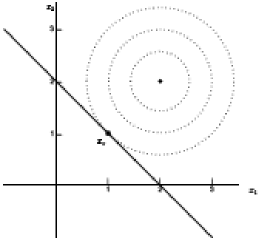
Optimization

Màster de Fonaments de Ciència de Dades

Lecture 1. Optimization. First examples and background

First introductory examples

Problem. *Find the point on the line $x_1 + x_2 = 2$ that is closest to the point $(2,2)^T$.*



The problem can be written as

$$\begin{array}{ll} \text{minimize} & f(x,y) = (x-2)^2 + (y-2)^2, \\ \text{subject to} & x + y = 2. \end{array}$$

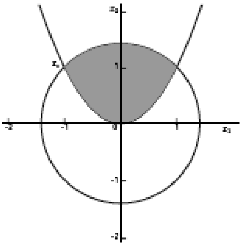
The solution is $(x,y)^T = (1,1)^T$.

First introductory examples

Problem. *Find the point such that:*

$$\begin{array}{ll} \text{minimize} & f(x,y) = x, \\ \text{subject to} & x^2 \leq y, \\ & x^2 + y^2 \leq 2. \end{array}$$

In this example, the (feasible) set where we must look for the solution is defined by multiple constraints.



The solution (optimal point) is $(x,y)^T = (-1,1)^T$.

First introductory examples

Problem. *Find the solution of:*

$$\text{minimize} \quad f(x, y) = (e^x - 1)^2 + (y - 1)^2.$$

This is an example of an **unconstrained** optimization problem.

The **feasible set** here is the entire two-dimensional space.

The solution is $(x, y)^T = (0, 1)^T$, since the function value is zero only at this point and is positive elsewhere.

Introduction

- **What is Optimization?** Given a system or process, find the best solution to this process within (or not) constraints.
- **Objective Function:** Indicator of "goodness" of the solution, e.g., cost, profit, time, etc. In the above examples, the function f.
- **Decision Variables:** Variables that influence process behavior and can be adjusted for optimization. In the above examples, the variables x and y.

- We are interested in a **systematic approach** to the optimization process, and to make it as efficient as possible.

- **Optimization** is also called: *Mathematical Programming*, or *Operations Research.*

Current applications

- In modern times, (linear and nonlinear) optimization is used in optimal engineering design, finance, statistics and many other fields.
- Think of:
  - designing a car with minimal air resistance,
  - designing a bridge of minimal weight that still meets essential specifications,
  - defining a stock portfolio where the risk is minimal and the expected return high,...
- **Rule of thumb:** If you can make a mathematical model of your decision problem, then you can *try to optimize* it!

Optimization viewpoints

- **Mathematician** - characterization of theoretical properties of optimization, convergence, existence, local convergence rates.
- **Numerical Analyst** - implementation of optimization method for efficient and "practical" use. Concerned with fast computations, numerical stability, performance.
- **User** - applies optimization method to real problems. Concerned with reliability, robustness, efficiency, diagnosis, and recovery from failure.
- Optimization is a **fast moving research field**. Currently, there are over 30 journals devoted to optimization with roughly 200 published papers/month.
- In **this course**, we will see only the most **basic concepts, results, and procedures.**

Some classical optimization problems - I

1. Dido's (or isoperimetric) problem. Among all closed plain curves of a given length, find the one that encloses the largest area.
2. Heron's problem. Given two points A and B on the same side of a line L, find a point D on L such that the sum of the distances form A to D and from D to B is a minimum.
3. Snell's law of refraction. Given two points A and B on either side of a horizontal line L separating two (homogeneous) different media, find a point D on L such that the time it takes for a light ray to traverse the path ADB is a minimum.
   Note: In an inhomogeneous medium, light travels from one point to another along the path requiring the shortest time ($v_i = c/n_i$).
4. Euclid (Elements, 4th cent. B.C.). In a given triangle ABC inscribe a parallelogram $ADEF$ ($EF||AB, DE||AC$) of maximal area.
5. Steiner. In the plane of a triangle, find a point (Fermat point) such that the sum of its distances to the vertices of the triangle is minimal

Some classical optimization problems - II

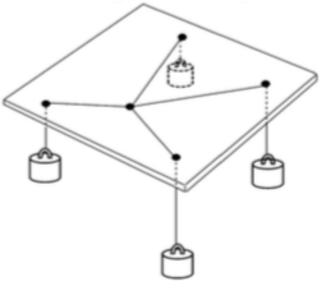
6. Find the maximum of the product of two numbers whose sum is given.
7. Find the maximal area of a right triangle whose small sides have constant sum.
8. In a given circle find a rectangle of maximal area.
9. In a given sphere find a cylinder of maximal volume.
10. Of all rectangular parallelepipeds inscribed in a sphere find the one of maximal volume.
11. Of all rectangular parallelepipeds with square base inscribed in a sphere find the one of maximal volume.
12. The Brachistochrone. Let two points A and B be given in a vertical plane. Find the curve that a point M, moving on a path AMB must follow such that, starting from A with zero velocity, it reaches B in the shortest time under its own gravity.

Some classical optimization problems - III

13. The Fermat point of a set of points. *Given set of points $y_1,\ldots,y_m$ in the plane, find a point x^* whose sum of weighted distances to the given set of points is minimized. Mathematically, the problem is*

$$\min \sum_{i=1}^{m} w_i \|x^* - y_i\|, \quad \textit{subject to } x^* \in \mathbb{R}^2,$$

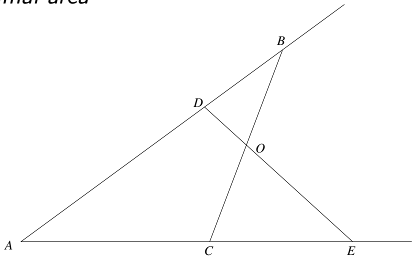
where $w_1, \ldots, w_m$ are given positive real numbers.



