4.4 Algorithms for Minimizing Smooth Functions

4.4.1 Steepest Descent Method

Consider $f : \mathbb{R}^n \to \mathbb{R}$ a differentiable function on its domain.

Steepest Descent Method	
Choose:	$\boldsymbol{x}_0 \in \mathbb{R}^n$
Iterate:	$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - h_k \boldsymbol{\nabla f}(\boldsymbol{x}_k),\ \ k = 0, 1, \ldots$

We consider four strategies for the step-size h_k:

1. **Constant Step**

   The sequence $\{h_k\}_{k=0}^{\infty}$ is chosen in *advance*. For example

   $$h_k := h > 0,$$

   $$h_k := \frac{h}{\sqrt{k+1}}.$$

   This is the simplest strategy.

2. **Exact Line Search (Cauchy Step-Size)**

   The sequence $\{h_k\}_{k=0}^{\infty}$ is chosen such that

   $$h_k := \arg\min_{h \geq 0} f(\boldsymbol{x}_k - h \boldsymbol{\nabla f}(\boldsymbol{x}_k)).$$

   This choice is only theoretical since even for the one dimensional case, it is very difficult and expensive.

3. **Goldstein-Armijo Rule**

   Find a sequence $\{h_k\}_{k=0}^{\infty}$ such that

   $$\begin{aligned} \alpha \langle \boldsymbol{\nabla f}(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{x}_{k+1} \rangle &\leq f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}), \\ \beta \langle \boldsymbol{\nabla f}(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{x}_{k+1} \rangle &\geq f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}), \end{aligned}$$

   where $0 < \alpha < \beta < 1$ are fixed parameters.

   Since $f(\boldsymbol{x}_{k+1}) = f(\boldsymbol{x}_k - h_k \boldsymbol{\nabla f}(\boldsymbol{x}_k))$,

   $$f(\boldsymbol{x}_k) - \beta h_k \|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2^2 \leq f(\boldsymbol{x}_{k+1}) \leq f(\boldsymbol{x}_k) - \alpha h_k \|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2^2.$$

   The acceptable steps exist unless $f(\boldsymbol{x}_{k+1}) = f(\boldsymbol{x}_k - h \boldsymbol{\nabla f}(\boldsymbol{x}_k))$ is not bounded from below.

4. **Barzilai-Borwein Step-Size**[1]

   Let us define $\boldsymbol{s}_{k-1} := \boldsymbol{x}_k - \boldsymbol{x}_{k-1}$ and $\boldsymbol{y}_{k-1} := \boldsymbol{\nabla f}(\boldsymbol{x}_k) - \boldsymbol{\nabla f}(\boldsymbol{x}_{k-1})$. Then, we can define the Barzilai-Borwein (BB) step sizes $\{h_k^1\}_{k=1}^{\infty}$ and $\{h_k^2\}_{k=1}^{\infty}$:

   $$h_k^1 := \frac{\|\boldsymbol{s}_{k-1}\|_2^2}{\langle \boldsymbol{s}_{k-1}, \boldsymbol{y}_{k-1} \rangle},$$

   $$h_k^2 := \frac{\langle \boldsymbol{s}_{k-1}, \boldsymbol{y}_{k-1} \rangle}{\|\boldsymbol{y}_{k-1}\|_2^2}.$$

   The first step-size is the one which minimizes the following secant condition $\|\frac{1}{h}\boldsymbol{s}_{k-1} - \boldsymbol{y}_{k-1}\|_2^2$ while the second one minimizes $\|\boldsymbol{s}_{k-1} - h\boldsymbol{y}_{k-1}\|_2^2$.

[1] J. Barzilai and J. M. Borwein, "Two-point step size gradient methods," *IMA Journal of Numerical Analysis*, **8** (1988), pp. 141–148.

Now, consider the problem

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x})$$

where $f \in \mathcal{C}_L^{1,1}(\mathbb{R}^n)$, and $f(\boldsymbol{x})$ is bounded from below.

