Warsaw University of Technology

FACULTY OF BUILDING SERVICES,
HYDRO AND ENVIRONMENTAL ENGINEERING

Assignment 04 –Curve fitting and interpolation

Computational Methods in Environmental Engineering

08.12.2019
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4.1 Growth rate of bacteria

Determine the growth rate of bacteria, k, as a function of oxygen concentration, c.

c (mg/L)	0.5	0.8	1.5	2.5	4.0
k (per day)	1.1	2.5	5.3	7.6	8.9

- As we know the modeling equation is:

$$k = \frac{k_{max}c^2}{c_s + c^2}$$

Reform this equation,

$$\frac{1}{k} = \frac{c_s + c^2}{k_{max}c^2} = \frac{c_s}{k_{max}c^2} + \frac{1}{k_{max}} = \frac{c_s}{k_{max}}\frac{1}{c^2} + \frac{1}{k_{max}}$$

As we assume $y = \frac{1}{k}, x = \frac{1}{c^2}, a = \frac{c_s}{k_{max}}, b = \frac{1}{k_{max}}$, so this equation can be seen in the linear equation form: y=ax+b

Use the MATLAB

```
%Assignment04_1
c=[0.5 0.8 1.5 2.5 4];
k=[1.1 2.5,5.3 7.6 8.9];
x=1./(c.^2.);
y=1./k;
figure, plot(x,y,'o');
a=polyfit(x,y,1);
xt=0:0.2:4;
yt=polyval(a,xt);
hold on
plot(xt,yt,'r-')
legend('data','fitting')
```

When we modeling this equation, we know that P1=0.20201, P2=0.096666, as we know: $P_1 = a = \frac{c_s}{k_{max}}, P_2 = b = \frac{1}{k_{max}}$

Hence, $k_{max} = \frac{1}{P_2} = \frac{1}{0.096666} = 10.3449$

$c_s = k_{max} \cdot P_1 = 10.3449 \times 0.096666 = 2.0898$

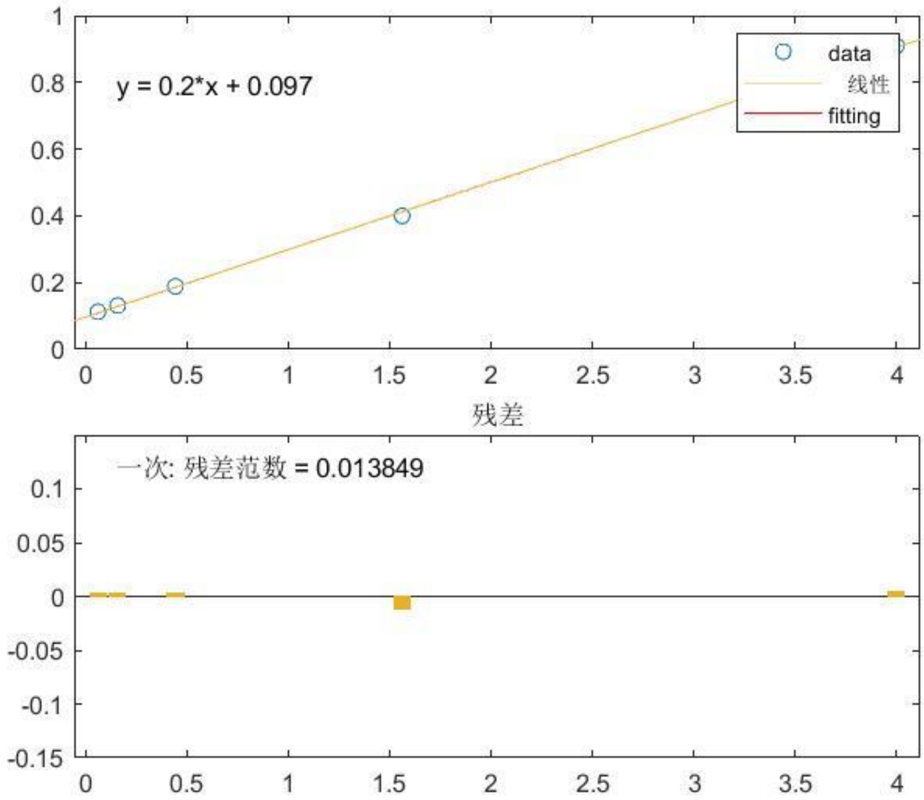


Fig 1 – the linear equation of the growth rate of bacteria

So the linear equation we got is: $y = 0.20201x + 0.096666$

If we bring c=2mg/L into this equation, we got the growth rate of bacteria k_1:

$$\frac{1}{k_1} = 0.20201 \times \frac{1}{4} + 0.096666 = 0.501$$

$$k_1 = 6.803$$

4.2 Reaction rate coefficient – Arrhenius equation

T(K)	595	623	761	849	989	1076	1146	1202	1382	1445	1562
k$\times 10^{20}(m^3/s)$	2.12	3.12	14.4	30.6	80.3	131	186	240	489	604	868

