

Optimization Algorithms: Theory and Software Implementation

Prof. Thirumulanathan D

Department of Mathematics

Institute of IIT Kanpur

Lecture: 37

Hello everyone, this is the second lecture in week 8. Recall that in the previous lecture, we introduced the augmented Lagrangian method. We discussed the differences between the quadratic penalty method and the augmented Lagrangian method, noting that while the procedural steps are similar, the augmented Lagrangian method resolves the issues associated with the quadratic penalty method.

Let us now consider an example to illustrate the augmented Lagrangian method. We will use the same example from earlier:

$$\text{minimize } f(\mathbf{x}) = x_1^2 + x_2^2 + x_3^2$$

subject to the constraints

$$h_1(\mathbf{x}) = 3x_1 + x_2 + x_3 - 5 = 0 \text{ and } h_2(\mathbf{x}) = x_1 + x_2 + x_3 - 1 = 0.$$

We already know the solution is

$$\mathbf{x}^* = (2, -0.5, -0.5) \text{ and the Lagrange multipliers are } \lambda^* = (-2.5, 3.5).$$

Notation: $\nabla_2 f(\mathbf{x}) = \nabla^2 f(\mathbf{x}) = \text{Hessian}$, $\mu_{k+1} = \mu^{k+1}$, $\lambda_k = \lambda^k$, $\mathbf{x}_k = \mathbf{x}^k$, $\lambda_{m,k} = \lambda_m^{(k)}$, $\mu_{n,k} = \mu_n^{(k)}$

The augmented Lagrangian function is defined as:

$$L_\gamma(\mathbf{x}, \lambda) = f(\mathbf{x}) + \sum_j \lambda_j h_j(\mathbf{x}) + \gamma \sum_j [h_j(\mathbf{x})]^2.$$

The gradient is:

$$\nabla L_\gamma(\mathbf{x}, \lambda) = \nabla f(\mathbf{x}) + \sum_j \lambda_j \nabla h_j(\mathbf{x}) + 2\gamma \sum_j h_j(\mathbf{x}) \nabla h_j(\mathbf{x}).$$

The Hessian is:

$$\nabla^2 L_\gamma(\mathbf{x}, \lambda) = \nabla^2 f(\mathbf{x}) + \sum_j \lambda_j \nabla^2 h_j(\mathbf{x}) + 2\gamma \sum_j [h_j(\mathbf{x}) \nabla^2 h_j(\mathbf{x}) + \nabla h_j(\mathbf{x}) \nabla h_j(\mathbf{x})^T].$$

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$$\min_{x_1, x_2, x_3} x_1^2 + x_2^2 + x_3^2$$

$$\text{s.t.} \quad 3x_1 + x_2 + x_3 = 5$$

$$x_1 + x_2 + x_3 = 1$$

$$(x_1^*, x_2^*, x_3^*, \lambda_1^*, \lambda_2^*) = (2, -\frac{1}{2}, -\frac{1}{2}, -2.5, 3.5)$$

$$L_\eta(x, \lambda) = f(x) + \sum_{j=1}^m \lambda_j h_j(x) + \eta \sum_{j=1}^m [h_j(x)]^2$$

$$\nabla L_\eta(x, \lambda) = \nabla f(x) + \sum_{j=1}^m \lambda_j \nabla h_j(x) + 2\eta \sum_{j=1}^m h_j(x) \nabla h_j(x)$$

$$\nabla_x^2 L_\eta(x, \lambda) = \nabla_x^2 f(x) + \sum_{j=1}^m \lambda_j \nabla_x^2 h_j(x) + 2\eta \sum_{j=1}^m [h_j(x) \nabla_x^2 h_j(x) + \nabla h_j(x) \nabla h_j(x)^T]$$

We can implement this in Python by modifying the code for the quadratic penalty method. The key changes are:

1. Define $L_\gamma(x, \lambda) = f(x) + \lambda \cdot h(x) + \gamma (h \cdot h)$
2. Define $\nabla L_\gamma(x, \lambda) = \nabla f(x) + \lambda @ \nabla h(x) + 2\gamma h(x) @ \nabla h(x)$
3. Define the Hessian as $2I + 2\gamma \nabla h(x)^T \nabla h(x)$

We initialize x_0 , set $\gamma = 1$, and initialize $\lambda_0 = [0, 0]$.

We then iterate until $|L_\gamma(x, \lambda) - f(x)| > 1e-6$ and $\|\nabla L_\gamma(x, \lambda)\| > 1e-6$.

