Team Control Number 12833

Problem Chosen

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2022 HiMCM/MidMCM Summary Sheet

Quantitatively Modelling CO₂ and Global Warming

Atmospheric carbon dioxide levels, in parts per million (ppm), have been increasing consistently over several decades of observation. This has had considerable implications for the global climate, leading to increases in land-ocean temperatures over time. The purpose of this report is to examine trends in carbon dioxide concentration and land-ocean temperatures over a period of time, and further to explore the relationship between carbon dioxide concentration and land-ocean temperatures. Furthermore, these relationships are discussed and analyzed in the context of current claims and projections.

To assess the change in carbon dioxide concentration as a time series, we adopted a variety of regression models, with the intention of identifying the most accurate one. Linear regression was first used, however the residual graph shape was curved, so it was found that the next model, exponential, better fit to the data. Although this yielded an acceptable predictive model for the historical data available, it failed to account for the existence of natural limiting factors for growth. For this reason, we implemented a sigmoid regression that closely matched the exponential function up to a defined upper limit. We then employed the Facebook-developed Prophet model to further assess the reliability of this regression through comparative evaluation. This yielded a more advanced, multi-part analysis that better reflected the nuances of the CO₂ system; we obtained a more representative piecewise function that accounted for exponential growth, while maintaining predictions based on the most recent linear trend. Additionally, an attempted alternative prediction model was ARIMA (Auto Regressive Integrated Moving Average), which was rejected as the data set was unsuitable for the model's requirements. The data's unsuitability was demonstrated through ACF and PACF graphs, as well as an ADF test, which determines the stationarity of the dataset and the order of differencing required. Following correlation analysis, we determined that the Prophet, exponential and sigmoid models resulted in the most reliable future projections and corroborated each other's predictions for existing data within reasonable bounds of error.

Furthermore, we calculated the Pearson's Correlation Coefficient for temperature against CO2 concentration, which yielded an R^2 value of approximately 0.924. This suggested a strong linear correlation that matched the distinctive positive trend of the available data. Similarly, a linear regression of temperature against time resulted in an R^2 value of 0.898, indicating a reasonably accurate linear model. An analysis of error metrics revealed that although both relationships could be modelled linearly, the temperature- CO_2 relationship was the more strongly and verifiably linear of the two. Finally, we undertook factor analysis to examine the influences of carbon sources and sinks on future CO_2 levels, further comparing our predictions with existing literature values in order to evaluate the reliability of our models.

Keywords: Global Warming, Greenhouse Gases, CO_2 , Forecast, Predictions, Environment, Temperature

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CARBON DIOXIDE: TOO LATE TO STOP A SILENT KILLER?

A new report hints at problems with current assumptions and reveals we're headed down a dangerous path.

arbon dioxide: an invisible, odorless gas, and perhaps the greatest threat mankind has ever faced. In recent years, a rapid increase in carbon emissions has led many scientists to predict catastrophic climate change within our lifetimes. But this change is by no means inevitable. Understanding current predictions is the first step to changing our relationship with the planet for the better.

Challenging current assumptions

Until recently, atmospheric carbon dioxide levels in March 2004, at 377.7 ppm, were considered to follow the largest decade-spanning increase recorded until then, at a startling 4.63% higher than the 1994 value.

However, a new report for Scientific Today indicates that this wasn't the case: in fact, it was a drop from the 1993-2003 increase (4.74%). This is little consolation; since then, the annual increase in carbon dioxide concentration (ppm), has only risen year-on-year at an alarming rate.

Fossil fuel consumption is the largest contributor to global CO₂ emissions.

Still, oil-based infrastructure continues to account for most of our energy use today.

According to the report, current projections for CO2 levels are also mistaken. Readings likely won't reach 685 ppm by 2050, as was previously thought. Conservative estimates suggest we won't reach this until about 2081 or even as late as 2095. We're starting to change things, but not nearly fast enough. It's important to consider, too, that this 685 ppm figure included multiple greenhouse gases - so it was an overestimate for CO2 levels to begin with. By the end of the century, CO2 levels are expected to reach a devastating 701 ppm. This means we're on track for rapid increases in the average global temperature: by 2058, it'll have risen by 1.5 degrees Celsius. By 2100, the world will be 2.2 degrees hotter.

The promises of the 1.5-degree target, long-forgotten, will haunt us all too soon. 2.2 degrees means irreversible species loss, an unpredictable and violent climate, and thousands of square kilometers lost under a rising sea. This must serve as a jarring reminder that our current systems are not endlessly sustainable. Far from it. We are in urgent need of change.

Understanding the data: sources and sinks

The carbon dioxide system is complex. Huge quantities of CO₂ constantly enter the atmosphere through sources like energy consumption and transportation, and are absorbed by sinks, including the oceans and forests. To change our CO₂ future, we need to address human sources and protect carbon sinks.

Finding a way forward

Most importantly, the report underlines the importance of recommendations for the future. At a micro-level, individuals and communities should minimize their carbon footprints. This calls for significant reductions in waste, whether that's through recycling efforts or more responsible consumption. Try, for example, to buy food that was sourced locally – not moved halfway around the world on a petroleum-guzzling cargo ship.

But carbon emissions have reached a scale where individual actions are no longer enough. First and foremost, the issue needs to be addressed through policy changes. We need to reduce our reliance on coal, oil, and gas, gradually replacing them with a combination of renewable resources. Transportation infrastructure must also shift, in favor of clean electric vehicles. As fires ravage the Amazon, protecting our rainforests has never been more important. And marine pollution, which reduces the oceans' effectiveness as a CO2 sink, must be addressed. This calls for nothing short of a global collaborative effort one that stretches across countries, continents, and beyond simple greed and economic progress. The idea is a daunting one; nothing of this scale has ever been done before. But unless we can manage it, the threat of human extinction looms large. The data foretells a difficult century ahead. We have the means to counter this change, to alter our ways of life. What will we do with them? ■

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2 Introduction

2.1 Background

The most significant greenhouse gas on Earth is carbon dioxide, which both absorbs and radiates heat. In contrast to oxygen and nitrogen, which together make up the majority of our atmosphere, greenhouse gases absorb heat emitted from the Earth's surface and re-emit it in all directions, including back toward the planet's surface. The natural greenhouse effect that keeps the Earth's atmosphere above freezing would be insufficient without carbon dioxide. People are accelerating the natural greenhouse effect and raising the earth's temperature by releasing more carbon dioxide into the atmosphere. The NOAA Global Monitoring Lab found that in 2021, carbon dioxide accounted for nearly two thirds of the total heating influence of all greenhouse gases created by humans.

