Numerical Optimization with applications: Homework 01

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Exercise 1. *Compute the gradient $\nabla f(x)$ and Hessian $\nabla^2 f(x)$ of the Rosenbrock function*

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

Show that $x^* = (1,1)^T$ is the only local minimizer of this function, and that the Hessian matrix at that point is positive definite.

Proof. Calculating the gradient of $f(x)$

$$\nabla f(x) = \begin{bmatrix} f_{x_1} \\ f_{x_2} \end{bmatrix} = \begin{bmatrix} 200(x_2 - x_1^2)(2x_1) + 2(1-x_1)(-1) \\ 200(x_2 - x_1^2) \end{bmatrix} = \begin{bmatrix} -400x_1(x_2 - x_1^2) + 2(x_1 - 1) \\ 200(x_2 - x_1^2) \end{bmatrix}$$

Solving $\nabla f(x) = 0$, we obtain that $\nabla f(x) = 0$ if and only if x equals to $x^* = (1,1)^T$.

On the other hand, calculating the Hessian of $f(x)$

$$\nabla^2 f(x) = \begin{bmatrix} f_{x_1x_1} & f_{x_1x_2} \\ f_{x_2x_1} & f_{x_2x_2} \end{bmatrix} = \begin{bmatrix} 400(x_2 - x_1^2) - 400x_1(2x_2) + 4 & 400x_1 \\ -400x_1 & 200 \end{bmatrix}$$

Observe that

$$\begin{aligned} P^T \nabla^2 f(x^*) P &= \begin{bmatrix} p_1 & p_2 \end{bmatrix} \begin{bmatrix} 804 & 400 \\ -400 & 200 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} \\ &= 804p_1^2 + 400p_1p_2 - 400p_1p_2 + 200p_2^2 \\ &= 804p_1^2 + 200p_2^2 \end{aligned}$$

Therefore, $P^T \nabla^2 f(x^*) P > 0$ for all nonzero vector P. *i.e. the Hessian matrix at x^* is positive definite.* By Theorem2.4 (Second-Order Sufficient Conditions), $x^* = (1,1)^T$ is the only local minimizer of this function. □

Exercise 7. *Suppose that $f(x) = x^T Q x$, where Q is an $n \times n$ symmetric positive semidefinite matrix. Show using the definition (1.4) that $f(x)$ is convex on the domain $\mathbb{R}^n$.Hint: It may be convenient to prove the following equivalent inequality:*

$$f(y + \alpha(x-y)) - \alpha f(x) - (1-\alpha) f(y) \le 0$$

for all $\alpha \in [0,1]$ and all $x, y \in \mathbb{R}$.

Proof. By the definition of f and (1.4), for any $x, y \in \mathbb{R}^n$

$$\begin{aligned} & f(y + \alpha(x-y)) - \alpha f(x) - (1-\alpha) f(y) \\ &= (y + \alpha(x-y))^T Q (y + \alpha(x-y)) - \alpha x^T Q x - (1-\alpha) y^T Q y \\ &= y^T Q y + \alpha y^T Q (x-y) + \alpha (x-y)^T Q y + \alpha^2 (x-y)^T Q (x-y) - \alpha x^T Q x - (1-\alpha) y^T Q y \\ &= \alpha [y^T Q y + y^T Q (x-y) - x^T Q x + (x-y)^T Q y] + \alpha^2 (x-y)^T Q (x-y) \\ &= \alpha [y^T Q x - x^T Q x + (x-y)^T Q y] + \alpha^2 (x-y)^T Q (x-y) \\ &= \alpha [-(x-y)^T Q x + (x-y)^T Q y] + \alpha^2 (x-y)^T Q (x-y) \\ &= -\alpha (x-y)^T Q (x-y) + \alpha^2 (x-y)^T Q (x-y) \\ &= (\alpha - \alpha^2)(x-y)^T Q (x-y) \le 0 \end{aligned}$$

since $\alpha \in [0,1]$ and Q is positive semidefinite. This completes the proof. □

Exercise 8. *Suppose that f is a convex function. Show that the set of global minimizer of f is a convex set.*

Proof. Let E denotes the set of global minimizer of f.
For any $x^*, y^* \in E$, $f(x^*) \leq f(y^*)$ and $f(y^*) \leq f(x^*)$. i.e. $f(x^*) = f(y^*)$
Then for any $\alpha \in [0,1]$

$$f(\alpha x^* + (1-\alpha)y^*) \leq \alpha f(x^*) + (1-\alpha)f(y^*) = f(x^*) \leq f(x) \qquad \forall x \in \mathbb{R}^n$$

since x^* is a global minimizer.
By above, $f(\alpha x^* + (1-\alpha)y^*) \leq f(x), \forall x \in \mathbb{R}, \alpha \in [0,1]$.
E is a convex set. □

Exercise 16. *Consider the sequence x_k defined by*

$$x_k = \begin{cases} \left(\frac{1}{4}\right)^{2^k}, & k \text{ even}, \\ (x_{k-1})/k, & k \text{ odd}. \end{cases}$$

Is this sequence Q-superlinearly convergent? Q-quadratically convergent? R-quadratically convergent?

Proof. Clearly, x_k converges to $x^* = 0$

(i) Q-superlinearly:
If k is even: $\lim\limits_{k\to\infty} \dfrac{|x_{k+1} - x^*|}{|x_k - x*|} = \lim\limits_{k\to\infty} \dfrac{\frac{x_k}{k+1}}{x_k} = \lim\limits_{k\to\infty} \dfrac{1}{k+1} = 0$
If k is odd: $\lim\limits_{k\to\infty} \dfrac{|x_{k+1} - x^*|}{|x_k - x*|} = \lim\limits_{k\to\infty} \dfrac{x_{k+1}}{\frac{x_{k-1}}{k}} = \lim\limits_{k\to\infty} \dfrac{k(\frac{1}{4})^{2^k}}{(\frac{1}{4})^{2^{k-1}}} = \lim\limits_{k\to\infty} k(\dfrac{1}{4})^{2^{k-1}} = 0$
This implies x_k is Q-superlinearly convergence.

(ii) Q-quadratically:
If k is even: $\lim\limits_{k\to\infty} \dfrac{|x_{k+1} - x^*|}{|x_k - x*|^2} = \lim\limits_{k\to\infty} \dfrac{\frac{x_k}{k+1}}{x_k^2} = \lim\limits_{k\to\infty} \dfrac{1}{kx_k} = \lim\limits_{k\to\infty} \dfrac{1}{k(\frac{1}{4})^{2^k}} = +\infty$ This implies x_k is not Q-quadratically convergent.

(iii) R-quadratically:
Let $\epsilon_k = \begin{cases} \left(\frac{1}{4}\right)^{2^k}, & \text{k even}, \\ \left(\frac{1}{4}\right)^{2^{k-1}}, & \text{k odd}. \end{cases}$
When k is even, $|x_k - x^*| = |x_k| = (\frac{1}{4})^{2^k} \leq \epsilon_k$
When k is odd, $|x_k - x^*| = |x_k| = x_{k-1}/k = (\frac{1}{4})^{2^{k-1}}(\frac{1}{k}) \leq (\frac{1}{4})^{2^{k-1}} = \epsilon_k$
By the above, $|x_k - x^*| \leq \epsilon_k \quad \forall k$
If k is even: $\lim\limits_{k\to\infty} \dfrac{|\epsilon_{k+1} - 0|}{|\epsilon_k - 0|^2} = \lim\limits_{k\to\infty} \dfrac{(\frac{1}{4})^{2^k}}{(\frac{1}{4})^{2^k}} = 1$
If k is odd: $\lim\limits_{k\to\infty} \dfrac{|\epsilon_{k+1} - 0|}{|\epsilon_k - 0|^2} = \lim\limits_{k\to\infty} \dfrac{(\frac{1}{4})^{2^{k+1}}}{(\frac{1}{4})^{2^{k-1}}} = \lim\limits_{k\to\infty} [(\dfrac{1}{4})^{2^{k-1}}]^3 = 0$
This implies ϵ_k is Q-quadratically convergent.
And therefore, x_k is R-quadratically convergent.

□

Numerical Optimization with applications: Homework 02

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Exercise 5. *Prove that* $\|Bx\| \geq \frac{\|x\|}{\|B^{-1}\|}$ *for any nonsingular matrix* B*. Use this fact to establish* (3.19)*.*

Proof. For simplicity, we drop the iteration index k in the proof.
Note that from (3.2) we use the fact $P = -B^{-1}\nabla f$. Thus by multiplying both sides by B and taking transport, we have $BP = -\nabla f$ and $P^T B^T = -\nabla f^T$. We are now prepared to estimate $\cos\theta$:

$$\begin{aligned}
\cos\theta &= \frac{-\nabla f^T P}{\|\nabla f\|\|P\|} \\
&= \frac{\left(P^T B^T\right) P}{\|\nabla f\|\|B^{-1}BP\|} \\
&= \frac{P^T BP}{\|BP\|\|B^{-1}BP\|} \\
&\geq \frac{P^T BP}{\|B\|\|P\|\|B^{-1}\|\|BP\|} \\
&= \left(\frac{P^T BP}{\|P\|\|BP\|}\right)\frac{1}{\|B\|\|B^{-1}\|} \\
&\geq \frac{1}{\|B\|\|B^{-1}\|} \\
&\geq \frac{1}{M},
\end{aligned}$$

where the last two inequality hold by the assumption that B is positive definite and has a uniformly bounded condition number. Therefore, (3.19) follows. □

