

AE 6310-A: Assignment #3

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Problem 1

Part A: Finding constrained optimum and Lagrange multipliers

The function is defined as follows

$$f: (x_1 + 2)^2 + 10(x_2 + 3)^2$$

$$c: x_1^2 + x_2^2 \leq 2$$

Before proceeding further, it is important to point out that the unconstrained minimum of the objective function is $[-2, -3]$. This point does not satisfy the constraint function, so we know that the constraint must be active.

Note that `scipy.minimize` requires the gradient as one of the inputs.

$$\nabla f: \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 + 4 \\ 20x_2 + 60 \end{bmatrix}$$

Additionally, `scipy.minimize` assumes the constraints are of the form $C(x) \geq 0$ and requires a Jacobian for each constraint. Therefore, the constraint is restructured as

$$c: -x_1^2 - x_2^2 + 2 \geq 0$$

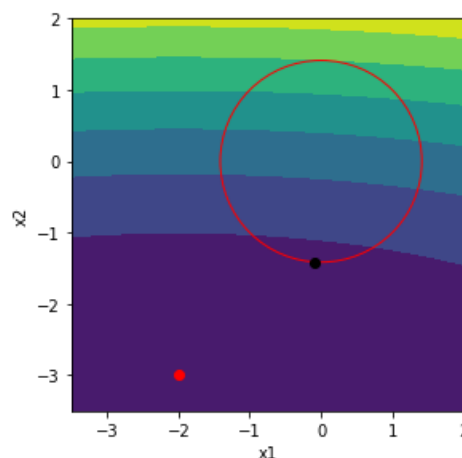
$$A(x) = \begin{bmatrix} \frac{\partial c}{\partial x_1} & \frac{\partial c}{\partial x_2} \end{bmatrix} = [-2x_1 \quad -2x_2]$$

Additionally, `scipy.minimize` only returns the constrained optimum (x^*). In order to calculate the Lagrange multipliers, we can use the following, derived from the KKT conditions:

$$\nabla f(x^*) = -A(x^*)^T \lambda \Rightarrow \lambda = \frac{A(x^*) \nabla f(x^*)}{-A(x^*) A(x^*)^T}$$

Note that if using $A(x)$ from the `scipy` definition, λ will be negative so be sure to multiply by -1 .

Using this method, we find the **constrained min to be $[-0.1619, -1.4049]$, Lagrange multiplier= 11.3536**



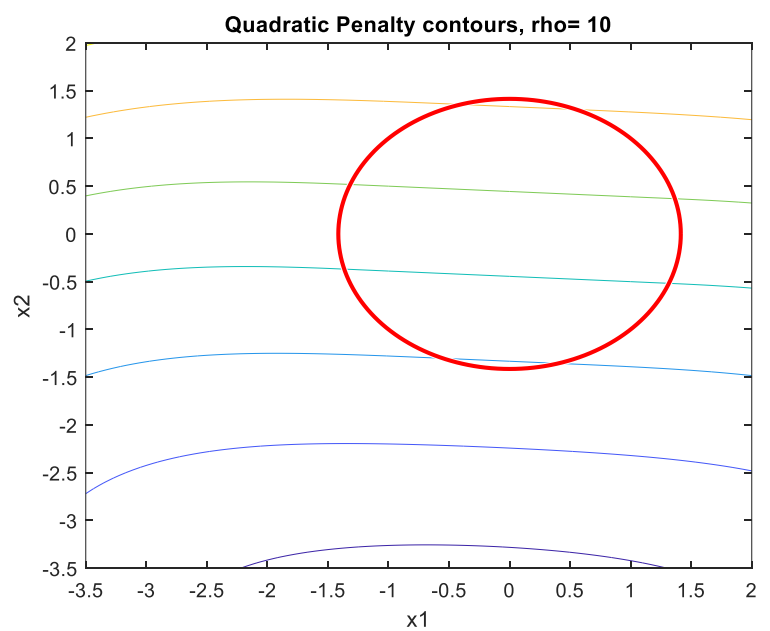
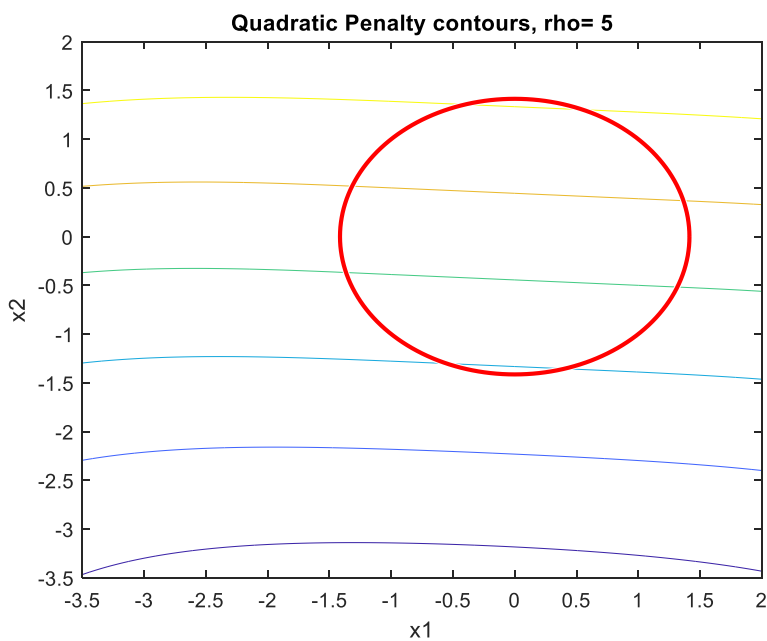
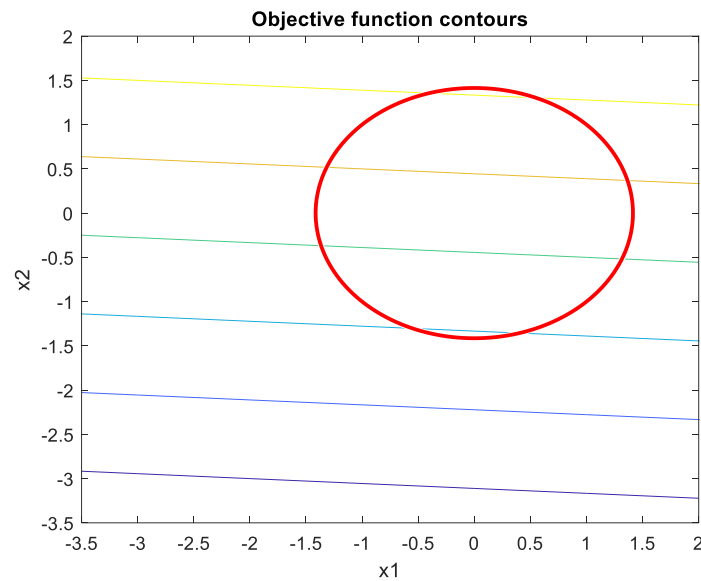
Constraint boundary = red circle, Unconstrained min = red point, Constrained min = black point

