Course notes for MATH 524: Non-Linear Optimization

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CHAPTER 1

Background

Our starting point is, for any positive integer $d \in \mathbb{N}$, the Cartesian products:

$$\mathbb{R}^d = \mathbb{R} \times \stackrel{(d)}{\cdots} \times \mathbb{R} = \{(x_1, \dots, x_d) : x_k \in \mathbb{R} \text{ for } 1 \le k \le d\}.$$

These sets, endowed with the operations of addition and scalar multiplication, have the structure of a *vector field*:

Addition: For $\boldsymbol{x} = (x_1, \dots, x_d), \boldsymbol{y} = (y_1, \dots, y_d) \in \mathbb{R}^d$,

$$\boldsymbol{x} + \boldsymbol{y} = (x_1 + y_1, \dots, x_d + y_d) \in \mathbb{R}^d.$$

Scalar multiplication: For $\boldsymbol{x} \in \mathbb{R}^d$ and $\lambda \in \mathbb{R}$,

$$\lambda \cdot \boldsymbol{x} = \lambda \boldsymbol{x} = (\lambda x_1, \dots, \lambda x_d) \in \mathbb{R}^d.$$

Given $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in \mathbb{R}^d$, $\lambda, \mu \in \mathbb{R}$,

- (a) The addition is commutative: x + y = y + x.
- (b) Existence of identity elements for addition: Let $\mathbf{0} = (0, \dots, 0)$. $\mathbf{x} + \mathbf{0} = \mathbf{x}$.
- (c) The addition is associative: x + (y + z) = (x + y) + z.
- (d) Existence of inverse elements for addition: If $\mathbf{x} = (x_1, \dots, x_d)$, the element $-\mathbf{x} = (-x_1, \dots, -x_d)$ satisfies $\mathbf{x} + (-\mathbf{x}) = \mathbf{0}$. We write $\mathbf{x} \mathbf{y}$ instead of $\mathbf{x} + (-\mathbf{y})$.
- (e) Scalar multiplication is compatible with field multiplication: $\lambda(\mu x) = (\lambda \mu)x$.
- (f) Existence of identity for scalar multiplication: $1 \cdot x = x$.
- (g) Scalar multiplication is distributive with respect to addition: $\lambda(x + y) = \lambda x + \lambda y$.
- (h) Scalar multiplication is distributive with respect to field addition: $(\lambda + \mu)x = \lambda x + \mu x$.

A basis of \mathbb{R}^d is any finite set $\{b_k : 1 \le k \le d\}$ satisfying two properties:

Spanning property: For all $\boldsymbol{x} \in \mathbb{R}^d$ there exist d scalars $\{\lambda_1, \dots, \lambda_d\}$ so that $\boldsymbol{x} = \sum_{k=1}^d \lambda_k \boldsymbol{b}_k$.

Linear independence: If $\{\lambda_1, \ldots, \lambda_d\}$ satisfy $\sum_{k=1}^d \lambda_k \boldsymbol{b}_k = \boldsymbol{0}$, then it must be $\lambda_k = 0$ for all $1 \le k \le d$.

PROBLEM 1.1. Define in \mathbb{R}^d , for each $1 \leq k \leq d$, the element e_k to be the ordered d-tuple with k-th entry equal to one, and zeros on all other entries.

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- (a) Prove that $\{e_k : 1 \le k \le d\}$ is a basis for \mathbb{R}^d .
- (b) Set $\boldsymbol{b}_k = \boldsymbol{e}_k \boldsymbol{e}_{k+1}$ for $1 \le k < d$, $\boldsymbol{b}_d = \boldsymbol{e}_d$. Is $\{\boldsymbol{b}_k : 1 \le k \le d\}$ a basis for

1. Functions

Given sets X, Y, we define a function $f: X \to Y$ to be a subset of $X \times Y$ subject to the following condition: for every $x \in X$ there is exactly one element $y \in Y$ such that the ordered pair (x, y) is contained in the subset defining f. The sets X and Y are called respectively the *domain* and *codomain* of f.

