Application: Unconstrained optimization

Stationary points

Consider $f: \mathbb{R}^N \mapsto \mathbb{R}$. The unconstrained optimization problem

$$\max_{\boldsymbol{x} \in \mathbb{R}^N} f(\boldsymbol{x}) \qquad \left(\text{or } \min_{\boldsymbol{x} \in \mathbb{R}^N} f(x) \right) \tag{1}$$

is about finding the maximum or minimum of $f(\boldsymbol{x})$ over the whole space $\mathbb{R}^N$. In the following we will present the theory for minima/miniimizers. The theory for maxima/maximizers can be obtained through obvious changes.

The general strategy is the following:

1. Find all local minima/minimizers;
2. Pick the miniima/minimizer from these local minima/minimizers.

Recall that $\boldsymbol{x}_0$ is a local minimizer if and only if $\exists r > 0$, $\forall \boldsymbol{x} \in B(\boldsymbol{x}_0, r)$, $f(\boldsymbol{x}_0) \leqslant f(\boldsymbol{x})$.

Previously we have derived the following necessary condition:

Theorem 1. *Let $\boldsymbol{x}_0$ be a local minimizer for f: $\mathbb{R}^N \mapsto \mathbb{R}$ and assume f is differentiable at $\boldsymbol{x}_0$. Then $(D f)(\boldsymbol{x}_0) = 0$. In particular* $(\text{grad } f)(\boldsymbol{x}_0) = \mathbf{0}$.

It is clear that the condition $(D f)(\boldsymbol{x}_0) = 0$ (or $(\text{grad } f)(\boldsymbol{x}_0) = \mathbf{0}$ is not sufficient, for example it does not distinguishi between local maximizers and local minimizers. Furthermore there are $\boldsymbol{x}_0$ could be neither.

Example 2. Consider $f(x, y) = x\, y$. Then we have $(\text{grad } f)(x, y) = \begin{pmatrix} y \\ x \end{pmatrix}$. Thus $(\text{grad } f)(0, 0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$. Since the partial derivatives are continuous, this also means $(D f)(0, 0) = 0$.

Now we show that $(0, 0)$ is neither local maximizer nor local minimizer. For any $r > 0$, set $x = y = r/2$, then we have $(x, y) \in B((0, 0), r)$ and

$$f(x, y) = \frac{r^2}{4} > 0 = f(0, 0) \tag{2}$$

so $(0, 0)$ is not a local maximizer.

Similarly setting $-x = y = r/2$ we have $(x, y) \in B((0, 0), r)$ and

$$f(x, y) = -\frac{r^2}{4} < 0 = f(0, 0) \tag{3}$$

so $(0, 0)$ is not a local minimizer.

Definition 3. *Let $f: \mathbb{R}^N \mapsto \mathbb{R}$ be differentiable. Then a point $\boldsymbol{x}_0 \in \mathbb{R}^N$ is called a* stationary point *of f if and only if* $(\text{grad } f)(\boldsymbol{x}_0) = \mathbf{0}$.

Exercise 1. Find all stationary points for $f(\boldsymbol{x}) := x_1 \cdots x_N$ and discuss whether each of them is a local maximizer, local minimizer, or neither.

Thus solving $(\text{grad } f) = 0$ only gives us all stationary points. Previously we compare the values of f at each stationary point to find global minimizer – note that we cannot find local minimizers this way. In the following we will develop sufficient conditions for $\boldsymbol{x}_0$ to be a local minimizer using the theory of Taylor expansion.

Remark 4. The above theory still applies in the case $f\colon U \mapsto \mathbb{R}$ where $U \subseteq \mathbb{R}^N$ is open.

Quadratic functions

Consider a twice differentiable function $f\colon \mathbb{R}^N \mapsto \mathbb{R}$ and a stationary point $\boldsymbol{x}_0$. The idea is to approximate $f\colon \mathbb{R}^N \mapsto \mathbb{R}$ at $\boldsymbol{x}_0$ be a quadratic polynomial

$$F(\boldsymbol{x}) := \sum_{i=1, j=1}^{N} a_{ij} x_i\, x_j + \sum_{i=1}^{N} b_i\, x_i + c. \tag{4}$$

Thus we have to first fully understand local minimizers of quadratic functions.

First we simplify the formula for F.

- Notice that $x_i\, x_j = x_j\, x_i$. Thus only $a_{ij} + a_{ji}$ is determined. So we take $a_{ij} = a_{ji}$. From now on we always assume this.

  Exercise 2. Let $F(x, y) = 3\,x^2 + 2\,x\,y + y^2$. Find $a_{11}, a_{12}, a_{21}, a_{22}$.

