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Additional Information

1       **AIR QUALITY AND URBAN SUSTAINABLE DEVELOPMENT: THE APPLICATION OF**  
2                                       **MACHINE LEARNING TOOLS**

3  
4                       **Nidia Isabel Molina-Gómez<sup>1,2</sup>, José Luis DíazArévalo<sup>3</sup>, P. Amparo López-Jiménez<sup>2</sup>**

5  
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9  
10                                       **ABSTRACT**

11       Air quality has an effect on a population's quality of life. As a dimension of sustainable urban development, governments have  
12       been concerned about this indicator. This is reflected in the references consulted that have demonstrated progress in forecasting  
13       pollution events to issue early warnings using conventional tools which, as a result of the new era of big data, are becoming  
14       obsolete. There is a limited number of studies with applications of machine learning tools to characterize and forecast behavior  
15       of the environmental, social, and economic dimensions of sustainable development as they pertain to air quality. This article  
16       presents an analysis of studies that developed machine learning models to forecast sustainable development and air quality.  
17       Additionally, this paper sets out to present research that studied the relationship between air quality and urban sustainable de-  
18       velopment to identify the reliability and possible applications in different urban contexts of these machine learning tools. To that  
19       end, a systematic review was carried out, revealing that machine learning tools have been primarily used for clustering and  
20       classifying variables and indicators according to the problem analyzed, while tools such as artificial neural networks and sup-  
21       port vector machines are the most widely used to predict different types of events. The non-linear nature and synergy of the  
22       dimensions of sustainable development are of great interest for the application of machine learning tools.

23       **Key words:** air pollution, sustainability, forecasting, sustainable development goals, and influencing variables.

## 24 1 INTRODUCTION

25 Compatible, socially just, and economically viable ecological development is at the heart of the concept of sustainable de-  
26 velopment (Mellos 1988). This term has been more widely recognized since the Earth Summit, where it was established that  
27 it is essential for development to meet the needs of the present without compromising the ability of future generations to  
28 meet their own needs (WCED 1987). Sustainable development is a goal of the global agenda, which nations have pursued  
29 since the Millennium Development Goals and currently with the Sustainable Development Goals (SDGs). These set targets  
30 that should be integrated into countries' national development plans. In this regard, considering that it is of special concern  
31 for nations to achieve the SDGs, there is great interest in forecasting SD behavior. Nations need to make progress in fore-  
32 casting their territorial behavior and consider indicators' variability in the scope of sustainable development. A future vision  
33 of this behavior for the cities and regions that comprise nations is a valuable tool for decision-makers.

34  
35 Sustainable development (SD henceforth) is supported by three encompassing dimensions; the environmental, social, and  
36 economic dimensions. This concept includes environmental health, social equality and economic growth as part of the di-  
37 mensions' interactions, which on balance, are difficult to measure (Lubell et al. 2009). Any change of any one of those inter-  
38 actions could impact SD, demonstrating that balancing and integrating these dimensions is challenging in the quest for sus-  
39 tainability. In this sense, it is important to mention that greater than 55% of the world population lives in urban zones  
40 (United Nations 2019). As a result, air, water and soil quality, species extinctions, worsening health of populations, poverty,  
41 among others, all impact SD, specifically urban sustainable development.

42  
43 Air pollution is one of the effects of great concern at the global level. It is included in the SDGs and may become the main  
44 environmental cause of premature mortality (Cruz et al. 2017). A study performed by Krzyzanowski et al. (2014) identified  
45 that at least 96% of the population of large cities is exposed to particulate matter smaller than 2.5 micron ( $PM_{2.5}$ ). This study  
46 also identified that cities with higher concentrations of particulate matter and the lowest air quality improvement rates over  
47 the last decade, tend to be countries with lower levels of economic development. Furthermore, 92% of the world's popula-  
48 tion lives in places where the air quality exceeds standards established by the World Health Organization (WHO) (WHO  
49 2016). Moreover, the annual global mortality of nearly 3 million people is related to exposure to outdoor air pollution (WHO  
50 2016). Instruments have been developed to monitor and forecast atmospheric pollutants in order to control these correlations.  
51 Several studies have applied machine learning (ML) tools to forecast air quality and certain pollutants, primarily particulate  
52 matter smaller than 10 and 2.5 micrometers ( $PM_{10}$  and  $PM_{2.5}$ ). For example, Antanasijević et al. (2013) and Paas et al.

53 (2017) applied artificial neural networks (ANN), Karimian et al. (2019) and Zhou et al. (2019) used deep neural networks  
54 (DNN), and Oprea et al. (2016) and Wang (2019) utilized decision trees (DT) or their ensembles. Furthermore, support vec-  
55 tor machine (SVM) models were developed for the spatio-temporal predictions of PM<sub>2.5</sub> (Song et al. 2014; de Hoogh et al.  
56 2018).

57

58 Machine learning tools are instruments that forecast the behavior of different variables considering large volumes of data and  
59 in many cases, substantial quantities of predictors. With several advantages over conventional models, the use of ML has  
60 advanced. Different documents on data mining and ML extensively describe the algorithms and their applications (Brink et  
61 al. 2016; Lässig et al. 2016). Those studies, which applied conventional models and ML tools, analyzed and forecasted the  
62 behavior of pollutants for certain regions and territories. The principal aim has been to provide useful technological tools and  
63 results for decision-makers in order to protect populations' health. Nevertheless, these studies have not identified air pollu-  
64 tion's impacts on SD. Learning the influence of air pollution on nations' sustainability, with respect to mortality rates and the  
65 impacts of air pollution on the world population is of great interest.

66

67 Machine learning tools are useful for understanding the impacts of air pollution on the sustainable development of territories.  
68 As such, the primary objective of this paper is to analyze the work developed in prior studies, which have used ML tools to  
69 forecast air quality and SD. This study aims to identify tools that can closely relate both concepts in order to identify the  
70 state of the art ML applications, existing gaps in the field, and determine aspects that can be addressed in the future. This  
71 research paper develops its analysis on the following questions: which machine learning tools have been applied to forecast  
72 the sustainable development behavior of territories, and which machine learning tools could be applied to identify the influ-  
73 ence of air pollution on sustainable development?

74

75 This study is of special interest for governments, scientific communities, and societies. It is innovative in that it provides  
76 tools for environmental governance. Sustainable development is a challenge for governments as it requires an understanding  
77 of each component's behavior, the sustainability dimensions and the territories' evolution in terms of the SDGs. Addition-  
78 ally, this study provides specific information for decision-makers by analyzing the application of machine learning tools where  
79 technology and development issues meet.

80

81 This paper is structured into four sections; following this introduction, the second section *Materials and Methods*, describes  
82 the procedures applied in the systematic revision. The next section introduces the results through a description of the differ-

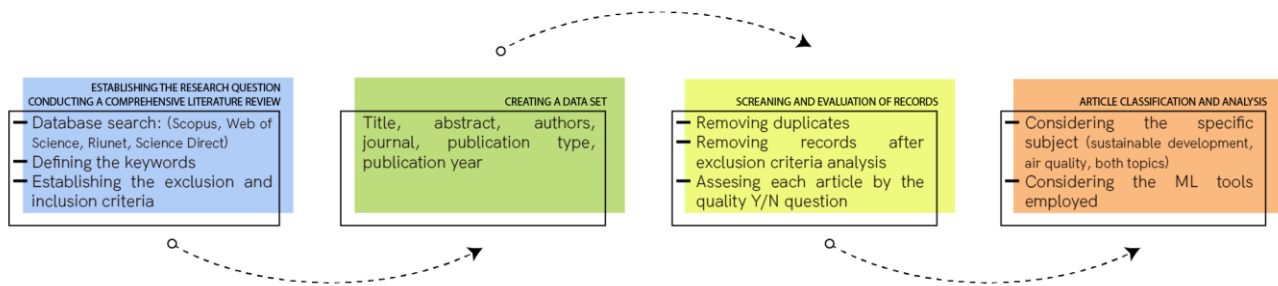
83 ent ML tools employed in various studies to forecast air quality and SD levels. This section contains the results and subse-  
 84 quent discussion of this review, evaluating the tools' functionality based on the requirements for their application in the  
 85 integration of both concepts. This is followed by a section that analyzes the gaps and proposed future developments. The  
 86 paper closes with the conclusions section.