<u>(a) Determine the constants C, b and D by curve fitting a linear combination</u>

➢ (a) We know that in question a, the form of the rate coefficient k is:

$$ln(k) = C + b \cdot ln(T) - \frac{D}{T}$$

Frist step is to change the form of k:

Assume the formula:

$$y = C_1 \cdot f_1(T) + C_2 \cdot f_2(T) + C_3 \cdot f_3(T)$$

Then we can bring this formula to the form of k, where:

Prescribed function: $f_1(T) = 1;\ f_2(T) = lnT;\ f_3(T) = \frac{1}{T}$

Unknow coefficients: $C = C_1 ;\ b = C_2;\ -D = C_3$

As in linear regression, we minimize the total error E between the data points and values of function F(x), then we can get the equation:

$$E = \sum_{i=1}^{n} (y_i - C_1 \cdot f_1(T) - C_2 \cdot f_2(T) - C_3 \cdot f_3(T))^2 \rightarrow min$$

Then the partial derivatives of E with respect to each of the coefficients are equal to zero:

$$\frac{\partial E}{\partial C_1} = -2 \sum_{i=1}^{n} \left(y_i - C_1 - C_2 \cdot ln(T_i) - C_3 \cdot \left(\frac{1}{T_i} \right) \right) = 0$$

$$\frac{\partial E}{\partial C_2} = -2 \sum_{i=1}^{n} \left(y_i - C_1 - C_2 \cdot ln(T_i) - C_3 \cdot \left(\frac{1}{T_i} \right) \right) \cdot ln(T_i) = 0$$

$$\frac{\partial E}{\partial C_3} = -2 \sum_{i=1}^{n} \left(y_i - C_1 - C_2 \cdot ln(T_i) - C_3 \cdot \left(\frac{1}{T_i} \right) \right) \cdot (\frac{1}{T_i}) = 0$$

Next, these three equations can be rewritten in the form:

$$\sum_{i=1}^{n} C_1 + C_2 \cdot \sum_{i=1}^{n} ln(T_i) + C_3 \cdot \sum_{i=1}^{n} \left(\frac{1}{T_i} \right) = \sum_{i=1}^{n} y_i$$

$$C_1 \cdot \sum_{i=1}^{n} ln(T_i) + C_2 \cdot \sum_{i=1}^{n} (ln(T_i))^2 + C_3 \cdot \sum_{i=1}^{n} \left(\frac{1}{T_i} \cdot ln(T_i) \right) = \sum_{i=1}^{n} y_i \cdot ln(T_i)$$

$$C_1 \cdot \sum_{i=1}^{n} \left(\frac{1}{T_i} \right) + C_2 \cdot \sum_{i=1}^{n} \left(\frac{1}{T_i} \cdot ln(T_i) \right) + C_3 \cdot \sum_{i=1}^{n} \left(\frac{1}{T_i} \right)^2 = \sum_{i=1}^{n} y_i \cdot \left(\frac{1}{T_i} \right)$$

In this system of equations, $ln(T_i), \frac{1}{T_i}, y_i$ are all known quantities, and the coefficients C_1, C_2, C_3 are the unknowns, then we can solve these three expressions from the perspective of the matrix.

The known quantities on the left side of these equations can be expressed as matrix A, and the known quantities on the right side of these equations are expressed as b, so we can get the following matrix equation:

$$A \cdot \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = b$$

As we know the $\sum_{i=1}^{n} 1 = n = 11,\ y_i = ln(k_i)$, bringing all the known values into the following matrix:

$$\begin{bmatrix} 11 & \sum_{i=1}^{n} ln(T_i) & \sum_{i=1}^{n} \left(\frac{1}{T_i}\right) \\ \sum_{i=1}^{n} ln(T_i) & \sum_{i=1}^{n} (ln(T_i))^2 & \sum_{i=1}^{n} \left(\frac{1}{T_i} \cdot ln(T_i)\right) \\ \sum_{i=1}^{n} \left(\frac{1}{T_i}\right) & \sum_{i=1}^{n} \left(\frac{1}{T_i} \cdot ln(T_i)\right) & \sum_{i=1}^{n} \left(\frac{1}{T_i}\right)^2 \end{bmatrix} \cdot \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} ln(k_i) \\ \sum_{i=1}^{n} ln(k_i) \cdot ln(T_i) \\ \sum_{i=1}^{n} ln(k_i) \cdot \left(\frac{1}{T_i}\right) \end{bmatrix}$$