Exercise 7. *Prove the result (3.28) by working through the following steps. First, use (3.26) to show that*

$$\|x_k - x^*\|_Q^2 - \|x_{k+1} - x^*\|_Q^2 = 2\alpha_k \nabla f_k^T Q(x_k - x^*) - \alpha_k^2 \nabla f_k^T Q \nabla f_k$$

where $\|\cdot\|_Q$ *is defined by (3.27). Second, use the fact that* $\nabla f_k = Q(x_k - x^*)$ *to obtain*

$$\|x_k - x^*\|_Q^2 - \|x_{k+1} - x^*\|_Q^2 = \frac{2(\nabla f_k^T \nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)} - \frac{(\nabla f_k^T \nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)}$$

and

$$\|x_k - x^*\|_Q^2 = \nabla f_k^T Q^{-1} \nabla f_k.$$

Proof. (1)

$$\begin{aligned}
&\|x_k - x^*\|_Q^2 - \|x_{k+1} - x^*\|_Q^2 \\
&= \ 2f(x_k) - 2f(x_{k+1}) \\
&= \ x_k^T Q x_k - 2b^T x_k - (x_k - \alpha_k \nabla f_k)^T Q (x_k - \alpha_k \nabla f_k) + 2b^T (x_k - \alpha_k \nabla f_k) \\
&= \ x_k^T Q(\alpha_k \nabla f_k) + (\alpha_k \nabla f_k)^T Q x_k - \alpha_k^2 \nabla f_k^T Q \nabla f_k - 2\alpha_k b^T \nabla f_k \\
&= \ 2\alpha_k \nabla f_k^T Q x_k - \alpha_k^2 \nabla f_k^T Q \nabla f_k - 2\alpha_k (Qx^*)^T \nabla f_k \\
&= \ 2\alpha_k \nabla f_k^T Q(x_k - x^*) - \alpha_k^2 \nabla f_k^T Q \nabla f_k
\end{aligned}$$

(2) Combining the result of (1) and the fact that $\nabla f_k = Q(x_k - x^*)$, we have

$$\begin{aligned}
&\|x_k - x^*\|_Q^2 - \|x_{k+1} - x^*\|_Q^2 \\
=\ & 2\alpha_k \nabla f_k^T \nabla f_k - \alpha_k^2 \nabla f_k^T Q \nabla f_k \\
=\ & 2(\frac{\nabla f_k^T \nabla f_k}{\nabla f_k^T Q \nabla f_k}) \nabla f_k^T \nabla f_k - (\frac{\nabla f_k^T \nabla f_k}{\nabla f_k^T Q \nabla f_k})^2 \nabla f_k^T Q \nabla f_k \\
=\ & \frac{2(\nabla f_k^T \nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)} - \frac{(\nabla f_k^T \nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)}
\end{aligned}$$

(3) The definition of the weight norm: $\|x\|_Q^2 = x^T Q x$, therefore

$$\begin{aligned}
\|x_k - x^*\|_Q^2 &= (x_k - x^*)^T Q (x_k - x^*) \\
&= (x_k - x^*) T (Q Q^{-1}) Q (x_k - x^*) \\
&= (Q(x_k - x^*))^T Q^{-1} Q (x_k - x^*) \\
&= \nabla f_k^T Q^{-1} \nabla f_k
\end{aligned}$$

Since Q is symmetric and nonsingular.

(4) Now we turn to prove (3.28) by using the result of (2) and (3).

$$\begin{aligned}
\|x_{k+1} - x^*\|_Q^2 &= \|x_k - x^*\|_Q^2 - \frac{(\nabla f_k^T \nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)} \\
&= \|x_k - x^*\|_Q^2 - \frac{(\nabla f_k^T \nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)(\nabla f_k^T Q^{-1} \nabla f_k)} (\nabla f_k^T Q^{-1} \nabla f_k) \\
&= (1 - \frac{(\nabla f_k^T \nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)(\nabla f_k^T Q^{-1} \nabla f_k)}) \|x_k - x^*\|_Q^2
\end{aligned}$$

Therefore the proof is completed.

□

Exercise 8. *Let Q be a positive definite symmetric matrix. Prove that for any vector x, we have*

$$\frac{(x^T x)^2}{(x^T Q x)(x^T Q^{-1} x)} \geq \frac{4\lambda_n \lambda_1}{(\lambda_n + \lambda_1)^2}$$

where λ_n and λ_1 are, respectively the largest and smallest eigenvalues of Q. (This relation, which is known as the Kantorovich inequality, can be used to deduce (3.29) from (3.28).)

Proof. Since Q is positive definite and symmetric, we have eigenvalue decompsition $Q = U \Lambda U^T$. Let $x = Uy$. Then

$$\frac{(x^T x)^2}{(x^T Q x)(x^T Q^{-1} x)} = \frac{(y^T y)^2}{(y^T \Lambda y)(y^T \Lambda^{-1} y)} = \frac{(\sum_{i=1}^n y_i^2)^2}{(\sum_{i=1}^n \lambda_i y_i^2)(\sum_{i=1}^n y_i^2/\lambda_i)}$$

Let $\eta_i = \dfrac{y_i^2}{\sum_{j=1}^n y_j^2}$ and $f(\lambda) = \frac{1}{\lambda}$. Then

$$\frac{(x^T x)^2}{(x^T Q x)(x^T Q^{-1} x)} = \frac{1}{(\sum_{i=1}^n \lambda_i \eta_i)(\sum_{i=1}^n f(\lambda_i)\eta_i)}$$

Let $\lambda = \displaystyle\sum_{i=1}^n \lambda_i \eta_i$, $\quad \lambda_f = \displaystyle\sum_{i=1}^n f(\lambda_i)\eta_i$

Since $\eta_i \geq 0 \quad \forall i$ and $\sum_{i=1}^n \eta_i = 1$, $\lambda_1 \leq \lambda \leq \lambda_n$

Write $\lambda_i = \dfrac{\lambda_n - \lambda_i}{\lambda_n - \lambda_1}\lambda_1 + \dfrac{\lambda_i - \lambda_1}{\lambda_n - \lambda_1}\lambda_n$. This shows λ_i is a convex combination of λ_1 and λ_n $\quad \forall i$

$\because f$ is convex $\quad \therefore f(\lambda_i) \le \dfrac{\lambda_n - \lambda_i}{\lambda_n - \lambda_1} f(\lambda_1) + \dfrac{\lambda_i - \lambda_1}{\lambda_n - \lambda_1} f(\lambda_n)$

Therefore,

$$\lambda_f \le \sum_{i=1}^{n} \left[\frac{\lambda_n - \lambda_i}{\lambda_n - \lambda_1} f(\lambda_1) + \frac{\lambda_i - \lambda_1}{\lambda_n - \lambda_1} f(\lambda_n)\right]\eta_i = \sum_{i=1}^{n} \left[\frac{\lambda_n - \lambda_i}{\lambda_n - \lambda_1}\frac{1}{\lambda_1} + \frac{\lambda_i - \lambda_1}{\lambda_n - \lambda_1}\frac{1}{\lambda_n}\right]\eta_i$$

$$= \sum_{i=1}^{n} \frac{\eta_i}{\lambda_n - \lambda_1}\left[\frac{\lambda_n - \lambda_i}{\lambda_1} + \frac{\lambda_i - \lambda_1}{\lambda_n}\right] = \sum_{i=1}^{n} \frac{\eta_i}{\lambda_n - \lambda_1}\left[\frac{\lambda_n^2 - \lambda_i\lambda_n + \lambda_i\lambda_1 - \lambda_1^2}{\lambda_n\lambda_1}\right]$$

$$= \sum_{i=1}^{n} \frac{\eta_i}{\lambda_n - \lambda_1}\left[\frac{(\lambda_n + \lambda_1)(\lambda_n - \lambda_1) - \lambda_i(\lambda_n - \lambda_1)}{\lambda_n\lambda_1}\right] = \sum_{i=1}^{n} \frac{\lambda_n + \lambda_1 1 - \lambda_i}{\lambda_n\lambda_1}\eta_i$$

$$= \frac{\lambda_n \sum_{i=1}^{n}\eta_i + \lambda_1\sum_{i=1}^{n}\eta_i - \sum_{i=1}^{n}\lambda_i\eta_i}{\lambda_n\lambda_1} = \frac{\lambda_n + \lambda_1 - \lambda}{\lambda_n\lambda_1}$$

We conclude that

$$\frac{(x^T x)^2}{(x^T Q x)(x^T Q^{-1} x)} = \frac{1}{\lambda\lambda_f} \ge \frac{\lambda_n\lambda_1}{\lambda(\lambda_n + \lambda_1 - \lambda)} \ge \frac{\lambda_n\lambda_1}{\max_{\lambda\in[\lambda_1,\lambda_n]} \lambda(\lambda_n + \lambda_1 - \lambda)}$$

Let $g(\lambda) = \lambda(\lambda_n + \lambda_1 - \lambda) = -\lambda^2 + (\lambda_n + \lambda_1)\lambda$. Then $g(\lambda)$ has maxmun at $\bar{\lambda} = \dfrac{\lambda_n + \lambda_1}{2} \in [\lambda_1, \lambda_n]$.

$$g(\bar{\lambda}) = -\frac{(\lambda_n + \lambda_1)^2}{4} + \frac{(\lambda_n + \lambda_1)^2}{2} = \frac{(\lambda_n + \lambda_1)^2}{4}$$

This implies that

$$\frac{(x^T x)^2}{(x^T Q x)(x^T Q^{-1} x)} \ge \frac{\lambda_n\lambda_1}{g(\bar{\lambda})} = \frac{4\lambda_n\lambda_1}{(\lambda_n + \lambda_1)^2}$$

$\square$

Exercise 13. *Show that the quadratic function that interpolates $\phi(0)$, $\phi'(0)$, and $\phi(\alpha_0)$ is given by (3.57). Then, make use of the fact that the sufficient decrease condition (3.6a) is not satisfied at $\alpha(0)$ to show that this quadratic has positive curvature and that the minimizer satisfies*

$$\alpha_1 < \frac{\alpha_0}{2(1 - c_1)}.$$

Since c_1 is chosen to be quite small in practice, this inequality indicates that α_1 cannot be much greater than $\frac{1}{2}$ (and may be smaller), which gives us an idea of the new step length.

