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Wine Quality Analysis Using Newton Interpolation: Applying Computational Physics in the Food Industry

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Abstract

This study aims to analyze wine quality based on computational physics using the Newton Interpolation method. This method is applied to estimate the quality value of wine based on certain values of variables such as sulphates, alcohol, citric acid, and the average of several physicochemical variables. Data were obtained from a red wine dataset commonly used in food product quality studies. Each variable was analyzed separately using strategically selected observation data points, then the interpolation value was calculated to predict the quality of wine at certain variable values. The interpolation results showed that the Newton method was able to produce quality value estimates that were consistent with data trends, such as quality predictions of 4.52 for sulphates = 0.61 and 2.97 for alcohol = 9.2. However, in some cases such as citric acid and the average of the variable, extreme fluctuations appeared in the high-degree divided difference values, indicating the potential for overfitting due to uneven data distribution or outliers. Nevertheless, the Newton interpolation method proved effective in providing initial estimates of wine quality, especially when data is limited.

Keywords: computational physics, newton interpolation, wine quality

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INTRODUCTION

Wine is an alcoholic beverage made from the fermentation of grape juice, and it comes in various types such as Red Wine, Rose Wine, and White Wine. The quality of wine is influenced by various characteristics including density, pH, alcohol content, and acidity. Wine quality assessment is usually done by experts with sensitive taste buds, but not everyone possesses this ability (Parga-

Dans et al., 2022). Wine quality is a crucial factor in the food and beverage industry, assessed thru sensory testing by experts. However, this approach has limitations in subjectivity and requires a significant amount of time and cost. As technology advances, various computational methods have been applied to predict wine quality more efficiently and objectively.

In the context of the food and beverage industry, particularly wine, alcohol content is one of the key parameters in determining product quality. Research by Mukubesa et al. (2022) utilized data-driven chemical predictive methods (such as alcohol, pH, and sulfates) to classify red wine using machine learning and multivariate statistics. The study results indicate that alcohol content has a significant impact on wine quality and consumer preferences, making it an important variable in the quantitative modeling of wine quality.

Several previous studies have applied a data-driven approach to model wine quality. One of these is the study by Bondarev (2023), which used data mining techniques such as neural networks and support vector machines to predict wine flavor preferences based on physicochemical data. This study shows that variables such as alcohol and sulfates have a significant impact on the final quality of wine. Recent studies also confirm that a data-driven approach can improve efficiency and accuracy in controlling the quality of food and beverage products (Dahal et al., 2021).

However, most previous approaches used regression or classification-based prediction methods. Researchers adopted a numerical approach using Newton's interpolation method, which allows for estimating values between available experimental data points. This method is very useful in the industrial context, especially when quality values need to be estimated from limited measurements without direct sensory testing.

As technology advances, data-driven quantitative approaches are becoming a more objective alternative. An and Zhang (2025) research shows that data mining techniques such as neural networks and support vector machines are capable of modeling wine taste preferences based on physicochemical parameters. However, this approach tends to be complex and difficult to trace mathematically (a black box). Therefore, a numerical method is needed that is not only accurate, but also transparent and easy to apply.

Newton's interpolation is a crucial numerical method in computational physics for forming an approximation polynomial from discrete experimental data (Varin, 2025). This method recursively uses divided differences, making it easier to update the polynomial without rebuilding the entire function, unlike the Lagrange approach, which is unflexible when adding new data (Patil & Kadoli, 2025).

In the context of computational physics, Newton's interpolation is not just a numerical technique, but also a fundamental approach to approximating continuous functions based on discrete experimental data. Newton's polynomial is constructed using divided differences, which are recursive and stable, and suitable for small to medium-sized datasets (Wei et al., 2025). Compared to other methods like splines, Newton's polynomial is more reliable in handling sparse and uneven datasets (Bak et al., 2025). Furthermore, recent numerical stability analysis indicates that divided difference calculations using Newton's structure can be performed with high relative accuracy if the data point nodes are specifically ordered and the function being represented has an alternating sign structure. This is confirmed by Yan (2025), who shows that this algorithm, with node conditions met, successfully maintains high stability and accuracy even in floating-point arithmetic.

From a practical implementation perspective, Newton's interpolation has been widely used in food industry quality control, including for wine (Liakos et al., 2025). One recent study shows that a combination of numerical methods and infrared spectroscopy-based chemometrics can be used to predict wine quality quickly and accurately without sensory testing. The results of that research even showed that the estimation of wine quality and geographical origin classification can achieve an accuracy of over 99%.

