Course notes for MATH 524: Non-Linear Optimization

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CHAPTER 1

Review of Optimization from Vector Calculus

The starting point of these notes is the concept of *optimization* as developed in MATH 241 (see e.g. [**1**, Chapter 14])

DEFINITION. Let $D \subseteq \mathbb{R}^2$ be a region on the plane containing the point (x_0, y_0). We say that the real-valued function $f\colon D \to \mathbb{R}$ has a *local minimum* at (x_0, y_0) if $f(x_0, y_0) \leq f(x, y)$ for all domain points (x, y) in an open disk centered at (x_0, y_0). In that case, we also say that $f(x_0, y_0)$ is a *local minimum value* of f in D.

Emphasis was made to find conditions on the function f to guarantee existence and characterization of minima:

THEOREM 1.1. *Let $D \subseteq \mathbb{R}^2$ and let $f\colon D \to \mathbb{R}$ be a function for which first partial derivatives $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$ exist in D. If $(x_0, y_0) \in D$ is a local minimum of f, then $\nabla f(x_0, y_0) = 0$.*

The local minima of these functions are among the zeros of the equation $\nabla f(x, y) = 0$, the so-called *critical points* of f. More formally:

DEFINITION. An interior point of the domain of a function $f(x, y)$ where both directional derivatives are zero, or where at least one of the directional derivatives do not exist, is a *critical point* of f.

We employed the *Second Derivative Test for Local Extreme Values* to characterize some minima:

THEOREM 1.2. *Suppose that $f\colon \mathbb{R}^2 \to \mathbb{R}$ and its first and second partial derivatives are continuous throughout a disk centered at the point (x_0, y_0), and that $\nabla f(x_0, y_0) = 0$. If the two following conditions are satisfied, then $f(x_0, y_0)$ is a local minimum value:*

$$\frac{\partial^2 f(x_0, y_0)}{\partial x^2} > 0 \tag{1}$$

$$\det \underbrace{\begin{bmatrix} \dfrac{\partial^2 f(x_0, y_0)}{\partial x^2} & \dfrac{\partial^2 f(x_0, y_0)}{\partial x \partial y} \\[2ex] \dfrac{\partial^2 f(x_0, y_0)}{\partial y \partial x} & \dfrac{\partial^2 f(x_0, y_0)}{\partial y^2} \end{bmatrix}}_{\operatorname{Hess} f(x_0, y_0)} > 0 \tag{2}$$

REMARK 1.1. The restriction of this result to univariate functions is even simpler: Suppose f'' is continuous on an open interval that contains x_0. If $f'(x_0) = 0$ and $f''(x_0) > 0$, then f has a local minimum at x_0.

EXAMPLE 1.1 (Rosenbrock Functions). Given strictly positive parameters $a, b > 0$, consider the Rosenbrock function

$$\mathcal{R}_{a,b}(x, y) = (a - x)^2 + b(y - x^2)^2.$$

It is easy to see that Rosenbrock functions are polynomials (prove it!). The domain is therefore the whole plane. Figure 1.1 illustrates a contour plot with several level lines of $\mathcal{R}_{1,1}$ on the domain $D = [-2, 2] \times [-1, 3]$, as well as its graph.

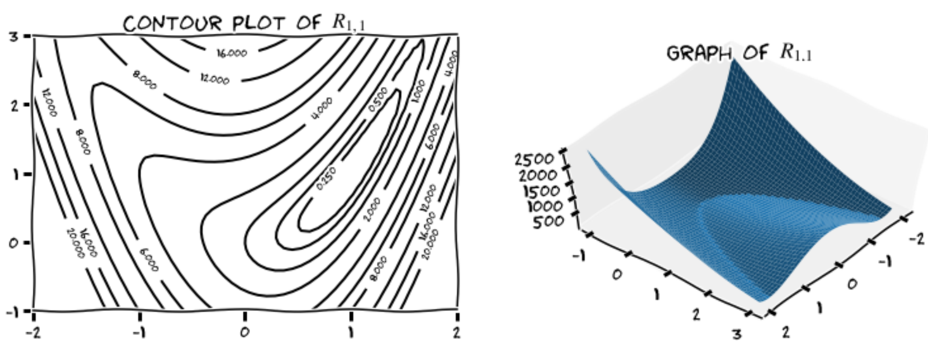

FIGURE 1.1. Details of the graph of $\mathcal{R}_{1,1}$

It is also easy to verify that the image is the interval $[0, \infty)$. Indeed, note first that $\mathcal{R}_{a,b}(x, y) \geq 0$ for all $(x, y) \in \mathbb{R}^2$. Zero is attained: $\mathcal{R}_{a,b}(a, a^2) = 0$. Note also that $\mathcal{R}_{a,b}(0, y) = a^2 + by^2$ is a polynomial of degree 2, therefore unbounded.

Let's locate all local minima:

- The gradient and Hessian are given respectively by

$$\nabla\mathcal{R}_{a,b}(x, y) = \big[2(x - a) + 4bx(x^2 - y), b(y - x^2)\big]$$

$$\text{Hess}\mathcal{R}_{a,b}(x, y) = \begin{bmatrix} 12bx^2 - 4by + 2 & -4bx \\ -4bx & 2b \end{bmatrix}$$

- The search for critical points $\nabla\mathcal{R}_{a,b} = \mathbf{0}$ gives only the point (a, a^2).
- $\frac{\partial^2 \mathcal{R}_{a,b}}{\partial x^2}(a, a^2) = 8ba^2 + 2 > 0$.
- The Hessian at that point has positive determinant:

$$\det \text{Hess}\mathcal{R}_{a,b}(a, a^2) = \det \begin{bmatrix} 8ba^2 + 2 & -4ab \\ -4ab & 2b \end{bmatrix} = 4b > 0$$

There is only one local minimum at (a, a^2), which happens also to be a global minimum.

The second step was the notion of *global (or absolute) minima*: points (x_0, y_0) that satisfy $f(x_0, y_0) \leq f(x, y)$ for any point (x, y) in the domain of f. We always started with the easier setting, in which we placed restrictions on the domain of our functions:

THEOREM 1.3. *A continuous real-valued function always attains its minimum value on a* compact *set K. If the function is also differentiable in the* interior *of K, to search for global minima we perform the following steps:*

Interior Candidates: *List the critical points of f located in the interior of K.*

Boundary Candidates: *List the points in the boundary of K where f may have minimum values.*

Evaluation/Selection: *Evaluate f at all candidates and select the one(s) with the smallest value.*

EXAMPLE 1.2. A flat circular plate has the shape of the region $x^2+y^2 \leq 1$. The plate, including the boundary, is heated so that the temperature at the point (x, y) is given by $f(x, y) = 100(x^2 + 2y^2 - x)$ in Celsius degrees. Find the temperature at the coldest point of the plate.

We start by searching for critical points. The equation $\nabla f(x, y) = 0$ gives $x = \frac{1}{2}$, $y = 0$. The point $(\frac{1}{2}, 0)$ is clearly inside of the plate. This is our first candidate.

The border of the plate can be parameterized by $\varphi(t) = (\cos t, \sin t)$ for $t \in [0, 2\pi)$. The search for minima in the boundary of the plate can then be coded as an optimization problem for the function $h(t) = (f \circ \varphi)(t) = 100(\cos^2 t + 2\sin^2 t - \cos t)$ on the interval $[0, 2\pi)$. Note that $h'(t) = 0$ for $t \in \{0, \frac{2}{3}\pi\}$ in $[0, 2\pi)$. We thus have two more candidates:

$$\varphi(0) = (1, 0) \qquad \varphi(\tfrac{2}{3}\pi) = \big(-\tfrac{1}{2}, \tfrac{1}{2}\sqrt{3}\big)$$

Evaluation of the function at all candidates gives us the solution to this problem:

$$f(\tfrac{1}{2}, 0) = -25^\circ\text{C}.$$

On a second setting, we remove the restriction of boundedness of the function. In this case, global minima will only be guaranteed for very special functions.

EXAMPLE 1.3. Any polynomial $p_n(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_0$ with even degree $n \geq 2$ and positive leading coefficient satisfies $\lim_{|x|\to\infty} p_n(x) = +\infty$. To see this, we may write

$$a_n x^n + a_{n-1}x^{n-1} + \cdots + a_0 = a_n x^n \big(1 + \tfrac{a_{n-1}}{a_n x} + \cdots + \tfrac{a_0}{a_n x^n}\big)$$

The behavior of each of the factors as the absolute value of x goes to infinity leads to our claim.

$$\lim_{|x|\to\infty} a_n x^n = +\infty,$$

$$\lim_{|x|\to\infty} \left(1 + \tfrac{a_{n-1}}{a_n x} + \cdots + \tfrac{a_0}{a_n x^n}\right) = 1.$$

It is clear that a polynomial of this kind must attain a minimum somewhere in its domain. The critical points will lead to them.

EXAMPLE 1.4. Find the global minima of the function $f(x) = \log(x^4 - 2x^2 + 2)$ in $\mathbb{R}$.

Note first that the domain of f is the whole real line, since $x^4-2x^2+2 = (x^2-1)^2+1 \geq 1$ for all $x \in \mathbb{R}$. Note also that we can write $f(x) = (g \circ h)(x)$ with $g(x) = \log(x)$ and $h(x) = x^4 - 2x^2 + 1$. Since g is one-to-one and increasing, we can focus on h to obtain the requested solution. For instance, $\lim_{|x|\to\infty} f(x) = +\infty$, since $\lim_{|x|\to\infty} h(x) = +\infty$. This guarantees the existence of global minima. To look for it, h again points to the possible locations by solving for its critical points: $h'(x) = 0$. We have then that f attains its minima at $x = \pm 1$.

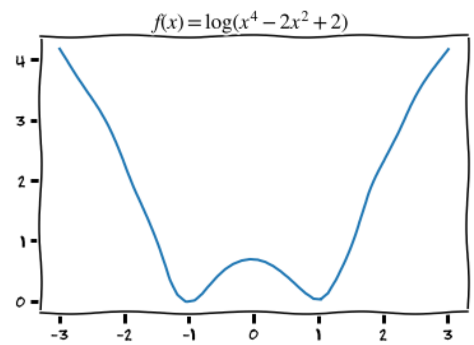

FIGURE 1.2. Global minima in unbounded domains

We learned other useful characterizations for extrema, when the domain could be expressed as solutions of equations:

THEOREM 1.4 (Orthogonal Gradient). *Suppose $f(x, y)$ is differentiable in a region whose interior contains a smooth curve $C\colon \boldsymbol{r}(t) = \big(x(t), y(t)\big)$. If P_0 is a point on C where f has a local extremum relative to its values on C, then ∇f is orthogonal to C at P_0.*

This result leads to the *Method of Lagrange Multipliers*

THEOREM 1.5 (Lagrange Multipliers on one constraint). *Suppose that $f(x, y)$ and $g(x, y)$ are differentiable and $\nabla g \neq 0$ when $g(x, y, z) = 0$. To find the local extrema of f subject to the constraint $g(x, y) = 0$ (if these exist), find the values of x, y and λ that simultaneously satisfy the equations*

$$\nabla f = \lambda \nabla g, \text{ and } g(x, y) = 0$$

EXAMPLE 1.5. Find the minimum value of the expression $3x + 4y$ for values of x and y on the circle $x^2 + y^2 = 1$.