If A is any subset of the domain X, then f(A) is the subset of the codomain Y consisting of all images of elements of A. We say that f(A) is the *image* of A under f. The image of f is given by f(X).

If $Y \subset \mathbb{R}$, we say that the function f is real-valued. For a real-valued function $f: \mathbb{R}^d \to \mathbb{R}$, we may regard the corresponding ordered pairs $(\boldsymbol{x}, y) \in \mathbb{R}^d \times \mathbb{R}$ as points in a (d+1)-dimensional space. We call this set the *graph* of f.

The *inverse image* of a subset B of the codomain Y under a function f is the subset of the domain X defined by $f^{-1}(B) = \{x \in X : f(x) \in B\}$.

For sets X, Y, Z, the function composition of $f: X \to Y$ with $g: Y \to Z$ is the function $g \circ f: X \to Z$ defined by $(g \circ f)(x) = g(f(x))$.

Unless specifically stated otherwise, all functions in these notes are real-valued functions $f: \mathbb{R}^d \to \mathbb{R}$.

EXAMPLE 1.1 (Linear Functions). We say that a real-valued function is *linear* if it preserves the operations in \mathbb{R}^d :

$$f(\boldsymbol{x} + \lambda \boldsymbol{y}) = f(\boldsymbol{x}) + \lambda f(\boldsymbol{y}) \text{ for } \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d, \lambda \in \mathbb{R}.$$

With this definition, the function f(x) = 3x is indeed a linear function, but g(x) = 3x + 5 is not! It is not hard to see that the only linear constant function is f(x) = 0 (since f(0) = f(x - x) = f(x) - f(x) = 0). For a non-constant linear function f(x), it is also easy to see that the image is the whole real line.

EXAMPLE 1.2 (Convex Functions). A subset $C \subset \mathbb{R}^d$ is said to be *convex* if for every $\boldsymbol{x}, \boldsymbol{y} \in C$, and every $\lambda \in [0,1]$, the point $\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}$ is also in C. Given such a convex set, we say that a real-valued function $f: C \to \mathbb{R}$ is *convex* if

$$f(\lambda x + (1 - \lambda)y) \le \lambda f(x) + (1 - \lambda)f(y)$$

If instead we have $f(\lambda x + (1-\lambda)f(y)) < \lambda f(x) + (1-\lambda)f(y)$ for $0 < \lambda < 1$, we say

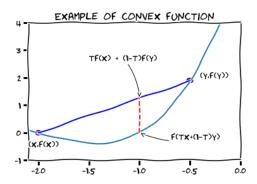


FIGURE 1. In convex functions, the segment joining two points of the graph is always above the graph.

that the function is *strictly convex*. A function f is said to be *concave* (resp. *strictly concave*) if -f is convex (resp. strictly convex).

EXAMPLE 1.3 (Rosenbrock Functions). Given strictly positive parameters a, b > 0, consider the (a, b)-Rosenbrock function $\mathcal{R}_{a,b} \colon \mathbb{R}^2 \to \mathbb{R}$ defined by:

$$\mathcal{R}_{a,b}(x_1, x_2) = (a - x_1)^2 + b(x_2 - x_1^2)^2.$$

The image of $\mathcal{R}_{a,b}$ is the interval $[0,\infty)$. Indeed, note first that $\mathcal{R}_{a,b}(x) \geq 0$ for all $x \in \mathbb{R}^2$. Zero is attained: $\mathcal{R}_{a,b}(a,a^2) = 0$. Note also that $\mathcal{R}_{a,b}(x_1,0) = (a-x_1)^2 + bx_1^4$ is a polynomial of degree 4, hence unbounded for $x_1 \in \mathbb{R}$. Figure 2 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