Let us evaluate the result of one step of the steepest descent method.
Consider $\boldsymbol{y} = \boldsymbol{x} - h\boldsymbol{\nabla f}(\boldsymbol{x})$. From Lemma 3.6,

$$\begin{aligned} f(\boldsymbol{y}) &\leq f(\boldsymbol{x}) + \langle \boldsymbol{\nabla f}(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x}\rangle + \frac{L}{2}\|\boldsymbol{y} - \boldsymbol{x}\|_2^2 \\ &= f(\boldsymbol{x}) - h\|\boldsymbol{\nabla f}(\boldsymbol{x})\|_2^2 + \frac{h^2 L}{2}\|\boldsymbol{\nabla f}(\boldsymbol{x})\|_2^2 \\ &= f(\boldsymbol{x}) - h\left(1 - \frac{h}{2}L\right)\|\boldsymbol{\nabla f}(\boldsymbol{x})\|_2^2. \end{aligned} \tag{5}$$

Thus, one step of the steepest descent method decreases the value of the objective function at least as follows for $h^* = 1/L$.

$$f(\boldsymbol{y}) \leq f(\boldsymbol{x}) - \frac{1}{2L}\|\boldsymbol{\nabla f}(\boldsymbol{x})\|_2^2.$$

Now, for the Goldstein-Armijo Rule, since $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - h_k\boldsymbol{\nabla f}(\boldsymbol{x}_k)$, we have:

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) \leq \beta h_k \|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2^2,$$

and from (5)

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) \geq h_k\left(1 - \frac{h_k}{2}L\right)\|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2^2.$$

Therefore, $h_k \geq 2(1-\beta)/L$.

Also, substituting in

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) \geq \alpha h_k \|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2^2 \geq \frac{2}{L}\alpha(1-\beta)\|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2^2.$$

Thus, in the three step-size strategies excepting the BB step size considered here, we can say that

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) \geq \frac{\omega}{L}\|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2^2$$

for some positive constant ω.

Summing up the above inequality we have:

$$\frac{\omega}{L}\sum_{k=0}^{N}\|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2^2 \leq f(\boldsymbol{x}_0) - f(\boldsymbol{x}_{N+1}) \leq f(\boldsymbol{x}_0) - f^*$$

where f^* is the optimal value of the problem.

As a simple consequence we have

$$\|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2 \to 0 \quad \text{as} \quad k \to \infty.$$

Finally,

$$g_N^* := \min_{0\leq k\leq N}\|\boldsymbol{\nabla f}(\boldsymbol{x}_k)\|_2 \leq \frac{1}{\sqrt{N+1}}\left[\frac{L}{\omega}(f(\boldsymbol{x}_0) - f^*)\right]^{1/2}. \tag{6}$$

Remark 4.14 $g_N^* \to 0$, but we cannot say anything about the rate of convergence of the sequence $\{f(\boldsymbol{x}_k)\}$ or $\{\boldsymbol{x}_k\}$.

Example 4.15 Consider the function $f(x,y) = \frac{1}{2}x^2 + \frac{1}{4}y^4 - \frac{1}{2}y^2$. $(0,-1)^T$ and $(0,1)^T$ are local minimal solutions, but $(0,0)^T$ is a stationary point.

If we start the steepest descent method from $(1,0)^T$, we will only converge to the stationary point.

We focus now on the following problem class:

Model:	1. $\min\limits_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x})$ 2. $f \in \mathcal{C}_L^{1,1}(\mathbb{R}^n)$ 3. $f(\boldsymbol{x})$ is bounded from below
Oracle:	Only function and gradient values are available
Approximate solution:	Find $\bar{\boldsymbol{x}} \in \mathbb{R}^n$ such that $f(\bar{\boldsymbol{x}}) \leq f(\boldsymbol{x}_0)$ and $\|\boldsymbol{\nabla f}(\bar{\boldsymbol{x}})\|_2 < \epsilon$

From (6), we have

$$g_N^* < \varepsilon \quad \text{if} \quad N+1 > \frac{L}{\omega\varepsilon^2}(f(\boldsymbol{x}_0) - f^*).$$

Remark 4.16 This is much better than the result of Theorem 4.6, since *it does not depend on* n.

Finally, consider the following problem under Assumption 4.17.

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x})$$

Assumption 4.17

1. $f \in \mathcal{C}_M^{2,2}(\mathbb{R}^n)$;
2. There is a local minimum $\boldsymbol{x}^*$ of the function $f(\boldsymbol{x})$;
3. We know some bound $0 < \ell \leq L < \infty$ for the Hessian at $\boldsymbol{x}^*$:
$$\ell \boldsymbol{I} \preceq \boldsymbol{\nabla}^2 \boldsymbol{f}(\boldsymbol{x}^*) \preceq L\boldsymbol{I};$$
4. Our starting point $\boldsymbol{x}_0$ is close enough to $\boldsymbol{x}^*$.

