Project 1

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1 Problem 1

(a) Let

$$J(\theta^{n-1}) = \begin{bmatrix} \frac{dx(t_1, \theta^{n-1})}{d\theta^{n-1}} \\ \frac{dx(t_2, \theta^{n-1})}{d\theta^{n-1}} \\ \frac{dx(t_3, \theta^{n-1})}{d\theta^{n-1}} \\ \vdots \\ \frac{dx(t_n, \theta^{n-1})}{d\theta^{n-1}} \end{bmatrix}$$

and

$$G(\theta^{n-1}) = \begin{bmatrix} y_1 - x(t_1, \theta^{n-1}) \\ y_2 - x(t_2, \theta^{n-1}) \\ y_3 - x(t_3, \theta^{n-1}) \\ \vdots \\ y_n - x(t_n, \theta^{n-1}) \end{bmatrix}$$

where y_i is the data at t_i and $x(t_i, \theta^{n-1})$ is the approximate at t_i using θ^{n-1} as the parameter (i = 1, ..., n).

Then for each iteration step:

$$\begin{split} H(\theta^{n-1}) &= J(\theta^{n-1})^T J(\theta^{n-1}) \\ g(\theta^{n-1}) &= J(\theta^{n-1})^T G(\theta^{n-1}) \\ \theta^n &= \theta^{n-1} + H(\theta^{n-1})^{-1} g(\theta^{n-1}) \end{split}$$

(b) Sensitivity System:

$$D \begin{bmatrix} x \\ \partial_{\theta} x \end{bmatrix} = \begin{bmatrix} x^{2}\theta \\ x^{2} + 2x\theta u \end{bmatrix}$$
$$\begin{bmatrix} x \\ u \end{bmatrix} (1) = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$$

(c) See code at the end of this document.

- (d) Using the built-in **fminsearch** function, we get $\theta \approx 1.8433$. The optimal parameter found by Gauss-Newton method was $\theta \approx 1.8319$.
- (e) The following figure shows the convergence of θ and SSE:

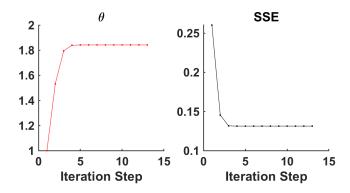


Figure 1: Convergence of θ and SSE

2 Problem 2

(a) Let

$$J(\theta^{n-1}) = \begin{bmatrix} \frac{dx(t_1, \theta^{n-1}, x_0)}{d\theta^{n-1}} & \frac{dx(t_1, \theta^{n-1}, x_0)}{dx_0} \\ \frac{dx(t_2, \theta^{n-1}, x_0)}{d\theta^{n-1}} & \frac{dx(t_2, \theta^{n-1}, x_0)}{dx_0} \\ \frac{dx(t_3, \theta^{n-1}, x_0)}{d\theta^{n-1}} & \frac{dx(t_3, \theta^{n-1}, x_0)}{dx_0} \\ \vdots & \vdots \\ \frac{dx(t_n, \theta^{n-1}, x_0)}{d\theta^{n-1}} & \frac{dx(t_n, \theta^{n-1}, x_0)}{dx_0} \end{bmatrix}$$

and

$$G(\theta^{n-1}) = \begin{bmatrix} y_1 - x(t_1, \theta^{n-1}, x_0) \\ y_2 - x(t_2, \theta^{n-1}, x_0) \\ y_3 - x(t_3, \theta^{n-1}, x_0) \\ \vdots \\ y_n - x(t_n, \theta^{n-1}, x_0) \end{bmatrix}$$

where y_i is the data at t_i and $x(t_i, \theta^{n-1})$ is the approximate at t_i using θ^{n-1} as the parameter (i = 1, ..., n).