This research uses physicochemical data from red wine experiments, with the data source kept confidential for licensing and copyright protection reasons. Variables such as alcohol content, citric acid, sulfates, and the average of eleven physicochemical parameters were analyzed to determine the extent to which Newton's interpolation can be used to predict wine quality. This research also aims to examine the stability of the method when used in a practical context in the food industry, as well as its relevance as teaching material for students in applied computational physics learning.

METHOD

The method used in this study is a descriptive quantitative method that uses a numerical approach to analyze wine quality. This type of data was obtained by the researcher from the open-source data platform Kaggle. The data used is secondary data from laboratory experiments on red wine samples.

fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
7.4	0.7	0	1.9	0.076	11	34	0.9978	3.51	0.56	9.4	5
7.8	0.88	0	2.6	0.098	25	67	0.9968	3.2	0.68	9.8	5
7.8	0.76	0.04	2.3	0.092	15	54	0.997	3.26	0.65	9.8	5
11.2	0.28	0.56	1.9	0.075	17	60	0.998	3.16	0.58	9.8	6
7.4	0.7	0	1.9	0.076	11	34	0.9978	3.51	0.56	9.4	5
7.4	0.66	0	1.8	0.075	13	40	0.9978	3.51	0.56	9.4	5
7.9	0.6	0.06	1.6	0.069	15	59	0.9964	3.3	0.46	9.4	5
7.3	0.65	0	1.2	0.065	15	21	0.9946	3.39	0.47	10	7
7.8	0.58	0.02	2	0.073	9	18	0.9968	3.36	0.57	9.5	7
7.5	0.5	0.36	6.1	0.071	17	102	0.9978	3.35	0.8	10.5	5
6.7	0.58	0.08	1.8	0.097	15	65	0.9959	3.28	0.54	9.2	5
7.5	0.5	0.36	6.1	0.071	17	102	0.9978	3.35	0.8	10.5	5
5.6	0.615	0	1.6	0.089	16	59	0.9943	3.58	0.52	9.9	5
7.8	0.61	0.29	1.6	0.114	9	29	0.9974	3.26	1.56	9.1	5
8.9	0.62	0.18	3.8	0.176	52	145	0.9986	3.16	0.88	9.2	5
8.9	0.62	0.19	3.9	0.17	51	148	0.9986	3.17	0.93	9.2	5
8.5	0.28	0.56	1.8	0.092	35	103	0.9969	3.3	0.75	10.5	7
8.1	0.56	0.28	1.7	0.368	16	56	0.9968	3.11	1.28	9.3	5
7.4	0.59	0.08	4.4	0.086	6	29	0.9974	3.38	0.5	9	4

Figure 1. Wine Data Set

The data includes physicochemical values such as sulfates, alcohol, citric acid, and combinations of several variables like fixed acidity, volatile acidity, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, and others.

The steps in this research involve the Newton interpolation process, also known as Newton polynomial interpolation, which is used to make predictions about function values when given a large amount of data (Mohammed et al., 2022; Qin et al., 2025; Yingnan & Xiaowei, 2025). Newton's interpolation uses divided differences to construct an n-th order polynomial that approximates the function being analyzed. The program created also accepts input values for x from the user, then calculates and displays the predicted value of f(x) along with the accompanying divided difference structure using the formula :

$$f(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1) + \ldots + b_n(x - x_0)(x - x_1)\ldots(x - x_{n-1}). \quad (1)$$

with the coefficient bi obtained thru the process of divided differences, according to the equation:

$$b_i = f[x_0, x_1, \ldots, x_i] = \frac{f[x_1, \ldots, x_i] - f[x_0, \ldots, x_{i-1}]}{x_i - x_0} \quad (2)$$

The values of the coefficients b_n are calculated iteratively based on divided differences and are then substituted into the polynomial to compute the function value at the desired point x. This method is flexible and efficient because the polynomial coefficients can be updated without recalculating the entire structure if new data is added. In the context of this research, Newton's interpolation is used to predict wine quality values based on physicochemical data without the need for direct sensory testing.

The things or tools used in this research are Google Collab as the platform where the model is built and the Python programming language. In this study, Google Collab is used as a medium for training data and forming the model. Next, prepare the Python libraries that will be used. Once the media or tools are ready, the researcher will input the Python libraries into the algorithm model. The libraries used in Python are Pandas for data processing and Pretty Table for displaying calculation results in table format.