Theorem 4.18 Let $f(\boldsymbol{x})$ satisfy our assumptions above and let the starting point $\boldsymbol{x}_0$ be close enough to a local minimum:

$$r_0 = \|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2 < \bar{r} := \frac{2\ell}{M}.$$

Then, the steepest descent method with step-size $h^* = 2/(L+\ell)$ converges as follows:

$$\|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2 \leq \frac{\bar{r}r_0}{\bar{r} - r_0}\left(1 - \frac{2\ell}{L+3\ell}\right)^k.$$

This rate of convergence is called (R-)*linear*.

Proof:
In the steepest descent method, the iterates are $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - h_k \boldsymbol{\nabla f}(\boldsymbol{x}_k)$.
Since $\boldsymbol{\nabla f}(\boldsymbol{x}^*) = 0$,

$$\nabla \boldsymbol{f}(\boldsymbol{x}_k) = \nabla \boldsymbol{f}(\boldsymbol{x}_k) - \nabla \boldsymbol{f}(\boldsymbol{x}^*) = \int_0^1 \nabla^2 \boldsymbol{f}(\boldsymbol{x}^* + \tau(\boldsymbol{x}_k - \boldsymbol{x}^*))(\boldsymbol{x}_k - \boldsymbol{x}^*) d\tau = \boldsymbol{G}_k(\boldsymbol{x}_k - \boldsymbol{x}^*),$$

and therefore,

$$\boldsymbol{x}_{k+1} - \boldsymbol{x}^* = \boldsymbol{x}_k - \boldsymbol{x}^* - h_k \boldsymbol{G}_k(\boldsymbol{x}_k - \boldsymbol{x}^*) = (\boldsymbol{I} - h_k \boldsymbol{G}_k)(\boldsymbol{x}_k - \boldsymbol{x}^*).$$

Let $r_k = \|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2$. From Lemma 3.8,

$$\nabla^2 \boldsymbol{f}(\boldsymbol{x}^*) - \tau M r_k \boldsymbol{I} \preceq \nabla^2 \boldsymbol{f}(\boldsymbol{x}^* + \tau(\boldsymbol{x}_k - \boldsymbol{x}^*)) \preceq \nabla^2 \boldsymbol{f}(\boldsymbol{x}^*) + \tau M r_k \boldsymbol{I}.$$

Integrating all parts from 0 to 1 and using our hypothesis,

$$(\ell - \frac{r_k}{2} M)\boldsymbol{I} \preceq \boldsymbol{G}_k \preceq (L + \frac{r_k}{2} M)\boldsymbol{I}.$$

Therefore,

$$\left(1 - h_k(L + \frac{r_k}{2} M)\right) \boldsymbol{I} \preceq \boldsymbol{I} - h_k \boldsymbol{G}_k \preceq \left(1 - h_k(\ell - \frac{r_k}{2} M)\right) \boldsymbol{I}.$$

We arrive at

$$\|\boldsymbol{I} - h_k \boldsymbol{G}_k\|_2 \leq \max\{|a_k(h_k)|, |b_k(h_k)|\}$$

where $a_k(h) = 1 - h(\ell - \frac{r_k}{2} M)$ and $b_k(h) = h(L + \frac{r_k}{2} M) - 1$.

Notice that $a_k(0) = 1$ and $b_k(0) = -1$.

Now, let us use our hypothesis that $r_0 < \bar{r}$.

When $a_k(h) = b_k(h)$, we have $1 - h(\ell - \frac{r_k}{2} M) = h(L + \frac{r_k}{2} M) - 1$, and therefore

$$h_k^* = \frac{2}{L + \ell}.$$

(Surprisingly, it does not depend neither on M nor r_k). Finally,

$$r_{k+1} = \|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|_2 \leq \left(1 - \frac{2}{L + \ell}\left(\ell - \frac{r_k}{2} M\right)\right) \|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2.$$

That is,

$$r_{k+1} \leq \left(\frac{L - \ell}{L + \ell} + \frac{r_k M}{L + \ell}\right) r_k.$$

and $r_{k+1} < r_k < \bar{r}$.

