Chapter 2: Unconstrained Extrema

Math 368

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Types of Sets

Definition

For $\mathbf{p} \in \mathbb{R}^n$ and $r > 0$, the **open ball about p of radius** r is the set

$$\mathbf{B}(\mathbf{p}, r) = \{ \mathbf{x} \in \mathbb{R}^n : \|\mathbf{x} - \mathbf{p}\| < r \}.$$

The **closed ball about p of radius** r is the set

$$\overline{\mathbf{B}}(\mathbf{p}, r) = \{ \mathbf{x} \in \mathbb{R}^n : \|\mathbf{x} - \mathbf{p}\| \leq r \}.$$

Definition

The **complement** of a set $\mathbf{S}$ in $\mathbb{R}^n$ are the points not in $\mathbf{S}$,

$$\mathbf{S}^c = \mathbb{R}^n \smallsetminus \mathbf{S} = \{ \mathbf{x} \in \mathbb{R}^n : \mathbf{x} \notin \mathbf{S} \}.$$

Boundary

Definition

The **boundary** of **S** is the set of all points which have

points arbitrarily close in both **S** and $\mathbf{S}^c$,

$\partial(\mathbf{S}) = \{\, \mathbf{x} \in \mathbb{R}^n : \mathbf{B}(\mathbf{x}, r) \cap \mathbf{S} \neq \emptyset \;\; \& \;\; \mathbf{B}(\mathbf{x}, r) \cap \mathbf{S}^c \neq \emptyset \;\; \text{for all} \;\; r > 0 \,\}$.

Example

The boundary of an open or a closed ball is the same

$$\partial(\mathbf{B}(\mathbf{p}, r)) = \partial(\overline{\mathbf{B}}(\mathbf{p}, r)) = \{\, \mathbf{x} \in \mathbb{R}^n : \|\mathbf{x} - \mathbf{p}\| = r \,\}.$$

Example

S bounded polyhedral set $x_1 + x_2 \leq 100$, $5x_1 + 10x_2 \leq 800$,

$2x_1 + x_2 \leq 150$, $0 \leq x_1$, $0 \leq x_2$.

Boundary is the polygonal closed curve made up of five line segments.

Closed and Open Sets

Definition

A set $\mathbf{S} \subset \mathbb{R}^n$ is **open** p.t.

for each point $\mathbf{x}_0 \in \mathbf{S}$, all nearby points are also in $\mathbf{S}$,

i.e., there exists an $r > 0$ s.t. $\mathbf{B}(\mathbf{x}_0, r) \subset \mathbf{S}$.

Same as: $\mathbf{S} \cap \partial(\mathbf{S}) = \emptyset$, none of boundary of $\mathbf{S}$ is in $\mathbf{S}$.

Definition

A set $\mathbf{S} \subset \mathbb{R}^n$ is said to be **closed** p.t.

all its boundary is a contained in $\mathbf{S}$, $\partial(\mathbf{S}) \subset \mathbf{S}$,

Same as: $\mathbf{S} = \{\, \mathbf{p} : \mathbf{B}(\mathbf{p}, r) \cap \mathbf{S} \neq \emptyset$ for all $r > 0 \,\}$.

Since $\partial(\mathbf{S}) = \partial(\mathbf{S}^c)$, it follows that $\mathbf{S}$ is open iff $\mathbf{S}^c$ is closed.

Examples of Open and Closed Sets, continued

Example

In $\mathbb{R}$, the intervals (a, b), (a, ∞), and $(-\infty, b)$ are open;

$[a, b]$, $[a, \infty)$, and $(-\infty, b]$ are closed.

$[a, b)$ and $(a, b]$ are neither open nor closed.

$(-\infty, \infty)$ is both open and closed in $\mathbb{R}$.

Example

$\mathbb{R}^n$ and $\emptyset$ are both open and closed in $\mathbb{R}^n$.

Examples of Open and Closed Sets

Example

An open ball $\mathbf{B}(\mathbf{p}, r)$ is open:

$\partial(\mathbf{B}(\mathbf{p}, r)) \cap \mathbf{B}(\mathbf{p}, r) = \emptyset$, so open.

Or: For $\mathbf{x}_0 \in \mathbf{B}(\mathbf{p}, r)$, let $r' = r - \|\mathbf{x}_0 - \mathbf{p}\| > 0$.

If $\mathbf{x} \in \mathbf{B}(\mathbf{x}_0, r')$,

$\|\mathbf{x} - \mathbf{p}\| \leq \|\mathbf{x} - \mathbf{x}_0\| + \|\mathbf{x}_0 - \mathbf{p}\| < r' + \|\mathbf{x}_0 - \mathbf{p}\| = r$,

$\mathbf{x} \in \mathbf{B}(\mathbf{p}, r)$, and $\mathbf{B}(\mathbf{x}_0, r') \subset \mathbf{B}(\mathbf{p}, r)$.

This shows that $\mathbf{B}(\mathbf{p}, r)$ is open.

Therefore, $\mathbf{B}(\mathbf{p}, r)^c$ is closed.

Examples of Open and Closed Sets, continued

Example

Since $\partial(\overline{\mathbf{B}}(\mathbf{p}, r)) \subset \overline{\mathbf{B}}(\mathbf{p}, r)$, closed ball $\overline{\mathbf{B}}(\mathbf{p}, r)$ is closed.

Or: For $\mathbf{x}_0 \in \overline{\mathbf{B}}(\mathbf{p}, r)^c$, let $r' = \|\mathbf{p} - \mathbf{x}_0\| - r > 0$.