Programming Algorithm for Wine Quality Analysis using Newton's Interpolation: Application of Computational Physics in the Food Industry as follows:

1. Initial data definition
   1.1 Defining the initial data printing function
   1.2 Printing the initial data table framework
   1.3 For i to be within the range (len(x)):
      1.3.1 Print ("| {:^4} | {:^15} |".format(x[i], fx[i]))
   1.4 Print Table

2. Definition of the calculation table

   2.1 Defining the calculation_table()
   2.2 Print ("\nCalculation Table :")
   2.3 Initializing the table = PrettyTable()
   2.4 Initializing table.field_names = ["x", "f(x)"] + ["d" + str(i)
   2.5 For i in range (1, len(x)):
   2.6 Initializing n = len(fa)
   2.7 For i in range (len(fa) - 1):
      2.7.1 Initializing the row = [x[i], fx[i]] + [format(fa[j + 1][i], '.6f')
      2.7.2 For j in range (n - 1):
      2.7.3 Conditioning if len(row) < len(table.field_names):

2.7.3.1 Initializing row += [''] * (len(table.field_names) - len(row))
2.7.4 Initializing table.add_row(row)

2.7.5 Decrement n by 1
2.8 Print Table

3. Calculation Definitions

3.1 Defining the calculation function (xa)
3.2 For i in range (len(x) - 1):
3.2.1 Initializing Lfd = []
3.2.2 Initializing n = i
3.2.3 For j in range (len(fa[i]) - 1):
3.2.3.1 Calculating fd = (fa[i][j + 1] - fa[i][j]) / (x[n + 1] - x[j])
3.2.3.2 Adding fd to Lfd using Lfd.append(fd)
3.2.3.3 Adding 1 to n
3.2.4 Adding Lfd to fa using fa.append (Lfd)
3.3 Initializing fxb = fa[len(fa) - 1][0]
3.4 For i in range (1, len(fa)):
3.4.1 Updating fxb = fa[len(fa) - 1 - i][0] + (xa - x[len(fa) - 1 - i]) * fxb
3.5 Returning fxb

4. Main Program
4.1 Start
4.2 Adding data
4.2.1 Initiate import pandas as pd
4.2.2 Initiate df = pd.read_csv('Data variabel x.csv')
4.3 Print "Kelompok 3"
4.4 Printing "Title: Analysis of Wine Quality Using Newton Interpolation: Application of Computational Physics in the Food Industry"
4.5 Print " Method : NEWTON INTERPOLATION'
4.6 Print "\n"
4.7 Initializing x = df['Variabel x'].values
4.8 Initializing fx = df['Variabel x'].values
4.9 Creating an empty list for fa
4.10 Adding List (fx) to List (fa)
4.11 Calling print_initial_data()
4.12 Initialize variable y = input("Value of variable x = ")
4.13 Initiating xa = float(variable x)
4.14 Calling the calculation fxb = calculation(xa)
4.15 Calling the calculation table()
4.16 Print "Quality Value: "
4.17 Print "N("+variable x+") =",fxb

4.18	End

Flowchart for Wine Quality Analysis using Newton's Interpolation: Application of Computational Physics in the Food Industry as follows:

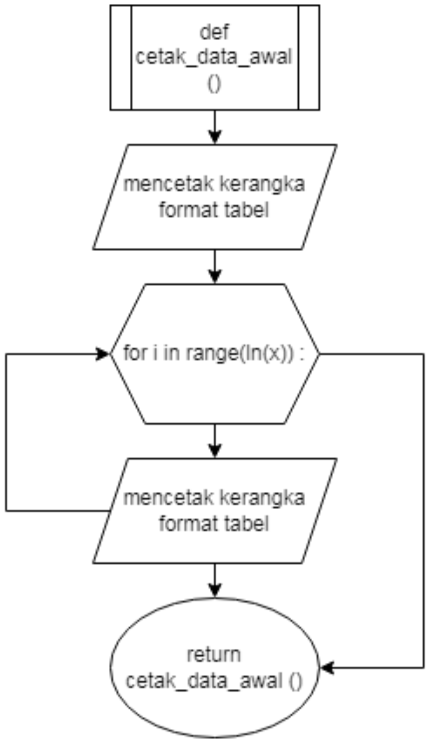

Figure 2. Initial data definition Flowchart

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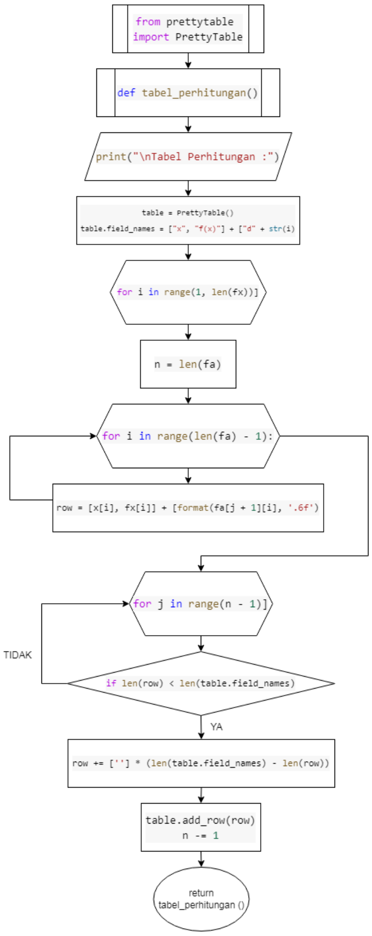

Figure 3. Definition of the calculation table Flowchart

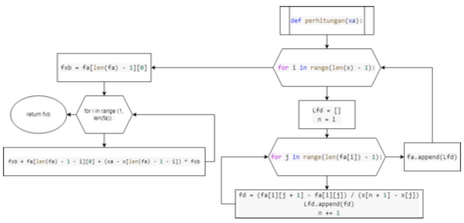

Figure 4. Calculation Definitions Flowchart

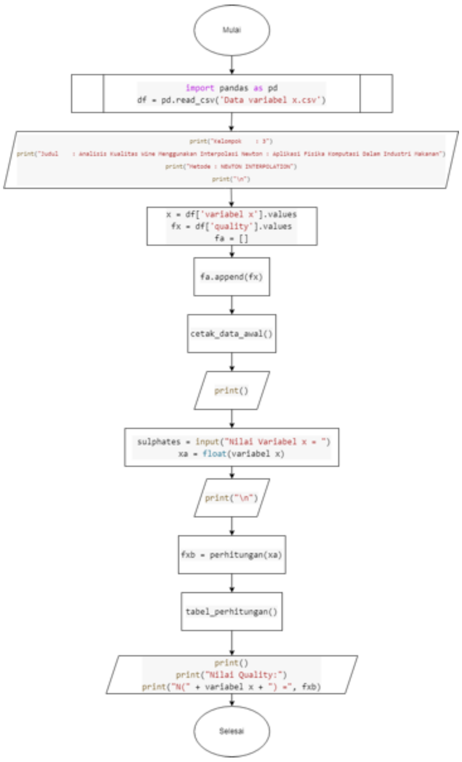

Figure 5. Main Program Flowchart

Source code for Wine Quality Analysis using Newton's Interpolation: Application of Computational Physics in the Food Industry as follows:

```
# Mulai
def print_initial_data():
    print("Quality Value Table:")
    table = PrettyTable(["Variable x", "Quality"])
    for i in range(len(x)):
        table.add_row([x[i], fx[i]])
    print(table)

def calculation (xa):
    for i in range(len(x) - 1):
        Lfd = []
        n = i
        for j in range(len(fa[i]) - 1):
            fd = (fa[i][j + 1] - fa[i][j]) / (x[n + 1] - x[j])
            Lfd.append(fd)
            n += 1
        fa.append(Lfd)
    fxb = fa[len(fa) - 1][0]
```

```
    for i in range(1, len(fa)):
        fxb = fa[len(fa) - 1 - i][0] + (xa - x[len(fa) - 1 - i]) * fxb
    return fxb

from prettytable import PrettyTable
def Calculation_table():
    print("\nTabel Perhitungan :")
    table = PrettyTable()
    table.field_names = ["x", "f(x)"] + ["d" + str(i)
    for i in range(1, len(fx))]
    n = len(fa)
    for i in range(len(fa) - 1):
        row = [x[i], fx[i]] + [format(fa[j + 1][i], '.6f')
        for j in range(n - 1)]
        if len(row) < len(table.field_names):
            row += [''] * (len(table.field_names) - len(row))
        table.add_row(row)
        n -= 1
    print(table)

import pandas as pd
df = pd.read_csv('Data variable x.csv')

print("Kelompok    : 3")
print("Title   : Analysis of Wine Quality Using Newton Interpolation:
Application of Computational Physics in the Food Industry ")
print("Method : NEWTON INTERPOLATION")
print("\n")

x = df['variabel x'].values
fx = df['quality'].values
fa = []
fa.append(fx)

Print_ initial_data()

print()
sulphates = input("Variable Value x = ")
xa = float(sulphates)
print("\n")
```

```
fxb = Calculation(xa)

Calculation_table()

print()
print("Quality Value:")
print("N(" + variable x + ") =", fxb)
# end
```