87

## 88 2 MATERIALS AND METHODS

89

90 This study was developed based on the following four relevant stages: 1) determining the research question and establishing  
 91 the criteria for exhaustive literature selection; 2) preparing a dataset with the research documents collected in stage 1; 3)  
 92 researching and evaluating records, and 4) analyzing the selected literature. Figure 1 presents the methodological framework  
 93 used for this research study.



94

95 **Fig. 1 Methodological framework to understand the relationship between air quality and sustainable development for**  
 96 **forecasting.**

97

### 98 2.1 ESTABLISHING THE RESEARCH QUESTION AND CONDUCTING A COMPREHENSIVE LITERATURE 99 REVIEW

100

101 Sustainable urban development encompasses the integration of three fundamental pillars and their interactions. Identifying  
 102 the machine learning tools used to forecast sustainable development in territories will enable the identification of a set of  
 103 tools that could be implemented in other territories with similar characteristics. Furthermore, this identification would be  
 104 able to guide the combination of ML methods to solve specific problems in each SD dimension, particularly related to air  
 105 pollution. Therefore, to answer the research question, the criteria for searching and choosing scientific literature have been  
 106 established as is described in Table 1.

107

**Table 1.** Primary aspects to identify scientific literature in the framework of this study

| Database   | Keywords and equation used in the search  | Inclusion and exclusion criteria  |
|--|---|---|
| <ul style="list-style-type: none"> <li>- Scopus</li> <li>- Web of Science (WoS)</li> <li>- Riunet</li> </ul> | (((("machine learning" OR "data mining" OR "pattern recognition") AND ("air quality" OR "air pollution" OR "atmospheric pollution" OR "atmosphere" OR "atmosph*") AND ("sustainable development" OR "sustainability" OR "sustainable" OR "sustain*")))) | <b>Date:</b> Last 20 years (2000-2019)<br><b>Publication type:</b> Articles, reviews, doctoral theses, conference papers.<br><b>Language:</b> English<br><b>Peer reviewed publications:</b> Articles, reviews, doctoral |

| Database       | Keywords and equation used in the search  | Inclusion and exclusion criteria   |
|----------------|---|--|
| Science Direct | ((( "machine learning" OR "data mining" ) AND ( "air quality" OR "air pollution" OR "atmospheric pollution" OR atmsp ) AND ( "sustainable development" OR sustain ))) | theses, conference papers published in a peer reviewed journals or conference proceedings.<br><b>Publications' objective:</b> The primary goal of the publication is forecasting sustainable development OR air quality OR atmospheric pollution with machine learning tools. Only studies that strictly entailed the use of machine learning tools in both sustainable development and air quality were included. |

108

109 The databases identified in Table 1 were the primary sources for data collection. Additionally, the search engine of the Uni-  
110 versitat Politècnica de València was used based on the criteria outlined in Table 1.

111

## 112 2.2 CREATING A DATA SET FOR THE RECORDED INFORMATION

113

114 A template was designed for the inclusion of each of the records gathered by the searches. In addition to specific information  
115 identifying each record, the information base included the identification of the machine learning tools used in the studies,  
116 their use in each case, the tools utilized in processes to train and validate the data for forecasting, and each study's analysis  
117 objective: sustainable development, air quality according to pollutants or sustainable development dimensions, in the event  
118 that the study focused on specific dimensions.

119

## 120 2.3 SCREENING AND EVALUATION OF RECORDS

121

122 Once the data set was created based on the criteria established in Table 1, the identified records were reviewed. The infor-  
123 mation was verified by reading abstracts of each study. Duplicate records in the databases were eliminated, as well as rec-  
124 ords that did not meet the quality criteria established for inclusion in the data set to be analyzed.

125

## 126 2.4 ARTICLE CLASSIFICATION AND ANALYSIS

127

128 The set of records was then analyzed by reading each document and identifying essential information to answer the follow-  
129 ing research questions: which machine learning tools have been applied to forecast the sustainable development behavior of  
130 territories, and which machine learning tools could be applied to identify air pollution's impact on sustainable development?  
131 The classification and analysis of the scientific literature were guided by the subjects covered in the documents, the machine  
132 learning tools applied, how they were used, the evaluation metrics employed, and their performance.

133

# 134 3 RESULTS AND DISCUSSION

135

136 Following the methodological framework described above, a great number of scientific works were found, mainly in the  
137 fields of forecasting air pollutants, air quality indexes to issue early warnings, ensembles of tools to identify future spatio-  
138 temporal behavior of pollutants, as well as the identification of factors that induce the presence of atmospheric pollutants at a

139 specific level. Although scientific production has increased with the integration of sustainable development goals, research  
140 on the application of machine learning tools in this field is limited. The following are the results found in each case.

### 141 142 3.1 APPLICATION OF MACHINE LEARNING TOOLS IN THE FRAMEWORK OF SUSTAINABLE DEVELOP- 143 MENT

144 Different studies have evaluated the state of progress of the environmental, social, and economic dimensions of SD and their  
145 respective indicators. Machine learning tools have analyzed the behavioral patterns of conjugate variables, as well as the lack  
146 of a self-learning capacity, the treatment of non-linear relationships, and possible bias to estimate the weight of each dimen-  
147 sions of sustainable development (Zhang and Huan 2006; Zhang et al. 2009).

149 Machine learning encompasses tools and techniques to identify patterns within data or process time series in some cases. ML  
150 is an integral piece of predictive modeling; whose principal aim is developing reliable models to forecast variable behavior  
151 or that of specific problems. A model's reliability and accuracy are determined by specific metrics whose application is  
152 closely tied the model's purpose. The root mean square error (RMSE), mean square error (MSE), mean absolute error  
153 (MAE), maximum mean absolute error (MMAE), mean percentage error (MPE), mean absolute percentage error (MAPE),  
154 mean bias error (MBE), accuracy (Acc), relative error ratio (RER), correlation coefficient (R), and index of agreement (IA)  
155 are among the metrics used to evaluate the performance of ML models. ML has been successfully applied to specific sub-  
156 jects regarding the dimensions of SD. Certain studies have examined the dimensions and specific indicators to a greater  
157 degree (Li et al. 2006; Gounaridis et al. 2018), while others employ a more holistic vision (Zhang and Huan 2006; Zhang et  
158 al. 2009). Studies that assessed environmental, social and economic policies are included, and their results provide an under-  
159 standing of the variables to be reinforced to achieve certain SDGs and increase eco-efficiency and socio-efficiency levels in  
160 the territory analyzed. The application of ML tools depends on the objectives established and information availability.

