Optimization Techniques (MA-526)

Variable Metric Method For Constrained Optimization

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1 Introduction

In the unconstrained optimization problems the desirable improved convergence rate of Newton's method could be approached by using suitable update formulas to approximate the matrix of second derivatives. Thus, with the wisdom of hindsight, it is not surprising that, as first shown by Garcia- Palomares and Mangasarian [1], similar constructions can be applied to approximate the quadratic portion of our Lagrangian subproblems. The idea of approximating $\nabla^2 L$ using quasi-Newton update formulas that only require differences of gradients of the Lagrangian function was further developed by Han [2, 3] and Powell [4, 5]. The basic variable metric strategy proceeds as follows.

1.1 Description of the problem

P :

$$\begin{array}{ll} \text{Minimize} & f(x) \\ \text{Subject to} & h_k(x) = 0,\ k = 1, \dots, K \\ & g_j(x) \geq 0,\ j = 1, \dots, J \end{array}$$

1.2 Assumptions

The following assumptions are taken into account:

- f, g_i and h_j are differentiable.
- g_i is continuous at x^*.

2 Algorithm

Given initial estimates x^0 , u^0 , v^0 and a symmetric positive-definite matrix H^0.

Step 1. Solve the problem

$$\begin{array}{ll} \text{Minimize} & \nabla f(x^{(t)})^T d + \frac{1}{2} d^T \mathbf{H}^{(t)} d \\ \text{Subject to} & h_k(x^{(t)}) + \nabla h_k(x^{(t)})^T d = 0,\ k = 1, \dots, K \\ & g_j(x^{(t)}) + \nabla g_j(x^{(t)})^T d \geq 0,\ j = 1, \dots, J \end{array}$$

Step 2. Select the step size α along $d^{(t)}$ and set $x^{(t+1)} = x^{(t)} + \alpha d^{(t)}$.
Step 3. Check for convergence.
Step 4. Update $\mathbf{H}^{(t)}$ using the gradient difference

$$\nabla_x L(x^{(t+1)}, u^{(t+1)}, v^{(t+1)}) - \nabla_x L(x^{(t)}, u^{(t+1)}, v^{(t+1)})$$

in such a way that $\mathbf{H}^{(t+1)}$ remains positive definite.

The key choices in the above procedure involve the update formula for $\mathbf{H}^{(t)}$ and the manner of selecting α . Han [1, 2] considered the use of several well-known update formulas, particularly DFP. He also showed [1] that if the initial point is sufficiently close, then convergence will be achieved at a superlinear rate without a step-size procedure or line search by setting $\alpha = 1$. However, to assure convergence from arbitrary points, a line search is required. Specifically, Han [2] recommends the use of the penalty function

$$P(x, R) = f(x) + R\{\sum_{k=1}^{K} |h_k(x)| - \sum_{j=1}^{J} min(0, g_j(x))\}$$

to select α^* so that

$$P(x(\alpha^*)) = \min_{0 \leq \alpha \leq \delta} P(x^{(t)} + \alpha d^{(t)}), R)$$

where R and δ are suitably selected positive numbers.

Powell [4], on the other hand, suggests the use of the BFGS formula together with a conservative check that ensures that $\mathbf{H}^{(t)}$ remains positive definite. Thus, if

$$z = x^{(t+1)} - x^{(t)}$$

and

$$y = \nabla_x L(x^{(t+1)}, u^{(t+1)}, v^{(t+1)}) - \nabla_x L(x^{(t)}, u^{(t+1)}, v^{(t+1)})$$

Then define

$$\theta = \begin{cases} 1 & \text{if } z^T y \geq 0.2 z^T \mathbf{H}^{(t)} z \\ \frac{0.8 z^T \mathbf{H}^{(t)} z}{z^T \mathbf{H}^{(t)} z - z^T y} & \text{otherwise} \end{cases}$$

and calculate

$$w = \theta y + (1 - \theta) \mathbf{H}^{(t)} z$$

Finally, this value of w is used in the BFGS updating formula,

$$\mathbf{H}^{(t+1)} = \mathbf{H}^{(t)} - \frac{\mathbf{H}^{(t)} z z^T \mathbf{H}^{(t)}}{z^T \mathbf{H}^{(t)} z^T} + \frac{w w^T}{z^T w}$$

Note that the numerical value 0.2 is selected empirically and that the normal BFGS update is usually stated in terms of y rather than w.

