2022

High School Mathematical Contest in Modeling (HiMCM)

Summary Sheet

Team Control Number: **12465**

Problem Chosen: **B**

Prior to the Industrial Revolution, carbon dioxide (CO2) content in the atmosphere was almost constant at about 280 parts per million (ppm). After the Industrial Revolution, however, atmospheric CO2 levels increased dramatically. According to National Oceanographic and Atmospheric Administration (NOAA), the monthly mean CO2 concentration peaked at 421 ppm in May 2022. The main possible consequence of the increase in CO2 concentration is the enhanced greenhouse effect leading to rising air temperature. According to the 2022 report of Intergovernmental Panel on Climate Change (IPCC), air temperature will increase by 1.5ºC within the next two decades. Based on the assumption that the statistical trend of change obtained from historical data also applies to future changes, in this work we created three models based on historical data of CO2 and land-ocean temperature, projected their future changes, and investigated the relationship between these two variables.

Based on a trend analysis over the 10-year moving averages of CO2 by a modified Mann-Kendall test for autocorrelated data, we confirmed the claim that the CO2 increase in 2004 is greater than the averages over any previous 10-year period. Linear, quadratic and exponential models were fitted to describe CO2 changes over time. Among them, the quadratic model proves to be the most accurate through a 10-fold cross validation for time series. None of our models support the claim that the CO2 concentration level will reach 685 ppm by 2050. The highest CO2 level in 2050 is predicted to be around 497 ppm and the quadratic model estimates CO2 concentration level of 685 ppm in 2097.

As there is obvious increase trend, strong autocorrelation, but without periodicity in the land-ocean temperature anomaly time series, we innovatively propose a univariate forecasting model combining the seasonal-component-free Holt-Winters method and bootstrap-aggregated residuals, which reflects well the fluctuations present in the observed temperature time series with a correlation coefficient of 0.971. The projection shows an increase in average land-ocean temperature of 1.25, 1.50, and 2°C will occur in 2032 [2027, 2037], 2042 [2038, 2047], and 2063 [2058, 2067], respectively.

We used a linear regression model and ARIMA errors to investigate the relationship between CO2 and temperature. Given limited data, we assessed the models' forecast ability through multiple ways, including creating various training-testing scenarios. The relationship model with CO2 as input shows a more robust performance under any scenarios than the univariate model but it underrepresents the fluctuations in long-term forecast. Limited evidence shows the models perform better forecasts in the first 10-20 years. While increased CO2 has been shown to be a major contributor to rising temperature, fluctuations of temperature are in fact related to many intervening factors and complex interactions within the climate system.

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Solution for Problem B of HiMCM 2022

1 Introduction

1.1 Background

For most of the time in earth's history, the carbon dioxide (CO2) concentration in the atmosphere changed very slowly and nearly constantly, which is about 280 ppm (parts per million) prior to the Industrial Revolution in the 1760s [1]. Most living things, including humans, animals, plants, require oxygen (O2) and produce carbon dioxide (CO2) when respirating. Most plants carry out photosynthesis under sunlight. In the chloroplasts in their leaves, CO2 and H2O turned into O2 and glucose. The rate of production of CO2 and the rate of conversion of CO2 into O2 were roughly equal, leading to a relatively equilibrium state of concentration level of CO2 in the atmosphere. However, after the Industrial Revolution, the atmospheric CO2 level rose dramatically. Three types of fossil fuels, i.e., coal, oil and natural gas, support our industry and make our life better. Combustion of all sorts of fuels greatly increased as demands of human beings for energy soared [1]. Further, the total forest area decreased globally because a great deal of forests had been turned into cultivated or urban areas to sustain a rapidly increasing population [2]. Every year, large amounts of CO2 are emitted into the atmosphere beyond the converting ability of CO2. According to National Oceanographic and Atmospheric Administration (NOAA), the monthly mean CO2 concentration level peaked at 421 ppm in May 2022 [3].

The most prominent consequence of CO2 concentrations is the enhanced greenhouse effect. Together with other greenhouse gases, CO2 in the atmosphere traps some of the heat that Earth might have otherwise radiated out into space, causing the air temperature to rise. According to the report of Intergovernmental Panel on Climate Change (IPCC) in 2022, the air temperature rise will reach 1.5ºC within the next two decades [4]. Global warming is altering the earth's climate system, leading to many disastrous consequences, such as more frequent and sever weather, higher sea level, more acidic oceans, higher death rates, dirtier air, and higher wildlife extinction rates. Only the most drastic cuts in carbon emissions from now would help decrease environmental disasters.

The connections between CO2 and temperature changes are very complex and the scientists simulated their responses and feedback through state-of-the-art climate models and earth system models. In this contest, we are to create empirical models based on historical data of CO2 and land-ocean temperature provided, investigate the relationship between these two variables, and predict future changes in CO2 concentration and land-ocean temperature. The solution to this simplified task will help in understanding climate change and its causes.

1.2 Problem restatement

First of all, we would like to point out an error in the original problem text. Based on the link provided to the source of the CO2 Data Set 1 [5], the values in the CO2 Data Set

1 provided represent annual means of Mauna Loa CO2 concentrations, rather than monthly means. The value of 377.7 ppm quoted in the text is the annual mean of 2004, not the monthly mean of March of 2004, and the correct value for March 2004 is 379.06 ppm. We split the problem into the following three questions.

Question 1: How does CO2 level change over time? Analyze and model the changes of CO2 concentrations using the CO2 Data Set 1 provided.

1a. Is the increase in CO2 in 2004 (relative to pre-industrial levels) greater than the record over any previous 10-year period. Provide explanations.

1b. Fit the changes of concentration levels of CO2 in the atmosphere using various mathematical models in different forms.

1c. Use each of the proposed models to predict the CO2 concentrations in the year 2100. Determine the CO2 concentration level by 2050 using the models. If the predicted level for 2050 is not equal to 685 ppm, determine when the 685 ppm threshold will be reached.

1d. Evaluate the performance of those proposed models and determine which is most accurate. Provide a justification.

Question 2: How is mean ocean-land temperature evolving over time? Analyze and model land-ocean temperatures changes using Temps Data Set 2.

2a. Create a model that reflects historical land-ocean temperatures changes and predicts future changes.

2b. Estimate when the increase of the average land-ocean temperature will reach 1.25°C, 1.50°C, and 2°C compared to the base period of 1951-1980, which is about 14°C.

Question 3: What's the relationship between CO2 concentration and temperature change? Model and evaluate the relationship between CO2 concentrations and land-ocean temperatures.

3a. Build a model to analyze the relationship between CO2 concentrations and land-ocean temperatures since 1959 and explain the possible relationship.

3b. Evaluate the model's ability to predict future changes and figure out what factors affect this model's ability.

2 Problem analysis

Question 1a: The question is essentially about the trend of CO2 changes over time. We can perform a trend analysis over the 10-year running averages of CO2, which can be derived from the annual CO2 mean data provided. If the smoothed time series is indicated by a trend analysis method to be monotonical increase through 2004, this answer to this question is yes. Compared to a threshold approach, where the 2004 level is directly compared to any previous levels, this approach has an advantage in solving the problem from a statistical point of view. We also note that autocorrelation should be considered when performing trend analysis.