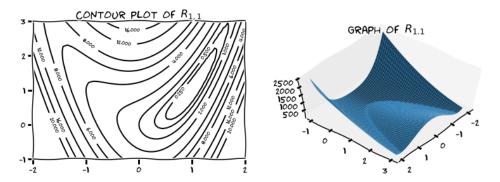


FIGURE 2. Details of the graph of $\mathcal{R}_{1,1}$

This is a good spot to introduce the goal of these notes. The main purpose of *optimization* is the search for *extrema* of real-valued functions. Given a set $D \subset \mathbb{R}^d$, and a real-valued function $f: D \to \mathbb{R}$, we say that a point $x^* \in D$ is:

- (a) A global minimum for f on D if $f(x^*) \leq f(x)$ for all $x \in D$.
- (b) A global maximum for f on D if $f(\mathbf{x}^*) \geq f(\mathbf{x})$ for all $\mathbf{x} \in D$.
- (c) A strict global minimum for f on D if $f(\mathbf{x}^*) < f(\mathbf{x})$ for all $\mathbf{x} \in D \setminus \{\mathbf{x}^*\}$.
- (d) A strict global maximum for f on D if $f(\mathbf{x}^*) > f(\mathbf{x})$ for all $\mathbf{x} \in D \setminus \{\mathbf{x}^*\}$.
- (e) A local minimum for f on D if there exists $\delta > 0$ so that $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in B_{\delta}(\mathbf{x}^*) \cap D$.
- (f) A local maximum for f on D if there exists $\delta > 0$ so that $f(\mathbf{x}^*) \geq f(\mathbf{x})$ for all $\mathbf{x} \in B_{\delta}(\mathbf{x}^*) \cap D$.
- (g) A local minimum for f on D if there exists $\delta > 0$ so that $f(x^*) < f(x)$ for all $x \in B_{\delta}(x^*) \cap D$, $x \neq x^*$.
- (h) A local maximum for f on D if there exists $\delta > 0$ so that $f(\mathbf{x}^*) > f(\mathbf{x})$ for all $\mathbf{x} \in B_{\delta}(\mathbf{x}^*) \cap D$, $\mathbf{x} \neq \mathbf{x}^*$.

Let's play around with some more examples of functions, before we proceed to techniques for finding extrema:

EXAMPLE 1.4 (Bilinear Forms). Let $\mathbf{A} = \begin{bmatrix} a_{jk} \end{bmatrix}_{j,k=1}^d$ be a square matrix with real coefficients. Considering elements in \mathbb{R}^d as horizontal matrices, and by means of matrix products, we construct functions $\mathcal{B}_{\mathbf{A}} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ given by

$$\mathcal{B}_{\boldsymbol{A}}(\boldsymbol{x},\boldsymbol{y}) = \begin{bmatrix} x_1 \cdots x_d \end{bmatrix} \begin{bmatrix} a_{11} & \cdots & a_{1d} \\ \vdots & \ddots & \vdots \\ a_{d1} & \cdots & a_{dd} \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_d \end{bmatrix}$$

We call functions constructed in this way bilinear forms.

PROBLEM 1.2. Prove that, if the associated matrix is symmetric $(A = A^{\mathsf{T}})$, then $\mathcal{B}_{A}(x,y) = \mathcal{B}_{A}(y,x)$ for all $x,y \in \mathbb{R}^{d}$.