Then for each iteration step:

$$\begin{split} H(\theta^{n-1}) &= J(\theta^{n-1})^T J(\theta^{n-1}) \\ g(\theta^{n-1}) &= J(\theta^{n-1})^T G(\theta^{n-1}) \\ \theta^n &= \theta^{n-1} + H(\theta^{n-1})^{-1} g(\theta^{n-1}) \end{split}$$

(b) Sensitivity System:

$$D \begin{bmatrix} x \\ \partial_{\theta} x \\ \partial_{x_0} x \end{bmatrix} (1) = \begin{bmatrix} -0.9 \\ 0 \\ 1\theta v \end{bmatrix}$$

- (c) See code at the end of this document.
- (d) Using the build in function **fminsearch**, we get $\theta \approx 1.7553$ and $x_0 \approx -0.8963$. Using the Gauss-Newton method, we get $\theta \approx 1.7543$ and $x_0 \approx -0.8963$.
- (e) The following figure shows the convergence of θ , x_0 and SSE:

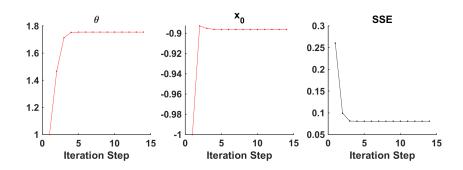


Figure 2: Convergence of θ , x_0 and SSE

3 Problem 3

(a) This problem is similar to problem 1 (a), just replace the Jacobian matrix with the one below:

$$J(a^{n-1},b^{n-1}) = \begin{bmatrix} \frac{dx(t_1,a^{n-1},b^{n-1})}{da^{n-1}} & \frac{dy(t_1,a^{n-1},b^{n-1})}{da^{n-1}} & \frac{dx(t_1,a^{n-1},b^{n-1})}{da^{n-1}} & \frac{dx(t_1,a^{n-1},b^{n-1})}{dx(t_2,a^{n-1},b^{n-1})} & \frac{dx(t_1,a^{n-1},b^{n-1})}{dx(t_2,a^{n-1},b^{n-1})} & \frac{dy(t_1,a^{n-1},b^{n-1})}{dx(t_2,a^{n-1},b^{n-1})} & \frac{dy(t_1,a^{n-1},b^{n-1})}{dy(t_2,a^{n-1},b^{n-1})} & \frac{dy(t_1,a^{n-1},b^{n-1})}{dx(t_2,a^{n-1},b^{n-1})} & \frac{dy(t_1,a^{n-$$

In each iteration step, the first two columns are added with the last two columns to create the gradient matrix with respect to a and b.

(b)
$$D\begin{bmatrix} x \\ y \\ \partial_a x \\ \partial_a y \\ \partial_b x \\ \partial_b y \end{bmatrix} = \begin{bmatrix} -axy \\ axy - by \\ -xy - ay\partial_a x - ayx\partial_a y \\ xy + ay\partial_a x + (ax - b)\partial_a y \\ -ay\partial_b x - ax\partial_b y - y + ay\partial_b x + (ax - b)\partial_b y \end{bmatrix}$$
$$D\begin{bmatrix} x \\ y \\ \partial_a x \\ \partial_a y \\ \partial_b x \\ \partial_b y \end{bmatrix} (0) = \begin{bmatrix} 0.9 \\ 0.1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

- (c) See code at the end of this document.
- (d) Using the built-in **fminsearch** function, we get $a \approx 0.5023$ and $b \approx 0.1031$. The optimal parameters found by Gauss-Newton method was $a \approx 0.5132$ and $b \approx 0.1091$.
- (e) The following figure shows the convergence of a, b and SSE:

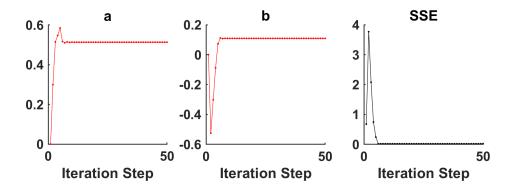
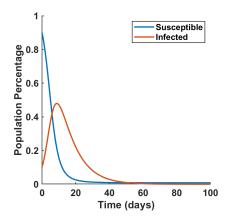


Figure 3: Convergence of a, b and SSE

(f) The figure below shows the population percentage over time: As shown in Figure (f), the susceptible population levels off to around 0.0085 while the infected population goes to zero.



