《机械工程中的数值分析技术》

作业

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Catalog

Lec14 Curve Fitting

1.1 Question 14.11

14.11 Determine an equation to predict metabolism rate as a function of mass based on the following data. Use it to predict the metabolism rate of a 200-kg tiger.

Animal	Mass (kg)	Metabolism (watts)
Cow	400	270
Human	70	82
Sheep	45	50
Hen	2	4.8
Rat	0.3	1.45
Dove	0.16	0.97

The Matlab code is below:

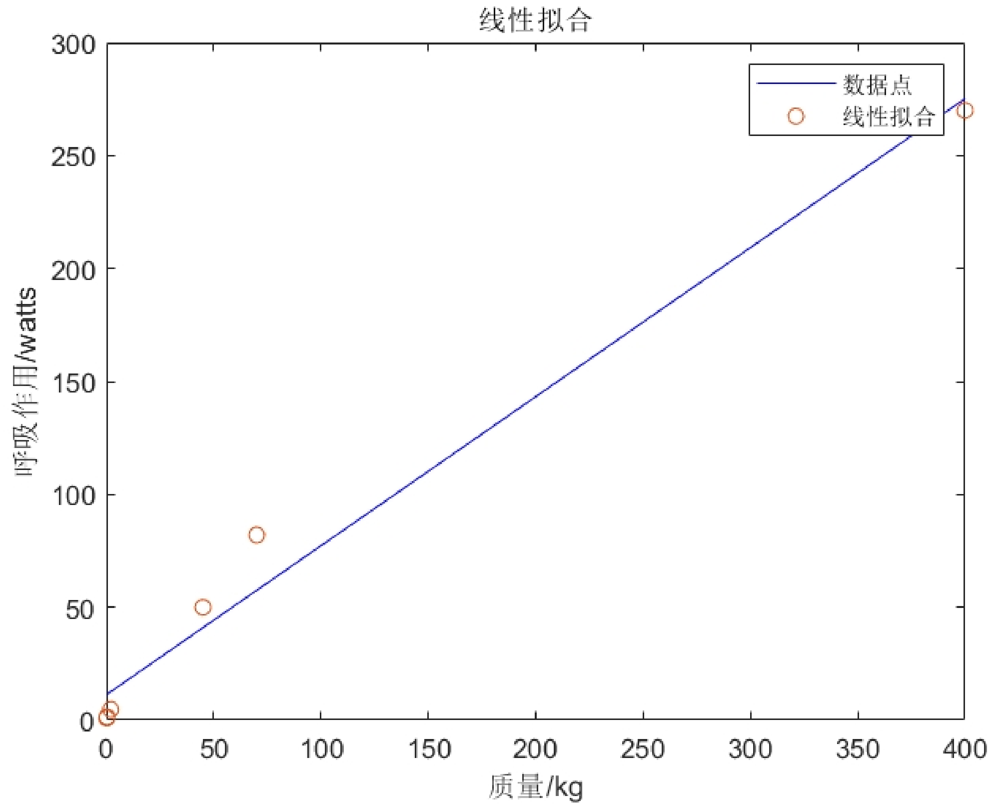
```
%% 14.11
clc;clear all;close all;
M = [400, 70, 45, 2, 0.3, 0.16];
Met = [270, 82, 50, 4.8, 1.45, 0.97];
e = exp(1);
xp = linspace(min(M),max(M),200);

% 线性拟合
[a_lin, r2_lin] = linear_regression(M, Met);
yp = a_lin(1)*xp+a_lin(2);
figure
plot(xp, yp, '-b')
hold on
plot(M, Met, 'o')
legend("数据点", "线性拟合")
title("线性拟合")
xlabel("质量/kg")
ylabel("呼吸作用/watts")

% 幂方拟合
[a_log, r2_log] = linear_regression(log(M), log(Met));
yp = e^a_log(2)*xp.^(a_log(1));
```