- Denote

$$A = (\ a_{ij}\ ) \in \mathbb{R}^{N \times N}, \qquad \boldsymbol{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix} \in \mathbb{R}^N. \tag{5}$$

  Then

$$F(\boldsymbol{x}) = \boldsymbol{x}^T A\, \boldsymbol{x} + \boldsymbol{b}^T \boldsymbol{x} + c. \tag{6}$$

  Note that $A = A^T$ is symmetric.

Now we calculate

$$\operatorname{grad} F = 2\, A\, \boldsymbol{x} + \boldsymbol{b} \tag{7}$$

therefore if $\boldsymbol{x}_0$ is a stationary point, then $2\, A\, \boldsymbol{x}_0 + \boldsymbol{b} = \boldsymbol{0}$.

Next let $\boldsymbol{y} := \boldsymbol{x} - \boldsymbol{x}_0$. We have

$$\begin{aligned} F(\boldsymbol{y}) &= (\boldsymbol{y} + \boldsymbol{x}_0)^T A\, (\boldsymbol{y} + \boldsymbol{x}_0) + \boldsymbol{b}^T (\boldsymbol{y} + \boldsymbol{x}_0) + c \\ &= \boldsymbol{y}^T A\, \boldsymbol{y} + \boldsymbol{y}^T A\, \boldsymbol{x}_0 + \boldsymbol{x}_0^T A\, \boldsymbol{y} + \boldsymbol{x}_0^T A\, \boldsymbol{x}_0 + \boldsymbol{b}^T \boldsymbol{y} + \boldsymbol{b}^T \boldsymbol{x}_0 + c \\ &= \boldsymbol{y}^T A\, \boldsymbol{y} + 2\, \boldsymbol{y}^T A\, \boldsymbol{x}_0 + \boldsymbol{y}^T \boldsymbol{b} + \boldsymbol{x}_0^T A\, \boldsymbol{x}_0 + c \\ &= \boldsymbol{y}^T A\, \boldsymbol{y} + \boldsymbol{y}^T (2\, A\, \boldsymbol{x}_0 + \boldsymbol{b}) + \boldsymbol{x}_0^T A\, \boldsymbol{x}_0 + c \\ &= \boldsymbol{y}^T A\, \boldsymbol{y} + (\boldsymbol{x}_0^T A\, \boldsymbol{x}_0 + c). \end{aligned} \tag{8}$$

Note that $\boldsymbol{x}_0^T A\, \boldsymbol{x}_0 + c$ is a constant. Thus $\boldsymbol{x}_0$ being a local minimizer for $F(\boldsymbol{x})$ is equivalent to $\boldsymbol{0}$ being a local minimizer for $G(\boldsymbol{y}) := \boldsymbol{y}^T A\, \boldsymbol{y}$.

Lemma 5. *Let $G(\boldsymbol{y}) := \boldsymbol{y}^T A\, \boldsymbol{y}$. Then $\boldsymbol{0}$ is a local minimizer for G if and only if $G(\boldsymbol{y}) \geqslant 0$ for all $\boldsymbol{y} \in \mathbb{R}^N$.*

Proof. "If" is obvious. For "only if", assume $\boldsymbol{0}$ is a local minimizer, that is $\exists r > 0$, $\forall \|\boldsymbol{y}\| < r$, $G(\boldsymbol{y}) \geqslant 0$. Now take any $\boldsymbol{y} \in \mathbb{R}^N$. If $\boldsymbol{y} = \boldsymbol{0}$ then obviously $G(\boldsymbol{y}) \geqslant 0$. Otherwise set

$$\boldsymbol{v} := \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|} \frac{r}{2}. \tag{9}$$

Then $\boldsymbol{y} = \frac{2\,\|\boldsymbol{y}\|}{r}\,\boldsymbol{v}$ and

$$G(\boldsymbol{y}) = \boldsymbol{y}^T A\,\boldsymbol{y} = \frac{4\,\|\boldsymbol{y}\|^2}{r^2}\,\boldsymbol{v}^T A\,\boldsymbol{v} \geqslant 0. \tag{10}$$

Thus ends the proof. □

From the above lemma we have

Lemma 6. *Let $F(\boldsymbol{x}) = \boldsymbol{x}^T A\,\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x} + c$ be quadratic and $\boldsymbol{x}_0$ be its critical point. Then $\boldsymbol{x}_0$ is a local minimizer of F if and only if for all $\boldsymbol{v} \in \mathbb{R}^N$, $\boldsymbol{v}^T A\,\boldsymbol{v} \geqslant 0$.*