If $\mathbf{x} \in \mathbf{B}(\mathbf{x}_0, r')$,

$$\|\mathbf{x} - \mathbf{p}\| \geq \|\mathbf{p} - \mathbf{x}_0\| - \|\mathbf{x}_0 - \mathbf{x}\| > \|\mathbf{p} - \mathbf{x}_0\| - r' = r,$$

$\mathbf{x} \in \mathbf{B}(\mathbf{p}, r)^c$, $\mathbf{B}(\mathbf{x}_0, r') \subset \overline{\mathbf{B}}(\mathbf{p}, r)^c$, and $\overline{\mathbf{B}}(\mathbf{p}, r)^c$ is open.

Therefore, $\overline{\mathbf{B}}(\mathbf{p}, r)$ is closed.

Interior and Closure

Definition

interior of $\mathbf{S} \subset \mathbb{R}^n$ is set with boundary removed,

$$\text{int}(\mathbf{S}) = \mathbf{S} \smallsetminus \partial(\mathbf{S}) = \{\mathbf{p} : \mathbf{p} \in \mathbf{S} \ \ \& \ \ \mathbf{p} \notin \partial(\mathbf{S})\}.$$

$$= \{\, \mathbf{p} \in \mathbf{S} : \exists \ r > 0 \ \text{ with } \ \mathbf{B}(\mathbf{p}, r) \subset \mathbf{S} \,\}.$$

Largest open set contained in $\mathbf{S}$.

Definition

The **closure** of $\mathbf{S} \subset \mathbb{R}^n$,

$$\text{cl}(\mathbf{S}) = \overline{\mathbf{S}} = \mathbf{S} \cup \partial(\mathbf{S}) = \{\, \mathbf{p} : \mathbf{B}(\mathbf{p}, r) \cap \mathbf{S} \neq \emptyset \ \text{ for all } \ r > 0 \,\}.$$

Smallest closed set containing $\mathbf{S}$.

$\mathbf{S}$ is closed iff $\mathbf{S} = \text{cl}(\mathbf{S})$.

$\partial(\mathbf{S}) = \text{cl}(\mathbf{S}) \smallsetminus \text{int}(\mathbf{S})$.

Examples of Interior and Closure

Example

Intervals in $\mathbb{R}$: $\quad \text{int}([0,1]) = (0,1)$,

$$\text{cl}((0,1)) = [0,1],$$

$$\partial([0,1]) = \partial((0,1)) = \{0,1\},$$

$$\text{cl}\,(\mathbb{Q} \cap (0,1)) = [0,1], \qquad \mathbb{Q} \text{ rationals}$$

$$\text{int}\,(\mathbb{Q} \cap (0,1)) = \emptyset,$$

$$\partial\,(\mathbb{Q} \cap (0,1)) = [0,1].$$

Example

In $\mathbb{R}^n$,

$$\text{int}\,\overline{\mathbf{B}}(\mathbf{a}, r) = \mathbf{B}(\mathbf{a}, r) \quad \text{and} \quad \text{cl}\,\mathbf{B}(\mathbf{a}, r) = \overline{\mathbf{B}}(\mathbf{a}, r).$$

Bounded and Compact Sets

To be certain that a max exists, domain cannot “go off to infinity”.

Definition

A set $\mathbf{S} \subset \mathbb{R}^n$ is **bounded** p.t. there exists $r > 0$ s.t. $\mathbf{S} \subset \overline{\mathbf{B}}(\mathbf{0}, r)$,

i.e., $\|\mathbf{x}\| \leq r$ for all $\mathbf{x} \in \mathbf{S}$.

Definition

A set $\mathbf{S} \subset \mathbb{R}^n$ is called **compact** p.t. it is closed and bounded.

In analysis, a compact set is defined in terms of convergent sequences

Then a theorem says a closed bounded subsets of $\mathbb{R}^n$ are compact.

Empty set is compact because the hypothesis is satisfied vacuously.

Discontinuous functions

For $f : \mathbb{R} \to \mathbb{R}$, intuitive defn of continuous fn is that

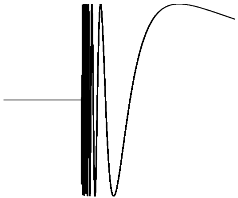
its graph can be drawn without lifting the pen.

$$f(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0, \end{cases}$$

has a **jump** at $x = 0$, so is discontinuous at $x = 0$.

Discontinuous functions

$$g(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ \sin\left(\frac{1}{x}\right) & \text{if } x > 0, \end{cases}$$



$$g\left(\tfrac{1}{n\pi}\right) = 0 \;\;\&\;\; g\left(\frac{2}{(2n+1)\pi}\right) = (-1)^n.$$

oscillates as x approaches 0 and is discontinuous at $x = 0$.

Example in $\mathbb{R}^2$

$$F(x,y) = \begin{cases} \dfrac{y^2}{x^2+y^2} & \text{if } (x,y) \neq (0,0) \\ 0 & \text{if } (x,y) = (0,0) \end{cases}$$

approaches different values along different directions into origin:

$$\lim_{y\to 0} F(0,y) = \lim_{y\to 0} \frac{y^2}{y^2} = 1.$$

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

Limits

Definition

Let $f : \mathbf{S} \subset \mathbb{R}^n \to \mathbb{R}^m$ and $\mathbf{p} \in \mathrm{cl}(\mathbf{S})$.