Question 1b-c: CO2 Data Set 1 contains only a time series of annual CO2 concentration at Mauna Loa. Visual inspection shows changes continue to increase with what appears to be linear trend throughout the time period. However, the data points in the low value end and high value end appear to be above the linear trend line, suggesting it is not a prefect linear trend. We therefore test quadratic and exponential models in addition to the linear fit. The abscissa is unified to the years to the beginning year (1959) to remove the potential effect of using the year as the x-value in regression models.

Question 1d: The CO2 data provided is not very long (only 63 points). We prefer n-fold cross validation for time series to assess the model performance, in order to maximize the benefits of limited data.

Question 2a-b: A quick look at the annual ocean-land temperature data indicates an obvious increase trend throughout the entire period. A common time series model breaks a non-stationary time series into trend, periodicity/seasonality and remainder components. Trend is obvious, but periodicity for yearly temperatures needs attention. Although some materials indicate some periods such as 11 years and 9.3 years in the global temperature data [6], they are based on much longer time series. We performed seasonality test and spectral analysis, as well as autocorrelation test, on the given temperature data. Based on the findings (no obvious periodicity and strong autocorrelation), we propose a novel method, which is a combination of Holt-Winters method (exponential smoothing based) with no seasonality component and bootstrapping for residuals. The question 2b can be answered using this model.

Question 3a: Given the finding in Question 1b that CO2 changes follow a steadily increasing trend, we decompose the temperature time series into a linear trend component and the residuals component. Informed by physics, we can deduce that the linear component of temperature anomalies can be regressed from the log-transformed CO2 changes, and the residuals are more related to past temperature anomalies and can be estimated by an ARIMA approach.

Question 3b: We use the historical data to evaluate the model's ability in predicting future temperature changes. The whole historical data is divided into a training set and validation set. We create scenarios with different sizes of training set and validate using the validation set consisting of the remaining data. By this means, the impacts of training set size on the model ability and how the prediction accuracy changes over time into the future are quantified. The temperature prediction model developed in question 2 does not depend on external variables, while the relationship model in this question additionally includes CO2 concentration as an independent external variable. Therefore, we also investigate any benefits of using CO2 concentration in the model in terms of predicting future changes.

3 Assumptions

Assumption 1: A common disadvantage of empirical/statistical models is that in most cases they are applicable only for the conditions the data were collected, thus they are often not able to predict beyond this particular condition. In our case, we assume the statistical trend of change obtained from historical data applies to future changes. In other words, we simulate future changes under a business-as-usual scenario.

Justification: Since we don't know how exactly CO2 levels will change in the future, a plausible solution is to simulate different scenarios describing all kinds of possibilities. This approach is also taken by IPCC, in whose annual report many scenarios were created and simulated. One of the scenarios is a business-as-usual scenario where the current trend continues into the end of 21st century. However, we must avoid overfitting during the training stage. In addition, we validate model ability against the validation data set, which was specifically left out from historical data for validation purposes.

Assumption 2: The link between temperature and CO2 is very complex. We assume a rise in CO2 precedes a rise in temperature in a short period and the trend of change in CO2 primarily affects a long-term trend of land-ocean temperature. However, temperature fluctuations between years can be caused by many factors and thus expressed as an autoregressive process.

Justification: Considering physics behind the link, changes in temperature are roughly proportional to changes in radiative forcing as a function of changing concentration of CO2 [7]. Strong correlations present between the trends of temperature anomalies and CO2 levels also support this assumption.

Assumption 3: The CO2 concentration data provided come from the Mauna Loa site and may differ from other CO2 sampling sites. We assume these data have sufficient representativeness for the global average condition in our attempts to investigate the relationship between CO2 levels and land-ocean temperatures.

Justification: The team at Mauna Loa has confidence that CO2 measurements made at the Mauna Loa Observatory reflect truth about global atmosphere [8]. The site is located 3400 m high enough to represent very large areas. All measurements are rigorously calibrated with a very high accuracy.

4 Methodology

4.1 Trend analysis for autocorrelated annual CO2 time series (Question 1a)

In response to Question 1a, we first computed 10-year running averages for the annual CO2 data sequence. We evaluated the exceedance of the considered threshold of CO2 level in 2004.

Then, a modified Mann-Kendall (M-K) trend test [9] was conducted for monotonicity on the annual CO2 level data sequence. M-K test is a commonly used non-parametric trend analysis method based on rank correlation, but its null hypotheses is that the data are independent and randomly ordered so the effect of autocorrelation in the CO2 level data provided should be considered. The modified method is based on the modified variance of the data and shows robust in the presence of autocorrelation in the data. In absence of correlation in the data, the power of the modified M-K trend test is also comparable to that of the original M-K test.

The M-K test computes the statistic S for observations X with a dimension of n in Eq. (1) where sgn() is a sign function:

$$S = \sum_{i<j} a_{ij} = \sum_{i<j} sgn(x_j - x_i) \tag{1}$$

where

$$a_{ij} = sgn(x_j - x_i) = \begin{cases} 1, & x_i < x_j \\ 0, & x_i = x_j \\ -1, & otherwise \end{cases} \tag{2}$$

For a large n, the statistic S tends to normality with a mean of 0, and a variance given by:

$$\mathrm{var}(S) = n(n-1)(2n+5)/18 \tag{3}$$

In the case of autocorrelation between the values of X, the mean is still zero while the variance can be computed by:

$$\mathrm{var}(S) = E(S^2) = \sum_{i<j_{k<l}} E(a_{ij}a_{kl}) = \sum_{i<j_{k<l}} \frac{2}{\pi} \sin^{-1}(r_{ijkl}) \tag{4}$$

where

$$r_{ijkl} = corr(Y, Z) = \frac{\rho(j-l) - \rho(i-l) - \rho(j-k) + \rho(i-k)}{2\sqrt{[1-\rho(j-i)][1-\rho(l-k)]}} \tag{5}$$

and $Y = x_j - x_i$ and $Z = x_l - x_k$. i, j, l, k indicates the element index in X. ρ denotes a correlation function.

M-K Z statistic is used to transform S to a normally distribution, as computed by:

$$Z_{\mathrm{MK}} = \begin{cases} \frac{S-1}{\sqrt{\mathrm{VAR(S)}}} (S > 0) \\ 0 \quad (S = 0) \\ \frac{S+1}{\sqrt{\mathrm{VAR}(S)}} (S < 0) \end{cases} \tag{6}$$

For an upward monotonic trend, the null hypothesis is rejected if $|Z_{mk}| \geq Z_{1-\alpha/2}$ where α is confidence level. For more details about the modified M-K method and its derivation, refer to the literature [9]. We applied the modified M-K trend test to the annual CO2 level data by using R package modifiedmk.

4.2 Models for predicting CO2 concentrations (Question 1b-d)

Mathematical models are required to fit annual CO2 concentrations. We observed good increasing monotonicity, but with data points above the linear trend line in the low end and high end. Therefore, we fit linear, quadratic and exponential forms (Equations 7-9) of models to this time series, and compared their performances.

Linear form: $cc = a \times y + b$ (7)

Quadratic form: $cc = a \times y^2 + b \times y + c$ (8)

Exponential form: $cc = a \times e^{b \times y}$ (9)

where cc denotes CO2 concentration [ppm], y represents the number of years to the beginning year 1959. Coefficients a, b, and c were optimized by using observation data.

To answer Question 1d, we performed n-fold cross validation for time series to evaluate the models' skill in view of very limited data samples in the CO2 dataset. There is a temporal dependency between observations in a time series, the traditional n-fold cross validation must be modified to preserve that dependency during test. The procedure consists of the following steps.

