CMA	MAS	MET	WYN				
	0.0320	0.0000	0.0000	0.0130	0.0080	0.0000				

The desirability optimization graphic of the CMO method with clusters and financial ratios is shown in Fig. 4.

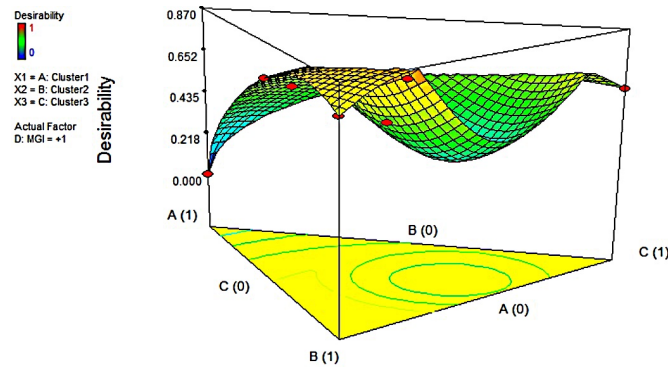


Fig. 4: 3D Desirability optimization of the CMO method with clusters and financial ratios

## CONCLUSION

In this research, the proposed CMO method is exemplified and validated using real world data of Green Companies. Computational results show that it can help investors to analyze market exchange scenarios more robustly. The diversification seems better when the calculated ratios is considered from the annual financial reports.

The results shown in Table 4 demonstrate that there are considerable differences between the returns and risks of each model. Observing, the proposed method mitigates the risk of negative returns or losses, although the Markowitz model allows it. In the series where the Markowitz model is being used, there are negative values. Observing the CMO and CM-DOE series, in any case of the simulations, there are non-positive returns, meaning that in any case using the proposals the risk of capital loss exists, but only with reduced gain. This pioneering approach makes the proposed models more robust and viable. In the CMO model, the best portfolio will be clustered in a new one, and this new cluster will be optimized. In the other hand, on the CM-DOE model, there is the simultaneous optimization of mixtures of portfolios and companies considering their financial indicators. The graph shown in Fig. 5 illustrates the simulation of a US\$ 100,000.00 investment comparing the different methods. Observing the data provided by the simulation, it can be concluded that the best investment is the one which considers the CMO model with MGI process variables. The Markowitz method applied (de Oliveira et al., 2011) shows to be the second best method, followed by the CM-DOE. The portfolios of companies that were excluded by proposed method and an equal distributed capital portfolio (Equal Investment) is also shown.



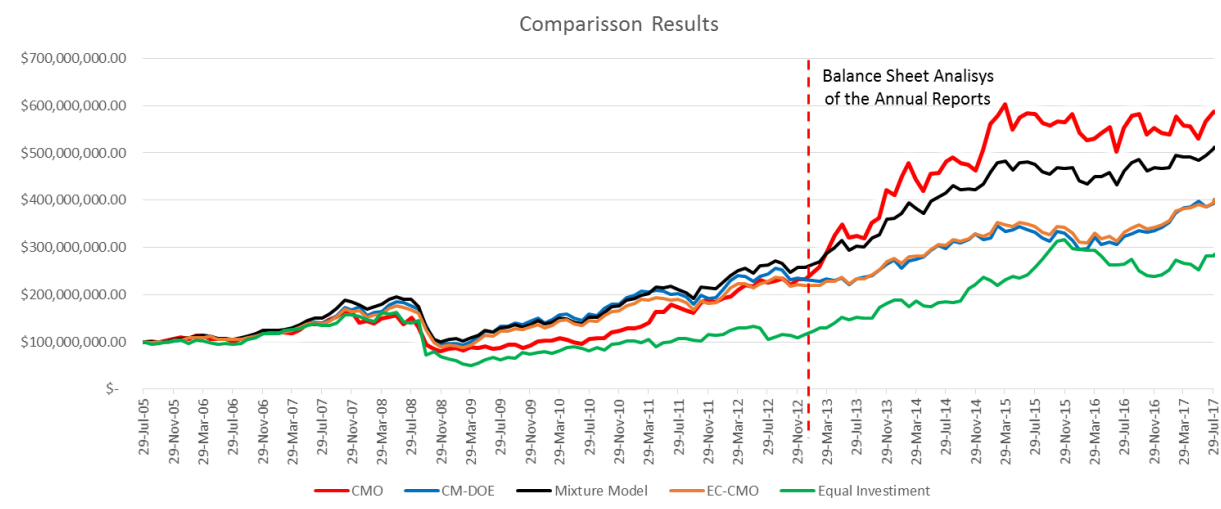


Fig. 5: Simulation result of US\$ 100,000.00 investment.

This is the first attempt in the literature to combine principal components analysis, mixture of mixture and crossed mixtures design of experiments into a single analysis tool that is capable of providing robust results with a minimal computational cost. For future work, the inclusion of several different years of the annual reports and comparing return-risk is proposed. Another proposal would be to use constraints at all levels, to increase the diversification. All the datasets are available at Mendeley Data according to the references.

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