EXAMPLE 1.5 (Quadratic Forms). Each symmetric bilinear form has an associated quadratic form: A function $Q_A : \mathbb{R}^d \to \mathbb{R}$ constructed as follows:

$$Q_{\mathbf{A}}(\mathbf{x}) = \mathcal{B}_{\mathbf{A}}(\mathbf{x}, \mathbf{x}) = \begin{bmatrix} x_1 \cdots x_d \end{bmatrix} \begin{bmatrix} a_{11} & \cdots & a_{1d} \\ \vdots & \ddots & \vdots \\ a_{1d} & \cdots & a_{dd} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$

We say that the quadratic form (or the associated matrix) is:

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

EXAMPLE 1.6 (Inner products). We say that a symmetric bilinear form \mathcal{B}_{A} is an *inner product* if its associated quadratic form is positive definite. By extension, we call an inner product any function $\mathcal{F} \colon \mathbb{R}^{d} \times \mathbb{R}^{d} \to \mathbb{R}$ that satisfies the following four properties for all $x, y, z \in \mathbb{R}^{d}, \lambda \in \mathbb{R}$:

- (a) $\mathcal{F}(x + y, z) = \mathcal{F}(x, z) + \mathcal{F}(y, z)$.
- (b) $\mathcal{F}(\lambda \boldsymbol{x}, \boldsymbol{y}) = \lambda \mathcal{F}(\boldsymbol{x}, \boldsymbol{y}).$
- (c) $\mathcal{F}(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{F}(\boldsymbol{y}, \boldsymbol{x}).$
- (d) $\mathcal{F}(\boldsymbol{x}, \boldsymbol{x}) \geq 0$, $\mathcal{F}(\boldsymbol{x}, \boldsymbol{x}) = 0$ if and only if $\boldsymbol{x} = \boldsymbol{0}$.

PROBLEM 1.3. Prove that $\langle \cdot, \cdot \rangle \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ given by

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \sum_{k=1}^{d} x_k y_k$$

is an inner product. What is the matrix associated to its corresponding bilinear form?

PROBLEM 1.4. Prove that, if f is a linear function, then there exist a unique $a_0 \in \mathbb{R}^d$ so that $f(x) = \langle a_0, x \rangle$ for all $x \in \mathbb{R}^d$.

PROBLEM 1.5. We say that $\tau \colon \mathbb{R}^d \to \mathbb{R}^d$ is a translation if there exist a fixed $\boldsymbol{x}_0 \in \mathbb{R}^d$ so that $\tau(\boldsymbol{x}) = \boldsymbol{x} + \boldsymbol{x}_0$ for all $\boldsymbol{x} \in \mathbb{R}^d$.

An affine function $h: \mathbb{R}^d \to \mathbb{R}$ is a composition of a linear function $f: \mathbb{R}^d \to \mathbb{R}$ with a translation $\tau: \mathbb{R} \to \mathbb{R}$.

Prove that for each affine function h there exist a unique $\mathbf{a}_0 \in \mathbb{R}^d$ and a unique $\lambda_0 \in \mathbb{R}$ so that $h(\mathbf{x}) = \lambda_0 + \langle \mathbf{a}_0, \mathbf{x} \rangle$ for all $\mathbf{x} \in \mathbb{R}^d$. Use this result to prove that the graph of an affine function is a hyperplane in \mathbb{R}^{d+1} .

EXAMPLE 1.7 (Norms). A norm in \mathbb{R}^d is a function $\|\cdot\| \colon \mathbb{R}^d \to \mathbb{R}$ that satisfies the following properties: For all $x, y \in \mathbb{R}^d$, and for all $\lambda \in \mathbb{R}$,

- (a) $\|x\| \ge 0$.
- (b) $\|\boldsymbol{x}\| = 0$ if and only if $\boldsymbol{x} = \boldsymbol{0}$
- (c) $\|\lambda \boldsymbol{x}\| = |\lambda| \|\boldsymbol{x}\|$.
- (d) Triangle inequality: $\|x + y\| \le \|x\| + \|y\|$.