#### 161 162 3.1.1 Information required for the studies 163

164 The application of ML tools both in the scope of the indicator and in a broader vision of SD, requires information from mac-  
165 roeconomic indicators, such as gross domestic product (GDP), level of financial development, education, rate of employ-  
166 ment generated by industry, and environmental quality indexes (Li et al. 2006; Zhang et al. 2009; Pérez-Ortíz et al. 2014).  
167 This information is centered on indexes, indicators, and variables according to the dimension analyzed. To illustrate, for the  
168 environmental dimension; the concentration of atmospheric pollutants, water consumption and volume of waste-water per  
169 unit of GDP, the biochemical oxygen demand, noise level, the rate of treated industrial water, solid waste use, and reforested

170 areas are taken into consideration (Li et al. 2006; Zhang and Huan 2006). With respect to the social dimension; the student  
171 rate, population density, unemployment rate, distance to hospitals and transportation stations are used (Zhang and Huan  
172 2006; Gounaridis et al. 2018). To analyze the economic dimension; the GDP, the ratio of industry to GDP, foreign invest-  
173 ment, energy consumption per unit of GDP, among others, are taken into account (Zhang and Huan 2006; Zhang et al. 2009;  
174 Wang and Xiao 2017). However, this data is not available in every territory with the necessary quality and timeliness, and it  
175 is generally recorded at the national level. Most studies in this field analyze the behavior of cities and provinces in China,  
176 others performed behavioral analysis of different European Union nations, primarily applying SVM, with ANNs and DTs  
177 employed to a lesser degree.

178 SD assessments are limited due to the scarcity and quality of data (Toumi et al. 2017), as it tends to present atypical values,  
179 additional noise, missing data and even errors (Gibert et al. 2016). Countries in Latin America and the Caribbean have defi-  
180 ciencies in the standardized information management and collection. Some cities in the region are characterized by high  
181 population densities, disjointed urban development, and interesting geographic conditions for the study of air quality and  
182 sustainable urban development. Forecasting the behavior in a territory as it pertains to SD in these types of urban areas calls  
183 for the application of tools to understand their growth and development, as well as to complete and standardize the infor-  
184 mation to be included in a ML model.

185 The scarcity of information on the characteristics required to calculate and forecast sustainability progress, demonstrates the  
186 need to use tools to assign data to the evaluated territories, as presented in the study developed by Phillis et al. (2017). Other  
187 studies have proposed the spatial identification of different variables (Holloway and Mengersen 2018), but they are condi-  
188 tioned upon the information visible in satellite images or georeferenced data. These studies provide useful tools to solve the  
189 problem of data quality and territorial scope. Nevertheless, it is important to solve the problem of data frequency generation  
190 to feed and validate machine learning models. In this sense, intervention from, and synergy with, the government sector  
191 plays an important role.

192 Data capturing, recording and quality assurance is another challenge that impacts SD as it limits the effectiveness and accu-  
193 racy of ML application results. Territories have centralized their information through reports or international management  
194 platforms. There are different types of software and programs that provide support for informed decision-making (Gibert et  
195 al. 2012; Kadiyala and Kumar 2017a), but a minimum quality standard must be ensured for the information used.

196

### 197 **3.1.2 Machine learning models**



198 A selected group of machine learning tools is described below. This group of tools focuses on classification and regression  
 199 problems in the framework of sustainability analysis and air quality forecasting. Through an analysis of different studies  
 200 developed in the last 20 years related to forecasting sustainable development, it was found that SVMs, ANNs, Random For-  
 201 est (RF), and DNNs are the primary machine learning tools used to forecast sustainable development or their dimensions in  
 202 different territories.

203

204 - Support Vector Machine (SVM)

205 SVMs are a group of supervised learning algorithms related to classification and regression problems (Sierra 2006). The  
 206 classification categorizes new objects in two or more separate groups based on their properties and a set of observations (de  
 207 Hoogh et al. 2018). SVM draws a vector to separate classes; the greater their separation, the greater the recognition of differ-  
 208 ent groups. For problems regarding more than two dimensions, SMV finds a hyperplane that maximizes the separation mar-  
 209 gin between classes. The classification could be supported by Kernel functions. The regression, referred to as support vector  
 210 regression (SVR), enables it to be applied to forecast continuous variables; as such, the data needs to be trained (Suárez et al.  
 211 2011). Both classification and regression require data for validation and testing purposes.

212 SVMs have advantages in treating small samples and non-linear data patterns (Wang and Xiao 2017; de Hoogh et al. 2018).  
 213 They are used to predict nations' progress levels in terms of the environmental, social, economic, and institutional dimen-  
 214 sions of SD, and to forecast eco-efficiency, including the analysis of spatial data behavior and mixed frequency data model-  
 215 ing (Li et al. 2006; Pérez-Ortíz et al. 2014; Wang and Xiao 2017). Table 2 summarizes the principal studies developed in the  
 216 framework of SD forecasting by SVM methods. It is important to note that the studies compared different ML tools to find a  
 217 reliable model for their defined objective.

218

219 **Table 2.** Applications of SVM in the field of sustainable development

| Specific tools and applications in the machine learning model  | Objective  | Information regarding the training process  | Model accuracy metrics  | Study                            |
|--|--|---|---|----------------------------------|
| <p>Cobweb algorithm for hierarchical clustering to identify regions with similar indicator behavior in the framework of social, economic, environmental, and institutional dimensions, followed by an ordinal classifier: SVM or logistic regression (LR)</p> <p>SVM and LR classifiers and their reformulation to ordinal regression, were compared with their ensemble versions.</p> <p>The Gaussian function was applied as a kernel function</p> | <p>Classification and ranking countries according to its SD level.</p> | <p>Two methods developed for the training process:</p> <ol style="list-style-type: none"> <li>1. A dataset with 75% of the patterns for training and 25% for testing, applied 30 times.</li> <li>2. Three different data partitions were used with different years for training and testing.</li> </ol> | <p>MMAE= 0.28<br/>           Acc= 92.5 for the SVM trainable ensemble with ordinal coding</p> | <p>(Pérez-Ortíz et al. 2014)</p> |
| <p>Principal component analysis (PCA): for the dimension to reduce of environmental indicators, which was followed by SVR or ANN.</p>  | <p>Forecast model for eco-efficiency up to 1 year in advance.</p>      | <p>A training dataset with 13 environmental indicators measured over 13 years and a</p>   | <p>RER= 1) 0.48%;<br/>           2) 2.9%</p>  | <p>(Li et al. 2006)</p>          |

| Specific tools and applications in the machine learning model  | Objective   | Information regarding the training process                           | Model accuracy metrics   | Study                |
|--|---|--|--|----------------------|
| 1. SVM-SVR, the Gaussian radial basis function was applied as a kernel function and, a sequential minimal optimization algorithm for data training.<br>2. ANN - radial basis neural network function (●)   |   | validation dataset with 13 indicators measured for 1 year            |  |                      |
| Support vector spatial dynamic and mixed data sampling (SVSD-MIDAS) to consider spatial correlation, sampling data frequency, and the non-linear relationship between eco-efficiency and the factors. Additionally, the radial basis function kernels were adopted | Prediction of the regional eco-efficiency with spatial mixed-frequency panel data | A training and validation dataset with information from 1998 to 2013 | Average MPE = <1% in different spatial settings<br>Average MSE = <1% in different spatial settings | (Wang and Xiao 2017) |

220 The dots (●) in Table 2 identify the machine learning tool(s) that are not support vector machines. This type of ML was  
221 compared with the SVM employed in the study of interest.  
222

223 - Artificial Neural Networks (ANN)

224 ANNs are non-linear operators formed by a set of neurons connected to each other and to an external environment through  
225 weight-determined connections (Sierra 2006). They generalize non-linear relationship patterns between input and output  
226 variables with noise information (Kadiyala and Kumar 2017b), and are used for industrial, energy, agriculture, environmen-  
227 tal, transportation, economic and water conservation purposes (Chen et al. 2018). ANNs are composed of the following three  
228 layers: 1) an input layer that receives the predictor variables; 2) one or more hidden layers, which usually share the same  
229 information, and are interconnected in different ways; and 3) an output layer; for regression, the output layer may be a single  
230 layer while in a classification case the output will consist of a node of possible output classes (Holloway and Mengersen  
231 2018). It is important to mention that each node or neuron in the hidden layers represents an activation function that acts on a  
232 weighted input of the previous layers' outputs (Holloway and Mengersen 2018). Neural networks can be classified based on  
233 their number of layers (monolayer or multilayer networks) and according to the direction that the information flows (recur-  
234 rent networks, feedforward networks). The most widely known ANN is the multilayer perceptron (MLP). The back-  
235 propagation (BP) algorithm performs better the ANN given its capacity to identify the correct weight of the nodes in the  
236 ANN.