On the basis of empirical testing, Powell [5] proposed that the step-size procedure be carried out using the penalty function

$$P(x, \mu, \sigma) = f(x) + \sum_{k=1}^{K} \mu_k |h_k(x)| - \sum_{j=1}^{J} \sigma_j min(0, g_j(x))$$

where for the first iteration

$$\mu_k = |v_k|, \sigma_j = |u_j|$$

and for all subsequent iterations t

$$\mu_k^{(t)} = max(|v_k^{(t)}|, \frac{1}{2}(\mu_k^{(t-1)} + |v_k^{(t)}|))$$

$$\sigma_j^{(t)} = max(|u_j^{(t)}|, \frac{1}{2}(\sigma_j^{(t-1)} + |u_j^{(t)}|))$$

The line search could be carried out by selecting the largest value of $\alpha, 0 \leq \alpha \leq 1$, such that

$$P(x(\alpha)) < P(x(0))$$

However, Powell [5] prefers the use of quadratic interpolation to generate a sequence of values of α_k until the more conservative condition

$$P(x(\alpha_k)) \leq P(x(0)) + 0.1\alpha_k \frac{dP}{d\alpha}(x(0))$$

is met. It is interesting to note, however, that examples have been found for which the use of Powell's heuristics can lead to failure to converge [6]. Further refinements of the step-size procedure have been reported [7], but these details are beyond the scope of the present treatment.

3 Implementation

The code was written in Python language, using Numpy, Scipy and Matplotlib libraries.

Environment Setup

- Python 2.7.14
- matplotlib 2.1.0
- numpy 1.13.3
- scipy 1.0.0

The code can be found in Appendix in Section 6.

4 Evalution and Results

Example 1

Problem Statement

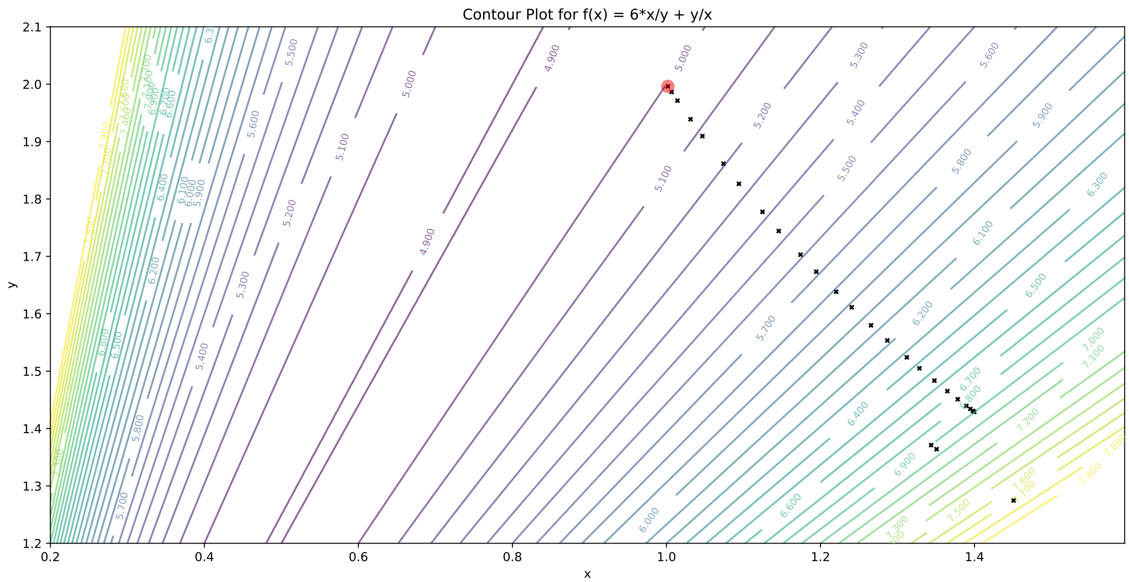
$$\begin{array}{ll} \text{Minimize} & f(x) = 6x_1x_2^{-1} + x_2x_1^{-1} \\ \text{Subject to} & h(x) = x_1x_2 - 2 = 0 \\ & g(x) = x_1 + x_2 - 1 \geq 0 \\ \text{Initialisation} & x^0 = (2,1), H^0 = I \end{array}$$

