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A hybrid model for predicting air quality combining Holt–Winters and Deep Learning Approaches: A novel method to identify ozone concentration peaks

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Ozone (O_3) from the troposphere is one of the substances that has a strong effect on air pollution in the city of Tanger. Prediction of this pollutant can have positive improvements in air quality. This paper presents a new approach combining deep-learning algorithms and the Holt–Winters method in order to detect pollutant peaks and obtain a more accurate forecasting model. Given that LSTM is an extremely powerful algorithm, we hybridized with the Holt–Winters method to enhance the model. Making use of multiple accuracy metrics, the models' efficiency is investigated. Empirical findings reveal the superiority of the hybrid model by providing forecasts that are more accurate with an index of agreement equal to 0.91.

Keywords: *Air quality forecasting; Ozone (O_3); Long Short-Term Memory (LSTM); Holt–Winters method; Recurrent Neural Network (RNN); Artificial Neural Networks.*

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1. Introduction

The atmosphere is one of the main components of the environment. Furthermore, the emissions of pollutants into the atmosphere are the main source of air pollution, which is an extremely important threat because the quality of the air has a direct influence on our health and our environment. For that reason, predicting the air pollution levels of the coming day is the first and most crucial step in air quality management.

Air pollution has been a major source of worry for both the public and authorities, due to its potentially harmful effects. To avoid the negative impacts of exposure to these pollutants and to give the authorities the information they need in time to take action to minimize the short-term peak of pollution, an advanced model founded on correct forecasting techniques must be put in place.

Due to recent growth in economic status and rapid urbanization, ozone levels have grown in the atmosphere. Tangier, a city in northern Morocco, is one of the cities that has experienced significant changes in several business sectors. However, this development has had an impact on both the environment and population health [1].

Human health is negatively impacted by the rise in ozone concentration, which can cause suffocation, breathing problems, serious respiratory disorders, and eye irritation. High ozone concentrations prevent plants from performing photosynthesis normally, which causes them to wither [2]. Additionally, the risk of mortality has increased, especially for people living in hot climates, since the exposure to O_3 was strongly related to death from cardiovascular and respiratory disorders [3]. Then, in order to better effectively safeguard public health from exposure to ambient O_3, it is crucial to correctly estimate the ozone concentration in advance, and establish a typical data science work, because forecasting supports organizations with goal-setting, capacity planning, and anomaly detection, especially the national air quality monitoring network who strive to measure, forecast, and inform the public and governments about air quality. Despite its importance, producing high quality forecasts is a serious challenge. Actually, there are numerous time series of different types and relatively few analysts specializing in time series modeling. To deal with these difficulties, we suggest a useful method for forecasting that mixes Deep Learning approaches with the classical times series forecasting techniques.

In this study, we will compare the Holt–Winters approach and the Long Short-Term Memory model in order to come up with a good prediction of daily ozone in Tangier City. Then we develop three original approaches. The first two approaches are based on: LSTM as a specific type of recurrent neural networks and the different types of exponential smoothing methods, respectively. Lastly, the coupling of the LSTM algorithm and Holt–Winters will represent our suggested methodology.

The National Direction of Meteorology works every day and collects huge databases from the air quality measurement of each region. In this paper, the dataset provides the number of daily concentrations of the O_3 air pollutant from January 2010 to April 2014. The values are a count of concentrations, and there are 1556 observations. We divided the dataset into two parties, one for model development (dataset) and the other for validation (validation), dataset: Observations from January 2010 to December 2013. Validation: Observations from January 2014 to April 2014.

The prediction of ozone has grown in importance as a research area in the subject of air quality management in recent years. Prediction precision is a key component of air quality forecasting. As a result, numerous initiatives have been undertaken to improve the accuracy of this procedure. For that reason, within this study, the accuracy is determined by comparing the actual concentrations of pollutants with the predicted results and then utilizing several error measurement methods like RMSE, MAPE, and the index of agreement to assess our suggested model.

The application of artificial intelligence and machine learning techniques has expanded in forecasting as a replacement for the old models a consequence of the explosion of technology and the rise in the amount of measurable data [2]. It helps programmers design and implement intelligent computer systems, as well as provide useful and reliable applications [4]. Deep learning and machine learning methods are effective instruments for precise forecasting [5].