Matlab Code

Problem 1

```
close all;
   clear all;
   format long;
   plotting=1;
   global xexp
   global texp
   global xt0
   %Experimental data
   xexp = \begin{bmatrix} -0.9 & -0.3 & -0.28 & -0.15 & -0.13 \end{bmatrix}';
   texp = [1:5];
   xt0 = -1;
13
   a_{pt_init} = 1;
14
15
   method = 2; % 1=fminsearch, 2=Newton
16
17
   if (method==1)
        % Finding the parameter values minimizing SSE error
19
             using built-in function
         [\,a\_opt\,,fval\,,exitflag\,,output\,]\,\,=\,\,fminsearch\,(@SSE\,,[
20
             a_opt_init])
21
   _{\rm else}
22
        %Newton-Raphson method
23
        aa(1) = [a_opt_init];
         \operatorname{error}(1) = \operatorname{SSE}(\operatorname{aa}(1));
```

```
delta1 = 1e-16;
26
        delta2 = 1e-16;
27
        Nsteps = 200;
28
        for k=1:Nsteps
30
31
            %Need to solve ODE on a finer grid
32
            tt = linspace(texp(1), texp(end), 1000);
33
            zt0 = [xt0, 0]; %initial data for the sensitivity
34
                system
            [tspan, zz] = ode45(@(t,z)sens(t,z,aa(k)),tt,zt0);
35
            z = interp1(tt,zz,texp); %getting back to the
36
                 coarser grid to compare with xexp
37
            %Jacobian calculation
            J1 = [z(:,2)];
39
40
            %Hessian with weights
41
            H = J1' * J1;
            g = J1'*(xexp - z(:,1));
43
45
            %Newton direction = inv(H)*g, but
46
            %Better to use slash command for a more stable
47
                 calculation
            aa(k+1) = aa(k) + (H\backslash g);
48
            a_{-}opt = aa(k+1);
            \operatorname{error}(k+1) = \operatorname{SSE}(a_{-}\operatorname{opt});
50
51
             if (norm(aa(k+1)-aa(k)) < delta1) | (abs(SSE(aa(k+1)-aa(k)) < delta1) |
52
                 +1))-SSE(aa(k)))<delta2)
                 % Plotting convergence of parameters
53
                 figure(2);
54
                 subplot(1,2,1);
                 set (gca, 'FontName', 'Arial', 'FontSize', 14, '
56
                     FontWeight', 'Bold', 'LineWidth', 1);
                 hold on;
57
                 title('\theta')
58
                 xlabel("Iteration Step")
59
                 axis square;
                 plot (1: length (aa), aa, 'r.-');
                 subplot(1,2,2);
63
                 set (gca, 'FontName', 'Arial', 'FontSize', 14, '
64
                     FontWeight', 'Bold', 'LineWidth', 1);
                 hold on;
65
```

```
title('SSE');
66
                 xlabel("Iteration Step")
67
                 axis square;
68
                  plot (1: length (aa), error, 'k.-');
                 break;
70
             end
71
        end
72
   end
73
74
    if (plotting == 1)
76
        [tspan,x] = ode45(@(t,x)system(t,x,a_opt),texp,xt0);
77
78
        figure (1);
79
        set (gca, 'FontName', 'Arial', 'FontSize', 14, 'FontWeight'
            , 'Bold', 'LineWidth', 1);
        hold on;
81
        axis square;
82
        title ('x vs. t');
        plot(tspan, x, 'r'.;');
84
        plot(texp,xexp,'bo');
        legend('ODE', 'data');
86
   end
88
    function z = SSE(a)
    global texp
    global xexp
    global xt0
    [tspan, x] = ode45(@(t,x)system(t,x,a),texp,[xt0]);
95
   z = norm(x-xexp, 2);
97
98
   end
99
100
    function dxdt=system(t,x,a)
101
   dxdt = a*x^2;
103
104
   end
105
106
    function dzdt = sens(t,z,a)
107
   dzdt(1)=a*z(1)^2;
109
   dzdt(2)=z(1)^2+2*a*z(1)*z(2);
```

```
111
   dzdt = dzdt;
112
   end
113
   Problem 2
   close all;
    clear all;
    format long;
    plotting=1;
    global xexp
    global texp
   %Experimental data
   xexp = \begin{bmatrix} -0.9 & -0.3 & -0.28 & -0.15 & -0.13 \end{bmatrix}';
    texp = [1:5];