Proof. By assuming a quadratic function

$$\phi_q(\alpha) = a\alpha^2 + b\alpha + c$$

and solving coefficients through standard calculations, we have

$$\phi_q(0) = c = \phi(0).$$

Also, since

$$\phi_q'(\alpha) = 2a\alpha + b,$$

we find

$$\phi_q'(0) = b = \phi'(0).$$

On the other hand,

$$\phi_q(\alpha_0) = \phi(\alpha_0) = a\alpha_0^2 + \phi'(0)\alpha_0 + \phi(0),$$

we obtain

$$a = \frac{\phi(\alpha_0) - \phi(0) - \phi'(0)\alpha_0}{\alpha_0^2}.$$

By assumptions, we now discuss a senario that (3.6a) is not satisfied at α_0. Thus we have

$$\phi(\alpha_0) > \phi(0) + c_1\alpha_0\phi'(0).$$

Hence, a minor manipulation of this inequality gives

$$a = \frac{\phi(\alpha_0) - \phi(0) - \phi'(0)\alpha_0}{\alpha_0} > 0,$$

which guarantees that the quadratic has positive curvature. Moreover, since the minimizer of a quadratic is $-b/2a$, we obtain

$$\begin{aligned}
\alpha_1 = \frac{-b}{2a} &= \frac{-\alpha_0^2\phi'(0)}{2[\phi(\alpha_0) - \phi(0) - \phi'(0)\alpha_0]} \\
&= \frac{\alpha_0}{2[1 - \frac{\phi(\alpha_0)-\phi(0)}{\alpha_0\phi'(0)}]} \\
&\leq \frac{\alpha_0}{2(1-c_1)},
\end{aligned}$$

where the second equality holds by dividing $-\alpha_0\phi'(0)$ both upper and lower sides, and the last inequality follows from the given senario.

□

Numerical Optimization with applications: Homework 03

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Exercise 6. *The Cauchy-Schwarz inequality states that for any vectors u and v, we have*

$$|u^T v|^2 \leq (u^T u)(v^T v),$$

with equality only when u and v are parallel. When B is positive definite, use this inequality to show that

$$\gamma := \frac{\|g\|^4}{(g^T B g)(g^T B^{-1} g)} \leq 1,$$

with equality only if g and Bg (and $B^{-1}g$) are parallel.

Proof. B is a positive definite matrix, so there exists an orthonormal matrix Q and a diagonal matrix $\Lambda = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix}$ s.t. $B = Q\Lambda Q^T$.

Define the matrix $\sqrt{B} = Q\sqrt{\Lambda}Q^T$ where $\sqrt{\Lambda} = \begin{pmatrix} \sqrt{\lambda_1} & & & \\ & \sqrt{\lambda_2} & & \\ & & \ddots & \\ & & & \sqrt{\lambda_n} \end{pmatrix}$

Obviously, $\sqrt{B}$ is also symmetric.
Claim:$(\sqrt{B})^{-1} = \sqrt{B^{-1}}$
proof of claim:
$(\sqrt{B})^{-1} = Q(\sqrt{\Lambda})^{-1}Q^T = Q\sqrt{\Lambda^{-1}}Q^T = \sqrt{B^{-1}}$
We proved the claim.
Now we use the claim above, the symmetricity of $\sqrt{B}$ and Cauchy-Schwarz inequality. We have the following statement:

$$\begin{aligned}
\|g\|^4 &= (g^T g)^2 = (g^T\sqrt{B}(\sqrt{B})^{-1}g)^2 = ((\sqrt{B}g)^T(\sqrt{B^{-1}}g))^2 \\
&\leqslant (\sqrt{B}g)^T(\sqrt{B}g)(\sqrt{B^{-1}}g)^T(\sqrt{B^{-1}}g) \\
&= (g^T\sqrt{B}\sqrt{B}g)(g^T\sqrt{B^{-1}}\sqrt{B^{-1}}g) \\
&= (g^T B g)(g^T B^{-1} g)
\end{aligned}$$

When the equality holds only if $\sqrt{B}g$ and $\sqrt{B^{-1}}g$ are parallel.
i.e.$\sqrt{B}g = k\sqrt{B^{-1}}g$ for some constant k.
1. Multiplying both side by $\sqrt{B}$.
$Bg = kg \Longrightarrow Bg$ and g are parallel.

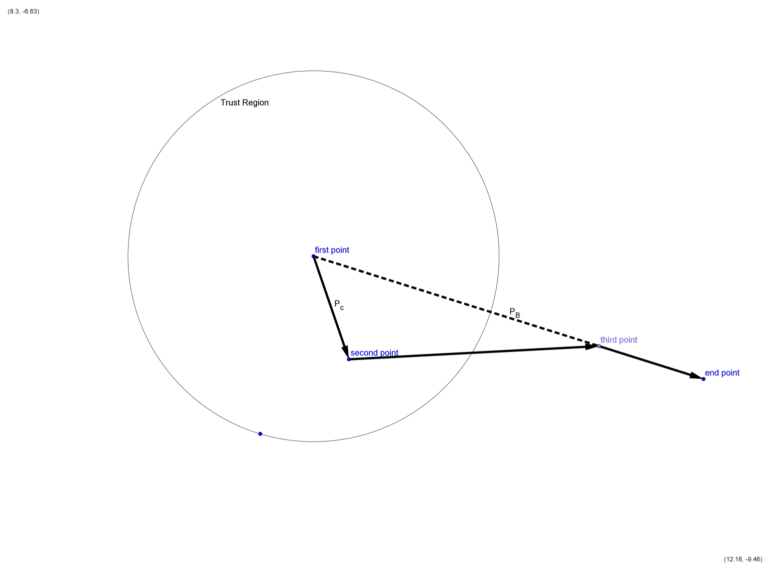
2. Multiplying both side by $\sqrt{B^{-1}}$.
$g = kB^{-1}g \Longrightarrow B^{-1}g$ and g are parallel.

□

Exercise 7. *When B is positive definite, the double-dog leg method constructs a path with three line segments from the origin to the full step. The four points that define the path are*

- *the origin;*
- *the unconstrained Cauchy step $p^c = -(g^T g)/(g^T Bg)g$;*
- *a fraction of the full step $\bar{\gamma} p^B = -\bar{\gamma} B^{-1} g$, for some $\bar{\gamma} \in (\gamma, 1]$, where γ is defined in the previous question; and*
- *the full step $p^B = -B^{-1} g$*

Show that $\|p\|$ increases monotonically along this path.
(Note: The double-dogleg method, as discussed in Dennis and Schnabel [92, Section 6.4.2], was for some time thought to be superior to the standard dogleg method, but later testing has not shown much difference in performance.)



Proof. It is obviously that $\|p\|$ increases monotonically along the first segment and the last segment because $\alpha\|v\|$ increases as α increases, where $\alpha \in (0, 1)$. Now we consider the second segment. Let $P^A = -\bar{\gamma} B^{-1} g$, and $P^U = -(g^T g)/(g^T Bg)g$, then the parametrization of the second segment is

$$P(\alpha) = \alpha(P^A - P^U) + P^U.$$

Define

$$\begin{aligned}
h(\alpha) &= (1/2)\|P(\alpha)\|^2 \\
&= (1/2)\|\alpha(P^A - P^U) + P^U\|^2 \\
&= (1/2)\|P^U\|^2 + \alpha(P^U)^T(P^A - P^U) + (1/2)\alpha^2\|P^A - P^U\|^2
\end{aligned}$$

Then we have

$$\begin{aligned}
h'(\alpha) &= -(P^U)^T(P^U - P^B) + \alpha\|P^U - P^B\|^2 \\
&\geq -(P^U)^T(P^U - P^A) \\
&= \frac{g^T g}{g^T Bg} g^T \left(-\frac{g^T g}{g^T Bg} g + \bar{\gamma} B^{-1} g \right) \\
&= g^T g \frac{gB^{-1}g}{gBg} \left(\bar{\gamma} - \frac{(g^T g)^2}{(g^T Bg)(g^T B^{-1} g)} \right) \\
&> 0
\end{aligned}$$

Since $h'(\alpha) > 0$ for all $\alpha \in (0, 1)$, $h(\alpha)$ is increasing monotonically on $(0, 1)$, that is, $\|p(\alpha)\|$ is increasing monotonically on $(0, 1)$.Therefore, the $\|p\|$ increases monotonically along this segament.

□

Exercise 8. *Show that*

$$\lambda^{(l+1)} = \lambda^{(l)} - \frac{\phi_2(\lambda^{(l)})}{\phi_2'(\lambda^{(l)})}, \quad \textit{and} \quad \lambda^{(l+1)} = \lambda^{(l)} + \left(\frac{\|p_l\|}{\|q_l\|}\right)^2 \left(\frac{\|p_l\| - \Delta}{\Delta}\right)$$

are equivalents.

Proof. First,we caculate

$$\phi_2'(\lambda) = \frac{d}{d\lambda}\left(\frac{1}{\|p(\lambda)\|}\right) = \frac{d}{d\lambda}\left(\|p(\lambda)\|^2\right)^{-1/2} = -\frac{1}{2}\left(\|p(\lambda)\|^2\right)^{-3/2}\frac{d}{d\lambda}\|p(\lambda)\|^2$$

Since B is symmetric, there is an orthonormal matrix U and a diagonal matrix Λ such that $B = U\Lambda U^T$, where

$$\Lambda = diag(\lambda_1, \lambda_2, \cdots, \lambda_n)$$

Then, $B + \lambda I = U(\Lambda + \lambda I)U^T$. We have,

$$p(\lambda) = -U(\Lambda + \lambda I)U^T g = -\sum_{j=1}^{n} -\frac{u_j^T g}{\lambda_j + \lambda} u_j$$

where u_j denotes the jth column of U. Therefore, by orthonormality of $u_1, u_2, \cdots, u_n$, we have

$$\|p(\lambda)\|^2 = \sum_{j=1}^{n} \frac{(u_j^T g)^2}{(\lambda_j + \lambda)^2}$$

Hence, we can caculate

$$\frac{d}{d\lambda}\|p(\lambda)\|^2 = -2\sum_{j=1}^{n} \frac{(u_j^T g)^2}{(\lambda_j + \lambda)^3}$$