Prior to the Industrial Revolution, carbon dioxide in the atmosphere was consistently around 280 parts per million (ppm). The concentration of CO_2 in the atmosphere reached 377.7 ppm in March 2004, resulting in the largest 10-year average increase up to that time. According to scientists from National Oceanographic and Atmospheric Administration (NOAA) and Scripps Institution of Oceanography (SIO) the monthly mean CO_2 concentration level peaked at 421 ppm in May 2022. An Organisation for Economic Co-Operations and Development (OECD) report predicts a CO_2 level of 685 ppm by 2050.

2.2 Problem Analysis

Problem 1: CO₂ level Forecasting

Modelling.

Prodice models that reflect existing CO_2 data and extrapolates to reasonable predictions.

Choose suitable mathematical models and fit each one to existing data.

Evaluate each model... Use different evaluation approaches including statistical accuracy, contextual reasoning, comparison with external predictions, etc.

Generate a conclusive model based on results obtained... Either pick the "best" model, or create new model based on multiple sub-parts.

Verify External Claims.

Whether CO_2 levels in 2004 had a "larger increase than observed over any previous 10-year period".

Determine how exactly the comparison is done with "any previous 10-year period"... Find supporting evidence from existing literature or make the best interpretation.

Whether CO₂ levels will reach 685ppm by 2050.

Testify this statement against all models.

Draw Conclusions.

Real-world implications based on predictions and results.

Problem 2: Temperature vs CO₂

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Modelling.

Produce models that reflect existing temperature data and extrapolates to reasonable predictions.

Direct relationship between CO₂ and temperature.

Temperature as a time series, and compare with CO_2 models from Problem 1.

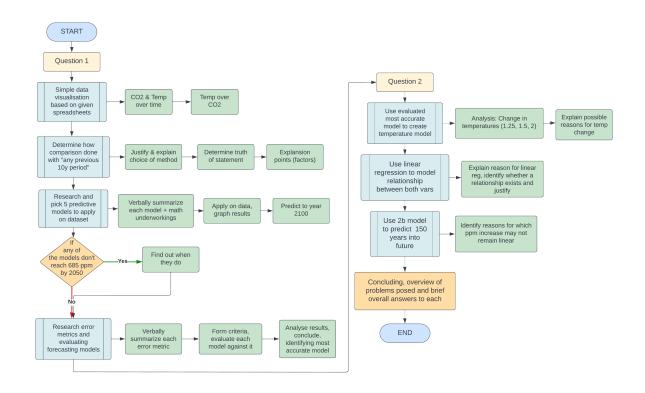
Predictions.

Predict points in time where global temperature will have an average increase of 1.25°C, 1.5°C, and 2°C compared to the base period of 1951–1980.

Evaluation.

Longevity & Confidence; discuss the distance into the future that the model can still predict with reasonable accuracy.

Our thought process and plan is presented here below as a flowchart:



2.3 Keyword Definitions

 CO_2 Level/Content: Global average concentration of CO_2 in the atmosphere, in parts-permillion (ppm).

Relative Temperature: Global average temperature, relative to the baseline average temperature from 1951 to 1980, in degrees Celsius.

Error and Relationship Metric Abbreviations: See Table 2.1.

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Abb.	Full Name
MSE	Mean Squared-Error
RMSE	Square Root of MSE
MAE	Mean Absolute Error
PCC	Pearson's Correlation Coefficient
R^2	Coefficient of Determination, or PCC Squared
CVAR	Covariance

Table 2.1: Abbreviations of Important Metrics

2.4 Assumptions and Justifications

Assumption 1: CO_2 , as a greenhouse gas, has a true case-and-effect relationship with temperature.

Justification: Most existing literature and evidence suggest that CO_2 is a greenhouse gas, and that greenhouse gases traps heat and leads to increases in temperature on a global scale. This fact is taken for granted to make more confident predictions that relate temperature to CO_2 levels.

Assumption 2: Both datasets provided for CO₂ emissions and temperatures are reliable and accurate.

Justification: Accurate predictions are always based on accurate data. Since official data is given along the problem, they will be taken and treated assuming the absence of mistakes and errors.

2.5 General Variables

See table 2.2:

Variable	Definition
$\overline{C_i}$	CO_2 level at year i , in ppm
T_i	Temperature at year i , in °C
$C_i^{-1} \\ T_i^{-1}$	Year where (predicted) CO_2 is at i ppm
T_i^{-1}	Year where (predicted) Temperature is at i °C

Table 2.2: General Variables

3 The Generic Modelling Procedure

In this section, the generic procedure to produce specific models for a given task is stated and explained. All relevant information; such as metrics, concepts, and terms; are explained and directly referred to later. This section helps avoid bloat in the paper by isolating generic baseline information to prevent repetition and confusion.

Modelling, Conceptually

"A mathematical model is a description of a *system* using mathematical concepts and language." (wikipedia reference) A completed math model should describe/simulate it's target system to the best of its ability. All models behave like a (complex) function (3.1) - it produces

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outputs when given inputs. For this problem, the *systems* to be modelled are atmospheric CO_2 and global warming. y = f(x) (3.1) where y is the output, x is the input, and f is the model itself.

Time Series

Inputs and outputs differ depending on the type of the model, but one type relevant to this paper is are time-series'. In a time-series model, the input is a timeframe, and the output describes the state of a system it is modelling; conceptually, a time-series models the evolution of a possibly boundless dynamic system over time (3.2). This will be useful later to, for example, model the change of CO_2 levels over time. Time-series' belong to the family of relationship models, which produces outputs based on an input variable, effectively translation values between two variables. This will be useful later to model the relationship between CO_2 levels and temperature change. $t \rightarrow y$

$$\begin{array}{c}
t \to y \\
\Delta t \to \Delta y + y_0
\end{array} \tag{3.2}$$

where y is the output, t is the time or input, and y_0 is the initial state (when modelling relative evolution over time).

Quantitative Data

Because math models are strictly quantitative, a pre-defined procedure must exist to translate between real-world parameters and numeric values. For most systems, this can be done using existing scientific measurements and units. Otherwise, custom metrics have to be defined. With the given problem, there are simple metrics for both CO_2 levels in the atmosphere and global warming, concentration in parts-per-million and temperature in degrees Celsius, respectively. In terms of time, years are already represented numerically.

Once the system can be represented quantitatively and a quantitative output can be interpreted as a state of the system, a math model can be constructed. There are many different approaches to construct a model from numerical representations of a system, but this paper focuses on "fitting" "generic models" to true/historical numeric data.

Function Regression

In short, a "generic model" is a mathematical function parameterized by a variable amount of constants within its definition (3.3). The function exhibits specific characteristics regardless of the values of its parameters. The end goal of modelling is to adjust these parameters such that the function can produce the most accurate output (compared to the real system) for each given input. In the case of modelling CO_2 levels as a time-series, the model function should produce ppm values for a given year.

$$\beta = [p_1, p_2, p_3, p_4, \dots]$$

$$f(x) = g(x, \beta)$$

$$y = f(x)$$
(3.3)

where g is the generic model, and f is a constructed model by finding specific values for each of the parameters p_i . β is simply a vector that encapsulates all of the parameters.