Some classical optimization problems - III

Exercise 1. To be delivered before 29-X-2019 as: `Ex01-YourSurname.pdf`.

13. Smallest area problem. *Given an angle with vertex A and a point O in its interior. Pass a line BC through the point O that cuts off from the angle a triangle of minimal area*



Hint: proof that for a triangle of minimal area the segments OB and OC should be equal.

The general optimization problem

Definition:
The general nonlinear optimization (NLO) problem can be written as follows:

$$\begin{array}{lll} \min & f(x), & \\ \text{subject to} & g_i(x) = 0, & i \in I = \{1, ..., m\}, \\ & h_j(x) \leq 0, & j \in J = \{1, ..., p\}, \\ & x \in \mathcal{C}, & \end{array}$$

where $x \in \mathbb{R}^n$, $\mathcal{C} \subset \mathbb{R}^n$ is a certain set, and $f, g_1, ..., g_m, h_1, ..., h_p$ are real-valued functions defined on $\mathcal{C}$.

Terminology:

- The function f is called the objective function of the NLO.
- The set $\mathcal{F}$ defined by:

$$\mathcal{F} = \{x \in \mathcal{C} \ : \ g_i(x) = 0, i = 1, ..., m, \ h_j(x) \leq 0, j = 1, ..., p\},$$

  is called the feasible set (or feasible region).
- If $\mathcal{F} = \emptyset$ then we say that the optimization problem is infeasible.
- If the infimum of f over $\mathcal{F}$ is attained at $x^* \in \mathcal{F}$, then we call x^* an optimal solution of the NLO, and $f(x^*)$ the the optimal (objective) value of the NLO.

Classification of optimization problems

- Unconstrained Optimization: The index sets I and J are empty:

$$g_1 = \ldots = g_m = h_1 = \ldots = h_p = 0,$$

  and $\mathcal{C} = \mathbb{R}^n$.

- Linear Optimization (LO) (Linear programming): The functions $f, g_1, \ldots, g_m, h_1, \ldots, h_p$ are linear (affine: $F(\boldsymbol{x}) = A\boldsymbol{x} + \boldsymbol{b}$) and the set $\mathcal{C}$ either equals to $\mathbb{R}^n$, the positive (negative) orthant $\mathbb{R}^n_+$, or is polyhedral.

- Quadratic Optimization (QO): The objective function f is quadratic:

$$f(\boldsymbol{x}) = \boldsymbol{x}^T Q\boldsymbol{x} + \boldsymbol{c}^T\boldsymbol{x} + \boldsymbol{d},$$

  all the constraint functions $g_1, \ldots, g_m, h_1, \ldots, h_p$ are linear and the set $\mathcal{C}$ is $\mathbb{R}^n$ or the positive (negative) orthant $\mathbb{R}^n_+$, and Q is a $n \times n$ real matrix ($Q \in \mathbb{R}^{n\times n}$).

- Quadratically Constrained Quadratic Optimization: Same as QO, except that the constraint functions are quadratic.

- Convex Quadratic Optimization (CQO).

- Convex Quadratically Constrained Quadratic Optimization:

- ...

A well known application of Quadratic Optimization: Regression problems

- If a system
$$A\boldsymbol{x} = \boldsymbol{b}, \quad A \in \mathbb{R}^{m\times n}, \quad \boldsymbol{x} \in \mathbb{R}^n, \quad \boldsymbol{b} \in \mathbb{R}^m,$$
has more equations than unknowns ($m > n$), then, in general, it has no solution, but we can compute the least squares solution
$$\boldsymbol{x}^* = \min_{\boldsymbol{x}\in\mathbb{R}^n} \|A\boldsymbol{x} - \boldsymbol{b}\|,$$
for the Euclidean norm $\|\boldsymbol{x}\| = \sqrt{\sum_{i=1}^n x_i^2} = \sqrt{\boldsymbol{x}^T\boldsymbol{x}} \geq 0$.
- Note that
$$\begin{aligned} \|A\boldsymbol{x} - \boldsymbol{b}\|^2 &= (A\boldsymbol{x} - \boldsymbol{b})^T(A\boldsymbol{x} - \boldsymbol{b}) \\ &= \boldsymbol{x}^T A^T A\boldsymbol{x} - 2\boldsymbol{b}^T A\boldsymbol{x} + \|\boldsymbol{b}\|^2. \end{aligned}$$
- Note also that if $A \in \mathbb{R}^{m\times n}$, then $A^T A \in \mathbb{R}^{n\times n}$, $\boldsymbol{b}^T A \in \mathbb{R}^n$, and introducing $\boldsymbol{z} = A\boldsymbol{x}$:
$$\boldsymbol{x}^T A^T A\boldsymbol{x} = \boldsymbol{z}^T\boldsymbol{z} = \|\boldsymbol{z}\|^2 \geq 0, \quad \forall \boldsymbol{x} \in \mathbb{R}^n.$$
According to this last inequality, $A^T A$ will be positive definite if and only if for all $\boldsymbol{x} \neq 0$ then $A\boldsymbol{x} \neq 0$, which is equivalent to say that the rank of A is n.

Example of regression problem: Concrete mixing

Mix concrete using n different gravel sizes $s_1, s_2, \ldots, s_n$.