237 In SD modeling, artificial neural networks simulate non-linear relationships among indexes and prevent bias found in tradi-  
238 tional weight design methods (Zhang et al. 2009). They have been used in evaluating SD by applying the BP algorithm to  
239 establish the degree of relationship between indexes (Zhang and Huan 2006; Zhang et al. 2009), and to determine the behav-  
240 ior of the environmental dimension and activity levels in an emissions inventory through the use of sustainability indicators  
241 (Antanasijević et al. 2013). Table 3 outlines the aforementioned studies and indicates the reliability of the machine learning  
242 structures employed.

243

244 Deep neural networks (DNNs) are ANN, which cover complex architectures and have more than one layer of hidden units,  
245 which improves the computer’s learning capacity. They are used in the energy field through multivariate analyses of envi-  
246 ronmental, social and economic factors with big data (Ifaei et al. 2017). They are also employed in the field of greenhouse  
247 gas mitigation, as a basis for developing SD plans (Ifaei et al. 2017; Madu et al. 2017), and as a key tool for air quality fore-  
248 casts that considers particulate matter (Karimian et al. 2019; Zhou et al. 2019).

249

250 A little number of publications that employed ANN to predict sustainable development, or a combination of its dimensions,  
251 was found in the studies analyzed. Table 3 summarizes those studies and the application of ANN over the last 20 years,  
252 indicating their use and the resulting metrics used to evaluate the performance of the developed ML models.

253

254 **Table 3.** Applications of ANN in the field of sustainable development

| Specific tools and applications in the machine learning model  | Objective  | Information regarding the training process  | Model accuracy metrics | Study                 |
|--|--|---|------------------------|-----------------------|
| BP neural network: definition of the degree of relationship among indexes in the same layer.   | Evaluation of sustainable development levels for society, economy, zoology, resource, science, and technological factors   | 10 years of statistical data used in the evaluation (1993-2003)                               |                        | (Zhang and Huan 2006) |
| BP neural network to estimate the index weight of sustainable development and forecasting SD factors.  | Forecasting sustainable development factors  | A training dataset with 33 factors from 8 years, and another with 1 year of data for testing. | Average error 0.037    | (Zhang et al. 2009)   |
| Six annual hourly consumption variables predicted by recurrent and deep neural networks as machine learning tools. The prediction was part of the information of the Techno-Econo-Socio-Environmental Multivariate Analysis (TESEMA) model which additionally encompassed:<br>1. PCA: Identifying linear modeling between variables.<br>2. k-Nearest Neighbors (k-NN): Clustering zones according to modeling results.<br>3. Multivariate data analysis (TESEMA): Reducing data variability.<br>4. Partial least squares (PLS): investigate any correlation between major variables of TESEMA and population density | DNN: prediction of annual hourly electrical demand load using the maximum domestic power consumption at peak intervals, industrial power consumption, stored power at power plants, and total energy trade.<br><br>TESEMA model: Analyzing the correlation between variables and population density in the study zone. | Two-thirds of available data as a training set and the rest as the testing set.               | RSME = 73.15% for DNN  | (Ifaei et al. 2017)   |

255

256 - Decision Trees

257 Decision trees (DT) are an inductive inference method of machine learning that develops classification rules or regression  
 258 tasks. The former consists of a supervised learning method that uses class-labeled training examples; the leaves are the la-  
 259 beled classes and the branches are the features that conduct the classification tasks. This kind of tree creates classification  
 260 rules to be applied for new observations to be classified. Decision tree regression enables the forecasting of continuous vari-  
 261 ables based on input predictors. For example, decision trees can to be applied for pattern recognition with regard to specific  
 262 characteristics of an area, which was the case in a study developed by Zeng et al. (2019), or to forecast pollution levels ac-  
 263 cording to the behavior of pollution sources (Zalakeviciute et al. 2020). M5P, C4.5 and random forests are decision tree  
 264 algorithms employed in studies reviewed. The C4.5 algorithm can be used for classification tasks and builds decision trees  
 265 using the information gain concept (Tzima 2011), while the M5P algorithm combines trees with linear regression models at  
 266 the leaves (Shaban 2016). The C5.0 algorithm considers the information entropy to select the best classification method. To  
 267 improve the robustness of the model, C5.0 introduces boosting technology that consists of repeating sampling simulation of  
 268 existing weighted samples (Zeng et al. 2019).

269  
 270 Random forests (RF) correspond to a collection of DT that are applied to classification and regression problems (Brink et al.  
 271 2016). They make statistical predictions by averaging a set of non-correlated regression or classification trees, and are capa-  
 272 ble of computing non-linear relationships and interaction effects (Zhan et al. 2018). For example, they can be used to create  
 273 potential land use transition maps by applying the RF classification algorithm to satellite images, combining dynamic, bio-  
 274 physical, socioeconomic and legislative factors (Gounaridis et al. 2018). Table 4 outlines the aforementioned studies and the  
 275 application of DT over the last 20 years.

276  
 277 **Table 4.** Applications of decision trees in the field of sustainable development

| <b>Specific tools and applica-<br/>tions in the machine learn-<br/>ing model</b>  | <b>Objective</b>  | <b>Information regarding the<br/>training process</b>                               | <b>Model accuracy met-<br/>rics</b>                              | <b>Study</b>       |
|---|---|---|--|--------------------|
| Two decision tree models that applied the C5.0 growth and pruning algorithm for the 1) development stage target and 2) region target. | Identifying patterns and characteristics of sustainability of coal-mining cities considering data from 55 prefectures and 34 indicators | The development stage of the 55 coal-mining cities was the classification attribute | Acc= 92.73% for the stage model,<br>Acc=94.55% for region model. | (Zeng et al. 2019) |

| Specific tools and applications in the machine learning model  | Objective  | Information regarding the training process   | Model accuracy metrics  | Study                    |
|--|--|--|---|--------------------------|
| 1. Remote sensors and Landsat images: determining changes in urban dynamics.<br>2. Random forests: 3 predictor variables randomly sampled at each decision tree split and 500 trees to be built<br>3. Cellular automata: Forecasting land use changes through 2045 | Development of potential transition surfaces by combining 20 dynamic, biophysical, socio-economic and legislative factors. | A set of randomly distributed points was plotted against the Landsat images and high-resolution images available via Google Earth. | Acc= 90.9-93.1% with respect to the resulting yearly map compared against reference samples | (Gounaridis et al. 2018) |

278

279 Combining ML with other tools, such as those presented in Tables 2 – 4, has improved pattern recognition efficiency and  
 280 data clustering to more accurately forecast the behavior of an analyzed data set.