First, split the dataset into *n* equal-size subsets (in this work, n takes 10). Take the first subset as a training data set and the second subset as a testing data set. In the next iteration, take the first and second subsets as a training set, and the third sunset as a testing set, and so on to the end of the training set. In other words, the same forecasted subset is then included as part of the next training dataset and subsequent subset is forecasted. In this way temporal dependency is respected. At last, we summarize the skill of the model using the average of model evaluation scores, which in this work include coefficient of determination (R-squared), root mean square error (RMSE) and mean absolute error (MAE).

4.3 Modeling changes of land-ocean temperatures (Question 2)

The land-ocean temperature anomalies included in Temps Data Set 2 show fluctuation but have an increasing trend over time, with an evolving pattern that is much more complex than CO2 changes over the same period. We utilize the time series decomposition approach to model the changes. A time series can be decomposed to a trend component, a periodicity component and a remainder component. For our annual temperature data, we first test for the presence of a periodic component using STL (Seasonal and Trend decomposition using Loess) method and a spectral analysis.

The STL has an advantage in that the seasonal component is allowed to change over time and provides facilities for additive decompositions [10]. It is implemented in R package known as stl() function. The seasonal() function returns the seasonal component. Our work indicates no obvious seasonal component present in the annual land-ocean temperature anomalies. On the other hand, spectral analysis involves the calculation of oscillations in a set of sequenced data by breaking down a signal into its components at various frequencies. A previous material [6] based on spectral analysis indicates annual global temperatures may exist frequencies of 60 years, 11 years and 9.3 years. Therefore, despite the failure of detecting seasonality by STL, we also performed spectral analysis on our temperature anomalies (1958-2021) using R function spec.pgram(), which calculates the periodogram using a fast Fourier transform. The resulting periodogram shows very weak spectrum (c. 0.050 for the largest) present in the data sequence considered.

Next, we estimated the autocorrelation using R function acf(), which returns strong autocorrelation present in the temperature time series. Based on these findings (no obvious periodicity and strong autocorrelation), we modelled the temperature time series based on a decomposition framework with autocorrelation considered. One option is a linear regression combined with an ARIMA (autoregressive integrated moving average) model for residuals. However, this option relies on ARIMA to represent variability over the entire forecast period, and the performance tends to deteriorate in the distant future due to ARIMA's well-known poorer performance for long term forecasts. Bearing this in mind, we turn to choose an exponential smoothing approach, which is more explainable than ARIMA, to decompose the temperature time series, with the residuals estimated by a bootstrap method. Our novel model is based on the Holt-Winters method (exponential smoothing based) with no seasonality component [11] and formulated as Equation 10.

$$\Delta T' = hw(\Delta T) + \epsilon' \tag{10}$$
$$\epsilon' = E(bootstrap(E(\epsilon), var(\epsilon)) \tag{11}$$

where hw() is the Holt-Winters method with no seasonal component applied to temperature anomalies series (ΔT); bootstrap() is a bootstrap function for the remainder series (ϵ) while maintaining expected value ($E(\epsilon)$ and variance ($var(\epsilon)$) of the remainder component. $\Delta T'$ and ϵ' are the predicted temperature anomalies series and the remainder series.

The Holt-Winters method has been implemented as an R function HoltWinters() in the stats package. It involves a forecast equation and two smoothing equations if no seasonality is considered:

$$\text{Forecast equation: } \hat{y}_{t+h|t} = \ell_t + hb_t \tag{12}$$
$$\text{Level equation: } \ell_t = \alpha y_t + (1-\alpha)(\ell_{t-1} + b_{t-1}) \tag{13}$$
$$\text{Trend equation: } b_t = \beta(\ell_t - \ell_{t-1}) + (1-\beta)b_{t-1} \tag{14}$$

where ℓ_t denotes an estimate of the level of the series at time t, and b_t denotes an estimate of the trend of the series at time t. α, β are smoothing parameters for the level ($0 \leq \alpha \leq 1$) and the trend ($0 \leq \beta \leq 1$), respectively.

Bootstrap is used to simulate the residual component from an estimated distribution of the residual component. The basic idea underlying the bootstrap is to estimate the residuals by operating a resampling with replacement from the sample at the disposal. To reduce the effect of autocorrelation in the residual, we applied moving block bootstrap [12] to our work. Besides, bootstrap aggregating (bagging) consisting of 100 runs is used to overcome overfitting. The mathematical details and procedures can be found in the literature [12]. In this work, we used R function bld.mbb.bootstrap() in the forecast package to implement our task.

Once the model is determined by fitting observed temperature data, it is used for predicting the future changes of temperature anomaly. One merit of using this newly proposed model is the capability of quantifying uncertainty during the estimation.

4.4 Modeling the relationship between CO2 concentration and land-ocean temperature (Question 3a)

The model proposed for solving Question 2 works only for univariate time series, so a new model needs to be created to represent the relationship between the two variables: CO2 concentration and land-ocean temperature. In physics, the primary effect of increased CO2 concentration is to raise the height to which the atmosphere is relatively opaque to the infrared radiation from the earth's surface [7]. Thus, changes in temperature are roughly proportional to changes in radiative forcing as a function of changing concentration of CO2. A logarithmic function of increased CO2 concentration is suggested to best fit the mean temperature anomaly. However, annual temperature anomalies exhibit strong fluctuations over time. We speculate CO2 changes may play an important role in affecting the change trend of temperature, rather than the detailed fluctuations that are likely resulted from numerous exogenous factors and interactions within the climate system. To establish a link between CO2 concentrations and land-ocean temperatures, we decomposed the temperature time series into a linear trend component and a residual component in the hope that the first component would be estimated by the linear increase of CO2 concentrations and the residuals by an ARIMA model. This model is known as regression with ARIMA errors and can be solved by the R function Arima().

Suppose that y_t and x_t are time series variables. A linear regression model with autoregressive errors can be written as:

$$y_t = \beta_0 + \beta_1 x_t + \epsilon_t \qquad (15)$$

If an autoregressive model $\Phi(B)$ is defined, and let $\Phi(B)\epsilon_t = \omega_t$, then $\epsilon_t = \Phi^{-1}(B)\omega_t$ if the inverse operator, $\Phi^{-1}(B)$, exists. Then, the model of regression with ARIMA error can be written:

$$y_t = \beta_0 + \beta_1 x_t + \Phi^{-1}(B)\omega_t \qquad (16)$$

where ω_t is white noise series. In this work, x_t represents log-transformed increased CO2 concentration at time t.

4.5 Evaluating robustness of CO2 prediction models (Question 3b)

We have established a univariate model combining the seasonal-component-free Holt-Winters method and bootstrap (HW+Bootstrap) and a bivariate model of linear regression with ARIMA errors (Trend+ARIMA) for predicting future CO2 level changes. To answer Question 3b, we assessed the models' forecast ability from two aspects and figured out what factors may affect the ability.

1) Quantify the model ability based on scenarios configured with different training dataset and test set created from historical data, as listed in Table 1.

By comparing S1, S3 and S5, we can investigate changes of the performance of HW+Bootstrap univariate model as the forecast moves forward. Likewise, comparison among S2, S4 and S6 helps investigate that of Trend+ARIMA model.

Alternatively, comparing S1 and S2, S3 and S4, and S5 and S6, allows us to look into the performance distinction between the two models with the same configuration of training and test datasets.

Model performance is measured by correlation coefficient (R) and RMSE.