On the other hand, we have

$$\begin{aligned}\|q_l\|^2 = \left\|R^{-T}p_l\right\|^2 = p_l^T R^{-1}R^{-T}p_l = [-(R^TR)^{-1}g]^T(R^TR)^{-1}[-(R^TR)^{-1}g] = g^T[(R^TR)^{-1}]^3 g \\ = g^T[(B + \lambda^{(l)}I)^{-1}]^3 g = g^T U(\Lambda + \lambda^{(l)}I)^{-3}U^T g = \sum_{j=1}^{n} \frac{(u_j^T g)^2}{(\lambda_j + \lambda^{(l)})^3}\end{aligned}$$

We conclude that

$$\phi_2'(\lambda^{(l)}) = -\frac{1}{2}\left\|p(\lambda^{(l)})\right\|^{-3}\left(-2\sum_{j=1}^{n}\frac{(u_j^T g)^2}{(\lambda_j + \lambda^{(l)})^3}\right) = \|p_l\|^{-3}\|q_l\|^2$$

Finally, we get

$$-\frac{\phi_2(\lambda^{(l)})}{\phi_2'(\lambda^{(l)})} = \left(\frac{1}{\Delta} - \frac{1}{\|p(\lambda^{(l)})\|}\right)\left(\frac{\|p_l\|^3}{\|q_l\|^2}\right) = \left(\frac{\|p_l - \Delta\|}{\Delta\|p_l\|}\right)\left(\frac{\|p_l\|^3}{\|q_l\|^2}\right) = \left(\frac{\|p_l\|}{\|q_l\|}\right)^2\left(\frac{\|p_l\| - \Delta}{\Delta}\right)$$

Therefore, the two equations above are equivalent. $\square$

Numerical Optimization with applications: Homework 04

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Exercise 1. *Implement Algorithm 5.2 and use to it solve linear systems in which A is the Hilbert matrix, whose elements are $A_{i,j} = 1/(i+j-1)$. Set the right-hand-side to $b = (1, 1, ..., 1)^T$ and the initial point to $x_0 = 0$. Try dimensions $n = 5, 8, 12, 20$ and report the number of iterations required to reduce the residual below 10^{-6}.*

Solution. The numbers of iterations as the table below.

n	5	8	12	20
number of iteration	6	19	38	73
condition number	4.766E+05	1.526E+10	1.633E+16	2.596E+18

Observe that the condition number in the case $n = 20$ is greater than the others. By(5.36), the rate of convergence should be less than the others. ◀

Exercise 2. *Show that if the nonzero vectors $p_0, p_1, ..., p_l$ satisfy (5.5), where A is symmetric and positive definite, then these vectors are linearly independent. (This result implies that A has at most n conjugate direction.)*

Proof. Suppose $a_0 p_0 + a_1 p_1 + ... + a_l p_l = 0$. For any p_j, we have the following argument.

$$\begin{aligned} 0 &= p_j^T A(a_0 p_0 + a_1 p_1 + ... + a_l p_l) \\ &= a_0(p_j^T A p_0) + a_1(p_j^T A p_1) + ... + a_j(p_j^T A p_j) + ... + a_l(p_j^T A p_l) \\ &= a_0 \cdot 0 + a_1 \cdot 0 + ... + a_j \cdot (p_j^T A p_j) + ... + a_l \cdot 0 \\ &= a_j \cdot (p_j^T A p_j) \end{aligned}$$

Since A is positive definite, $p_j^T A p_j > 0$, this implies $a_j = 0$. $\forall j$
Consequently, $p_0, p_1, ..., p_l$ are linearly independent.

□

Exercise 4. *Show that if $f(x)$ is a strictly convex quadratic, then the function $h(\sigma) \overset{def}{=} f(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1} p_{k-1})$ also is a strictly convex quadratic in the variable $\sigma = (\sigma_0, \sigma_1, \cdots, \sigma_{k-1})^T$.*

Proof. By the definition of strictly convex quadratic function, we can assume

$$f(x) = \frac{1}{2} x^T A x - b^T x,$$

where A is a positive definite symmetric matrix and b is a constant vector. We want prove that $h(\sigma)$ is also a strictly convex quadratic function by showing

$$h(\sigma) = \frac{1}{2} \sigma^T B \sigma - c^T \sigma + d,$$

where B is a positive definite symmetric matrix and c, d are constant vectors. Since $p_i^T A p_j = 0$ for all

$i \neq j$, we obtain that

$$
\begin{aligned}
h(\sigma) &= f(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) \\
&= \frac{1}{2}(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1})^T A(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) - b^T(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) \\
&= \frac{1}{2}x_0^T A(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) + \frac{1}{2}(\sigma_0 p_0)^T A(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) + \cdots \\
&\quad + \frac{1}{2}(\sigma_{k-1}p_{k-1})^T A(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) - b^T(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) \\
&= \frac{1}{2}(\sigma_0 p_0)^T A(\sigma_0 p_0) + \frac{1}{2}(\sigma_1 p_1)^T A(\sigma_1 p_1) + \cdots + \frac{1}{2}(\sigma_{k-1}p_{k-1})^T A(\sigma_{k-1}p_{k-1}) \\
&\quad + \frac{1}{2}x_0^T A(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) - b^T(x_0 + \sigma_0 p_0 + \cdots + \sigma_{k-1}p_{k-1}) \\
&= \frac{1}{2}\sigma^T B\sigma + \frac{1}{2}x_0^T AP\sigma - b^T P\sigma + \frac{1}{2}x_0^T Ax_0 - b^T x_0 \\
&= \frac{1}{2}\sigma^T B\sigma + (\frac{1}{2}x_0^T AP - b^T P)\sigma + \frac{1}{2}x_0^T Ax_0 - b^T x_0
\end{aligned}
$$

where $B = \begin{bmatrix} p_0^T A p_0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & p_{k-1}^T A p_{k-1} \end{bmatrix}$ is positive definite sysmmetric matrix and $P = (p_0, p_1, \cdots, p_{k-1})$ and $\sigma = (\sigma_0, \sigma_1, \cdots, \sigma_{k-1})^T$. Hence, $h(\sigma)$ is also a strictly convex quadratic function. □

Exercise 7. *Let $\{\lambda_i, v_i\}$ $i = 1, 2, \cdots, n$ be the eigenpairs of the symmetric matrix A. Show that the eigenvalues and eigenvectors of $[I + P_k(A)A]^T A[I + P_k(A)A]$ are $\lambda_i[1 + \lambda_i P_k(\lambda_i)]^2$ and v_i, respectively.*

Proof. We first show that

$$P_k(A)v_i = P_k(\lambda_i)v_i$$

for any polynomials $P_k(x)$ of degree k.

Let $P_k(x) = \sum_{j=0}^{k} a_j x^j$. Then

$$P_k(A)v_i = \sum_{j=0}^{k} a_j A^j v_i = \sum_{j=0}^{k} a_j A^{j-1}(\lambda_i v_i) = \sum_{j=0}^{k} a_j A^{j-2}(\lambda_i^2 v_i) = \cdots = \sum_{j=0}^{k} a_j \lambda_i^j v_i = P_k(\lambda_i)v_i$$

Since $[I + P_k(x)x]$ is a ploynomial, we have

$$[I + P_k(A)A]v_i = [1 + \lambda_i P_k(\lambda_i)]v_i$$

A is symmetric, therefore, $[I + P_k(A)A]^T = [I + P_k(A)A]$

Now,we are ready to compute

$$
\begin{aligned}
[I + P_k(A)A]^T A[I + P_k(A)A]v_i &= [I + P_k(A)A]A[I + P_k(A)A]v_i \\
&= [I + P_k(A)A]A[1 + \lambda_i P_k(\lambda_i)]v_i \\
&= [I + P_k(A)A](Av_i)[1 + \lambda_i P_k(\lambda_i)] \\
&= [I + P_k(A)A]\lambda_i v_i[1 + \lambda_i P_k(\lambda_i)] \\
&= [I + P_k(A)A]v_i \lambda_i[1 + \lambda_i P_k(\lambda_i)] \\
&= [1 + \lambda_i P_k(\lambda_i)]v_i \lambda_i[1 + \lambda_i P_k(\lambda_i)] \\
&= \lambda_i[1 + \lambda_i P_k(\lambda_i)]^2 v_i
\end{aligned}
$$

We conclude that $\{\lambda_i[1 + \lambda_i P_k(\lambda_i)]^2, v_i\}$ $i = 1, 2, \cdots, n$ are the eigenpairs of $[I + P_k(A)A]^T A[I + P_k(A)A]$. □

Numerical Optimization with applications: Homework 05

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Exercise 6. *The square root of a matrix A is a matrix $A^{1/2}$ such that $A^{1/2}A^{1/2} = A$. Show that any symmetric positive definite matrix A has a square root, and that this square root is itself symmetric and positive definite.(Hint: factorization $A = UDU^T$ (A.16), where U is orthogonal and D is diagonal with positive diagonal elements.)*

Proof. First, we show that a real symmetric matrix A is diagonalizable. Prove it by contradiction, which means there is a generalized eigenvector v of order 2, that is $(A - \lambda I)v \neq 0$ and $(A - \lambda I)^2 = 0$, and we have the following statement.

$$\begin{aligned} 0 &= v^T(A - \lambda I)^2 v = v^T(A - \lambda I)^T(A - \lambda I)v \\ &= \|(A - \lambda I)v\|^2 \neq 0 \rightarrow\leftarrow \end{aligned}$$

Thus, every eigenvector of A is of order 1 and A is diagonalizable. We may Assume $A = UDU^T$, where U is orthogonal and by $A > 0$, $D = diag(\lambda_1, \lambda_2, ..., \lambda_n)$ is diagonal with positive diagonal elements. Define the square root of A

$$A^{1/2} := U\sqrt{D}U^T = U diag(\sqrt{\lambda_1}, \sqrt{\lambda_2}, ...\sqrt{\lambda_n})U^T$$

Obviously, $A^{1/2}$ is symmetric, and positive number $\sqrt{\lambda_i}$ is the eigenvalue correspond to the ith column vector of U. Hence $A^{1/2}$ is also positive definite.