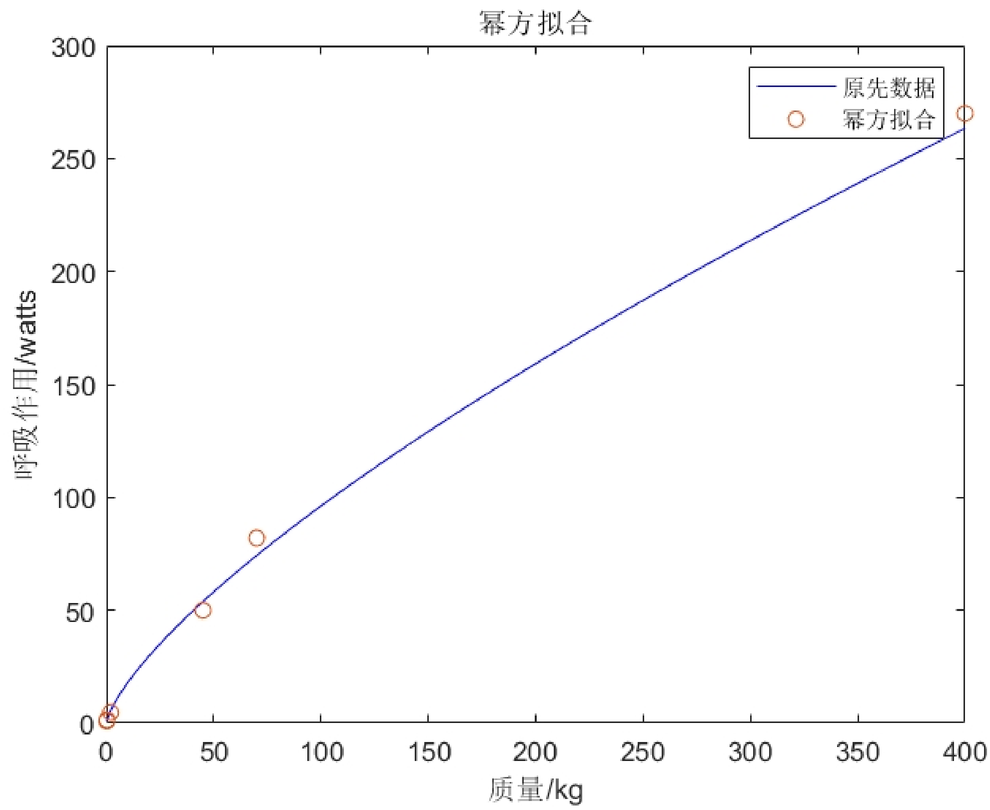
```
figure
plot(xp, yp, '-b')
hold on
plot(M, Met, 'o')
legend("原先数据", "幂方拟合")
title("幂方拟合")
xlabel("质量/kg")
ylabel("呼吸作用/watts")

fprintf("线性拟合决定系数: %f\n", r2_lin)
fprintf("幂方拟合决定系数: %f\n", r2_log)
fprintf("线性拟合200kg老虎的呼吸作用的预估: %f watts\n",
a_lin(1)*200+a_lin(2))
fprintf("幂方拟合200kg老虎的呼吸作用的预估: %f watts\n",
e^a_log(2)*200.^(a_log(1)))

function [a, r2] = linear_regression(x,y)
% linear_regression: 用于线性回归拟合
% input:
% x      自变量
% y      应变量
% output:
% a      包含两个元素，斜率和交点
% r2     决定系数，用于考量拟合效果
    n = length(x);
    if length(y) ~= n
        error('x and y must be same length');
    end
    x = x(:);
    y = y(:);
    sx = sum(x);
    sy = sum(y);
    sx2 = sum(x.*x);
    sxy = sum(x.*y);
    sy2 = sum(y.*y);
    a(1) = (n*sxy - sx*sy) / (n*sx2 - sx^2);
    a(2) = sy/n - a(1)*sx/n;
    r2 = ((n*sxy- sx*sy)/sqrt(n*sx2 - sx^2)/sqrt(n*sy2 - sy^2))^2;
end
```

The output is below:

```
线性拟合决定系数: 0.981926
幂方拟合决定系数: 0.998241
```

```
线性拟合 200kg 老虎的呼吸作用的预估: 143.272140 watts
幂方拟合 200kg 老虎的呼吸作用的预估: 159.204721 watts
```





1.2 Question 14.14

14.14 An investigator has reported the data tabulated below for an experiment to determine the growth rate of bacteria k (per d) as a function of oxygen concentration c (mg/L). It is known that such data can be modeled by the following equation:

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

where c_s and k_{max} are parameters. Use a transformation to linearize this equation. Then use linear regression to estimate c_s and k_{max} and predict the growth rate at $c = 2$ mg/L.