Results

Table 1: Values of $\mathbf{x_1}$, $\mathbf{x_2}$ and $\mathbf{f(x)}$ after each iteration

Iteration	$\mathbf{x_1}$	$\mathbf{x_2}$	$\mathbf{f(x)}$
1	1.450	1.274	7.43474
2	1.350	1.363	6.68951
3	1.343	1.371	6.63966
4	1.399	1.428	6.60628
5	1.397	1.430	6.59488
6	1.394	1.434	6.57176
7	1.389	1.439	6.53692
8	1.378	1.451	6.46293
9	1.364	1.465	6.37562
10	1.347	1.483	6.26813
11	1.328	1.504	6.14924
12	1.312	1.524	6.05084
13	1.286	1.553	5.90833
14	1.265	1.579	5.79306
15	1.240	1.611	5.66654
16	1.220	1.638	5.56931
17	1.194	1.673	5.45614
18	1.174	1.702	5.37209
19	1.145	1.744	5.27006
20	1.124	1.777	5.20153
21	1.094	1.826	5.12007
22	1.074	1.861	5.07568
23	1.046	1.909	5.03189
24	1.031	1.938	5.01439
25	1.014	1.971	5.00332
26	1.006	1.986	5.00074
27	**1.001**	**1.996**	**5.00007**

Graph



Example 2

Problem Statement

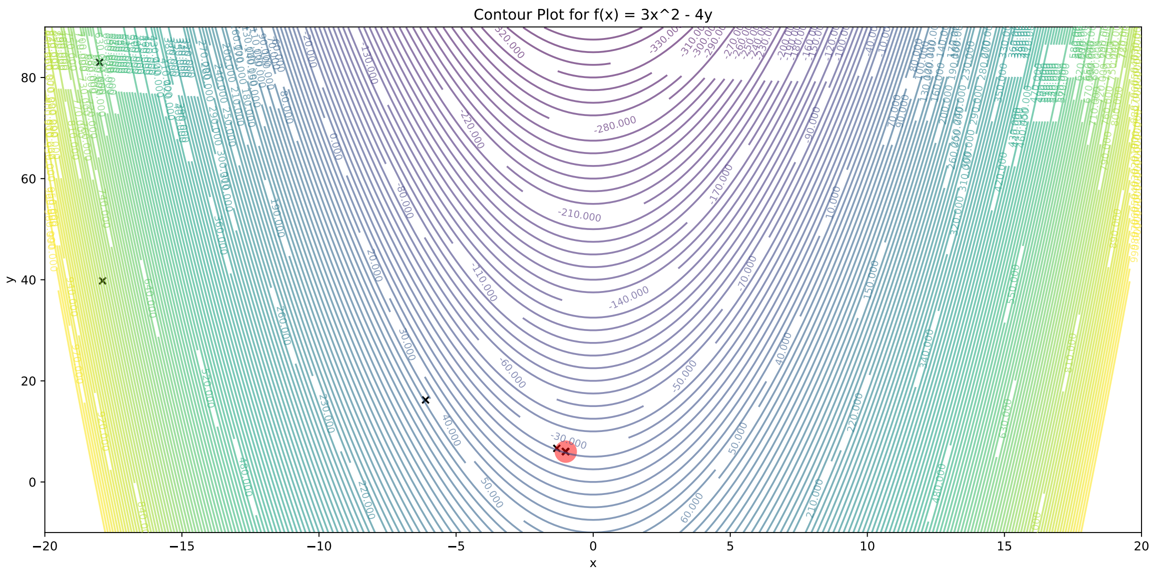
$$
\begin{aligned}
&\text{Minimize} && f(x) = 3x_1^2 - 4x_2 \\
&\text{Subject to} && h(x) = 2x_1 + x_2 - 4 = 0 \\
& && g(x) = 37 - x_1^2 - x_2^2 \geq 0 \\
&\text{Initialisation} && x^0 = (50, 50), H^0 = I
\end{aligned}
$$

Results

Table 2: Values of $\mathbf{x_1}$, $\mathbf{x_2}$ and $\mathbf{f(x)}$ after each iteration

Iteration	$\mathbf{x_1}$	$\mathbf{x_2}$	$\mathbf{f(x)}$
1	-18.005	82.983	640.69981
2	-17.892	39.785	801.31495
3	-6.114	16.228	47.23222
4	-1.326	6.653	-21.33320
5	-1.018	6.036	-21.03549
6	**-1.000**	**6.000**	**-21.00012**

Graph



5 References

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[8] Bartholemew-Biggs, M. C., "Recursive Quadratic Programming Based on Penalty Functions for Constrained Minimization," in Nonlinear Optimization: Theory and Algorithms (L. C. W. Dixon, E. Spedicato, and G. P. Szego, Eds.), Birkhauser, Boston, 1980.

