

Lecture 5: Unconstrained smooth optimization



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1. Taylor's theorem

- Taylor's theorem shows how smooth functions can be locally approximated by low-order (e.g., linear or quadratic) functions.

定理 12.3.1 (Taylor 公式) 设 $f(x, y)$ 在点 (x_0, y_0) 的邻域 $U = O((x_0, y_0), r)$ 上具有 $k+1$ 阶连续偏导数, 那么对于 U 内每一点 $(x_0 + \Delta x, y_0 + \Delta y)$ 都成立

$$\begin{aligned} & f(x_0 + \Delta x, y_0 + \Delta y) \\ &= f(x_0, y_0) + \left(\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y} \right) f(x_0, y_0) \\ & \quad + \frac{1}{2!} \left(\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y} \right)^2 f(x_0, y_0) + \cdots \\ & \quad + \frac{1}{k!} \left(\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y} \right)^k f(x_0, y_0) + R_k, \end{aligned}$$

其中 $R_k = \frac{1}{(k+1)!} \left(\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y} \right)^{k+1} f(x_0 + \theta \Delta x, y_0 + \theta \Delta y) (0 < \theta < 1)$
称为 **Lagrange 余项**.

Theorem 1

Given a continuously differentiable function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, we have

$$f(\mathbf{x} + \mathbf{p}) = f(\mathbf{x}) + \nabla f(\mathbf{x} + \xi \mathbf{p})^\top \mathbf{p}, \text{ for some } \xi \in (0, 1),$$

$$f(\mathbf{x} + \mathbf{p}) = f(\mathbf{x}) + \int_0^1 \nabla f(\mathbf{x} + t\mathbf{p})^\top \mathbf{p} dt,$$

$$f(\mathbf{x} + \mathbf{p}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^\top \mathbf{p} + o(\|\mathbf{p}\|).$$

If f is twice continuously differentiable, we have for some $\xi \in (0, 1)$,

$$f(\mathbf{x} + \mathbf{p}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^\top \mathbf{p} + \frac{1}{2} \mathbf{p}^\top \nabla^2 f(\mathbf{x} + \xi \mathbf{p}) \mathbf{p},$$

and

$$\nabla f(\mathbf{x} + \mathbf{p}) = \nabla f(\mathbf{x}) + \int_0^1 \nabla^2 f(\mathbf{x} + t\mathbf{p}) \mathbf{p} dt,$$

$$f(\mathbf{x} + \mathbf{p}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^\top \mathbf{p} + \frac{1}{2} \mathbf{p}^\top \nabla^2 f(\mathbf{x}) \mathbf{p} + o(\|\mathbf{p}\|^2).$$

2. Global and local solutions of $\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x})$

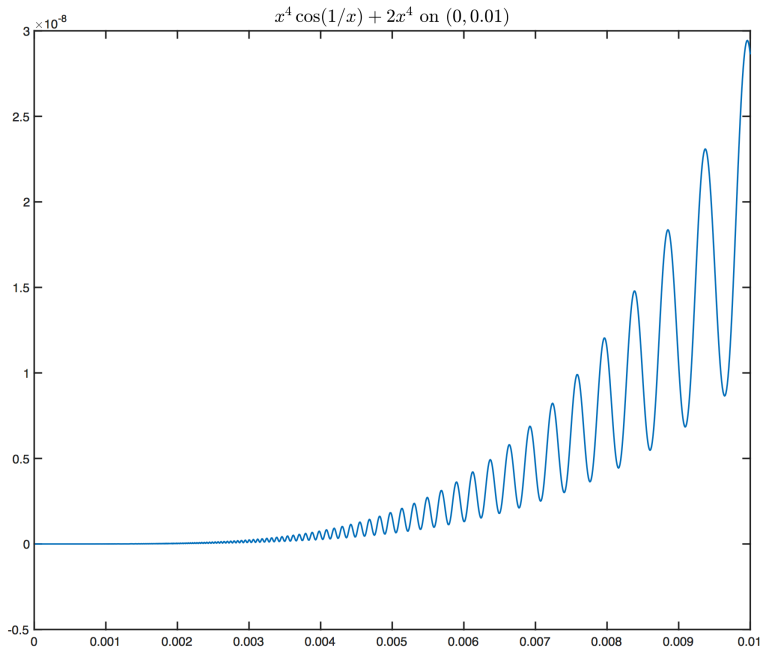
- \mathbf{x}_\star is a *local minimizer* of f if there is a neighborhood \mathcal{N} of \mathbf{x}_\star such that $f(\mathbf{x}) \geq f(\mathbf{x}_\star)$ for all $\mathbf{x} \in \mathcal{N}$.
- \mathbf{x}_\star is a *strict local minimizer* if it is a local minimizer on some neighborhood \mathcal{N} and in addition $f(\mathbf{x}) > f(\mathbf{x}_\star)$ for all $\mathbf{x} \in \mathcal{N}$ with $\mathbf{x} \neq \mathbf{x}_\star$.
- \mathbf{x}_\star is an *isolated local minimizer* if there is a neighborhood \mathcal{N} of \mathbf{x}_\star such that $f(\mathbf{x}) \geq f(\mathbf{x}_\star)$ for all $\mathbf{x} \in \mathcal{N}$ and in addition, \mathcal{N} contains no local minimizers other than \mathbf{x}_\star .