We start by modeling this problem to adapt the technique of Lagrange multipliers:

$$f(x,y) = \underbrace{3x+4y}_{\text{target}} \qquad\qquad g(x,y) = \underbrace{x^2+y^2-1}_{\text{constraint}}$$

Look for the values of x, y and λ that satisfy the equations $\nabla f = \lambda \nabla g$, $g(x,y) = 0$

$$3 = 2\lambda x, \qquad\qquad 4 = 2\lambda y \qquad\qquad 1 = x^2 + y^2$$

Equivalently, $\lambda \neq 0$ and x, y satisfy

$$x = \frac{3}{2\lambda}, \qquad\qquad y = \frac{2}{\lambda}, \qquad\qquad 1 = \frac{9}{4\lambda^2} + \frac{4}{\lambda^2}$$

These equations lead to $\lambda = \pm\frac{5}{2}$, and there are only two possible candidates for minimum. Evaluation of f on those gives that the minimum is at the point $\big(-\frac{3}{5}, -\frac{4}{5}\big)$.

This method can be extended to more than two dimensions, and more than one constraint. For instance:

Theorem 1.6 (Lagrange Multipliers on two constraints). *Suppose that $f(x,y,z)$, $g_1(x,y,z)$, $g_2(x,y,z)$ are differentiable with ∇g_1 not parallel to ∇g_2. To find the local extrema of f subject to the constraint $g_1(x,y,z) = g_2(x,y,z) = 0$ (if these exist), find the values of x, y, λ and μ that simultaneously satisfy the equations*

$$\nabla f = \lambda \nabla g_1 + \mu \nabla g_2, \qquad g_1(x,y,z) = 0, \qquad g_2(x,y,z) = 0$$

Example 1.6. The cylinder $x^2+y^2 = 1$ intersects the plane $x+y+z = 1$ in an ellipse. Find the points on the ellipse that lie closest to the origin.

We again model this as a Lagrange multipliers problem:

$$\begin{aligned} f(x,y,z) &= \overbrace{x^2+y^2+z^2}^{\text{target}}, \\ g_1(x,y,z) &= \underbrace{x^2+y^2-1}_{\text{constraint}}, \qquad\qquad g_2(x,y,z) = \underbrace{x+y+z-1}_{\text{constraint}}. \end{aligned}$$

The gradient equation $\nabla f = \lambda \nabla g_1 + \mu \nabla g_2$ gives

$$2x = 2\lambda x + \mu, \qquad\qquad 2y = 2\lambda y + \mu, \qquad\qquad 2z = \mu$$

These equations are satisfied simultaneously only in two scenarios:

(a) $\lambda = 1$ and $z = 0$
(b) $\lambda \neq 1$ and $x = y = z/(1-\lambda)$

Resolving each case we find four candidates:

$$(1,0,0), \quad (0,1,0), \quad (\sqrt{2}/2, \sqrt{2}/2, 1-\sqrt{2}), \quad (-\sqrt{2}/2, -\sqrt{2}/2, 1+\sqrt{2}).$$

The first two are our solution.

The Theory of Optimization

The purpose of these notes is the development of a theory to deal with optimization in a more general setting.

- We start in an Euclidean d–dimensional space with the usual topology based on the distance

$$\mathrm{d}(\boldsymbol{x},\boldsymbol{y}) = \|\boldsymbol{x}-\boldsymbol{y}\| = \langle \boldsymbol{x}-\boldsymbol{y}, \boldsymbol{x}-\boldsymbol{y}\rangle^{1/2} = \sqrt{\sum_{k=1}^{d}(x_k-y_k)^2}.$$

  For instance, the *open ball* of radius $r>0$ centered at a point $\boldsymbol{x}^\star$ is the set $B_r(\boldsymbol{x}^\star) = \{\boldsymbol{x}\in\mathbb{R}^d : \|\boldsymbol{x}-\boldsymbol{x}^\star\| < r\}$.
- Given a real-valued function $f\colon D\to\mathbb{R}$ on a domain $D\subseteq\mathbb{R}^d$, we define the concept of *extrema*:

  Definition. Given a real-valued function $f\colon D\to\mathbb{R}$ on a domain $D\subseteq\mathbb{R}^d$, we say that a point $\boldsymbol{x}^\star\in D$ is a:
  global minimum: $f(\boldsymbol{x}^\star)\le f(\boldsymbol{x})$ for all $\boldsymbol{x}\in D$.
  global maximum: $f(\boldsymbol{x}^\star)\ge f(\boldsymbol{x})$ for all $\boldsymbol{x}\in D$.
  strict global minimum: $f(\boldsymbol{x}^\star) < f(\boldsymbol{x})$ for all $\boldsymbol{x}\in D\setminus\{\boldsymbol{x}^\star\}$.
  strict global maximum: $f(\boldsymbol{x}^\star) > f(\boldsymbol{x})$ for all $\boldsymbol{x}\in D\setminus\{\boldsymbol{x}^\star\}$.
  local minimum: There exists $\delta>0$ so that $f(\boldsymbol{x}^\star)\le f(\boldsymbol{x})$ for all $\boldsymbol{x}\in B_\delta(\boldsymbol{x}^\star)\cap D$.
  local maximum: There exists $\delta>0$ so that $f(\boldsymbol{x}^\star)\ge f(\boldsymbol{x})$ for all $\boldsymbol{x}\in B_\delta(\boldsymbol{x}^\star)\cap D$.
  strict local minimum: There exists $\delta>0$ so that $f(\boldsymbol{x}^\star) < f(\boldsymbol{x})$ for all $\boldsymbol{x}\in B_\delta(\boldsymbol{x}^\star)\cap D$, $\boldsymbol{x}\ne\boldsymbol{x}^\star$.
  strict local maximum: There exists $\delta>0$ so that $f(\boldsymbol{x}^\star) > f(\boldsymbol{x})$ for all $\boldsymbol{x}\in B_\delta(\boldsymbol{x}^\star)\cap D$, $\boldsymbol{x}\ne\boldsymbol{x}^\star$.

In this setting, the objective of *optimization* is the search for extrema in the following two scenarios:

Unconstrained Optimization: if D is an open set (usually the whole space $\mathbb{R}^d$)

Constrained Optimization: if D can be described as a set of *constraints*: $\boldsymbol{x}\in D$ if there exist $m,n\in\mathbb{N}$ and functions $g_k\colon\mathbb{R}^d\to\mathbb{R}$ $(1\le k\le m)$, $h_j\colon\mathbb{R}^d\to\mathbb{R}$ $(1\le j\le n)$ so that

$$\begin{aligned} g_k(\boldsymbol{x}) &\le 0 & (1\le k\le m)\\ h_j(\boldsymbol{x}) &= 0 & (1\le j\le n)\end{aligned}$$

For each of these problems, we follow a similar program:

Existence of extrema: Establish results that guarantee the existence of extrema depending on the properties of D and f.

Characterization of extrema: Establish results that describe conditions for points $\boldsymbol{x}\in D$ to be extrema of f.

Tracking extrema: Design robust numerical algorithms that find the extrema for scientific computing purposes.

The development of existence and characterization results for unconstrained optimization will be covered in chapter 2. The design of algorithms to track extrema will be covered in chapter 3.

Exercises

PROBLEM 1.1 (Advanced). State and prove similar statements as in Definition 1, Theorems 1.1, 1.2 and 1.3, but for *local* and *global maxima*.

PROBLEM 1.2 (Basic). Find and sketch the domain of the following functions.

(a) $f(x,y) = \sqrt{y-x-2}$
(b) $f(x,y) = \log\left(x^2+y^2-4\right)$
(c) $f(x,y) = \frac{(x-1)(y+2)}{(y-x)(y-x^3)}$
(d) $f(x,y) = \log(xy+x-y-1)$

PROBLEM 1.3 (Basic). Find and sketch the level lines $f(x,y) = c$ on the same set of coordinate axes for the given values of c.

(a) $f(x,y) = x+y-1$, $c \in \{-3,-2,-1,0,1,2,3\}$.
(b) $f(x,y) = x^2+y^2$, $c \in \{0,1,4,9,16,25\}$.
(c) $f(x,y) = xy$, $c \in \{-9,-4,-1,0,1,4,9\}$

PROBLEM 1.4 (CAS). Use a Computer Algebra System of your choice to produce contour plots of the given functions on the given domains.

(a) $f(x,y) = (\cos x)(\cos y)e^{-\sqrt{x^2+y^2}/4}$ on $[-2\pi, 2\pi] \times [-2\pi, 2\pi]$.
(b) $g(x,y) = \dfrac{xy(x^2-y^2)}{x^2+y^2}$ on $[-1,1] \times [-1,1]$
(c) $h(x,y) = y^2-y^4-x^2$ on $[-1,1] \times [-1,1]$
(d) $k(x,y) = e^{-y}\cos x$ on $[-2\pi, 2\pi] \times [-2,0]$

PROBLEM 1.5 (Intermediate). Find the points of the hyperbolic cylinder $x^2-z^2-1=0$ in $\mathbb{R}^3$ that are closest to the origin.

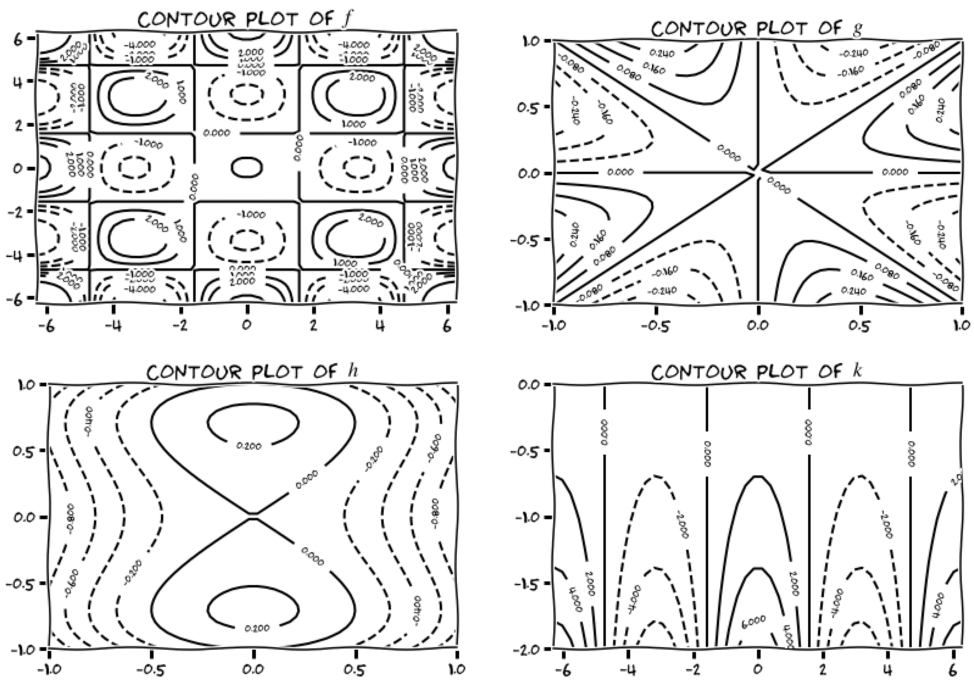

FIGURE 1.3. Contour plots for problem 1.4

CHAPTER 2

Existence and Characterization of Extrema

In this chapter we will study different properties of functions and domains that guarantee existence of extrema. Once we have them, we explore characterization of those points. We start with a reminder of the definition of continuous and differentiable functions, and then we proceed to introduce other functions with advantageous properties for optimization purposes.