    a_{pt_i} = 1;
    xt0_init = -1;
   method =2; % 1=fminsearch, 2=Newton
15
16
    if (method == 1)
17
        % Finding the parameter values minimizing SSE error
18
            using built-in function
        [a_opt, fval, exitflag, output] = fminsearch(@SSE,[
19
            a_opt_init xt0_init])
20
    {\rm else}
21
        %Newton-Raphson method
22
        aa(1,:) = [a_opt_init xt0_init];
23
        \operatorname{error}(1) = \operatorname{SSE}(\operatorname{aa}(1,:));
        delta1 = 1e-16;
        delta2 = 1e-16;
26
        Nsteps = 200;
        for k=1:Nsteps
30
             %Need to solve ODE on a finer grid
31
             tt = linspace(texp(1), texp(end), 100);
             zt0 = [aa(k,2);0;1]; %initial data for the
33
                 sensitivity system
             [tspan, zz] = ode45(@(t,z)sens(t,z,aa(k,1)),tt,zt0
34
                 );
             z = interp1(tt, zz, texp); % getting back to the
35
                 coarser grid to compare with xexp
```

```
36
            %Jacobian calculation
37
            J1 = [z(:,2:3)];
38
            %Hessian with weights
40
            H = J1'*J1;
41
            g = J1'*(xexp - z(:,1));
42
43
44
            %Newton direction = inv(H)*g, but
            %Better to use slash command for a more stable
46
                calculation
            aa(k+1,:) = aa(k,:) + (H\backslash g)';
47
            a_{-}opt = aa(k+1,:);
48
            \operatorname{error}(k+1) = \operatorname{SSE}(a_{-}\operatorname{opt});
49
50
             if (norm(aa(k+1,:)-aa(k,:)) < delta1) \mid (abs(SSE(aa))) < delta1)
51
                (k+1,:))-SSE(aa(k,:))<delta2)
                 % Plotting convergence of parameters
                 figure (2);
53
                 subplot(1,3,1);
                 set (gca, 'FontName', 'Arial', 'FontSize', 14, '
                     FontWeight', 'Bold', 'LineWidth', 1);
                 hold on;
56
                 title ('\theta')
57
                 xlabel("Iteration Step")
                 axis square;
                 plot(1: length(aa(:,1)), aa(:,1), 'r.-');
60
61
                 subplot(1,3,2);
62
                 set (gca, 'FontName', 'Arial', 'FontSize', 14, '
63
                     FontWeight', 'Bold', 'LineWidth', 1);
                 hold on;
64
                 title ('x_0')
                 xlabel("Iteration Step")
66
                 axis square;
                 plot(1: length(aa(:,2)), aa(:,2), 'r.-');
68
                 subplot(1,3,3);
70
                 set (gca, 'FontName', 'Arial', 'FontSize', 14, '
71
                     FontWeight', 'Bold', 'LineWidth', 1);
                 hold on;
                 title ('SSE');
73
                 xlabel("Iteration Step")
74
                 axis square;
75
                 plot (1: length (aa(:,1)), error, 'k.-');
```

```
break;
77
             end
78
        end
79
   end
80
81
    if (plotting==1)
82
        [tspan,x] = ode45(@(t,x)system(t,x,a_opt(1)),texp,
84
            a_opt(2));
        figure (1);
86
        set (gca, 'FontName', 'Arial', 'FontSize', 14, 'FontWeight'
87
            , 'Bold', 'LineWidth', 1);
        hold on;
88
        axis square;
        title ('x vs. t');
90
        plot(tspan,x,'r.');
91
        plot(texp, xexp, 'bo');
92
        legend('ODE', 'data');
94
   end
96
    function z = SSE(a)
    global texp
    global xexp
100
   xt0 = a(2);
101
    [tspan, x] = ode45(@(t,x)system(t,x,a(1)),texp,xt0);
102
103
   z = norm(x-xexp, 2);
104
105
   end
106
107
    function dxdt=system(t,x,a)
108
109
   dxdt = a*x^2;
110
111
   end
113
    function dzdt = sens(t,z,a)
114
115
   dzdt(1)=a*z(1)^2;
   dzdt(2)=z(1)^2+2*a*z(1)*z(2);
   dzdt(3)=2*a*z(1)*z(3);
   dzdt = dzdt;
119
   end
120
```

