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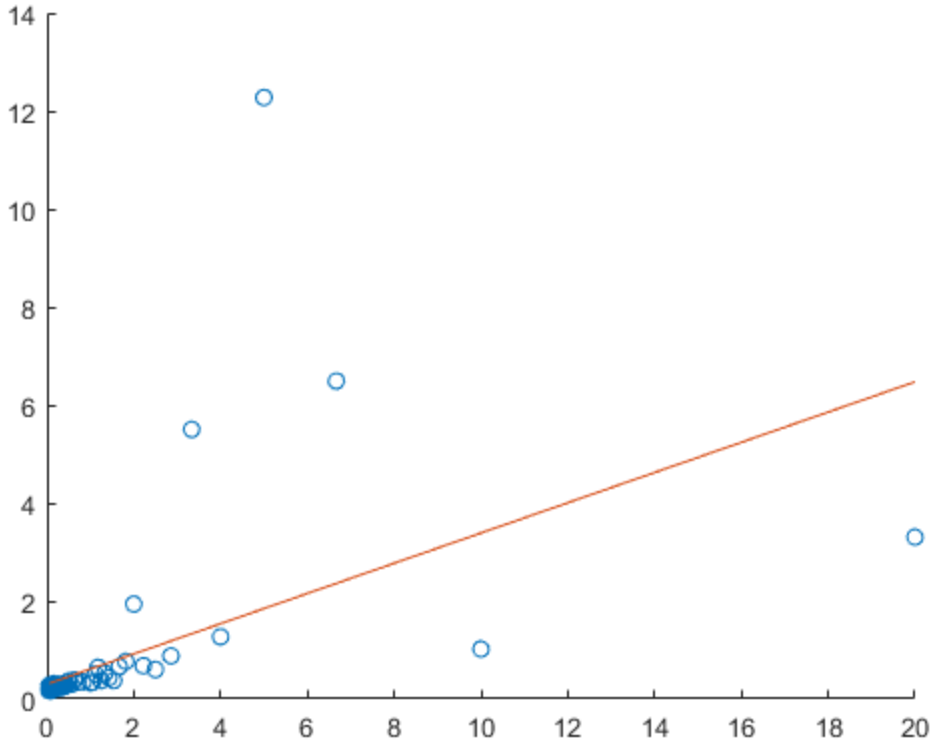
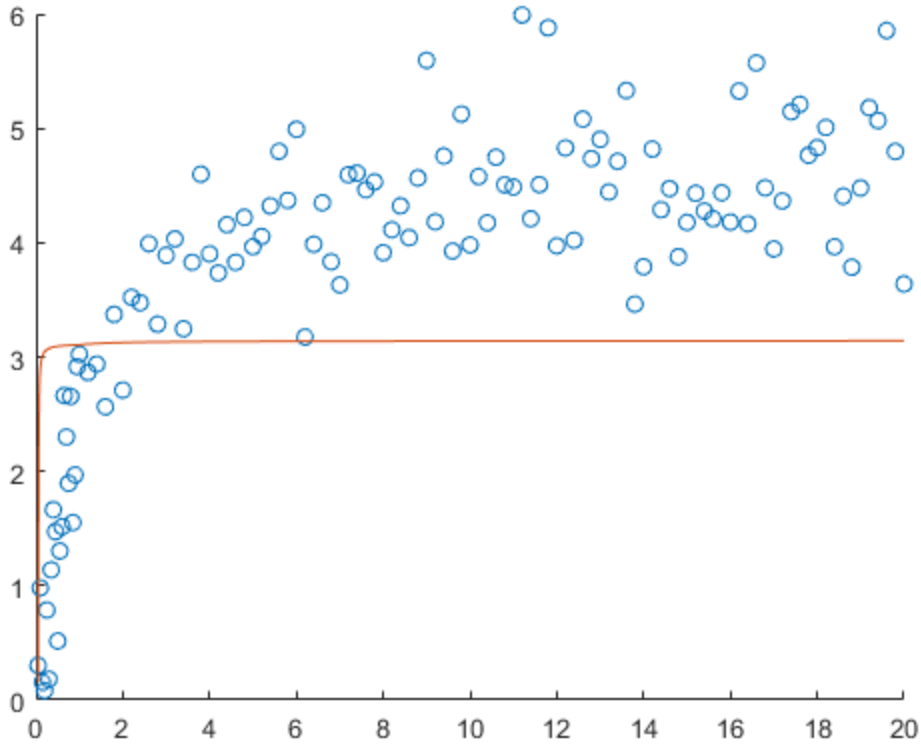
```
close all
clear all
```