Strict local minimizers are not always isolated: for example,

$$f(x) = x^4 \cos(1/x) + 2x^4, \quad f(0) = 0.$$

All isolated local minimizers are strict.

- \mathbf{x}_\star is a *global minimizer* of f if $f(\mathbf{x}) \geq f(\mathbf{x}_\star)$ for all $\mathbf{x} \in \mathbb{R}^n$.



3. Optimality conditions for smooth functions

Theorem 2 (First-order necessary condition)

If \mathbf{x}_\star is a local minimizer of f and f is continuously differentiable in an open neighborhood of \mathbf{x}_\star , then $\nabla f(\mathbf{x}_\star) = \mathbf{0}$.

Proof. Suppose for contradiction that $\nabla f(\mathbf{x}_\star) \neq \mathbf{0}$. Define the vector $\mathbf{p} = -\nabla f(\mathbf{x}_\star)$ and note that $\mathbf{p}^\top \nabla f(\mathbf{x}_\star) = -\|\nabla f(\mathbf{x}_\star)\|^2 < 0$. Because ∇f is continuous near \mathbf{x}_\star , there is a scalar $T > 0$ such that

$$\mathbf{p}^\top \nabla f(\mathbf{x}_\star + t\mathbf{p}) < 0, \quad \text{for all } t \in [0, T].$$

For any $s \in (0, T]$, we have by Taylor's theorem that

$$f(\mathbf{x}_\star + s\mathbf{p}) = f(\mathbf{x}_\star) + s\mathbf{p}^\top \nabla f(\mathbf{x}_\star + \xi s\mathbf{p}) \quad \text{for some } \xi \in (0, 1).$$

Therefore, $f(\mathbf{x}_\star + s\mathbf{p}) < f(\mathbf{x}_\star)$ for all $s \in (0, T]$. We have found a direction leading away from \mathbf{x}_\star along which f decreases, so \mathbf{x}_\star is not a local minimizer, and we have a contradiction. \square

Theorem 3 (Second-order necessary conditions)

If \mathbf{x}_\star is a local minimizer of f and $\nabla^2 f$ is continuous in an open neighborhood of \mathbf{x}_\star , then $\nabla f(\mathbf{x}_\star) = \mathbf{0}$ and $\nabla^2 f(\mathbf{x}_\star) \succeq \mathbf{0}$.

Proof. We know from Theorem 2 that $\nabla f(\mathbf{x}_\star) = \mathbf{0}$. Assume that $\nabla^2 f(\mathbf{x}_\star)$ is not positive semidefinite. Then we can choose a vector \mathbf{p} such that $\mathbf{p}^\top \nabla^2 f(\mathbf{x}_\star) \mathbf{p} < 0$, and because $\nabla^2 f$ is continuous near \mathbf{x}_\star , there is a scalar $T > 0$ such that

$$\mathbf{p}^\top \nabla^2 f(\mathbf{x}_\star + t\mathbf{p}) \mathbf{p} < 0, \quad \text{for all } t \in [0, T].$$