6 Appendix

```
import numpy as np
from scipy import optimize
from sympy import *
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm

x_values = []

def list_to_array(x):
    return np.array(x, dtype = np.float64).reshape(2, 1)

def calculate_function_value(fx, xvars, xcurr):
    return fx.subs(zip(xvars,xcurr))

def find_dk(curr_fx, curr_hx, curr_gx, curr_grad_fx, curr_grad_hx,
    curr_grad_gx, H):
    curr_grad_fx = list_to_array(curr_grad_fx)
    curr_grad_gx = list_to_array(curr_grad_gx)
    curr_grad_hx = list_to_array(curr_grad_hx)

    new_hx = lambda d : curr_hx + np.matmul(np.transpose(
    curr_grad_hx), list_to_array(d))
    new_gx = lambda d : curr_gx + np.matmul(np.transpose(
    curr_grad_gx), list_to_array(d))
    objective = lambda d :  np.matmul(np.transpose(curr_grad_fx),
    list_to_array(d)) + (np.matmul(np.transpose(list_to_array(d)),
    np.matmul(H, list_to_array(d))))/2

    constraints = ({'type': 'eq', 'fun': new_hx},
                   {'type': 'ineq', 'fun': new_gx})

    result = optimize.minimize(objective, [1.0, 1.0], constraints =
     constraints)
    return result.x

def find_lagrange_multipliers(curr_fx, curr_hx, curr_gx,
    curr_grad_fx, curr_grad_hx, curr_grad_gx, H, d):
    A = np.array( ( [ curr_grad_hx[0], curr_grad_gx[0] ], [
    curr_grad_hx[1], curr_grad_gx[1]] ), dtype = np.float64)
```

```
    B = np.array( [ curr_grad_fx[0] + H[0][0]*d[0] + (H[0][1] + H[1][0])*d[1] , curr_grad_fx[1] + H[1][1]*d[1] + (H[0][1] + H[1][0])*d[0] ], dtype = np.float64 ).reshape(2,1)
    A_inverse = np.linalg.inv(A)
    X = np.matmul(A_inverse,B)
    return X[0][0], X[1][0]

def calculate_mu_sigma(k, u, v, mu_k_1, sigma_k_1):
    if k==1:
        mu_k = abs(v)
        sigma_k = abs(u)
    else:
        mu_k = max(abs(v),(mu_k_1+abs(v))/2)
        sigma_k = max(abs(u), (sigma_k_1+abs(u))/2)
    return mu_k, sigma_k


def minimize_alpha_through_penalty_function(fx, hx, gx, mu_k, sigma_k, x_k_1, d_k):
    alpha = symbols('alpha')
    Px = fx + mu_k*abs(hx) - sigma_k*Min(0, gx)
    P_alpha = Px.subs([(x1,x_k_1[0]+alpha*d_k[0]), (x2,x_k_1[1]+alpha*d_k[1])])
    call_P = lambda alpha : P_alpha.subs([('alpha',alpha)])
    constraints = ({'type': 'ineq', 'fun': lambda alpha: alpha},
                   {'type': 'ineq', 'fun': lambda alpha: 1-alpha})
    alpha_k = optimize.minimize(call_P, 0, constraints = constraints).x
    return alpha_k

def calculate_y(grad_L, x_k, x_k_1):
    return np.array([i.subs([(x1,x_k[0]),(x2,x_k[1])]) for i in grad_L]) - np.array([i.subs([(x1,x_k_1[0]),(x2,x_k_1[1])]) for i in grad_L])

def calculate_theta(z, y, H):
    z = z.reshape(2,1).astype(np.float64)
    y = y.reshape(2,1).astype(np.float64)
    a1 = np.matmul(np.transpose(z),y)
    a2 = 0.2*np.matmul(np.transpose(z), np.matmul(H,z))
    if(a1>=a2):
        return np.array([[1]])
    else:
        return (0.8*np.matmul(np.transpose(z), np.matmul(H,z)))/(np.matmul(np.transpose(z), np.matmul(H,z)) - np.matmul(np.transpose(z),y))

def calculate_w(theta, H, z, y):
    z = z.reshape(2,1).astype(np.float64)
    y = y.reshape(2,1).astype(np.float64)
    theta = theta[0][0]
    return theta*y + (1-theta)*np.matmul(H,z)

def updateH(H, z, w):
    z = z.reshape(2,1).astype(np.float64)
    w = w.reshape(2,1).astype(np.float64)
```

```
    a1 = np.matmul(H , np.matmul(z, np.matmul(np.transpose(z) , H ))) / np.matmul(np.transpose(z) , np.matmul(H, z) )
    a2 = np.matmul(w, np.transpose(w)) / np.matmul(np.transpose(z), w)
    return H - a1 + a2

def constrained_variable_metric_method(fx, hx, gx, x_0, H_0, xvars, no_of_iterations):
    d1, d2 = symbols('d1 d2')
    dvars = [d1, d2]

    grad_fx = np.array([ diff(fx, x) for x in xvars ])
    grad_hx = np.array([ diff(hx, x) for x in xvars ])
    grad_gx = np.array([ diff(gx, x) for x in xvars ])

    x_k_1 = x_0
    H_k_1 = H_0

    mu_k_1 = 0
    sigma_k_1 = 0

    for k in range(1,no_of_iterations+1):

        xcurr = x_k_1
        H_k = H_k_1

        curr_fx = np.array([ fx.subs(zip(xvars,xcurr)) ])
        curr_hx = np.array([ hx.subs(zip(xvars,xcurr)) ])
        curr_gx = np.array([ gx.subs(zip(xvars,xcurr)) ])

        curr_grad_fx = np.array([ dfx.subs(zip(xvars,xcurr)) for dfx in grad_fx ])
        curr_grad_hx = np.array([ dhx.subs(zip(xvars,xcurr)) for dhx in grad_hx ])
        curr_grad_gx = np.array([ dgx.subs(zip(xvars,xcurr)) for dgx in grad_gx ])

        d_k = find_dk(curr_fx, curr_hx, curr_gx, curr_grad_fx, curr_grad_hx, curr_grad_gx, H_k)

        v, u = find_lagrange_multipliers(curr_fx, curr_hx, curr_gx, curr_grad_fx, curr_grad_hx, curr_grad_gx, H_k, d_k)

        mu_k, sigma_k = calculate_mu_sigma(k, u, v, mu_k_1, sigma_k_1)

        alpha_k = minimize_alpha_through_penalty_function(fx, hx, gx, mu_k, sigma_k, x_k_1, d_k)

        x_k = x_k_1 + alpha_k*d_k.reshape(2)

        z = x_k - x_k_1

        grad_L = grad_fx - v*grad_hx - u*grad_gx

        y = calculate_y(grad_L, x_k, x_k_1)