Part B: Quadratic penalty function plots

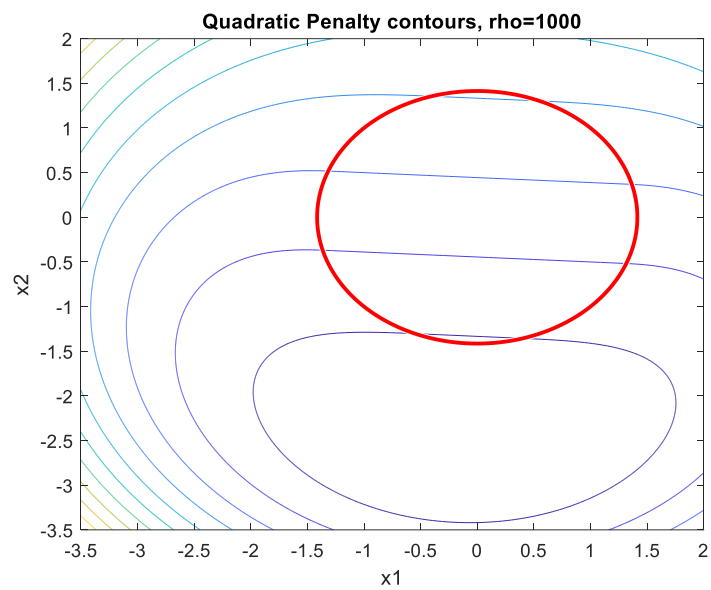
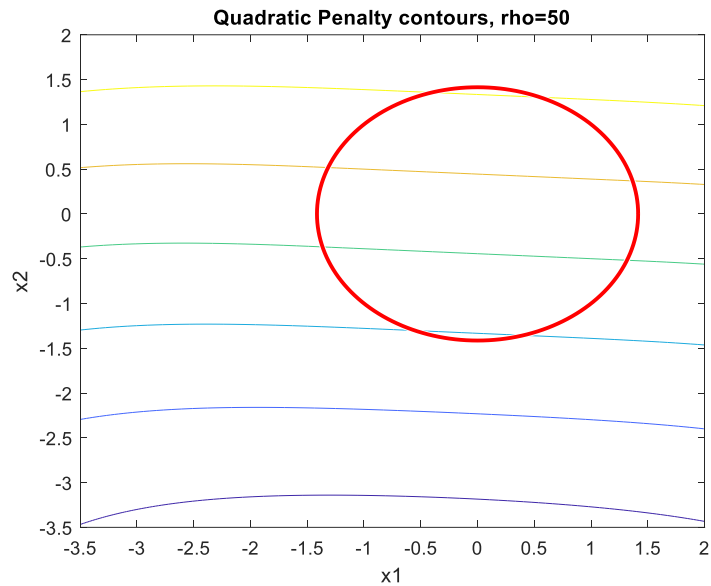
The quadratic penalty is an exterior penalty method, defined everywhere. It modifies the problem to

$$\min_x \left\{ f(x) + \frac{\rho}{2} \sum_i (c_i(x), 0)^2 \right\}$$

In both of the following plots, the original constraint boundary is marked by a red circle. As rho increases, the minimizer approaches the constrained minimizer from the infeasible space.



If the contours are hard to view, consider two extreme cases where the difference between the rho is increased significantly. In this case, it is much easier to see as rho increases, the minimizer approaches the constrained minimizer from the *infeasible* space.

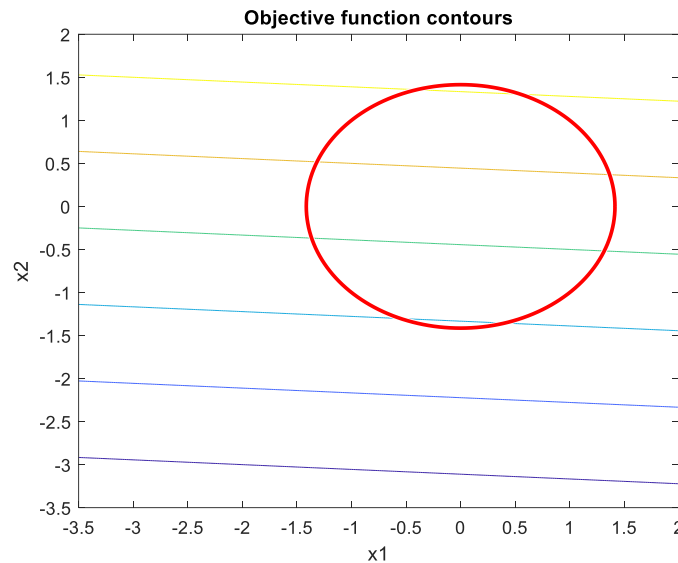


Part C: Log-barrier penalty function plots

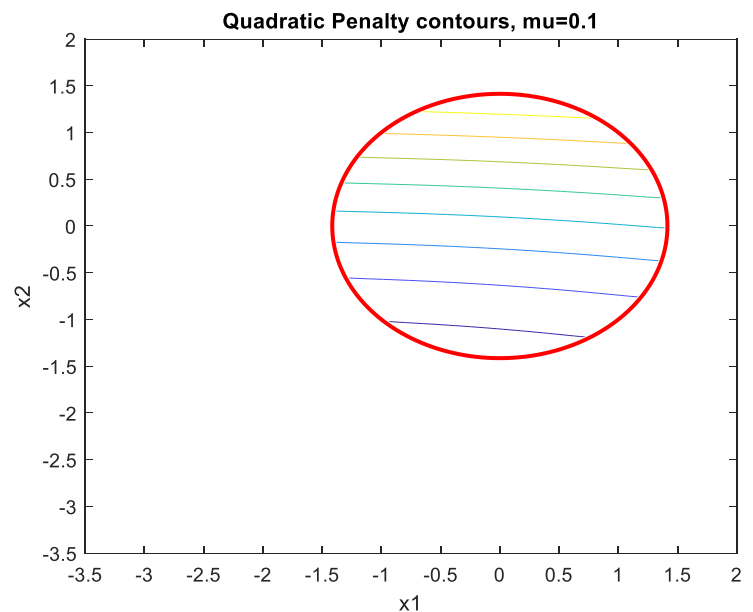
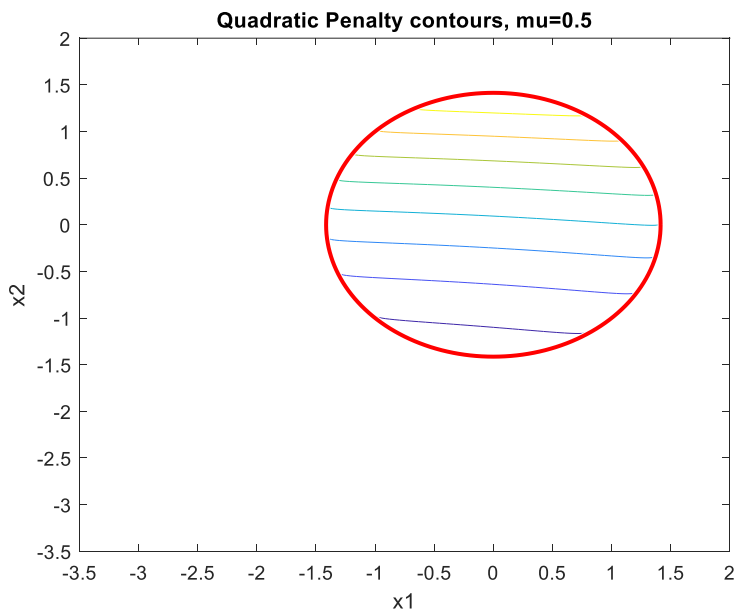
The log-barrier penalty is an interior penalty method, defined only within the feasible space. It modifies the problem to