Exercise 3. Let $F(\boldsymbol{x}) = \boldsymbol{x}^T A\,\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x} + c$ be quadratic and $\boldsymbol{x}_0$ be its critical point. Then $\boldsymbol{x}_0$ is a local maximizer if and only if for all $\boldsymbol{v} \in \mathbb{R}^N$, $\boldsymbol{v}^T A\,\boldsymbol{v} \leqslant 0$. If there are $\boldsymbol{v}_1, \boldsymbol{v}_2$ such that $\boldsymbol{v}_1^T A\,\boldsymbol{v}_1 > 0$ but $\boldsymbol{v}_2^T A\,\boldsymbol{v}_2 < 0$, then $\boldsymbol{x}_0$ is neither local maximizer nor local minimizer.

We notice that the condition is in fact independent of $\boldsymbol{x}_0$ – it is purely a condition on A.

Definition 7. *Let $A \in \mathbb{R}^{N\times N}$ by symmetric: $A = A^T$. Then A is called* positive semi-definite *if and only if all $\boldsymbol{v} \in \mathbb{R}^N$, $\boldsymbol{v}^T A\,\boldsymbol{v} \geqslant 0$; It is called* positive definite *if and only if all nonzero $\boldsymbol{v} \in \mathbb{R}^N$, $\boldsymbol{v}^T A\,\boldsymbol{v} > 0$. A is called* negative semi-definite *if and only if all $\boldsymbol{v} \in \mathbb{R}^N$, $\boldsymbol{v}^T A\,\boldsymbol{v} \leqslant 0$; It is called* negative definite *if and only if all nonzero $\boldsymbol{v} \in \mathbb{R}^N$, $\boldsymbol{v}^T A\,\boldsymbol{v} < 0$.*

Exercise 4. Let $F(\boldsymbol{x}) = \boldsymbol{x}^T A\,\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x} + c$ be quadratic and $\boldsymbol{x}_0$ be its critical point. Then $\boldsymbol{x}_0$ is a strict local minimizer of F, in the sense that there is $r > 0$, for all $\boldsymbol{x} \in B(\boldsymbol{x}_0, r)$, $\boldsymbol{x} \neq \boldsymbol{x}_0$, if and only if A is positive definite.

Sufficient conditions for local optima

We try to apply the above understanding to general nonlinear functions. First notice: If $F(\boldsymbol{x}) = \boldsymbol{x}^T A\,\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x} + c$, then

$$a_{ij} = \frac{\partial^2 F}{\partial x_i \partial x_j}. \tag{11}$$

Definition 8. (Hessian matrix) *Let $f: \mathbb{R}^N \mapsto \mathbb{R}$ have continuous second order derivatives at $\boldsymbol{x}_0$. Then the symmetric matrix $\left(\frac{\partial^2 f}{\partial x_i \partial x_j}(\boldsymbol{x}_0)\right)$ is called the* Hessian matrix *of f at $\boldsymbol{x}_0$.*

Theorem 9. (Second order sufficient conditions) *Let $f: \mathbb{R}^N \mapsto \mathbb{R}$ have continuous second derivatives at $\boldsymbol{x}_0$. Further assume that $\boldsymbol{x}_0$ is a stationary point. Then $\boldsymbol{x}_0$ is a local minimizer if the Hessian matrix at $\boldsymbol{x}_0$ is positive definite.*

Proof. By continuity of the second derivatives of f, the Hessian matrix $H(\boldsymbol{x})$ is continuous in $\boldsymbol{x}$. Thus there is $r > 0$ such that for all $\boldsymbol{x} \in B(\boldsymbol{x}_0, r)$ and all nonzero $\boldsymbol{v} \in \mathbb{R}^N$, $\boldsymbol{v}^T H(\boldsymbol{x})\,\boldsymbol{v} > 0$.

Now for any $\boldsymbol{x} \in B(\boldsymbol{x}_0, r)$, $\boldsymbol{x} \neq \boldsymbol{x}_0$, the Taylor expansion theorem gives (note that $(\text{grad } f)(\boldsymbol{x}_0) = \boldsymbol{0}$ by the assumption that $\boldsymbol{x}_0$ is a critical point)

$$\begin{aligned} f(\boldsymbol{x}) &= f(\boldsymbol{x}_0) + (\text{grad } f)(\boldsymbol{x}_0) \cdot (\boldsymbol{x} - \boldsymbol{x}_0) + \frac{1}{2}\,(\boldsymbol{x} - \boldsymbol{x}_0)^T H(\boldsymbol{\xi})\,(\boldsymbol{x} - \boldsymbol{x}_0) \\ &= f(\boldsymbol{x}_0) + \frac{1}{2}\,(\boldsymbol{x} - \boldsymbol{x}_0)^T H(\boldsymbol{\xi})\,(\boldsymbol{x} - \boldsymbol{x}_0) > f(\boldsymbol{x}_0). \end{aligned} \tag{12}$$