RESULTS AND DISCUSSION

Predicting Wine Quality Based on Sulfate Content

In this study, Newton's interpolation method was used to predict wine quality based on sulfate content. The data used is taken from the wine quality-red dataset, with the following six data points:

Table 1. Six data points

Sulphates	Quality
0.57	3
0.60	4
0.62	5
0.68	6
0.74	7
0.76	8

The selection of these data points is based on the distribution of sulfate values, which ranges from low to high, so that the interpolation can represent the overall trend.

Newton's interpolation is performed in several steps (1) The initial data table is displayed to show the pairs of sulfate values and quality from the dataset used and (2) Newton's Divided Differences are calculated to form tables d1, d2, ..., d5. This is the basis for the Newton polynomial, which will be constructed recursively.

From the calculation results shown in the table, it can be seen that the first-order (d1) to fifth-order (d5) divided differences are arranged systematically. These values represent the coefficients of the Newton interpolating polynomial. Interpolation is performed for the sulfate value $x = 0.61$, which lies between the two data points 0.60 and 0.62. The interpolation result is

$$\boldsymbol{N(0.61) = 4.5211889220877145}$$

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This means that, based on Newton's interpolation model, the predicted wine quality for a sulfate content of 0.61 is approximately 4.52. The interpolation value of 4.52 indicates that wine quality increases gradually as the sulfate level increases.

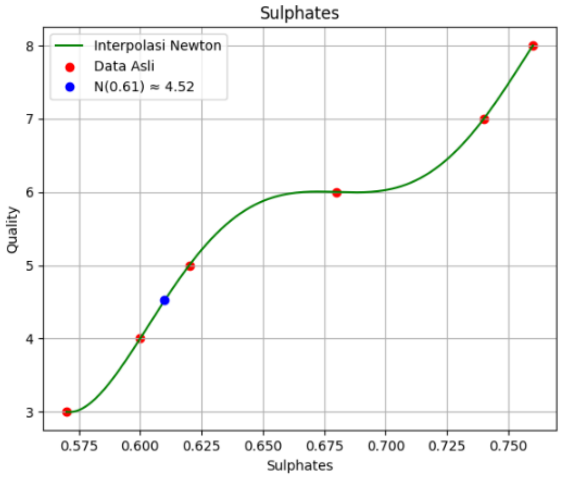

Figure 6. Sulphates graph and quality

The pattern of quality improvement is initially relatively linear, but higher-order coefficients (d3, d4, d5) show greater fluctuations. This indicates that the data has little irregularity or deviation from a simple polynomial function. Negative values at d3, d5, and other large values reflect sensitivity to small changes in the data; this is typical in high-degree interpolation and can lead to overfitting if not controlled.

The predicted wine quality with a sulfate content of 0.61 is 4.52, while the actual value is 5. An error percentage of 9.60% is considered low, indicating that Newton's interpolation method is capable of closely approximating the quality values, although there is a slight deviation likely caused by the irregularity of the local data. The resulting interpolation polynomial shows good numerical stability, with coefficients that are not too fluctuating. This indicates that the data distribution for the sulfates variable is quite linear and supports the accuracy of medium-degree interpolation.

The training loss curve (Figure 2) further confirms the effective learning and convergence of the proposed model. Initially, the loss was high due to significant prediction errors. However, as training continued, the loss dropped quickly and eventually leveled off at a very low value. This indicates that the model successfully learned the underlying patterns in the dataset. The smooth convergence also shows that the model did not suffer from overfitting or underfitting, which are common challenges in neural network training.