Error Metrics

"Fitting" a model, also known as "optimization", is a systematic approach to find parameters that "best" models the given system. Usually, an error function is defined to quantitatively

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gauge how accurate or good the model is by calculating a metric based on the difference between the actual output and expected output for a given input (3.4). The optimization process tries to produce the "best" model by minimizing the error function across all available data values. For example, (3.5) is a square-error function that gives the sum of square-error for all data points. $E(y) \approx y - \hat{y} \tag{3.4}$

$$E_{sum} = \sum_{i=1}^{n} (f(x_i) - \hat{y}_i)^2$$
 (3.5)

Optimization

The optimization process aims to minimize the (sum of the) error function. A generic approach is to take partial derivatives of the summed error with respect to every parameter in the model. This allows the minimum to be calculated by equating the differential functions to 0. Generally, the partial derivative of error E with respect to parameter β_i is:

$$\frac{\partial E}{\partial \beta_{j}} = 2 \sum_{i} e_{i} \frac{\partial e_{i}}{\partial \beta_{j}}$$

$$\frac{\partial E}{\partial \beta_{j}} = -2 \sum_{i} e_{i} \frac{\partial f(x_{i}, \beta)}{\partial \beta_{j}}$$
(3.6)

where e is the error, and j = 1, ..., m for m parameters in β .

4 CO₂ - Modelling

This section includes a walk through of all mathematical models used to model the CO_2 levels as a time series and how they specifically apply to the given data.

4.1 Pre-Analysis

Firstly, this problem takes the form of a single-variable time series; CO_2 levels evolve as time passes, and we are trying to model the relationship between time and CO_2 . Based on simple logic and scientific reasoning, there is no cause-and-effect relationship between time and carbon dioxide levels, so the models will assume a relationship that is purely a statistical correlation.

The given CO_2 data is graphed to visualize the rough correlation and trend present in the data (Figure 4.1). It is very apparent that there is a strong correlation with minimal variance between time and carbon dioxide levels. The shape of the curve seems exponential. These ideas will be help guide future mathematical modelling. Auto-correlation is calculated to identify any seasonality within the data (Figure 4.2). However, it is apparent that there is no clear seasonality within the data, as shown by the lack of an oscillating correlation. This is expected since the data comes in annual resolutions; yearly seasonality could be expected due to seasonal effects, but would only be observed with monthly data.

4.2 Linear

A linear regression is performed first due to its simplicity and ability to help pick more complex models.

Linear regression is an approach used to model a linear relationship between an independent variable x and a dependent variable y by finding the slope of the trend and initial value (y when x is 0). It is used to represent existing data and predict future values; linear models are

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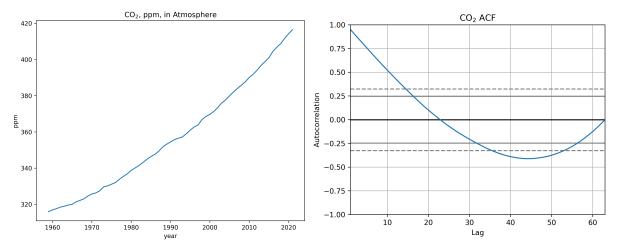


Figure 4.1: Graph of given CO₂ data

Figure 4.2: CO₂ Auto-correlation

used both for interpolation and extrapolation. In this case, the model will be fit to existing data and used to predict future CO_2 levels. A linear growth function takes the general form of (4.1): $f(x) = \alpha x + \beta$ (4.1)

where α is the coefficient, or growth rate; and β is the y-intercept, or initial value. The values of α and β are "optimized" using an algorithm to model a given dataset with the minimum "error".

One of the most common and simplest methods used to calculate the coefficient and intercept of the regression line is the Ordinary Least Square (OLS) optimization method. In short, OLS minimizes the Square-Error for each point against a given linear function by adjusting the function's parameters, which in the end produces optimal parameters for a equation in the form of a linear line of best fit.

The Square-*Error* function, which is what OLS *optimizes*, is simply a summation of the squares of the difference between actual values and predicted values, over all data points (4.2):

$$E = \sum (y - \hat{y})^2 \tag{4.2}$$

Because the predicted values \hat{y} for a linear model is modelled as $\alpha x + \beta$, the Square-Error function for a linear model can be more specific (4.3):

$$E = \sum (y - (\alpha x + \beta))^2 \tag{4.3}$$

OLS calculates the values of α and β which minimize S in the summation above. Unlike the generic differential method described above, OLS is specialized for linear functions and can calculate the optimal parameters in one stop, using summation ratios. The coefficient α , or the linear trend of the dataset can be calculated with (4.4):

$$\alpha = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - (\sum x_i)^2}$$
(4.4)

where n is the number of data points.

After calculating the slope of the trend, the intercept β , is calculated by (4.5):

$$\beta = \bar{y} - \alpha \bar{x} \tag{4.5}$$

OLS was applied to the given data set to obtain the coefficient α and the y-intercept β

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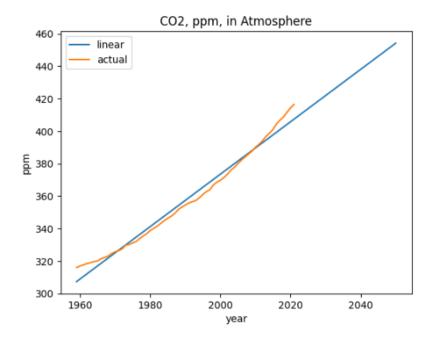
- 1.6140361 and -2854.59326421, respectively - which corresponds to the following linear equation: $\hat{C}_i = 1.6140361i - 2854.59326421 \tag{4.6}$ where i is the year.

The inverse of the function is derived by solving for i in terms of C:

$$\hat{C}_i^{-1} = \frac{C + 2854.59326421}{1.6140361} \tag{4.7}$$

C was then set to 685 to find the year at which CO_2 emissions would reach 685ppm; it was found that it would reach this level at the year 2193. The regression line was then graphed and used to predict the next 30 years of CO_2 emissions; the actual data is also plotted for comparison (Figure 4.3).

Linear regression is useful in relation to the problem as it is simple to interpret and portray, allowing the prediction of data to be accurate during interpolation. However, if the data to be predicted is outside of the range, such as predicting future CO_2 levels, extrapolation may be inaccurate due to a false assumption of the trend. Furthermore, if the variables plotted provide a non-linear relationship, a linear regression line may inaccurately represent and predict values, which is the case in the data provided. Statistical error of the linear regression model against existing data shows a good but not perfect accuracy (Table 4.1).