1. Relevant Functions

1.1. Continuity and Differentiability.

Definition. We say that a real-valued function $f\colon D \to \mathbb{R}$ is continuous at a point $\boldsymbol{x}^\star \in D$ if for all $\varepsilon > 0$ there exists $\delta > 0$ so that for all $\boldsymbol{x} \in D$ satisfying $\|\boldsymbol{x} - \boldsymbol{x}^\star\| < \delta$, it is $|f(\boldsymbol{x}) - f(\boldsymbol{x}^\star)| < \varepsilon$.

Example 2.1. Let $f\colon \mathbb{R}^2 \to \mathbb{R}$ be given by

$$f(x,y) = \begin{cases} \frac{2xy}{x^2+y^2}, & (x,y) \neq (0,0) \\ 0, & (x,y) = (0,0) \end{cases}$$

This function is trivially continuous at any point $(x,y) \neq (0,0)$. However, it fails to be continuous at the origin. Notice how we obtain different values as we approach $(0,0)$ through different generic lines $y = mx$ with $m \in \mathbb{R}$:

$$\lim_{x\to 0} f(x,mx) = \lim_{x \to 0} \frac{2mx^2}{(1+m^2)x^2} = \frac{2m}{1+m^2}.$$

Definition. A real-valued function f is said to be *differentiable* at $\boldsymbol{x}^\star$ if there exists a *linear function* $J\colon \mathbb{R}^d \to \mathbb{R}$ so that

$$\lim_{\boldsymbol{h}\to\boldsymbol{0}} \frac{|f(\boldsymbol{x}^\star + h) - f(\boldsymbol{x}^\star) - J(\boldsymbol{h})|}{\|\boldsymbol{h}\|} = 0$$

Remark 2.1. A function is said to be *linear* if it satisfies $J(\boldsymbol{x} + \lambda \boldsymbol{y}) = J(\boldsymbol{x}) + \lambda J(\boldsymbol{y})$ for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$, $\lambda \in \mathbb{R}$. For each real-valued linear function $J\colon \mathbb{R}^d \to \mathbb{R}$ there exists $\boldsymbol{a} \in \mathbb{R}^d$ so that $J(\boldsymbol{x}) = \langle \boldsymbol{a}, \boldsymbol{x}\rangle$ for all $\boldsymbol{x} \in \mathbb{R}^d$. For this reason, the graph of a linear function is a hyperplane in $\mathbb{R}^d$.

Remark 2.2. For any differentiable real-valued function f at a point $\boldsymbol{x}$ of its domain, the corresponding linear function in the definition above guarantees a tangent hyperplane to the graph of f at $\boldsymbol{x}$.

EXAMPLE 2.2. Consider a real-valued function $f\colon \mathbb{R} \to \mathbb{R}$ of a real variable. To prove differentiability at a point $x^\star$, we need a linear function: $J(h) = ah$ for some $a \in \mathbb{R}$. Notice how in that case,

$$\frac{|f(x^\star + h) - f(x^\star) - J(h)|}{|h|} = \left| \frac{f(x^\star + h) - f(x^\star)}{h} - a \right|;$$

therefore, we could pick $a = \lim_{h\to 0} h^{-1}\big(f(x^\star + h) - f(x^\star)\big)$—this is the definition of derivative we learned in Calculus: $a = f'(x^\star)$

A *friendly* version of the differentiability of real-valued functions comes with the next result (see, e.g. [**1**, p.818])

THEOREM 2.1. *If the partial derivatives* $\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_d}$ *of a real-valued function* $f\colon \mathbb{R}^d \to \mathbb{R}$ *are continuous on an open region* $G \subseteq \mathbb{R}^d$*, then* f *is differentiable at every point of* $\mathbb{R}$.

EXAMPLE 2.3. Let $f\colon \mathbb{R}^d \to \mathbb{R}$. To prove that f is differentiable at a point $\boldsymbol{x}^\star \in \mathbb{R}^d$ we need a linear function $J(h) = \langle \boldsymbol{a}, h\rangle$ for some $\boldsymbol{a} \in \mathbb{R}^d$. Under the conditions of Theorem 2.1 we may use

$$\boldsymbol{a} = \nabla f(\boldsymbol{x}^\star) = \left(\frac{\partial f(\boldsymbol{x}^\star)}{\partial x_1}, \dots, \frac{\partial f(\boldsymbol{x}^\star)}{\partial x_d} \right).$$

It is a simple task to prove that all differentiable functions are continuous. Is it true that all continuous functions are differentiable?

EXAMPLE 2.4 (Weierstrass Function). For any positive real numbers a, b satisfying $0 < a < 1 < b$ and $ab \geq 1$, consider the Weierstrass function $\mathcal{W}_{a,b}\colon \mathbb{R} \to \mathbb{R}$ given by

$$\mathcal{W}_{a,b}(x) = \sum_{n=0}^\infty a^n \cos(b^n \pi x)$$

This function is continuous everywhere, yet *nowhere* differentiable! For a proof, see e.g. [**2**]

A few more useful results about higher order derivatives follow:

THEOREM 2.2 (Clairaut). *If* $f\colon \mathbb{R}^d \to \mathbb{R}$ *and its partial derivatives of orders 1 and 2,* $\frac{\partial f}{\partial x_k}$, $\frac{\partial^2 f}{\partial x_k \partial x_j}$, $(1 \leq k, j \leq d)$ *are defined throughout an open region containing the point* $\boldsymbol{x}^\star$*, and are all continuous at* $\boldsymbol{x}^\star$*, then*

$$\frac{\partial^2 f(\boldsymbol{x}^\star)}{\partial x_k \partial x_j} = \frac{\partial^2 f(\boldsymbol{x}^\star)}{\partial x_j \partial x_k}, \quad (1 \leq k, j \leq d).$$

DEFINITION (Hessian). Given a twice-differentiable function $f\colon \mathbb{R}^d \to \mathbb{R}$, we define the *Hessian* of f at $\boldsymbol{x}$ to be the following matrix of second partial

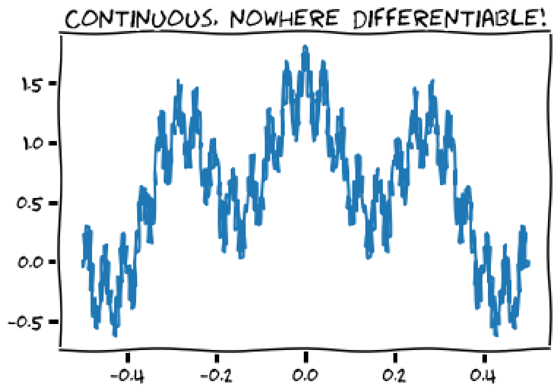

FIGURE 2.1. Detail of the graph of $\mathcal{W}_{0.5,7}$

derivatives:

$$\operatorname{Hess} f(\boldsymbol{x}) = \begin{bmatrix} \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_1^2} & \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_2} & \cdots & \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_d} \\ \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_d \partial x_1} & \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_d \partial x_2} & \cdots & \dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_d^2} \end{bmatrix}$$

Functions that satisfy the conditions of Theorem 2.2 have symmetric Hessians. We shall need some properties in regard to symmetric matrices.

DEFINITION. Given a symmetric matrix $\boldsymbol{A}$, we define its associated *quadratic form* as the function $\mathcal{Q}_{\boldsymbol{A}} \colon \mathbb{R}^d \to \mathbb{R}$ given by

$$\mathcal{Q}_{\boldsymbol{A}}(\boldsymbol{x}) = \boldsymbol{x}\boldsymbol{A}\boldsymbol{x}^\intercal = \begin{bmatrix} x_1 \cdots x_d \end{bmatrix} \begin{bmatrix} a_{11} & \cdots & a_{1d} \\ \vdots & \ddots & \vdots \\ a_{1d} & \cdots & a_{dd} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$

We say that a symmetric matrix is:

positive definite: if $\mathcal{Q}_{\boldsymbol{A}}(\boldsymbol{x}) > 0$ for all $\boldsymbol{x} \in \mathbb{R}^d \setminus \{\boldsymbol{0}\}$.
positive semidefinite: if $\mathcal{Q}_{\boldsymbol{A}}(\boldsymbol{x}) \geq 0$ for all $\boldsymbol{x} \in \mathbb{R}^d$.
negative definite: if $\mathcal{Q}_{\boldsymbol{A}}(\boldsymbol{x}) < 0$ for all $\boldsymbol{x} \in \mathbb{R}^d \setminus \{\boldsymbol{0}\}$.
negative semidefinite: if $\mathcal{Q}_{\boldsymbol{A}}(\boldsymbol{x}) \leq 0$ for all $\boldsymbol{x} \in \mathbb{R}^d$.
indefinite: if there exist $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$ so that $\mathcal{Q}_{\boldsymbol{A}}(\boldsymbol{x})\mathcal{Q}_{\boldsymbol{A}}(\boldsymbol{y}) < 0$.

EXAMPLE 2.5. Let $\boldsymbol{A}$ be the 3×3–symmetric matrix

$$\boldsymbol{A} = \begin{bmatrix} 2 & -1 & 2 \\ -1 & 3 & 0 \\ 2 & 0 & 5 \end{bmatrix}$$

The associated quadratic form is given by

$$\begin{aligned} \mathcal{Q}_{\boldsymbol{A}}(x,y,z) &= \begin{bmatrix} x & y & z \end{bmatrix} \begin{bmatrix} 2 & -1 & 2 \\ -1 & 3 & 0 \\ 2 & 0 & 5 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \\ &= \begin{bmatrix} x & y & z \end{bmatrix} \begin{bmatrix} 2x - y + 2z \\ -x + 3y \\ 2x + 5z \end{bmatrix} \\ &= x(2x - y + 2z) + y(-x + 3y) + z(2x + 5z) \\ &= 2x^2 + 3y^2 + 5z^2 - 2xy + 4xz \end{aligned}$$

To easily classify symmetric matrices, we usually employ any of the following two criteria:

THEOREM 2.3 (Principal Minor Criteria). *Given a general square matrix* $\boldsymbol{A}$*, we define for each* $1 \le \ell \le d$*,* Δ_ℓ *(the* ℓ*th* principal minor *of* $\boldsymbol{A}$*) to be the determinant of the upper left-hand corner* $\ell \times \ell$*–submatrix of* $\boldsymbol{A}$*.*

$$\begin{array}{c} \begin{array}{ccc} \Delta_1 & \Delta_2 & \Delta_3 \end{array} \\ \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \end{array}$$

A symmetric matrix $\boldsymbol{A}$ *is:*

- *Positive definite if and only if* $\Delta_\ell > 0$ *for all* $1 \le \ell \le d$*.*
- *Negative definite if and only if* $(-1)^\ell \Delta_\ell > 0$ *for all* $1 \le \ell \le d$*.*

THEOREM 2.4 (Eigenvalue Criteria). *Given a general square* $d \times d$ *matrix* $\boldsymbol{A}$*, consider the function* $p_{\boldsymbol{A}} \colon \mathbb{C} \to \mathbb{C}$ *given by* $p_{\boldsymbol{A}}(\lambda) = \det\big(\boldsymbol{A} - \lambda \boldsymbol{I}_d\big)$*. This is a polynomial of (at most) degree* d *in* λ*. We call it the* characteristic polynomial *of* $\boldsymbol{A}$*. The roots (in* $\mathbb{C}$*) of the characteristic polynomial are called the* eigenvalues *of* $\boldsymbol{A}$*. Symmetric matrices enjoy the following properties:*

(a) *The eigenvalues of a symmetric matrix are all real.*
(b) *If* $\lambda \in \mathbb{R}$ *is a root of multiplicity* n *of the characteristic polynomial of a (non-trivial) symmetric matrix, then there exist* n *linearly independent vectors* $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_n\}$ *satisfying* $\boldsymbol{A}\boldsymbol{x}_k = \lambda \boldsymbol{x}_k$ *(*$1 \le k \le n$*).*
(c) *If* $\lambda_1 \ne \lambda_2$ *are different roots of the characteristic polynomial of a symmetric matrix, and* $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{R}^d$ *satisfy* $\boldsymbol{A}\boldsymbol{x}_k = \lambda_k \boldsymbol{x}_k$ *(*$k = 1, 2$*), then* $\langle \boldsymbol{x}_1, \boldsymbol{x}_2 \rangle = 0$*.*

(d) *A symmetric matrix is positive definite (resp. negative definite) if and only if all its eigenvalues are positive (resp. negative).*

(e) *A symmetric matrix is positive semidefinite (resp. negative semidefinite) if and only if all its eigenvalues are non-negative (resp. non-positive)*

(f) *A symmetric matrix is indefinite if there exist two eigenvalues $\lambda_1 \neq \lambda_2$ with different sign.*

1.2. Coercive Functions. Other set of functions that play an important role in optimization are the kind of functions we explored in Example 1.3.