Limit of $f(\mathbf{x})$ at $\mathbf{p}$ is $\mathbf{L}$, $\lim_{\mathbf{x}\to\mathbf{p}} f(\mathbf{x}) = \mathbf{L}$, p.t.

for every $\epsilon > 0$ there exists a $\delta > 0$ s.t.

$$\|f(\mathbf{x}) - \mathbf{L}\| < \epsilon \text{ whenever } \|\mathbf{x} - \mathbf{p}\| < \delta \text{ and } \mathbf{x} \in \mathbf{S} \smallsetminus \{\mathbf{p}\}.$$

Definition

Limit as x goes to infinity of $f : \mathbb{R} \to \mathbb{R}$:

$$\lim_{x\to\infty} f(x) = L \text{ p.t.}$$

for every $\epsilon > 0$ there exists K s.t.

$$|f(x) - L| < \epsilon \text{ whenever } x \geq K.$$

Continuity

Definition

$f : \mathbf{S} \subset \mathbb{R}^n \to \mathbb{R}^m$ is **continuous at** $\mathbf{p} \in \mathbf{S}$ p.t.

$\lim_{\mathbf{x}\to\mathbf{p}} f(\mathbf{x}) = f(\mathbf{p})$,

i.e., for every $\epsilon > 0$ there exists a $\delta > 0$ such that

$\|f(\mathbf{x}) - f(\mathbf{p})\| < \epsilon$ whenever $\|\mathbf{x} - \mathbf{p}\| < \delta$ and $\mathbf{x} \in \mathbf{S}$.

This definition means that given a tolerance $\epsilon > 0$ in the values,

there is a tolerance $\delta > 0$ in the input such that

all points within δ of $\mathbf{p}$ have values within ϵ of $f(\mathbf{p})$.

Definition

f is **continuous on a set S** p.t. it is continuous at each $\mathbf{x} \in \mathbf{S}$.

Discussion of Continuity

Consider $g(x) = \sin\left(\frac{1}{x}\right)$,

$$g(0) = 0 = g(x_n) \text{ for } x_n = \frac{1}{n2\pi} > 0,$$

$$g(x_n') = 1 \neq g(0) \text{ for } x_n' = \frac{1}{n2\pi + \frac{\pi}{2}} > 0$$

For arb small $\delta > 0$, $\exists$ both x_n and x_n' within δ of 0.

Not all values close to $g(0) = 0$.

Theorem

$\mathbf{F} : \mathbf{S} \subset \mathbb{R}^n \to \mathbb{R}^m$ *is continuous at* $\mathbf{p}$ *iff*

all coordinate functions F_i *are continuous at* $\mathbf{p}$.

Inverse Images of Sets and Points

Definition

If $f : \mathscr{D} \subset \mathbb{R}^n \to \mathbb{R}^m$ is a function, then

the **inverse image of a subset $\mathbf{U} \subset \mathbb{R}^m$** is

$$f^{-1}(\mathbf{U}) = \{\, \mathbf{x} \in \mathscr{D} : f(\mathbf{x}) \in \mathbf{U} \,\} \subset \mathscr{D}.$$

In this context, f^{-1} is not the inverse function,

but $f^{-1}(\mathbf{U})$ merely denotes points that map into $\mathbf{U}$.

Also consider **inverse image of a point $\mathbf{b} \in \mathbb{R}^m$** or **level set**, which is

$$\begin{aligned} f^{-1}(\mathbf{b}) &= \{\, \mathbf{x} \in \mathscr{D} : f(\mathbf{x}) = \mathbf{b} \,\} \subset \mathscr{D}. \\ &= \{\, \mathbf{x} \in \mathscr{D} : f_i(\mathbf{x}) = b_i \ \text{ for } \ i = 1, \dots, m \,\}. \end{aligned}$$

Continuity in terms of Open and Closed Sets

Theorem

Let $f : \mathscr{D} \subset \mathbb{R}^n \to \mathbb{R}^m$*. Then the following are equivalent.*

(i) f *is continuous on* $\mathscr{D}$*.*

(ii) *For each open set* $\mathbf{V} \subset \mathbb{R}^m$*, there is an open set* $\mathbf{U} \subset \mathbb{R}^n$ *such that* $f^{-1}(\mathbf{V}) = \mathbf{U} \cap \mathscr{D}$*,*

i.e., the inverse image of an open set $f^{-1}(\mathbf{V})$ *is open relative to* $\mathscr{D}$*.*

(iii) *For each closed set* $\mathbf{C} \subset \mathbb{R}^m$*, there is an closed set* $\mathbf{B} \subset \mathbb{R}^n$ *such that* $f^{-1}(\mathbf{C}) = \mathbf{B} \cap \mathscr{D}$*,*

i.e., the inverse image of a closed set $f^{-1}(\mathbf{C})$ *is closed relative to* $\mathscr{D}$*.*

The Simplex is Compact

Let $p_i > 0$ for $1 \le i \le n$ be fixed prices and $w > 0$ be the wealth.

Simplex

$$\mathbf{S} = \{\, \mathbf{x} \in \mathbb{R}^n_+ : p_1 x_1 + \cdots + p_n x_n \le w \,\} \qquad \text{is compact.}$$

Each coordinate $0 \le x_j \le \frac{w}{p_j}$, so $\|\mathbf{x}\| \le \sqrt{n}\, \max_i\{\, |x_i| \,\} \le \sqrt{n}\, \max_i\{\frac{w}{p_i}\}$,

and the set is bounded.

Intuitively, the set is closed because the inequalities are non-strict,

"less than or equal to" or "greater than or equal to".

More formally, $f(\mathbf{x}) = p_1 x_1 + \cdots + p_n x_n$ is linear so continuous.