Time-series forecasting problems cannot be solved with a single optimum method [6], each issue might be resolved differently. One of the easiest prediction methods for time series with no discernible seasonal pattern is moving average (MA) [7]. In addition, various articles also employed the Autoregressive Integrated Moving Average (ARIMA) approach, and the results show that it is dependable for time-series modeling. Moreover, the combined models with ARIMA have a better level of robustness and accurately capture all series patterns [9].

SVM regression approaches are another class of models that have been effectively applied in a variety of applications, such as [8] where they predicted daily CO levels and the performance was superior.

Several other regression models have been tested in some research to anticipate daily ozone levels. These forecasts are often based on statistical connections between meteorological variables and pollution levels in the surrounding air. Furthermore, to achieve the same objective, the multivariate regression model has been successfully applied and produced accurate findings [10]. However, interactions between pollution and weather are often complicated and nonlinear, particularly for ozone qualities, which neural networks may be better able to model [11].

Another potential technique for predicting is artificial neural networks (ANN). It is compared in a study to more well-known methods, including the Box-Jenkins ARIMA model, multivariate regression, and even Winters exponential smoothing methods. The results demonstrated that the neural network model is typically more accurate than other approaches; moreover, it can record patterns of seasonality, nonlinear trends, and how they interact [12]. For instance, with data collected locally in Corsica, Artificial Neural Networks (ANNs) have produced good predictions of ozone levels one hour in advance [13].

Recently, an alternative method, called the recurring neural network (RNN), is attracting a lot of interest. RNNs are essentially networks made up of loops, which enable them to retain memories of prior events. Therefore, they are quite helpful in time-series prediction [14]. One of the special

RNN variants that provides a temporary storage solution is the Long Short-Term Memory (LSTM) approach [15]. When predicting ozone, it has received a great deal of attention because of its capability to simulate long-term dependency. However, to create a more accurate model, some studies suggested a novel hybridization method that combines deep learning techniques with other traditional models [16]. Then, the results obtained can more clearly demonstrate how the suggested strategy can forecast a high level of ozone concentration [17].

Exponential smoothing has shown to be a successful forecasting technique for prediction due to its simplicity of usage and overall high performance. Business tasks and environmental studies are two examples of typical applications that incorporate the Holt–Winters exponential smoothing approach. Due to its ease of use and overall strong performance, exponential smoothing has shown to be a successful forecasting technique for prediction. Business tasks and environmental studies are examples of common applications [18] and [19], which integrate the Holt–Winters exponential smoothing to boost precision beyond the usual model [20].

2. Methodology

2.1. Forecasting with Exponential Smoothing Methods

Exponential Smoothing has become very popular due to its success as an effective forecasting method. Three broad categories can be made out of it [21]. Forecasting time series without trend or seasonality is done by employing Single Exponential Smoothing (SES), a weighted average of the current observation y_t and the prior forecast $\hat{y_{t-1}}$ is what the forecast $\hat{y_{t+1}}$ represents according to Equation (1):

$$\hat{y}_{t+1} = \alpha y_t + (1-\alpha)\hat{y}_{t-1}, \tag{1}$$

where $0 \leqslant \alpha \leqslant 1$ is the smoothing parameter.

The type of double exponential smoothing (DES), which incorporates the trend component with an additional parameter, is an extension of the simple method. DES can be explained mathematically with Equation (2),

$$\begin{aligned} \hat{y}_{t+1} &= \alpha y_t + (1-\alpha)(y_{t-1} + b_{t-1}), \\ b_t &= \beta(y_t - y_{t-1}) + (1-\beta)b_{t-1}, \end{aligned} \tag{2}$$

where $0 \leqslant \alpha \leqslant 1$ and $0 \leqslant \beta \leqslant 1$ represent the smoothing parameter, $\hat{y}_{t+1}$ represents a time-series' level estimate, b_t represents time series growth at the moment t.