$$\min_x \left\{ f(x) - \mu \sum_i \ln(-c_i(x)) \right\}$$

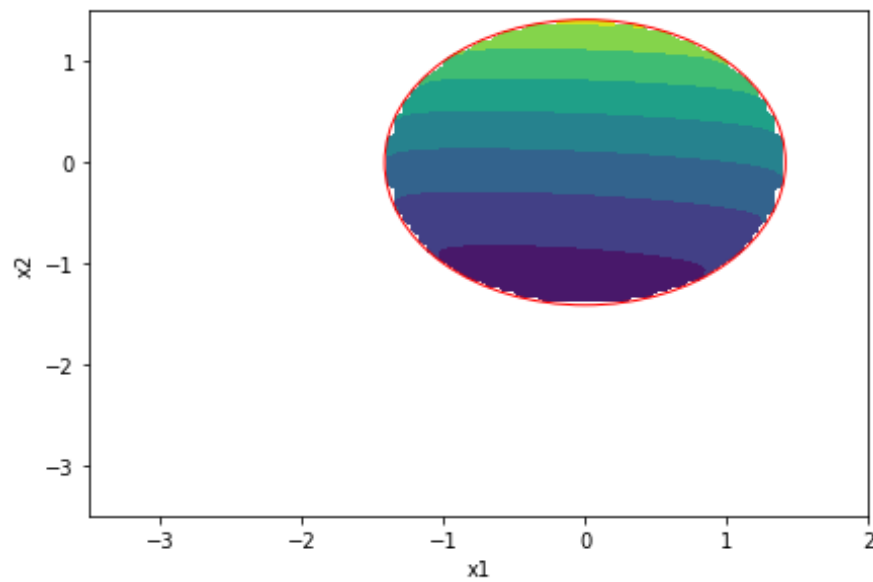
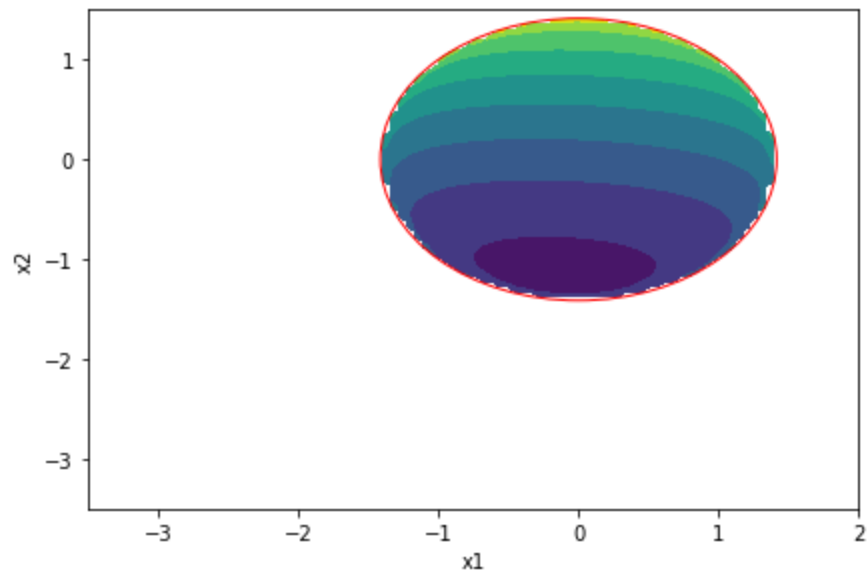
In both of the following plots, the original constraint boundary is marked by a red circle. As μ decreases, the minimizer approaches the constrained minimizer from the feasible space.



There is a small difference between the μ values, but the contour change is there.

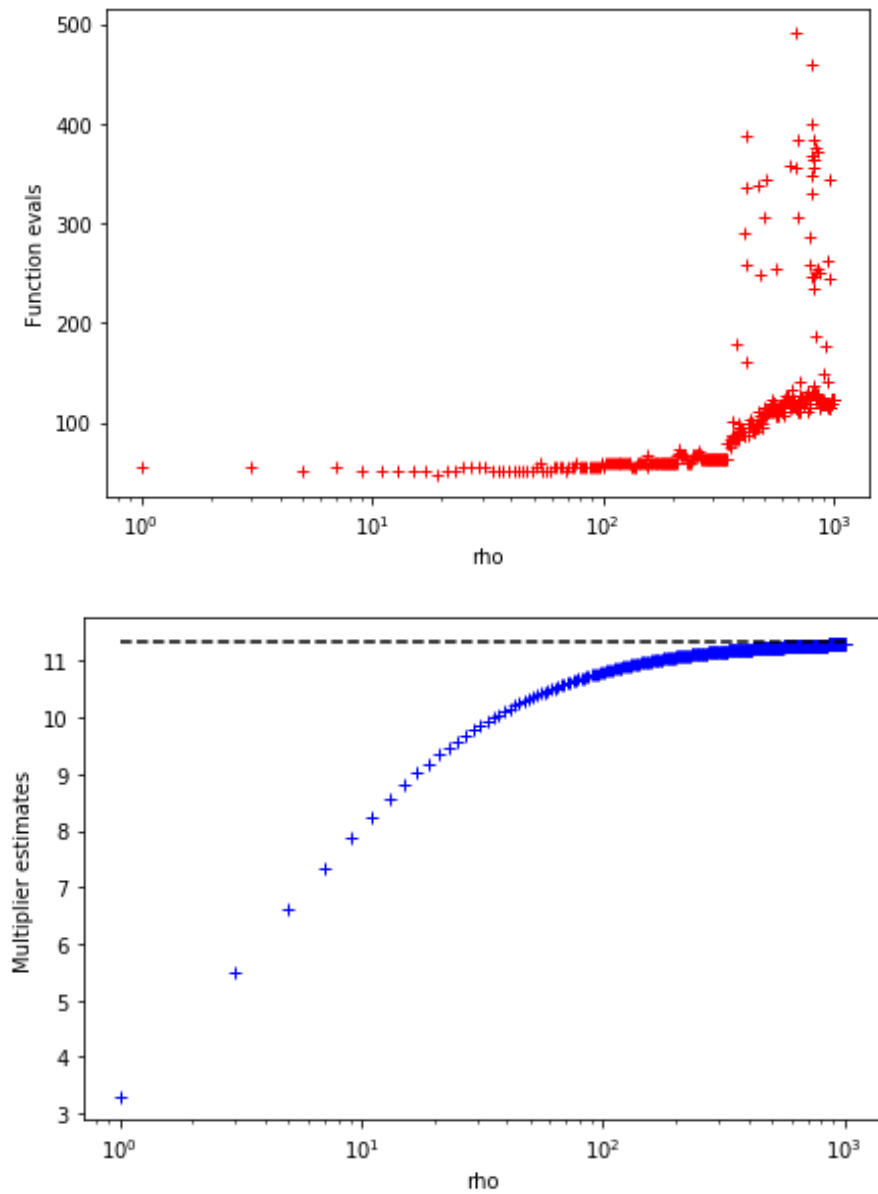


If the contours are hard to view, consider two extreme cases where the difference between the μ is increased significantly. In this case, it is much easier to see as μ decreases, the minimizer approaches the constrained minimizer from the *feasible* space.