```

```python
        theta = calculate_theta(z, y, H_k)

        w = calculate_w(theta, H_k, z, y)

        H_k_1 = updateH(H_k, z, w)

        print('Iteration: '+str(k)+' '+str(x_k)+' '+str(calculate_function_value(fx, xvars, x_k)))
        x_values.append(list(x_k))

        x_k_1 = x_k
        mu_k_1 = mu_k
        sigma_k_1 = sigma_k

    print('****************************************')
    print('Final x: '+str(x_k))
    print('f(x): '+str(calculate_function_value(fx, xvars, x_k)))
    print('****************************************')
    return




x1, x2 = symbols('x1 x2')
xvars = [x1, x2]

case = 1 # 1 or 2

if case == 1:
    fx = 6*x1*(x2**-1) + x2*(x1**-2)
    hx = x1*x2 - 2
    gx = x1 + x2 -1

    x_0 = np.array([2.0,1.0])
    H_0 = np.eye(2)

    num_iterations = 27
elif case == 2:
    fx = 3*x1**2 - 4*x2
    hx = 2*x1 + x2 -4
    gx = 37 - x1**2 - x2**2

    x_0 = np.array([50,50])
    H_0 = np.eye(2)

    num_iterations = 7

constrained_variable_metric_method(fx,hx,gx,x_0,H_0,xvars,num_iterations)

X_list1 = [i[0] for i in x_values]
Y_list1 = [i[1] for i in x_values]
print(X_list1)
print(Y_list1)
```

Listing 1: main.py