To address the data's trends and seasonality, Holt and Winters developed a more sophisticated version of exponential smoothing called triple exponential smoothing method (Holt–Winters method); it can be explained mathematically with Equation (3),

$$\begin{aligned} l_t &= \alpha\left(y_t - s_{t-m}\right) + (1-\alpha)\left(l_{t-1} + b_{t-1}\right), \\ b_t &= \beta\left(l_t - l_{t-1}\right) + (1-\beta)b_{t-1}, \\ s_t &= \gamma\left(y_t - l_{t-1} - b_{t-1}\right) + (1-\gamma)s_{t-m}, \\ \hat{y}_{t+h} &= l_t + hb_t + s_{t-m+h}, \end{aligned} \tag{3}$$

where $0 \leqslant \alpha \leqslant 1$ and $0 \leqslant \beta \leqslant 1$ and $0 \leqslant \gamma \leqslant 1$ represents the factors of smoothing factors, l_t represents the level at moment t, b_t represents the trend at moment t, s_t represents the seasonal moment t, $\hat{y}_{t+h}$ represents a time series level estimate, m represents the period of the seasonality, h represents the forecast horizon.

2.2. Forecasting with LSTM model

A more advanced variant of the conventional recurrent neural network is the long-short-term memory (LSTM), which excels at time series prediction. The particularity of LSTMs lies in how the hidden layer is managed [6]. Figure 1 shows the architecture of the LSTM model. As seen, a set of neurons and repeated cells that present its hidden layer. Inside each cell there are forgot gate, input gate, and output gate. Each of the three gates has activation functions that determine the amount of information that will be included in the process, such as the sigmoid function (σ) or the tanh function [22]. In general, it is a set of mathematical calculations that will be applied to some incoming information to get an output according to the following equations.

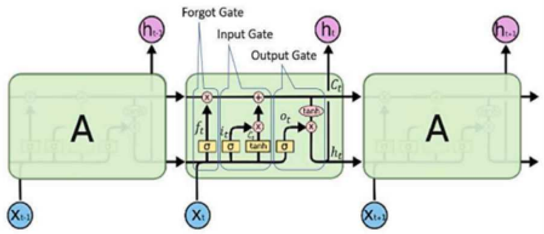

Fig. 1. The process of Long Short-Term Memory Network (LSTM).

Input gate: It obviously controls the amount of information that goes through the cell, and the tanh and sigmoid functions detect the value that needs to be updated and generate new potential values to be added, according to Equation (4),

$$\begin{aligned} i_t &= \sigma\left(w_t \cdot [h_{t-1}, x_t] + b_t\right), \\ \tilde{C}_t &= \tanh\left(w_c \cdot [h_{t-1}, x_t] + b_c\right), \\ C_t &= f_t \cdot C_{t-1} + i_t \cdot \tilde{C}_t, \end{aligned} \tag{4}$$

where w_t, w_c are weight vectors, and b_t, b_c are vectors of deviation.

Forget gate: By selectively analyzing historical data, it is feasible to determine which information in the cell state has to be destroyed and which information needs to be remembered with the help of the sigmoid function to calculate the forgot gate with the inputs h_{t-1} and x_t (Equation (5))

$$f_t = \sigma\left(w_f \cdot [h_{t-1}, x_t] + b_f\right), \tag{5}$$

where w_f is a vector of weights, and b_f is a deviation vector.

Output gate: By using the state of the cell at the instant t, it is possible to define the state of the cell at the instant $t-1$, integrate the new information, and erase the information that had to be forgotten, according to these equations (Equations (6)).

$$\begin{aligned} o_t &= \sigma\left(w_o \cdot [h_{t-1}, x_t] + b_o\right), \\ h_t &= o_t \cdot \tanh\left(C_t\right). \end{aligned} \tag{6}$$

Here w_o is a vector of weights and b_o is a vector of deviation.

2.3. Selection of evaluation criteria

Performance metrics for time-series forecasting show how well the model performs. A model can be assessed using a variety of techniques. To evaluate the efficiency of our presented methodology, three commonly used measures are used, such as Mean Squared Error (MSE), Mean Absolute Error (MAPE), and Root Mean Squared Error (RMSE). The expression of these evaluation metrics indicates that as the three values decrease, the prediction error of the model also decreases.