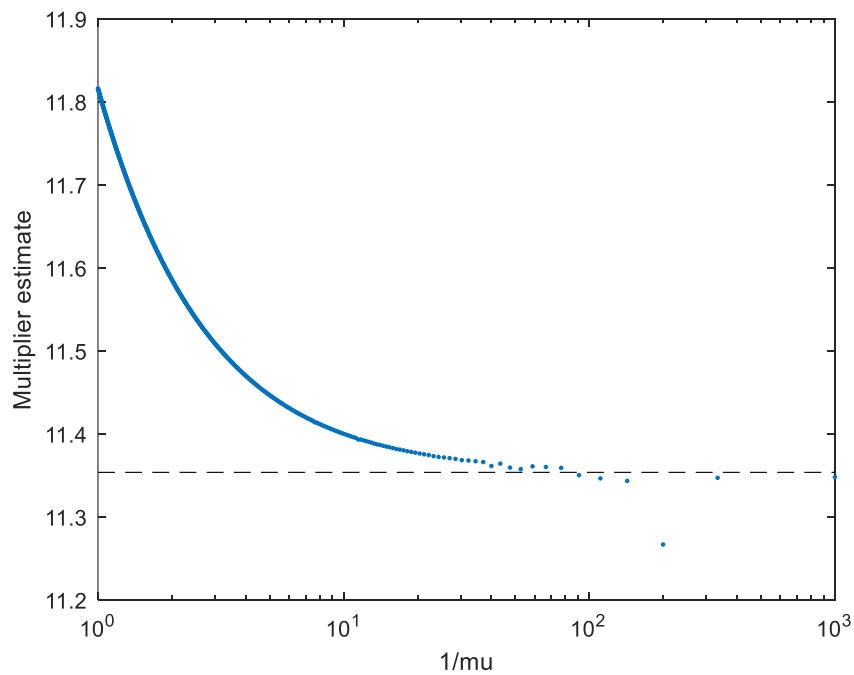
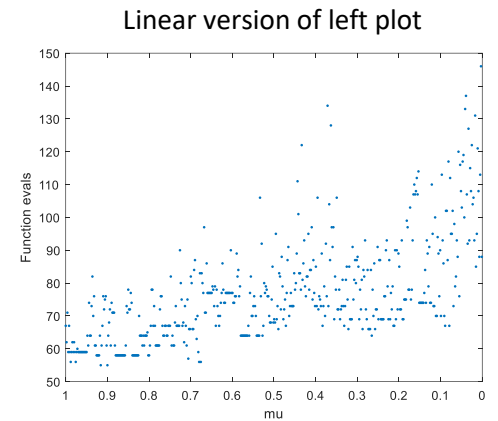
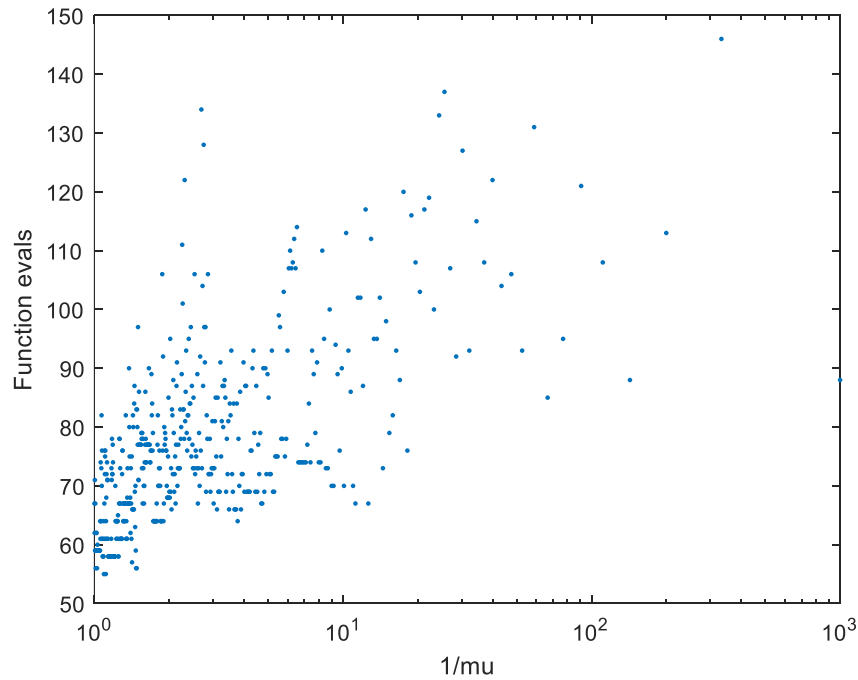


Part D: Plots for varying rho and mu

Varying rho between [1,1000] shows that increasing rho increases the number of function evaluations, but provides a better estimate of the multiplier estimates.



Varying μ between $[1, 0.001]$ shows that decreasing μ (i.e. increasing $1/\mu$) increases the number of function evaluations, but provides a better estimate of the multiplier estimates. Note that MATLAB handles the log-barrier method a bit better than Python.



Problem 2

For this problem, consider the design variables x_1, x_2, x_3 and the state variables u_1, u_2 . The design variables must be positive. The governing equations are given as

$$R(x, u) = \begin{bmatrix} (x_1 + x_2)u_1 + (x_3 - x_2)u_2 - 1 \\ (x_3 - x_2)u_1 + (x_1 + x_2 - x_3)u_2 - 1 \end{bmatrix} = 0$$

$$R(x, u) = \begin{bmatrix} (x_1 + x_2) & (x_3 - x_2) \\ (x_3 - x_2) & (x_1 + x_2 - x_3) \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 0$$

The state variables must have the same sign. The output function of interest is given as

$$f(x, u) = x_1 x_2 + \sqrt{u_1 u_2}$$

The adjoint method makes use of several derivatives which are detailed below.