$[0, w]$ is closed, so the set

$$f^{-1}([0, w]) = \{\, \mathbf{x} \in \mathbb{R}^n : 0 \le f(\mathbf{x}) \le w \,\} \quad \text{is closed.}$$

For $1 \le i \le n$, $g_i(\mathbf{x}) = x_i$ is continuous and $[0, \infty)$ is closed, so

$$g_i^{-1}([0, \infty)) = \{\, \mathbf{x} \in \mathbb{R}^n : 0 \le x_i \,\} \quad \text{is closed.}$$

Combining, $\mathbf{S} = f^{-1}([0, w]) \cap \bigcap_{i=1}^n g_i^{-1}([0, \infty))$ is closed and compact.

Extreme Value Theorem

Similarly, all the feasible sets in linear programming are closed.

If bounded, then compact.

Theorem (Extreme Value Theorem)

Assume that $\mathscr{F} \subset \mathbb{R}^n$ *is a nonempty compact set (closed and bounded), and* $f : \mathscr{F} \to \mathbb{R}$ *is a continuous real valued function.*

Then f *attains a maximum and a minimum on* $\mathscr{F}$*,*

i.e., there exist points $\mathbf{x}_m, \mathbf{x}_M \in \mathscr{F}$ *such that*

$$f(\mathbf{x}_m) \leq f(\mathbf{x}) \leq f(\mathbf{x}_M) \qquad \text{for all } \mathbf{x} \in \mathscr{F}, \qquad \text{so}$$

$$f(\mathbf{x}_m) = \min_{\mathbf{x} \in \mathscr{F}} f(\mathbf{x}), \qquad \text{and}$$

$$f(\mathbf{x}_M) = \max_{\mathbf{x} \in \mathscr{F}} f(\mathbf{x}).$$

Why must $\mathscr{F}$ be compact?

1. $f(x) = x^3$ is unbounded on $\mathbb{R}$

and has neither a maximum nor a minimum.

$f(x)$ is continuous, but $\mathbb{R}$ is not bounded.

2. Same $f(x) = x^3$ on $(-1, 1)$ is bounded, $-1 < f(x) < 1$,

but has no maximum nor minimum on $(-1, 1)$.

$(-1, 1)$ is bounded but not closed.

Examples related to Extreme Value Theorem, 2

3. $g(x) = \tan(x)$ is unbounded on $(-\frac{\pi}{2}, \frac{\pi}{2})$,

does not have a minimum or maximum value,.

$tan(x)$ is not bounded above or below on $(-\frac{\pi}{2}, \frac{\pi}{2})$.

$(-\frac{\pi}{2}, \frac{\pi}{2})$ is bounded but not closed.

4. $h(x) = \arctan(x)$ is bounded on $\mathbb{R}$, $-\frac{\pi}{2} < \arctan(x) < \frac{\pi}{2}$.

limiting values are finite but are not attained,

$$\lim_{x \to \pm\infty} arctan(x) = \pm\frac{\pi}{2}.$$

so $h(x)$ does not have a maximum or minimum.

$\mathbb{R}$ is closed but not bounded and

the image is bounded but not closed.

Why must the function be continuous?

$$f(x) = \begin{cases} \frac{1}{x} & \text{if } x \neq 0 \\ 0 & \text{if } x = 0 \end{cases}$$

is not continuous at $x = 0$ and

has no maximum nor minimum on $[-1, 1]$.

even though $[-1, 1]$ is compact.

Definition

$f : \mathscr{D} \subset \mathbb{R}^n \to \mathbb{R}^m$ is **continuously differentiable on** $\text{int}(\mathscr{D})$, $\mathbf{C^1}$, p.t. all 1st order partial derivatives $\frac{\partial f_i}{\partial x_j}(\mathbf{p})$ exist and are continuous on $\text{int}(\mathscr{D})$.

Derivative of f at $\mathbf{p} \in \text{int}(\mathscr{D})$ is the matrix

$$Df(\mathbf{p}) = \left(\frac{\partial f_i}{\partial x_j}(\mathbf{p}) \right).$$

Definition

For $f : \mathscr{D} \subset \mathbb{R}^n \to \mathbb{R}$, **gradient** of $f(\mathbf{x})$ at $\mathbf{p}$ is

$$\nabla f(\mathbf{p}) = Df(\mathbf{p})^{\mathsf{T}}.$$

Transpose makes derivative (row vector) into a column vector.

Derivative of a Function on Real Variable

For $f : \mathbb{R} \to \mathbb{R}$

$$\lim_{x\to p} \frac{f(x) - f(p)}{x - p} = f'(p) \qquad \text{or}$$

$$\lim_{x\to p} \frac{f(x) - f(p) - f'(p)(x-p)}{|x-p|} = 0.$$

$f(p) + f'(p)(x-p)$ is best affine approximation.

An **affine** function is a constant plus a linear function.

For $x > p$,

$$-\epsilon < \frac{f(x) - f(p) - f'(p)(x-p)}{x-p} < \epsilon$$

$$f(p) + [f'(p) - \epsilon]\,(x-p) < f(x) < f(p) + [f'(p) + \epsilon]\,(x-p)$$

Limit for Differentiation

Theorem

If $f : \mathscr{D} \subset \mathbb{R}^n \to \mathbb{R}^m$ *is* C^1 *on* $\text{int}(\mathscr{D})$ *and* $\mathbf{p} \in \text{int}(\mathscr{D})$, *then*

$$\lim_{\mathbf{x}\to\mathbf{p}} \frac{f(\mathbf{x}) - f(\mathbf{p}) - Df(\mathbf{p})(\mathbf{x}-\mathbf{p})}{\|\mathbf{x}-\mathbf{p}\|} = \mathbf{0}, \quad \textit{or}$$

$$f(\mathbf{x}) = f(\mathbf{p}) + Df(\mathbf{p})\,(\mathbf{x}-\mathbf{p}) + \widetilde{R}_1(\mathbf{p},\mathbf{x})\,\|\mathbf{x}-\mathbf{p}\| \quad \textit{where}$$

$$\lim_{\mathbf{x}\to\mathbf{p}} \widetilde{R}_1(\mathbf{p},\mathbf{x}) = \mathbf{0}.$$

Limit equal $\mathbf{0}$ in the last theorem means that

$$f(\mathbf{p}) + Df(\mathbf{p})(\mathbf{x}-\mathbf{p})$$

is **best affine approximation** of $f(\mathbf{x})$ near $\mathbf{p}$.