As a standardized method for evaluating the degree of model prediction error, Willmott [23] created an index of agreement (d) that clarifies the link between prospective error and mean square error. An agreement score of 1 shows an ideal match, while a value of 0 indicates no agreement at all.

These metrics are calculated using Equations (7)–(10).

$$\mathrm{MSE} = \frac{1}{n} \sum_{t=1}^{n} \left(y_t - \hat{y}_t\right)^2, \tag{7}$$

$$\mathrm{MAPE} = \frac{100}{n} \sum_{t=1}^{n} \left| \frac{(y_t - \hat{y}_t)}{y_t} \right|, \tag{8}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n} \sum_{t=1}^{n} \left(y_t - \hat{y}_t\right)^2}, \tag{9}$$

$$d = 1 - \frac{\sum_{t=1}^{n} \left(y_t - \hat{y}_t\right)^2}{\sum_{t=1}^{n} \left(\left|y_t - \bar{\hat{y}}_t\right| + \left|\hat{y}_t - \bar{\hat{y}}_t\right|\right)}, \tag{10}$$

where y_t represents the observed value, $\hat{y_t}$ represents the forecasted value, $\bar{\hat{y_t}}$ represents the average of forecasted values, n represents the number of total observations.

3. Experiments

3.1. Applied machine learning process

To achieve our main goal, namely to forecast ozone (O_3) concentration time series, this work introduces three approaches, which are the prediction using the three types of Exponential Smoothing as a classical method, the Architecture of LSTM (Long Short-Term Memory) as a specific type of Recurrent Neural Network (RNN), and finally an alternative approach that integrates the Holt–Winters model with the LSTM.

Following a few steps is essential for the success of our machine learning application. The initial phase is the preparation of the data, which involves normalizing and scaling the data in the range of 0 and 1 to accelerate the training. Then, datasets may have missing values for a variety of reasons, which can significantly lower the quality of the model and affect the outcomes. To solve this problem in the current study, the K-Nearest Neighbor method was used. Subsequently, the database must be divided into training and test datasets. After performing multiple tests, we found that 70% is the ideal percentage to use as a training database. Finally, to run the LSTM, each dataset will be separated into input and output samples.

The next stage is creating an LSTM model, after applying the three types of Exponential Smoothing method to our data. Then, we specify the input layer of the LSTM by using the fitted values of the previous methods (SES, DES, and TES). Certain different factors, among them the number of hidden layers, the number of neurons in each layer, and the functions of activation, are to be initialized.

The model is trained in the third stage using the LSTM training procedure which requires defining some parameters including a loss function e.g., (MSE) and an algorithm of optimization like gradient descent. Coming to the most important stage, during which we make predictions, several plots must be generated in order to compare predicted results with actual data. Finally, in the validation model stage, we used our hybrid model to forecast a period of three months in advance, then we examined those forecasts with the actual data for the same time period, and we watch to see how that appears [6].

3.2. Exploring times series data

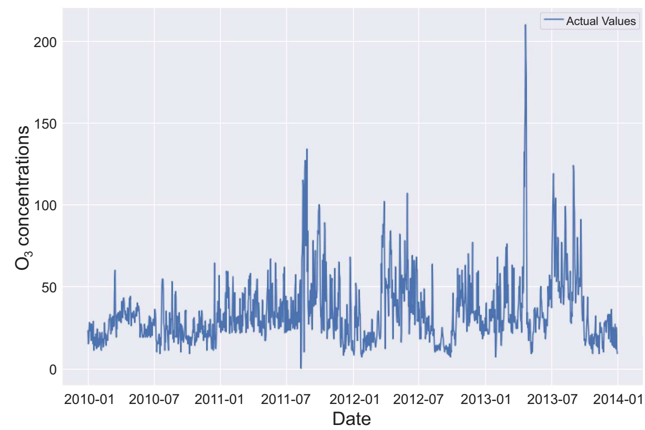

Fig. 2. Line plot of distribution of O_3.