Definition (Coercive functions). A continuous real-valued function f is said to be *coercive* if for all $M > 0$ there exists $R = R(M) > 0$ so that $f(\boldsymbol{x}) \geq M$ if $\|\boldsymbol{x}\| \geq R$.

Remark 2.3. This is equivalent to the limit condition

$$\lim_{\|\boldsymbol{x}\| \to \infty} f(\boldsymbol{x}) = +\infty.$$

Example 2.6. We saw in Example 1.3 how even-degree polynomials with positive leading coefficients are coercive, and how this helped guarantee the existence of a minimum.

We must be careful assessing coerciveness of polynomials in higher dimension. Consider for example $p_2(x,y) = x^2 - 2xy + y^2$. Note how $p_2(x,x) = 0$ for any $x \in \mathbb{R}$, which proves p_2 is not coercive.

To see that the polynomial $p_4(x,y) = x^4 + y^4 - 4xy$ is coercive, we start by factoring the leading terms:

$$x^4 + y^4 - 4xy = \big(x^4 + y^4\big)\left(1 - \frac{4xy}{x^4 + y^4}\right)$$

Assume $r > 1$ is large, and that $x^2 + y^2 = r^2$. We have then

$$\begin{aligned} x^4 + y^4 &\geq \frac{r^4}{2} && \text{(Why?)} \\ |xy| &\leq \frac{r^2}{2} && \text{(Why?)} \end{aligned}$$

therefore,

$$\begin{aligned} \frac{4xy}{x^4 + y^4} &\leq \frac{4}{r^2} \\ 1 - \frac{4xy}{x^4 + y^4} &\geq 1 - \frac{4}{r^2} \\ \big(x^4 + y^4\big)\left(1 - \frac{4xy}{x^4 + y^4}\right) &\geq \frac{r^2(r^2 - 4)}{2} \end{aligned}$$

We can then conclude that given $M > 0$, if $x^2 + y^2 \geq 2 + \sqrt{4 + 2M}$, then $p_4(x,y) \geq M$. This proves p_4 is coercive.

There is one more kind of functions we should explore.

1.3. Convex Functions.

DEFINITION (Convex Sets). A subset $C \subseteq \mathbb{R}^d$ is said to be *convex* if for every $\boldsymbol{x}, \boldsymbol{y} \in C$, and every $\lambda \in [0,1]$, the point $\lambda \boldsymbol{y} + (1-\lambda)\boldsymbol{x}$ is also in C.

The following result is an interesting characterization of convex sets that allows us to actually construct any convex set from a family of points.

THEOREM 2.5. *Let $C \subseteq \mathbb{R}^d$ be a convex set and let $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_n\} \subset C$ be a family of points in C. The convex combinations $\lambda_1\boldsymbol{x}_1 + \lambda_2\boldsymbol{x}_2 + \cdots + \lambda_n\boldsymbol{x}_n$ are also in C, provided $\lambda_k \geq 0$ for all $1 \leq k \leq n$ and $\lambda_1 + \lambda_2 + \cdots + \lambda_n = 1$.*

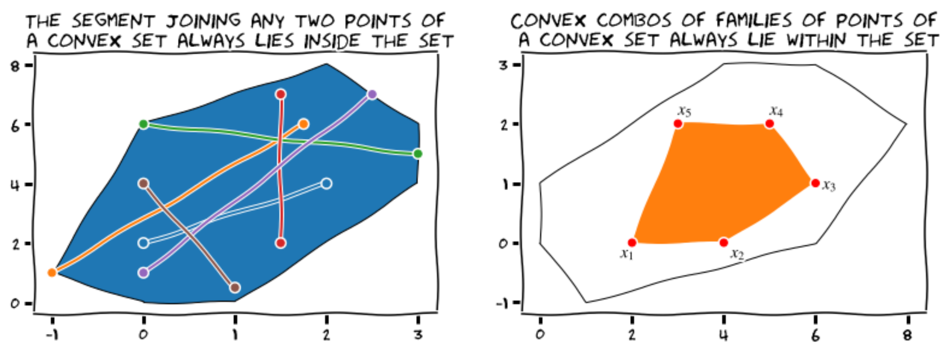

FIGURE 2.2. Convex sets.

DEFINITION (Convex Functions). Given a convex set $C \subseteq \mathbb{R}^d$, we say that a real-valued function $f\colon C \to \mathbb{R}$ is *convex* if

$$f\big(\lambda \boldsymbol{y} + (1-\lambda)\boldsymbol{x}\big) \leq \lambda f(\boldsymbol{y}) + (1-\lambda) f(\boldsymbol{x})$$

If instead we have $f\big(\lambda \boldsymbol{x} + (1-\lambda) f(\boldsymbol{y})\big) < \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y})$ for $0 < \lambda < 1$, we say that the function is *strictly convex*. A function f is said to be *concave* (resp. *strictly concave*) if $-f$ is convex (resp. strictly convex).

REMARK 2.4. There is an alternative definition of convex functions using the concept of *epigraph* of a function. Given a convex function $f\colon C \to \mathbb{R}$ on a convex set C, the epigraph of f is a set $\operatorname{epi}(f) \subset \mathbb{R}^{d+1}$ defined by

$$\operatorname{epi}(f) = \{(\boldsymbol{x}, y) \in \mathbb{R}^{d+1} : \boldsymbol{x} \in C, y \in \mathbb{R}, f(\boldsymbol{x}) \leq y\}.$$

The function f is convex if and only if its epigraph is a convex set.

Convex functions have many pleasant properties:

THEOREM 2.6. *Convex functions are continuous.*

THEOREM 2.7. *Let $f\colon C \to \mathbb{R}$ be a real-valued convex function defined on a convex set $C \subseteq \mathbb{R}^d$. If $\lambda_1, \dots, \lambda_n$ are nonnegative numbers satisfying $\lambda_1 + \cdots + \lambda_n = 1$ and $\boldsymbol{x}_1, \dots, x_n$ are n different points in C, then*

$$f\big(\lambda_1 \boldsymbol{x}_1 + \cdots + \lambda_n x_n\big) \leq \lambda_1 f(\boldsymbol{x}_1) + \cdots + \lambda_n f(\boldsymbol{x}_n).$$

Theorem 2.8. *If $f\colon C \to \mathbb{R}$ is a function on a convex set $C \subseteq \mathbb{R}^d$ with continuous first partial derivatives on C, then*

(a) *f is convex if and only if for all $\boldsymbol{x}, \boldsymbol{y} \in C$,*

$$f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle \leq f(\boldsymbol{y}).$$

(b) *f is strictly convex if for all $\boldsymbol{x} \neq \boldsymbol{y} \in C$,*

$$f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle < f(\boldsymbol{y}).$$

Remark 2.5. Theorem 2.8 implies that the graph of any (strictly) convex function always lies over the tangent hyperplane at any point of the graph.

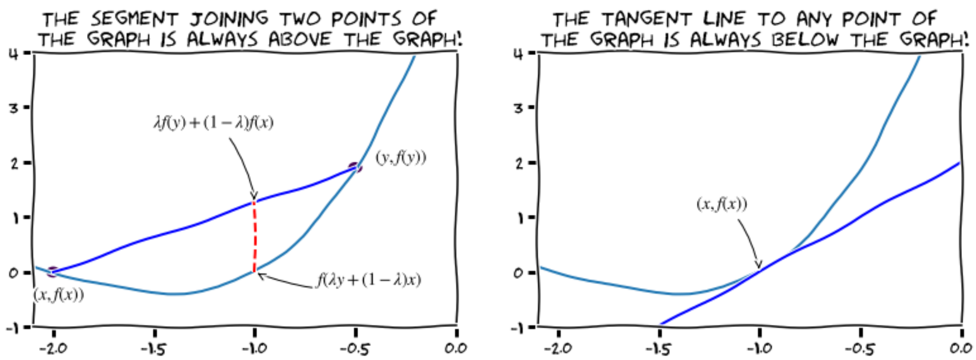

Figure 2.3. Convex Functions.

Two more useful characterization of convex functions.

Theorem 2.9. *Suppose that $f\colon C \to \mathbb{R}$ is a function with second partial derivatives on an open convex set $C \subseteq \mathbb{R}^d$. If the Hessian is positive semidefinite (resp. positive definite) on C, then f is convex (resp. strictly convex).*

Theorem 2.10. *Let $C \subseteq \mathbb{R}^d$ be a convex set.*

(a) *If $f_k\colon C \to \mathbb{R}$ are convex functions for $1 \leq k \leq n$, then so is the sum $f\colon C \to \mathbb{R}$:*

$$f(\boldsymbol{x}) = \sum_{k=1}^{n} f_k(\boldsymbol{x}).$$

If at least one of them is strictly convex, then so is f.

(b) *If $f\colon C \to \mathbb{R}$ is convex (resp. strictly convex) on C, then so is λf for any $\lambda > 0$.*

(c) *If $f\colon C \to \mathbb{R}$ is convex (resp. strictly convex) on C, and $g\colon f(C) \to \mathbb{R}$ is an increasing convex function (resp. strictly increasing convex), then so is $g \circ f$.*

(d) *If $f, g\colon C \to \mathbb{R}$ are convex functions on C, then so is $\max\{f, g\}$.*

EXAMPLE 2.7. Consider the function $f(x, y, z)$ defined on $\mathbb{R}^3$ by

$$f(x, y, z) = 2x^2 + y^2 + z^2 + 2yz.$$

Notice that for all $(x, y, z) \in \mathbb{R}^3$,

$$\text{Hess}f(x, y, z) = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 2 & 2 \\ 0 & 2 & 2 \end{bmatrix}, \qquad \Delta_1 = 4 > 0, \qquad \Delta_2 = 8 > 0, \qquad \Delta_3 = 0.$$

By virtue of Theorem 2.9, we infer that the function f is convex, but not strictly convex.