By doing a Taylor series expansion around \mathbf{x}_\star , we have for all $s \in (0, T]$ and some $\xi \in (0, 1)$ that

$$f(\mathbf{x}_\star + s\mathbf{p}) = f(\mathbf{x}_\star) + s\mathbf{p}^\top \nabla f(\mathbf{x}_\star) + \frac{1}{2}s^2 \mathbf{p}^\top \nabla^2 f(\mathbf{x}_\star + \xi s\mathbf{p}) \mathbf{p} < f(\mathbf{x}_\star).$$

As in Theorem 2, we have found a direction from \mathbf{x}_\star along which f is decreasing, and so again, \mathbf{x}_\star is not a local minimizer. □

Theorem 4 (Second-order sufficient conditions)

Suppose that $\nabla^2 f$ is continuous in an open neighborhood of \mathbf{x}_\star and that $\nabla f(\mathbf{x}_\star) = \mathbf{0}$ and $\nabla^2 f(\mathbf{x}_\star) \succ \mathbf{0}$. Then \mathbf{x}_\star is a strict local minimizer of f .

Proof. Because the Hessian $\nabla^2 f$ is continuous and positive definite at \mathbf{x}_\star , we can choose a radius $r > 0$ so that $\nabla^2 f(\mathbf{x})$ remains positive definite for all \mathbf{x} in the open ball $\mathcal{B} = \{\mathbf{z} \mid \|\mathbf{z} - \mathbf{x}_\star\| < r\}$. Taking any nonzero vector \mathbf{p} with $\|\mathbf{p}\| < r$, we have $\mathbf{x}_\star + \mathbf{p} \in \mathcal{B}$ and

$$\begin{aligned} f(\mathbf{x}_\star + \mathbf{p}) &= f(\mathbf{x}_\star) + \mathbf{p}^\top \nabla f(\mathbf{x}_\star) + \frac{1}{2} \mathbf{p}^\top \nabla^2 f(\mathbf{x}_\star + \xi \mathbf{p}) \mathbf{p} \\ &= f(\mathbf{x}_\star) + \frac{1}{2} \mathbf{p}^\top \nabla^2 f(\mathbf{x}_\star + \xi \mathbf{p}) \mathbf{p}, \end{aligned}$$

for some $\xi \in (0, 1)$. Since $\mathbf{x}_\star + \xi \mathbf{p} \in \mathcal{B}$, we have

$$\mathbf{p}^\top \nabla^2 f(\mathbf{x}_\star + \xi \mathbf{p}) \mathbf{p} > 0,$$

and therefore $f(\mathbf{x}_\star + \mathbf{p}) > f(\mathbf{x}_\star)$, giving the result. □

- A point \mathbf{x} is called a *stationary point* if

$$\nabla f(\mathbf{x}) = \mathbf{0}.$$

- A stationary point \mathbf{x} is called a *saddle point* if there exist \mathbf{u} and \mathbf{v} such that

$$f(\mathbf{x} + \alpha \mathbf{u}) < f(\mathbf{x}) \quad \text{and} \quad f(\mathbf{x} + \alpha \mathbf{v}) > f(\mathbf{x})$$

for all sufficiently small $\alpha > 0$.

- Stationary points are not necessarily local minimizers. Stationary points can be *local maximizers* or *saddle points*.
- If $\nabla f(\mathbf{x}) = \mathbf{0}$, and $\nabla^2 f(\mathbf{x})$ has both strictly positive and strictly negative eigenvalues, then \mathbf{x} is a saddle point.
- If $\nabla^2 f(\mathbf{x})$ is positive semidefinite or negative semidefinite, then $\nabla^2 f(\mathbf{x})$ alone is insufficient to classify \mathbf{x} .

4. Line search methods

- Consider an iterative method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + t_k \mathbf{d}_k, \quad k = 0, 1, 2, \dots,$$

where \mathbf{d}_k is the *direction* and $t_k > 0$ is the *stepsize*.

- Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a continuously differentiable function over \mathbb{R}^n . A nonzero vector $\mathbf{d} \in \mathbb{R}^n$ is called a *descent direction* of f at \mathbf{x} if the directional derivative $f'(\mathbf{x}; \mathbf{d})$ is negative, meaning that

$$f'(\mathbf{x}; \mathbf{d}) = \nabla f(\mathbf{x})^\top \mathbf{d} < 0.$$

Lemma 5 (descent property of descent directions)

Let f be a continuously differentiable function over an open set U , and let $\mathbf{x} \in U$. Suppose that \mathbf{d} is a descent direction of f at \mathbf{x} . Then there exists $\varepsilon > 0$ such that

$$f(\mathbf{x} + t\mathbf{d}) < f(\mathbf{x}) \quad \text{for any } t \in (0, \varepsilon].$$

4.1 Choices for stepsize selection rules

- Assume that \mathbf{d}_k is a descent direction. Three popular choices:

(1) **constant**. $t_k = \bar{t} > 0$ for any k

(2) **exact line search**. t_k is a minimizer of f along the ray $\mathbf{x}_k + t\mathbf{d}_k$, i.e.,

$$t_k \in \operatorname{argmin}_{t \geq 0} f(\mathbf{x}_k + t\mathbf{d}_k)$$

(3) **backtracking**. Three parameters $s > 0$, $\alpha \in (0, 1)$, $\beta \in (0, 1)$. First, set $t_k = s$. Then, while

$$f(\mathbf{x}_k) - f(\mathbf{x}_k + t_k\mathbf{d}_k) < -\alpha t_k \nabla f(\mathbf{x}_k)^\top \mathbf{d}_k,$$

set $t_k \leftarrow \beta t_k$. In other words, $t_k = s\beta^{i_k}$, where i_k is the smallest nonnegative integer satisfying ([the sufficient decrease condition](#))

$$f(\mathbf{x}_k) - f(\mathbf{x}_k + s\beta^{i_k}\mathbf{d}_k) \geq -\alpha s\beta^{i_k} \nabla f(\mathbf{x}_k)^\top \mathbf{d}_k.$$

Lemma 6 (validity of the sufficient decrease condition)

Let f be a continuously differentiable function over \mathbb{R}^n . Suppose that $\mathbf{0} \neq \mathbf{d} \in \mathbb{R}^n$ is a descent direction of f at \mathbf{x} and let $\alpha \in (0, 1)$. Then there exists $\varepsilon > 0$ such that the inequality

$$f(\mathbf{x}) - f(\mathbf{x} + t\mathbf{d}) \geq -\alpha t \nabla f(\mathbf{x})^\top \mathbf{d}$$

holds for all $t \in [0, \varepsilon]$.

Proof. It follows from \mathbf{d} is a descent direction that

$$\lim_{t \rightarrow 0^+} \frac{(1 - \alpha)t \nabla f(\mathbf{x})^\top \mathbf{d} + o(t)\|\mathbf{d}\|}{t} = (1 - \alpha)\nabla f(\mathbf{x})^\top \mathbf{d} < 0.$$

Hence, there exists $\varepsilon > 0$ such that for all $t \in (0, \varepsilon]$ the inequality $(1 - \alpha)t \nabla f(\mathbf{x})^\top \mathbf{d} + o(t)\|\mathbf{d}\| < 0$ holds. The statement follows from

$$f(\mathbf{x}) - f(\mathbf{x} + t\mathbf{d}) = -\alpha t \nabla f(\mathbf{x})^\top \mathbf{d} - (1 - \alpha)t \nabla f(\mathbf{x})^\top \mathbf{d} - o(t)\|\mathbf{d}\|. \quad \square$$

4.2 The gradient method

- Set $\mathbf{d}_k = -\nabla f(\mathbf{x}_k)$, the steepest descent direction.

Proposition 7

Let f be a continuously differentiable function over \mathbb{R}^n , and let \mathbf{x} be a nonstationary point ($\nabla f(\mathbf{x}) \neq \mathbf{0}$). Then we have

$$-\frac{\nabla f(\mathbf{x})}{\|\nabla f(\mathbf{x})\|} = \operatorname{argmin}_{\mathbf{d} \in \mathbb{R}^n, \|\mathbf{d}\|=1} \nabla f(\mathbf{x})^\top \mathbf{d}.$$

Proposition 8 (“zig-zag”)