In each iteration, we update x using Newton's method and update λ as $\lambda_{k+1} = \lambda_k + 2\gamma h(x)$.

After running the code, we obtain $x^* = (2, -0.5, -0.5)$ and $\lambda^* = (-2.5, 3.5)$, which matches the expected solution.

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+ Code + Text
import numpy as np

def f(x):
    return x[0]**2+x[1]**2+x[2]**2

def h(x):
    return np.array([3*x[0]+x[1]+x[2]-5,x[0]+x[1]+x[2]-1])

def grad_h(x):
    return np.array([[3,1,1],[1,1,1]])

def L(x,l,gm):
    return f(x)+l.dot(h(x))+gm*h(x).dot(h(x))

def grad(x,l,gm):
    return 2*x+l@grad_h(x)+2*gm*h(x)@grad_h(x)

def H(x,l,gm):
    return 2*np.eye(3)+2*gm*grad_h(x).T@grad_h(x)

x,l,gm,k=np.array([0,0,0]),np.array([0,0]),1,0
while(np.abs(L(x,l,gm)-f(x))>1e-6):
    while(np.linalg.norm(grad(x,l,gm))>1e-6):
        x=-np.linalg.inv(H(x,l,gm))@grad(x,l,gm) # Newton's method
        print("%1.3e,%1.3e,%1.3e,%1.3e"%(x[0],x[1],x[2],np.linalg.norm(grad(x,l,gm))))
    l=1+2*gm*h(x)
    k=k+1

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+ Code + Text
def grad_h(x):
    return np.array([[3,1,1],[1,1,1]])

def L(x,l,gm):
    return f(x)+l.dot(h(x))+gm*h(x).dot(h(x))

def grad(x,l,gm):
    return 2*x+l@grad_h(x)+2*gm*h(x)@grad_h(x)

def H(x,l,gm):
    return 2*np.eye(3)+2*gm*grad_h(x).T@grad_h(x)

x,l,gm,k=np.array([0,0,0]),np.array([0,0]),1,0
while(np.abs(L(x,l,gm)-f(x))>1e-6):
    @while(np.linalg.norm(grad(x,l,gm))>1e-6):
        x=-np.linalg.inv(H(x,l,gm))@grad(x,l,gm) # Newton's method
        print("%1.3e,%1.3e,%1.3e,%1.3e"%(x[0],x[1],x[2],np.linalg.norm(grad(x,l,gm))))
    l=1+2*gm*h(x)
    k=k+1
    print("k=%d,%1.3e,%1.3e,%1.3e"%(k,l[0],l[1],np.abs(L(x,l,gm)-f(x))))

k=4,-2.218e+00,2.913e+00,7.353e-01
1.919e+00,-4.045e-01,-4.045e-01,1.804e-15
k=5,-2.323e+00,3.132e+00,4.812e-01
1.949e+00,-4.402e-01,-4.402e-01,2.882e-15
k=6,-2.389e+00,3.270e+00,3.095e-01
1.968e+00,-4.626e-01,-4.626e-01,2.081e-15

