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Modeling in Physical Sciences Problems by Single Python Program

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Abstract- A Python program was first developed for multiple regression, but it is equally good for modeling of physical sciences phenomena through linear regression, non-linear, and polynomial fitting. The program was implemented on three problems from three disciplines. An example from environmental science is used to implement multiple regression; relative humidity was predicted from daily temperatures and Dew point. The polynomial fitting example was taken from Physics, in which a quadratic polynomial was fitted. The non-linear fitting example was taken from Chemistry, in which the reaction rate is a non-linear function of the product's concentration. Good results have been obtained in each case. The program can do multiple tasks, can easily be understood, and can easily be operated. Another important feature of the program is that it calculates the coefficients through a single line code.

Keywords- Multiple Regression, Relative Humidity, Polynomial Fitting, Non-linear Fitting, Electron Transfer Reaction, Chaplygin gas pressure, Cosmology

I. INTRODUCTION

Digitalization has influenced almost everything; researchers have also switched to computing. The present era is a time for big data activities. Scientists in every field need software and computer program to pursue research. Large and heavy software have been developed, but scientists still need simple and easily accessible software and computer program. The present study attempts to develop a complete program without any additional library. Researchers need a single computer program capable of doing multiple tasks. Following are a few examples from three disciplines, Environmental Science, Physics, and Chemistry, where scientists require software to conduct research.

The invisible concentration of water vapor in the atmosphere is Relative Humidity which indicates the likelihood of the different forms of condensation like cloud/fog, which further lead to precipitation/snowfall or dew/frost etc. As this parameter is temperature dependent, scientists tried to reproduce it through daily air temperatures of a few stations in Italian snow-covered area [1]. Others added precipitation to the temperature and relative humidity to observe the relationship between these three variables across Australia [2-3]. Four variables, temperature, pressure, detrainment rates, and fractional entrainment also considered to model the equations to predict relative humidity and temperature Lapse rate [4]. surface relative humidity is an attempt at theoretical modeling of relative humidity on contact electrification of sand particles was also investigated in which charge moved between sand particles in a solitary crash under various stickiness conditions was researched [5-6]. Scientists utilize the neural networks using a feed-forward counterfeit neural system (FFNN) Nonlinear AutoRegressive with external input (NNARX) model, and genetic algorithms were employed to construct networks and were detailed [7-8]. An applied box model with examining the reaction of relative surface land relative humidity to changes in the atmosphere [9]. An electron transfer reaction is a reaction in which a single electron is transferred from one molecule to another. Scientists have used several fluorometric and calorimetric probes in the last decade to detect moisture and humidity. These probes are classified based on the signaling unit used. The application and mechanism of electron transfer for these sensors were highlighted in literature [10]. Moisture content and humidity monitoring by optical sensing have now been adopted by many process industries, hospitals, climate science, automated machines, intelligence systems, etc. In power generation cycles, an electron transfer reaction between a ferroelectric hybrid semiconductor and the super-hygroscopic metal hydrogel is carried

out and serves as a humidity harvester for the continuous water supply to the hybrid. [11]. The influence of relative humidity on chlorinated-polycyclic-hydrocarbons and observed electronic paramagnetic resonance (EPR) spectra [12]. He. J. Zheng et al. discover the electron transfer method of pairing silver nano lines arrays as a nanoscale humidity sensor are discovered by [13-14]. The effect of different relative humidity conditions for the triboelectric nanogenerators (TENG) capsule within a humid environment is also investigated [15]. Electron transfer between 2D metal oxide nanosheets has been employed for real-time breath humidity data collection by application of the sensors [16]. A theoretical model which relates the electron transfer mechanism with relative humidity, and simulated results verified the universal experimental results that charge transfer initially increases and then decreases with an increase in relative humidity is also proposed [17].