c	0.5	0.8	1.5	2.5	4
k	1.1	2.5	5.3	7.6	8.9

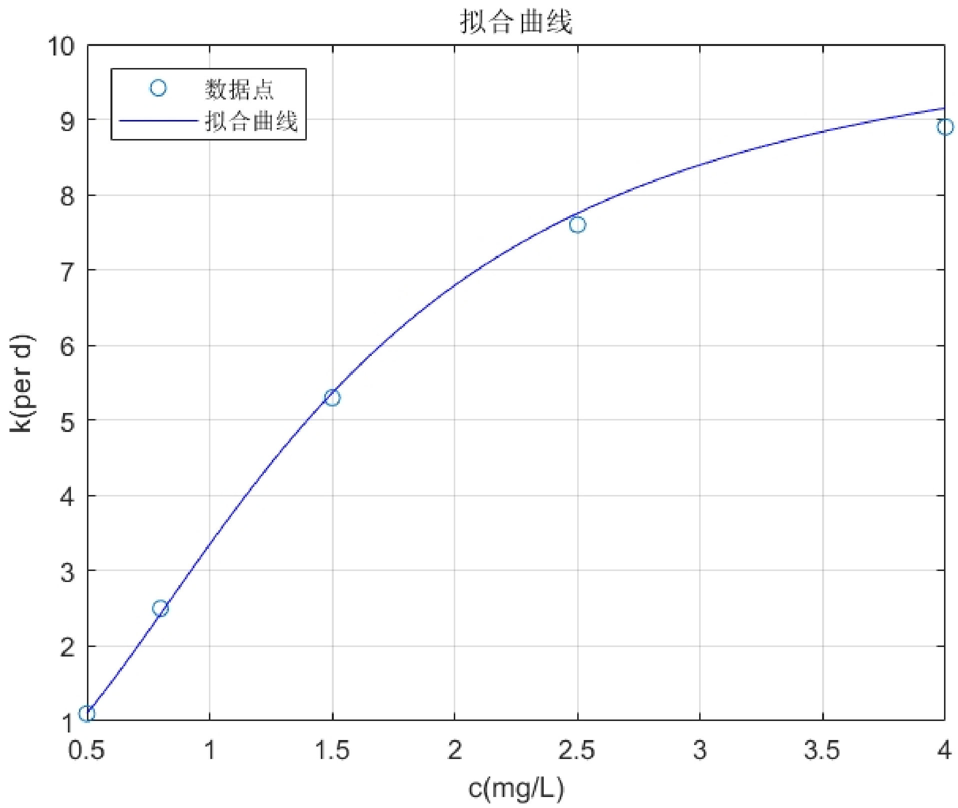
The Matlab code is below:

```
%% 14.14
clc; clear all; close all;
c = [0.5, 0.8, 1.5, 2.5, 4];
k = [1.1, 2.5, 5.3, 7.6, 8.9];
c_ = 1./c.^2;
k_ = 1./k;
[a, r2] = linear_regression(c_, k_);
kmax = 1/a(2);
cs = a(1)*kmax;
xp = linspace(min(c),max(c),200);
yp = (kmax*xp.^2)./(cs+xp.^2);
plot(c, k, 'o');
hold on
plot(xp, yp, '-b');
grid on
legend("数据点", "拟合曲线")
title("拟合曲线")
xlabel("c(mg/L)")
ylabel("k(per d)")
fprintf("拟合决定系数： %f\n", r2)
fprintf("kmax = %f\ncs = %f\n", kmax, cs)
fprintf("c = 2mg/L预测: k = %f\n", (kmax*2.^2)./(cs+2.^2))
```

```
function [a, r2] = linear_regression(x,y)
% linear_regression: 用于线性回归拟合
% input:
% x      自变量
% y      应变量
% output:
% a      包含两个元素，斜率和交点
% r2     决定系数，用于考量拟合效果
    n = length(x);
    if length(y) ~= n
        error('x and y must be same length');
    end
    x = x(:);
    y = y(:);
    sx = sum(x);
    sy = sum(y);
    sx2 = sum(x.*x);
    sxy = sum(x.*y);
    sy2 = sum(y.*y);
    a(1) = (n*sxy - sx*sy) / (n*sx2 - sx^2);
    a(2) = sy/n - a(1)*sx/n;
    r2 = ((n*sxy- sx*sy)/sqrt(n*sx2 - sx^2)/sqrt(n*sy2 - sy^2))^2;
end
```

The output is below:

```
拟合决定系数： 0.999569
kmax = 10.344931
cs = 2.089730
c = 2mg/L 预测：k = 6.795002
```



1.3 Question 14.21

14.21 The following data were taken from a stirred tank reactor for the reaction $A \rightarrow B$. Use the data to determine the best possible estimates for k_{01} and E_1 for the following kinetic model:

$$-\frac{dA}{dt} = k_{01} e^{-E_1/RT} A$$

where R is the gas constant and equals 0.00198 kcal/mol/K.