Limit in theorem is usually taken as definition of derivative.

Does not calculate matrix $Df(\mathbf{p})$ but is matrix that satisfies this limit

Chain Rule

Theorem (Chain Rule)

If $f : \mathbb{R}^n \to \mathbb{R}^m$ *and* $g : \mathbb{R}^m \to \mathbb{R}^k$ *are* C^1, $\mathbf{p} \in \mathbb{R}^n$ *and* $\mathbf{q} = f(\mathbf{p}) \in \mathbb{R}^m$, *then* $g \circ f : \mathbb{R}^n \to \mathbb{R}^k$ *is* C^1 *and*

$$D(g \circ f)(\mathbf{p}) = Dg(\mathbf{q})\, Df(\mathbf{p}).$$

(order of matrix multiplication matters)

This chain rule agrees with the usual chain rule for partial derivatives:

$$w = g(\mathbf{x}) \in \mathbb{R} \quad \text{and} \quad \mathbf{x} = \mathbf{r}(t) \in \mathbb{R}^n$$

$$\frac{dw}{dt} = Dw(\mathbf{x}(t))\,\frac{d\,\mathbf{r}}{d\,t}(t) = \left(\frac{\partial w}{\partial x_1}, \dots, \frac{\partial w}{\partial x_n}\right)\left(\frac{dx_1}{dt}, \dots, \frac{dx_n}{dt}\right)^{\mathsf{T}}$$

$$= \frac{\partial w}{\partial x_1}\frac{dx_1}{dt} + \cdots + \frac{\partial w}{\partial x_n}\frac{dx_n}{dt} = \sum_i \frac{\partial w}{\partial x_i}\frac{dx_i}{dt} \qquad = \nabla g \cdot \mathbf{r}'(t)$$

Second Derivative or Hessian Matrix

Definition

Let $\mathscr{D} \subset \mathbb{R}^n$ be an open set and $f : \mathscr{D} \to \mathbb{R}$.

f is said to be **twice continuously differentiable** or C^2 p.t.

all second order partial derivatives $\dfrac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{p})$ exists

and are continuous for all $\mathbf{p} \in \mathscr{D}$.

Matrix of second partial derivatives $\left(\dfrac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{p})\right)$ is called

second derivative and is denoted by $D^2 f(\mathbf{p})$.

Some call it **Hessian matrix of f at $\mathbf{p}$**, and denote it by $\mathbf{H}(\mathbf{p})$.

Equality of Cross Partials

Theorem

If $\mathscr{D} \subset \mathbb{R}^n$ *is open and* $f : \mathscr{D} \to \mathbb{R}$ *is* C^2, *then*

$$\frac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{p}) = \frac{\partial^2 f}{\partial x_j \partial x_i}(\mathbf{p}), \qquad \text{for all } 1 \leq i, j \leq n \text{ and all } \mathbf{p} \in \mathscr{D}.$$

i.e., $D^2 f(\mathbf{p})$ *is a symmetric matrix.*

$D^2 f(\mathbf{p})$ defines a quadratic form for $\mathbf{x} \in \mathbb{R}^n$,

$$(\mathbf{x} - \mathbf{p})^{\mathsf{T}} D^2 f(\mathbf{p}) (\mathbf{x} - \mathbf{p}) = \sum_{i,j} \frac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{p})(x_j - p_j)(x_i - p_i)$$

which is used in Taylor's Theorem for several variables.

Taylor's Theorem for Several Variables

Theorem

Assume that $F : \mathscr{D} \subset \mathbb{R}^n \to \mathbb{R}$ *is* C^2 *on* $\text{int}(\mathscr{D})$ *and* $\mathbf{p} \in \text{int}(\mathscr{D})$.

Then

$$F(\mathbf{x}) = F(\mathbf{p}) + DF(\mathbf{p})\,(\mathbf{x} - \mathbf{p}) + \tfrac{1}{2}\,(\mathbf{x} - \mathbf{p})^{\mathsf{T}}\, D^2F(\mathbf{p})\ (\mathbf{x} - \mathbf{p}) + R_2(\mathbf{p}, \mathbf{x})$$

where

$$\lim_{\mathbf{x} \to \mathbf{p}} \frac{R_2(\mathbf{p}, \mathbf{x})}{\|\mathbf{x} - \mathbf{p}\|^2} = 0.$$

If $R_2(\mathbf{p}, \mathbf{x}) = \widetilde{R}_2(\mathbf{p}, \mathbf{x}) \|\mathbf{x} - \mathbf{p}\|^2$ *then,*

$$\lim_{\mathbf{x} \to \mathbf{p}} \widetilde{R}_2(\mathbf{p}, \mathbf{x}) = 0.$$

Remainder $R_2(\mathbf{p}, \mathbf{x})$ goes to zero faster than quadratic term.

Proof of Taylor's Theorem

Let $\mathbf{x}_t = \mathbf{p} + t(\mathbf{x} - \mathbf{p})$ and $g(t) = F(\mathbf{x}_t)$, so

$g(0) = F(\mathbf{p})$, and $g(1) = F(\mathbf{x})$.

For $\mathbf{x}$ near enough to $\mathbf{p}$, $\mathbf{x}_t \in \mathscr{D}$ for $0 \le t \le 1$.