PROBLEM 1.6. Consider the function $\|\cdot\|: \mathbb{R}^d \to \mathbb{R}$ defined by

$$\|\boldsymbol{x}\| = \langle \boldsymbol{x}, \boldsymbol{x} \rangle^{1/2}.$$

- (a) Prove that $\|\cdot\|$ is a norm
- (b) Prove the Cauchy-Schwartz inequality: For all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$,

$$|\langle \boldsymbol{x}, \boldsymbol{y} \rangle| \leq ||\boldsymbol{x}|| ||\boldsymbol{y}||.$$

2. Topology

The norm introduced in Example 1.7 induces a metric d: $\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ on the space \mathbb{R}^d :

$$d(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\| \text{ for any } \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d.$$

Metrics allow us to measure distance between elements. These are the four main properties of these objects: Given $x, y, z \in \mathbb{R}^d$,

Separation property: $d(x, y) \ge 0$.

Identity of indiscernibles: d(x, y) = 0 if and only if x = y.

Symmetry: d(x, y) = d(y, x).

Triangle inequality: $d(x, z) \le d(x, y) + d(y, z)$.

Metric spaces like $(\mathbb{R}^d, d(\cdot, \cdot))$ inherit a topology in a natural manner, as explained below.

We define the *open ball* of radius r > 0 about \boldsymbol{x} as the set $B_d(\boldsymbol{x}, r) = \{\boldsymbol{y} \in \mathbb{R}^d : \|\boldsymbol{x} - \boldsymbol{y}\| < r\}$. We say \boldsymbol{x} is an interior point of $D \subset \mathbb{R}^d$ if $\boldsymbol{x} \in D$ and there exists r > 0 so that $B_d(\boldsymbol{x}, r) \subset D$. A subset $G \subset \mathbb{R}^d$ is said to be open if all its points are interior.

A neighborhood of the point x is any subset of \mathbb{R}^d that contains an open ball about x as subset.

A sequence $(\boldsymbol{x}_n)_{n\in\mathbb{N}}$ in \mathbb{R}^d is an enumerated collection of elements of \mathbb{R}^d in which repetitions are allowed. A sequence is said to *converge* to the limit $\boldsymbol{x}\in\mathbb{R}^d$ if and only if for every $\varepsilon>0$ there exists $N=N(\varepsilon)\in\mathbb{N}$ so that $\|\boldsymbol{x}_n-\boldsymbol{x}\|<\varepsilon$ for all $n\geq N$. We write then

$$x = \lim_{n \to \infty} x_n = \lim_n x_n$$
, or $\lim_{n \to \infty} ||x_n - x|| = \lim_n ||x_n - x|| = 0$.

We say that $(\boldsymbol{x}_n)_{n\in\mathbb{N}}$ is a Cauchy sequence if for every $\varepsilon > 0$ there exists $N = N(\varepsilon) \in \mathbb{N}$ so that for any $m, n \geq N$, $\|\boldsymbol{x}_n - \boldsymbol{x}_m\| < \varepsilon$.

PROBLEM 1.7 (Completeness of Euclidean spaces). Prove that all Cauchy sequences converge in \mathbb{R}^d (**Hint**: this is direct consequence of the completeness of \mathbb{R} , which you should also prove).

The complement of an open set is called *closed*. In \mathbb{R}^d , all subsets F are closed if and only if they are *sequentially closed*: If $\mathbf{x}_n \in F$ for all $n \in \mathbb{N}$ and $\lim_n ||\mathbf{x}_n - \mathbf{x}|| = 0$, then $\mathbf{x} \in F$.

We say D is bounded if there exists M > 0 so that $D \subset B_d(\mathbf{0}, M)$. A bounded and closed subset of \mathbb{R}^d is called *compact*.

Theorem 2.1 (Bolzano-Weierstrass). Every sequence in a compact subset $K \subset \mathbb{R}^d$ contains a convergent subsequence.

PROBLEM 1.8. Prove Theorem 2.1 for a closed interval $K = [a, b] \subset \mathbb{R}$.

3. Analysis

A real-valued function f is said to be *continuous* at \mathbf{x}_0 if for any $\varepsilon > 0$ there exists $\delta = \delta(\varepsilon) > 0$ so that $|f(\mathbf{x}) - f(\mathbf{x}_0)| < \varepsilon$ for all $x \in B_d(\mathbf{x}_0, \delta)$.