2) Comparing the forecast ability of the models for 2021-2100. Since no true data are present for 2021-2100, we examined predicted temperature changes estimated from both HW+Bootstrap and Trend+ARIMA models in terms of projected trend, evolution pattern over time and uncertainty propagation as time progresses.

Table 1 Scenarios for evaluating models' forecasting ability. 'HW+Bootstrap' represents the method combining the seasonal-component-free Holt-Winters method and bootstrapped residuals and 'Trend+ARIMA' represents the method combining the linear regression and ARIMA errors.

# of scenario	Training set	Testing set	Method
S1	1959-1979	1980-2000	HW+Bootstrap
S2	1959-1979	1980-2000	Trend+ARIMA
S3	1959-1979	2001-2021	HW+Bootstrap
S4	1959-1979	2001-2021	Trend+ARIMA
S5	1980-2000	2001-2021	HW+Bootstrap
S6	1980-2000	2001-2021	Trend+ARIMA

5 Results and analyses

5.1 Trends in historical CO2 concentrations

Figure 1 shows decadal running averages of CO2 concentrations during 1959-2021 in a steadily increasing trend that starts from about 320 ppm in the 1960s to ca. 405 ppm in the 2010s. The CO2 concentration level in 2004 is 377.7 ppm, which intersects the running averages curve at almost 2008 (which indicates an average of the interval 1999 to 2008), and it seems to be higher than CO2 concentrations in any previous 10-years averages. The highest decadal average CO2 concentration before 2004 was at 367.24 ppm occurring in the period of 1994 to 2003.

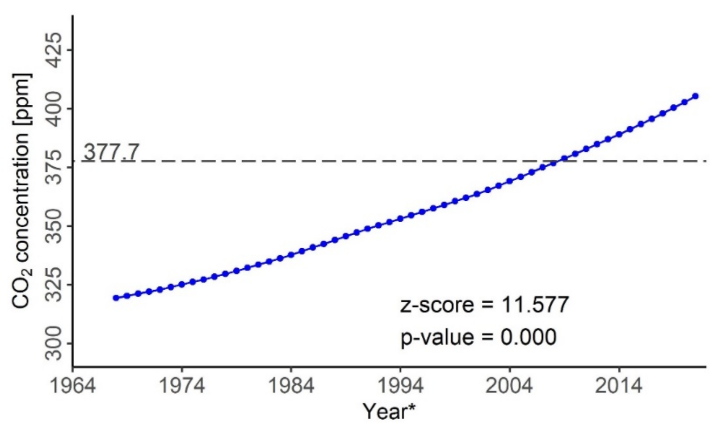


Figure 1 Decadal running averages of CO2 concentrations. The abscissa (Year) indicates the last year of each 10-year window.*

Since the running averages are highly autocorrelated, a modified M-K trend developed specially for autocorrelated time series [9] was applied to test monotonicity in the data sequence. The test showed a p-value close to zero and a z-score of 11.577, much greater than the threshold of 2.807 at 99% significant level, indicating a statistically significant monotonic increasing trend present in the time series. It thus confirms the claim in Question 1a that the increase in CO2 in 2004 (relative to pre-industrial levels) is greater than the record over any previous 10-year period.

5.2 CO2 concentration forecast models and predictions

Based on the historical data provided, we fitted three models, i.e., linear, quadratic, and exponential models (Equations 17-18, respectively) for CO_2 concentration changes over time:

Linear form: $cc = 1.614\,y + 307.303$ (17)

Quadratic form: $cc = 0.013\,y^2 + 0.806\,y + 315.522$ (18)

Exponential form: $cc = 309.839\,e^{0.00449\,y}$ (19)

where cc denotes CO2 concentration in ppm and y denotes the years to 1959. Figure 2 shows the fitted models together with the historical CO2 level data. The fits are all statistically significant with *p*-values lower than 0.001. All three models well capture the increasing trend in CO2 concentration with very high R-square values. Among them, the quadratic model (Figure 2b) performs the best with an R-square of 0.999, showing perfect agreement with the observations. Both the linear (Figure 2a) and exponential (Figure 2c) models show some defects at the lower and upper ends of the x axis, where the fit values deviate downward from the observations.

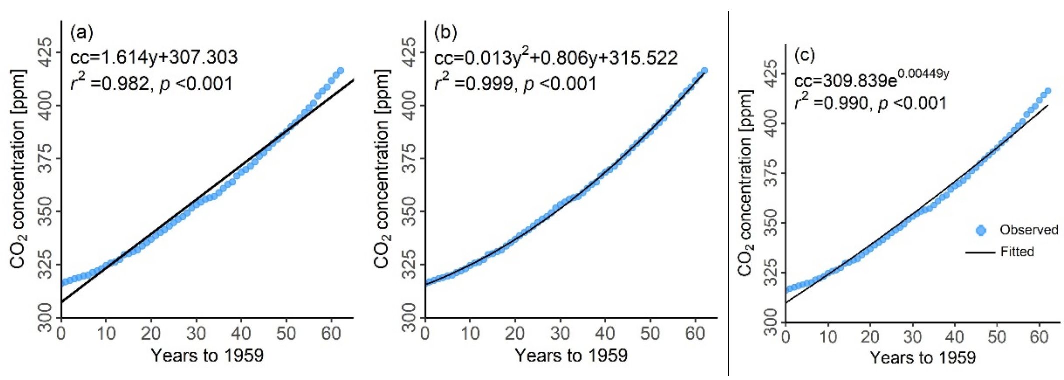


Figure 2. Three fitted models for CO2 changes over time. (a) linear model, (b) quadratic model, and (c) exponential model.

We verified the performance of the models by performing a 10-fold cross validation for time series (Table 2). The overall high R-square values (>0.98) indicate that these models agree pretty well with the observations. However, the quadratic equation has tiny MAE and RMSE values (<0.08 ppm), which are much smaller than the values of the linear and exponential models. Therefore, the quadratic model (Equation 18) proves to be the most accurate model, in prefect agreement with the available observations.

Based on the fitted models, CO2 concentrations are projected to increase steadily in the future, hitting the levels of 535, 688, and 584 ppm, respectively, by 2100. However, compared to the Organization for Economic Co-Operations and Development (OECD) report, which predicts a CO2 concentration level of 685 ppm in 2050, our fitted models appear to be much more conservative. The highest CO2 concentration in 2050 predicted by the quadratic equation is around 497 ppm, well below 685 ppm. The linear and exponential models predicted that CO2 levels in 2050 at 454 and 466 ppm, respectively, which may somewhat underestimate the acceleration in CO_2 concentration changes. Based on our fitted models, the years when the CO_2 level reaches 685 ppm are much later than predicted in the OECD report. The quadratic model estimates CO2 concentration reaching 685 ppm in 2097, close to the end of this century, while the estimates from the linear and exponential models are even later (by 2193 and 2134, respectively).

Table 2. Averaged skill scores of fitted models measured by cross validation for time series

Equations	R-square	MAE [ppm]	RMSE [ppm]
Linear	0.983	3.584	4.237
Quadratic	0.999	0.681	0.777
Exponential	0.991	2.541	3.078

Table 3. Forecasts of CO_2 concentration in 2050 and 2100, and the year predicted to reach a CO_2 concentration of 685 ppm.