EXAMPLE 2.8. To prove that $f(x, y, z) = e^{x^2+y^2+z^2}$, rather than computing the Hessian and address if it is positive (semi)definite, it is easier to realize that we can write $f = g \circ h$ with

$$\begin{aligned} &g\colon \mathbb{R} \to \mathbb{R} && h\colon \mathbb{R}^3 \to \mathbb{R} \\ &g(x) = e^x && h(x, y, z) = x^2 + y^2 + z^2 \end{aligned}$$

The function g is trivially strictly increasing and convex (since $g'(x) = g''(x) = e^x > 0$ for all $x \in \mathbb{R}$). The function h is strictly convex, since (by Theorem 2.9)

$$\text{Hess}h(x, y, z) = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \quad \Delta_1 = 2 > 0, \quad \Delta_2 = 4 > 0, \quad \Delta_3 = 8 > 0.$$

By virtue of (c) in Theorem 2.10, we infer that f is strictly convex.

EXAMPLE 2.9. Set $C = \{(x, y) \in \mathbb{R}^2 : x > 0, y > 0\}$. Consider the function $f\colon C \to \mathbb{R}$ given by

$$f(x, y) = x^2 - 4xy + 5y^2 - \log(xy)$$

Notice we may write $f = g + h$ with $g, h\colon C \to \mathbb{R}$ given respectively by $g(x, y) = x^2 - 4xy + 5y^2$ and $h(x, y) = -\log(xy)$. Note also that both functions are strictly convex, since for all $(x, y) \in C$:

$$\begin{aligned} \text{Hess}g(x, y) &= \begin{bmatrix} 2 & -4 \\ -4 & 10 \end{bmatrix}, && \Delta_1 = 2 > 0, && \Delta_2 = 4 > 0, \\ \text{Hess}h(x, y) &= \begin{bmatrix} x^{-2} & 0 \\ 0 & y^{-2} \end{bmatrix}, && \Delta_1 = x^{-2} > 0, && \Delta_2 = (xy)^{-2} > 0. \end{aligned}$$

By virtue of part (a) in Theorem 2.10, we infer that f is strictly convex.

We are now ready to explore existence and characterization of extrema in a wide variety of situations.

2. Existence

2.1. Continuous functions on compact domains. The existence of global extrema is guaranteed for continuous functions over compact sets thanks to the following two basic results:

THEOREM 2.11 (Bounded Value Theorem). *The image $f(K)$ of a continuous real-valued function $f\colon \mathbb{R}^d \to \mathbb{R}$ on a compact set K is bounded: there exists $M > 0$ so that $|f(\boldsymbol{x})| \leq M$ for all $\boldsymbol{x} \in K$.*

THEOREM 2.12 (Extreme Value Theorem). *A continuous real-valued function $f\colon K \to \mathbb{R}$ on a compact set $K \subset \mathbb{R}^d$ takes on minimal and maximal values on K.*

2.2. Continuous functions on unbounded domains. Extra restrictions must be applied to the behavior of f in this case, if we want to guarantee the existence of extrema.

THEOREM 2.13. *Coercive functions always have a global minimum.*

PROOF. Since f is coercive, there exists $r > 0$ so that $f(\boldsymbol{x}) > f(\boldsymbol{0})$ for all $\boldsymbol{x}$ satisfying $\|\boldsymbol{x}\| > r$. On the other hand, consider the closed ball $K_r = \{\boldsymbol{x} \in \mathbb{R}^2 : \|\boldsymbol{x}\| \leq r\}$. The continuity of f guarantees a global minimum $\boldsymbol{x}^\star \in K_r$ with $f(\boldsymbol{x}^\star) \leq f(\boldsymbol{0})$. It is then $f(\boldsymbol{x}^\star) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^d$ trivially. $\square$

3. Characterization

Differentiability is key to guarantee characterization of extrema. Critical points lead the way:

THEOREM 2.14 (First order necessary optimality condition for minimization). *Suppose $f\colon \mathbb{R}^d \to \mathbb{R}$ is differentiable at $\boldsymbol{x}^\star$. If $\boldsymbol{x}^\star$ is a local minimum, then $\nabla f(\boldsymbol{x}^\star) = 0$.*

To be able to classify possible extrema $\boldsymbol{x}^\star$ for a properly differentiable function, we take into account the behavior of the function around $f(\boldsymbol{x}^\star)$ with respect to the tangent hyperplane at the point $\big(\boldsymbol{x}^\star, f(\boldsymbol{x}^\star)\big)$. Second derivatives make this process very easy.

THEOREM 2.15. *Suppose $f\colon \mathbb{R}^d \to \mathbb{R}$ is coercive and continuously differentiable at a point $\boldsymbol{x}^\star$. If $\boldsymbol{x}^\star$ is a global minimum, then $\nabla f(\boldsymbol{x}^\star) = \boldsymbol{0}$.*

THEOREM 2.16 (Second order necessary optimality condition for minimization). *Suppose that $f\colon \mathbb{R}^d \to \mathbb{R}$ is twice continuously differentiable at $\boldsymbol{x}^\star$.*

- *If $\boldsymbol{x}^\star$ is a local minimum, then $\nabla f(\boldsymbol{x}^\star) = 0$ and* $\operatorname{Hess} f(\boldsymbol{x}^\star)$ *is* positive semidefinite.
- *If $\boldsymbol{x}^\star$ is a strict local minimum, then $\nabla f(\boldsymbol{x}^\star) = 0$ and* $\operatorname{Hess} f(\boldsymbol{x}^\star)$ *is* positive definite.

THEOREM 2.17 (Second order sufficient optimality conditions for minimization). *Suppose $f\colon D \subseteq \mathbb{R}^d \to \mathbb{R}$ is twice continuously differentiable at a point $\boldsymbol{x}^\star$ in the interior of D and $\nabla f(\boldsymbol{x}^\star) = 0$. Then $\boldsymbol{x}^\star$ is a:*

Local Minimum: *if* $\operatorname{Hess} f(\boldsymbol{x}^\star)$ *is* positive semidefinite.
Strict Local Minimum: *if* $\operatorname{Hess} f(\boldsymbol{x}^\star)$ *is* positive definite.

If $D = \mathbb{R}^d$ and $\boldsymbol{x}^\star \in \mathbb{R}^d$ satisfies $\nabla f(\boldsymbol{x}^\star) = 0$, then $\boldsymbol{x}^\star$ is a:

Global Minimum: *if* $\operatorname{Hess} f(\boldsymbol{x})$ *is* positive semidefinite *for all* $\boldsymbol{x} \in \mathbb{R}^d$.
Strict Global Minimum: *if* $\operatorname{Hess} f(\boldsymbol{x})$ *is* positive definite *for all* $\boldsymbol{x} \in \mathbb{R}^d$.

THEOREM 2.18. *Any local minimum of a convex function $f\colon C \to \mathbb{R}$ on a convex set $C \subseteq \mathbb{R}^d$ is also a global minimum. If f is a strict convex function, then any local minimum is the unique strict global minimum.*

THEOREM 2.19. *Suppose $f\colon C \to \mathbb{R}$ is a convex function with continuous first partial derivatives on a convex set $C \subseteq \mathbb{R}^d$. Then, any critical point of f in C is a global minimum of f.*

Examples

EXAMPLE 2.10. Find a global minimum in $\mathbb{R}^3$ (if it exists) for the function

$$f(x,y,z) = e^{x-y} + e^{y-x} + e^{x^2} + z^2.$$

This function has continuous partial derivatives of any order in $\mathbb{R}^3$. Its continuity does not guarantee existence of a global minimum initially since the domain is not compact, but we may try our luck with its critical points. Note $\nabla f(x,y,z) = \big[e^{x-y} - e^{y-x} + 2xe^{x^2}, -e^{x-y} + e^{y-x}, 2x\big]$. The only critical point is then $(0,0,0)$ (Why?). The Hessian at that point is positive definite:

$$\operatorname{Hess} f(0,0,0) = \begin{bmatrix} 4 & -2 & 0 \\ -2 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \quad \Delta_1 = 4 > 0, \quad \Delta_2 = 4 > 0, \quad \Delta_3 = 8 > 0.$$

By Theorem 2.17, $f(0,0,0) = 3$ is a priori a strict local global minimum value. To prove that this point is actually a strict global minimum, notice that

$$\operatorname{Hess} f(x,y,z) = \begin{bmatrix} e^{x-y} + e^{y-x} + 4x^2e^{x^2} + 2e^{x^2} & -e^{x-y} - e^{y-x} & 0 \\ -e^{x-y} - e^{y-x} & e^{x-y} + e^{y-x} & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

The first principal minor is trivially positive: $\Delta_1 = e^{x-y} + e^{y-x} + 4x^2e^{x^2} + 2e^{x^2}$, since it is a sum of positive terms. The second principal minor is also positive:

$$\Delta_2 = \det \begin{bmatrix} e^{x-y} + e^{y-x} + 4x^2e^{x^2} + 2e^{x^2} & -e^{x-y} - e^{y-x} \\ -e^{x-y} - e^{y-x} & e^{x-y} + e^{y-x} \end{bmatrix}$$

$$= (e^{x-y} + e^{y-x})^2 + (e^{x-y} + e^{y-x})(4x^2 e^{x^2} + 2e^{x^2}) - (e^{x-y} + e^{y-x})^2$$
$$= (e^{x-y} + e^{y-x})(4x^2 e^{x^2} + 2e^{x^2}) > 0$$

The third principal minor is positive too: $\Delta_3 = 2\Delta_2 > 0$. We have just proved that $\text{Hess}f(x, y, z)$ is positive definite for all $(x, y, z) \in \mathbb{R}^3$, and thus $(0, 0, 0)$ is a strict global minimum.

EXAMPLE 2.11. Find global minima in $\mathbb{R}^2$ (if they exist) for the function

$$f(x, y) = e^{x-y} + e^{y-x}.$$

This function also has continuous partial derivatives of any order, but no extrema is guaranteed a priori. Notice that all points (x, y) satisfying $y = x$ are critical. For such points, the corresponding Hessians and principal minors are given by

$$\text{Hess}f(x, x) = \begin{bmatrix} 2 & -2 \\ -2 & 2 \end{bmatrix}, \qquad \Delta_1 = 2 > 0, \qquad \Delta_2 = 0;$$

therefore, $\text{Hess}f(x, x)$ is positive semidefinite for each critical point. By Theorem 2.17, $f(x, x) = 2$ is a local minimum for all $x \in \mathbb{R}$. To prove they are global minima, notice that for each $(x, y) \in \mathbb{R}^2$:

$$\text{Hess}f(x, y) = \begin{bmatrix} e^{x-y} + e^{y-x} & -e^{x-y} - e^{y-x} \\ -e^{x-y} - e^{y-x} & e^{x-y} + e^{y-x} \end{bmatrix},$$
$$\Delta_1 = e^{x-y} + e^{y-x} > 0, \quad \Delta_2 = 0.$$

The Hessian is positive semidefinite for all points, hence proving that any point in the line $y = x$ is a global minimum of f.