The derivatives of g in terms of partial derivatives of F are

$$g'(t) = \sum_{i=1}^{n} \frac{\partial F}{\partial x_i}(\mathbf{x}_t)(x_i - p_i),$$

$$g'(0) = DF(\mathbf{p})(\mathbf{x} - \mathbf{p}),$$

$$g''(t) = \sum_{\substack{i=1,\dots,n \\ j=1,\dots,n}} \frac{\partial^2 F}{\partial x_j \partial x_i}(\mathbf{x}_t)(x_i - p_i)(x_j - p_j),$$

$$g''(0) = (\mathbf{x} - \mathbf{p})^{\top} D^2 F(\mathbf{p})(\mathbf{x} - \mathbf{p}).$$

Thm follows from Taylor's Thm for a fn of one variable. **QED**

Quadratic Forms

The second derivative determines a quadratic form.

Definition

If $\mathbf{A} = (a_{ij})$ is an $n \times n$ symmetric matrix, then

$$\mathbf{x}^\top \mathbf{A} \mathbf{x} = \sum_{i,j=1}^{n} a_{ij} x_i x_j \qquad \text{for } \mathbf{x} \in \mathbb{R}^n$$

is called a **quadratic form**.

Definition

The quadratic form is called

- **positive definite** p.t. $\mathbf{x}^\top \mathbf{A} \mathbf{x} > 0$ for all $\mathbf{x} \neq \mathbf{0}$,
- **positive semidefinite** p.t. $\mathbf{x}^\top \mathbf{A} \mathbf{x} \geq 0$ for all $\mathbf{x}$,
- **negative definite** p.t. $\mathbf{x}^\top \mathbf{A} \mathbf{x} < 0$ for all $\mathbf{x} \neq \mathbf{0}$,
- **negative semidefinite** p.t. $\mathbf{x}^\top \mathbf{A} \mathbf{x} \leq 0$ for all $\mathbf{x}$.
- **indefinite** p.t. $\mathbf{x}^\top \mathbf{A} \mathbf{x}$ is > 0 for some $\mathbf{x}$ and < 0 for other $\mathbf{x}$.

Principal Submatrices

For symmetric matrix $n \times n$ $\mathbf{A}$, a criteria for positive definite in terms of determinants of $k \times k$ **principal submatrices**

$\mathbf{A}_k = (a_{ij})_{1 \le i,j \le k}$ for $1 \le k \le n$.

$$
\begin{array}{cccc}
\mathbf{A}_1 & \mathbf{A}_2 & \mathbf{A}_3 & \mathbf{A}_4
\end{array}
$$

$$
\left(\begin{array}{c|c|c|c}
a_{11} & a_{12} & a_{13} & a_{14} \\
\cline{1-1}
a_{21} & a_{22} & a_{23} & a_{24} \\
\cline{1-2}
a_{31} & a_{32} & a_{33} & a_{34} \\
\cline{1-3}
a_{41} & a_{42} & a_{43} & a_{44}
\end{array}\right)
$$

$\Delta_k = \det(\mathbf{A}_k)$, $\Delta_1 = a_{11}$, $\Delta_2 = a_{11}a_{22} - a_{12}a_{21}$, ...

Theorem (Test for Definiteness)

Let $\mathbf{A}$ *be an* $n \times n$ *symmetric matrix.*

a. *Following are equivalent:*

- **(i)** $\mathbf{A}$ *is positive definite.*
- **(ii)** *All eigenvalues of* $\mathbf{A}$ *are positive.*
- **(iii)** *Determinant of every principal submatrices is positive,* $\Delta_k = \det(\mathbf{A}_k) > 0$ *for* $1 \leq k \leq n$.
- **(iv)** $\mathbf{A}$ *can be row reduced to triangular matrix with all n positive pivots without row exchanges or scalar multiplications of rows.*

b. *Following are equivalent:*

- **(i)** $\mathbf{A}$ *is negative definite.*
- **(ii)** *All eigenvalues of* $\mathbf{A}$ *are negative.*
- **(iii)** *Determinants of principal submatrices alternate sign,* $(-1)^k \Delta_k = (-1)^k \det(\mathbf{A}_k) > 0$ *for* $1 \leq k \leq n$. $\Delta_1 < 0,\ \Delta_2 > 0,\ \dots$
- **(iv)** $\mathbf{A}$ *can be row reduced to triangular matrix with all n negative pivots without row exchanges or scalar multiplications of rows.*

Theorem (Test for Indefiniteness)

Let $\mathbf{A}$ *be an* $n \times n$ *symmetric matrix.*

c. *(i) and (ii) are equivalent;*
(iii) or (iv) or (v) implies (i) and (ii):

- **(i)** $\mathbf{A}$ *is indefinite.*
- **(ii)** $\mathbf{A}$ *has at least one positive and one negative eigenvalue.*
- **(iii)** $\det(\mathbf{A}) = \det(\mathbf{A}_n) \neq 0$ *and pattern of signs of* $\Delta_k = \det(\mathbf{A}_k)$ *are different than those of both part (a) and (b) (allowing one of other* $\Delta_k = \det(\mathbf{A}_k) = 0$ *).*
- **(iv)** $\mathbf{A}$ *can be row reduced without row exchanges or scalar multiplications of rows and there is some pivot* $p_j > 0$ *and another* $p_k < 0$*.*
- **(v)** $\mathbf{A}$ *cannot be row reduced to an upper triangular matrix without row exchanges.*

Test for Definiteness, continued

A proof of all this theorem except about row reduction is given in
Linear Algebra and Its Applications by Gilbert Strang.