Equations	CO_2 in 2100 [ppm]	CO_2 in 2050 [ppm]	Year to reach 685 ppm
Linear	534.9	454.2	2193
Quadratic	687.6	496.5	2097
Exponential	583.6	466.2	2134

5.3 Forecast of land-ocean temperature changes using Holt-Winters model and bootstrap residuals model

The level weight α and trend weight β of the seasonal-component-free Holt-Winters method (HW) for land-ocean temperature anomalies were estimated to be 0.283 and 0.173, respectively. The results show the fitted temperature anomalies can well represent the variability trend of the observations (Figure 3a), while they do not reproduce peaks and troughs in the time series. Figure 3b presents the residuals, which appear to conform to a normal distribution with a mean close to zero. No seasonality was observed in the residual series. We applied a bootstrap aggregation approach (also known as bagging) to reproduce the residuals as shown in Figure 4a. The resampled residuals by bagging can explain the upward and downward variabilities present in the original residuals. Therefore, when the mean residuals from the 100 runs were added to the fitted values of the HW model, the additive result was found to reflect well the fluctuations present in the observation time series (Figure 4b). The correlation coefficient between the observed time series and the HW estimates was 0.947, which increased to 0.971 with the HW+bootstrap model as a result of the addition of the bootstrapped residuals. Similarly, the RMSE value was reduced from 0.107 °C to 0.081 °C.

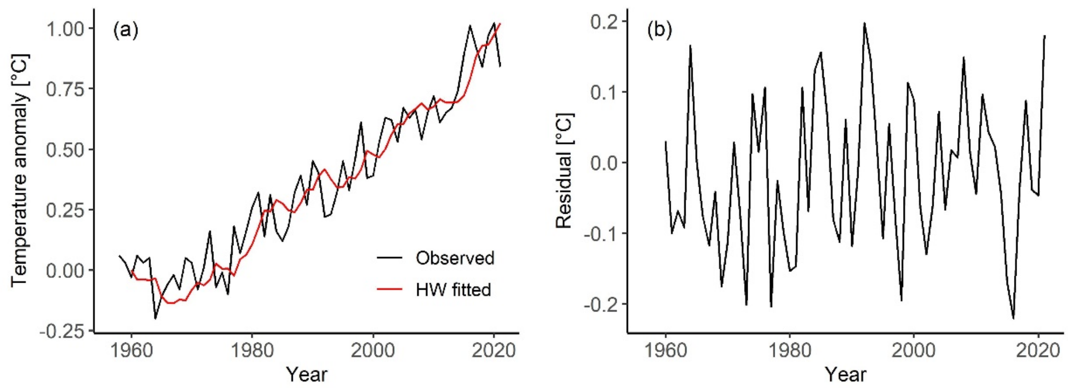


Figure 3. Fits of the seasonal-component-free Holt-Winters method (HW) to the annual mean land-ocean temperature anomalies. (a) shows the fitted anomalies and the observations; (b) shows the residuals.

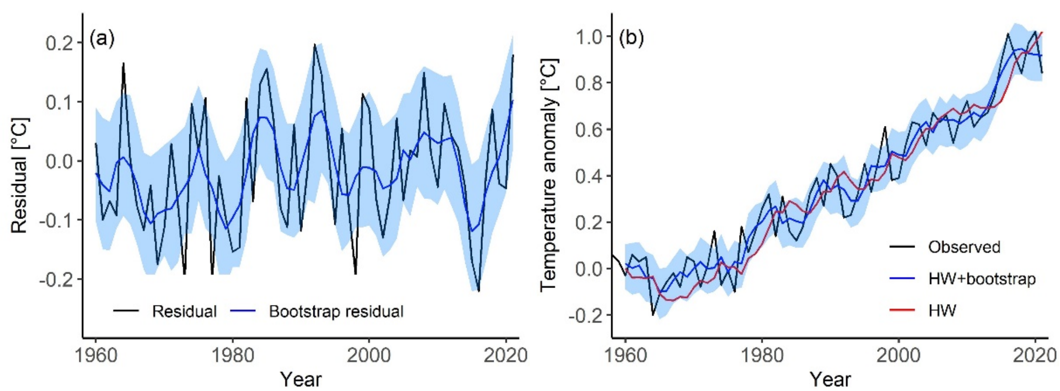


Figure 4. Fitted temperature anomalies by a seasonal-component-free Holt-Winters method (HW) with bootstrapped residuals (HW+bootstrap). (a) Residuals computed by removing HW fits from the observations and the residuals reproduced by the bootstrap approach. The solid blue line represents the mean value of 100 times bootstrapped residuals, while the blue shade represents 10% to 90% quantiles of them. (b) Observed temperature anomalies and forecasts by HW and HW+bootstrap.

The HW-bootstrap model was used to project future changes of land-ocean temperature anomalies. The results are shown in Figure 5. According to our model, land-ocean temperature is projected to increase at a rate of about 0.24°C/decade in the future. The average land-ocean temperature will change by 1.25°C in 2032, 1.5°C in 2042, and 2°C in 2063 compared to the base period of 1951-1980. If we take into account the uncertainties arising from bootstrapping, an increase in average land-ocean temperature of 1.25, 1.50, and 2°C will occur successively in the intervals: [2027, 2037], [2038, 2047], and [2058, 2067], respectively.

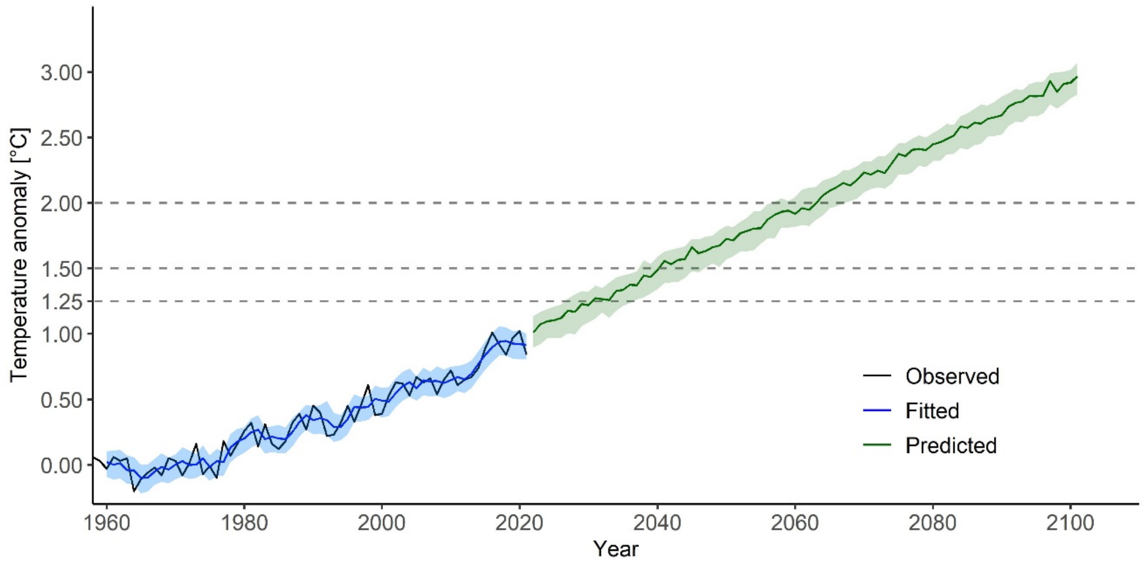


Figure 5. Simulations of the proposed HW-bootstrap model for 1958 to 2100. Both observed land-ocean temperature anomalies (labelled as Observed) and the model estimates (labelled as Fitted) are shown for 1958-2021. Temperature anomalies for 2022-2100 were projected by HW-bootstrap (labelled as Predicted). Levels of 1.25, 1.50 and 2.00°C are marked.