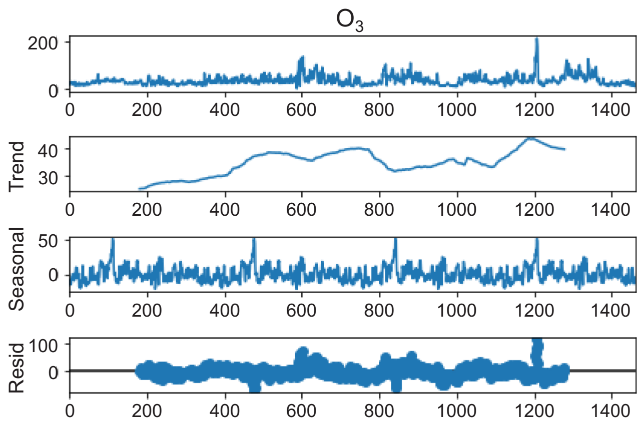

Fig. 3. Decomposing of the O_3 time series.

In this paper, three approaches of Exponential Smoothing methods are tested using databases of daily concentrations of the O_3 air pollutant, measured by the National Direction of Meteorology, from

01 January 2010 to December 2013 in Tangier. In time series analysis and forecasting, visualization is crucial. It can offer helpful diagnostics to spot temporal structures that may affect model choice. In Figure 2, we can visualize the distribution of the daily concentration of ozone time series, this plot is obtained after handling missing data using the K-Nearest-Neighbor algorithm. The O_3 time series indicates an increasing pattern of behavior over time, with a small repeating pattern that represents low seasonality.

The analysis of time series is of the utmost importance in achieving the aim of this study. It involves building models that most accurately represent or describe our observed time series to be able to comprehend the underlying causes of the data. This frequently necessitates making assumptions about the structure of the data and requires decomposing the time series into its four component parts: Level, Trend, Seasonality and Noise, according to Figure 3.

4. Results and Discussion

4.1. Forecasting of O_3 concentrations using the Single Exponential Smoothing (SES)

We must understand that Single Exponential Smoothing produces a forecast time series without a trend or seasonality and allows us to smooth only the level, where α is the weight used in the level component of the smoothed estimate [18]. α is similar to a moving average of the observations. After applying the SES method, the results look like Figure 4 in which we represent the actual observations and the forecasting values given by the SES method. According to the summary of the method used, we obtained an optimal value of α which is equal to 0.825.

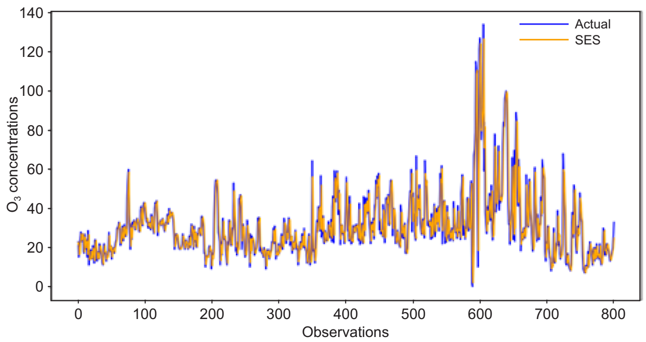

Fig. 4. Graphical representation of current and forecasted values of the O_3 applying the SES method.

4.2. Forecasting of O_3 concentrations using the double exponential smoothing (DES)

As noted previously, single smoothing struggles to follow trends in the data. This problem can be resolved by adding another equation containing a supplementary constant β that should be selected according to α. The Double Exponential Smoothing type is an extended of the simple method that includes the trend component. After applying the DES method, the results look like in Figure 5, in which we represent the current observations and the predicted values given by the DES method. According to the summary of the method used, we obtained an optimal value of α and β which are equal to 0.794 and 0.02 respectively. Here, the smoothing factors for the level and the trend are α and β, respectively.