Problem 3

```
close all;
   clear all;
  format long;
   plotting=1;
   global xexp
   global texp
   global xt0
  %Experimental data
10
  xexp = [0.9 \ 0.858 \ 0.78 \ 0.7 \ 0.6 \ 0.5;]
11
       0.1 \ 0.14 \ 0.2 \ 0.25 \ 0.3 \ 0.38;
  texp = [0:5];
   xt0 = [0.9 \ 0.1];
14
  method =2; % 1=fminsearch, 2=Newton
16
   if (method == 1)
18
       % Finding the parameter values minimizing SSE error
           using built-in function
       [a_opt, fval, exitflag, output] = fminsearch(@SSE, [0 0])
20
21
   else
22
       %Newton-Raphson method
23
       aa(1,:) = [0 \ 0];
       \mathbf{error}(1) = SSE(aa(1,:));
25
       delta1 = 1e-16;
       delta2 = 1e-16;
       Nsteps = 200;
28
29
       for k=1:Nsteps
30
           %Need to solve ODE on a finer grid
32
            tt = linspace(texp(1), texp(end), 300);
            zt0 = [xt0 \ 0 \ 0 \ 0 \ 0]; %initial data for the
34
                sensitivity system
            [tspan, zz] = ode45(@(t,z)sens(t,z,aa(k,:)),tt,zt0
35
               );
            z = interp1(tt,zz,texp); %getting back to the
36
               coarser grid to compare with xexp
37
           %Jacobian calculation
38
            J1 = [z(:,3:4)];
39
            J2 = [z(:,5:6)];
```

```
41
           %Hessian with weights
42
           H = J1'*J1 + J2'*J2;
43
            g = J1'*(xexp(:,1) - z(:,1)) + J2'*(xexp(:,2) - z
44
                (:,2));
45
46
           %Newton direction = inv(H)*g, but
47
           %Better to use slash command for a more stable
48
                calculation
            aa(k+1,:) = aa(k,:) + (H\backslash g);
49
            a_{-}opt = aa(k+1,:);
50
            error(k+1) = SSE(a_opt);
51
52
            if (norm(aa(k+1,:)-aa(k,:)) < delta1) | (abs(SSE(aa))
                (k+1,:) -SSE (aa(k,:)) < delta 2)
                 tt = [0:100];
54
                 [tspan, xd] = ode45(@(t,x)system(t,x,a_opt),tt]
55
                     ,xt0);
                 figure (3)
56
                 set (gca, 'FontName', 'Arial', 'FontSize', 14, '
57
                    FontWeight', 'Bold', 'LineWidth', 1);
                 hold on;
58
                 xlabel("Time (days)")
59
                 ylabel("Population Percentage")
60
                 axis square;
                 plot (tspan, xd, 'LineWidth', 2)
                 legend("Susceptible","Infected")
63
64
                % Plotting convergence of parameters
                 figure (2);
66
                 subplot(1,3,1);
67
                 set (gca, 'FontName', 'Arial', 'FontSize', 14, '
68
                    FontWeight', 'Bold', 'LineWidth', 1);
                 hold on;
69
                 title ('a')
70
                 xlabel("Iteration Step")