281

282 3.1.3 Important variables that influence sustainable development

283

284 The relationship between the atmospheric component and SD has been demonstrated through the development of sustainable  
 285 energy plans based on dimensional impact analyses and energy consumption (Ifaei et al. 2017), in addition to forecasting air  
 286 quality by using certain sustainability indicators (Antanasijević et al. 2013). Studies predict and/or analyze atmospheric pol-  
 287 lutant behavior based on information registered by monitoring stations and other sources, while advancing the integration of  
 288 geospatial information, which includes the relationship between geospatial data and mixed frequency data analysis through  
 289 SVM (Wang and Xiao 2017). The same occurs with the application of the BP algorithm in ANNs, establishing the degree of  
 290 relationship of indexes in the same layer (Zhang et al. 2009). The results of the relationship between different variables and  
 291 information characteristics are emphasized in order to understand future land use behavior in a territory (Gounaridis et al.  
 292 2018).

293

294 The scope of most studies is both from a holistic vision of SD and the specific analysis of a variable or indicator in the  
 295 framework of SD. There is a lack of studies that identify the most influencing variables or indicators of SD progress. Urban  
 296 territories are influenced by different variables and identifying the progress of each and their synergetic behavior in the  
 297 scope of SD is necessary for decision-makers. Identifying variables' level of importance should consider the data that feeds  
 298 the models. In this vein, tools like analytic hierarchy process and clustering could guide the knowledge of influencing varia-  
 299 bles in sustainability categories. Hybrids or ensembles of tools offer an improvement of the models' exactitude or reduced  
 300 computational costs, as demonstrated in the studies developed by Peng et al. (2017) and Zhan et al. (2018). Therefore, the

301 ensembles, which include hierarchical and clustering tools, could support the identification of important variables regarding  
302 the sustainable development behavior of territories, as well as its forecast.

303

304 Even though there are a limited number of studies associated with the forecast of SD and its influential variables, research  
305 for air quality forecasting through ML tools provides guidelines for causality analyses of urban sustainable development  
306 progress. Tools like proportion-based causality tests and sequential forward feature selection applied by Wang (2019) facili-  
307 tate the evaluation and forecasting of urban sustainable development.

308

### 309 3.2 APPLICATION FOR AIR QUALITY

310 ANNs, SVMs and DTs have been utilized to forecast air quality and their influencing variables. Studies primarily focus on  
311 Asia and Europe. Countries such as India, China and Saudi Arabia, which according to the WHO have higher registered  
312 levels of pollution, stand out due to their application of ML tools to forecast future pollution events.

313

314 ANNs have been employed for air quality and atmospheric emission applications, with MLP and BP predominantly used as  
315 training algorithm. To identify the best forecasting tool, ANNs have been compared with conventional statistical models,  
316 DTs, and SVMs. Multilayer perceptron neural networks have been extensively analyzed and have been combined with the  
317 Manhattan propagation algorithm (Souza et al. 2015), with self-organizing map (SOM) and hierarchical clustering (Tamas et  
318 al. 2016), linear regression statistical techniques, or in comparison with an extreme learning machine (ELM) (Peng et al.  
319 2017). Hybrid models provide synergetic results, in particular to establish early warnings, and have improved behavior in  
320 forecasting specific atmospheric pollutants. The application of ELM has surpassed the limitations of MLP with respect to the  
321 non-linearity of data and operational costs of traditional ANN methods (Peng et al. 2017).

322 To identify pollution risk, clustering algorithms such as the K-means algorithm have been used by applying the AQ algo-  
323 rithm to defined groups (Cervone et al. 2008). Furthermore, MLP was applied to forecast  $PM_{10}$  and  $PM_{2.5}$ , while the K-mean  
324 and PCA algorithms facilitated the identification of input variables for the model (Franceschi et al. 2018).

325 For the ozone ( $O_3$ ) and  $PM_{10}$  forecasts, lazy learning networks (LL) perform better than pruned neural networks (PNN) and  
326 feed-forward neural networks (FFNN), while PNNs effectively detect the increase of alarm and attention thresholds for the  
327 pollutants analyzed (Corani 2005). To forecast the concentration of nanoparticles, FFNNs are combined with BP, in which  
328 the inclusion of all types of variables enabled the ANN to precisely map the non-linear relationship between the measured  
329 and expected nanoparticles (Al-Dabbous et al. 2017). However, to predict  $PM_{2.5}$ , it was concluded that increasing the num-

330 ber of data points does not necessarily result in better estimates, as it is more a correlation between the main factor and those  
 331 related to it (Ni et al. 2017).  
 332 Additionally, the effectiveness of different ML algorithms was compared, as well as integration with the Gaussian dispersion  
 333 model for an emission source, establishing excellent behavior in forecasting the dispersion of atmospheric pollutants, which  
 334 is an applicable method for predicting and identifying source parameters (Ma and Zhang 2016). Table 5 lists the results of  
 335 the studies analyzed and how ANNs have been applied and combined with algorithms, see the artificial neural network mod-  
 336 el in Table 5 for model training and selecting input variables, while also presenting that a single study compared different  
 337 tools.

338

339 **Table 5.** Application of ANNs to air quality and atmospheric pollutants

| Study                    | Artificial neural network model   | Objective  | Information regarding the training process   | Model accuracy metrics   |
|--------------------------|---|--|--|--|
| (Souza et al. 2015)      | MLP configured with hyperbolic tangent activation function + Manhattan propagation algorithm  | Forecast daily concentrations of PM <sub>10</sub> .  | 80% of data used for training (daily samples collected from 0.7/2009-06/2013) and 20% for testing the data set (daily samples collected from 07.2013-06.2014).   | Improvements of MSE compare with individual MPL and ensembles = 8.85% (4 neurons in the hidden layer).   |
| (Tamas et al. 2016)      | 1. MLP + Levenberg-Marquardt training algorithm + hybridized with hierarchical clustering.  | Hourly concentrations of O <sub>3</sub> , NO <sub>2</sub> and PM <sub>10</sub> , 24 hours in advance.  | Clustering methods were used to subdivide the data set, with MLP trained on each subset: 60% for training data (3 years of data), 20% for validation (1 year of data), and 20% for testing (1 year of data). | RMSE = 18.65 (O <sub>3</sub> ); 12.1 (NO <sub>2</sub> ); 7.4 (PM <sub>10</sub> ) µg/m <sup>3</sup>   |
|                          | 2. MLP hybridized with SOM and k-mean clustering.   |  |  | MAE = 14.69 (O <sub>3</sub> ); 8.58 (NO <sub>2</sub> ); 5.77 (PM <sub>10</sub> ) µg/m <sup>3</sup><br>IA = 0.87 (O <sub>3</sub> ); 0.8 (NO <sub>2</sub> ); 0.74 (PM <sub>10</sub> )  |
| (Peng et al. 2016)       | ELM based on MLP+ hill-climbing algorithm to determine the optimal number of hidden nodes. ELM conducted the training task, followed by an online sequential ELM (OSELM) which updated the model. The input data of the model consisted of meteorological variables, O <sub>3</sub> , PM <sub>2.5</sub> , NO <sub>2</sub> , and physical variables. An online sequential multiple linear regression and the MLP configured with hyperbolic tangent activation function were compared together with the OSELM. | Hourly concentrations of O <sub>3</sub> , NO <sub>2</sub> and PM <sub>2.5</sub> , 48 hours in advance. | 2 years of information for training and validation (2009/07-2011/07), three for testing (2011/08-2014/07) as well as model updating.   | The models were ranked using the forecast scores averaged over all forecast lead times, for each pollutant. For MAE and correlation scores the OSELM outperformed MLP and MLR for O <sub>3</sub> , NO <sub>2</sub> and PM <sub>2.5</sub> |
| (Franceschi et al. 2018) | A combination of PCA to identify the most influencing predictors, K-means for data grouping, and MLP neural network + BP as the training algorithm.   | Hourly and daily prediction of PM <sub>10</sub> and PM <sub>2.5</sub> .                                | Ratios for training and validating the data set: 80% for training and 20% for validation.  | RSME = 15.62 (PM <sub>10</sub> ); 5.79 (PM <sub>2.5</sub> ) µg/m <sup>3</sup><br>MAE = 13.39 (PM <sub>10</sub> ); 4.72 (PM <sub>2.5</sub> ) µg/m <sup>3</sup>  |