- The ideal mixture is given by $\boldsymbol{c} = (c_1, c_2, \ldots, c_n)$, where c_i $(0 \leq c_i \leq 1)$ is the fraction of size s_i in the mix, and $\sum_{i=1}^{n} c_i = 1$.
- Gravel mixtures come from m different mines.
- The gravel composition at each mine M_j given by $A_j = (a_{1j}, \ldots, a_{nj})$ where $0 \leq a_{ij} \leq 1$ for all $i = 1, \ldots, n$ and $\sum_{i=1}^{n} a_{ij} = 1$

	s_1	$\ldots$	s_n	
M_1	a_{11}	$\ldots$	a_{n1}	$x_1 =$ fraction from M_1 in the mix
$\vdots$	$\vdots$		$\vdots$	$\vdots$
M_m	a_{1m}	$\ldots$	a_{nm}	$x_m =$ fraction from M_m in the mix

In the mix, the amount of grave with size k should be close to c_k.

Concrete mixing: mathematical formulation

Exercise 2. To be delivered before 29-X-2019 as: `Ex02-YourSurname.pdf`.

Find the best possible approximation $x_1, ..., x_m$ of the ideal mixture, $c_1, ..., c_n$, by using the material from the m mines.

Show that the optimal mixture will be the point $\boldsymbol{x}$ such that:

$$\min \ (A\boldsymbol{x} - \boldsymbol{c})^T(A\boldsymbol{x} - \boldsymbol{c}),$$

$$s.t. \quad \sum_{j=1}^{m} x_j = 1, \quad \text{and} \quad x_j \geq 0,$$

where the matrix $A = (A_1, ..., A_m)$ has A_j as columns.

Some mathematical notation and background

Notation and background

- Scalar and cross product
- Lines and planes
- Continuity
- Derivatives
- Gradients
- Approximation of functions

Scalar and cross product

Let $\boldsymbol{x} = (x_1, \dots, x_n)^T, \boldsymbol{y} = (y_1, \dots, y_n)^T \in \mathbb{R}^n$, we define:

- Scalar (dot) product: $\boldsymbol{x} \cdot \boldsymbol{y} = \boldsymbol{x}^T \boldsymbol{y} = x_1 y_1 + \cdots + x_n y_n \in \mathbb{R}$.
- Euclidean norm: $\|\boldsymbol{x}\| = \sqrt{\boldsymbol{x} \cdot \boldsymbol{x}} = \sqrt{\boldsymbol{x}^T \boldsymbol{x}} = \sqrt{x_1^2 + \cdots + x_n^2}$.
- Euclidean distance: $d(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{y} - \boldsymbol{x}\| = \sqrt{(y_1 - x_1)^2 + \cdots + (y_n - x_n)^2}$.
- Cosinus of the angle: $\cos(\widehat{\boldsymbol{x}, \boldsymbol{y}}) = \dfrac{\boldsymbol{x} \cdot \boldsymbol{y}}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|}$.
- Perpendicularity (orthogonality): $\boldsymbol{x} \perp \boldsymbol{y} \quad \Leftrightarrow \quad \boldsymbol{x} \cdot \boldsymbol{y} = 0$.

Let $\boldsymbol{x} = (x_1, x_2, x_3), \boldsymbol{y} = (y_1, y_2, y_3) \in \mathbb{R}^3$, we define:

- Cross product:

$$\boldsymbol{x} \times \boldsymbol{y} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{vmatrix} = \begin{pmatrix} x_2 y_3 - x_3 y_2 \\ x_3 y_1 - x_1 y_3 \\ x_1 y_2 - x_2 y_1 \end{pmatrix}.$$

Note that

$$\boldsymbol{x} \times \boldsymbol{y} \perp \boldsymbol{x} \quad \text{and} \quad \boldsymbol{x} \times \boldsymbol{y} \perp \boldsymbol{y}.$$

Lines and planes

- In $\mathbb{R}^2$: The line determined by the point $\boldsymbol{a} = (a_1, a_2)^T$ and the vector $\boldsymbol{v} = (v_1, v_2)^T$ is

$$\boldsymbol{x} = \boldsymbol{a} + t\boldsymbol{v},\ t \in \mathbb{R} \quad \Leftrightarrow \quad \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} + t \begin{pmatrix} v_1 \\ v_2 \end{pmatrix},\ t \in \mathbb{R},$$

  that can also be written as

$$\frac{x - a_1}{v_1} = \frac{y - a_2}{v_2} \quad \Leftrightarrow \quad Ax + By + C = 0,$$

  with $A = v_2,\ B = -v_1,\ C = -a_1 v_2 + a_2 v_1.$

- In $\mathbb{R}^3$: The line determined by the point $\boldsymbol{a} = (a_1, a_2, a_3)^T$ and the vector $\boldsymbol{v} = (v_1, v_2, v_3)^T$ is

$$\boldsymbol{x} = \boldsymbol{a} + t\boldsymbol{v},\ t \in \mathbb{R} \quad \Leftrightarrow \quad \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} + t \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix},\ t \in \mathbb{R},$$

  that can also be written as

$$\frac{x - a_1}{v_1} = \frac{y - a_2}{v_2} = \frac{z - a_3}{v_3}.$$

Lines and planes

- In $\mathbb{R}^3$: The plane determined by the point $\boldsymbol{a} = (a_1, a_2, a_3)^T$ and the vectors $\boldsymbol{u} = (u_1, u_2, u_3)^T$ and $\boldsymbol{v} = (v_1, v_2, v_3)^T$ is

$$\boldsymbol{x} = \boldsymbol{a} + t\boldsymbol{u} + s\boldsymbol{v} \quad \Leftrightarrow \quad \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} + t \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} + s \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix},$$

  with $t, s \in \mathbb{R}$.