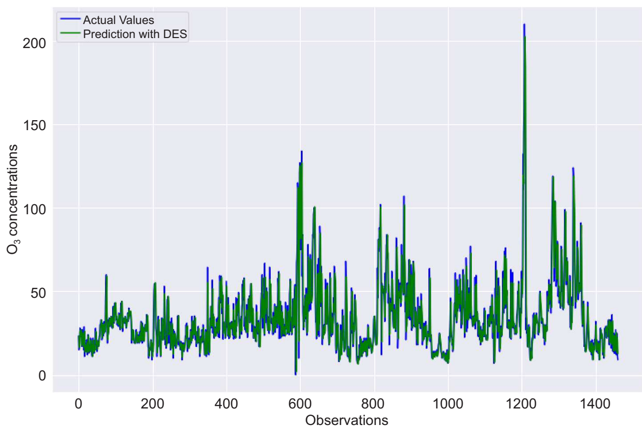

Fig. 5. Graphical representation of observed and predicted values of the O_3 time series for the DES method.

4.3. Forecasting of O_3 concentrations using the third exponential smoothing (Holt–Winters)

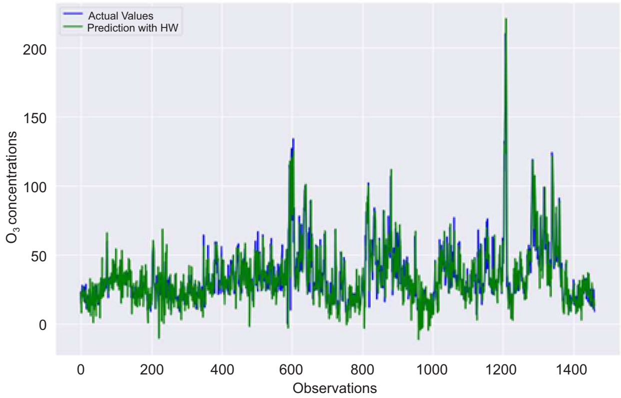

Fig. 6. Graphical representation of observed and anticipated values of the O_3 using the HW method.

As the Holt–Winters method is the more sophisticated version of Exponential Smoothing. We employ it with our data and the results look like in Figure 6 in which we graphically represent the recent data and the anticipated values given by the HW technique. In accordance with the summary of the approach utilized, we achieved optimal values of α, β and γ which are 0.828, 0.092 and 0.089 respectively. Where the smoothing factors with respect to the level, trend, and seasonality are α, β and γ respectively.

4.4. Comparison with three types of exponential smoothing methods

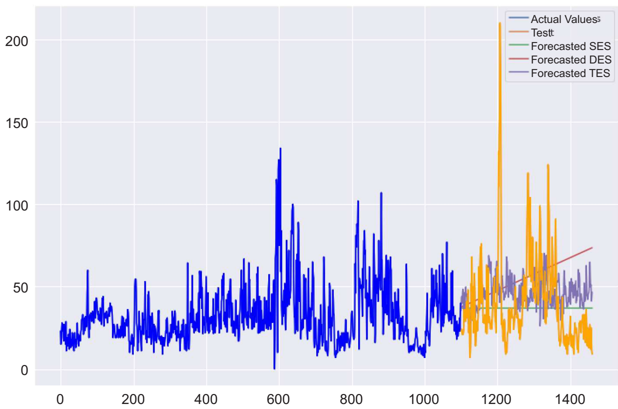

Fig. 7. Graphical representation of observed and predicted values of the O_3 time series using SES, DES and HW methods.

If we plot our three forecast structure of three kinds of Exponential smoothing, then we will see that we have a times series looking like illustrated in Figure 7. We can see that the green, red, and purple curves plotted above represent, respectively, our forecasts made using the SES, DES, and HW approaches. From the plot we can concluded that the best forecast is that given by the purple curve because it is the closest to the test curve (in orange) and which represents the forecasting with the Holt–Winters method.

4.5. The Hybridization with LSTM Technique

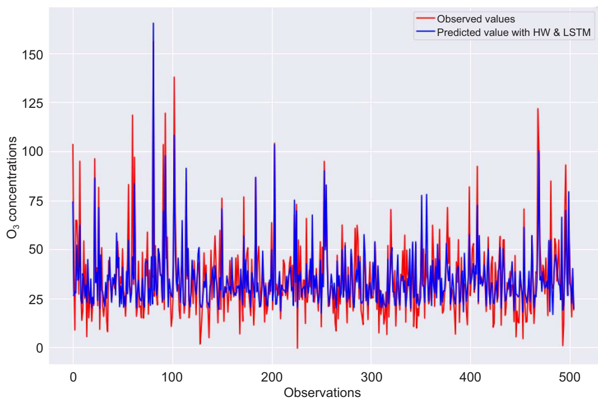

Fig. 8. Graphical representation of observed and predicted values of the O_3 time series using the hybrid model: HW and LSTM model.