Problem 2 Part 1

```
[data_ID, S, reactionrate] = textread('Problem2_kineticsData.txt', '%f
%f%f', 'headerlines', 1);
t = S;
y = reactionrate;

%take reciprocal to build A and b
t_recip = 1./S;
y_recip = 1./reactionrate;

%take reciprocal to build A and b
z = ones(115, 1);
A = [t_recip z];
b = y_recip;
G = A' * A;
b_new = A' * b;
x_ster = G\b_new;

yrecipfit = x_ster(1) .* t_recip + x_ster(2);

f0 = figure('Name', 'Reciprocal-Transformed Data');

h1 = scatter(t_recip, y_recip);
hold on
plot(t_recip, yrecipfit)
% xlabel(1/S)
% ylabel(1/y) %when i run this the plots just become single points
% title('Initial fit on reciprocal transformed data')

Vmax = 1/x_ster(2);
Km = x_ster(1) * Vmax;


f1 = figure('Name', 'Original Data');

h2 = scatter(t, y);
hold on
yorigfit = Vmax * (S)./(S + Km);
```

```
plot(t_recip, flip(yorigfit))
% ylabel(y)
% xlabel(S)
% title('Initial fit on original data')
```



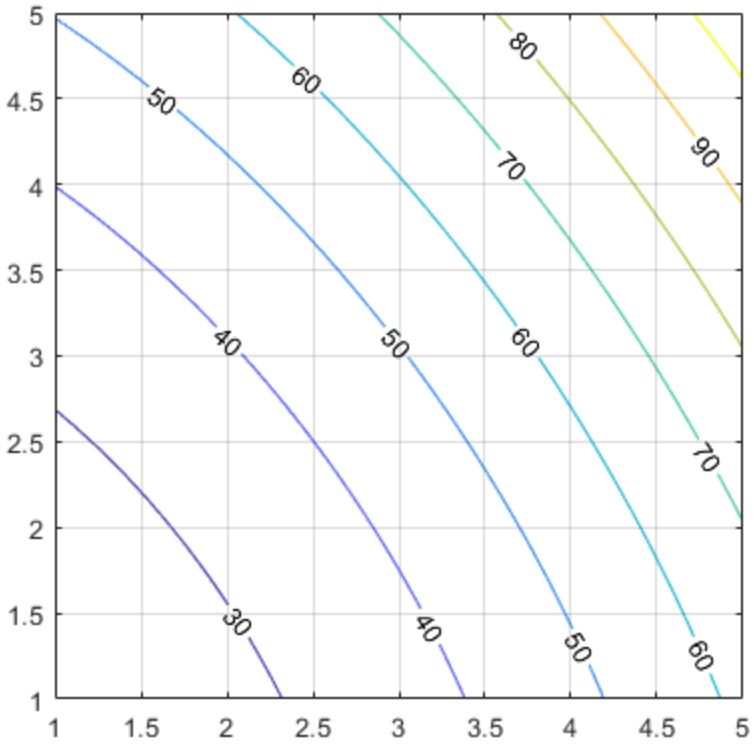


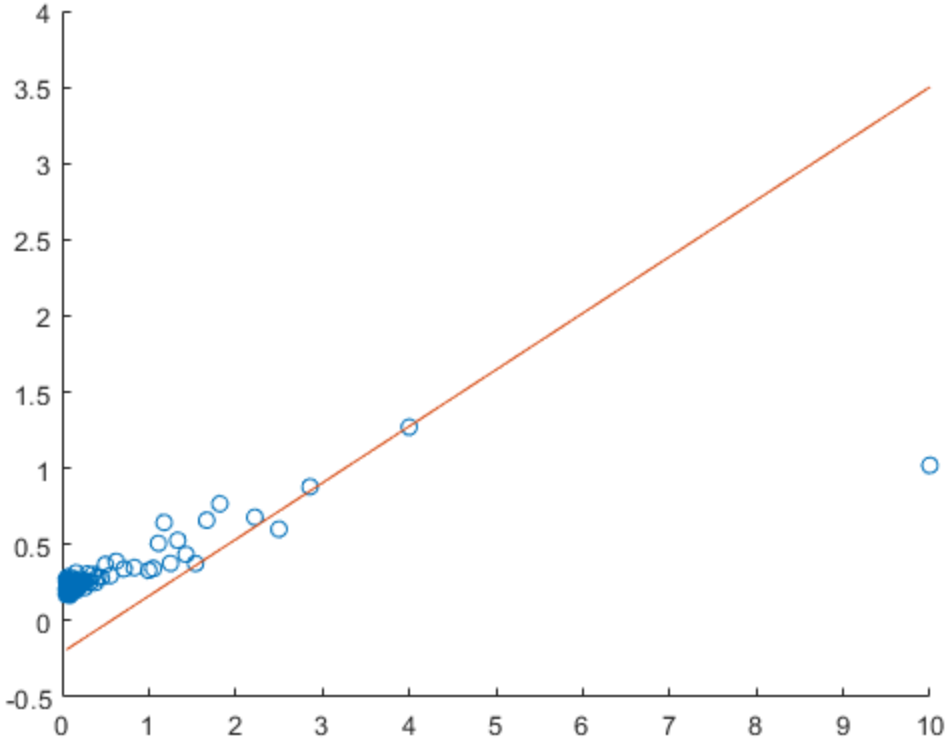
Task 2

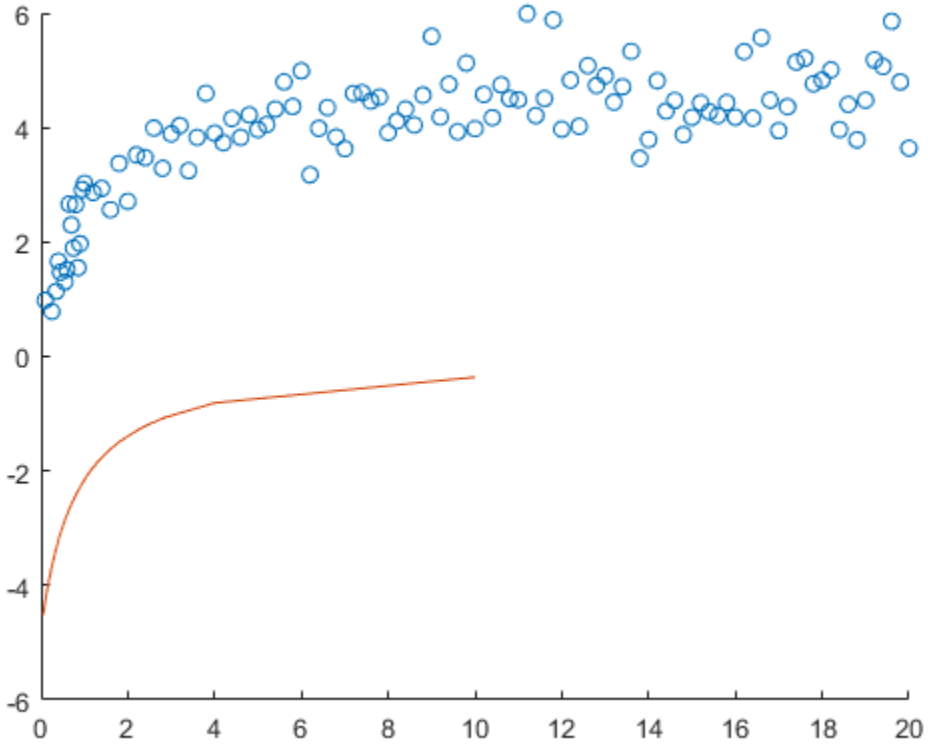
```
data_IDnew=data_ID(6:end);
t_new=[t(2); t(5); t(7:9); t(11:end)];
y_new=[y(2); y(5); y(7:9); y(11:end)];
tn_recip = 1./t_new;
yn_recip = 1./y_new;
z=ones(1,110);
An=[tn_recip z'];
bn=[yn_recip];
Gn=An'*An;
b_newn=An'*bn;
xn=Gn\b_newn;

x1 = 1:0.05:5;
x2 = 1:0.05:5;

[X1, X2] = meshgrid(x1, x2);