- The above equation of the plane can also be written as

$$\begin{vmatrix} x - a_1 & y - a_2 & z - a_3 \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix} = 0$$

  or as

$$Ax + By + Cz + D = 0,$$

  with $(A, B, C)^T = \boldsymbol{u} \times \boldsymbol{v}$.

Continuity

Consider the function

$$f : \mathcal{C} \subset \mathbb{R}^n \longrightarrow \mathbb{R},$$

we define:

- The domain $\mathcal{C}$ of f as the set of points $\boldsymbol{x} \in \mathbb{R}^n$ where f is defined.
- The graph of f, as the subset of $\mathbb{R}^{n+1}$ defined by:

$$\{(\boldsymbol{x}, z) \in \mathbb{R}^{n+1} : \boldsymbol{x} = (x_1, \ldots, x_n)^T \in \mathcal{C} \subset \mathbb{R}^n,\ z = f(\boldsymbol{x}) \in \mathbb{R}\} \subset \mathbb{R}^{n+1}\}.$$

- For each $c \in \mathbb{R}$, the level set c of f as:

$$f^{-1}(c) = \{\boldsymbol{x} \in \mathcal{C} \ : \ f(\boldsymbol{x}) = c\} \subset \mathbb{R}^n.$$

- We say that f is continuous at a point $\boldsymbol{a} \in \mathcal{C}$ if and only if

$$\lim_{\boldsymbol{x} \to \boldsymbol{a}} f(\boldsymbol{x}) = f(\boldsymbol{a}).$$

Continuity

Some fundamental properties of continuous functions are:

- The elementary functions of one variable $e^x, \log x, \sin x, \cos x, \ldots$ and the coordinate functions

$$\begin{array}{rccc} x_i : & \mathbb{R}^n & \longrightarrow & \mathbb{R} \\ & \boldsymbol{x} = (x_1, \ldots, x_n)^T & \longrightarrow & x_i \end{array}$$

  are continuous in their domain.

- Addition, substraction, product, division (except at the points where the denominator vanishes) and composition of continuous functions are also continuous functions.

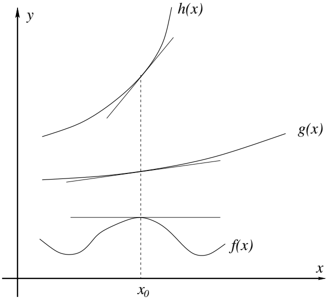
- Given a continuous function

$$f : \mathcal{C} \subset \mathbb{R}^n \longrightarrow \mathbb{R},$$

  such that $\mathcal{C}$ is compact (closed and bounded), then f is bounded and f attaints its maximum and minimum values on $\mathcal{C}$.

Derivatives

- The derivative of a function $y = f(x)$ of a variable x is a measure of the rate at which the value y of the function changes with respect to the change of the variable x.
- If x and y are real numbers, and if the graph of f is plotted against x, the derivative is the slope of this graph at each point.



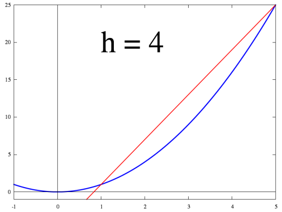
Derivatives

Let f be a real valued function defined in an open neighborhood of a real number a, then:

- The derivative of $y = f(x)$ with respect to x at a is, geometrically, the slope of the tangent line to the graph of f at $(a, f(a))^T$.
- The slope of the tangent line is very close to the slope of the line through $(a, f(a))$ and a nearby point on the graph, for example $(a + h, f(a + h))^T$.
- The slope m of the secant line is

$$m = \frac{\Delta f(a)}{\Delta a} = \frac{f(a+h) - f(a)}{(a+h) - (a)} = \frac{f(a+h) - f(a)}{h}.$$

- A value of h close to zero gives, in general, a good approximation to the slope of the tangent line



Derivatives. Rigorous definition

- Geometrically, the limit of the secant lines is the tangent line. Therefore, the limit of the difference quotient as h approaches zero, if it exists, should represent the slope of the tangent line to $(a, f(a))$.
- This limit is defined to be the derivative of the function f at a:

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}.$$

- When the limit exists, f is said to be differentiable at a.
- Equivalently, the derivative satisfies the property that

$$\lim_{h \to 0} \frac{f(a+h) - f(a) - f'(a) \cdot h}{h} = 0,$$

which has the intuitive interpretation that the tangent line to f at a gives the best linear approximation

$$f(a+h) \approx f(a) + f'(a)h,$$

to f near a.

Derivatives in higher dimensions

- A vector-valued function $\boldsymbol{y}(t)$ of a real variable sends real numbers to vectors in some vector space ($\mathbb{R}^n$).

$$\begin{array}{rccc} \boldsymbol{y}: & \mathbb{R} & \longrightarrow & \mathbb{R}^n \\ & t & \longrightarrow & \boldsymbol{y}(t). \end{array}$$

- A vector-valued function can be split up into its coordinate functions

$$\boldsymbol{y}(t) = (y_1(t), ..., y_n(t))^T.$$

- The derivative of the curve $\boldsymbol{y}(t)$ is defined to be the vector, called the tangent vector, whose coordinates are the derivatives of the coordinate functions

$$\boldsymbol{y}'(t) = (y_1'(t), \ldots, y_n'(t))^T, \quad \text{or equivalently} \quad \boldsymbol{y}'(t) = \lim_{h\to 0} \frac{\boldsymbol{y}(t+h) - \boldsymbol{y}(t)}{h},$$

if the limit exists.