Interpolation Based on Alcohol Content

At this stage, Newton's interpolation is applied to predict wine quality based on its alcohol content. The data used consists of six observation points taken from the red wine dataset, with the following distribution of alcohol content and quality values:

Table 2. Alcohol Table and Quality

Sulphates	Quality
9.0	3
9.3	4
9.4	5
9.8	6
10.0	7
12.8	8

These points were chosen because they represent the variation in alcohol content from low to high values in the dataset, allowing interpolation to estimate quality at values between two data points with adequate representation.

Interpolation was performed on an alcohol content value of 9.2%, which falls between two data points: 9.0% and 9.3%. Using the Newton Divided Difference method, a Newton polynomial up to the fifth degree was obtained, and the estimated wine quality at that alcohol content is: This result indicates that at an alcohol content of 9.2%, the wine quality is estimated to be approximately 2.98, which is lower than the value at an alcohol content of 9.0% (quality value of 3). This indicates local irregularities in the data, as it is generally expected that increasing alcohol content will improve wine quality. Additionally, the calculation table shows that the coefficients of higher-order divided differences (e.g., at d3, d4, and d5) have fluctuating and significant values, such as:

This fluctuation indicates that high-degree interpolation can lead to numerical instability, particularly if the data used has an uneven distribution or contains outliers. In this context, a data point with 12.8% alcohol can be considered a leverage point because its value is quite far from the other points.

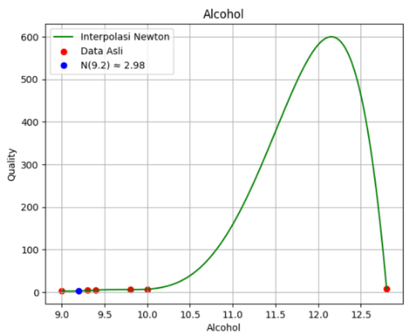

Figure 7. Alcohol graph and quality

The prediction at an alcohol content of 9.20% is 2.98, while the actual value is 4, resulting in an error of 25.50%, which is quite high and indicates the possibility of overfitting or the influence of outliers, such as the data point at an alcohol content of 12.8%. The uneven distribution of data affects the stability of high-degree interpolation.

Overall, Newton interpolation successfully provided an estimate of wine quality at alcohol levels not explicitly present in the data. However, these estimated values require further analysis considering the possibility of overfitting effects due to the high degree of interpolation and the non-linear distribution of the data. Large differences indicate the sensitivity of the interpolation to extreme points in the dataset. Alcohol is a variable with high variation and potential outliers, making Newton's interpolation less stable in this case.

Interpolation Based on Citric Acid Content

In this section, Newton's interpolation is used to predict wine quality based on the citric acid content, one of the chemical compounds that contribute to the taste and acidity of wine. Four data points are used to form the interpolation polynomial as follows:

Table 3. Citric Acid Table and Quality

Sulphates	Quality
0.66	3
0.56	6
0.47	7
0.46	8

Interpolation was performed for a Citric Acid content of 0.57. Calculations based on Newton's method yielded the following wine quality estimate:

$$N(0.57) = 6.2342$$

These results indicate that at a Citric Acid concentration of 0.57, the estimated wine quality is 6.23. This value falls between the observation points with a quality of 6 (at 0.56) and a quality of 7 (at 0.47), demonstrating logical consistency in the interpolation results. However, it should be noted that the values of higher-order divided differences show large fluctuations, such as:

$$d_2 = -99.415$$
$$d_3 = -4941.520$$

These extreme values indicate irregularities in the data structure, or could signify the presence of outliers or a non-smooth distribution between points. This is a strong indication of potential overfitting, especially if interpolation is performed with high-degree polynomials on small or unevenly distributed datasets.

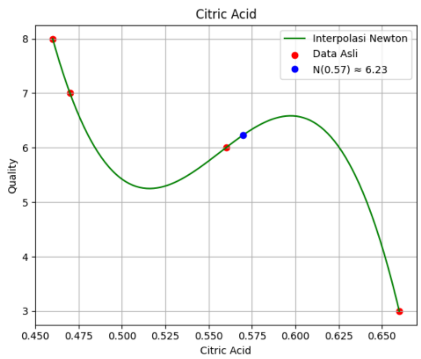

Figure 8. Citric Acid graph and quality

At a citric acid level of 0.57, the predicted quality result is 6.23, while the actual data shows a value of 6 with an error of 3.83%, indicating that the interpolation results are quite precise. However, the presence of extreme points like 0.66 (with a quality of 3) can still affect the overall stability of the prediction.