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k=25, -2.500e+00, 3.500e+00, 4.439e-05
2.000e+00, -5.000e-01, -5.000e-01, 4.955e-15
k=26, -2.500e+00, 3.500e+00, 2.780e-05
2.000e+00, -5.000e-01, -5.000e-01, 7.364e-15
k=27, -2.500e+00, 3.500e+00, 1.741e-05
2.000e+00, -5.000e-01, -5.000e-01, 4.710e-16
k=28, -2.500e+00, 3.500e+00, 1.090e-05
2.000e+00, -5.000e-01, -5.000e-01, 6.896e-15
k=29, -2.500e+00, 3.500e+00, 6.827e-06
2.000e+00, -5.000e-01, -5.000e-01, 4.021e-15
k=30, -2.500e+00, 3.500e+00, 4.275e-06
2.000e+00, -5.000e-01, -5.000e-01, 7.833e-15
k=31, -2.500e+00, 3.500e+00, 2.677e-06
k=32, -2.500e+00, 3.500e+00, 2.677e-06
2.000e+00, -5.000e-01, -5.000e-01, 2.412e-15
k=33, -2.500e+00, 3.500e+00, 6.758e-07

```

[] Start coding or [generate](#) with AI.

Now, we extend the method to problems with inequality constraints. Consider the problem:

$$\min f(x)$$

subject to

$$g_i(x) \leq 0 \text{ for } i = 1 \text{ to } p,$$

and

$$h_j(x) = 0 \text{ for } j = 1 \text{ to } m.$$

We convert inequality constraints to equality constraints by introducing slack variables s_i :

Which is equivalent to

$$\min_{\{x, s_i\}} f(x)$$

s.t.

$$g_i(x) + s_i^2 = 0 \text{ for all } i=1,2,\dots,p \text{ and } h_j(x)=0 \text{ for } j=1,2,\dots,m.$$

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$$\min_{x_1, x_2, x_3} x_1^2 + x_2^2 + x_3^2$$

$$\text{s.t. } 3x_1 + x_2 + x_3 = 5$$

$$x_1 + x_2 + x_3 = 1$$

$$(x_1^*, x_2^*, x_3^*, \lambda_1^*, \lambda_2^*) = (2, -\frac{1}{2}, -\frac{1}{2}, -2.5, 3.5) \checkmark$$

$$L_q(x, \lambda) = f(x) + \sum_{j=1}^m \lambda_j h_j(x) + q \sum_{j=1}^m [h_j(x)]^2$$

$$\nabla L_q(x, \lambda) = \nabla f(x) + \sum_{j=1}^m \lambda_j \nabla h_j(x) + 2q \sum_{j=1}^m h_j(x) \nabla h_j(x)$$

$$\nabla_x^2 L_q(x, \lambda) = \nabla_x^2 f(x) + \sum_{j=1}^m \lambda_j \nabla_x^2 h_j(x) + 2q \sum_{j=1}^m [h_j(x) \nabla_x^2 h_j(x) + \nabla h_j(x) \nabla h_j(x)^T]$$

Inequality constraints:

$$\min_x f(x)$$

$$\text{s.t. } g_i(x) \leq 0 \quad \forall i=1, \dots, p$$

$$h_j(x) \geq 0 \quad \forall j=1, \dots, m.$$

$$\equiv \min_{(x, s_i)} f(x)$$

$$\text{s.t. } g_i(x) + s_i^2 = 0 \quad \forall i=1, \dots, p$$

$$h_j(x) \geq 0 \quad \forall j=1, \dots, m$$

The augmented Lagrangian becomes:

$$L_\gamma(x, \lambda, \mu) = f(x) + \sum_{j=1}^m \lambda_j h_j(x) + \sum_{i=1}^p \mu_i (g_i(x) + s_i^2) + \gamma [\sum_{j=1}^m (h_j(x))^2 + \sum_{i=1}^p (g_i(x) + s_i^2)^2].$$

We minimize over s_i analytically. The optimal s_i^* is given by:

$$L_\gamma(x, \lambda, \mu) = f(x) + \sum_{j=1}^m \lambda_j h_j(x) + \gamma \sum_{j=1}^m (h_j(x))^2 + \gamma [\sum_{i=1}^p (g_i(x) + s_i^2 + \mu_i/(2\gamma))^2 - \mu_i^2/(4\gamma^2)].$$

This implies that

$$(g_i(x) + s_i^2 + \mu_i/(2\gamma))^2 = (g_i(x) + s_i^2)^2 + \mu_i^2/(4\gamma^2) + (g_i(x) + s_i^2) \cdot \mu_i/\gamma$$

$$s_i^* = \operatorname{argmin}_{s_i} L_\gamma(x, \lambda, \mu) = \begin{cases} \sqrt{g_i(x) + \mu_i/(2\gamma)} & \text{if } g_i(x) + \mu_i/(2\gamma) \leq 0 \\ 0 & \text{if } g_i(x) + \mu_i/(2\gamma) > 0 \end{cases}$$

$$g_i(x) + s_i^{*2} + \mu_i/(2\gamma) = (g_i(x) + \mu_i/(2\gamma)) \text{ if } g_i(x) + \mu_i/(2\gamma) \leq 0, \text{ and } 0 \text{ otherwise.}$$