- If $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n$ is the standard basis for $\mathbb{R}^n$, then

$$\boldsymbol{y}(t) = y_1(t)\boldsymbol{e}_1 + \cdots + y_n(t)\boldsymbol{e}_n,$$

and since each of the basis vectors is a constant

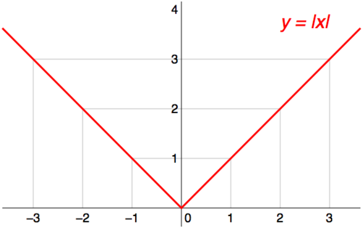
$$\boldsymbol{y}'(t) = y_1'(t)\boldsymbol{e}_1 + \cdots + y_n'(t)\boldsymbol{e}_n.$$

Continuity and differentiability

- **Property:** If
$$\begin{array}{rccc} \boldsymbol{f}: & \mathbb{R}^n & \longrightarrow & \mathbb{R} \\ & \boldsymbol{x} & \longrightarrow & f(\boldsymbol{x}) \end{array}$$
is differentiable at $\boldsymbol{a}$, then f must also be continuous at $\boldsymbol{a}$.

- **Property:** If a function is continuous at a point it may not be differentiable there.

- **Example:** The absolute value function $f(x) = |x|$ is continuous at $x = 0$, but it is not differentiable there, since the tangent slopes do not approach the same value from the left as they do from the right.



Partial derivatives

- If f is a real value function that depends on n variables

$$\begin{array}{rccc} \boldsymbol{f}: & \mathbb{R}^n & \longrightarrow & \mathbb{R} \\ & \boldsymbol{x} & \longrightarrow & f(\boldsymbol{x}) = f(x_1, \ldots, x_n), \end{array}$$

  the partial derivative of $f(\boldsymbol{x})$ in the direction x_i at the point $\boldsymbol{a} = (a_1, \ldots, a_n)^T$ is defined to be:

$$\frac{\partial f}{\partial x_i}(\boldsymbol{a}) = \lim_{h \to 0} \frac{f(a_1, \ldots, a_i + h, \ldots, a_n) - f(a_1, \ldots, a_i, \ldots, a_n)}{h}.$$

- In the above difference quotient, all the variables except x_i are held fixed. That choice of fixed values determines a function of one variable

$$f_{a_1,\ldots,a_{i-1},a_{i+1},\ldots,a_n}(x_i) = f(a_1, \ldots, a_{i-1}, x_i, a_{i+1}, \ldots, a_n),$$

  and, by definition:

$$\frac{df_{a_1,\ldots,a_{i-1},a_{i+1},\ldots,a_n}}{dx_i}(a_i) = \frac{\partial f}{\partial x_i}(\boldsymbol{a}).$$

First and second partial derivatives

Let $\boldsymbol{a} \in \mathcal{C} \subset \mathbb{R}^n$ be a point where the real function

$$f : \mathcal{C} \longrightarrow \mathbb{R},$$

is differentiable.

- **Property:** If a real-valued function f is differentiable at an interior point $\boldsymbol{a} \in \mathcal{C}$, then its first partial derivatives exist at $\boldsymbol{a}$.
- **Definition:** If the partial derivatives are continuous at $\boldsymbol{a}$, then f is said to be continuously differentiable at $\boldsymbol{a}$.
- **Property:** If f is twice differentiable at $\boldsymbol{a} \in \mathcal{C}$, then the second partial derivatives exist there.
- **Definition:** If the second partial derivatives are continuous at $\boldsymbol{a}$, then f is said to be twice continuously differentiable at $\boldsymbol{a}$.
- **Definition:** If f is twice continuously differentiable at $\boldsymbol{a}$ we define the Hessian matrix of f at $\boldsymbol{a}$ as the $n \times n$ symmetric matrix $\nabla^2 f(\boldsymbol{a})$ given by:

$$\nabla^2 f(\boldsymbol{a}) = \left(\frac{\partial^2 f(\boldsymbol{a})}{\partial x_i \partial x_j} \right), \quad i, j = 1, \dots, n.$$

Directional derivatives

- If f is a real-valued function on $\mathbb{R}^n$, then the partial derivatives of f measure its variation in the direction of the coordinate axes.
- If f is a function of x and y ($x, y \in \mathbb{R}$), then its partial derivatives measure the variation in f in the x direction and the y direction. They do not, however, directly measure the variation of f in any other direction, such as along the diagonal line $y = x$.
- These are measured using directional derivatives. Choose a vector

$$\boldsymbol{v} = (v_1, \ldots, v_n)^T.$$

The directional derivative of f in the direction of $\boldsymbol{v}$ at the point $\boldsymbol{x}$ is defined by

$$D_{\boldsymbol{v}} f(\boldsymbol{x}) = \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{v}) - f(\boldsymbol{x})}{h} = \frac{d}{dt}\bigg|_{t=0} f(\boldsymbol{x} + t\boldsymbol{v}) = \sum_{j=1}^{n} \frac{\partial f(\boldsymbol{x})}{\partial x_j} v_j,$$

where we have used the chain rule to get the last equality.