$$\frac{\partial R}{\partial u} = \begin{bmatrix} (x_1 + x_2) & (x_3 - x_2) \\ (x_3 - x_2) & (x_1 + x_2 - x_3) \end{bmatrix}$$

$$\frac{\partial R}{\partial x} = \begin{bmatrix} \frac{\partial R_1}{\partial x_1} & \frac{\partial R_1}{\partial x_2} & \frac{\partial R_1}{\partial x_3} \\ \frac{\partial R_2}{\partial x_1} & \frac{\partial R_2}{\partial x_2} & \frac{\partial R_2}{\partial x_3} \end{bmatrix} = \begin{bmatrix} u_1 & u_1 - u_2 & u_2 \\ u_2 & u_2 - u_1 & u_1 - u_2 \end{bmatrix}$$

$$\frac{\partial f}{\partial u} = \begin{bmatrix} \frac{u_2}{2\sqrt{u_1 u_2}} & \frac{u_1}{2\sqrt{u_1 u_2}} \end{bmatrix}$$

$$\frac{\partial f}{\partial x} = [x_2 \quad x_1 \quad 0]$$

Part A: Forward difference and complex step

Both methods work by evaluating the function at a point then comparing it to another point after taking a step. Calculation of the output function value is done through the following process:

1. Pick a point for the design variables $[x_1, x_2, x_3]$
2. Solve the governing equations for the state variables $[u_1, u_2]$
3. Evaluate the output function of interest

After stepping to the next point and finding the value of the function of interest at that new point, we can then create an estimate for the derivate.

For the forward-difference method, the derivative is estimated as

$$\frac{df}{dx} \approx \frac{f(x + h) - f(x)}{h} + \mathcal{O}(h)$$

For the complex step method, the derivative is estimated as

$$\frac{df}{dx} \approx \frac{\text{Im}\{f(x + i h)\}}{h} + \mathcal{O}(h^2)$$

Note that relative error is defined as

$$\text{relative error} = \frac{|\text{method} - \text{adjoint}|}{|\text{adjoint}|}$$

Consider a design point of [1.1, 1.2, 1.3] looking at two different step sizes:

```

Design x0 point: [1.1 1.2 1.3]
Function value: 1.9344649467017594

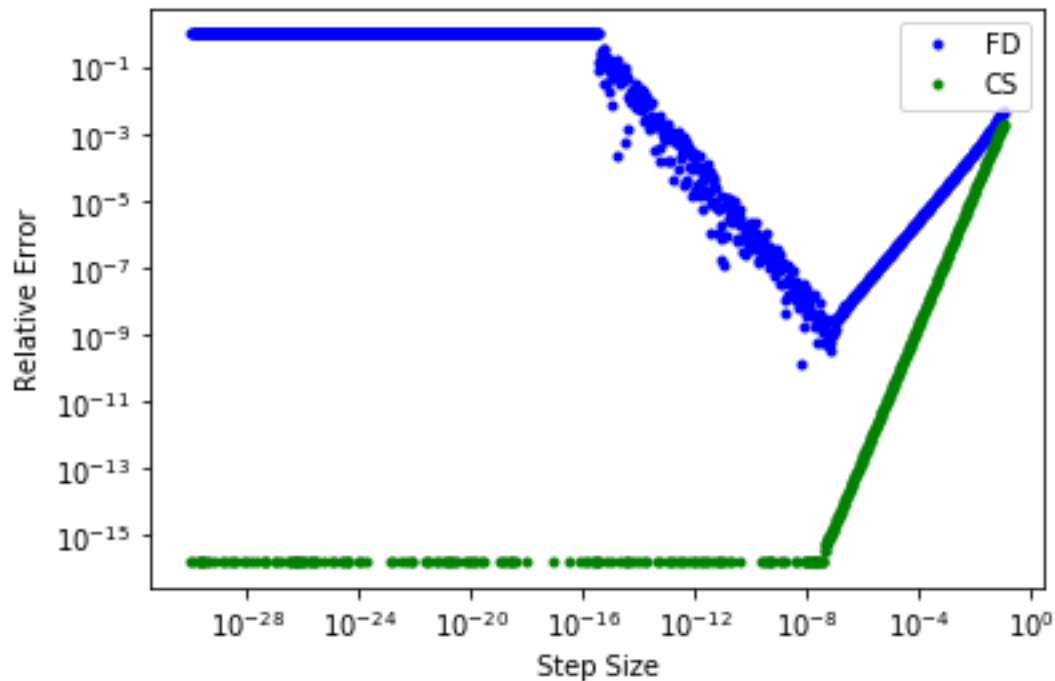
Step size: 1e-30
Forward-difference approximation: [0. 0. 0.]
Complex-step approximation: [ 0.79554704  1.12290251 -0.15157669]
Adjoint based total derivative: [ 0.79554704  1.12290251 -0.15157669]
Magnitude of relative FD error: 1.0
Magnitude of relative CS error: 1.6038140697726189e-16

-----
Design x0 point: [1.1 1.2 1.3]
Function value: 1.9344649467017594

Step size: 1e-06
Forward-difference approximation: [ 0.79554732  1.12290235 -0.15157683]
Complex-step approximation: [ 0.79554704  1.12290251 -0.15157669]
Adjoint based total derivative: [ 0.79554704  1.12290251 -0.15157669]
Magnitude of relative FD error: 2.9361459771228685e-08
Magnitude of relative CS error: 2.2966617479143904e-13

```

Now consider a range of different step sizes, keeping the same design point:



Part B: Adjoint and complex step comparison

The adjoint equations are defined as follows

$$\left(\frac{\partial R}{\partial u}\right)^T \Psi = -\left(\frac{\partial f}{\partial u}\right)^T$$

$$\begin{bmatrix} (x_1 + x_2) & (x_3 - x_2) \\ (x_3 - x_2) & (x_1 + x_2 - x_3) \end{bmatrix}^T \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix} = -\begin{bmatrix} \frac{u_2}{2\sqrt{u_1 u_2}} & \frac{u_1}{2\sqrt{u_1 u_2}} \end{bmatrix}^T$$

The total derivative is then given by

$$\nabla f = \frac{\partial f}{\partial x} + \Psi^T \frac{\partial R}{\partial x}$$

$$\nabla f = [x_2 \quad x_1 \quad 0] + [\Psi_1 \quad \Psi_2] \begin{bmatrix} u_1 & u_1 - u_2 & u_2 \\ u_2 & u_2 - u_1 & u_1 - u_2 \end{bmatrix}$$

Therefore, the function to compute the total derivative using the adjoint method goes through the following set of steps:

1. Pick a point for the design variables $[x_1, x_2, x_3]$
2. Solve the governing equations for the state variables $[u_1, u_2]$
3. Solve for the adjoint variables
4. Take derivative of the interest function with respect to x (design variables)
5. Add the result of step 4 to the transpose of the adjoint variables times the derivative of the governing equations with respect to x (design variables)

Once the total derivative has been computed, we estimate the value at the new point by simply taking the dot product of the perturbation and the total derivative. The relative error between the complex step and adjoint method is simply $(\text{adj} - \text{cs})/\text{cs}$ where adj and cs are the estimations at the x_1 point using the adjoint and complex step methods respectively.