EXAMPLE 2.12. Find local and global minima in $\mathbb{R}^2$ (if they exist) for the function

$$f(x, y) = x^3 - 12xy + 8y^3.$$

This is a polynomial of degree 3, so we have continuous partial derivatives of any order. It is easy to see that this function has no global minima:

$$\lim_{x \to -\infty} f(x, 0) = \lim_{x \to -\infty} x^3 = -\infty.$$

Let's search instead for local minima. From the equation $\nabla f(x, y) = \mathbf{0}$ we obtain two critical points: $(0, 0)$ and $(2, 1)$. The corresponding Hessians and their eigenvalues are:

$$\text{Hess}f(0, 0) = \begin{bmatrix} 0 & -12 \\ -12 & 0 \end{bmatrix}, \quad \lambda_1 = -12 < 0, \quad \lambda_2 = 12 > 0,$$
$$\text{Hess}f(2, 1) = \begin{bmatrix} 12 & -12 \\ -12 & 48 \end{bmatrix}, \quad \lambda_1 = 30 - 6\sqrt{13} > 0, \quad \lambda_2 = 30 + 6\sqrt{30} > 0.$$

By Theorem 2.17, we have that $f(2, 1) = -8$ is a local minimum, but $f(0, 0) = 0$ is not.

EXAMPLE 2.13. Find local and global minima in $\mathbb{R}^2$ (if they exist) for the function

$$f(x,y) = x^4 - 4xy + y^4.$$

This is a polynomial of degree 4, so we do have continuous partial derivatives of any order. There are three critical points: $(0,0)$, $(-1,-1)$ and $(1,1)$. The latter two are both strict local minima (by virtue of Theorem 2.17).

$$\operatorname{Hess} f(-1,-1) = \operatorname{Hess} f(1,1) = \begin{bmatrix} 12 & -4 \\ -4 & 12 \end{bmatrix}, \quad \Delta_1 = 12 > 0, \quad \Delta_2 = 128 > 0.$$

We proved in Example 2.6 that f is coercive. By Theorems 2.13 and 2.15 we have that $f(-1,-1) = f(1,1) = -2$ must be strict global minimum values.

EXAMPLE 2.14. Find local and global minima in $\mathbb{R}^2$ (if they exist) for the function

$$f(x,y) = 2x^2 + y^2 + \frac{1}{2x^2 + y^2}.$$

The simplest way is to realize that f is a convex function on $\mathbb{R}^2$. We prove this by re-writing $f = g \circ h$ as a composition of $g(x) = x + 1\boldsymbol{x}$ on $(0, \infty)$ with $h(x,y) = 2x^2 + y^2$ on $\mathbb{R}^2$. Note that both functions are strictly convex (Why?).

The only critical point of g in $(0,\infty)$ lies at $x = 1$. By Theorem 2.19, $g(1) = 2$ must be a strict global minimum value of g. That being the case, any point (x,y) satisfying $h(x,y) = 1$ is a global minimum of f. These are all the points on the ellipse $2x^2 + y^2 = 1$.

Exercises

PROBLEM 2.1 (Basic). Consider the function

$$f(x,y) = \frac{x+y}{2 + \cos x}$$

At what points $(x,y) \in \mathbb{R}^2$ is this function continuous?

PROBLEM 2.2 (Intermediate). Give an example of a 2×2 symmetric matrix of each kind below:

(a) positive definite,
(b) positive semidefinite,
(c) negative definite,
(d) negative semidefinite,
(e) indefinite.

PROBLEM 2.3 (Basic). [**3**, p.31, #2] Classify the following matrices according to whether they are positive or negative definite or semidefinite or indefinite:

$$\text{(a)} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{bmatrix} \qquad \text{(b)} \begin{bmatrix} -1 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} \qquad \text{(c)} \begin{bmatrix} 7 & 0 & 0 \\ 0 & -8 & 0 \\ 0 & 0 & 5 \end{bmatrix}$$

(d) $\begin{bmatrix} 3 & 1 & 2 \\ 1 & 5 & 3 \\ 2 & 3 & 7 \end{bmatrix}$ (e) $\begin{bmatrix} -4 & 0 & 1 \\ 0 & -3 & 2 \\ 1 & 2 & -5 \end{bmatrix}$ (f) $\begin{bmatrix} 2 & -4 & 0 \\ -4 & 8 & 0 \\ 0 & 0 & -3 \end{bmatrix}$

Problem 2.4 (Basic). [**3**, p.31, #3] Write the quadratic form $\mathcal{Q}_{\boldsymbol{A}}(\boldsymbol{x})$ associated with each of the following matrices $\boldsymbol{A}$:

(a) $\begin{bmatrix} -1 & 2 \\ 2 & 3 \end{bmatrix}$ (b) $\begin{bmatrix} 1 & -1 & 0 \\ -1 & -2 & 2 \\ 0 & 2 & 3 \end{bmatrix}$

(c) $\begin{bmatrix} 2 & -3 \\ -3 & 0 \end{bmatrix}$ (d) $\begin{bmatrix} -3 & 1 & 2 \\ 1 & 2 & -1 \\ 2 & -1 & 4 \end{bmatrix}$

Problem 2.5 (Basic). [**3**, p.32, #4] Write each of the quadratic forms below in the form $\boldsymbol{x}\boldsymbol{A}\boldsymbol{x}^\intercal$ for an appropriate symmetric matrix $\boldsymbol{A}$:

(a) $3x^2 - xy + 2y^2$.
(b) $x^2 + 2y^2 - 3z^2 + 2xy - 4xz + 6yz$.
(c) $2x^2 - 4z^2 + xy - yz$.

Problem 2.6 (Intermediate). Identify which of the following real-valued functions are coercive. Explain the reason.

(a) $f(x, y) = \sqrt{x^2 + y^2}$.
(b) $f(x, y) = x^2 + 9y^2 - 6xy$.
(c) $f(x, y) = x^4 - 3xy + y^4$.
(d) Rosenbrock functions $\mathcal{R}_{a,b}$.

Problem 2.7 (Advanced). [**3**, p.36, #32] Find an example of a continuous, real-valued, non-coercive function $f\colon \mathbb{R}^2 \to \mathbb{R}$ that satisfies, for all $t \in \mathbb{R}$,

$$\lim_{x\to\infty} f(x, tx) = \lim_{y\to\infty} f(ty, y) = \infty.$$

Problem 2.8 (Basic). [**3**, p.77, #1,2,7] Determine whether the given functions are convex, concave, strictly convex or strictly concave on the specified domains:

(a) $f(x) = \log(x)$ on $(0, \infty)$.
(b) $f(x) = e^{-x}$ on $\mathbb{R}$.
(c) $f(x) = |x|$ on $[-1, 1]$.
(d) $f(x) = |x^3|$ on $\mathbb{R}$.
(e) $f(x, y) = 5x^2 + 2xy + y^2 - x + 2x + 3$ on $\mathbb{R}^2$.
(f) $f(x, y) = x^2/2 + 3y^2/2 + \sqrt{3}xy$ on $\mathbb{R}^2$.
(g) $f(x, y) = 4e^{3x-y} + 5e^{x^2+y^2}$ on $\mathbb{R}^2$.
(h) $f(x, y, z) = x^{1/2} + y^{1/3} + z^{1/5}$ on $C = \{(x, y, z) : x > 0, y > 0, z > 0\}$.

Problem 2.9 (Intermediate). [**3**, p.79 #11] Sketch the epigraph of the following functions

(a) $f(x) = e^x$.
(b) $f(x, y) = x^2 + y^2$.

PROBLEM 2.10 (Intermediate). For the following optimization problems, state whether existence of a solution is guaranteed:

(a) $f(x) = (1 + x)/x$ over $[1, \infty)$
(b) $f(x) = 1/x$ over $[1, 2)$
(c) The following piecewise function over $[1, 2]$

$$f(x) = \begin{cases} 1/x, & 1 \leq x < 2 \\ 1, & x = 2 \end{cases}$$

PROBLEM 2.11 (Advanced). State and prove equivalent results to Theorems 2.14, 2.16 and 2.17 to describe necessary and sufficient conditions for the characterization of *maxima*.

PROBLEM 2.12 (Basic). [**3**, p.32, #7] Use the *Principal Minor Criteria* (Theorem 2.3) to determine—if possible—the nature of the critical points of the following functions:

(a) $f(x, y) = x^3 + y^3 - 3x - 12y + 20$.
(b) $f(x, y, z) = 3x^2 + 2y^2 + 2z^2 + 2xy + 2yz + 2xz$.
(c) $f(x, y, z) = x^2 + y^2 + z^2 - 4xy$.
(d) $f(x, y) = x^4 + y^4 - x^2 - y^2 + 1$.
(e) $f(x, y) = 12x^3 + 36xy - 2y^3 + 9y^2 - 72x + 60y + 5$.

PROBLEM 2.13 (Intermediate). [**3**, p.35 #26] Show that the function

$$f(x, y, z) = e^{x^2+y^2+z^2} - x^4 - y^6 - z^6$$

has a global minimum on $\mathbb{R}^3$.

PROBLEM 2.14 (Intermediate). [**3**, p.36 #33] Consider the function

$$f(x, y) = x^3 + e^{3y} - 3xe^y.$$

Show that f has exactly one critical point, and that this point is a local minimum but not a global minimum.

PROBLEM 2.15 (Basic). Let $f(x, y) = -\log(1 - x - y) - \log x - \log y$.

(a) Find the domain D of f.
(b) Prove that D is a convex set.
(c) Prove that f is strictly convex on D.
(d) Find the strict global minimum.

PROBLEM 2.16 (Basic). [**3**, p.81 #27] Find local and global minima in $\mathbb{R}^3$ (if they exist) for the function

$$f(x, y) = e^{x+z-y} + e^{y-x-z}$$

CHAPTER 3

Numerical Approximation for Unconstrained Optimization

Although technically any characterization result finds the exact value of the extrema of a function, computationally this is hardly feasible (specially for functions of very high dimension). See the following session based on problem 2.13 for an example, where we try to find the critical points of the function $f(x, y, z) = e^{x^2+y^2+z^2} - x^4 - y^y - z^6$ symbolically in Python with the `sympy` libraries:

```
# Importing necessary symbols/libraries/functions
from sympy.abc import x,y,z
from sympy import Matrix, solve, exp
from sympy.tensor.array import derive_by_array

# Description of f, computation of its gradient and Hessian
f = exp(x**2 + y**2 + z**2) - x**4 -y**6 - z**6
gradient = derive_by_array(f, [x,y,z])
hessian  = Matrix([derive_by_array(gradient, a) for a in [x,y,z]])
```

While the correct expressions for ∇f and $\operatorname{Hess} f$ are quickly computed, trying to find critical points results in an error:

```
# Search of critical points by solving ∇f = 0
solve(gradient)
```

```
NotImplementedError: could not solve
4*x**2*sqrt(-log(exp(x**2)/(2*x**2))) - 6*(-log(exp(x**2)/(2*x**2)))**(5/2)
```

Too complex a task to be performed symbolically, although the obvious answer is $(0, 0, 0)$. A better way to approach this is by trying to approximate this minimum using the structure of the graph of f. In these notes we are going to explore several strategies to accomplish this task, based on the concept of *iterative methods for finding zeros of real-valued functions.*

1. Newton's Method

EXAMPLE 3.1 (The Newton-Raphson method). In order to find a good estimation of $\sqrt{2}$ with mani decimal places, we allow a computer to find better and better approximations of the solution of the equation $f(x) = x^2 - 2$. We start with an initial guess, say $x_0 = 3$. We construct a sequence $\{x_n\}_{n \in \mathbb{N}}$ that converges to $\sqrt{2}$ as follows:

(a) Find the tangent line to the graph of f at x_0,

$$y - f(x_0) = f'(x_0)(x - x_0)$$

(b) Provided this line is not horizontal ($f'(x_0) \neq 0$), report the intersection of this line with the x–axis. Call this intersection x_1