5.4 Relationships between CO2 concentration and land-ocean temperature

The fit of annual land-ocean temperature anomalies and CO2 concentrations yielded the equation:

$$\Delta T_{trend} = -21.835 + 3.776\, ln(cc) \quad (20)$$

where ΔT_{trend} denotes the increased temperature anomaly, and cc denotes CO2 concentration. The R-square is 0.922 and the p-value < 0.001. If we eliminate the constant terms in Equation 20 by adding a divisor in the logarithm, the equation is transformed to:

$$\Delta T_{trend} = 3.776\, ln\left(\frac{cc}{324.594}\right) \quad (21)$$

where the value 324.594 can be considered as a reference concentration level. Equation 21 implies a proportional relationship between increased temperature and CO2 concentration that has physical basis.

The fit shown in Figure 6 indicates the logarithm model can well interpret the increasing trend in temperature anomaly time series. However, the fluctuations over time were missed, so an ARIMA model was used to reproduce the fluctuations. We first stationarized the fluctuation time series by first differencing (Figure 7a). Then, we determined an ARIMA(6, 1, 0) model because the PACF (Figure 7b) generally cuts off after six while the ACF (Figure 7b) varies sinusoidally. After running the ARIMA model, the autocorrelation values are all within the confidence interval, indicating white noise, while the *p*-value is greater than 0.1, which means that the null hypothesis is rejected, and we could regard this residual series as white noise. Figure 8a shows the fluctuations estimated by the ARIMA model compared to the observed fluctuations calculated by subtracting the trend component from the observed temperature anomalies, demonstrating acceptable skill of the model. Figure 8b exhibits the final results of combining ARIMA-simulated fluctuations with the trend component predicted by CO2 concentrations. Comparison of the simulation of the Trend-ARIMA model with the observed tempearutre anomalies show good agreement between them, with an R value of 0.965, which is slightly better than the value (r = 0.960) measured between the observations and the separate trend component. Adding the ARIMA-estimated fluctuations to the trend component also resulted in a reduction of RMSE from 0.090 to 0.085.

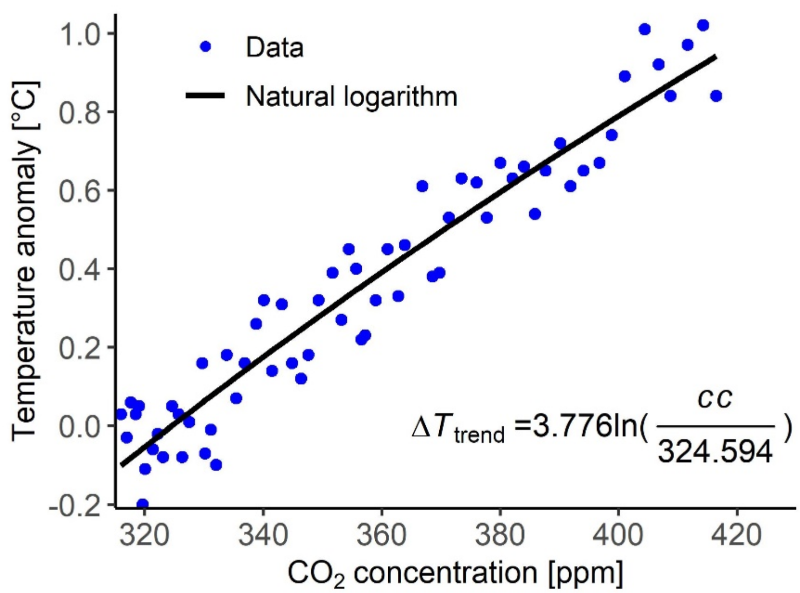


Figure 6. A proportional relationship between annual land-ocean temperature anomalies and log-transformed CO2 concentrations.

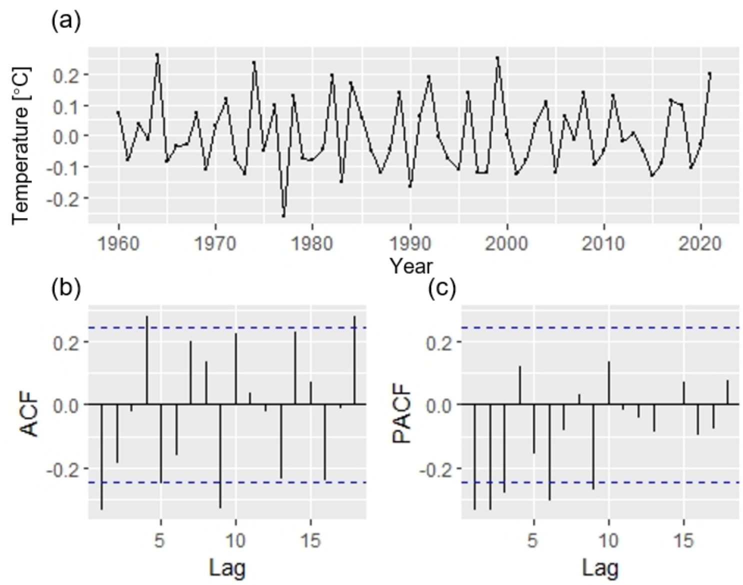


Figure 7. First-differenced fluctuations in annual temperature anomalies after subtracting the long-term trend from the time series. (a) First-differenced fluctuations; (b) Autocorrelation Function (ACF) plot; and (c) Partial Autocorrelation Function (PACF).

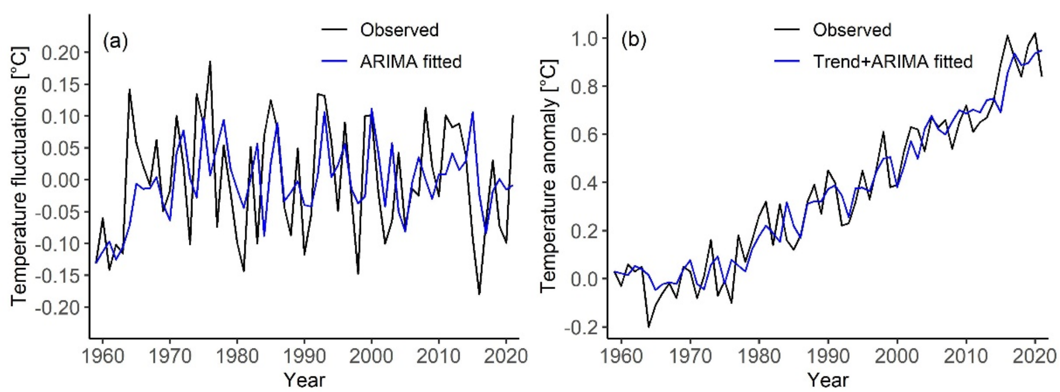


Figure 8. Fluctuations estimated by an ARIMA model (a) and the estimates of temperature anomalies from the linear regression and ARIMA errors model (b). The observed fluctuations in (a) were computed by subtracting the linear trend component as a function of log-transformed CO2 concentrations from the historical temperature anomalies. The observed time series in (b) represents the historical land-ocean temperature anomalies. The Trend+ARIMA fitted anomaly time series is the result of adding ARIMA-estimated fluctuations to the trend component predicted by CO2 concentration.