To simplify this matrix, I assume $ln(T_i) = a,\ \frac{1}{T_i} = b$, thus the matrix can be expressed as:

$$\begin{bmatrix} 11 & \sum_{i=1}^{n} a & \sum_{i=1}^{n} b \\ \sum_{i=1}^{n} a & \sum_{i=1}^{n} a^2 & \sum_{i=1}^{n} ab \\ \sum_{i=1}^{n} b & \sum_{i=1}^{n} ab & \sum_{i=1}^{n} b^2 \end{bmatrix} \cdot \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} ln(k_i) \\ \sum_{i=1}^{n} ln(k_i) \cdot a \\ \sum_{i=1}^{n} ln(k_i) \cdot b \end{bmatrix}$$

Then I present the Gauss elimination method without pivoting in the MATLAB, create a m.file named “assignment04_2_Gauss0.m”, then create my main script named “assignment04_2a”, add the matrix A and matrix b in it, then call the Gauss0 function from the main script.
The result I have got from MATLAB is:

$$A = \begin{bmatrix} 11 & 76.0761 & 0.0115 \\ 76.0761 & 527.2348 & 0.0782 \\ 0.0115 & 0.0782 & 0 \end{bmatrix}$$

$$b = \begin{bmatrix} 47.307 \\ 333.9751 \\ 0.042 \end{bmatrix}$$

$$\begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{bmatrix} -6.4 \\ 2.1 \\ -3815.3 \end{bmatrix}$$

Ultimately, we can conclude that the constants C, b and D are:

$$C = -6.4;\ b = 2.1;\ D = -3815.3$$

(b) Having the constants C, b, D, deduce the values of A (m^3/s) and E_a (J/mole) in the Arrhenius.

- As we know the Arrhenius equation is:

$$k = AT^b e^{-Ea/(RT)}$$

And from part (a), we already know k is the variable y, T is the variable x, we also know the value of C, b and D, R=8.314 J/mole/K.

In order to calculate the constant A and the activation energy E_a, I assume a(1)=A, a(2)=E_a, then we can reform the Arrhenius to the following equation,

$$y = a(1) \cdot x^{2.1} \cdot e^{-a(2)/(8.314x)}$$

Hence, using the function "lsqcurvefit" from *Optimization Toolbox* in MATLAB to calculate A and E_a.

The results obtained from MATLAB are:

A= 0(m^3/s), E_a = 31.834 (kJ/mole)

```
>> assignment04_2b

Local minimum possible.
lsqcurvefit stopped because the final change in the sum of squares relative
to its initial value is less than the value of the function tolerance.
<stopping criteria details>
a =
   1.0e+04 *
    0.0000    3.1834
```

From this result, we know that A is ignored because its value is too small, and it can be reduced to zero, where E_a=31.834 kJ/mole. Following is the fig 2 we got after the calculation.