Here the last step follows from $\boldsymbol{\xi} \in B(\boldsymbol{x}_0, \delta)$ which is a consequence of $\boldsymbol{x} \in B(\boldsymbol{x}_0, \delta)$ and the Taylor expansion theorem. Therefore $\boldsymbol{x}_0$ is a local minimizer of f. □

Remark 10. Note that the above proof actually shows that $\boldsymbol{x}_0$ has to be strict local minimizer.

Corollary 11. (Second order necessary conditions) *Let $f: \mathbb{R}^N \mapsto \mathbb{R}$ have continuous second derivatives at $\boldsymbol{x}_0$. Further assume that $\boldsymbol{x}_0$ is a local minimizer, then the Hessian matrix H at $\boldsymbol{x}_0$ is positive semi-definite.*

Proof. Assume not. Then there is $\boldsymbol{v} \in \mathbb{R}^N$ such that $\boldsymbol{v}^T H(\boldsymbol{x}_0)\, \boldsymbol{v} < 0$. By continuity of $H(\boldsymbol{x})$, there is $\delta > 0$ such that for all $\boldsymbol{x} \in B(\boldsymbol{x}_0, \delta)$, $\boldsymbol{v}^T H(\boldsymbol{x})\, \boldsymbol{v} < 0$.

Now consider $\boldsymbol{x} := \boldsymbol{x}_0 + t\, \boldsymbol{v}$ with $t < \frac{\delta}{\|\boldsymbol{v}\|}$. Then by Taylor expansion theorem we have

$$\begin{aligned} f(\boldsymbol{x}) &= f(\boldsymbol{x}_0) + (\operatorname{grad} f)(\boldsymbol{x}_0) \cdot (\boldsymbol{x} - \boldsymbol{x}_0) + \frac{1}{2} (\boldsymbol{x} - \boldsymbol{x}_0)^T H(\boldsymbol{\xi})\, (\boldsymbol{x} - \boldsymbol{x}_0) \\ &= f(\boldsymbol{x}_0) + \frac{t^2}{2} \boldsymbol{v}^T H(\boldsymbol{\xi})\, \boldsymbol{v} < f(\boldsymbol{x}_0). \end{aligned} \tag{13}$$

Here the last step follows from $\boldsymbol{\xi} \in B(\boldsymbol{x}_0, \delta)$ which is a consequence of $\boldsymbol{x} \in B(\boldsymbol{x}_0, \delta)$ and the Taylor expansion theorem.

Thus we reach contradiction. □

Note that positive semi-definiteness of the Hessian matrix is not sufficient for $\boldsymbol{x}_0$ to be a local minimizer.

Example 12. Consider $f(x, y) = (y - x^2)\,(y - 3\,x^2)$. We have

$$(\operatorname{grad} f)(0, 0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{14}$$

so $(0, 0)$ is a critical point of f. Furthermore we have the Hessian matrix at $(0, 0)$ to be $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ which is clearly positive semi-definite. But clearly $(0, 0)$ is neither local minimizer nor local maximizer.

Exercise 5. Prove that $(0, 0)$ is neither local minimizer nor local maximizer.

Exercise 6. Prove by definition that $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ is positive semi-definite.

Exercise 7. Give three other examples illustrating the insufficiency of positive semi-definiteness of the Hessian matrix.

Exercise 8. Find the extreme points of

$$f(x, y) = x^3 + y^3 + 2\,x^2 + 4\,y^2 + 5. \tag{15}$$

Question 13. *Let $A \in \mathbb{R}^{N \times N}$ be symmetric. Denote by $A_1, \ldots, A_N$ the sub-matrices:*

$$A_1 = (\ a_{11}\ ), A_2 = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \ldots, A_{N-1} = \begin{pmatrix} a_{11} & \cdots & a_{1(N-1)} \\ \vdots & & \vdots \\ a_{(N-1)1} & \cdots & a_{(N-1)(N-1)} \end{pmatrix}, A_N = A \tag{16}$$

Prove that

a) A is positive semi-definite if and only if $\det A_k \geqslant 0$ for all $k = 1, 2, \ldots, N$;

b) A is positive definite if and only if $\det A_k > 0$ for all $k = 1, 2, \ldots, N$;

c) A is negative definite if and only if $\det A_k > 0$ for all even k's and <0 for all odd k's.