In a previous paper, we examined the Simple RNN and the Long-Short-Term Memory (LSTM) architecture as two time-series prediction approaches. Since the LSTM is the most effective, we combined it with the Holt–Winters method, a traditional time series forecasting, to enhance the model.

After applying the LSTM architecture to the fitted values produced by the Holt–Winters methodology, we obtained a representation of the predicted and observed values. As seen in Figure 8, our hybrid model performs very well, especially at the peak level because these two curves are very close to each other.

Several of the performance metrics mentioned above, including Mean Squared Error (MSE), Mean Absolute percentage Error (MAPE), Root Mean Squared Error (RMSE), and the Index of Agreement, are used to assess the performance of our model; see Table 1. These measures are given after using all forecasting methods and hybrid models. We observe that there is a decrease in the calculated errors and an increase in the index of agreement when we opt for the HW and LSTM hybrid model, which shows that it is the best.

Table 1. Error indices.

Models	MSE	RMSE	MAPE	d
SES	824	28.7	460	0.32
DES	167	12.95	460	0.89
HW	154.9	12.4	440	0.89
LSTM	0.55	0.74	450	0.86
SES LSTM	0.0032	0.056	420	0.86
DES LSTM	0.0039	0.063	496	0.87
HW LSTM	0.0030	0.055	410	0.91

In Figures 9a and 9b, we have the plot of the error function and the function of the mean absolute percentage error. We note that it decreases during the training and the validation step, which indicates the capability of the proposed model.

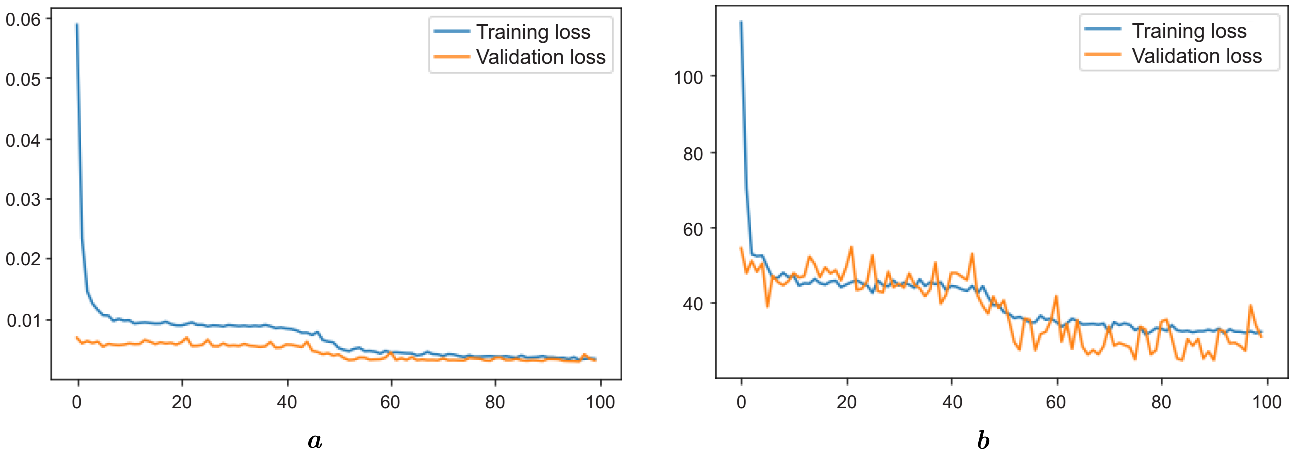

Fig. 9. Training and validation error Training and validation MAPE.