Equivalently, f is continuous at x_0 if $\lim_n f(x_n) = f(x_0)$ for any sequence $(x_n)_{n\in\mathbb{N}}$ satisfying $\lim_n x_n = x_0$.

We say that f is continuous in $D \subset \mathbb{R}^d$ if f is continuous at all points $x \in D$. The image of a continuous functions enjoys nice properties, which are key to the pursue of extrema. Let's start with two basic Theorems.

THEOREM 3.1 (Bounded Value Theorem). The image f(K) of a continuous real-valued function $f: \mathbb{R}^d \to \mathbb{R}$ on a compact set K is bounded: there exists M > 0 so that $|f(\mathbf{x})| \leq M$ for all $\mathbf{x} \in K$.

THEOREM 3.2 (Extreme Value Theorem). A continuous real-valued function $f: K \to \mathbb{R}$ on a compact set $K \subset \mathbb{R}^d$ takes on minimal and maximal values on K.

Theorem 3.2 guarantees the existence of global *extrema* (maxima/minima) for continuous real-valued functions over compact subsets. What if we do not have compactness?

EXAMPLE 1.8 (Coercive Functions). A continuous real-valued function $f: \mathbb{R}^d \to \mathbb{R}$ is said to be *coercive* if the values of $f(\boldsymbol{x})$ cannot remain bounded on any non-bounded set $A \subset \mathbb{R}^d$:

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

A coercive function always has a global minimum. Indeed: 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, the set $K_r = \{\boldsymbol{x} \in \mathbb{R}^d : \|\boldsymbol{x}\| \le r\}$ is compact. The continuity of f guarantees a global minimum $\boldsymbol{x}^* \in K_r$ with $f(\boldsymbol{x}^*) \le f(\boldsymbol{0})$. It is then $f(\boldsymbol{x}^*) \le f(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^d$ trivially.

How about local extrema? Continuity may not be enough:

A real-valued function f is said to be differentiable at \mathbf{x}_0 if there exists a linear function $J \colon \mathbb{R}^d \to \mathbb{R}$ so that

$$\lim_{h \to 0} \frac{|f(x_0 + h) - f(x_0) - J(h)|}{\|h\|} = 0$$

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} . It is the behavior of the interaction of the rest of the graph with this hyperplane what will give us clues to the nature of possible extrema.

EXAMPLE 1.9. Consider a real-valued function $f: \mathbb{R} \to \mathbb{R}$ of a real variable. To prove differentiability at a point x_0 , we need a linear function: J(h) = ah for some $a \in \mathbb{R}$. Notice how in that case,

$$\frac{|f(x_0+h)-f(x_0)-J(h)|}{|h|} = \left|\frac{f(x_0)-f(x_0)}{h}-a\right|;$$

therefore, we could pick $a = \lim_{h\to 0} h^{-1} (f(x_0 + h) - f(x_0))$ —this is the definition of derivative we learned in Calculus.

3. ANALYSIS

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PROBLEM 1.9. Let $f: \mathbb{R}^d \to \mathbb{R}$ be a real-valued function. To prove that f is differentiable at a point $\mathbf{x}_0 \in \mathbb{R}^d$ we need a linear function $J(h) = \langle \mathbf{a}, h \rangle$ for some $\mathbf{a} \in \mathbb{R}^d$. Prove that in this case, we can use

$$\boldsymbol{a} = \nabla f(\boldsymbol{x}_0) = \left(\frac{\partial f}{\partial x_1}(\boldsymbol{x}_0), \dots, \frac{\partial f}{\partial x_d}(\boldsymbol{x}_0)\right).$$