| Study                       | Artificial neural network  | Objective  | Information regarding   | Model accuracy metrics  |
|-----------------------------|--|--|---|---|
| (Paas et al. 2017)          | MLP configured with a hyperbolic tangent transfer function + BP training algorithm.  | Prediction of (PM <sub>0.25-10</sub> ) mass concentrations and particle number concentrations.   | Data split through stratified random sampling with self-organizing map. 70% of the subset was used for training, 20% for validation, and 10% for testing. | RMSE= 7.78 µg/m <sup>3</sup>  |
| (Ni et al. 2017)            | Back propagation neural network.   | A correlation analysis of PM <sub>2.5</sub> , meteorological data, pollutant concentration data and social media.  | Ratios for modeling and testing the data set: 70% for training and 30% for testing.   | RMSE=24.06 µg/m <sup>3</sup>  |
| (Chen et al. 2018)          | Measurement of partial mutual information to select significant variables + ensemble ANN-based output estimation + KNN regression output estimation error. | Forecasting an air quality index one day in advance considering the following predictors: PM <sub>10</sub> , PM <sub>2.5</sub> , and SO <sub>2</sub>   | 2 years of information for training, one for validation.  | The model cannot simulate well for large AQI values, but has good precision for medium and small AQI values   |
| (Antanasijević et al. 2013) | General regression neural network + genetic algorithm for training.  | Forecasting PM <sub>10</sub> up to two years in the future with the following predictors: GDP, gross inland energy consumption, wood incineration factor, motorization rate, paper production, and processing of certain minerals. | 5 years of data from 26 countries for training and validation, 2 years for testing.   | MAE = 10%   |
| (Corani 2005)               | 1. FFNN configured with a hyperbolic tangent transfer function and the Levenberg-Marquardt training algorithm.<br>2. LL<br>3. PNN                          | Prediction of O <sub>3</sub> and PM <sub>10</sub> at 9:00 am for the current day and detection of exceedance.  | Cross-validation approach   | True/predicted correlation=0.85 (O <sub>3</sub> ); 0.9 (PM <sub>10</sub> )<br>Success index=0.6 (O <sub>3</sub> ); 0.75 (PM <sub>10</sub> )<br>MAE=15.87 (O <sub>3</sub> ) and 8.25 for LL which outperformed the FFNN and PNN in the prediction. |
| (Al-Dabbous et al. 2017)    | FFNN configured with a hyperbolic sigmoid transfer function + BP training algorithm based on Levenberg Marquardt optimization.                             | Prediction of nanoparticles regarding different input variables.   | Ratios for modeling and testing the data set: 80% for training and 20% for testing.   | R <sup>2</sup> value = 0.79<br>IA = 0.94  |
| (Ma and Zhang 2016)         | 1. RBF + Gaussian dispersion model   | Emission source parameters identification and pollutant dispersion forecasting.  | Ratios for modeling and testing the data set: 47% for training and 53% for testing.   | MSE=482.78 R=0.89   |
|                             | 2. BP + Levenberg-Marquardt training algorithm + Gaussian  |  |   | MSE=371.82 R=0.91   |
|                             | 3. SVR+ Gaussian dispersion model  |  |   | MSE=300.37 R=0.92   |
| (Zhou et al. 2019)          | 1. Shallow multi-output long short-term neural network memory (SM-LSTM)  | Regional multi-step-ahead air quality (PM <sub>2.5</sub> , PM <sub>10</sub> , NO <sub>x</sub> ) forecast horizon: t+1 up to t+4  | Mini-batch gradient descent algorithm, dropout neuron algorithm, and L2 regularization algorithm for the training process.                                | MSE= 0.87   |
|                             | 2. Deep multi-output LSTM (DM-LSTM) neural network   |  |   | MSE= 0.72   |
| (Karimian et al. 2019)      | 1. Long short-term neural network (LSTM)   | Prediction of PM <sub>2.5</sub> up to 48 hours.  | Ratios for training and validating the data set: 60% for training, 20% for validation, and 20% for testing.   | RMSE=8.91µg/m <sup>3</sup><br>MAE= 6.21 µg/m <sup>3</sup><br>R <sup>2</sup> = 0.8   |
|                             | 2. DNN: Deep feed forward neural network (DFNN)  |  |   | RMSE=19.45 µg/m <sup>3</sup><br>MAE= 14.52 µg/m <sup>3</sup><br>R <sup>2</sup> = 0.49   |



| Study | Artificial neural network                 | Objective | Information regarding | Model accuracy metrics   |
|-------|---|-----------|-----------------------|--|
|       | 3. Multiple additive regression trees (●) |           |                       | RMSE=12.83 $\mu\text{g}/\text{m}^3$<br>MAE= 8.99 $\mu\text{g}/\text{m}^3$<br>R <sup>2</sup> = 0.56 |

340 The dots (●) in Table 5 identify the machine learning tool(s) that are not artificial neural networks. This type of ML was  
 341 compared with the ANN employed in the study of interest.

342  
 343 MLP was compared with SVR, in which the generalization capacity acquired in a relatively small amount of learning data  
 344 and a large number of entry nodes demonstrated better behavior for SVR (Suárez et al. 2011; García et al. 2013; Shaban et  
 345 al. 2016). This capacity was also demonstrated in forecasting air quality indexes (Liu et al. 2017; Weizhen et al. 2014) (see  
 346 Table 6). Furthermore, SVR was utilized for spatio-temporal modeling of PM<sub>2.5</sub>, taking into account missing information  
 347 (Song et al. 2014), and to forecast atmospheric pollutants by developing an online method (Wang et al. 2008). SVR and the  
 348 Gaussian function kernel have been used to capture the non-linearity and interaction between predictors (Wang et al. 2008;  
 349 Weizhen et al. 2014). In the prediction of hourly and daily levels of carbon monoxide (CO), the hybrid model of SMV and  
 350 partial least squares (PLS), which was used to reduce input data, performed better with less modeling time and better per-  
 351 formance metrics than the just SVM (Yeganeh et al. 2012).