71
                 axis square;
                 plot(1: length(aa(:,1)), aa(:,1), 'r.-');
73
                 subplot(1,3,2);
75
                 set (gca, 'FontName', 'Arial', 'FontSize', 14, '
76
                    FontWeight', 'Bold', 'LineWidth', 1);
                 hold on;
77
                 title ('b')
78
                 xlabel("Iteration Step")
79
```

```
axis square;
80
                   plot(1: length(aa(:,2)), aa(:,2), 'r.-');
81
82
                   subplot(1,3,3);
                   set (gca, 'FontName', 'Arial', 'FontSize', 14, '
84
                       FontWeight', 'Bold', 'LineWidth', 1);
                   hold on;
85
                   title ('SSE');
86
                   xlabel("Iteration Step")
87
                   axis square;
                   plot(1: length(aa(:,1)), error, 'k.-');
                   break;
90
              end
91
         end
92
    end
93
94
    if (plotting == 1)
95
96
         [tspan, x] = ode45(@(t,x)system(t,x,a_opt),texp,xt0);
98
         figure (1);
         subplot(1,2,1);
100
         set (gca, 'FontName', 'Arial', 'FontSize', 14, 'FontWeight'
101
             , 'Bold', 'LineWidth', 1);
         hold on;
102
         axis square;
103
         title ('x vs. t');
104
         plot(tspan(:,1),x(:,1),'r.');
105
         plot (texp, xexp(:,1), 'bo');
106
         legend('ODE', 'data');
107
108
         subplot(1,2,2);
109
         set (gca, 'FontName', 'Arial', 'FontSize', 14, 'FontWeight'
110
             , 'Bold', 'LineWidth', 1);
         hold on;
111
         axis square;
112
         title ('y vs. t');
113
         plot (tspan, x(:,2), 'r.');
         \operatorname{plot}(\operatorname{texp},\operatorname{xexp}(:,2),\operatorname{'bo'});
115
         legend ('ODE', 'data');
116
117
    end
118
119
    function z = SSE(a)
    global texp
121
    global xexp
```

```
global xt0
123
124
    [tspan,x] = ode45(@(t,x)system(t,x,a),texp,xt0);
125
126
    z = norm(x-xexp, 2);
127
128
    end
129
130
    function dxdt=system(t,x,a)
131
132
    dxdt(1) = -a(1)*x(1)*x(2);
133
    dxdt(2) = a(1)*x(1)*x(2) - a(2)*x(2);
134
135
    dxdt = dxdt;
136
137
    end
138
139
140
    function dzdt = sens(t,z,a)
    dzdt(1) = -a(1)*z(1)*z(2);
142
    dzdt(2) = a(1)*z(1)*z(2)-a(2)*z(2);
    dzdt\left(3\right) \; = \; -z\left(1\right)*z\left(2\right) \; - \; a\left(1\right)*z\left(2\right)*z\left(3\right) \; - \; a\left(1\right)*z\left(2\right)*z\left(4\right) \; ;
    dzdt(4) = z(1)*z(2) + a(1)*z(2)*z(3) + (a(1)*z(1)-a(2))*z
         (4);
    dzdt(5) = -a(1)*z(2)*z(5) -a(1)*z(1)*z(6);
    dzdt(6) = -z(2) + a(1)*z(2)*z(5) + (a(1)*z(1)-a(2))*z(6);
    dzdt = dzdt;
    end
149
```