$$= \max(0, g_i(x) + \mu_i/(2\gamma))$$

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$$L_\gamma(x, \lambda, \mu) = f(x) + \sum_{j=1}^m \lambda_j h_j(x) + \sum_{i=1}^p \mu_i (g_i(x) + \lambda_i)^2$$

$$+ \gamma \left(\sum_{j=1}^m [h_j(x)]^2 + \sum_{i=1}^p (g_i(x) + \lambda_i)^2 \right)$$

$$\min_{\lambda_i} [L_\gamma(x, \lambda, \mu)]$$

$$L_\gamma(x, \lambda, \mu) = f(x) + \sum_{j=1}^m \lambda_j h_j(x) + \gamma \sum_{j=1}^m [h_j(x)]^2$$

$$+ \gamma \left[\sum_{i=1}^p \left(g_i(x) + \lambda_i + \frac{\mu_i}{2\gamma} \right)^2 - \frac{\mu_i^2}{4\gamma^2} \right]$$

$$\left(g_i(x) + \lambda_i + \frac{\mu_i}{2\gamma} \right)^2 = \left(g_i(x) + \lambda_i \right)^2 + \frac{\mu_i^2}{4\gamma^2} + \frac{\mu_i}{\gamma} \cdot (g_i(x) + \lambda_i)$$

$$\lambda_i^* = \underset{\lambda_i}{\operatorname{argmin}} L_\gamma(x, \lambda, \mu) = \begin{cases} -\left(g_i(x) + \frac{\mu_i}{2\gamma} \right) & \text{if } g_i(x) + \frac{\mu_i}{2\gamma} \leq 0 \\ 0 & \text{if } g_i(x) + \frac{\mu_i}{2\gamma} > 0 \end{cases}$$

$$g_i(x) + \left(\lambda_i^* \right)^2 + \frac{\mu_i}{2\gamma} = \begin{cases} g_i(x) + \frac{\mu_i}{2\gamma} & g_i(x) + \frac{\mu_i}{2\gamma} > 0 \\ 0 & g_i(x) + \frac{\mu_i}{2\gamma} \leq 0 \end{cases}$$

$$= \max\left(0, g_i(x) + \frac{\mu_i}{2\gamma}\right).$$

Substituting back, we obtain:

$$L_\gamma(x, \lambda, \mu) = f(x) + \sum_j \lambda_j h_j(x) + \gamma \sum_j (h_j(x))^2 + \gamma \sum_i \left[\left(\max\left(0, g_i(x) + \frac{\mu_i}{2\gamma}\right) \right)^2 - \frac{\mu_i^2}{4\gamma^2} \right].$$

The update for μ is:

$$\mu_{k+1} = \max(0, \mu_k + 2\gamma g(x)).$$

The algorithm is:

Initialize x_0 , $k = 0$, tolerance, $\gamma > 0$, $\lambda_0 = (\lambda_{1,0}, \lambda_{2,0}, \dots, \lambda_{m,0})$ (size m), μ_0 (size p) ($\mu_{1,0}, \mu_{2,0}, \dots, \mu_{p,0}$).

While $|L_\gamma(x_k, \lambda_k, \mu_k) - f(x_k)| > \text{tolerance}$:

$$x_{k+1} = \operatorname{argmin}_x L_\gamma(x, \lambda_k, \mu_k)$$

$$\lambda_{k+1} = \lambda_k + 2\gamma h(x_{k+1})$$

$$\mu_{k+1} = \max(0, \mu_k + 2\gamma g(x_{k+1}))$$

$$k = k + 1$$

Output $x^* = x_k$, $\lambda^* = \lambda_k$, $\mu^* = \mu_k$.

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$$L_{\eta}(x, \lambda, \mu) = f(x) + \sum_{j=1}^m \lambda_j h_j(x) + \eta \left(\sum_{j=1}^m [h_j(x)]^2 + \sum_{i=1}^p \left[\max\left(0, g_i(x) + \frac{\mu_i}{2\eta}\right) \right]^2 - \frac{\mu_i^2}{4\eta^2} \right)$$

$$\mu^{k+1} = \max(0, \mu^k + 2\eta g(x)), \quad \lambda^{k+1} = \lambda^k + 2\eta h(x)$$

Algorithm:

- (i) Initialize $x^{(0)}, k=0, \text{tol}, \eta > 0, \lambda^{(0)} = (\lambda_1^{(0)}, \dots, \lambda_m^{(0)}), \mu^{(0)} = (\mu_1^{(0)}, \dots, \mu_p^{(0)})$
- (ii) while $(|L_{\eta}(x^k, \lambda^k, \mu^k) - f(x^k)| > \text{tol})$:
 - * Find $x^{k+1} = \underset{x \in \mathbb{R}^n}{\text{argmin}} L_{\eta}(x, \lambda^k, \mu^k)$
 - * $\lambda^{k+1} = \lambda^k + 2\eta h(x^{k+1}), \mu^{k+1} = \max(0, \mu^k + 2\eta g(x^{k+1}))$
 - * $k = k+1$
- (iii) Output $(x^*, \lambda^*, \mu^*) = (x^k, \lambda^k, \mu^k)$.

This approach handles both equality and inequality constraints effectively.

We will continue with more details in the next lecture. Thank you.