Using a step of $1e-30$, the relative error is very small, approximately machine precision. Consider the design point of $[1.1, 1.2, 1.3]$ below:

```
Adjoint-based derivative @x0: [ 0.79554704  1.12290251 -0.15157669]
Complex-step approximation:  [ 0.79554704  1.12290251 -0.15157669]
Rel error between CS & Adjoint: [1.39554668e-16 1.97741658e-16 1.83112423e-16]
```

Code snippets

Problem 1A

```

109 def p1_ptA():
110     # Plot the function with constraint and unconstrained min
111
112     # find unconstrained min
113     res = sp.minimize(func, [0,0], method='BFGS', options={'disp':False})
114     uncon_min= res.x
115
116     # find constrained min
117     x0=[0,0]
118     cons= ({'type':'ineq',
119             'fun': con,
120             'jac': con_deriv})
121     res = sp.minimize(func, x0, jac=func_deriv, constraints=cons,
122                       method='SLSQP', options={'disp':False})
123     x_star=res.x
124     delta_fStar= res.jac
125     l_mult=lagrange_mult(x_star,delta_fStar)
126     cplot(func,False,uncon_min,x_star)
127
128     print('Constrained min= ',x_star)
129     print('Lagrange multiplier= ',l_mult)
130
131 def func(x):
132     #x=[x1,x2]
133     return (x[0]+2)**2 +10*(x[1]+3)**2
134
135 def quad_penalty(x, *args):
136
137 def log_barrier(x, *args):
138
139 def func_deriv(x):
140     res= np.zeros((1, 2))
141     dfdx1= 2*x[0]+4
142     dfdx2= 20*x[1]+60
143     return np.array([dfdx1,dfdx2])
144
145 def func_jac(x):
146     return np.array([[df2dx12,df2dx1x2],[df2dx2x1,df2dx22]])
147
148 def con(x):
149     #x1^2 +x2^2 <= 2
150     # scipy wants the form of c(x) >= 0
151     #-x1^2 -x2^2 +2 >= 0
152     return -x[0]**2 -x[1]**2 +2
153
154 def con_deriv(x):
155     res= np.zeros((1, 2))
156     dcdx1= -2*x[0]
157     dcdx2= -2*x[1]
158     return np.array([dcdx1,dcdx2])
159
160 def lagrange_mult(x_star,delta_fstar):
161     A_x= con_deriv(x_star)
162     l_mult= np.dot(A_x,delta_fstar)/(-np.dot(A_x,np.transpose(A_x)))*-1
163     return l_mult

```

Problem 1B and 1C

```

71 def cplot(fobj,line,*args):
72     n = 100
73     x1 = np.linspace(-3.5, 2, n)
74     x2 = np.linspace(-3.5, 1.5, n)
75     X1, X2 = np.meshgrid(x1, x2)
76     f = np.zeros((n, n))
77
78     if line:
79         for j in range(n):
80             for i in range(n):
81                 f[i, j] = fobj([X1[i, j], X2[i, j]])
82             fig, ax = plt.subplots(1, 1)
83             ax.contour(X1, X2, f)
84
85     else:
86         # Query the function at the specified locations
87         for i in range(n):
88             for j in range(n):
89                 f[i, j] = fobj([X1[i, j], X2[i, j]])
90
91         fig, ax = plt.subplots(1, 1)
92         ax.contourf(X1, X2, f)
93
94         #this is the constraint
95         circ = plt.Circle((0, 0), 2**0.5, color='r',fill=False,linestyle='-')
96         ax.add_artist(circ)
97
98     if len(args) !=0:
99         uncon_min=args[0]
100         x_star=args[1]
101         ax.plot(uncon_min[0],uncon_min[1], 'ro')
102         ax.plot(x_star[0],x_star[1], 'ko')
103
104     # ax.set_aspect('equal', 'box')
105     fig.tight_layout()
106     plt.xlabel('x1')
107     plt.ylabel('x2')

```

```

17 def quad_penalty(x, *args):
18     #defined everywhere
19     if len(args) !=0:
20         rho= args[0]
21     else:
22         rho= 5
23     f_val= func(x) #function value
24     c_val= con(x)*-1 #constraint value, have to *-1 to undo scipy
25     return f_val+ (0.5*rho)*(max(c_val,0)**2)
26
27 def log_barrier(x, *args):
28     #only defined in feasible space
29     if len(args) !=0:
30         mu= args[0]
31     else:
32         mu= 0.1
33     f_val= func(x)
34     c_val= con(x)*-1
35
36     if c_val < 0:
37         return f_val -(mu)*np.log(-c_val)
38     else:
39         return float('NaN')

```

```
128 - function quad_graphs(X1,X2)
129 -     figure()
130 -     rho= 50;
131 -     f2= quadPenalty(X1,X2,rho);
132 -     contour(X1,X2,f2)
133 -     hold on
134 -     viscircles([0,0],sqrt(2));
135 -     hold off
136 -     title_text= strcat('Quadratic Penalty contours, rho= ', num2str(rho));
137 -     title(title_text)
138 -     xlabel('x1'); ylabel('x2');
139 -
140 -     figure()
141 -     rho= 1000;
142 -     f2= quadPenalty(X1,X2,rho);
143 -     contour(X1,X2,f2)
144 -     hold on
145 -     viscircles([0,0],sqrt(2));
146 -     hold off
147 -     title_text= strcat('Quadratic Penalty contours, rho= ', num2str(rho));
148 -     title(title_text)
149 -     xlabel('x1'); ylabel('x2');
150 - end

152 - function log_graphs(X1,X2)
153 -     figure()
154 -     mu= 0.5;
155 -     f2= logBarrier_penalty(X1,X2,mu);
156 -     contour(X1,X2,f2)
157 -     hold on
158 -     viscircles([0,0],sqrt(2));
159 -     hold off
160 -     title_text= strcat('Quadratic Penalty contours, mu= ', num2str(mu));
161 -     title(title_text)
162 -     xlabel('x1'); ylabel('x2');
163 -
164 -     figure()
165 -     mu= 0.1;
166 -     f2= logBarrier_penalty(X1,X2,mu);
167 -     contour(X1,X2,f2)
168 -     hold on
169 -     viscircles([0,0],sqrt(2));
170 -     hold off
171 -     title_text= strcat('Quadratic Penalty contours, mu= ', num2str(mu));
172 -     title(title_text)
173 -     xlabel('x1'); ylabel('x2');
174 - end
```

```
180 - function f= quadPenalty(x1,x2,rho)
181 -     f=(x1+2)^2 +10.*(x2+3)^2;
182 -     con_val= x1.^2+x2.^2 -2;
183 -     dim= size(x1);
184 -     zero= zeros(dim(1));
185 -     f=f+ (rho/2)*(max(con_val,zero).^2);
186 - end
187
188 - function f= logBarrier_penalty(x1,x2,mu)
189 -     dim= size(x1);
190 -     f= ones(dim(1));
191 -     for i=1:dim(1) %iterate through x1 (cols)
192 -         for j=1:dim(1) %iterate through x2 (rows)
193 -             x1_curr= x1(1,i);
194 -             x2_curr= x2(j,1);
195
196 -             c= x1_curr^2 + x2_curr^2 -2;
197 -             if c<0 %feasible if c <0
198 -                 f(i,j)=(x1_curr+2)^2 +10.*(x2_curr+3)^2 +mu*log(-c);
199 -             else
200 -                 f(i,j)= NaN;
201 -             end
202 -         end
203 -     end
204 -     f= f';
205 - end
```