Metric	Value		
MSE	15.376		
RMSE	3.9212		
MAE	3.1920		
PCC	0.9912		
R^2	0.9825		
CVAR	875.32		

Table 4.1: Linear Model Statistics

Figure 4.3: Graph of given CO₂ data

4.3 Exponential

The second approach decided upon was exponential regression, which models the non-linear relationship between an independent variable x and dependent variable y, where the rate of change of y with respect to x at a given point is proportional to the quantity itself. This choice was made based on visual indicators of the data given's trend, where the line graph exhibited a possible exponential curve. Exponential growth functions take the general form of (4.8): $f(x) = \alpha^x \tag{4.8}$

where α is the exponential growth factor.

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However, in order to fit such a model to arbitrary (non-normalized) values, two additional parameters have to be added to allow for displacement translations of the function on both axis. This gives: $f(x) = \beta(\alpha)^{x+a} + b \tag{4.9}$

where a and b allows for offsets in the x and y axis, respectively.

An optimization can be made here - the equation can be rearranged to only have 3 parameters yet still be able to fit to any scale and offset of values:

$$f(x) = B^{b(x+a)} + c (4.10)$$

where B, the base, can be any positive constant, and the function is parameterized by a, b, and c.

a and b performs a linear transformation on the input, while c performs a translation on the output. The equation in this form expresses in the relationship in purely in terms of translations. This reduction in parameters allows for a higher efficiency when regressing the function to the dataset programmatically. In the actual regression, 2 was used for the value of B.

Unlike linear regression, trying to fit an exponential function to a data set would theoretically require complex methods such as partial derivatives. However, a programmatic approach was taken, and the function was "blindly" regressed using gradient descent (Alg. 1) from derivative estimates. The curve_fit() optimizer from the Python SciPy library can optimize any nonlinear function to a dataset blindly - without knowing the algebraic denotation of the function. It is able to optimize unknown functions by performing gradient estimates (4.11) of the error function with respect to the parameters using the basic definition of the derivative (at a given point, x): $\Delta f(x) = f(x + \Delta x) - f(x)$

point, x): $G = \frac{\Delta f(x)}{\Delta x} = \frac{f(x + \Delta x) - f(x)}{\Delta x}$ where G is the gradient of function f at point x. Δx is set to a very small value to increase accuracy for sensitive functions. (4.11)

After being able to calculate gradients of the error function at any point of the model function, a gradient descent algorithm (1) can be deployed to iteratively minimize the error function. The parameters are adjusted based the gradients of the error function:

$$\beta_j \longleftarrow \beta_j - \alpha \frac{E(x, \beta + \Delta \beta_j) - E(x, \beta)}{\Delta \beta_j}$$
 (4.12)

where parameter β_j is adjusted based the error function E's gradient - the parameter changes in to the opposite direction of the gradient in order to find the minimum of the error function. α , the learning rate, is usually a very small value to prevent the parameters from changing too much at once.

Algorithm 1 Gradient Descent

repeat $\begin{vmatrix} \epsilon \leftarrow E(f(x,\beta)) \\ \gamma \leftarrow \frac{\Delta E(f(x,\beta))}{\Delta \beta} \\ \beta \leftarrow \beta - \alpha \gamma \end{vmatrix}$

▷ E is the error function
 ▷ calculate current gradient
 ▷ α is the learning rate

until ϵ is sufficiently small

return β as the optimal parameters

The SciPy curve fit optimizer was applied to the given data to obtain the following model:

$$\hat{C}_i = 2^{0.023381(i-1707.690634)} + 256.024002 \tag{4.13}$$

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and i was solved for $\hat{C}_i = 685$ to find that CO_2 levels will reach 685ppm in 2081. The exponential model was graphed alongside the actual values and the linear model for comparison in Figure 4.4.

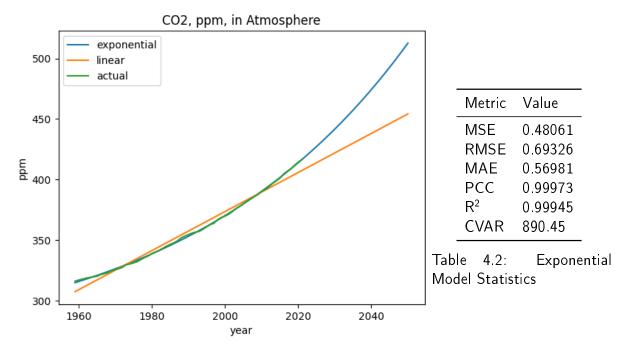


Figure 4.4: Graph of Exponential Regression

Visually, the exponential function better aligns with the actual values; the predicted values also seem to fit with the general trend, and this is confirmed by extremely good error metrics, as show in Table 4.2. An advantage of exponential regression as a predictive model is that it provides high quality forecasts, which increase the accuracy of predicted values during interpolation. However, a key drawback is that a large data set is necessary to carry this method out, as a reasonable amount of continuity is needed to accurately predict future values, especially during extrapolation.

4.4 Sigmoid

The third predictive model selected shares similarities with the exponential model. While most sigmoid functions, when the domain is restricted, may behave very similar to an exponential function, the difference is that sigmoid functions also have an upper asymptote. The function has a S-shaped curve, comparable to two exponential functions, one with a negative exponent and one with a positive exponent, that are joined at the point of inflection. Sigmoid functions are commonly used to model growth variables with a natrual limit. The most common sigmoid function is the logistic function, which takes the general form of:

$$f(x) = \frac{L}{1 + e^{-k(x - x_0)}} \tag{4.14}$$

where L is the curve's maximum value, k is the logistic growth rate, and x_0 is the x value of the sigmoid midpoint.

The standard logistic function is, however, pretty limited; the minimum asymptote is fixed at zero and the shape of the curve is fixed other than the growth rate, which reflects the gradient at the midpoint. In order to fit to the CO_2 dataset, a more generalized and

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adjustable sigmoid function is used:

$$f(x) = \frac{x - x_0}{\left(s^{-z} + \frac{2|x - x_0|}{y_{max} - y_{min}}^{z}\right)^{\frac{1}{z}}} + \frac{y_{max} - y_{min}}{2} + y_{min}$$
(4.15)

where x_0 is the x value of the sigmoid midpoint, s is the growth rate or slope at the midpoint, z governs the shape of the curve, y_{max} is the maximum y value, and y_{min} is the minimum y value.

Removing parameters that allow linear transformations, the sigmoid function can be simplified to: $f(x) = \frac{x}{\left(s^{-z} + \frac{|x|^z}{L}\right)^{\frac{1}{z}}}$ (4.16)

and by removing the z parameter, a basic algebraic sigmoid function remains:

$$f(x) = \frac{x}{s^{-1} + |x|/L} \tag{4.17}$$

where L is the curve's maximum value (also the negative minimum; the function is centered at the origin) and s is the growth rate or slope at the midpoint.