The chain rule

- Let

$$\begin{array}{rccl} \alpha: & I \subset \mathbb{R} & \longrightarrow & C \\ & t & \longrightarrow & \alpha(t) = (x_1(t), \dots, x_n(t))^T, \end{array}$$

be a differentiable curve in $C \subset D \subset \mathbb{R}^n$ and

$$\begin{array}{rccl} f: & D \subset \mathbb{R} & \longrightarrow & \mathbb{R}^n \\ & \boldsymbol{x} & \longrightarrow & f(\boldsymbol{x}) \end{array}$$

be a differentiable function. Then

$$f(\alpha(t)) = f(x_1(t), \dots, x_n(t)),$$

and

$$\frac{d}{dt} f(\alpha(t)) = \frac{\partial f}{\partial x_1}(\alpha(t)) x_1'(t) + \cdots + \frac{\partial f}{\partial x_n}(\alpha(t)) x_n'(t).$$

Directional derivatives

- We want to compute the directional derivative after changing the length of the vector $\boldsymbol{v}$.
- Suppose that $\boldsymbol{v} = \lambda \boldsymbol{u}$. If in
$$\frac{f(\boldsymbol{x} + h\boldsymbol{v}) - f(\boldsymbol{x})}{h},$$
we substitute $h = k/\lambda$ and $\boldsymbol{v} = \lambda \boldsymbol{u}$, we get
$$\frac{f(\boldsymbol{x} + (k/\lambda)(\lambda \boldsymbol{u})) - f(\boldsymbol{x})}{k/\lambda} = \lambda \cdot \frac{f(\boldsymbol{x} + k\boldsymbol{u}) - f(\boldsymbol{x})}{k}.$$
This is λ times the difference quotient that we had for the directional derivative of f with respect to $\boldsymbol{u}$.
- Taking the limit as h tends to zero is the same as taking the limit as k tends to zero, because h and k are multiples of each other.
- Therefore, $D_{\boldsymbol{v}}(f) = \lambda D_{\boldsymbol{u}}(f)$. Because of this rescaling property, directional derivatives are considered only for unit vectors: $\|\boldsymbol{v}\| = 1$.

The gradient

Consider the function

$$f : \mathcal{C} \subset \mathbb{R}^n \longrightarrow \mathbb{R}.$$

- If f has a partial derivatives $\partial f / \partial x_j$ with respect to each variable x_j, then at any point $\boldsymbol{a} \in \mathcal{C}$, these partial derivatives define the vector

$$\nabla f(\boldsymbol{a}) = \left(\frac{\partial f}{\partial x_1}(\boldsymbol{a}), \ldots, \frac{\partial f}{\partial x_n}(\boldsymbol{a}) \right)^T .$$

  This vector is called the gradient of f at $\boldsymbol{a}$.

- **Theorem:** If all the partial derivatives of f exist and are continuous at $\boldsymbol{a}$, then the function f is differentiable at $\boldsymbol{a}$ and the gradient of f at $\boldsymbol{a}$ exists

- From

$$D_{\boldsymbol{v}} f(\boldsymbol{a}) = \sum_{j=1}^{n} \frac{\partial f(\boldsymbol{a})}{\partial x_j} v_j,$$

  we get

$$D_{\boldsymbol{v}} f(\boldsymbol{a}) = (\nabla f(\boldsymbol{a})) \cdot \boldsymbol{v}.$$

Properties of the gradient

- **Property:** If $f : D \subset \mathbb{R}^n \longrightarrow \mathbb{R}$ is differentiable, $\boldsymbol{a} \in D$, and $\boldsymbol{u} \in \mathbb{R}^n$ is an unitary vector ($\|\boldsymbol{u}\| = 1$), then

$$D_{\boldsymbol{u}} f(\boldsymbol{a}) = (\nabla f(\boldsymbol{a})) \cdot \boldsymbol{u} = \|\nabla f(\boldsymbol{a})\| \cos\theta,$$

  where θ is the angle between $\boldsymbol{u}$ and $\nabla f(\boldsymbol{a})$.

- **Property:** The gradient vector $\nabla f(\boldsymbol{a})$ gives the maximum direction variation of f at the point $\boldsymbol{a}$ (since $\cos\theta$ is maximum $\Leftrightarrow \theta = 0$).

- **Property:** Gradients are orthogonal to the level curves and the level surfaces of a function f.
  Proof. Let $\boldsymbol{r}(t) = (x_1(t), x_2(t), \ldots, x_n(t))^T$ be a level curve (or a curve on a level furface) this means that $f(\boldsymbol{r}(t))$ is constant for any value of t. Then

$$\frac{d}{dt} f(\boldsymbol{r}(t)) = 0.$$

  Using the chain rule for the computation of the derivative, we get

$$\begin{aligned} \frac{d}{dt} f(\boldsymbol{r}(t)) &= \frac{d}{dt} f(x_1(t), x_2(t), \ldots, x_n(t)) \\ &= \frac{\partial f}{\partial x_1}(\boldsymbol{r}(t)) x_1'(t) + \ldots + \frac{\partial f}{\partial x_n}(\boldsymbol{r}(t)) x_n'(t) \;=\; \nabla f(\boldsymbol{r}(t))^T \, \boldsymbol{r}'(t), \end{aligned}$$

  and since $\boldsymbol{r}'(t)$ is the tangent vector to the curve, the property follows.

Properties of the gradient. Examples

- **Property:** The equations of the tangent plane and the normal line of the level set of f at $\boldsymbol{a}$ are:
  - Tangent plane
  $$(\nabla f(\boldsymbol{a})) \cdot (\boldsymbol{x} - \boldsymbol{a}) = 0 \quad \Leftrightarrow \quad \frac{\partial f}{\partial x_1}(x_1 - a_1) + \cdots + \frac{\partial f}{\partial x_n}(x_n - a_n) = 0.$$
  - Normal line
  $$\boldsymbol{x} = \boldsymbol{a} + \lambda \nabla f(\boldsymbol{a}), \quad \lambda \in \mathbb{R}.$$

- **Example:** Compute the tangent plane to the surface $3x^2y + z^2 - 4 = 0$ at the point $(1,1,1)^T$.