352

353 **Table 6.** Application of SVMs to forecast air quality and atmospheric pollutants

| Study                                    | SVM model   | Objective   | Information regarding the training process  | Model accuracy metrics  |
|--|---|---|---|---|
| (García et al. 2013; Suárez et al. 2011) | 1. MLP neural network configured with a sigmoid activation function (●)<br>2. SVR + sequential minimal optimization algorithm, and kernel function variants | Obtain a relationship between concentrations of CO, SO <sub>2</sub> , NO, NO <sub>2</sub> , PM <sub>10</sub> , O <sub>3</sub>   | 10-fold cross-validation  | SVM outperformed MLP with correlation coefficients that ranged from 0.62 to 0.9 for the pollutants. |
| (Liu et al. 2017)                        | SVR   | AQI forecasting up to 24 in advance, with information (PM <sub>2.5</sub> , PM <sub>10</sub> , SO <sub>2</sub> , CO, NO <sub>2</sub> and O <sub>3</sub> levels, AQI, temperature, weather, wind force and direction) on cities with similar urban air pollution. | 4 folds, each with 25% of the data. 3 folds were selected for training, the remaining fold was used for model testing.                                  | RMSE = 6.54<br>MAPE = 0.0534  |
| (Weizhen et al. 2014)                    | SVR + successive over relaxation algorithm + Gaussian kernel function   | Prediction of PM <sub>10</sub> and PM <sub>2.5</sub> for the following 24h and hourly forecasting based on daily average aerosol optical depths and meteorological parameters.  | k-fold cross validation. 83% of the data used as a training dataset, the remaining as a testing dataset.  | R <sup>2</sup> =0.87<br>Average error=12.66 $\mu\text{g}/\text{m}^3$                                |
| (Song et al. 2014)                       | Spatial data aided incremental SVR  | Daily average spatio-temporal prediction of PM <sub>2.5</sub> based on hourly PM <sub>10</sub> levels.  | The split for training and testing the ML model encompasses data from August 2006 to 2009 for training and data from 2011 to 2012 as a testing dataset. | RMSE= 1.0775<br>MAE = 0.81<br>MBE = 0.18<br>IA= (0.51-0.68)   |

| Study                 | SVM model  | Objective  | Information regarding                             | Model accuracy metrics                                     |
|-----------------------|--|--|---|--|
| (Wang et al. 2008)    | SVR model + Gaussian kernel function   | Prediction of respirable particulate matter, NO <sub>x</sub> and SO <sub>2</sub> concentrations, up to 24 hours and 1 week in advance by using data found online.  | 59% for training and 41% for testing the dataset. | RMSE=25.89ug/m <sup>3</sup><br>MAE=19.29 ug/m <sup>3</sup> |
| (Yeganeh et al. 2012) | Partial least square (PLS) for data selection and to reduce the amount of input data + SVR + radial-basis function as a kernel function. | Hourly and daily CO concentration forecast by using data on PM <sub>10</sub> , total hydrocarbons (THC), NO <sub>x</sub> , CH <sub>4</sub> , SO <sub>2</sub> , O <sub>3</sub> and meteorological parameters. | 75% for training and 25% for testing the model.   | RMSE = 0.711<br>R <sup>2</sup> =0.654                      |

354 The dots (●) in Table 6 identify the machine learning tool(s) that are not support vector machine. This type of ML was compared with the SVM employed in the study of interest.

357 On the other hand, the M5P decision tree algorithm outperformed both SVM and ANNs, given the efficiency of its tree structure and generalization capacity (Shaban et al. 2016) (see Table 7). The M5P algorithm performed well in forecasting PM<sub>10</sub>, when heuristic rules were applied (Oprea et al. 2016). A comparable situation was found when applying the RF algorithm, which performed better than the SVM algorithms (Pandey et al. 2013). RFs outperform other classifiers because of their capacity to assimilate forecasts from a variety of simple tree classifiers based on more predictive variables, resulting in low levels of bias and variance (Pandey et al. 2013). By applying different predictors, it was found that different variables have different types of impacts on the levels of ultrafine particulate matter in the atmosphere. The same case was presented in a comparison of five types of algorithms: LR, MLP, DT (C4.5 algorithm), SVM, and a variant of "ZCS-DM" decision trees, which belong to a class of ML tools, termed learning classifier systems, which use conditional rules. SVM and ZCS-DM performed well, the latter algorithm identified extreme cases and forecasted pollution episodes (Tzima et al. 2011). SVM has been used to compare ML algorithm performance. SVM was compared with single decision trees (SDT), decision tree forests (DTF), and decision tree boosting (DTB) for forecasting air quality indexes (Singh et al. 2013). It was concluded that as the result of incorporating aggregation and optimization algorithms, DTF and DTB outperformed SVM both in classification and regression (Singh et al. 2013). RFs outperform chemical transport models, which require input variable information from emission inventories that may not be accurate (Zhan et al. 2018).

372 DTB was used to forecast PM<sub>10</sub> concentrations, revealing that when comparing the multiple linear regression model (MLRM), the quantile regression model (QRM), and the generalized additive model (GAM), the capacity of the QRM to capture contributions from covariates in different quantiles produces better forecasting, when compared to procedures in which a single central trend is considered for a set of independent variables (Sayegh et al. 2014).

376 To improve the exactitude of the models and reduce computational costs in data treatment, analysis and forecasting, hybrids or ensembles of tools have been made (Peng et al. 2017; Zhan et al. 2018). The choice was made to combine DTs in their

378 different degrees of complexity, which have been compared to the performance of conventional statistical tools, SVMs and  
 379 ANNs. Furthermore, DTs have been combined with linear regression tools to improve their accuracy. Table 7 presents the  
 380 studies analyzed, including the decision tree model developed in each study, the objective of the ML model, information  
 381 regarding the training and testing datasets, and each model's performance. Some studies evaluated the performance of the  
 382 ML model in comparison with other learnings architectures.

383

384 **Table 7** Application of decision trees to air quality and/or atmospheric pollutants

| Study                | Decision tree model                     | Objective   | Information regarding the training process   | Model accuracy metrics  |
|----------------------|---|---|--|---|
| (Zhan et al. 2018)   | RF                                      | Prediction of the spatio-temporal distribution of daily 8h maximums of O <sub>3</sub> concentrations.                       | 10-fold cross-validation (9 groups for training and 1 for testing).  | RMSE=26 µg/m <sup>3</sup><br>R <sup>2</sup> = 0.69  |
| (Sayegh et al. 2014) | Boosted regression trees                | Prediction of hourly PM <sub>10</sub> concentration levels.   | 10-fold cross validation; 11 months of data used as a training data set; 1 month as a testing dataset.   | MBE=-41.1 µg/m <sup>3</sup><br>RMSE=125.6<br>MAE= 80.4<br>R=0.54<br>IA=0.66   |
| (Singh et al. 2013)  | 1. Decision tree forest                 | <ul style="list-style-type: none"> <li>Seasonal air quality discrimination</li> <li>Air quality index prediction</li> </ul> | Kennard-Stone approach for a uniform scatter of training data around the training domain (70% for training and 30% for testing), k-folds-cross validation. | Acc=96.68%<br>RMSE=6.58<br>MAE=5.24<br>R=0.90   |
|                      | 2. Decision tree boosting               |   |  | Acc=96.45%<br>RMSE=6.59<br>MAE=5.26<br>R=0.90   |
| (Tzima et al. 2011)  | 3. Tree induction algorithm C4.5        | Air quality episode forecasting   | 10-fold cross validation   | Overall average rank regarding the kappa coefficient for pollutants=4.25 (C4.5); 2.5 (ZCS-DM); 1.75 (SVM); 3.4(MLP) |
|                      | 4. Rule induction ZCS-DM algorithm      |   |  |   |
|                      | 5. SVM (●)                              |   |  |   |
|                      | 6. MLP (●)                              |   |  |   |
| (Shaban et al. 2016) | 1. M5P decision tree                    | Prediction of NO <sub>2</sub> , SO <sub>2</sub> , and O <sub>3</sub> concentrations up to 24 hours in advance.              | Time windowing (forecasting horizon) = 2 windows are used for training and testing.  | RMSE=5.8  |
|                      | 2. SVM (●)                              |   |  | RMSE=6.4  |
|                      | 3. ANN (●)                              |   |  | RMSE=16.4   |
| (Oprea et al. 2016)  | 1. M5P decision tree                    | Prediction of PM <sub>10</sub> concentrations levels up to 3 days in advance.   |  | RMSE=8.38; MAE=6.52; R=0.87   |
|                      | 2. Reduced error pruning tree algorithm |   |  | RMSE=12.74; MAE=9.34; R=0.65  |
| (Wang 2019)          | 1. DT                                   | Air quality classification  | k-cross validation   | Acc= 75.1%  |
|                      | 2. Ensemble (boosted and bagged trees)  |   |  | Acc= 90.2% and 89.1%  |
|                      | 3. k-NN                                 |   |  | Acc= 80.2%  |
|                      | 4. SVM (linear and gaussian) (●)        |   |  | Acc= 82.3% and 85.6%  |