Because the entire idea of a sigmoid function is that there is an upper limit, this limit has to be set before the other parameters defining the curve can be regressed against the dataset. If the limit left to the freedom of the optimizer, the output usually results in completely unreasonable limits, due to the fact that the optimizer will naively try to minimize the error function by adjusting any parameters necessary. This is demonstrated in Figure 4.6, where the limit was automatically regressed to beyond 2700ppm. The logistic function used was inflated so much that the sigmoid curve could only be seen on half-millennium time scales.

To avoid this issue which causes sigmoid functions to regress into practically exponential functions in a short time frame, the limit set to values between 420 and 960ppm before the optimizer was applied. The range of sigmoid curves for different limits is shown in Figure 4.7. As explored later, external sources predict a maximum CO_2 level within the near future (2070) to be around 565ppm, which is used as the limit of the final sigmoid model:

$$\hat{C}_{i} = \frac{x - 2016.8}{\left(2.2796^{-1.4953} + \frac{2|x - 2016.8|}{565 - 246.49}\right)^{\frac{1}{1.4953}}} + \frac{565 - 246.49}{2} + 246.49 \tag{4.18}$$

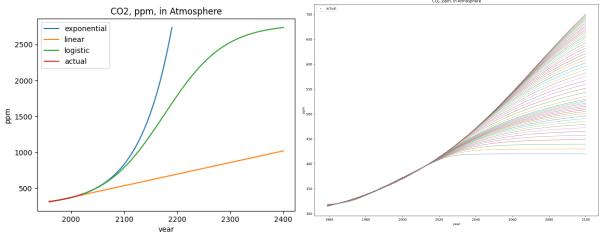


Figure 4.6: Blown up Logistic Regression

Figure 4.7: Sigmoid Functions with Different Limits

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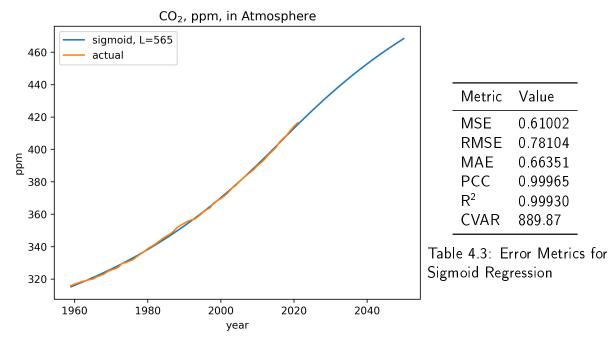


Figure 4.5: Graph of Sigmoid Regression

A limit at 565ppm obviously prevents the model from every reaching a 685ppm prediction. Therefore, a longer-term limit of 960ppm is used to predict the CO_2 level until 2100. This model predicts CO_2 levels to reach 685ppm in 2096. This is a reasonable limit because the predictions fall between the exponential and Prophet (explored below) models.

4.5 Prophet

Prophet is a an advanced time-series forecasting model developed by Facebook. Its selling points are the ability to produce multi-part models that fit complex trends as well as seasonality. Prophet is fast and generally maintains a high accuracy when predicting values. It can be used in a range of different contexts and it is robust to outliers, shifts in the overall trend and missing data. A Prophet model is similar to a Generalized Additive Model (reference):

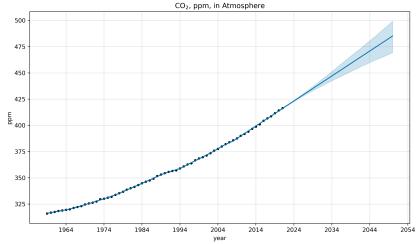
$$f(x) = g(x) + s(x) + h(x) + \epsilon \tag{4.19}$$

where g is the trend (made of piecewise linear or logistic functions), s captures seasonal patterns, h captures holiday (one-off) effects, and ϵ is the remaining noise-like error unaccounted for by the model.

The model follows a Bayesian approach, where the prior distribution is specified; the parameters are then tuned for the model to better fit the data set. The piecewise trend consists of change-points, which are automatically selected; an upper bound can be set with a logistic function. The seasonal patterns involve Fourier series, where the default orders for annual and weekly seasonality are set to 10 and 3 respectively. Holiday effects are extra parameters designed to take into account public holidays.

While Prophet is able to fit to existing data with near-perfect accuracy, its future predictions are a linear extension of the latest trend - a projection of approximately 2.4ppm increase per year. This is a reasonable prediction, but it does not reach 685ppm within the next century. Summary of the model is presented in Figure 4.8 and Table 4.4.

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Metric	Value
MSE	0.10309
RMSE	0.32108
MAE	0.25507
PCC	0.99994
R^2	0.99988
CVAR	890.82

Table 4.4: Error Metrics for Prophet

Figure 4.8: Graph of Prophet

4.6 ARIMA

An additional time-series prediction model that was investigated was ARIMA, which is based on ARMA (AutoRegressive Moving Average). These models are widely used in datasets that demonstrate non-stationarity, where the series'statistical properties such as mean, variance and autocorrelation change over time. ARMA assumes the input data to be stationary, so any non-stationary data has to be made stationary through a reversible process. Usually, the transformation involves finding the general trend with methods such as regression and then using differencing to remove the trend from the dataset. With the trend eliminated, an ARMA model can then be constructed and its optimal parameters found.

Another appropriate model to use in regards to the data set is ARIMA, which is an extension of ARMA. ARIMA models are generally denoted as ARIMA(p, d, q) where p is the number of Auto-Regressive (AR) terms, d is the orders of differencing, and q is the number of Moving Average (MA) terms.

The functions AR(p) and MA(q) are defined below as: AR(p):

AR(p):	MA(q):
$\phi(B)X_t = w_t$	$X_t = \theta(B)w_t$
Where	Where
$ullet$ $\phi(B)=$ Autoregressive operator	ullet $ heta(B)=$ Moving average operator
• $X_t = Inverse operator$	• $X_t = $ Inverse operator
• $w_t = White noise$	• $w_t = White noise$

Before tuning the parameters p and q, the number of differencing required to make the data stationary must be found out. To evaluate whether the current dataset is stationary, an Augmented Dickey-Fuller (ADF) test was performed.

ADF tests expand on the original Dickey-Fuller test by including higher-order autoregressive processes to form the equation:

$$\Delta y_t = \alpha + \beta t + \gamma y_{t-1} + \delta_1 \Delta y_{t-1} + \dots + \delta_{p-1} \Delta y_{t-p+1} + \varepsilon_t \tag{4.20}$$

where y_t is the value of the time series at time t, α is a constant, β is the coefficient of the trend, and p is the lag order of the autoregressive process.

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The results of the ADI	test applied	on the given	dataset is	presented below.
THE RESULTS OF THE ADI	test applied	OII LIIC EIVCII	uataset is	presented below.