Problem 1D

```
131 def var_rho(): #use python
132     n= 500
133     x1 = np.linspace(-3.5, 2, n)
134     x2 = np.linspace(-3.5, 2, n)
135     rho= np.linspace(1,1000,n)
136     f_evals= []
137     lambda_est= []
138     x0= [0,0]
139     for current_rho in rho:
140         res = sp.minimize(quad_penalty, x0, args=current_rho, method='BFGS', options={'disp':False})
141         f_evals.append(res.nfev)
142         current_L_est= current_rho*con(res.x)*-1
143         lambda_est.append(current_L_est)
144
145     fig, ax = plt.subplots(1, 1)
146     ax.set_xscale('log')
147     ax.plot(rho,f_evals,'r+')
148     fig.tight_layout()
149     plt.xlabel('rho')
150     plt.ylabel('Function evals')
151
152     fig, ax = plt.subplots(1, 1)
153     ax.plot(rho,lambda_est,'b+')
154     ax.plot(rho, 11.3536*np.ones([1,n])[0], 'k--')
155     ax.set_xscale('log')
156     fig.tight_layout()
157     plt.xlabel('rho')
158     plt.ylabel('Multiplier estimates')
159
160 def var_mu(): #use matlab
161     n= 500
162     x1 = np.linspace(-3.5, 2, n)
163     x2 = np.linspace(-3.5, 2, n)
164     mu= np.linspace(1,0.001,n)
165     f_evals= []
166     lambda_est= []
167     x0= [0,0]
168     for current_mu in mu:
169         res = sp.minimize(quad_penalty, x0, args=current_mu, method='BFGS', options={'disp':False})
170         f_evals.append(res.nfev)
171         current_L_est= -current_mu/(con(res.x)*-1)
172         lambda_est.append(current_L_est)
173
174     fig, ax = plt.subplots(1, 1)
175     ax.plot(1/mu,f_evals,'r+')
176     fig.tight_layout()
177     plt.xlabel('1/mu')
178     plt.ylabel('Function evals')
179
180     fig, ax = plt.subplots(1, 1)
181     ax.plot(1/mu,lambda_est,'b+')
182     fig.tight_layout()
183     plt.xlabel('1/mu')
184     plt.ylabel('Multiplier estimates')
```



```

58 - function quadPenalty_vary() %Use Python
59 - funcEvals= [];
60 - lambda_est= [];
61 - n= 500;
62 -
63 - for rho= linspace(1,1000,n)
64 -     fun_quad= @(x) (x(1)+2)^2 +10*(x(2)+3)^2 +...
65 -         (rho/2)*(max(x(1)^2+ x(2)^2 -2,0).^2);
66 -     nonlcon = @cons;
67 -     x0= [-1,-1];
68 -     A= []; b= [];
69 -     Aeq= []; beq= [];
70 -     lb= []; ub= [];
71 -     [x,fval,exitflag,output] = fmincon(fun_quad,x0,A,b,Aeq,beq,lb,ub,nonlcon);
72 -     funcEvals= [funcEvals, output.funcCount];
73 -
74 -     c= x(1)^2+ x(2)^2 -2;
75 -     lambda_est= [lambda_est, rho*c];
76 - end
77 - rho= linspace(1,1000,n);
78 - figure()
79 - plot(rho, funcEvals, '+')
80 - xlabel('rho')
81 - set(gca, 'XScale', 'log')
82 - ylabel('Function evals')
83 -
84 - figure()
85 - plot(rho, lambda_est, '+')
86 - xlabel('rho')
87 - set(gca, 'XScale', 'log')
88 - ylabel('Multiplier estimate')
89 - end
22 - function logBarrier_vary() %use MATLAB
23 - funcEvals= [];
24 - lambda_est= [];
25 - n= 500;
26 -
27 - for mu= linspace(1,0.001,n)
28 -     fun_quad= @(x) (x(1)+2)^2 +10*(x(2)+3)^2 -...
29 -         mu*log(-1*(x(1)^2+ x(2)^2 -2));
30 -     nonlcon = @cons;
31 -     x0= [-1,0];
32 -     A= []; b= [];
33 -     Aeq= []; beq= [];
34 -     lb= []; ub= [];
35 -     [x,fval,exitflag,output] = fmincon(fun_quad,x0,A,b,Aeq,beq,lb,ub,nonlcon);
36 -     funcEvals= [funcEvals, output.funcCount];
37 -
38 -     c= x(1)^2+ x(2)^2 -2;
39 -     lambda_est= [lambda_est, -mu/c];
40 - end
41 - mu= linspace(1,0.001,n);
42 - figure()
43 - plot(1./mu, funcEvals, '.')
44 - xlabel('mu')
45 - % set(gca, 'XScale', 'log')
46 - set(gca, 'xdir','reverse')
47 - ylabel('Function evals')
48 -
49 - figure()
50 - plot(1./mu, lambda_est, '.')
51 - hold on
52 - plot(1./mu, 11.3536.*ones(1,n), 'k--')
53 - xlabel('1/mu')
54 - set(gca, 'XScale', 'log')
55 - ylabel('Multiplier estimate')
56 - end

```

Problem 2

```

8 import numpy as np
9 import time
10 import matplotlib.pyplot as plt
11
12 def evaluate(x):
13     """
14     Evaluate the function of interest
15     Args: x (np.ndarray) Vector of Length 3. The design variables
16     Return: The value of the function of interest
17     """
18     # Fill in the values of the governing equation
19     #  $R(x,u) = K(x)u - F = 0$ 
20     K, F = evaluate_governing_eqns(x)
21     # Solve the governing equations to obtain u
22     u = np.linalg.solve(K, F)
23
24     # Evaluate the function of interest
25     f = x[0]*x[1] + np.sqrt(u[0]*u[1])
26     return f
27
28 def evaluate_governing_eqns(x):
29     #  $K(x)u - F$ 
30     K = np.zeros((2, 2), dtype=x.dtype)
31     F = np.zeros(2, dtype=x.dtype)
32
33     # x = [x1, x2, x3]
34     K[0,0] = x[0] + x[1] #  $x_1 + x_2$ 
35     K[0,1] = x[2] - x[1] #  $x_3 - x_2$ 
36     K[1,0] = x[2] - x[1] #  $x_3 - x_2$ 
37     K[1,1] = x[0] + x[1] - x[2] #  $x_1 + x_2 - x_3$ 
38
39     F[0] = 1.0
40     F[1] = 1.0
41     return K, F
42
43 def adjoint_total_derivative(x):
44     """ Use the adjoint method to evaluate the derivative of the function
45     of interest with respect to the design variables.
46     Args: x (np.ndarray) Vector of Length 3. The design variables
47     Return: dfdx (np.ndarray) Vector of Length 3. The total derivative
48     """
49     # Fill in the values of the governing equation
50     #  $R(x,u) = K(x)u - F = 0$ 
51     K, F = evaluate_governing_eqns(x)
52     # Solve the governing equations to obtain u
53     u = np.linalg.solve(K, F)
54
55     # define  $dR/du = K$ 
56     # define  $df/du$ 
57     dfdu = np.zeros((2), dtype=x.dtype)
58     dfdu[0] = u[1]/(2*np.sqrt(u[0]*u[1]))
59     dfdu[1] = u[0]/(2*np.sqrt(u[0]*u[1]))
60     # Solve for the adjoint variables
61     psi = -np.linalg.solve(K.T, dfdu.T)
62
63     # Define  $dR/dx$ 
64     dRdx = np.zeros((2, 3), dtype=x.dtype)
65     dRdx[0,0] = u[0] # first column
66     dRdx[1,0] = u[1]
67     dRdx[0,1] = u[0] - u[1] # column 2
68     dRdx[1,1] = u[1] - u[0]
69     dRdx[0,2] = u[1] # column 3
70     dRdx[1,2] = u[0] - u[1]
71
72     # define  $dF/dx$ 
73     dFdx = np.zeros((1, 3), dtype=x.dtype)
74     dFdx[0,0] = x[1]
75     dFdx[0,1] = x[0]
76     dFdx[0,2] = 0.0
77
78     return dFdx + np.dot(psi.T, dRdx)
79