  Let $f(\boldsymbol{x}) = 3x^2y + z^2 - 4$, since
  $$\begin{aligned} \nabla f(\boldsymbol{x})^T &= (6xy,\, 3x^2,\, 2z)^T, \\ \nabla f(1,1,1)^T &= (6,3,2)^T, \end{aligned}$$
  the plane is
  $$6(x-1) + 3(y-1) + 2(z-1) = 0 \quad \Leftrightarrow \quad 6x + 3y + 2z = 11.$$

Linear approximation of functions

- We have already seen that if f is a real function in one variable, the linear approximation of the function $f(x)$ at a point x_0 is defined by the linear function
$$L(x) = f(x_0) + f'(x_0)(x - x_0).$$
- In two dimensions, the linear approximation of the function $f(x, y)$ at the point $(x_0, y_0)^T$ is defined as the linear function
$$\begin{aligned} L(x,y) &= f(x_0,y_0) + \frac{\partial f}{\partial x}(x_0,y_0)(x-x_0) + \frac{\partial f}{\partial y}(x_0,y_0)(y-y_0) \\ &= f(x_0,y_0) + \left(\frac{\partial f}{\partial x}(x_0,y_0), \frac{\partial f}{\partial y}(x_0,y_0)\right)\begin{pmatrix} x-x_0 \\ y-y_0 \end{pmatrix} \\ &= f(x_0,y_0) + (\nabla f(x_0,y_0))^T \begin{pmatrix} x-x_0 \\ y-y_0 \end{pmatrix}. \end{aligned}$$
- In dimension n
$$L(\mathbf{x}) = f(\mathbf{x}_0) + (\nabla f(\mathbf{x}_0))^T(\mathbf{x} - \mathbf{x}_0).$$

Linear approximation of functions

- **Example:** Estimate the value of $f(0.01, 24.8, 1.02)$ for $f(x, y, z) = e^x \sqrt{y} z$.

  We take $\mathbf{x}_0 = (0, 5, 1)^T$ and we use the linear approximation of f to compute an estimation of $f(0.01, 24.8, 1.02)$.

  Clearly

$$
\begin{aligned}
f(\mathbf{x}_0) &= 5, \\
\nabla f(\mathbf{x})^T &= \left(e^x \sqrt{y} z,\ \frac{e^x z}{2\sqrt{y}},\ e^x \sqrt{y} \right)^T, \\
\nabla f(\mathbf{x}_0)^T &= (5,\ 1/10,\ 5)^T, \\
L(\mathbf{x}) &= f(\mathbf{x}_0) + (\nabla f(\mathbf{x}_0))^T (\mathbf{x} - \mathbf{x}_0) \\
&= 5 + (5,\ 1/10,\ 5) \begin{pmatrix} x - 0 \\ y - 5 \\ z - 1 \end{pmatrix} = 5 + 5x + \frac{y-5}{10} + 5(z-1)
\end{aligned}
$$

  We approximate $f(0.01, 24.8, 1.02) = 5.1306$ by $L(0.01, 24.8, 1.02) = 5.13$

The differential matrix

Let

$$\begin{array}{rccl} f: & \mathcal{C} \subset \mathbb{R}^n & \longrightarrow & \mathbb{R}^m \\ & \boldsymbol{x} & \longrightarrow & f(\boldsymbol{x}) = (f_1(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x})). \end{array}$$

- We say that f is differentiable if $f_1,\ldots,f_m$ are differentiable.
- The differential of f at an interior point $\boldsymbol{a} \in \mathcal{C}$ is

$$Df(\boldsymbol{a}) = \begin{pmatrix} \nabla f_1(\boldsymbol{a}) \\ \vdots \\ \nabla f_m(\boldsymbol{a}) \end{pmatrix} = \begin{pmatrix} \frac{\partial f_1(\boldsymbol{a})}{\partial x_1} & \cdots & \frac{\partial f_1(\boldsymbol{a})}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m(\boldsymbol{a})}{\partial x_1} & \cdots & \frac{\partial f_m(\boldsymbol{a})}{\partial x_n} \end{pmatrix}.$$

- If $g : \mathcal{D} \subset \mathbb{R}^p \longrightarrow \mathcal{C} \subset \mathbb{R}^n$ and $f : \mathcal{C} \subset \mathbb{R}^n \longrightarrow \mathbb{R}^m$ are both differentiable, then the composition $h = f \circ g$

$$\begin{array}{rcccccc} h: & \mathcal{D} & \longrightarrow & \mathcal{C} & \longrightarrow & \mathbb{R}^m \\ & \boldsymbol{x} & \longrightarrow & g(\boldsymbol{x}) = (g_1(\boldsymbol{x}), \ldots, g_n(\boldsymbol{x}))^T & \longrightarrow & h(\boldsymbol{x}) = f(g_1(\boldsymbol{x}), \ldots, g_n(\boldsymbol{x})) \end{array}$$

is also differentiable.

The differential matrix

If $g : \mathcal{D} \subset \mathbb{R}^p \longrightarrow \mathcal{C} \subset \mathbb{R}^n$ and $f : \mathcal{C} \subset \mathbb{R}^n \longrightarrow \mathbb{R}^m$ are both differentiable, then the differential of the composition $h = f \circ g$ at an interior point $\boldsymbol{a} \in \mathcal{D}$ is the product of the differentials

$$Dh(\boldsymbol{a}) = Df(g(\boldsymbol{a}))Dg(\boldsymbol{a})$$

$$Dh(\boldsymbol{a}) = \begin{pmatrix} \frac{\partial f_1(g(\boldsymbol{a}))}{\partial x_1} & \cdots & \frac{\partial f_1(g(\boldsymbol{a}))}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m(g(\boldsymbol{a}))}{\partial x_1} & \cdots & \frac{\partial f_m(g(\boldsymbol{a}))}{\partial x_n} \end{pmatrix} \begin{pmatrix} \frac{\partial g_1(\boldsymbol{a})}{\partial x_1} & \cdots & \frac{\partial g_1(\boldsymbol{a})}{\partial x_p} \\ \vdots & \ddots & \vdots \\ \frac{\partial g_n(\boldsymbol{a})}{\partial x_1} & \cdots & \frac{\partial g_n(\boldsymbol{a})}{\partial x_p} \end{pmatrix}.$$