ADF Test Statistic	5.506786113910213	Significance Level	Critical Value	
P-Value	1.0	1%	-3.5463945337644063	
No. of Lags Used	2	5%	-2.911939409384601	
No of Observations	59	10%	-2.5936515282964665	

The p-value obtained is greater than the significance level 0.05 and the ADF statistic is higher than any of the critical values, hence it can be concluded that the time series has a unit root and is non-stationary. The high p-value signifies that a high order of differencing will need to be used.

To further confirm the data's stationarity, autocorrelation and partial autocorrelation graphs were also used. AFC and PAFC functions are measures of correlation between past and present data, and indicate which past data values are most useful in predicting future ones. The results of these functions are then used to select the most optimal parameters for p and q. Both functions were applied on the given dataset and the graphed results displayed below:

For both graphs the x-axis represents lag, whereas the y-axis indicates the correlation strength. ACF graphs represent the correlation between data values that are n intervals apart. PACF graphs are similar in that they represent the same information, however they also account for the values of the intervals in between.

The correlation that can be seen in the ACF graph is negative, indicating that large current values correspond with small values at the specified lag. The absolute correlation values represent the strength of the relationship; to

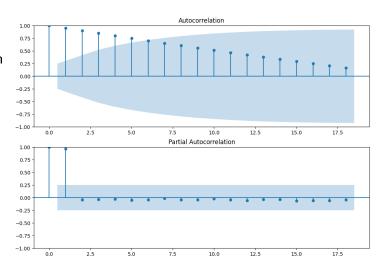


Figure 4.9: ACF and PACF of CO₂ data

construct an ARIMA model, the expected trend of these values should be random. In this case, the initial relationship between past and present values is strong, but gradually decreases over lags, indicating a clear trend of decreasing correlation strength.

If the autocorrelation follows a random non-linear trend, then AR(p) and MA(q) can be applied to the graphed functions to obtain the optimal parameter values for p and q. However, this is only assuming the data does not have a trend or seasonality component, which does not apply to the given dataset.

The autocorrelation trend as well as the high order of differencing required to transform the data to stationary (as seen in the ADF test) both demonstrate that the given dataset is unsuitable for constructing an ARIMA model, and therefore this prediction model has been rejected and will not be used as part of the predicted CO_2 and temperature values.

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5 CO₂ - Model Evaluation

5.1 Procedure

To rank the 4 accepted predictive models on their mathematical accuracy, the following error metrics are to be calculated for each model and then compared with each other:

Scale-dependent Errors	Forecast Errors
 MSE (Mean Squared Error) RMSE (Root Mean Squared Error) MAE (Mean Absolute Error) PCC (Pearson's Correlation Coefficient) R² (Coefficient of Determination) Covariance 	Seperation of known values into testing and training data

Separation of Known Values into Testing and Training data

75% of known data values are allocated to the testing data group, remaining 25% are allocated to the training group. The predictive model will take in the training group data values as its sole input, and will predict the remaining 25%. The model's predicted values are then to be compared with the training group's values and the forecast errors obtained. A forecast error is defined as the difference between an observed and its forecasted value; the formula for a single forecast error can be modified to suit multiple data values, and it is denoted by the following equation:

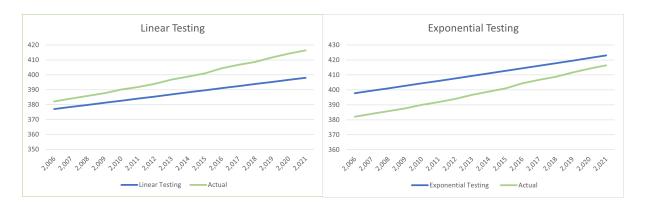
$$e_{T+h} = y_{T+h} - \hat{y}_{T+h|T} \tag{5.1}$$

where e_{T+h} is the forecast error, y_{T+h} is the actual value of the h-step observation, and $\hat{y}_{T+h|T}$ is the actual value of the h-step forecast.

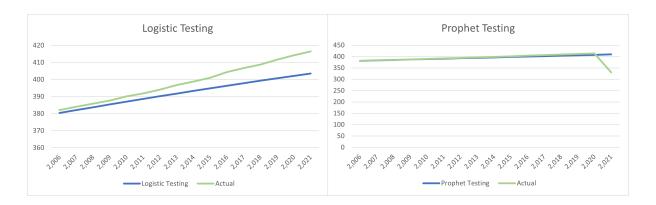
The equation was again modified to find the sum of all the forecast errors, this was then applied to each model to construct the table below:

	Linear	Exponential	Sigmoid	Prophet	
Forecast RMSE	11.660	0.37768	0.41312	3.5618	

It is important to note that although a model may fit the testing data well, it does not necessarily mean the model will forecast well, therefore it is important to take the other error metrics into consideration.



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5.2 Accuracy Analysis

MSE

Mean Squared Error (MSE) is a measure of the quality of a predictor or of an assessor, its definition differing accordingly. It is the average squared distance between the actual and predicted values, measuring the variance of the residuals. In this case, only the quality of the predictor is to be assessed. It involves taking the average squared distance between the actual and predicted values, measuring the variance of the residuals. The within-sample MSE of a predictor can then be denoted as:

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2$$
 (5.2)

where $\frac{1}{n}\sum_{i=1}^{n}$ calculates the mean (across all data points) and $\left(Y_{i}-\hat{Y}_{i}\right)^{2}$ is the squares of the difference between the actual and predicted values, or the error.

MSE also has a differentiable graph so it makes it easier to perform mathematical operations in comparison to MAE. MSE is more sensitive to outliers compared to MAE.

RMSE

Root Mean Squared Error (RMSE) is the square root of the MSE, measuring the standard deviation of the residuals. The higher the RMSE value, the larger the deviation between actual and predicted values. By proxy, the lower the RMSE value, the lower the deviation, hence the model is more accurate. Building on the MSE (5.2) formula, RMSE can be denoted as:

$$RMSE = \sqrt{MSE}$$
 (5.3)

When outliers are exponentially rare, such as this situation, RMSE is generally preferred over MSE as it provides a better evaluation of model performance, as it uses the same units as the Y axis (CO_2 emissions).

MAE

Mean Absolute Error (MAE) is the sum of the absolute difference between the actual and predicted values. A perfect prediction model would yield a 0 as its MAE value. The further away from 0 the MAE value is, the more errors the model makes and hence the less accurate the model is. The formula to calculate MAE is denoted as:

whate MAE is denoted as:
$$MAE = \frac{\sum_{i=1}^{n} |y_i - x_i|}{n}$$
(5.4)

where $\sum_{i=1}^{n} |y_i - x_i|$ is the sum of absolute error and n is the Number of data points.