Now, let us analyze the rate of convergence. Multiplying the above inequality by $M/(L + \ell)$,

$$\frac{M r_{k+1}}{L + \ell} \leq \frac{M(L - \ell)}{(L + \ell)^2} r_k + \frac{M^2 r_k^2}{(L + \ell)^2}.$$

Calling $\alpha_k = \frac{M r_k}{L + \ell}$ and $q = \frac{2\ell}{L + \ell}$, we have

$$\alpha_{k+1} \leq (1 - q)\alpha_k + \alpha_k^2 = \alpha_k(1 + \alpha_k - q) = \frac{\alpha_k(1 - (\alpha_k - q)^2)}{1 - (\alpha_k - q)}. \tag{7}$$

Now, since $r_k < \frac{2\ell}{M}$, $\alpha_k - q = \frac{M r_k}{L + \ell} - \frac{2\ell}{L + \ell} < 0$, and $1 + (\alpha_k - q) = \frac{L - \ell}{L + \ell} + \frac{M r_k}{L + \ell} > 0$. Therefore, $-1 < \alpha_k - q < 0$, and (7) becomes $\leq \frac{\alpha_k}{1 + q - \alpha_k}$.

$$\frac{1}{\alpha_{k+1}} \geq \frac{1 + q}{\alpha_k} - 1.$$

$$\frac{q}{\alpha_{k+1}} - 1 \geq \frac{q(1+q)}{\alpha_k} - q - 1 = (1+q)\left(\frac{q}{\alpha_k} - 1\right).$$

and then,

$$\frac{q}{\alpha_k} - 1 \geq (1+q)^k \left(\frac{q}{\alpha_0} - 1\right) = (1+q)^k \left(\frac{2\ell}{L+\ell}\frac{L+\ell}{Mr_0} - 1\right) = (1+q)^k \left(\frac{\bar{r}}{r_0} - 1\right).$$

Finally, we arrive at

$$r_k = \|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2 \leq \frac{\bar{r}r_0}{\bar{r} - r_0}\left(1 - \frac{2\ell}{L+3\ell}\right)^k.$$

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4.4.2 The Newton Method

Example 4.19 Let us apply the Newton method to find the root of the following function

$$g(x) = \frac{x}{\sqrt{1+x^2}}.$$

Clearly $x^* = 0$.

The Newton method will give:

$$x_{k+1} = x_k - \frac{g(x_k)}{g'(x_k)} = x_k - x_k(1+x_k^2) = -x_k^3.$$

Therefore, the method converges if $|x_0| < 1$, it oscillates if $|x_0| = 1$, and finally, diverges if $|x_0| > 1$.

Assumption 4.20

1. $f \in \mathcal{C}_M^{2,2}(\mathbb{R}^n)$;
2. There is a local minimum $\boldsymbol{x}^*$ of the function $f(\boldsymbol{x})$;
3. The Hessian is positive definite at $\boldsymbol{x}^*$:
$$\boldsymbol{\nabla}^2 \boldsymbol{f}(\boldsymbol{x}^*) \succeq \ell \boldsymbol{I}, \quad \ell > 0;$$
4. Our starting point $\boldsymbol{x}_0$ is close enough to $\boldsymbol{x}^*$.

Theorem 4.21 Let the function $f(\boldsymbol{x})$ satisfy the above assumptions. Suppose that the initial starting point $\boldsymbol{x}_0$ is close enough to $\boldsymbol{x}^*$:

$$\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2 < \bar{r} := \frac{2\ell}{3M}.$$

Then $\|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2 < \bar{r}$ for all k of the Newton method and it converges (Q-)quadratically:

$$\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|_2 \leq \frac{M\|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2^2}{2(\ell - M\|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2)}.$$

Proof:

Let $r_k = \|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2$. From Lemma 3.8 and the assumption, we have for $k = 0$,

$$\boldsymbol{\nabla}^2 \boldsymbol{f}(\boldsymbol{x}_0) \succeq \boldsymbol{\nabla}^2 \boldsymbol{f}(\boldsymbol{x}^*) - Mr_0 \boldsymbol{I} \succeq (\ell - Mr_0)\boldsymbol{I}. \tag{8}$$

Since $r_0 < \bar{r} = \frac{2\ell}{3M} < \frac{\ell}{M}$, we have $\ell - Mr_0 > 0$ and therefore, $\boldsymbol{\nabla}^2 \boldsymbol{f}(\boldsymbol{x}_0)$ is invertible.

Consider the Newton method for $k = 0$, $\boldsymbol{x}_1 = \boldsymbol{x}_0 - [\boldsymbol{\nabla}^2 \boldsymbol{f}(\boldsymbol{x}_0)]^{-1} \boldsymbol{\nabla} \boldsymbol{f}(\boldsymbol{x}_0)$.