Z = (Gn(1)*X1.^2 + Gn(4) * X2.^2 + 2 * Gn(2) * X1.*X2) - 2 * (31.5457
 * X1 + X2 *32) + norm(b_newn)^2;
z2 = Z./100;
% ZP=Gn(1).*X1.^2+(2*Gn(4)).*X1.*X2+Gn(2).*X2.^2-(2*b_newn(1)).*X1-
(2*b_newn(2)).*X2+norm(b_newn)^2;
```

```
f2 = figure('Name', 'Contour Plot');
contour(X1,X2,z2, 'ShowText', 'on')
axis square
grid on

%wo

x0 = [3;1];

zaxisaltitude = (b_newn-Gn*x0)'*(b_newn-Gn*x0);
w0 = 2*(b_newn - Gn * x0);
alph = 0.5 * (w0' * w0)/(w0' * Gn * w0);
x1 = x0 + alph*w0;

rvec = 1;
xk = x0;
n = 2;
zaxisalttot = zaxisaltitude;
wktot = w0;
xktot = x0;
alphktot = alph;
while rvec>1e-4
    zaxisaltk = (b_newn-Gn*xk)'*(b_newn-Gn*xk);
    zaxisalttot = [zaxisalttot zaxisaltk];
    wk = 2*(b_newn - Gn * xk);
    alphk = 0.5 * (wk' * wk)/(wk' * Gn * wk);
    xk = xk + alph*wk;
    rvec = abs(zaxisaltk - zaxisalttot(n-1));
    wktot = [wktot wk];
    alphktot = [alphktot alphk];

    xktot = [xktot xk];
    n = n+1;
end

%couldn't get the plot to work properly

optimumx_ster = xktot(:,2);

yrecipfitnew = optimumx_ster(1) .* tn_recip + optimumx_ster(2);

f3 = figure('Name', 'Reciprocal-Transformed Data');

h1 = scatter(tn_recip, yn_recip);
hold on
plot(tn_recip, yrecipfitnew)
% xlabel(1/S)
% ylabel(1/y)
% title('New fit on Reciprocal Transformed Data')

%this obviously isn't right, but i'm not sure where i'm wrong

Vmax_new = 1/optimumx_ster(2);