```

```
80 def ptA_compare(h):
81     # Set the perturbation vector. We perturb the design variables
82     pert = np.array([1,1,1])
83
84     # Compute the function of interest at the point x0
85     x0 = np.array([1.1, 1.2, 1.3])
86     f0 = evaluate(x0)
87     print('Design x0 point:', x0)
88     print('Function value: ', f0)
89
90     # forward difference approximation
91     print('\nStep size: ',h)
92     pert_x1= np.array([1,0,0])
93     pert_x2= np.array([0,1,0])
94     pert_x3= np.array([0,0,1])
95
96     x1_d= x0+ h*pert_x1
97     f1_d= evaluate(x1_d)
98     f1d = (f1_d - f0)/h
99
100    x2_d= x0+ h*pert_x2
101    f2_d= evaluate(x2_d)
102    f2d = (f2_d - f0)/h
103
104    x3_d= x0+ h*pert_x3
105    f3_d= evaluate(x3_d)
106    f3d = (f3_d - f0)/h
107    fd= np.array([f1d, f2d, f3d])
108    print('Forward-difference approximation: ', fd)
109    fd= np.linalg.norm(fd)
110
111    # complex step approximation
112    x1_c = x0 + h*1j*pert_x1
113    f1_c = evaluate(x1_c)
114    cs_1 = f1_c.imag/h
115
116    x2_c = x0 + h*1j*pert_x2
117    f2_c = evaluate(x2_c)
118    cs_2 = f2_c.imag/h
119
120    x3_c = x0 + h*1j*pert_x3
121    f3_c = evaluate(x3_c)
122    cs_3 = f3_c.imag/h
123
124    cs= np.array([cs_1,cs_2,cs_3])
125    print('Complex-step approximation: ', cs)
126    cs= np.linalg.norm(cs)
127
128    total_der = adjoint_total_derivative(x0)[0]
129    print('Adjoint based total derivative: ', total_der)
130    total_der= np.linalg.norm(total_der)
131
132    error_fd= abs(fd- total_der)/abs(total_der)
133    error_cs= abs(cs- total_der)/abs(total_der)
134    print('Magnitude of relative FD error: ', error_fd)
135    print('Magnitude of relative CS error: ', error_cs,'\n')
```

```

137 def ptA_graph():
138     pert = np.array([1,1,1])
139     x0 = np.array([1.1, 1.2, 1.3])
140     f0 = evaluate(x0)
141     n = 1000
142     exp = np.linspace(1,30,n)
143     h_list = 1*10**(-exp)
144     fd_error = []
145     cs_error = []
146
147     pert_x1 = np.array([1,0,0])
148     pert_x2 = np.array([0,1,0])
149     pert_x3 = np.array([0,0,1])
150
151     for h in h_list:
152         #forward step approx
153         x1_d = x0 + h*pert_x1
154         f1_d = evaluate(x1_d)
155         f1d = (f1_d - f0)/h
156         x2_d = x0 + h*pert_x2
157         f2_d = evaluate(x2_d)
158         f2d = (f2_d - f0)/h
159         x3_d = x0 + h*pert_x3
160         f3_d = evaluate(x3_d)
161         f3d = (f3_d - f0)/h
162
163         fd = np.array([f1d, f2d, f3d])
164         fd = np.linalg.norm(fd)
165
166         #complex step approximation
167         x1_c = x0 + h*1j*pert_x1
168         f1_c = evaluate(x1_c)
169         cs_1 = f1_c.imag/h
170         x2_c = x0 + h*1j*pert_x2
171         f2_c = evaluate(x2_c)
172         cs_2 = f2_c.imag/h
173         x3_c = x0 + h*1j*pert_x3
174         f3_c = evaluate(x3_c)
175         cs_3 = f3_c.imag/h
176
177         cs = np.array([cs_1, cs_2, cs_3])
178         cs = np.linalg.norm(cs)
179
180         total_der = adjoint_total_derivative(x0)[0]
181         total_der = np.linalg.norm(total_der)
182
183         fd_error.append(abs(fd - total_der)/abs(total_der))
184         cs_error.append(abs(cs - total_der)/abs(total_der))
185
186     fig, ax = plt.subplots()
187     ax.plot(h_list, fd_error, 'b.')
188     ax.plot(h_list, cs_error, 'g.')
189     ax.set_xscale('log')
190     ax.set_yscale('log')
191
192     ax.legend(['FD', 'CS'], loc='best')
193     plt.xlabel('Step Size')
194     plt.ylabel('Relative Error')

```

```
196 def ptB():
197     x0 = np.array([1.1, 1.2, 1.3])
198
199     total_der = adjoint_total_derivative(x0)[0]
200     print('Adjoint-based derivative @x0: ', total_der)
201
202     h= 1e-30
203     pert_x1= np.array([1,0,0])
204     x1_c = x0 + h*1j*pert_x1
205     f1_c = evaluate(x1_c)
206     cs_1 = f1_c.imag/h
207
208     pert_x2= np.array([0,1,0])
209     x2_c = x0 + h*1j*pert_x2
210     f2_c = evaluate(x2_c)
211     cs_2 = f2_c.imag/h
212
213     pert_x3= np.array([0,0,1])
214     x3_c = x0 + h*1j*pert_x3
215     f3_c = evaluate(x3_c)
216     cs_3 = f3_c.imag/h
217
218     cs= np.array([cs_1,cs_2,cs_3])
219     print('Complex-step approximation: ', cs)
220     diff= abs(cs- total_der)/abs(total_der)
221     print('Rel error between CS & Adjoint: ', diff)
222
```