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

(c) Repeat this process, to get the sequence

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

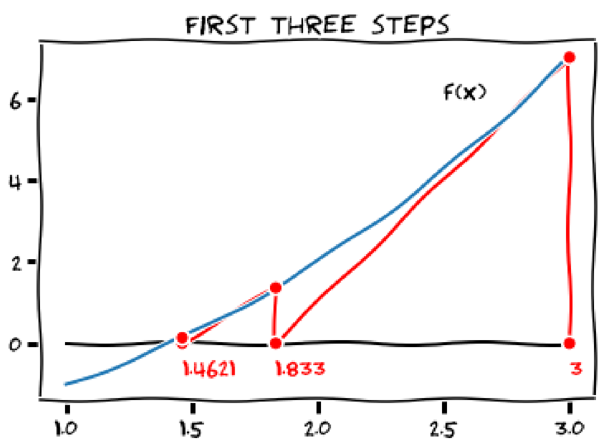

FIGURE 3.1. Newton-Raphson iterative method

Note the result of applying this process a few times:

n	x_n	$f(x_n)$
0	3.000000000000000	$7.0000E+00$
1	1.833333333333333	$1.3611E+00$
2	1.462121212121212	$1.3780E-01$
3	1.414998429894803	$2.2206E-03$
4	1.414213780047198	$6.1568E-07$
5	1.414213562373112	$4.7518E-14$
6	1.414213562373095	$-4.4409E-16$
7	1.414213562373095	$4.4409E-16$

TABLE 1. Convergence to $\sqrt{2}$ with 15-digit accuracy in 6 steps

EXAMPLE 3.2. Consider now the function $f(x) = 1 - \frac{1}{x}$ over $(0, \infty)$, which has the obvious root $x = 1$. The Newton-Raphson method gives the following iterates for any $x_0 \in (0, \infty)$:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n\big(2 - x_n\big).$$

Notice the two factors in the right-hand side of that expression: x_n, and $2 - x_n$. If the initial guess does not satisfy $0 < x_0 < 2$, then the next iteration gives a non-positive value (see Figure 3.2). The method will not work on those instances: convergence to a solution is not guaranteed.

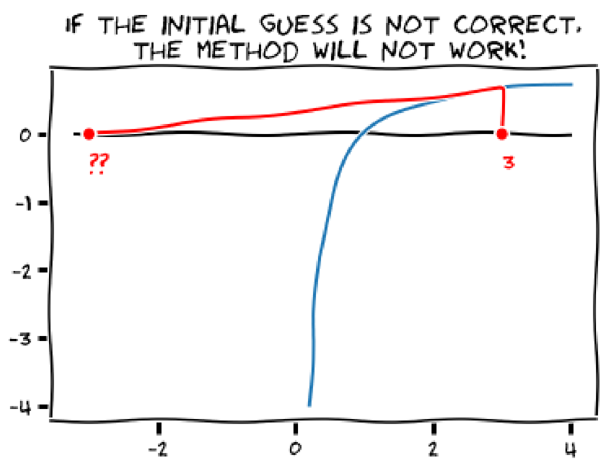

FIGURE 3.2. Initial guess must carefully be chosen in Newton-Raphson

EXAMPLE 3.3. Consider now $f(x) = \operatorname{sign}(x)\sqrt{\lvert x \rvert}$ over $\mathbb{R}$, with root at $x = 0$. The Newton-Raphson method fails miserably with this function: for any $x_0 \neq 0$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = x_0 - \frac{\operatorname{sign}(x_0)\lvert x_0 \rvert^{1/2}}{\frac{1}{2}\lvert x_0 \rvert^{-1/2}} = -x_0.$$

This sequence turns into a loop: $x_{2n} = x_0$, $x_{2n+1} = -x_0$ for all $n \in \mathbb{N}$ (see Figure 3.3).

Let's proceed to extend this process to functions $\boldsymbol{g} \colon \mathbb{R}^d \to \mathbb{R}^d$ as follows.

- Any function $\boldsymbol{g} \colon \mathbb{R}^d \to \mathbb{R}^d$ can be described in the form $\boldsymbol{g}(\boldsymbol{x}) = \big[g_1(\boldsymbol{x}), g_2(\boldsymbol{x}), \dots, g_d(\boldsymbol{x})\big]$ for d real-valued functions $g_k \colon \mathbb{R}^d \to \mathbb{R}$ $(1 \leq k \leq d)$.

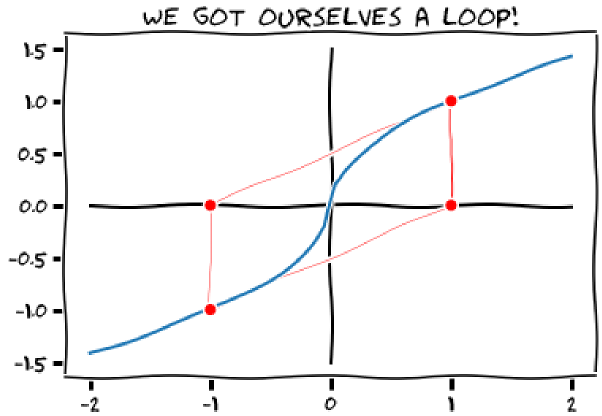

FIGURE 3.3. Newton-Raphson fails for some functions

- For such a function $\boldsymbol{g}$, we may express its gradient as a $d \times d$ matrix in the form

$$\nabla \boldsymbol{g} = \begin{bmatrix} \frac{\partial g_1}{\partial x_1} & \frac{\partial g_1}{\partial x_2} & \cdots & \frac{\partial g_1}{\partial x_d} \\ \frac{\partial g_2}{\partial x_1} & \frac{\partial g_2}{\partial x_2} & \cdots & \frac{\partial g_2}{\partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_d}{\partial x_1} & \frac{\partial g_d}{\partial x_2} & \cdots & \frac{\partial g_d}{\partial x_d} \end{bmatrix}$$

Start with a guess for the solution, $\boldsymbol{x}_0$, and on the n–th step of the algorithm compute the $(n+1)$–th term of the sequence by

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n - \big[\nabla \boldsymbol{g}(\boldsymbol{x}_n)\big]^{-1} \boldsymbol{g}(\boldsymbol{x}_n), \tag{3}$$

where $\big[\nabla \boldsymbol{g}(\boldsymbol{x}_n)\big]^{-1}$ represents the inverse matrix of the gradient at $\boldsymbol{x}_n$. This is equivalent to selecting in the tangent hyperplane to the graph of $\boldsymbol{g}$ at $\boldsymbol{g}(\boldsymbol{x}_n)$, the one line in the direction with the most rapid increase/decrease. The computation of $\boldsymbol{x}_{n+1}$ is therefore the intersection of that line with the hyperplane $x_d = 0$. We refer to $\big[\nabla \boldsymbol{g}(\boldsymbol{x}_n)\big]^{-1} \boldsymbol{g}(\boldsymbol{x}_n)$ as the *Newton direction* for $\boldsymbol{g}$ at $\boldsymbol{x}_n$.

EXAMPLE 3.4. Consider the function $\boldsymbol{g} \colon \mathbb{R}^2 \to \mathbb{R}^2$ given by

$$\boldsymbol{g}(x, y, z) = \big[x^3 - y, y^3 - x\big]$$

Its gradient at each (x, y) is given by

$$\nabla \boldsymbol{g}(x, y) = \begin{bmatrix} 3x^2 & -1 \\ -1 & 3y^2 \end{bmatrix}$$

Note the determinant of this matrix is $\det \nabla \boldsymbol{g}(x,y) = 9x^2y^2 - 1 = (3xy - 1)(3xy+1)$. For any point (x,y) that does not make this expression zero, this is an invertible matrix with

$$\left[\nabla \boldsymbol{g}(x,y)\right]^{-1} = \frac{1}{9x^2y^2-1}\begin{bmatrix} 3y^2 & 1 \\ 1 & 3x^2 \end{bmatrix}$$

For an initial guess (x_0, y_0), the sequence computed by the Newton method is then given by

$$\begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} = \begin{bmatrix} x_n \\ y_n \end{bmatrix} - \frac{1}{9x_n^2y_n^2-1}\begin{bmatrix} 3y_n^2 & 1 \\ 1 & 3x_n^2 \end{bmatrix}\begin{bmatrix} x_n^3 - y_n \\ y_n^3 - x_n \end{bmatrix}$$

Let's run this process with three different initial guesses:

(a) Starting at $(x_0, y_0) = (-1.0, 1.0)$, the sequence converges to $(0,0)$.

n	x_n	y_n
0	-1.00000000	1.00000000
1	-0.50000000	0.50000000
2	-0.14285714	0.14285714
3	-0.00549451	0.00549451
4	-0.00000033	0.00000033
5	-0.00000000	0.00000000
6	-0.00000000	0.00000000

TABLE 2. Convergence to $(0,0)$ with 8-digit accuracy in 5 steps

(b) Starting at $(x_0, y_0) = (3.5, 2.1)$, the sequence converges to $(1,1)$.

n	x_n	y_n
0	3.50000000	2.10000000
1	2.37631607	1.57961573
2	1.65945969	1.27476534
3	1.23996276	1.10419072
4	1.04837462	1.02274752
5	1.00260153	1.00133122
6	1.00000824	1.00000451
7	1.00000000	1.00000000
8	1.00000000	1.00000000

TABLE 3. Convergence to $(1,1)$ with 8-digit accuracy in 7 steps

(c) Starting at $(x_0, y_0) = (-13.5, -7.3)$, the sequence converges to $(-1,-1)$.

We can readily see how this process aids in the computation of critical points of twice continuously differentiable real-valued function $f\colon \mathbb{R}^d \to \mathbb{R}$:

n	x_n	y_n	n	x_n	y_n
0	-13.50000000	-7.30000000	7	-1.09518303	-1.04341362
1	-9.00900415	-4.92301873	8	-1.00932090	-1.00463507
2	-6.01982204	-3.36480659	9	-1.00010404	-1.00005571
3	-4.03494126	-2.36199873	10	-1.00000001	-1.00000001
4	-2.72553474	-1.73750959	11	-1.00000000	-1.00000000
5	-1.87830623	-1.36573112	12	-1.00000000	-1.00000000
6	-1.36121191	-1.15374930	13	-1.00000000	-1.00000000

TABLE 4. Convergence to $(-1, -1)$ with 8-digit accuracy in 11 steps

(a) Set $\boldsymbol{g}(\boldsymbol{x}) = \nabla f(\boldsymbol{x}) = \big[\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_d}\big]$
(b) It is then $\nabla \boldsymbol{g}(\boldsymbol{x}) = \operatorname{Hess} f(\boldsymbol{x})$
(c) Perform a Newton method (with initial guess $\boldsymbol{x}_0$) on $\boldsymbol{g} = \nabla f$ to obtain the recurrence formula

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n - \big[\operatorname{Hess} f(\boldsymbol{x}_n)\big]^{-1} \cdot \nabla f(\boldsymbol{x}_n) \tag{4}$$

EXAMPLE 3.5. Consider the polynomial $p_4(x, y) = x^4 - 4xy + y^4$. Notice $\nabla p_4(x, y) = \big[x^3 - y, y^3 - x\big]$—this is function $\boldsymbol{g}$ in Example 3.4. The critical points we found were $(0, 0)$, $(-1, -1)$ and $(1, 1)$. See Figure 3.4.