II. Data and Methodology

There are physical systems/ quantities which are a function of more than one variable. Such systems are dealt with in the field of Multivariate analysis. A function of several independent variables is given as:

$$y_i = f(x_i; A_i) \quad (1)$$

x_i are n independent variables $x_1, x_2, x_3, .., x_i$, and A_i are the parameters which are determined through multiple regression. The eq. (1) can also be written as

$$Y = AX + \epsilon \quad (2)$$

Here $X, Y, A,$ and ϵ are matrices of independent, dependent variables (are vectors), parameters, and errors, respectively. The parameters are found by

$$A = (X^T X)^{-1} X^T Y \quad (3)$$

This study aims to write a computer program for multiple regression in python so that the program for one of the research problems. We have made this program as simple as possible. The program is self-explanatory and does not have any additional library. In the first place, the program was developed for multiple regression, but it comes out that it is also can be used for linear regression, polynomial fitting, and non-linear fitting. Three examples from multiple regression, non-linear fitting, and polynomial fitting are presented in the following section.

III. Result and Conclusions

A python program is developed, which is capable of doing multiple tasks. The program was developed for multiple regression but can also be used for linear regression, non-linear, and polynomial fitting. Three environmental science, Chemistry, and physics examples show the program's implementation on multiple regression, non-linear, and polynomial fitting.

Multiple Regression: An application from environmental science

Relative humidity in the atmosphere depends on multiple factors. Here we assumed that two factors, temperature and Dew point, are more important. We developed the following relation of these variables with relative humidity.

$$RH = a_o + a_1 T + a_2 T_d \quad (4)$$

Where RH is relative humidity, T is temperature, T_d is dew point temperature while a_o, a_1, a_2 are regression coefficients which can be determined by the program. Multiple regression can be used to find coefficients in equation (4).

Data for 365 days of Karachi, taken from the Pakistan Meteorological Department to compute relative humidity by daily temperature and dew point. Fifty percent of the data was used in the training phase to find the regression coefficients, while the remaining fifty percent was used to test the model. Figures 1 and 2 show the training phase and testing of the coefficients, respectively.

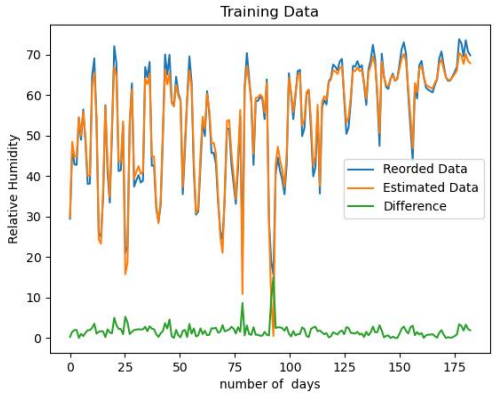

Figure 1: Recorded and estimated values of humidity for training phase

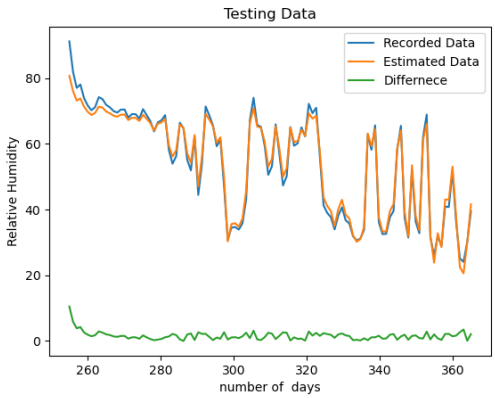

Figure 2: Recorded and estimated values of humidity for testing phase

The graph shows the variation of relative humidity calculated by multiple regression and recorded data for the number of days. From figure 1, it can be seen that the calculated values of humidity fit well with recorded values. However, the relative error shows a significant difference that might have occurred due to a recording error at one point. Where the relative error is more than 10%. However, the overall value of relative error is less than 8 percent.

In Figure 2, the graph shows recorded and estimated /calculated values obtained during the testing phase from the coefficients obtained in a training session. In this testing process, the fitting is better than the training process; here, the relative error is less than percent except at the starting point where it is more than 10% percent.

Non-linear fitting: An application from Chemistry

The developed program is also implemented on non-linear fitting; for example, equation (5) is fitted for reaction rate as a function of product concentration. The data was obtained from the PhD work of one of the authors. The author used Mathcad to fit the same equation.