The differential matrix. Linear approximations

- If $f : I \subset \mathbb{R} \longrightarrow \mathbb{R}$ is differentiable, then for $dx \approx 0$

$$f(x + dx) \approx f(x) + f'(x)dx$$

- If $f : \mathcal{C} \subset \mathbb{R}^n \longrightarrow \mathbb{R}$ is differentiable, $\boldsymbol{x} = (x_1, ..., x_n)^T$, $\boldsymbol{dx} = (dx_1, ..., dx_n)^T \approx \boldsymbol{0}$, then

$$f(\boldsymbol{x} + \boldsymbol{dx}) \approx f(\boldsymbol{x}) + (\nabla f(\boldsymbol{x})) \cdot \boldsymbol{dx}$$

- If $f : \mathcal{C} \subset \mathbb{R}^n \longrightarrow \mathbb{R}^m$ is differentiable, $\boldsymbol{x} = (x_1, ..., x_n)^T$, $\boldsymbol{dx} = (dx_1, ..., dx_n)^T \approx \boldsymbol{0}$, then

$$f(\boldsymbol{x} + \boldsymbol{dx}) \approx f(\boldsymbol{x}) + DF(\boldsymbol{x})\, \boldsymbol{dx}$$

Critical points

- **Definition.** Given a differentiable function $f : \mathcal{C} \subset \mathbb{R}^n \longrightarrow \mathbb{R}$, $\boldsymbol{a}$ is a critical point of f is

$$\nabla f(\boldsymbol{a}) = \mathbf{0} \quad \Leftrightarrow \quad \begin{cases} \dfrac{\partial f(\boldsymbol{a})}{\partial x_1} = 0, \\ \qquad \vdots \\ \dfrac{\partial f(\boldsymbol{a})}{\partial x_n} = 0. \end{cases}$$

- If $\boldsymbol{a}$ is not a critical point of f, then $\nabla f(\boldsymbol{a})$ gives the direction along which f increases or dicreases faster. In particular, if $\boldsymbol{a}$ is not a critical point of f then it can be not a maximum or minimum of f.

- The critical points of f are the candidates to be the local extrema (relative extrema) of f.

Quadratic approximation of functions

- We have already seen that, in dimension n, the linear approximation of the function $f(\boldsymbol{x})$ at a point $\boldsymbol{a}$ is defined by the function

$$L(\boldsymbol{x}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\boldsymbol{x} - \boldsymbol{a}).$$

- Is $\boldsymbol{a}$ is a critical point of f, then $\nabla f(\boldsymbol{a}) = 0$, and the linear approximation of f at $\boldsymbol{a}$ is constant.
- The second order approximation is obtained using Taylor's formula

$$f(\boldsymbol{x}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\boldsymbol{x} - \boldsymbol{a}) + \frac{1}{2}\nabla^2 f(\boldsymbol{a})(\boldsymbol{x} - \boldsymbol{a})^2 + \ldots$$

where the value of $\nabla^2 f(\boldsymbol{a})(\boldsymbol{x} - \boldsymbol{a})^2 \in \mathbb{R}$ is given by

$$(x_1 - a_1, \ldots, x_n - a_n)\begin{pmatrix} \frac{\partial^2 f(\boldsymbol{a})}{\partial x_1^2} & \cdots & \frac{\partial^2 f(\boldsymbol{a})}{\partial x_n \partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f(\boldsymbol{a})}{\partial x_1 \partial x_n} & \cdots & \frac{\partial^2 f(\boldsymbol{a})}{\partial x_n^2} \end{pmatrix}\begin{pmatrix} x_1 - a_1 \\ \vdots \\ x_n - a_n \end{pmatrix}.$$

- Denoting the Hessian $\nabla^2 f(\boldsymbol{a})$ by $H(\boldsymbol{a})$, the quadratic approximation of f at the point $\boldsymbol{a}$ is written as

$$Q(\boldsymbol{x}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\boldsymbol{x} - \boldsymbol{a}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{a})^T H(\boldsymbol{a})(\boldsymbol{x} - \boldsymbol{a}).$$

Quadratic functions

- For any $n \times n$ matrix Q ($Q \in \mathbb{R}^{n \times n}$) we have

  Q is symmetric $\Leftrightarrow$ $Q^T = Q$

  Q is skew-symmetric $\Leftrightarrow$ $Q^T = -Q$

  Q is positive semidefinite (PSD) $\Leftrightarrow$ $x^T Qx \geq 0$ for all $x \in \mathbb{R}^n$

  Q is positive definite (PD) $\Leftrightarrow$ $x^T Qx \geq 0$ for all $x \in \mathbb{R}^n$ and $x^T Qx = 0$ if and only if $x = 0$

- Let f be the quadratic function given by

$$f(x) = x^T Qx + c^T x + d$$

  where $Q \in \mathbb{R}^{n \times n}$, $c \in \mathbb{R}^n$ and $d \in \mathbb{R}$. Then f is:
  - linear $\Leftrightarrow$ $Q = 0$ and $d = 0$ $\Rightarrow$ $f(x) = c^T x$
  - affine $\Leftrightarrow$ $Q = 0$ $\Rightarrow$ $f(x) = c^T x + d$
  - convex $\Leftrightarrow$ Q is PSD $\Rightarrow$ $f(x) = x^T Qx + c^T x + d$