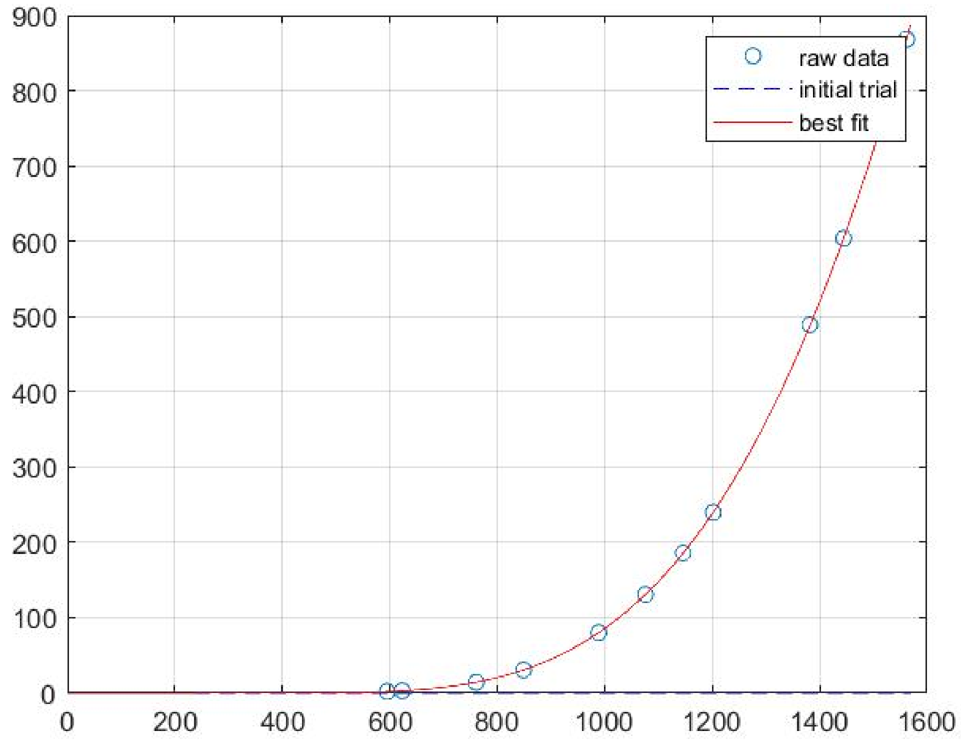


Fig 2 – the Arrhenius equation used in question 4.2(b)

4.3 Dissolved oxygen

Estimate the value of dissolved oxygen for T= 27℃ using:

(a) Linear interpolation

(b) Newton’s interpolation polynomial

(c) Cubic spline

T(℃)	0	8	16	24	32	40
o (mg/L)	14.621	11.843	9.87	8.418	7.305	6.413

I create a m.file named “assignment04_3.m” in MATLAB, then add the given data to the script and present the linear interpolation method, Newton’s interpolation polynomial and cubic splines method individually, the results I have got shows in following figure 3.

When we assume the temperature is 27 ℃, the result I got from different methods are:

method	**T [℃]**	**Dissolve oxygen [mg/L]**
linear interpolation	27	8.001
Newton’s interpolation polynomial	27	7.968
cubic splines	27	7.968

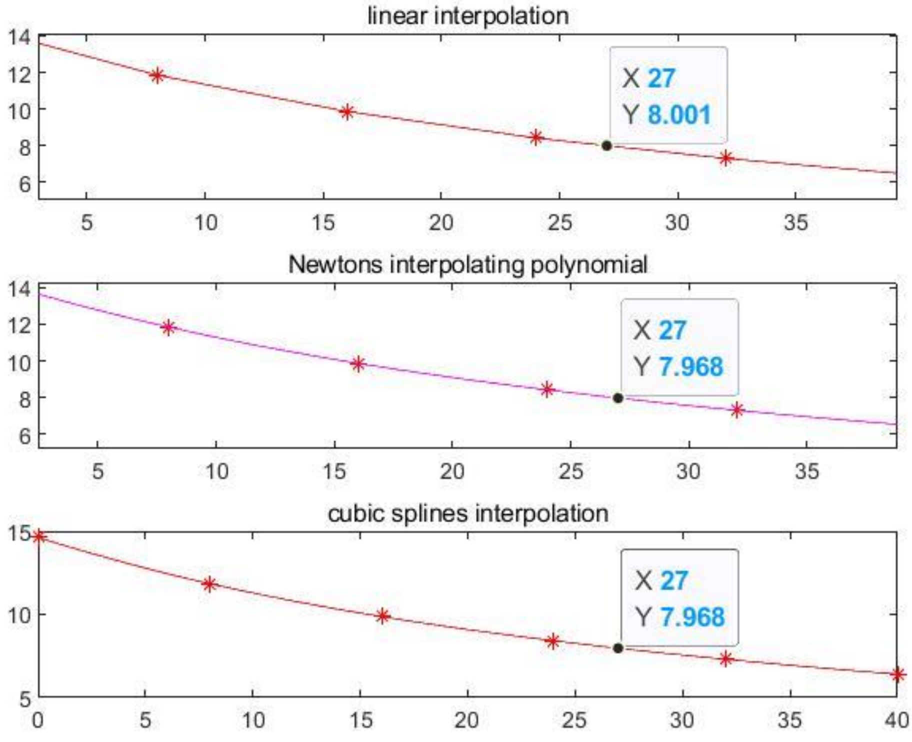


Fig 3 – compare the results of three different method to solve dissolve oxygen

From the figure, we can see clearly that the results from three methods are very similar, and the function images are basically the same. But as we know the exact value of dissolved oxygen is 7.968 mg/L, so both of Newton's interpolation method and cubic splines methods are outstanding and more accurate than the linear interpolation method.