5.5 Robustness of the temperature forecasting models

Until now, we have created a univariate model of HW+Bootstrap and a bivariate model of Trend+ARIMA, both having the capability of projecting future changes in temperature anomalies. Trend+ARIMA model relies on the changes of CO2 concentration to estimate future trend of temperature anomalies (Equation 21). We obtained future changes of CO2 concentration through the best-performed quadratic model (Equation 18). By the

Trend+ARIMA model, global land-ocean temperature anomalies are projected to continuously rise in the future and reach 2.5 °C at the end of this century (Figure 9). However, compared to the HW+Bootstrap projection (Figure 5), the fluctuations estimated by ARIMA fade away as time advances and only trend component remains. This is one of the known weaknesses of ARIMA, which performs poorly for long term forecasts. Moreover, Trend+ARIMA shows much broacher uncertainty bands than HW+Bootstrap.

Based on different scenarios configured with different training datasets and test sets created from historical data, we could investigate the performance of HW+Bootstrap and Trend+ARIMA models (Table 4) in forecasting. Taking data from 1959 to 1979 as the training set, the two models achieved close performances no matter what the testing set is. However, to our surprise, both two models performed better when predicting the temperature anomalies in the distant period of 2001~2021 (S3 and S4) than that in the near period of 1980-2000 (S1 and S2). Therefore, we can hardly infer whether the performance of these models will degrade when the forecast period goes on, based on our limited evidence.

The influence of the training set seems to override that of the departure of the testing period. When taking data from 1980 to 2000 as the training set, though HW+Bootstrap achieved a higher r value than Trend+ARIMA, its RMSE value is much larger (S5), while Trend+ARIMA achieved close performance regardless of scenarios (S2, S4, S6). It can be partially interpreted that while HW+Bootstrap depends solely on its own history, Trend+ARIMA is governed by an exogenous variable of CO2 concentration that can be reliably estimated. As a result, Trend+ARIMA shows a more robust performance under any train-test scenarios.

Annual temperature anomalies from 2022 to 2100 projected by the two models are shown in Figure 10. The contrast shows that the two trajectories evolve generally at a same rate, while the Trend+ARIMA trajectory is 0.1-0.2 °C lower than HW+Bootstrap and has less fluctuations due to the poor performance of ARIMA for long-term forecasts. Both models tend to perform better forecasts in the first 10-20 years than the period after.

It is difficult and irresponsible to determine how long into the future our models will lose its reliability, given the very limited information available and lack of comprehensive model validations. Though both models project a similar increasing trend in temperature, the fluctuations are often underrepresented. Trend+ARIMA uses CO2 concentration as an input, but CO2 concentration alone is far from sufficient to reproduce all details of the future time series of temperature anomaly. The fluctuations, which appear to be random and without apparent periodicity, are in fact controlled by many intervening factors and complex interactions within the climate system.

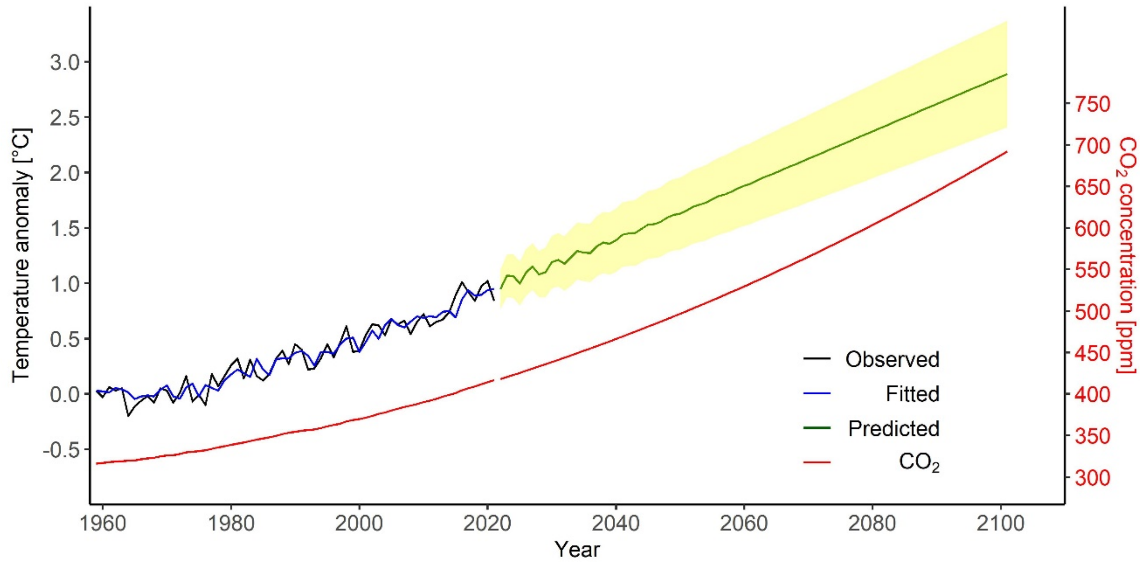


Figure 9. Simulations of annual land-ocean temperature anomalies in 1958 to 2100 by the Trend+ARIMA model with CO2 concentrations as input. CO2 concentrations in 1959-2021 are observed data while after 2021 they were predicted by the quadratic model (Equation 18). For temperature anomalies in 1959-2021, both observed data (labelled as observed) and the estimates by the Trend+ARIMA model (labelled as fitted) are shown. Temperature anomaly time series after 2021 was predicted by the Trend+ARIMA model while the future trend was calculated based on future projections of CO2 concentrations.

Table 4. Skill scores of two forecasting models (HW+Bootstrap univariate model and Trend+ARIMA bivariate model) under different train-test scenarios created from historical data.

# of scenario	Training set	Testing set	Approach	R [°C]	RMSE [°C]
S1	1959-1979	1980-2000	HW+Bootstrap	0.639	0.096
S2	1959-1979	1980-2000	Trend+ARIMA	0.633	0.097
S3	1959-1979	2001-2021	HW+Bootstrap	0.834	0.093
S4	1959-1979	2001-2021	Trend+ARIMA	0.848	0.082
S5	1980-2000	2001-2021	HW+Bootstrap	0.835	0.234
S6	1980-2000	2001-2021	Trend+ARIMA	0.793	0.097