The distribution of citric acid data supports a smoother polynomial interpolation form. The fluctuation of the coefficients is more controlled compared to the alcohol variable, indicating better model stability. Thus, although Newton's interpolation can provide a numerical estimate of wine quality, it is important to consider the distribution of the input data and the degree of interpolation.

Estimating Wine Quality Based on the Average of Computational Physics Variables

In an effort to obtain a wine quality estimate that comprehensively considers several parameters, Newton's interpolation approach is applied to the average values of several chemical variables. This step aims to illustrate the cumulative influence of these variables on wine quality.

Table 4. Quality Values Table

Average Variable	Quality
10.003938181818183	3
9.748918181818182	4
9.724250909090909	5
9.719854545454544	6
9.64448	7

Five observation data points were used as the basis for interpolation, with the average values of chemical variables as input and quality scores as output. Calculations were performed for an average value of 9.75, resulting in a predicted quality of:

$$N(9.75) = 4.1816$$

This result falls between the quality values at 9.74 (quality 4) and 9.72 (quality 5), indicating a logical prediction that aligns with the data trend.

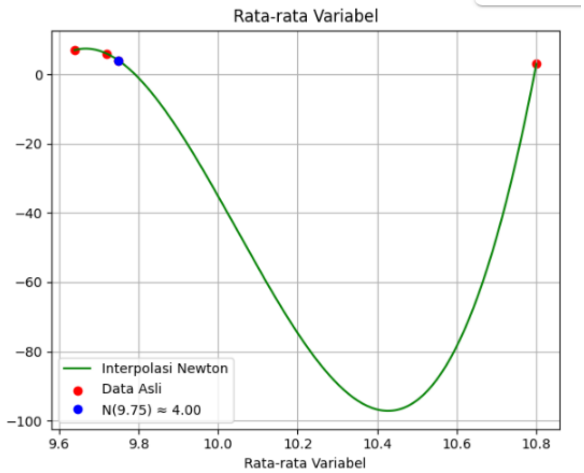

Figure 9. Average Variable Graph

However, the examination of the divided difference values indicated significant oscillations, including:

$$d_2 = 130{,}93$$
$$d_3 = -22{,}178$$
$$d_4 = -305{,}441$$

This high variation indicates a possible irregularity or disharmony in the data distribution, as well as potential overfitting due to using a high polynomial degree on a small dataset. Additionally, non-uniform spacing between points can affect the stability of Newton's polynomial.

The estimated quality value for an average variable of 9.75 is 4.00, which is also its actual value (4). Interpolation shows perfect precision in this case, indicating that combining the average variables provides better prediction stability, possibly due to the smoothing effect on individual variable fluctuations.

Although this approach offers a general overview of wine quality based on combined information, the accuracy of the estimation can be improved thru multivariate statistical methods, such as multiple linear regression or machine learning techniques that are more adaptable to non-linear data and the complexity of inter-variable relationships. This indicates that using the average of the variables is able to balance the fluctuations of each parameter, resulting in a more stable and accurate polynomial.

CONCLUSION

Newton's interpolation method was successfully used to estimate wine quality based on key chemical variables such as sulfates, alcohol, and citric acid. The interpolation results showed predictions consistent with the observed data, making this method effective as an initial approach in analyzing food product quality based on physicochemical parameters.

However, significant fluctuations in the high-degree difference value indicate potential overfitting due to uneven data distribution and a limited sample size. Therefore, Newton's interpolation is less than optimal when used on complex or large datasets.

This research contributes to the utilization of numerical methods for wine quality analysis and opens up opportunities for developing more complex and accurate quality prediction models in the future, particularly within the food and beverage industry. As emphasized by Dai et al. (2023), recursive structure-based interpolation approaches such as Newton polynomials have proven to have advantages in terms of numerical stability and computational efficiency, especially when dealing with imbalanced datasets or the high level of precision required in chemical experimental data processing.

This research is not only relevant in the context of the food industry but also has high educational value. The Newton interpolation method used in this study is highly suitable for introduction to students in computational physics learning because it involves understanding experimental data, the concept of variable change, and the application of numerical logic (Alabidi et al., 2023). Students can learn how real-world data, such as wine quality, can be modeled using physical and mathematical approaches, while also understanding the importance of data stability and point order in the numerical process. Therefore, the results of this research can be adapted into project-based learning materials to support numerical literacy.

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