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PCC, R², AND COVARIANCE

The last 3 error metrics are explained in further detail when exploring the relationship between temperature and CO_2 emissions

6 CO₂ - Results & Conclusions

6.1 Forecast Results

Figure 6.1 summarizes all above models in one graph. The horizontal line marks 685ppm.

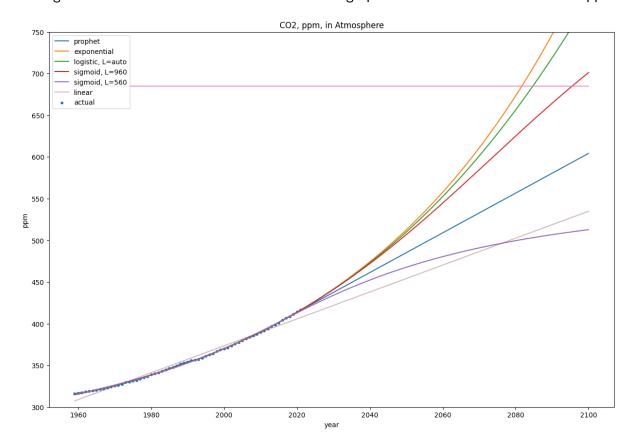


Figure 6.1: Graph of all Models

The MSE, RMSE, MAE, PCC, R² and covariance were calculated for each accepted model, rounded to 5 s.f., and compiled into a results table below. For each error metric, the model with the value closest to and furthest from a perfect value were highlighted:

	Linear	Exponential	Sigmoid	Prophet
MSE	15.376	0.47977	0.61002	0.10310
RMSE	3.9212	0.69266	0.78104	0.32109
MAE	3.1920	0.56081	0.66350	0.25507
PCC	0.99119	0.99973	0.99965	0.99994
R ²	0.98246	0.99945	0.99930	0.99990
Covariance	875.32	890.45	889.87	890.82

For each model, the year at which 685ppm was reached and the range from 2050 was found to construct the following table:

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	Linear	Exponential	Sigmoid	Prophet
Year (at which 685ppm is reached)	2193	2081	2096	2134
Range (from 2050)	+143	+31	+46	+84

Table 6.1: Different Models' Predictions to reach 685ppm

The train-test data split procedure demonstrated that the exponential model has the least amount of forecasting errors. However, Prophet has the best error metrics, such as the lowest MSE and highest R². However, this improvement is small over the exponential model and is explained by Prophet's ability to fit to arbitrary trends where it was able to capture irregularities in the data; essentially over-fitting.

Overall, even if by a small margin, as the Prophet model better fulfills the above criteria, it is deemed to be the most accurate out of the accepted models chosen and tested. This decision is reinforced by the model's use in major companies; additional studies have also demonstrated Prophet's high accuracy in predictions. A major disadvantage to the model however is its speed, as the run time to process a single item is 60ms. In this situation, this disadvantage can be overlooked, as the data set was small enough so as not to cause time issues.

6.2 Comparison with External Claims

With all relevant models fully constructed, a conclusion can be provided in response to claims by external sources.

NOAA: 2004 observed largest increase yet

Quoted from the problem statement: the "March 2004 increase of CO_2 resulted in a larger increase than observed over any previous 10-year period".

Before attempting to verify this claim, ambiguities in the meaning of a "larger increase than observed over any previous 10-year period" must be clearly defined. This statement contains two parts: "larger increase than [previously] observed" and "any previous 10 year period". How a comparative change metric for any 10-year period is left to interpretation. In the end, two reasonable quantitative approaches were adopted, both of which perform calculations on pre-2004 data, 10 consecutive years at a time, to generate a metric that encapsulates the change of CO_2 levels for that decade.

Comparing to decadal changes

In this approach, a simple method was used to calculate the net percentage change between any two years for CO_2 levels. The following equation was used,

$$\% \triangle CO_2 = \frac{C_f - C_i}{C_i} \times 100 \tag{6.1}$$

where C_f is the CO_2 level in the final year of the decade and C_i is the CO_2 level in the initial year of the decade.

This computation was carried out using a moving ten-year interval window, yielding a comparable measure of change for every preceding decade.

As indicated in Figure 6.2, the net percentage increase in atmospheric CO_2 levels over the ten-year period 1994–2004 (4.63%), while significant, was lower than that of the period1993–20033 (4.74%). With regard to the available data, the March 2004 increase was therefore

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only the second-highest recorded over any previous 10-year period.

Comparing to moving averages

In addition to direct interdecade comparisons, an analysis of change relative to the average values for each ten-year period was undertaken using the following methodology.

Using a moving ten-year window, the annual data was divided into 54 overlapping intervals. For each interval, the arithmetic average of the annual CO_2 levels was calculated. To create a ratio-based indicator, ∞ , for the extent of change, the following step was further applied:

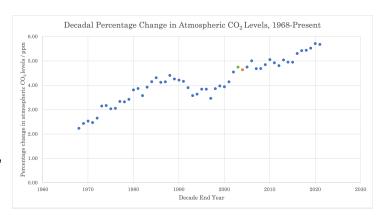


Figure 6.2: Moving Decadal Change

$$\propto = \frac{C_f}{\mu} \tag{6.2}$$

where C_f is CO_2 level in the decade end year μ is ten-year arithmetic average CO_2 level. The indicator thus provides a convenient and comparable measure for the increase in CO_2 levels at the end of each decade, relative to the ten-year average. A comparison of the-values calculated over the available data yielded the following result, represented visually in Figure 1.2, below.

Relative to previous years, the value of α for the decade ending in 2004 (1.0233) was the second-highest calculated, exceeded by that of 2003 (1.0238). This implies that the intradecade increase for March 2004, in comparison to previous decades, was not the highest.

A similar procedure was implemented to determine the relative annual increases, using the following formula to calculate a ratio β :

$$\beta = \frac{I_f}{\mu_i} \tag{6.3}$$

where I_f is the final increase, from the second-last to the last year in a given ten-year period; and μ_i is the arithmetic average yearly increase over the ten-year period.

This yielded a corroborating result, with the β -value for the decade ending in 2004 (1.217) lower than that of 14 other preceding decade groups.

Therefore, the intra-decade change for 1994–2004 is significantly smaller than that of multiple preceding decades.

In summary, both approaches yielded an identical conclusion; while the March 2004 increase of CO_2 was among the largest observed until that date, it was not the single largest. In terms of net change and increase from the decadal mean, it was exceeded by the change as of March 2003. Furthermore, its final increase relative to the average annual increase within the ten-year period was significantly smaller than several preceding decade intervals.

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OECD: reaching 685ppm by 2050

Quoted from the problem statement: "An Organisation for Economic Co-Operations and Development (OECD) report predicts a CO_2 level of 685ppm by 2050."