□

Exercise 10. *(a) Show that $\det(I + xy^T) = 1 + y^T x$, where x and y are n-vectors.*

(b) Using similar technique to prove that

$$\det(I + xy^T + uv^T) = (1 + y^T x)(1 + v^T u) - (x^T v)(y^T u).$$

(c) Use this relation to establish

$$\det(B_{k+1}) = \det(B_k)\frac{y_k^T s_k}{s_k^T B_k s_k}.$$

Proof. (a) Assuming $x \neq 0$, we can find vectors $q_1, q_2, \cdots, q_{n-1}$ such that the matrix Q defined by

$$Q = [x, q_1, q_2, \cdots, q_{n-1}]$$

is nonsingular and $x = Qe_1$.If we define

$$y^T Q = (w_1, w_2, \cdots, w_n)$$

then

$$w_1 = y^T Q e_1 = y^T x$$

and

$$\det(I + xy^T) = \det(Q^{-1}(I + xy^T)Q) = \det(I + Q^{-1}xy^T Q) = \det(I + e_1 y^T Q)$$

$$= \det\left(I + \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} (w_1, w_2, \cdots, w_n) \right) = \det\left(\begin{bmatrix} 1 + w_1 & w_2 & \cdots & w_{n-1} & w_n \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \right)$$

$$= \det\left(\begin{bmatrix} 1+w_1 & w_2 & \cdots & w_{n-1} \\ 0 & 1 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}\right) = \cdots = \det\left(\begin{bmatrix} 1+w_1 & w_2 \\ 0 & 1 \end{bmatrix}\right)$$
$$= 1 + w_1 = 1 + y^T x$$

(b) Assuming $x, u \neq 0$, we can find vectors $q_1, q_2, \cdots, q_{n-2}$ such that the matrix Q defined by

$$Q = [x, u, q_1, q_2, \cdots, q_{n-2}]$$

is nonsingular and $x = Qe_1$, $u = Qe_2$.If we define

$$y^T Q = (w_1, w_2, \cdots, w_n)$$
$$v^T Q = (z_1, z_2, \cdots, z_n)$$

then

$$w_1 = y^T Q e_1 = y^T x \qquad w_2 = y^T Q e_2 = y^T u$$
$$z_1 = v^T Q e_1 = v^T x \qquad z_2 = v^T Q e_2 = v^T u$$

and

$$\det(I + xy^T + uv^T) = \det\left(I + [x \quad u]\begin{bmatrix} y^T \\ v^T \end{bmatrix}\right) = \det\left(Q^{-1}(I + [x\ u]\begin{bmatrix} y^T \\ v^T \end{bmatrix})Q\right)$$
$$= \det\left(I + [Q^{-1}x \quad Q^{-1}u]\begin{bmatrix} y^T Q \\ v^T Q \end{bmatrix}\right) = \det\left(I + [e_1 \quad e_2]\begin{bmatrix} w_1 & w_2 & \cdots & w_n \\ z_1 & z_2 & \cdots & z_n \end{bmatrix}\right)$$
$$= \det\left(I + \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix}\begin{bmatrix} w_1 & w_2 & \cdots & w_n \\ z_1 & z_2 & \cdots & z_n \end{bmatrix}\right) = \det\left(\begin{bmatrix} 1+w_1 & w_2 & \cdots & w_{n-1} & w_n \\ z_1 & 1+z_2 & \cdots & z_{n-1} & z_n \\ \vdots & & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}\right)$$
$$= \det\left(\begin{bmatrix} 1+w_1 & w_2 & \cdots & w_{n-1} \\ z_1 & 1+z_2 & \cdots & z_{n-1} \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}\right) = \cdots = \det\left(\begin{bmatrix} 1+w_1 & w_2 \\ z_1 & 1+z_2 \end{bmatrix}\right)$$
$$= (1+w_1)(1+z_2) - z_1 w_2 = (1 + y^T x)(1 + v^T u) - (x^T v)(y^T u)$$

(c) We have $B_{k+1} = B_k - \dfrac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \dfrac{y_k y_k^T}{y_k^T s_k}$. So,

$$\det(B_{k+1}) = \det(B_k)\det\left(I + \left(\frac{-s_k}{s_k^T B_k s_k}\right)(s_k^T B_k)\left(\frac{B_k^{-1} y_k}{y_k^T s_k}\right)(y_k^T)\right)$$

Let

$$x = \left(\frac{-s_k}{s_k^T B_k s_k}\right) \quad y^T = (s_k^T B_k) \quad u = \left(\frac{B_k^{-1} y_k}{y_k^T s_k}\right) \quad v^T = (y_k^T)$$

Using (b), we can caculate

$$\det\left(I + \left(\frac{-s_k}{s_k^T B_k s_k}\right)(s_k^T B_k) + \left(\frac{B_k^{-1} y_k}{y_k^T s_k}\right)(y_k^T)\right)$$
$$= \left[1 + (s_k^T B_k)\left(\frac{-s_k}{s_k^T B_k s_k}\right)\right]\left[1 + (y_k^T)\left(\frac{B_k^{-1} y_k}{y_k^T s_k}\right)\right] - \left[(y_k^T)\left(\frac{-s_k}{s_k^T B_k s_k}\right)\right]\left[(s_k^T B_k)\left(\frac{B_k^{-1} y_k}{y_k^T s_k}\right)\right]$$
$$= 0 \times \left[1 + (y_k^T)\left(\frac{B_k^{-1} y_k}{y_k^T s_k}\right)\right] - \left[\frac{-y_k^T s_k}{s_k^T B_k s_k}\right] \times 1 = \frac{y_k^T s_k}{s_k^T B_k s_k}$$

We conclude that

$$\det(B_{k+1}) = \det(B_k)\frac{y_k^T s_k}{s_k^T B_k s_k}$$

□

Exercise 12. *Show that if f satisfies Assumption 6.1 and if the sequence of gradients satisfies* $\liminf \|\nabla f_k\| = 0$*, , then the whole sequence of iterates x converges to the solution x^*.*

Proof. Since $f(x_k)$ deceases at each step and by Assumption 6.1(ii) the convexity of the set $\mathcal{L} = \{x | f(x) \leq f(x_0)\}$, the fact $\liminf \|\nabla f_k\| = 0$ implies there exists a subsequence $\{x_{n_j}\}$ converges to the unique minimizer x^*. We are now proving the whole sequence $\{x_k\}$ converges to x^*. By Taylor's thm, for all $x \in \mathbb{R}^n$ we have

$$f(x) = f(x^* + (x - x^*)) = f(x^*) + \nabla f(x^*)^T (x - x^*) + \frac{1}{2}(x - x^*)^T \nabla^2 f(\xi)(x - x^*)$$

If x belongs to $\mathcal{L} = \{x | f(x) \leq f(x_0)\}$ and satisfies

$$f(x) \leq f(x^*) + \varepsilon$$

for some given $\varepsilon > 0$, we obtain following by using the fact $\nabla f(x^*) = 0$

$$\frac{1}{2}(x - x^*)^T \nabla^2 f(\xi)(x - x^*) \leq \varepsilon.$$

By Assumption 6.1(ii) again, we conclude that

$$m\|x - x^*\|_2^2 \leq (x - x^*)^T \nabla^2 f(\xi)(x - x^*) \leq 2\varepsilon.$$

So,

$$\|x - x^*\|_2^2 \leq (2\varepsilon/m)$$

On the other hand, the whole sequence $\{f(x_k)\}$ is nonincreasing by any descent direction Algorithm, and we already know that there exists a subsequence $\{f(x_{n_j})\}$ converges to the $f(x^*)$. So given $\varepsilon > 0$, we can find a $N \in \mathbb{N}$ such that

$$f(x_k) \leq f(x_{n_j}) \leq f(x*) + \varepsilon$$

for all $k \geq n_j \geq N$. Hence, combining the two inequality gives

$$\|x_k - x^*\|_2^2 \leq (2\varepsilon/m)$$

for for all $k \geq N$. So the whole sequence $\{x_k\}$ converges to x^*. □

Numerical Optimization with applications: Homework 06

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December 7, 2016

Exercise 1. *The following example from [268] with a single variable $x \in \mathbb{R}$ and a single equality constraint shows that strict local solutions are not necessarily isolated. Consider*

$$\min_x x^2 \quad \textit{subject to } c(x) = 0, \textit{where } c(x) = \begin{cases} x^6 \sin(1/x) & \textit{if } x \neq 0 \\ 0 & \textit{if } x = 0 \end{cases} \qquad (12.96)$$

(a) Show that the constraint function is twice continuously differentiable at all x (including at $x = 0$) and that the feasible points are $x = 0$ and $x = 1/(k\pi)$ for all nonzero integers k.

(b) Verify that each feasible point except $x = 0$ is an isolated local solution by showing that there is a neighborhood $\mathcal{N}$ around each such point within which it is the only feasible point.

Proof. (a) We first show directly that constraint function is twice continuously differentiable at all x.

If $x \neq 0$, then

$$\begin{aligned} c(x) &= x^6 \sin(1/x) \\ c'(x) &= 6x^5 \sin(1/x) - x^4 \cos(1/x) \\ c''(x) &= (30x^4 - x^2)\sin(1/x) - 10x^3 \cos(1/x) \end{aligned}$$

If $x = 0$, then by definition we obtain

$$\begin{aligned} c'(0) &= \lim_{h\to\infty} \frac{h^6 \sin(1/h) - 0}{h} = 0 \\ c''(0) &= \lim_{h\to\infty} \frac{\left[6h^5 \sin(1/h) - h^4 \cos(1/h)\right] - 0}{h} = 0 \end{aligned}$$

Hence, the constraint function is twice continuously differentiable at all x.

Second, we show that the feasible points are $x = 0$ and $x = 1/(k\pi)$ for all nonzero integers k.

If $x = 0$, then $c(x) = 0$ by definition. If $x = 1/(k\pi)$, then $\sin(1/x) = 0$ and thus we have $c(x) = 0$.

(b) If $x = 1/(k\pi)$ for some fixed nonzero integers k and we choose $r = \left|\frac{1}{k\pi} - \frac{1}{(k+1\pi)}\right|$, then the open interval $\mathcal{N} = (x - r, x + r)$ contains only a feasible point, which is x itself.

On the other hand, if $x = 0$, then for all $r > 0$ there exists nonzero positive integers k such that $x_k = 1/(k\pi) < r$. However, x_k are feasible points in the neighborhood $(-r, r)$.