EXAMPLE 1.10 (Weierstrass Function). For any positive real numbers a, b satisfying 0 < a < 1 < b and $ab \ge 1$, consider the Weierstrass function $W_{a,b} : \mathbb{R} \to \mathbb{R}$ given by

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

This function is continuous everywhere, yet *nowehere* differentiable! For a proof, see e.g. [1]

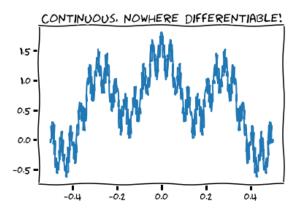


FIGURE 3. Detail of the graph of $W_{0.5,7}$

It is possible to extend the notion to higher derivatives. We would say, for instance, that a function is *twice differentiable* if the derivative is differentiable. For the case of such a real-valued function $f: \mathbb{R}^d \to \mathbb{R}$, this would mean in particular that all second partial derivatives exist, and are continuous over the domain of f.

We define for these functions the *Hessian* of f at $x \in D$ to be the following matrix of second partial derivatives:

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

The following three results aid in our search for local extrema for twice-differentiable real-valued functions of one variable.

THEOREM 3.3 (Rolle's Theorem). If $f:[a,b] \to \mathbb{R}$ is a continuous function on a closed interval [a,b], differentiable on (a,b), and f(a)=f(b), then there exists $c \in (a,b)$ so that f'(c)=0.

THEOREM 3.4 (Mean Value Theorem). If $f:[a,b] \to \mathbb{R}$ is a continuous function on the closed interval [a,b] and differentiable on (a,b), then there exists $c \in (a,b)$ so that

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$

THEOREM 3.5 (Extended Law of the Mean). If $f: D \to \mathbb{R}$ is a twice differentiable function on a domain $D \subset \mathbb{R}$ containing the closed interval [a,b], then there exists $c \in (a,b)$ so that

$$f(b) = f(a) + f'(a)(b-a) + \frac{1}{2}f''(c)(b-a)^2$$

This last result can be extended to a real-valued function $f: \mathbb{R}^{\to} \mathbb{R}$ as follows:

THEOREM 3.6 (Taylor). Given two points $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$, let $f: G \to \mathbb{R}$ be a twice-differentiable real-valued function on an open set $G \subset \mathbb{R}^d$ containing the segment $[\mathbf{a}, \mathbf{b}] = {\mathbf{a} + t(\mathbf{b} - \mathbf{a}) : t \in [0, 1]}$. There exists $\mathbf{c} \in [\mathbf{a}, \mathbf{b}]$ so that

$$f(x) = f(a) + \langle \nabla f(a), x - a \rangle + \frac{1}{2} \mathcal{Q}_{\mathbf{Hess}f(c)}(x - a)$$

EXAMPLE 1.11 (Rosenbrock functions, continued). In Example 1.3 we showed that the image of $\mathcal{R}_{a,b}$ is the interval $[0,\infty)$. We also found (by inspection) that the point (a,a^2) is a global minimum for this function. A straightforward computation shows that it is actually a strict global minimum. A different approach to obtain this result can be obtained using the previous technique:

• Notice $\mathcal{R}_{a,b}$ is twice differentiable. Its gradient and Hessian are given respectively by

$$\nabla \mathcal{R}_{a,b}(\mathbf{x}) = (2(x_1 - a) + 4bx(x_1^2 - x_2), b(x_2 - x_1^2))$$

$$\text{Hess} \mathcal{R}_{a,b}(\mathbf{x}) = \begin{bmatrix} 12bx_1^2 - 4bx_2 + 2 & -4bx_1 \\ -4bx_1 & 2b \end{bmatrix}$$

- The search for critical points $\nabla \mathcal{R}_{a,b} = \mathbf{0}$ gives only the point (a, a^2) .
- The Hessian at that point is positive definite:

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

4. Optimization

Notes

$CHAPTER \ 2$

Unconstrained Optimization via Calculus

Bibliography

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