Unlike the claim above, this one is straightforward to verify. According to data presented in Table 6.1, no models constructed were close to the year proposed by this claim; even the fastest-growing model, the exponential model, predicted a minimum of 2081 to reach 685ppm. All other models provide even further estimates.

There is a simple explanation for this discrepancy. The OECD never claimed a 686ppm level of *carbon dioxide* by 2050, but rather of *all greenhouse gases*. Naturally, this figure will be higher than CO_2 alone, because CO_2 only accounts for 76% of all greenhouse gases.

7 Temperature - Modelling

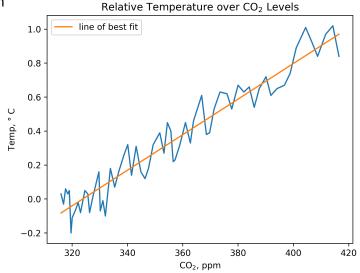
The model chosen to both forecast future temperature changes and to investigate whether a relationship exists between CO2 emissions and temperatures is a linear regression model. Although it was previously evaluated that Prophet and exponential regression were the most accurate models in forecasting future CO2 emissions, it will not be used for this section. The reason for the exponential model's success is mainly attributed to the data set's visibly curved trend, suggesting an exponential or power trend. An exponential relationship was confirmed after practical modelling.

On the other hand, temperature visually follows a more steadily linear trend; curves and deviations are not as apparent, hence the model was chosen to further investigate and confirm the trend. Additionally, to support this decision, linear regression is a popular and common approach used to model the relationship between an independent and a dependent variable (this case being CO2 emissions and temperature respectively), and hence would be the most optimal model to use for temperature/CO2 analysis.

To begin, the values for each variable are plotted onto a graph, and a regression line drawn which can be analysed, allowing other values to be predicted based on existing values. For simple regression, the form of model (trend line) can be defined as.

The regression line (Figure 7) demonstrates the relationship between the two variables, where PCC is used to measure the correlation The coefficient strength. determination was determined by squaring the PCC value. measures the proportion of variation in the temperatures and CO_2 levels. Covariance was also calculated. and this measures the directional relationship between the x and y variable. The definitions and results for PCC and covariance are denoted in Table 8.1





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obtained indicate a very strong positive correlation between CO₂

emissions and temperature. As for the R^2 value, it indicates that 92% of the variability observed in temperature can be explained by CO_2 emissions. Hence, the conclusion can be formed that there exists a strong positive relationship between CO_2 emissions and temperature.

As the existence of the relationship has been confirmed and justified, the regression line can be used to extrapolate future data. A temperature over time model was constructed and extended 30 years in the future to forecast future temperatures. The highlighted region indicates the margin of error and the black points indicate the actual observed values:

As can be observed, the regression line's margin of error extends to cover the vast majority of known value points. Additionally, what can be remarked is that the Prophet model was applied to the data to produce a completely identical trend-line to that of linear regression. It was previously argued in the introduction that Prophet and exponential modelling would not be used as visually, linear regression indicated the best fit. However, this argument applied mainly to the CO2 and temperature relationship. Prophet is capable of producing a more nuanced model that accounts for varying parameters; hence, the fact that its application yields an identical result to that of linear regression supports the initial argument that the best model option is linear regression.

As linear regression's accurate predictive ability has been confirmed, the equation line can then be used to obtain the years at which a temperature change of 1.25C, 1.5C and 2C will occur, compared to the base period. External predicted year values were obtained from carbonbrief.org as comparison. The results are presented in the table below:

	1.25C	1.5C	2C
Linear Regression	2043	2058	2088
External	N/A	2026-2042	22043-2052

The year values obtained are generally higher in comparison to the external values, which is possibly due to the spike in temperature from 2018–2021. The spike may have caused the gradient of the regression line to increase to accommodate for the sudden temperature increases, which in turn led to higher values.

8 Temperature - Model Evaluation

8.1 Error Metrics (cont.)

8.2 Predictive Ability

The linear model relating CO2 level to temperature is accurate and reliable when performing interpolation, since it fits existing data points with a very high coefficient of determination of 0.924. However, in order to predict future temperatures based on future CO2 levels, extrapolation must be performed on the CO2 model. By nature, extrapolation is less accurate than interpolation. This implies a lower forecast reliability of the model, as the assumption is made that the relationships remain unchanged.

Regardless, current data exhibits a very strong linear relationship between CO2 and temperature, as shown by a PCC of 0.961. Prophet, which is able to fit to complex trends

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$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2} \sqrt{\sum (y_i - \bar{y})^2}}$$

Where

• r = Correlation coefficient

• x_i = Values of the x-variable in a sample

• \overline{x} = Mean of the values of the x-variable

• y_i - Values of the y-variable in a sample

• \overline{y} = Mean of the values of the y-variable

$$cov_{x,y} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{N - 1}$$

Where

• $cov_{x,y}$ = Covariance between variable x and y

• x_i = Data value of x

• $y_i = Data value of y$

• $\bar{x} = \text{Mean of } x$

• $\bar{y} = \text{Mean of y}$

• N = Number of data values

Table 8.1: More Metrics

and perform highly accurate interpolation, simply produced a perfectly linear model. This supports the conclusion that the best model is a linear relationship, and that the relationship shows no sign of changing in the future.

The three linear regression models - CO2-time, CO2-temperature, and temperature-time - are linked together by the fact that the relationship between CO2 and temperature exhibits a strong statistical correlation. It is scientifically proven that CO2 and temperature have a cause-and-effect relationship, due to the greenhouse effect, where CO2 has a warming effect. This provides a link between the three models, where all three variables correlate strongly. This multi-variable correlation supports the accuracy of each individual model. On the contrary, if there is an unforeseen change in one of the relationships, all models will be incorrect.

Another approach to verify the accuracy and reliability of the models was to compare the predictions with external sources (existing literature). This can help us analyse the reliability of the forecast.

Values of CO2 concentration and Temperature Rise from secondary sources projected for 2100

CO ₂ (ppm)	Temperature Rise (C)	
701	2.2	

Data from:	CO ₂ (ppm)	Temperature Rise (C)
Confirmed Proposals (2011)	900	4.0
INDCs Strict (2015)	670	3.5
2C Pathway (2015)	475	2.0
1.8C Pathway (2015)	450	1.8
1.5C Pathway (2015)	425	1.5
2014 'Actuals'	397	0.9
Mean	536.16567	2.283333
Standard Deviation	161.49974	1.206681

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9 Temperature - Results & Conclusions

9.1 Forecast Results

PCC	R^2	Covariance	
0.9599812208926523	0.9215639444665472	9.20384156682028	

	1.25C	1.5C	2C
Linear Regression	2043	2058	2088
External	N/A	2026-2042	22043-2052

10 References

10.1 Program Code

Result data generated:

text data stuff

Python program code:

pass

10.2 Bibliography