Therefore, combining disscusion above, we have that each feasible point except $x = 0$ is an isolated local solution by showing that there is a neighborhood $\mathcal{N}$ around each such point within which it is the only feasible point.

□

Exercise 15. *Consider the following modification of (12.36), where t is a parameter to be fixed prior to solving the problem:*

$$\min_x (x_1 - \frac{3}{2})^2 + (x_2 - t)^4 \quad s.t. \quad \begin{bmatrix} 1 - x_1 - x_2 \\ 1 - x_1 + x_2 \\ 1 + x_1 - x_2 \\ 1 + x_1 + x_2 \end{bmatrix} \geq 0$$

(a)For what value of t does the point $x^* = (1,0)^T$ satisfy the KKT conditions?
(b)Show that when $t = 1$, only the first constraint is active at the solution, and find the solution.

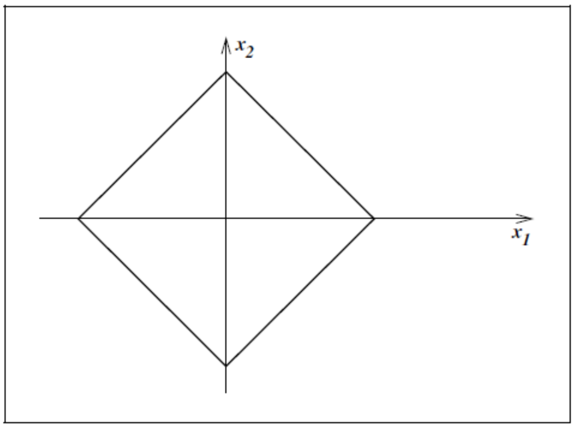
Proof. (a) First, we check the complementary condition of KKT, i.e. $\lambda_i c_i(x^*) = 0$ for $i = 1,2,3,4$.

$$\begin{cases} \lambda_1(1-1-0) = 0 \\ \lambda_2(1-1+0) = 0 \\ \lambda_3(1+1-0) = 0 \\ \lambda_4(1+1+0) = 0 \end{cases} \Rightarrow \begin{cases} \lambda_3 = 0 \\ \lambda_4 = 0 \end{cases} \tag{1}$$

Obviously, $c(x^*) \geq 0$ holds. Consider

$$\begin{aligned} \bigtriangledown_x L(x^*, \lambda) &= \bigtriangledown_x L((0,1)^T, \lambda) \\ &= \begin{bmatrix} -1 + \lambda_1 + \lambda_2 \\ -4t^3 + \lambda_1 - \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \end{aligned}$$

Since $\lambda_1, \lambda_2 \geq 0$ and $\lambda_1 + \lambda_2 = 1$, we have $\lambda_1 - \lambda_2 \in [-1,1]$. Hence, $4t^3 \in [-1,1]$, then $t \in [-\sqrt[3]{4}, \sqrt[3]{4}]$.



(b) We know the feasible set $E = \{x \in \mathbb{R}^2 \mid \|x\|_1 = 1\}$. Compute the gradient of $f(x)$

$$\bigtriangledown f(x) = \begin{bmatrix} 2(x_1 - \frac{3}{2}) \\ 4(x_2 - 1)^3 \end{bmatrix} \leq 0 \quad \forall x \in E$$

From above, $\forall x, y \in E$, if $x_1 \leq y_1$ and $x_2 \leq y_2$ then $f(y) \leq f(x)$. Therefore, we only have to consider the case that the first constraint is active: $1 - x_1 - x_2 = 0$. Substituting $x_2 = 1 - x_1$ into $f(x)$ and find the minimum of f:

$$\begin{aligned} f(x) &= (x_1 - \frac{3}{2})^2 + (-x_1)^4 \\ f'(x) &= 2(x_1 - \frac{3}{2}) + 4x_1^3 \\ &= 4x_1^3 + 2x_1 - 3 \end{aligned}$$

$f'(x^*) = 0$ if $x_1^* = \frac{\sqrt[3]{27+\sqrt{753}}}{2\times 3^{2/3}} - \frac{1}{\sqrt[3]{3(27+\sqrt{753})}}$. Consequently, the minimizer of f is $(x_1^*, 1 - x_1^*)$.

□

Exercise 19. *Consider the problem*

$$\min_{x\in R^2} = -2x_1 + x_2 \quad \textit{subject to} \quad \begin{cases} (1-x_1)^3 - x_2, & \geq 0 \\ x_2 + 0.25x_1^2 - 1, & \geq 0 \end{cases}$$

The optimal solution is $x^* = (0,1)^T$*, where both constraints are active.*

(a) Do the LICQ hold at this point?

(b) Are the KKT conditions satisfied?

(c) Write down the set $\mathcal{F}(x^*)$ *and* $\mathcal{C}(x^*, \lambda^*)$*.*

(d) Are the second-order necessary conditions satisfied? Are the second-order sufficient conditions satisfied?

Proof. (a)

$$A(x^*) = [\bigtriangledown C_i(x^*)]_{i\in\mathcal{A}(x^*)} = \begin{bmatrix} -3(1-x_1)^2 & 0.5x_1 \\ -1 & 1 \end{bmatrix}_{x=x*} = \begin{bmatrix} -3 & 0 \\ -1 & 1 \end{bmatrix}$$

$A(x^*)$ is nonsingular. Therefore, the LICQ holds.

(b)

$$\bigtriangledown f(x^*) = \begin{bmatrix} -2 \\ 1 \end{bmatrix}, \quad \bigtriangledown c_1(x^*) = \begin{bmatrix} -3 \\ -1 \end{bmatrix}, \quad \bigtriangledown c_2(x^*) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Therefore, the KKT conditions (12.34a)-(12.34e) are satisfied when we set

$$\lambda^* = \left(\frac{2}{3}, \frac{5}{3}\right)^T$$

(c)

$$\mathcal{F}(x^*) = \{d | \bigtriangledown c_i(x^*)^T d \geq 0\} = \{(d_1, d_2)^T | \begin{bmatrix} -3 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} \geq 0\} = \{(d_1, d_2)^T | d_2 \geq 0,\ 3d_1 + d_2 \leq 0\}$$

$$\begin{aligned} \mathcal{C}(x^*, \lambda^*) &= \{w \in \mathcal{F}(x^*) | \bigtriangledown c_i(x^*)^T w = 0\ \forall i \in \mathcal{A}(x^*) \cap I \text{ with } \lambda_i^* > 0\} \\ &= \{w \in \mathcal{F}(x^*) | \bigtriangledown c_i(x^*)^T w = 0 \text{ for } i = 1, 2\} \\ &= \{(w_1, w_2)^T \in \mathcal{F}(x^*) | \begin{bmatrix} -3 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = 0\} \\ &= \{(0,0)^T\} \end{aligned}$$

(d)

$$\forall w \in \mathcal{C}(x^*, \lambda^*) = \{(0,0)^T\} \qquad w^T \bigtriangledown_{xx} \mathcal{L}(x^*, \lambda^*) w = 0 \tag{2}$$

Since at x^* LICQ holds and (x^*, λ^*) satisfies KKT. By (2), the second-order necessary conditions is satisfied.
Since x^* is a feasible solution and (x^*, λ^*) satisfies KKT. By (2), the second-order sufficient conditions is satisfied.

□

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Exercise 2 (Chapter 7)**.** *Show that the matrix* $\widehat{H}_{k+1} = (I - \frac{s_k y_k^T}{y_k^T s_k})$ *is singular.*

Proof. Consider $\widehat{H}_{k+1} s_k$, then we have

$$\begin{aligned}
\widehat{H}_{k+1} s_k &= (I - \frac{s_k y_k^T}{y_k^T s_k}) s_k \\
&= s_k - \frac{s_k (y_k^T s_k)}{y_k^T s_k} \\
&= s_k - s_k \\
&= 0
\end{aligned}$$

Since $s_k = x_{k+1} - x_k \neq 0$, thus $\widehat{H}_{k+1}$ is singular. □

Exercise 5 (Chapter 10)**.** *Suppose that each residual function* r_j *and its gradient are Lipschitz continuous with Lipschitz constant L, that is ,*

$$\|r_j(x) - r_j(\widehat{x})\| \leq L\|x - \widehat{x}\|, \quad \| \bigtriangledown r_j(x) - \bigtriangledown r_j(\widehat{x})\| \leq L\|x - \widehat{x}\|$$

for all $j = 1, 2, ..., m$ *and all* $x, \widehat{x} \in \mathcal{D}$*, where* $\mathcal{D}$ *is a compact subset of* $\mathbb{R}^n$*. Assume also that the* r_j *are bounded on* $\mathcal{D}$*, that is there exist* $M > 0$ *such that* $|r_j(x)| \leq M$ *for all* $j = 1, 2, ..., m$ *and all* $x \in \mathcal{D}$*. Find Lipschitz constant for the Jacobian* J *and the gradient* $\bigtriangledown f$ *over* $\mathcal{D}$*.*

$$J(x) = \left[\frac{\partial r_j}{\partial x_i}\right]_{\substack{j=1,2,...,m \\ i=1,2,...,n}} = \begin{bmatrix} \bigtriangledown r_1(x)^T \\ \bigtriangledown r_2(x)^T \\ \vdots \\ \bigtriangledown r_m(x)^T \end{bmatrix}$$

$$\bigtriangledown f(x) = \Sigma_{j=1}^m r_j(x) \bigtriangledown r_j(x) = J(x)^T r(x)$$

Proof. Since all norms in $\mathbb{R}^n$ are equivalent.

$$\exists \alpha > 0 \quad \text{such that} \quad \|x\| \leq \alpha \|x\|_\infty \quad \forall x \in \mathbb{R}^n$$

We have,

$$\begin{aligned}
\|J(x_1) - J(x_2)\| &= \max_{\|y\|=1} \|(J(x_1) - J(x_2))y\| \\
&= \max_{\|y\|=1} \left\| \begin{bmatrix} (\bigtriangledown r_1(x_1) - \bigtriangledown r_1(x_2))^T y \\ \vdots \\ (\bigtriangledown r_m(x_1) - \bigtriangledown r_m(x_2))^T y \end{bmatrix} \right\| \\
&\leq \max_{\|y\|=1} \alpha \left\| \begin{bmatrix} (\bigtriangledown r_1(x_1) - \bigtriangledown r_1(x_2))^T y \\ \vdots \\ (\bigtriangledown r_m(x_1) - \bigtriangledown r_m(x_2))^T y \end{bmatrix} \right\|_\infty \\
&= \alpha \max_{\|y\|=1} \max_{1 \leq j \leq m} |(\bigtriangledown r_j(x_1) - \bigtriangledown r_j(x_2))^T y| \\
&\leq \alpha \max_{\|y\|=1} \max_{1 \leq j \leq m} |(\bigtriangledown r_j(x_1) - \bigtriangledown r_j(x_2))| \, |y| \\
&\leq \alpha \max_{\|y\|=1} \max_{1 \leq j \leq m} L \|x_1 - x_2\| \, |y| \\
&= \alpha L \|x_1 - x_2\|
\end{aligned}$$

We conclude that J is Lipschitz continuous with constant $\tilde{L} = \alpha L$.