$-dA/dt$ (moles/L/s)	460	960	2485	1600	1245
A (moles/L)	200	150	50	20	10
T (K)	280	320	450	500	550

The Matlab code is below:

```
%% 14.21
clc;clear all;
```

```
dAdt=[460 960 2485 1600 1245];
A=[200 150 50 20 10];
T=[280 320 450 500 550];
y=log(dAdt./A);
TI=1./T;
[a,r2]=linear_regression(TI,y) ;
k01=exp(a(2)) ;
E1=-a(1)*0.00198;
fprintf("k01预测值： %f\n", k01)
fprintf("E1预测值： %f\n", E1)
function [a, r2] = linear_regression(x,y)
% linear_regression: 用于线性回归拟合
% input:
% x      自变量
% y      应变量
% output:
% a      包含两个元素，斜率和交点
% r2     决定系数，用于考量拟合效果
    n = length(x);
    if length(y) ~= n
        error('x and y must be same length');
    end
    x = x(:);
    y = y(:);
    sx = sum(x);
    sy = sum(y);
    sx2 = sum(x.*x);
    sxy = sum(x.*y);
    sy2 = sum(y.*y);
    a(1) = (n*sxy - sx*sy) / (n*sx2 - sx^2);
    a(2) = sy/n - a(1)*sx/n;
    r2 = ((n*sxy- sx*sy)/sqrt(n*sx2 - sx^2)/sqrt(n*sy2 - sy^2))^2;

end
```

The output is below:

```
k01 预测值： 7620.498573
E1 预测值： 4.491309
```

Lec 15 General Linear Least-Squares and Nonlinear Regression

2.1 Question 15.8

15.8 Use multiple linear regression to fit

x_1	0	1	1	2	2	3	3	4	4
x_2	0	1	2	1	2	1	2	1	2
y	15.1	17.9	12.7	25.6	20.5	35.1	29.7	45.4	40.2

Compute the coefficients, the standard error of the estimate, and the correlation coefficient.

The Matlab code is below:

```
%% 15.8
clc; clear all; close all;
x1 = [0, 1, 1, 2, 2, 3, 3, 4, 4];
x2 = [0, 1, 2, 1, 2, 1, 2, 1 ,2];
y = [15.1, 17.9, 12.7, 25.6, 20.5, 35.1, 29.7, 45.4, 40.2];
a = MLR(x1, x2, y);
sr = sum((y-a(1)*x1-a(2)*x2-a(3)).^2);
st = sum((y-mean(y)).^2);
r = sqrt((st-sr)/st);
error = sqrt((sr/(length(x1)-(2+1))));

for i= 1:2
    fprintf("系数%d for x%d: %f\n", i, i, a(i))
end
fprintf("交点: %f\n", a(3))
fprintf("标准误差: %f\n", error)
fprintf("相关系数: %f\n", r)

function [a] = MLR(x1, x2, y)
% input:
% x1     自变量1
```

```
% x2    自变量2
% y     应变量
% output:
% a     包含三个元素，两个斜率和一个交点
    n = length(y);
    if length(x1) ~= n || length(x2) ~= n
        error('x and y must be same length');
    end
    x1 = x1(:);
    x2 = x2(:);
    y = y(:);
    x1m = mean(x1);
    x2m = mean(x2);
    ym = mean(y);
    x1 = x1-x1m;
    x2 = x2-x2m;
    y = y-ym;
    sx1x2 = sum(x1.*x2);
    sx1_2 = sum(x1.*x1);
    sx2_2 = sum(x2.*x2);
    sx1y = sum(x1.*y);
    sx2y = sum(x2.*y);
    a(1) = (sx1y*sx2_2-sx2y*sx1x2)/(sx1_2*sx2_2-sx1x2^2);
    a(2) = (sx2y*sx1_2-sx1y*sx1x2)/(sx1_2*sx2_2-sx1x2^2);
    a(3) = ym-a(1)*x1m-a(2)*x2m;
end
```