EXAMPLE 3.6. A similar process for the Rosenbrock function

$$\mathcal{R}_{1,1}(x, y) = (1 - x)^2 + (y - x^2)^2$$

gives the following recurrence formula:

$$\begin{aligned} \begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} &= \begin{bmatrix} x_n \\ y_n \end{bmatrix} - \big[\operatorname{Hess}\mathcal{R}_{1,1}(x_n, y_n)\big]^{-1} \cdot \nabla \mathcal{R}_{1,1}(x_n, y_n) \\ &= \frac{1}{2x_n^2 - 2y_n + 1} \begin{bmatrix} 2x_n^3 - 2x_n y_n + 1 \\ x_n(2x_n^3 - 2x_n y_n - x_n + 2) \end{bmatrix} \end{aligned}$$

For instance, starting with the initial guess $(x_0, y_0) = (-2, 2)$, the sequence converges to the critical point $(1, 1)$. See Figure 3.4.

REMARK 3.1. Newton's Method to solve $\boldsymbol{g} = \boldsymbol{0}$, as given by the recurrence formula in equation (3) in page 26, is very convenient to provide explicit descriptions of the different iterations. However, it is hardly suitable for practical purposes, due to the computational issues involving matrix inversion.

To avoid dealing with matrix inversion, we consider the following equivalent formula:

$$\nabla \boldsymbol{g}(\boldsymbol{x}_n) \cdot \big(\boldsymbol{x}_{n+1} - \boldsymbol{x}_n\big) = -\boldsymbol{g}(\boldsymbol{x}_n) \tag{5}$$

This is a simple system of linear equations, and thus much faster to solve.

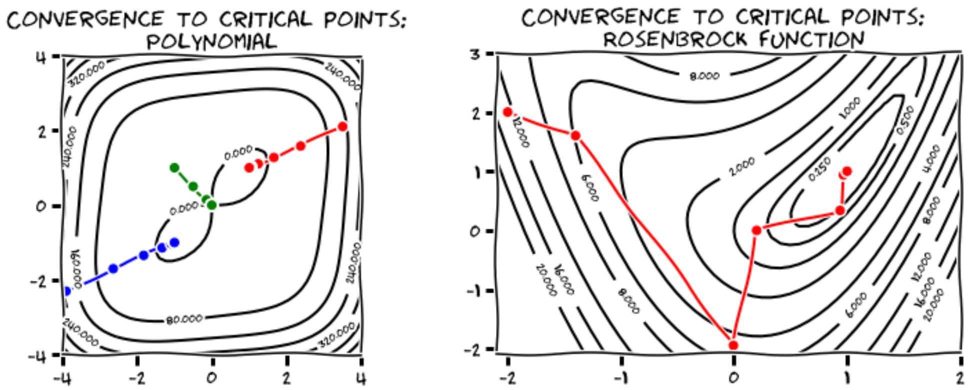

FIGURE 3.4. Newton method

The equivalent recurrence formula to search for critical points of a twice continuously differentiable real-valued function $f\colon \mathbb{R}^d \to \mathbb{R}$ is thus

$$\operatorname{Hess} f(\boldsymbol{x}_n) \cdot (\boldsymbol{x}_{n+1} - \boldsymbol{x}_n) = -\nabla f(\boldsymbol{x}_n). \tag{6}$$

EXAMPLE 3.7. The equivalent recurrence formula to the one we obtained in example 3.4 is as follows:

$$\begin{bmatrix} 3x_n^2 & -1 \\ -1 & 3y_n^2 \end{bmatrix} \begin{bmatrix} x_{n+1} - x_n \\ y_{n+1} - y_n \end{bmatrix} = \begin{bmatrix} x_n^3 - y_n \\ y_n^3 - x_n \end{bmatrix}$$

All we need to do is, at each step n, solve for X and Y the system of linear equations

$$\begin{cases} 3x_n^2(X - x_n) - (Y - y_n) = x_n^3 - y_n \\ -(X - x_n) + 3y_n^2(Y - y_n) = y_n^2 - x_n \end{cases}$$

or equivalently,

$$\begin{cases} 3x_n^2 X - Y = 4x_n^3 - 2y_n \\ -X + 3y_n^2 Y = 4y_n^2 - 2x_n \end{cases}$$

There are some theoretical results that aid in the search for a *good* initial guess:

THEOREM 3.1 (Quadratic Convergence Theorem). *Suppose $f\colon \mathbb{R}^d \to \mathbb{R}$ is a twice continuously differentiable real-valued function, and $\boldsymbol{x}^\star$ is a critical point of f. Let $\mathcal{N}(\boldsymbol{x}) = \boldsymbol{x} - \big[\operatorname{Hess} f(\boldsymbol{x})\big]^{-1} \cdot \nabla f(\boldsymbol{x})$. If there exists*

(a) *$h > 0$ so that*[1] $\big\| \big[\operatorname{Hess} f(\boldsymbol{x}^\star)\big]^{-1} \big\| \le \frac{1}{h}$,
(b) *$\beta > 0$, $L > 0$ for which $\|\operatorname{Hess} f(\boldsymbol{x}) - \operatorname{Hess} f(\boldsymbol{x}^\star)\| \le L\|\boldsymbol{x} - \boldsymbol{x}^\star\|$ provided $\|\boldsymbol{x} - \boldsymbol{x}^\star\| \le \beta$.*

[1]Recall the *norm* of a matrix M, defined by $\|M\| = \max\{\|M \cdot \boldsymbol{x}\| : \|\boldsymbol{x}\| = 1\}$.

In that case, for all $\boldsymbol{x} \in \mathbb{R}^d$ *satisfying* $\|\boldsymbol{x} - \boldsymbol{x}^\star\| \leq \min\{\beta, \frac{2h}{3L}\}$,

$$\frac{\|\mathcal{N}(\boldsymbol{x}) - \boldsymbol{x}^\star\|}{\|\boldsymbol{x} - \boldsymbol{x}^\star\|^2} \leq \frac{3L}{2h}$$

EXAMPLE 3.8. Consider the function $f(x) = x - \log x$ on $(0, \infty)$, which has a global minimum at $x^\star = 1$. Its gradient is $f'(x) = 1 - \frac{1}{x}$, the function we studied in Example 3.2 in page 25. We did establish then any initial guess x_0 should belong in the interval $(0, 2)$. We want to use Theorem 3.1 to improve the search, so we may guarantee *quadratic convergence* to the critical point.

- The Hessian is $f''(x) = x^{-2}$, and thus $\big\| \big[\operatorname{Hess} f(x^\star)\big]^{-1} \big\| = 1$.
- Notice that for all $0 < x < 2$,

$$\|\operatorname{Hess} f(x) - \operatorname{Hess} f(x^\star)\| = \big|\tfrac{1}{x^2} - 1\big| = \frac{1+x}{x^2}|x - 1|$$

  Choosing e.g. $\beta = \frac{1}{2}$, we readily obtain that $\frac{10}{9} \leq \frac{1+x}{x^2} \leq 6$; therefore, $\|\operatorname{Hess} f(x) - \operatorname{Hess} f(x^\star)\| \leq 6|x - 1|$, and we may choose $L = 6$ for $\beta = \frac{1}{2}$.

Theorem 3.1 guarantees that any initial guess $\boldsymbol{x}_0 \in \big(\frac{8}{9}, \frac{10}{9}\big)$ will give us good results.

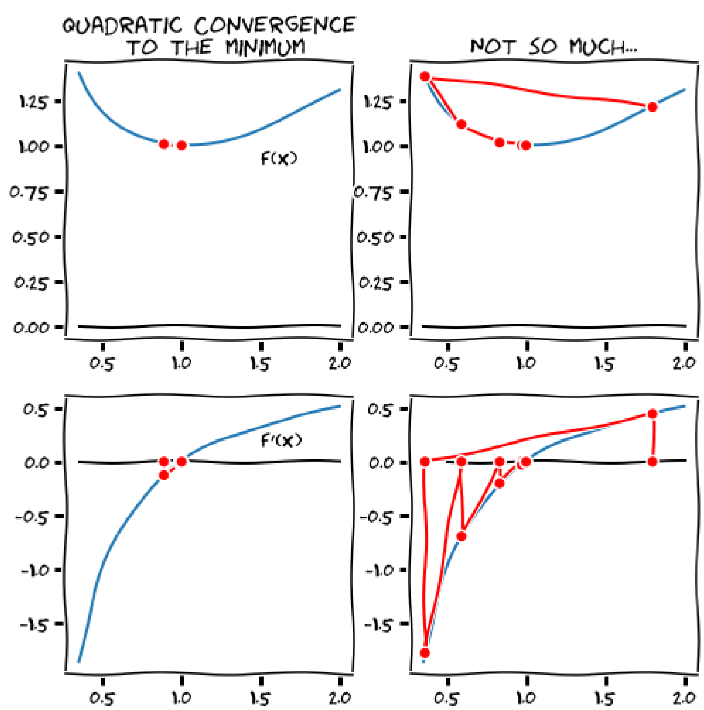

FIGURE 3.5. Quadratic Convergence of the Newton-Raphson method

2. Exercises

Problem 3.1 (Basic). Find an example of a function $f\colon \mathbb{R} \to \mathbb{R}$ (different from the function in Example 3.3) with a unique root at $x = 0$ for which the Newton-Raphson sequence is a loop no matter the initial guess $x_0 \neq 0$: $x_{2n} = x_0$, $x_{2n+1} = -x_0$ for all $n \in \mathbb{N}$.

Problem 3.2 (Intermediate). Consider the function

$$f(x) = 9x - 4\log(x - 7).$$

We wish to study the behavior of Newton-Raphson to find approximations to the critical points of this function.

(a) Find the domain D of f.
(b) Find the global minimum of f analytically.
(c) Compute an exact formula for the Newton-Raphson iterate x_{n+1} for an initial guess $x_0 \in D$.
(d) Compute five iterations of the Newton-Raphson method starting at each of the following initial guesses:
   (a) $x_0 = 7.4$.
   (b) $x_0 = 7.2$.
   (c) $x_0 = 7.01$.
   (d) $x_0 = 7.8$.
   (e) $x_0 = 7.88$.
(e) Prove that the Newton-Raphson method converges to the optimal solution for any initial guess $x_0 \in (7, 7.8888)$.
(f) What is the behavior of the Newton-Raphson method if the initial guess is not in the interval $(7, 7.8888)$?

Problem 3.3 (Intermediate). Consider the function

$$f(x) = 6x - 4\log(x - 2) - 3\log(25 - x).$$

We wish to study the behavior of Newton-Raphson to find approximations to the critical points of this function.

(a) Find the domain D of f.
(b) Find the global minimum of f analytically.
(c) Compute an exact formula for the Newton-Raphson iterate x_{n+1} for an initial guess $x_0 \in D$.
(d) Compute five iterations of the Newton-Raphson method starting at each of the following initial guesses:
   (a) $x_0 = 2.6$.
   (b) $x_0 = 2.7$.
   (c) $x_0 = 2.4$.
   (d) $x_0 = 2.8$.
   (e) $x_0 = 3$.
(e) Prove that the Newton-Raphson method converges to the optimal solution for any initial guess $x_0 \in (2, 3.05)$.

(f) What is the behavior of the Newton-Raphson method if the initial guess is not in the interval $(2, 3.05)$?

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