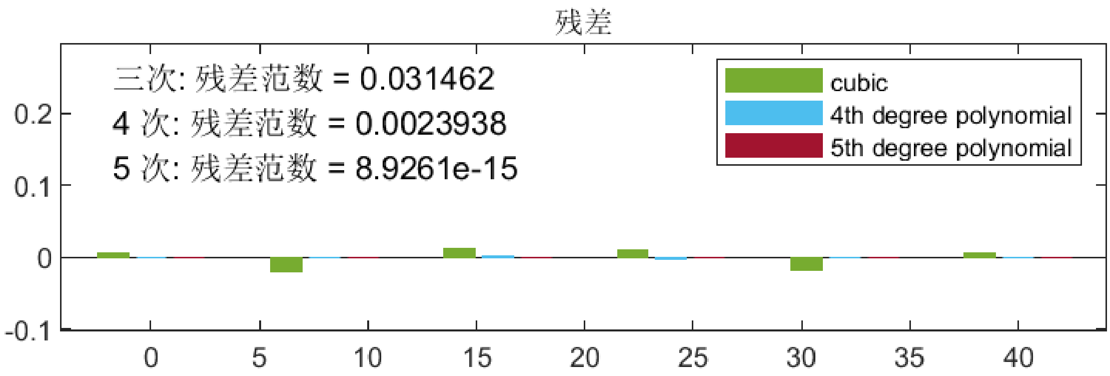
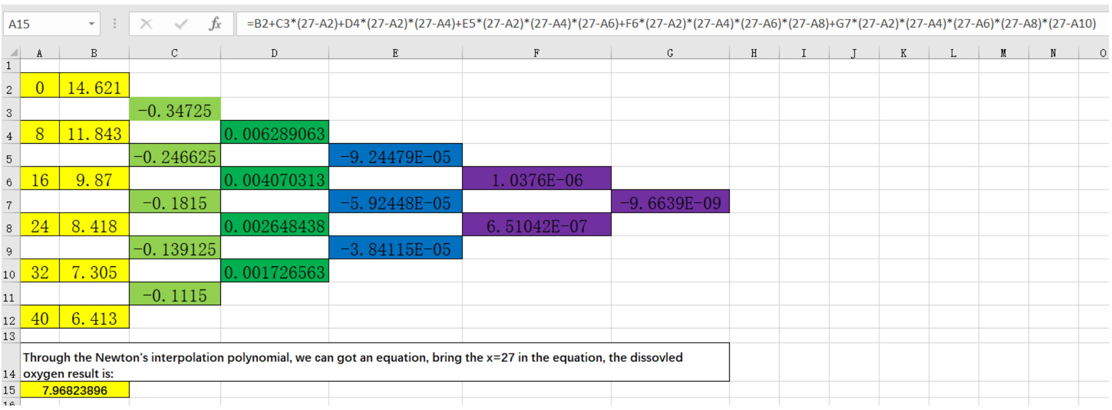


Fig 4 – the residuals of linear interpolation method

But as the figure 4 shows, when we calculate the residuals of the linear interpolation method, we find that the residuals of it 3rd, 4th, and 5th polynomials are getting smaller and smaller, which means that this formula is converge and higher the polynomial outcome, the more accurate it is.

As for the Newton's interpolation polynomial, I also determine it through the Excel, the result I get is 7.96823896, the steps t=shows in the following figure 5, which can prove that the result in the MATLAB is correct.



A15 =B2+C3*(27-A2)+D4*(27-A2)*(27-A4)+E5*(27-A2)*(27-A4)*(27-A6)+F6*(27-A2)*(27-A4)*(27-A6)*(27-A8)+G7*(27-A2)*(27-A4)*(27-A6)*(27-A8)*(27-A10)

	A	B	C	D	E	F	G
1							
2	0	14.621					
3			-0.34725				
4	8	11.843		0.006289063			
5			-0.246625		-9.24479E-05		
6	16	9.87		0.004070313		1.0376E-06	
7			-0.1815		-5.92448E-05		-9.6639E-09
8	24	8.418		0.002648438		6.51042E-07	
9			-0.139125		-3.84115E-05		
10	32	7.305		0.001726563			
11			-0.1115				
12	40	6.413					
13							
14	Through the Newton's interpolation polynomial, we can got an equation, bring the x=27 in the equation, the dissolved oxygen result is:						
15	7.96823896						

Fig 5 – determine the question4.3 under the Newton's interpolation method in Excel

After all I can conclude that the values calculated by the three methods are very accurate, the error between their result and the answer can be almost ignored, especially the Newton's interpolation method and cubic splines methods are the ideal way to solve the problem very easily and accurately.