The output is below:

```
系数 1 for x1: 9.025217
系数 2 for x2: -5.704348
交点: 14.460870
标准误差: 0.888787
相关系数: 0.997759
```

2.2 Question 15.10

15.10 Three disease-carrying organisms decay exponentially in seawater according to the following model:

$$p(t) = Ae^{-1.5t} + Be^{-0.3t} + Ce^{-0.05t}$$

Estimate the initial concentration of each organism (A, B, and C) given the following measurements:

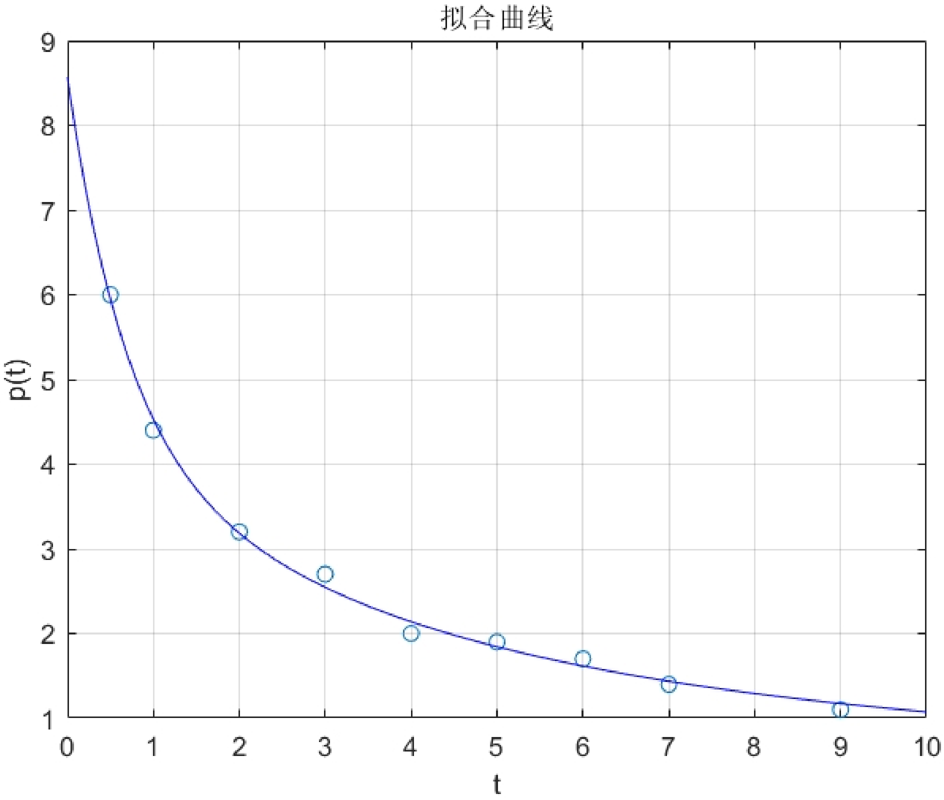
t	0.5	1	2	3	4	5	6	7	9
$p(t)$	6	4.4	3.2	2.7	2	1.9	1.7	1.4	1.1

The Matlab code is below:

```
%% 15.10
clc; clear all;
t = [0.5, 1, 2, 3, 4, 5, 6, 7, 9];
t = t(:);
p = [6, 4.4, 3.2, 2.7, 2, 1.9, 1.7, 1.4, 1.1];
p = p(:);
e = exp(1);
Z = [e.^(-1.5*t), e.^(-0.3*t), e.^(-0.05*t)];
a = (Z'*Z)\(Z'*p);
x = linspace(0, 10, 100);
y = a(1)*e.^(-1.5*x) + a(2)*e.^(-0.3*x) + a(3)*e.^(-0.05*x);
plot(t, p, 'o')
hold on
plot(x, y, '-b')
grid on
title("拟合曲线")
xlabel("t")
ylabel("p(t)")
string = ["A", "B", "C"];
fprintf("系数A，B，C分别为%f,%f,%f",a(1),a(2),a(3))
```

The output is below:

```
系数A，B，C分别为4.137497,2.895882,1.534920
```



2.3 Question 15.19

15.19 Environmental scientists and engineers dealing with the impacts of acid rain must determine the value of the ion product of water K_w as a function of temperature. Scientists have suggested the following equation to model this relationship:

$$-\log_{10} K_w = \frac{a}{T_a} + b\log_{10} T_a + cT_a + d$$

where T_a = absolute temperature (K), and a, b, c, and d are parameters. Employ the following data and regression to estimate the parameters with MATLAB. Also, generate a plot of predicted K_w versus the data.