Let $\{\mathbf{x}_k\}$ be the sequence generated by the gradient method with exact line search for solving a problem of minimizing a continuously differentiable function f . Then for any $k = 0, 1, 2, \dots$,

$$(\mathbf{x}_{k+2} - \mathbf{x}_{k+1})^\top (\mathbf{x}_{k+1} - \mathbf{x}_k) = 0.$$

- We assume that f is continuously differentiable and that ∇f is Lipschitz continuous over \mathbb{R}^n : there exists $L > 0$ such that

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\|, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n.$$

- Notation: $C_L^{1,1}(\mathbb{R}^n)$, $C^{1,1}(\mathbb{R}^n)$, $C_L^{1,1}(D)$, $C^{1,1}(D)$

Theorem 9

Let f be a twice continuously differentiable function over \mathbb{R}^n . Then $f \in C_L^{1,1}(\mathbb{R}^n) \Leftrightarrow \|\nabla^2 f(\mathbf{x})\| \leq L$ for any $\mathbf{x} \in \mathbb{R}^n$.

Lemma 10 (descent lemma)

Let $D \subseteq \mathbb{R}^n$ and $f \in C_L^{1,1}(D)$ for some $L > 0$. Then for any $\mathbf{x}, \mathbf{y} \in D$ satisfying $[\mathbf{x}, \mathbf{y}] \subseteq D$ it holds that

$$-\frac{L}{2}\|\mathbf{y} - \mathbf{x}\|^2 \leq f(\mathbf{y}) - f(\mathbf{x}) - \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) \leq \frac{L}{2}\|\mathbf{y} - \mathbf{x}\|^2.$$

Lemma 11 (sufficient decrease lemma)

Suppose that $f \in C_L^{1,1}(\mathbb{R}^n)$. Then for any $\mathbf{x} \in \mathbb{R}^n$ and $t > 0$, we have

$$f(\mathbf{x}) - f(\mathbf{x} - t\nabla f(\mathbf{x})) \geq t(1 - tL/2)\|\nabla f(\mathbf{x})\|^2.$$

Lemma 12 (sufficient decrease of the gradient method)

Let $f \in C_L^{1,1}(\mathbb{R}^n)$. Let $\{\mathbf{x}_k\}$ be the sequence generated by the gradient method for solving $\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x})$ with one of the following stepsize strategies: constant stepsize $\bar{t} \in (0, 2/L)$, exact line search, backtracking procedure with parameters $s > 0$, $\alpha \in (0, 1)$, and $\beta \in (0, 1)$. Then

$$f(\mathbf{x}_k) - f(\mathbf{x}_{k+1}) \geq M\|\nabla f(\mathbf{x}_k)\|^2,$$

where

$$M = \begin{cases} \bar{t}(1 - \bar{t}L/2), & \text{constant stepsize,} \\ 1/(2L), & \text{exact line search,} \\ \alpha \min\{s, 2(1 - \alpha)\beta/L\}, & \text{backtracking.} \end{cases}$$

Theorem 13 (convergence of the gradient method)

Let $f \in C_L^{1,1}(\mathbb{R}^n)$. Let $\{\mathbf{x}_k\}$ be the sequence generated by the gradient method for solving

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

with one of the following stepsize strategies: constant stepsize $\bar{t} \in (0, 2/L)$, exact line search, backtracking procedure with parameters $s > 0$, $\alpha \in (0, 1)$, and $\beta \in (0, 1)$. Assume that f is bounded below over \mathbb{R}^n , that is, there exists $m \in \mathbb{R}$ such that $f(\mathbf{x}) \geq m$ for all $\mathbf{x} \in \mathbb{R}^n$.

Then we have the following:

- (a) The sequence $\{f(\mathbf{x}_k)\}$ is nonincreasing. In addition, for any $k > 0$, $f(\mathbf{x}_{k+1}) < f(\mathbf{x}_k)$ unless $\nabla f(\mathbf{x}_k) = \mathbf{0}$.
- (b) The sequence $\{f(\mathbf{x}_k)\}$ converges, and $\nabla f(\mathbf{x}_k) \rightarrow \mathbf{0}$ as $k \rightarrow \infty$.
- (c) Let $f_\star = \lim_{k \rightarrow \infty} f(\mathbf{x}_k)$. Then

$$\min_{k=0,1,\dots,n} \|\nabla f(\mathbf{x}_k)\| \leq \sqrt{\frac{f(\mathbf{x}_0) - f_\star}{M(n+1)}}.$$