On the other hand, Given $x, \tilde{x}$ in $\mathcal{D}$, we estimate

$$\begin{aligned}
\|\nabla f(x) - \nabla f(\tilde{x})\| &= \|J(x)^T r(x) - J(\tilde{x})^T r(\tilde{x})\| \\
&= \| \left[J(x)^T r(x) - J(\tilde{x})^T r(x)\right] + \left[J(\tilde{x})^T r(x) - J(\tilde{x})^T r(\tilde{x})\right] \| \\
&= \| \left(J(x)^T - J(\tilde{x})^T\right) r(x) + J(\tilde{x})^T \left(r(x) - r(\tilde{x})\right) \| \\
&\le \|J(x)^T - J(\tilde{x})^T\| |r(x)| + \|J(\tilde{x})^T\| \|r(x) - r(\tilde{x})\| \\
&\le M\alpha L\|x - \tilde{x}\| + M'L\|x - \tilde{x}\| \\
&= \mathcal{L}\|x - \tilde{x}\|
\end{aligned}$$

where $\mathcal{L} = M\alpha L + M'L$ and $\|J(\tilde{x})^T\|$ is bounded since it is Lipschitz continuous on a compact set $\mathcal{D}$. $\square$

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Proof. Since all norms in $\mathbb{R}^n$ are equivalent.

$$\exists \alpha > 0 \quad \text{such that} \quad \|x\| \le \alpha \|x\|_\infty \quad \forall x \in \mathbb{R}^n$$

We have,

$$\begin{aligned}
\|J(x_1) - J(x_2)\| &= \max_{\|y\|=1} \|(J(x_1) - J(x_2))y\| \\
&= \max_{\|y\|=1} \left\| \begin{bmatrix} (\triangledown r_1(x_1) - \triangledown r_1(x_2))^T y \\ \vdots \\ (\triangledown r_m(x_1) - \triangledown r_m(x_2))^T y \end{bmatrix} \right\| \\
&\le \max_{\|y\|=1} \alpha \left\| \begin{bmatrix} (\triangledown r_1(x_1) - \triangledown r_1(x_2))^T y \\ \vdots \\ (\triangledown r_m(x_1) - \triangledown r_m(x_2))^T y \end{bmatrix} \right\|_\infty \\
&= \alpha \max_{\|y\|=1} \max_{1\le j\le m} |(\triangledown r_j(x_1) - \triangledown r_j(x_2))^T y| \\
&\le \alpha \max_{\|y\|=1} \max_{1\le j\le m} |(\triangledown r_j(x_1) - \triangledown r_j(x_2))| \; |y| \\
&\le \alpha \max_{\|y\|=1} \max_{1\le j\le m} L \|x_1 - x_2\| \; |y| \\
&= \alpha L \|x_1 - x_2\|
\end{aligned}$$

We conclude that J is Lipschitz continuous with constant $\tilde{L} = \alpha L$. □

Proof. Given $x, \tilde{x}$ in $\mathcal{D}$, we estimate

$$\begin{aligned}
\|\nabla f(x) - \nabla f(\tilde{x})\| &= \|J(x)^T r(x) - J(\tilde{x})^T r(\tilde{x})\| \\
&= \| \left[J(x)^T r(x) - J(\tilde{x})^T r(x)\right] + \left[J(\tilde{x})^T r(x) - J(\tilde{x})^T r(\tilde{x})\right] \| \\
&= \| \left(J(x)^T - J(\tilde{x})^T\right) r(x) + J(\tilde{x})^T \left(r(x) - r(\tilde{x})\right) \| \\
&\le \|J(x)^T - J(\tilde{x})^T\| |r(x)| + \|J(\tilde{x})^T\| \|r(x) - r(\tilde{x})\| \\
&\le M\alpha L \|x - \tilde{x}\| + M' L \|x - \tilde{x}\| \\
&= \mathcal{L} \|x - \tilde{x}\|
\end{aligned}$$

where $\mathcal{L} = M\alpha L + M'L$ and $\|J(\tilde{x})^T\|$ is bounded since it is Lipschitz continuous on a compact set $\mathcal{D}$. □

Numerical Optimization with applications
CHAPTER 17: Penalty and Augmented Lagrangian Methods

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17.1 THE QUADRATIC PENALTY METHOD

Given the original constrained optimization problem

$$\min_x f(x) \quad \text{subject to } c_i(x) = 0, \quad i \in \mathcal{E}, \quad c_i(x) \geq 0, \quad i \in \mathcal{I}, \tag{1}$$

we could define the corresponding quadratic penalty function as

$$Q(x;\mu) := f(x) + \frac{\mu}{2}\sum_{i\in\mathcal{E}} c_i^2(x) + \frac{\mu}{2}\sum_{i\in\mathcal{I}} \left([c_i(x)]^-\right)^2, \tag{2}$$

where $\mu > 0$ and $[y]^-$ is the abbreviated symbol of $\max(-y, 0)$.

If we take a sequence $\mu_k \nearrow \infty$ into the quadratic penalty function, we could find that $Q(x;\mu_k)$ deverges if x is infeasible. The larger μ_k is, the severer constraint violations we panalize. As a result, the minimizer of the quadratic penalty function $Q(x;\mu_k)$ is closer to the feasible region as k increases.

Framework 17.1 (Quadratic Penalty Method).

Given $\mu_0 > 0$, a nonnegative sequence $\{\tau_k\}$ with $\tau_k \to 0$, and a starting point x_0^s;
for $k = 0, 1, 2, \ldots$
  Find an approximate minimizer x_k of $Q(\cdot;\mu_k)$, starting at x_k^s,
    and terminating when $\|\nabla_x Q(x;\mu_k)\| \leq \tau_k$;
  if final convergence test satisfied
    stop with approximate solution x_k;
  end (if)
  Choose new penalty parameter $\mu_{k+1} > \mu_k$;
  Choose new starting point x_{k+1}^s;
end (for)

We have two theorems to support the convergence of Framework 17.1.

Theorm 17.1 states that the global minimizer x_k of quadratic penalty function $Q(x;\mu_k)$ converges to the constrained optimization problem x, i.e. $x_k \to x$.

Theorm 17.2 states that if $\tau_k \to 0$ and x_k only satisfies

$$\|\nabla_x Q(x;\mu_k)\| \leq \tau_k,$$

then

$$x_k \to x^*,$$

where x^* is a stationary point of $\|c(x)\|^2$. Besides, if $\nabla c_i(x^*)$ is linearly independent, then

$$\lim_{k\to\infty} -\mu_k c_i(x_k) = \lambda_i^* \quad \forall i \in \mathcal{E}$$

and (X^*, λ^*) satisfy the KKT conditions.

Practical problems

Even if $\nabla^2 f(x^*)$ is well-conditioned, the Hessian $\nabla^2_{xx} Q(x;\mu_k)$ might become ill-conditioned as $\mu_k \to \infty$.

By defining

$$A(x)^T = (\nabla c_i(x))_{i\in\mathcal{E}}$$

and considering equality constraints only, we have

$$\nabla^2_{xx}Q(x;\mu_k) = \nabla^2 f(x) + \sum_{i\in\mathcal{E}} \mu_k c_i(x)\nabla^2 c_i(x) + \mu_k A(X)^T A(X).$$

From **Theorem 17.2**, we have

$$\mu_k c_i(x) \approx -\lambda_i^*$$

for x near a minimizer. Hence, we obtain

$$\nabla^2_{xx}Q(x;\mu_k) \approx \nabla^2_{xx}\mathcal{L}(x,\lambda^*) + \mu_k A(X)^T A(X).$$

We find that $\nabla^2_{xx}Q(x;\mu_k)$ have problems with ill-conditioning since the second term diverges as $\mu_k \to \infty$.

For Newton's method step

$$\nabla^2_{xx}Q(x;\mu_k)p = \nabla_x Q(x;\mu),$$

we can apply a reformulation

$$\begin{pmatrix} \nabla^2 f(x) + \sum_{i\in\mathcal{E}} \mu_k c_i(x)\nabla^2 c_i(x) & A(x)^T \\ A(x) & -(1/\mu_k)I \end{pmatrix} \begin{pmatrix} p \\ \mu A(x)p \end{pmatrix} = \begin{pmatrix} -\nabla_x Q(x;\mu_k) \\ 0 \end{pmatrix}$$

to avoid the ill-conditioning since p solves both systems. Note that this system has dimension $n + |\mathcal{E}|$ rather than n.