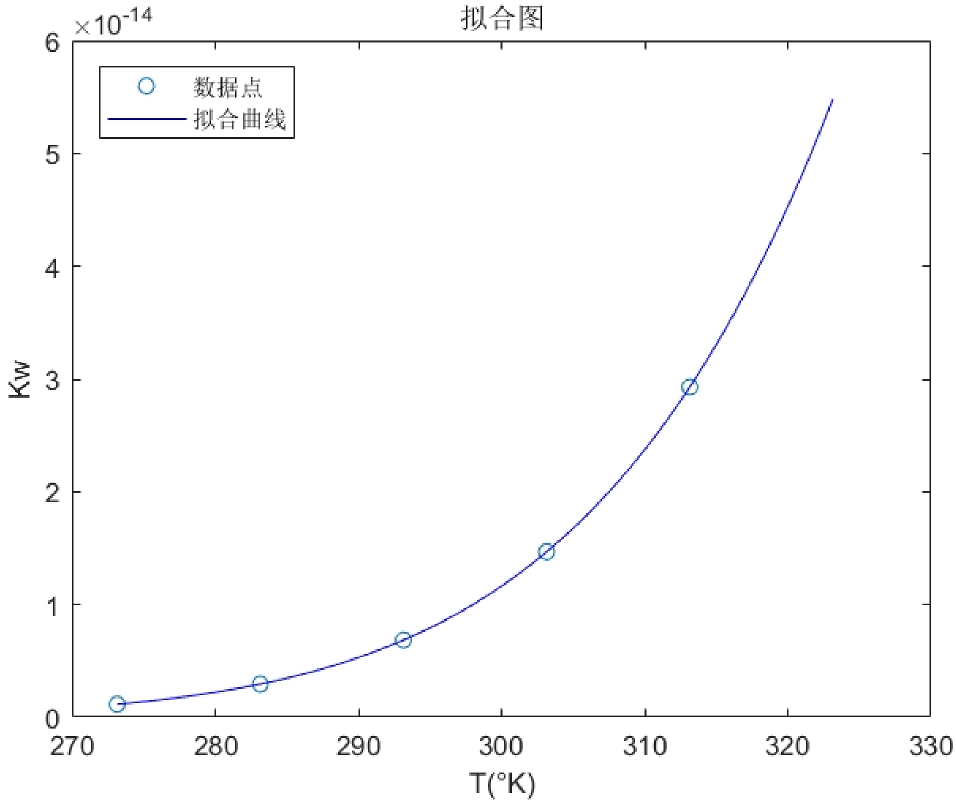
T (°C)	K_w
0	1.164×10^{-15}
10	2.950×10^{-15}
20	6.846×10^{-15}
30	1.467×10^{-14}
40	2.929×10^{-14}

The Matlab code is below:

```
%% 15.19
clc;clear all;close all;
T = [0, 10, 20, 30, 40];
T = T + 273.15;
T = T(:);
Kw = [1.164e-15, 2.95e-15, 6.846e-15, 1.467e-14, 2.929e-14];
Kw_ = -log10(Kw);
Kw_ = Kw_(:);
Z = [1./T, log10(T), T, ones(size(T))];
a = (Z'*Z)\(Z'*Kw_);
tp = linspace(0+273.15, 50+273.15, 100);
Kw_d = 10.^(-(a(1)./tp+a(2)*log10(tp)+a(3)*tp+a(4)));
plot(T, Kw, 'o')
hold on
plot(tp, Kw_d, "-b")
legend("数据点", "拟合曲线")
xlabel("T(°K)")
ylabel("Kw")
title("拟合图")
string = ["a", "b", "c", "d"];
fprintf("系数a,b,c,d分别为%f,%f,%f,%f", a(1),a(2),a(3),a(4));
```

The output is below:

```
系数 a,b,c,d 分别为 5180.685972,13.424329,0.005629,-38.276954
```


拟合图
×10^-14
6
5
4
3
2
1
0
Kw
数据点
拟合曲线
270
280
290
300
310
320
330
T(°K)