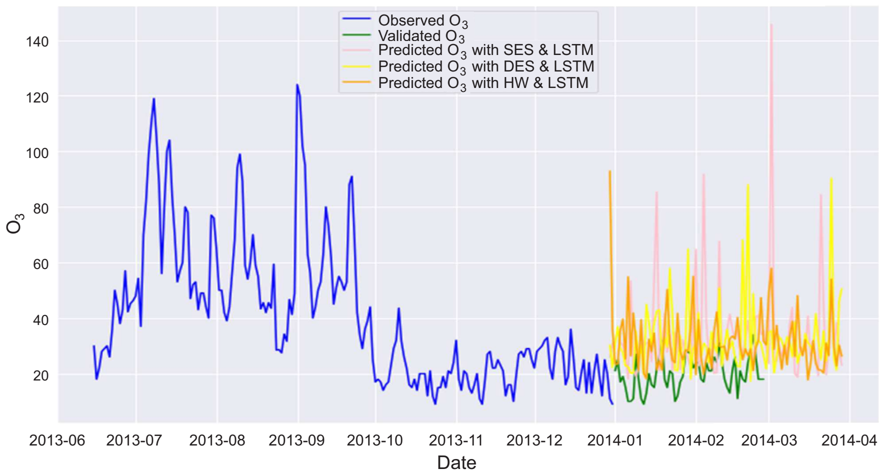

Fig. 10. Forecasting of O_3 concentrations using the hybrid model the three types of Exponential Smoothing.

To validate our suggested model, we applied it for a new period like three months starting with the first January 2014, then we compared the predictions with the validation data (observations from January 2014 to April 2014) in the same period. As shown in Figure 10, three curves (pink, yellow, and orange) are, respectively, the forecasts given by three hybrid models (SESLSTM, DESLSTM and HWLSTM). We can observe that the best forecast is produced by the orange curve which is the Holt–Winters LSTM because it is very close to the validated data represented by the green curve.

5. Conclusion

In this work, we focused on forecasting the levels of air pollution for the next day in Tangier City, caused by daily ozone, to prevent the negative consequences of exposure to this pollutant and identify the period of peaks.

In a previous study, two types were compared: Long-Short-Term Memory (LSTM) and simple RNN; LSTM performed better and produced positive empirical results. Then, we have chosen to develop three original approaches. The first two approaches are based on LSTM as a specific type of recurrent neural networks and different types of exponential smoothing methods. Finally, the LSTM and the Holt–Winters are merged in the third alternative, as a hybrid method.

The dataset used in this work comes from the National Direction of Meteorology and provides the number of daily concentrations of the O_3 air pollutant from January 2010 to April 2014. First, we applied and compared three different kinds of Exponential Smoothing, the resulting plots revealed that the Holt–Winters method provided the best forecasts. Next, we combined all three types with an LSTM architecture, and after that four statistical performance metric: MSE, RMSE, MAPE, and index of agreement are adopted to examine the results. By offering more precise predictions of O_3 concentration, the hybrid model generally outperforms the other methods, and the results indicate a good finding with an index of agreement equal to 0.91 and a lower value of the error indices MSE $= 0.0032$, RMSE $= 0.055$, and MAPE $= 410$.

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Гібридна модель для прогнозування якості повітря, що поєднує підходи Хольта–Вінтерса та глибинного навчання: новий метод визначення піків концентрації озону

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Озон (O_3) з тропосфери є однією з речовин, яка сильно впливає на забруднення повітря в місті Танжер. Прогнозування цього забруднювача може покращити якість повітря. У цій статті представлено новий підхід, який поєднує алгоритми глибинного навчання та метод Хольта–Вінтерса для виявлення піків забруднюючих речовин і отримання більш точної моделі прогнозування. З огляду на те, що LSTM є надзвичайно потужним алгоритмом, ми об'єднали його з методом Хольта–Вінтерса, щоб покращити модель. Використовуючи декілька показників точності, досліджено ефективність моделей. Емпіричні результати показують перевагу гібридної моделі, надаючи більш точні прогнози з індексом згоди, що дорівнює 0.91.

Ключові слова: *прогнозування якості повітря; озон (O_3); довга короткочасна пам'ять (LSTM); метод Хольта–Вінтерса; рекурентна нейронна мережа (RNN); штучні нейронні мережі.*