The non-linear ordinary differential equation (ODE) describes the simultaneous effect of temperature and concentration of product upon the rate of production of a product and has been used as the kinetic model (KM) during the study to fit the experimental kinetic data for product formation.

$$r = Ae^{-\frac{E}{RT}}\left(C_{A_o} - \frac{C_p}{6}\right)^{\alpha}\left(C_{B_o} - C_p\right)^{\beta} \qquad (5)$$

Where r is the reaction rate, A is the pre-exponential factor, E is the activation energy, T is temperature, R is gas constant, C_{A_o} & C_{B_o} are the initial concentration of reactants, C_p is the concentration of the product. α and β are the order of reaction for reactants A and B, and are described in [18]. The parameters may be estimated by the direct fitting of experimental kinetic data (experimentally regressed values of C_p and computed values of r for product formation to the K.M. (1). Equation (5) is a non-linear equation and can be converted into a linear equation by taking a logarithm. Equation (5) becomes

$$lnr = lnk + \alpha \ln\left(C_{A_o} - \frac{C_p}{6}\right) + \beta \ln\left(C_{B_o} - C_p\right) \quad (6)$$

Here k is $Ae^{-\frac{E}{RT}}$. The above equation can be written as

$$f(x_1, x_2) = lnk + \alpha x_1 + \beta x_2$$

Here $x_1 = \ln\left(C_{A_o} - C_p/6\right)$, and $x_2 = \ln\left(C_{B_o} - C_p\right)$, now the parameters can be found by multiple regression.

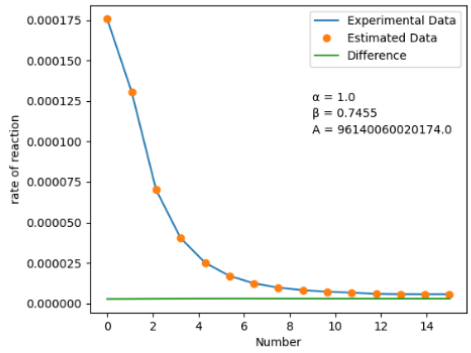

Figure 3: Hypothetical data for quadratic polynomial and estimated values through ANN for training and testing phases.

Polynomial fitting: An application from Physics

A second-degree polynomial is representative of the parabola; one such example is the equation of motion $S = vt + \frac{1}{2}gt^2$, which is quadratic in time variable; another example is from cosmology, where for Chaplygin gas pressure p is expressed as a function of energy density (ρ) by the equation, $p(\rho) = p_o + \omega\rho + \alpha\rho^2$, where ω and α are parameters. A general form of a second-degree polynomial is given by [18-20]

$$y = a_o + a_1 x + a_2 x^2$$

The parameters can be found by fitting second-degree polynomial, but here we assume that $y = f(x_1, x_2)$ is a function of two variables $x_1 = x$ and $x_2 = x^2$. Therefore, the coefficients a_o, a_1, and a_2 can also be found by multiple regression analysis. The hypothetical values of x are taken, and noise is introduced through random numbers. Some known values of the coefficients are taken to generate the values of y. The data is then used in a multiple regression program.

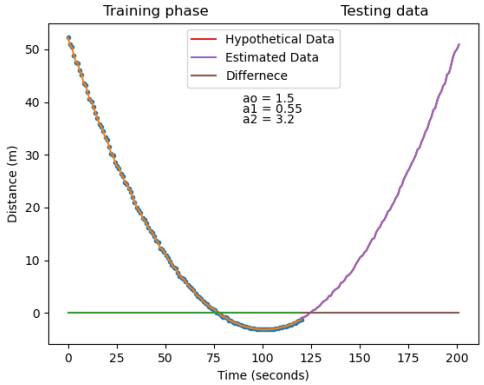

Figure 4: Hypothetical data for quadratic polynomial and estimated values through ANN for training and testing phases

IV. CONCLUSION

A multiple task Python program has been developed to test and predict the different type of models in physical sciences, viz. Multiple Regression, Non-Linear Polynomial fitting for Environmental Science, Chemistry, Physics in addition to Cosmology, respectively. The uniqueness of this program is that the main body of the program which calculates coefficients comprises of a single line. The data has been divided into two parts to conduct training and testing contain in commonly available excel file. The actual body of program is quite short; the whole calculation can be performed in two to three line's code which takes a second to produce output on Intel i-7 laptops. Moreover, the program does not require any additional library to keep. It is user friendly and self-explanatory.

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