Also see the presentation in online class book

Determinants of principal submatrices or row reduction test
are best methods of determining whether
a symmetric matrix is positive or negative definite.

2.2 Local/Global Extrema

Definition

Let $f : \mathscr{F} \subset \mathbb{R}^n \to \mathbb{R}$.

f has a **maximum** at $\mathbf{x}_M \in \mathscr{F}$ p.t. $f(\mathbf{x}) \leq f(\mathbf{x}_M)$ for all $\mathbf{x} \in \mathscr{F}$.

f has a **local maximum** at $\mathbf{x}_M \in \mathscr{F}$ p.t.

there exists an $r > 0$ such that

$$f(\mathbf{x}) \leq f(\mathbf{x}_M) \qquad \text{for all } \mathbf{x} \in \mathscr{F} \cap \mathbf{B}(\mathbf{x}_M, r).$$

f has a **strict local maximum** at $\mathbf{x}_M$ p.t.

there exists an $r > 0$ such that

$$f(\mathbf{x}) < f(\mathbf{x}_M) \qquad \text{for all } \mathbf{x} \in \mathscr{F} \cap \mathbf{B}(\mathbf{x}_M, r) \smallsetminus \{\mathbf{x}_M\}.$$

An **unconstrained local maximum** is a point $\mathbf{x}_M \in \text{int}(\mathscr{F})$

that is a local maximum of f

Extrema and Critical Points

Similarly, **minimum, local minimum, strict local minimum**,

unconstrained local minimum.

Definition

f has a **(local) extremum** at $\mathbf{p}$ p.t.

it has either a (local) maximum or a (local) minimum at $\mathbf{p}$.

Definition

For a continuous function $f : \mathscr{F} \to \mathbb{R}$, a **critical point** of f is a point $\mathbf{x}_c$

s.t. either (i) $Df(\mathbf{x}_c) = \mathbf{0}$ or (ii) f is not differentiable at $\mathbf{x}$.

Most of our functions are differentiable on the whole domain,

so concentrate on points at which $Df(\mathbf{x}) = \mathbf{0}$.

Extrema are Critical Points

Theorem

If $f : \mathscr{F} \subset \mathbb{R}^n \to \mathbb{R}$ *is* C^1 *on* $\text{int}(\mathscr{F})$ *and*

f *has a unconstrained local extremum at* $\mathbf{x}^* \in \text{int}(\mathscr{F})$,

then $\mathbf{x}^*$ *is a critical point,* $Df(\mathbf{x}^*) = \mathbf{0}$.

Extrema are Critical Points, contin.

Proof.

Assume that the point $\mathbf{x}^*$ is not a critical point and

prove that the f does not have a extremum at $\mathbf{x}^*$.

$\mathbf{v} = Df(\mathbf{x}^*)^{\mathsf{T}} \neq \mathbf{0}$, the gradient, is a nonzero (column) vector.

Line in the direction of the gradient is $\mathbf{x}_t = \mathbf{x}^* + t\,\mathbf{v}$.

Applying the remainder form of the first order approximation.

$$\begin{aligned} f(\mathbf{x}_t) &= f(\mathbf{x}^*) + Df(\mathbf{x}^*)\,(t\,\mathbf{v}) + \widetilde{R}_1(\mathbf{x}^*, \mathbf{x}_t)\,\|t\,\mathbf{v}\| \\ &= f(\mathbf{x}^*) + \mathbf{v}^{\mathsf{T}}(t\,\mathbf{v}) + \widetilde{R}_1(\mathbf{x}^*, \mathbf{x}_t)\,\|t\,\mathbf{v}\| \\ &= f(\mathbf{x}^*) + t\left[\|\mathbf{v}\|^2 + \widetilde{R}_1(\mathbf{x}^*, \mathbf{x}_t)\|\mathbf{v}\|\mathrm{sign}(t)\right] \end{aligned}$$

$$\begin{cases} < f(\mathbf{x}^*) & \text{if } t < 0 \text{ and } t \text{ small enough so that } |\widetilde{R}_1| < \frac{1}{2}\|\mathbf{v}\| \\ > f(\mathbf{x}^*) & \text{if } t > 0 \text{ and } t \text{ small enough so that } |\widetilde{R}_1| < \frac{1}{2}\|\mathbf{v}\| \end{cases}$$

This proves that $\mathbf{x}^*$ is neither a maximum nor a minimum. □

Theorem

Suppose that $f : \mathscr{F} \subset \mathbb{R}^n \to \mathbb{R}$ *is* C^2 *on* $\text{int}(\mathscr{F})$ *and* $\mathbf{x}^* \in \text{int}(\mathscr{F})$.

(a) *If* f *has a local min (resp. local max) at* $\mathbf{x}^*$, *then* $D^2 f(\mathbf{x}^*)$ *is positive (resp. negative) semidefinite.*

(b) *If* $Df(\mathbf{x}^*) = \mathbf{0}$ *and* $D^2 f(\mathbf{x}^*)$ *is positive (resp. negative) definite, then* f *has a strict local min (resp. strict local max) at* $\mathbf{x}^*$.