Km_new = optimumx_ster(1) * Vmax;
```

```
f4 = figure('Name', 'Original Data');

h5 = scatter(t_new, y_new);
hold on
ynewfit = Vmax_new * (t_new)./(t_new + Km_new);
plot(tn_recip, ynewfit)
% ylabel(y)
% xlabel(S)
% title('New fit on Original Data')
```




4
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
0
1
2
3
4
5
6
7
8
9
10


6
4
2
0
-2
-4
-6
0
2
4
6
8
10
12
14
16
18
20

Echoing Resuls

```
diary vjprob2.txt
echo on
disp('Part 1')
G
b_new
x_ster

data_ID(1)
data_ID(3)
data_ID(4)
data_ID(6)
data_ID(10)

Vmax
Km

disp('Part 2')

zaxisalttot
xktot
wktot
alphktot

Vmax_new
Km_new

echo off

disp('Part 1')
Part 1
G

G =

  642.7496   86.4750
   86.4750  115.0000

b_new

b_new =

  224.4653
   61.5112

x_ster

x_ster =

    0.3085
    0.3029
```

```
data_ID(1)

ans =

     1

data_ID(3)

ans =

     3

data_ID(4)

ans =

     4

data_ID(6)

ans =

     6

data_ID(10)

ans =

    10


Vmax

Vmax =

    3.3012

Km

Km =

    1.0183


disp('Part 2')
Part 2

zaxisalttot

zaxisalttot =

   1.0e+05 *
```

```
    2.9383    2.9383

xktot

xktot =

    3.0000    0.3710
    1.0000   -0.2086

wktot

wktot =

 -985.0231 -985.0231
 -452.8390 -452.8390

alphktot

alphktot =

    0.0027    0.0027


Vmax_new

Vmax_new =

   -4.7936

Km_new

Km_new =

    1.2248


echo off
```

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