17.2 NONSMOOTH PENALTY FUNCTIONS

A penalty function ia called *exact* if, for certains coice of penalty parameters, the minimizer $x^\star$ is the exact solution of the original constrained optimization problem. Nevertheless, the quadratical penalty function is not exact. In this section, we introduce the *nonsmooth* penalty functions.
A popular nonsmooth penalty function is the l_1 *penalty function* defined by

$$\phi_1(x;\mu) = f(x) + \mu\sum_{i\in\mathcal{E}}|c_i(x)| + \mu\sum_{i\in\mathcal{I}}[c_i(x)]^-. \tag{3}$$

The next two theorems establish the *exactness* of (3).
Theorm 17.3 states that if $x^\star$ is a strictly local minimizer of (1), with Lagrange miltipliers $\lambda^\star$. Then $x^\star$ is a local minimizer of (3) $\quad\forall\ \mu > \mu^\star$, where

$$\mu^\star = \|\lambda^\star\|_\infty \tag{4}$$

Theorm 17.4 states that if $\hat{x}$ is a stationary points of $\phi_1(x;\mu)$ for all μ large enouth. Then, $\hat{x}$ is either satisfying KKT conditions for (1) or it is an infeasible stationary points.
Define the measure of infeasibility

$$h(x) = sum_{i\in\mathcal{E}}|c_i(x)| + sum_{i\in\mathcal{I}}[c_i(x)]^- \tag{5}$$

Then, we can develope an algorithm framwork via the l_1 penalty funtion.
Framework 17.2 (Classical ℓ_1 Penalty Method).

Given $\mu_0 > 0$, tolerance $\tau > 0$, starting point x_0^s;
for $k = 0, 1, 2, \ldots$
    Find an approximate minimizer x_k of $\phi_1(x;\mu_k)$, starting at x_k^s;
    if $h(x_k) \le \tau$
        stop with approximate solution x_k;
    end (if)
    Choose new penalty parameter $\mu_{k+1} > \mu_k$;
    Choose new starting point x_{k+1}^s;
end (for)

Since $\phi_1(x;\mu)$ is nonsmooth, the minimization will be difficule. However, we can transform $\phi_1(x;\mu)$ into a smooth model.

A PRATICAL l_1 PENALTY METHOD

As we did for the unconstrained optimization problem, we can transform (3) into a smooth model by replacing f by its Taylor expension and c_i by its linearization,as follows:

$$q(p;\mu) = f(x) + \bigtriangledown f(x)^T p + \frac{1}{2}p^T W p + \mu \sum_{i \in \mathcal{E}} |c_i(x) + \bigtriangledown c_i(x)^T p| + \mu \sum_{i \in \mathcal{I}} [c_i(x) + \bigtriangledown c_i(x)^T p]^-$$

where W is an approximation of Hessian about f and c_i. The function $q(p;\mu)$ is still not smooth, but we can reformulate it into a smooth quadratic optimization problem by introducing some new variables, as follows:

$$\begin{aligned} \min_{p,r,s,t} \quad & f(x) + \frac{1}{2}p^T W p + \bigtriangledown f(x)^T p + \mu \sum_{i \in \mathcal{E}} |r_i + s_i| + \mu \sum_{i \in \mathcal{I}} t_i \\ \textit{subject to} \quad & \bigtriangledown c_i(x)^T p + c_i(x) = r_i - s_i, \quad i \in \mathcal{E} \\ & \bigtriangledown c_i(x)^T p + c_i(x) \geq -t_i, \quad i \in \mathcal{I} \\ & r, s, t \geq 0 \end{aligned} \tag{6}$$

Even after adding a trust region constraint $\|p\|_\infty \leq \triangle$, (6) is still a quadratic problem. It can be solved by a quadratic programming solver.

A GENERAL CLASS OF NONSMOOTH PENALTY METHODS

Exact nonsmooth penalty funtions can use other norms.

$$\phi(x;\mu) = f(x) + \mu \|c_{\mathcal{E}}(x)\| + \mu \left\|[c_{\mathcal{I}}(x)]^-\right\| \tag{7}$$

Framework 17.2 can work on these penalty functions by simply redefinind the measure of infeasibility (5) as $h(x) = \|c_{\mathcal{E}}(x)\| + \|[c_{\mathcal{I}}(x)]^-\|$.
The properties garguaranteed by Theorem 17.3 and Theorem 17.4 can be extended to the general class (7).In Theorem 17.3, we replace $\mu^\star$ in (4) by

$$\mu^\star = \|\lambda^\star\|_D \,,$$

where $\|\bullet\|_D$ is the dual norm of $\|\bullet\|$. Theorem 17.4 applies without modification.

17.3 AUGMENTED LAGRANGIAN METHOD: EQUALITY CONSTRAINTS

In section 17.1, we know that even μ_k is large, the approximate minimizer x_k of the quadratic penalty function $Q(x;\mu_k)$ may be infeasible, the violation of $c_i(x) \approx -\lambda_i^*/\mu_k$. To make the approximate solution x_k closer to the feasible region, we introduce the Augmented Lagrangian function:

$$\mathcal{L}_A(x,\lambda;\mu) := f(x) - \sum_{i \in \mathcal{E}} \lambda_i c_i(x) + \frac{\mu}{2} \sum_{i \in \mathcal{E}} c_i^2(x) \tag{8}$$

Use the fact of Theorem 2.2 and (17.17), and rearranging the expression, we have $c_i(x_k) \approx -\frac{1}{\mu_k}(\lambda_i^* - \lambda_i^k)$, the violent of x_k is much smaller than $\frac{1}{\mu_k}$. We can set the Lagrangian multiplier vector of the next step $\lambda_i^{k+1} = \lambda_i^k - \mu_k c_i(x_k)$, for all $i \in \mathcal{E}$.

Framework 17.3 (Augmented Lagrangian Method-Equality Constraints).

Given $\mu_0 > 0$, tolerance $\tau_0 > 0$, starting points x_0^s and λ^0;
for $k = 0, 1, 2, \ldots$
    Find an approximate minimizer x_k of $\mathcal{L}_A(\cdot, \lambda^k; \mu_k)$, starting at x_k^s,
        and terminating when $\|\nabla_x \mathcal{L}_A(x_k, \lambda^k; \mu_k)\| \le \tau_k$;
    if a convergence test for (17.1) is satisfied
        stop with approximate solution x_k;
    end (if)
    Update Lagrange multipliers using (17.39) to obtain λ^{k+1};
    Choose new penalty parameter $\mu_{k+1} \ge \mu_k$;
    Set starting point for the next iteration to $x_{k+1}^s = x_k$;
    Select tolerance τ_{k+1};
end (for)

Theorm 17.5 states that if we know the exact Lagrangian multiplier λ^*, then the solution of (1) is a strict minimizer of $\mathcal{L}_A(x, \lambda; \mu)$ for μ large enough. Even though we only have a "good" estimate of λ^*, we can still get a good estimate of x^* by minimizing $\mathcal{L}_A(x, \lambda; \mu)$ with large μ.
Theorm 17.6 states the advantage of the augmented Lagrangian method. Different from the quadratic penalty method, we can get a good approximation of x^* if λ_k is close to λ^* or if the penalty parameter μ_k is large. On the other hand, by (17.46), we can improve the accuracy of λ^* by choosing a large μ_k.

17.4 PRACTICAL AUGMENTED LAGRANGIAN METHOD

In section 17.3, we only discuss the problem with equality constrains. Now for the general case, there are three useful formulations.
Bound-Constrained Formulation
Use the slack variable s_i to turn inequalities into equalities. That is

$$c_i(x) - s_i = 0, \quad s_i \ge 0, \quad \forall i \in \mathcal{I}$$

We can reformulate the problem into

$$\min_{x \in \mathbb{R}^n} f(x) \quad s.t. \quad c_i(x) = 0, \quad i = 1, 2, ..., m, \quad l \le x \le u$$

The Bounded-constrained Lagrangian will be:

$$\min_x \mathcal{L}_A(x, \lambda; \mu) = f(x) - \sum_{i=1}^m \lambda_i c_i(x) + \frac{\mu}{2} \sum_{i=1}^m c_i^2(x) \quad s.t. \quad l \le x \le u$$

Solve this problem and update λ and μ repeatedly.
Linearly Constrained Formulation
LCL method is to solve the subproblem of minimizing the augmented Lagrangian function subject to linearization of the constrains.

$$\begin{aligned} \min_x \quad & F_k(x) \\ s.t. \quad & c(x_k) + A_k(x - x_k) = 0, \quad l \le x \le u. \end{aligned}$$

where

$$c_i^{-k}(x) = c_i(x) - c_i(x_k) - \triangledown c_i(x_k)^T (x - x_k).$$

Current Augmented Lagrangian funciton

$$F_k(x) = f(x) - \sum_{i=1}^m \lambda_i^k c_i^{-k}(x) + \frac{\mu}{2} \sum_{i=1}^m [c_i^{-k}(x)]^2$$

Unconstrained Formulation

Suppose the problem has no equality constrain, i.e. $\mathcal{E} = \emptyset$, then we can rewrite the problem as

$$\min_{x \text{ feasible}} f(x) = \min_{x \in \mathbb{R}^n} F(x)$$

where

$$F(x) = \max_{\lambda \geq 0} \{f(x) - \sum_{i \in \mathcal{I}} \lambda_i c_i(x)\}$$

Note that if x is feasible, $F(x) = f(x)$ and λ_i should be zero. Otherwise $F(x)$ turns to infinity, and λ_i can be chosen arbitrary large. Consequently, F is not smooth, so it is not practical to minimize directly. We replace F by a smooth approximated function

$$\widehat{F}(x; \lambda^k, \mu_k) = \max_{\lambda \geq 0} \{f(x) - \sum_{i \in \mathcal{I}} \lambda_i c_i(x) - \frac{1}{2\mu_k} \sum_{i \in \mathcal{I}} (\lambda_i - \lambda_i^k)^2$$

where the last term can enforce the mew maximizer λ close to the previous estimate λ^k.
By above, we can obtain the explicit maximization of λ. Then we have

$$\widehat{F}(x; \lambda^k, \mu_k) = f(x) + \sum_{i \in \mathcal{I}} \psi(c_i(x), \lambda_i^k; \mu_k)$$

where the functionψ is defined as

$$\psi(t, \sigma; \mu) := \begin{cases} -\sigma t + \frac{\mu}{2} t^2 & \text{if} t - \sigma/\mu \leq 0, \\ -\frac{1}{2\mu}\sigma^2 & \text{otherwise}, \end{cases}$$

Hence, we can obtain x_k by minimizing $\widehat{F}$, and update Lagrange multiplier estimates repeatedly.