4.3 The scaled gradient method

- Let $\mathbf{S} \in \mathbb{R}^{n \times n}$ be nonsingular. Consider the equivalent problem

$$\min\{g(\mathbf{y}) \equiv f(\mathbf{S}\mathbf{y}) : \mathbf{y} \in \mathbb{R}^n\}.$$

We have $\nabla g(\mathbf{y}) = \mathbf{S}^\top \nabla f(\mathbf{S}\mathbf{y}) = \mathbf{S}^\top \nabla f(\mathbf{x})$. The gradient method takes the form

$$\mathbf{y}_{k+1} = \mathbf{y}_k - t_k \mathbf{S}^\top \nabla f(\mathbf{S}\mathbf{y}_k).$$

Multiplying by \mathbf{S} from the left and using the notation $\mathbf{x}_k = \mathbf{S}\mathbf{y}_k$ and $\mathbf{D} = \mathbf{S}\mathbf{S}^\top$ yield

$$\mathbf{x}_{k+1} = \mathbf{x}_k - t_k \mathbf{D} \nabla f(\mathbf{x}_k).$$

The direction $-\mathbf{D} \nabla f(\mathbf{x}_k)$ is a descent direction.

- It is often beneficial to choose the scaling matrix \mathbf{D} differently at each iteration:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - t_k \mathbf{D}_k \nabla f(\mathbf{x}_k).$$

4.4 Newton's method

- We assume that f is twice continuously differentiable. Given \mathbf{x}_k ,

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\nabla^2 f(\mathbf{x}_k))^{-1} \nabla f(\mathbf{x}_k).$$

If $\nabla^2 f(\mathbf{x}_k)$ is positive definite, then \mathbf{x}_{k+1} is the minimizer of the following quadratic approximation of f around \mathbf{x}_k :

$$f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^\top (\mathbf{x} - \mathbf{x}_k) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_k)^\top \nabla^2 f(\mathbf{x}_k) (\mathbf{x} - \mathbf{x}_k).$$

- Damped Newton's method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - t_k (\nabla^2 f(\mathbf{x}_k))^{-1} \nabla f(\mathbf{x}_k),$$

where t_k is the stepsize.

- Hybrid gradient-Newton method:

$$\mathbf{d}_k = \begin{cases} -(\nabla^2 f(\mathbf{x}_k))^{-1} \nabla f(\mathbf{x}_k), & \text{if } \nabla^2 f(\mathbf{x}_k) \text{ is pd,} \\ -\nabla f(\mathbf{x}_k), & \text{otherwise.} \end{cases}$$

Theorem 14 (quadratic local convergence of Newton's method)

Suppose $f(\mathbf{x})$ is twice Lipschitz continuously differentiable with Lipschitz constant $M > 0$, i.e.,

$$\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\| \leq M\|\mathbf{x} - \mathbf{y}\|.$$

Suppose that (the second-order sufficient conditions)

$$\nabla f(\mathbf{x}_\star) = \mathbf{0}, \quad \text{and} \quad \nabla^2 f(\mathbf{x}_\star) \succeq \gamma \mathbf{I} \quad \text{for some } \gamma > 0,$$

which ensure that \mathbf{x}_\star is a local minimizer of $f(\mathbf{x})$. If

$$\|\mathbf{x}_0 - \mathbf{x}_\star\| \leq \frac{\gamma}{2M},$$

then the sequence $\{\mathbf{x}_k\}_0^\infty$ in Newton's method converges to \mathbf{x}_\star at a quadratic rate, with

$$\|\mathbf{x}_{k+1} - \mathbf{x}_\star\| \leq \frac{M}{\gamma} \|\mathbf{x}_k - \mathbf{x}_\star\|^2, \quad k = 0, 1, 2, \dots$$

5. Further reading

- Jorge Nocedal and Stephen J. Wright
Numerical Optimization
Second Edition, Springer, 2006
- Amir Beck
Introduction to Nonlinear Optimization: Theory, Algorithms, and Applications with Python and MATLAB
Second Edition, SIAM, 2023
- Amir Beck
First-Order Methods in Optimization
SIAM, 2017