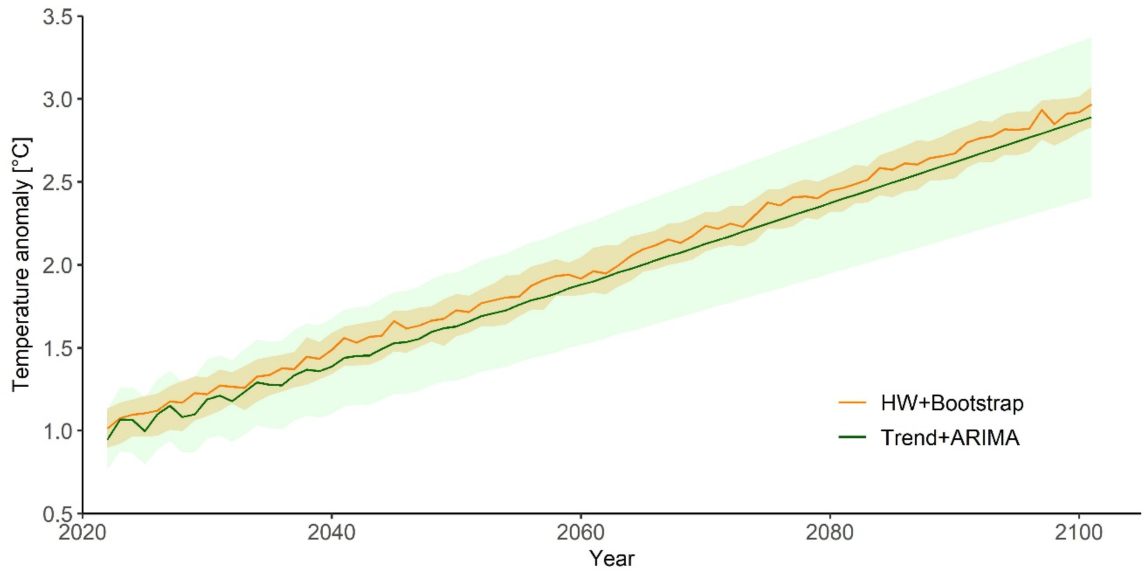


Figure 10. Projected annual temperature anomalies for the future period 2022 to 2100 by the HW+Bootstrap univariate model and the Trend+ARIMA bivariate model.

6 Strengths and Limitations

6.1 Strengths

We innovatively propose a univariate forecasting model (HW+bootstrap) combining the seasonal-component-free Holt-Winters model and bootstrap-aggregated residuals for forecasting annual land-ocean temperature variability. The results show that the model has high forecasting power that well preserves the trend of variability, prevents overfitting, and quantifies simulation uncertainties.

We show multiple ways to assess the reliability of the models based on a very limited length of data. We evaluated the models for CO2 changes using n-fold cross validation for time series. We ran multiple scenarios based on historical data to evaluate two models for temperature prediction, which we believe is one of the innovative points in this work. We also compared the performance of both models in simulating future time periods to determine the robustness of the models in extending into the future.

In this work, we follow rigorous modeling procedures, in which the studied data were first examined for stationarity, autocorrelation and seasonality, etc., before model building. This prevents the models from avoiding the model assumptions and ensures that the models have an excellent fit and safe future forecasting ability.

6.2 Limitations

All three models created in this work are based on historical data. They may not correctly predict the occurrence of turning points in the future. This is also a common problem of all the empirical/statistic models. Due to the nature of empirical/statistic models, our model can only simulate a business-as-usual CO2 emission scenario. For forecasts under other CO2 emission scenarios, physical models should be resorted to.

The data sets used in this work are not long enough, which may result in insufficient coverage of the patterns of the variables of interest. For example, some previous materials indicated the presence of periodicity in a long temperature data set that was more than a century long, but such periodicity was not tested in our data for the 1959-2021. This shows that consistent data sets are particularly crucial for making consistent forecasts from statistical models.

As noted in this work, our models are good at capturing the trend of change in temperature anomaly with a single CO2 input, not the detailed annual variations. Despite the better performance of HW+Bootstrap in predicting future changes with a narrower uncertainty band, its ability to reproduce annual fluctuations weakens over time. Moreover, HW+Bootstrap is likely to underestimate the uncertainty, especially in forecasts for the distant future.

7 Conclusions

In this work, we built three models based on historical data of CO2 and land-ocean temperature anomalies to describe past and future CO2 and temperature changes and to investigate the relationship between them. CO2 concentrations have increased steadily over the past six decades. Linear, quadratic, and exponential forms of mathematical models can well represent the overall trend of CO2 changes. 10-fold cross validation for time series showed that the quadratic model had the highest predictive accuracy. It is predicted that CO2 concentration will reach 685 ppm by the end of 21st century.

There is also a clear upward trend in the annual land-ocean temperature anomalies with evident fluctuations. The HW method can capture the increasing trend and levels in the time series, while a bootstrap approach can estimate the residual. Therefore, the combined HW+bootstrap model could provide a projection of future changes of temperature anomaly where the temperature will increase by 2°C and 3°C in around 2060 and 2100, respectively.

A logarithmic relationship between the increased temperature and CO2 concentration was found and can be used to account for long-term trends of changes in temperature. While the fluctuated signal in the temperature time series can be fitted and predicted by the ARIMA model, we thus created a linear regression model and ARIMA errors to investigate the relationship between CO2 and temperature. We assessed the model reliability through multiple ways. The Trend+ARIMA model shows a more robust performance under any scenarios than the HW+bootstrap model. Though both models project a similar increasing trend in temperature, the fluctuations are often underrepresented. While increased CO2 has been shown to be a major contributor to rising temperature, fluctuations in temperature are related to many intervening factors and complex interactions within the climate system and hard to be reproduced by both models in long term.

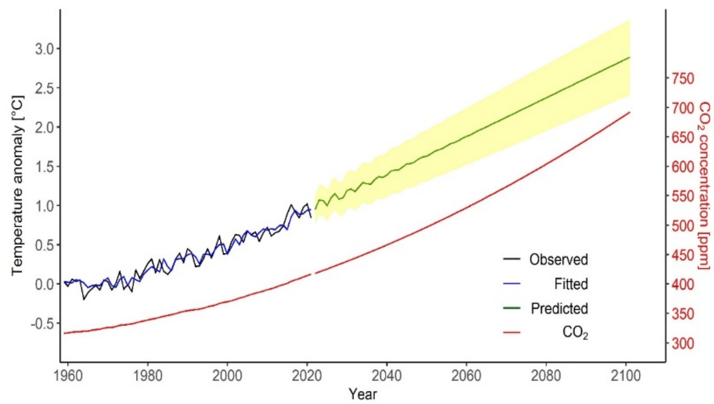
All questions concerned are answered in this work, and we highlight the development of the HW+bootstrap model for forecasting temperature variability and creation of scenarios based on historical data to evaluate model performance.

8 One-Page Non-Technical Article for Scientific Today

Act! Drastic temperature rise in response to massive carbon dioxide emissions

Carbon dioxide concentrations have increased dramatically over the past 60 years, with the trend accelerating. Currently, carbon dioxide concentration has increased by 30% compared to 60 years ago. If this trend continues in the future, the carbon dioxide concentration will be twice as high at the end of this century as it was 60 years ago.

Global temperature has also shown a clear upward trend over the past six decades, albeit with some fluctuations. If we do nothing, our modeling results indicate that global temperature will rise by 2°C in the middle of this century and by 3°C at the end of this century, compared to the baseline of the 1950s to the 1980s. This may lead to numerous environmental disasters in most regions of the world.



We have found that there is close relationship between increased carbon dioxide concentration and temperature. The increasing carbon dioxide concentration may be one of the main contributors to the temperature rising.

Global warming is one of the biggest threats of the 21st century. It is high time that we do something to stop climate change. First and easiest, we should raise our voices, talk to our friends and family to inform them of the risks of global warming, and get our representatives to make good decisions for our future. In addition, we could use renewable energy in our daily lives, reduce the waste of water and food since pumping, heating, and treating these stuffs consumes a lot of energy, drive a fuel-efficient vehicle to reduce carbon emissions while saving fuel, and so on. We should also protect forests, plant more trees and limit CO2 emission from factories. All in all, we must be aware of the urgent mission to cut down the carbon footprint. Governments of all countries should work together to solve the problem of global climate change. Last but not least, humans, animals and plants react to the global temperature rise —scientific studies matter! Scientific studies document these responses. In this way, science provides a basis for understanding how climate change affects our lives and what we can do to slow or reverse the changes.

9 References

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