385 The dots (●) in Table 7 identify the machine learning tool(s) that are not decision trees. This type of ML was compared with  
 386 the DT employed in the study of interest.  
 387

388 The machine learning tools presented above enabled the forecasting of air quality or specific indicators (see Tables 5 – 7).  
 389 Their performance and accuracy primarily depend on the data set and feature selection. Additionally, the machine learning

390 tools listed in Tables 2 – 4 showed the first advances related to forecasting sustainable development or its dimensions. Nev-  
391 ertheless, hybrid or ensembles like those used by Karimian et al. (2019) and Wang (2019) improve specific ML tools, and  
392 could be applied in forecasting sustainable development, possibly even to identify influencing variables.

393

394 However, a specific analysis of the influence of air quality or atmospheric pollution on sustainable development was not  
395 found in any of the studies analyzed; nor a study that identifies the degree of importance of variables on sustainable devel-  
396 opment to achieve the targets defined in the SDGs. Specific aspects and results of the reviewed studies provided an under-  
397 standing that there are two fundamental factors that need to be addressed in order to advance sustainable development fore-  
398 casting; the information required for training and model validation, and the identification of important variables that influ-  
399 ence sustainable development.

400

### 401 3.3 GAPS AND FUTURE DEVELOPMENTS

402 The application of ML must consider the characteristics of the data and its behavior. The atmosphere and reactions within it  
403 are non-linear complex processes, whose analysis is necessary to forecast SD and understand its impact. As such, SVMs and  
404 DTs are tools that can support this analysis.

405 The application of DNNs could be explored in conjunction with tools that have overcome data management difficulties. The  
406 majority of studies reviewed perform an analysis of redundancies to include variables with the most forecasting potential,  
407 avoiding the use of variables that introduce errors to the modeling results, which include over fitting.

408 One of the objectives in an air quality assessment is determining the environmental quality and reflecting human demands on  
409 the same (Chen et al. 2018). Some areas have geographic and atmospheric conditions that are not conducive to adequate air-  
410 circulation, coinciding with populations located in zones that are characterized by cities that are not optimally designed  
411 (Saeed et al. 2017). Given their effect on a population's health, these factors must be analyzed as they are part of the dynam-  
412 ic of SD.

413 As ultrafine particles are atmospheric pollutants that are not widely monitored, it is possible to learn their impact on the  
414 health of a population and on SD by applying ML and correlating them to other atmospheric pollutants.

415 Machine learning tools, their ensembles, and using techniques such as analyzing satellite imaging, offer decision-makers the  
416 possibility of having a better understanding of their territories. In the framework of sustainable development and its targets,  
417 decision-makers everywhere have the responsibility of identifying the most effective actions to achieve the SDGs. The eco-  
418 nomic, environmental, and social dimensions are not static and require continuous support to maintain or improve their be-  
419 havior. For example, any change to the environment and health dimensions of a population, both in an urban territory or

420 country, could influence every sustainability dimension. Furthermore, the use of ensembles of machine learning tools that  
421 include hierarchical and clustering tools applied by Franceschi et al. (2018) and Tamas et al. (2016) with MLP neural  
422 networks or by Oprea et al. (2016) and Singh et al. (2013) who used different kinds of decision trees, or by Peng et al. (2017)  
423 who applied SVR to identify subsets of the most relevant attributes for the prediccion taks, may facilitate early decisions  
424 from leaders.

425

426 Several studies have successfully applied machine learning tools to forecast air quality, with accuracies ranging from 70-  
427 95%. In this sense, the methodology and ML tools described by the studies mentioned above are a reference for the analysis  
428 of sustainability and its forecasting. Furthermore, research studies developed by Wang (2019) outline the relevant methods  
429 and tools replicable to evaluate the influence of air quality on urban sustainable development.

430

#### 431 **4 CONCLUSIONS**

432 Forecasting the level of SD and its variation in function of certain input parameters, enables decision-makers to establish the  
433 emphasis variable for increasing the sustainability of an analyzed territory. Through the analysis of the references consulted,  
434 the use of ML in defining sustainability indexes was evident, supporting the relevance of its application, as biases are pre-  
435 vented in determining the weights of parameters and indicators.

436 Regarding the research questions of this study, it is important to note that SVMs, ANNs, RFs, and DNNs were the machine  
437 learning tools used either to forecast sustainable development or their dimensions in different territories. The most widely  
438 used tools in the field of SD are SVMs and to a lesser degree, ANNs and DTs. However, it is important to note that no study  
439 was found which identified the influence of air quality on sustainable development. Nevertheless, different approaches and  
440 distinct machine learning tools have been applied, which enable further research to make progress in determining the influ-  
441 ence of air quality on sustainable urban development, as well as in its forecasting. In this vein, combining ML with other  
442 tools, such as hybrid systems or ensembles that include hierarchical and clustering tools, is useful in identifying the influence  
443 of different variables on urban sustainable development.

444 With respect to ML tools and the non-linearity of information that characterizes the dimensions of sustainable development,  
445 SVMs and DTs have performed the best in computing this type of data. However, despite the existence of ML approaches  
446 with certain characteristics that makes them suitable for forecasting, boundary conditions establish an opportunity for their  
447 use. It is necessary to consider the tools' favorable aspects, applying those that adjust to specific conditions, including the

448 availability of information with the required continuity and quality that enables the proper reflection of behavioral patterns of  
449 variables in a given territory, which is the key to forecasting.

450 Only the studies that applied ML in the field of air quality established the required time for forecasting or data treatment as  
451 an analytical value. This is a possible parameter of interest given the importance of making effective use of time in the de-  
452 velopment of these types of studies.

453

454 This study is useful in the field of environmental, social and economic dimension analysis, as it provides a map of different  
455 ML tools and the authors who have used them in specific case studies, either to address a specific challenge or in integrating  
456 the dimensions.

457 There is a need for studies that identify the behavior of territories concerning indicator variation and sustainable develop-  
458 ment variables. The environmental, social, and economic dimensions are interconnected, in which each all have an effect on  
459 the others. Furthermore, to understand and identify the most influencing actions on health, the environment, and economic  
460 effects, it is necessary to forecast behaviors and identify influencing variables, to develop scenarios and make the best deci-  
461 sions possible. The environmental dimension affects the social dimension in the framework of the population's health.

462

463 This study is unique and innovative, it recognizes the importance of air quality in sustainable development and seeks to iden-  
464 tify the behavior of the ML tools applied in different studies to forecast both concepts. It also identifies the tools used to  
465 understand the influence of variables on sustainable development or the dimensions of sustainability, in addition to those  
466 used to establish the association of predictors. Even when documentation was found regarding machine learning tools, it is  
467 necessary to collect the experiences developed for decision making. Few studies have taken the initiative of forecasting sus-  
468 tainable development and analyze its most-influencing possible variables. This work identifies the degree of progress in this  
469 sense, as it supports decision-making that could be undertaken by governments as part of their goals and objectives and those  
470 tied to the 2030 Agenda for Sustainable Development.

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