Proof

(**b**) Assume $D^2 f(\mathbf{x}^*)$ is positive definite. $\{\mathbf{u} : \|\mathbf{u}\| = 1\}$ is compact, so

$$m = \min_{\|\mathbf{u}\|=1} \mathbf{u}^\mathsf{T} D^2 f(\mathbf{x}^*)\, \mathbf{u} > 0,$$

For $\mathbf{x}$ near $\mathbf{x}^*$, let $\mathbf{v} = \mathbf{x} - \mathbf{x}^*$ & $\mathbf{u} = \frac{1}{\|\mathbf{v}\|}\mathbf{v}$,

$$\begin{aligned}(\mathbf{x} - \mathbf{x}^*)^\mathsf{T} D^2 f(\mathbf{x}^*)\, (\mathbf{x} - \mathbf{x}^*) &= (\|\mathbf{v}\|\mathbf{u})^\mathsf{T} D^2 f(\mathbf{x}^*)\, (\|\mathbf{v}\|\mathbf{u}) \\ &= \|\mathbf{v}\|^2 \mathbf{u}^\mathsf{T} D^2 f(\mathbf{x}^*)\, \mathbf{u} \geq m\, \|\mathbf{x} - \mathbf{x}^*\|^2.\end{aligned}$$

Since $Df(\mathbf{x}^*) = \mathbf{0}$, 2nd order Taylor's expansion is

$$f(\mathbf{x}) = f(\mathbf{x}^*) + \tfrac{1}{2}\, (\mathbf{x} - \mathbf{x}^*)^\mathsf{T} D^2 f(\mathbf{x}^*)\, (\mathbf{x} - \mathbf{x}^*) + \widetilde{R}_2(\mathbf{x}^*, \mathbf{x})\, \|\mathbf{x} - \mathbf{x}^*\|^2.$$

There exists a $\delta > 0$ such that

$$|\widetilde{R}_2(\mathbf{x}^*, \mathbf{x})| < \tfrac{1}{4} m \qquad \text{for } \|\mathbf{x} - \mathbf{x}^*\| < \delta.$$

For $\delta > \|\mathbf{x} - \mathbf{x}^*\| > 0$,

$$\begin{aligned} f(\mathbf{x}) &> f(\mathbf{x}^*) + \tfrac{1}{2} m\, \|\mathbf{x} - \mathbf{x}^*\|^2 - \tfrac{1}{4} m\, \|\mathbf{x} - \mathbf{x}^*\|^2 \\ &= f(\mathbf{x}^*) + \tfrac{1}{4} m\, \|\mathbf{x} - \mathbf{x}^*\|^2 > f(\mathbf{x}^*).\end{aligned}$$

QED

Example

Find the critical points and classify them as

local max, local min, or neither for

$$F(x, y, z) = 3x^2y + y^3 - 3x^2 - 3y^2 + z^3 - 3z.$$

A critical point satisfies

$$0 = \frac{\partial F}{\partial x} = 6xy - 6x = 6x(y - 1)$$
$$0 = \frac{\partial F}{\partial y} = 3x^2 + 3y^2 - 6y$$
$$0 = \frac{\partial F}{\partial z} = 3z^2 - 3.$$

From 3rd eq, $z = \pm 1$. From 1st eq, $x = 0$ or $y = 1$.

If $x = 0$, then 2nd eq $0 = 3y(y - 2)$, $y = 0$ or $y = 2$.

Pts: $(0, 0, \pm 1)$ $(0, 2, \pm 1)$.

If $y = 1$, then 2nd eq $0 = 3x^2 - 3$ $x = \pm 1$.

Pt: $(\pm 1, 1, \pm 1)$.

All the critical points: $(0, 0, \pm 1)$, $(0, 2, \pm 1)$, $(\pm 1, 1, \pm 1)$.

Example, continued

The second derivative is $$D^2F(x,y,z) = \begin{bmatrix} 6y-6 & 6x & 0 \\ 6x & 6y-6 & 0 \\ 0 & 0 & 6z \end{bmatrix}.$$

At the critical points

$$D^2F(0,0,\pm 1) = \begin{bmatrix} -6 & 0 & 0 \\ 0 & -6 & 0 \\ 0 & 0 & \pm 6 \end{bmatrix}$$

$$D^2F(0,2,\pm 1) = \begin{bmatrix} 6 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & \pm 6 \end{bmatrix}$$

$$D^2F(\pm 1,1,\pm 1) = \begin{bmatrix} 0 & \pm 6 & 0 \\ \pm 6 & 0 & 0 \\ 0 & 0 & \pm 6 \end{bmatrix}.$$

Example, continued

$$D^2F(x,y,z) = \begin{bmatrix} 6y-6 & 6x & 0 \\ 6x & 6y-6 & 0 \\ 0 & 0 & 6z \end{bmatrix}.$$

Let $\Delta_k = \det(\mathbf{A}_k)$.

$$\Delta_1 = F_{xx} = 6y - 6,$$

$$\Delta_2 = F_{xx}F_{yy} - F_{xy}^2 = (6y-6)^2 - 36x^2, \qquad \text{and}$$

$$\Delta_3 = F_{zz}\,\Delta_2 = 6z\,\Delta_2.$$

Example, continued

$$F_{xx} = 6y - 6, \quad F_{yy} = 6y - 6, \quad F_{xy} = 6x, \quad F_{zz} = 6z.$$

$$\Delta_1 = F_{xx}, \quad \Delta_2 = F_{xx}F_{yy} - F_{xy}^2, \quad \Delta_3 = F_{zz}\Delta_2$$

(x, y, z)	$\Delta_1 = F_{xx}$	F_{yy}	F_{xy}	Δ_2	F_{zz}	Δ_3	Type
$(0, 0, 1)$	-6	-6	0	36	6	216	saddle
$(0, 0, -1)$	-6	-6	0	36	-6	-216	local max
$(0, 2, 1)$	6	6	0	36	6	216	local min
$(0, 2, -1)$	6	6	0	36	-6	-216	saddle
$(\pm 1, 1, \pm 1)$	0	0	± 6	-36	± 6	∓ 216	saddle

$(0, 0, -1)$ is a local max,

$(0, 2, 1)$ is a local min,

other points are neither local max nor local min, saddle points.