Mathematics for Informatics

Multivariate optimization
(lecture 2 of 12)

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Winter 2024/2025

created: September 11, 2024, 14:20

What shall we do today?

- Multivariate optimization:
  - Gradient
  - Tangent plane
  - Critical points on two or more variables
  - Hessian (matrix)

Gradient of a function

The gradient of a function $f(x_1, x_2, \ldots, x_n)$ at the (n-dimensional) point $b \in \mathbb{R}^n$ is the n-dimensional vector function $\nabla f(b)$ defined by

$$\nabla f(b) = \left(\frac{\partial f}{\partial x_1}(b), \frac{\partial f}{\partial x_2}(b), \ldots, \frac{\partial f}{\partial x_n}(b) \right).$$

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Find the gradient of the function $f(x, y) = x^2 + xy + y^2$ *at the point* $(1, 1)$.

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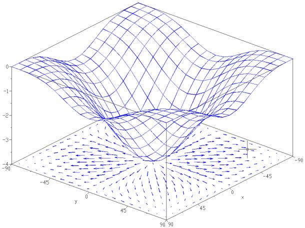
Geometrical meaning: the gradient points is the direction of the greatest rate of increase of the function. Its magnitude equals the rate of increase.



Gradient and the directional derivative

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Example

If we are on the graph of the fonction $f(x,y) = x^2 + xy + y^2$ *at the point* $(1,1)$ *and we start moving in the direction parallel to the* x*-axis, i.e., in the direction of the vector* $(1,0)$*, we will go "uphill" under the angle* $\arctan 3$ *since*

$$\frac{\partial f}{\partial x}(1,1) = 2 + 1 = 3.$$

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Theorem

Given a function $f(x) : \mathbb{R}^n \to \mathbb{R}$*, a point* $a \in \mathbb{R}^n$ *and a* ***unit*** *vector* $\vec{v} \in \mathbb{R}^n$*, the derivative in the direction of the vector* $\vec{v}$ *is the dot product of the gradient and* $\vec{v}$*, i.e,* $\nabla f(a_1, a_2, \ldots, a_n) \cdot \vec{v}$*.*

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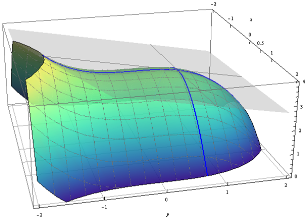
$$z = \frac{\partial f}{\partial x}(x_0, y_0) \cdot (x - x_0) \; + \; \frac{\partial f}{\partial y}(x_0, y_0) \cdot (y - y_0) \; + \; f(x_0, y_0).$$



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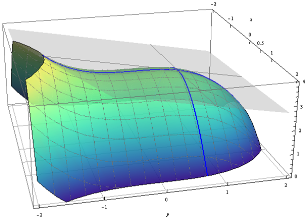

Example

Find the tangent plane to $f(x, y) = x^2 + xy + y^2$ *at* $(1, 1)$.

Critical points – two variables

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The first class of these points can be found as a solution of

$$\nabla f(x, y) = (0, 0)$$

which leads to the system of two equations for two variables

$$\begin{cases} \dfrac{\partial f}{\partial x}(x, y) & = & 0 \\ \dfrac{\partial f}{\partial y}(x, y) & = & 0 \end{cases}.$$

Critical points – more variables

For an n-variable function $f(x_1, x_2, \ldots, x_n)$ the situation is analogous:
The critical points of $f(x_1, x_2, \ldots, x_n)$ are points satisfying the equation

$$\nabla f(x_1, x_2, \ldots, x_n) = 0$$

i.e., points satisfying the system of n equations for n variables

$$\begin{cases} \dfrac{\partial f}{\partial x_1}(x_1, x_2, \ldots, x_n) & = & 0 \\ \dfrac{\partial f}{\partial x_2}(x_1, x_2, \ldots, x_n) & = & 0 \\ & \vdots & \\ \dfrac{\partial f}{\partial x_n}(x_1, x_2, \ldots, x_n) & = & 0 \end{cases},$$

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or where the gradient does not exist.
(Instead of a tangent plane, we have a tangent hyperplane.)

Critical points – example

Example

Find all critical points of

$$f(x_1, x_2, x_3) = x_1x_3 + x_1^2 - x_2 + x_2x_3 + x_2^2 + 3x_3^2,$$

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which always exists.

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which always exists. Thus the critical points are the solution of the system

$$\begin{cases} x_3 + 2x_1 & = & 0 \\ -1 + x_3 + 2x_2 & = & 0 \\ x_1 + x_2 + 6x_3 & = & 0 \end{cases},$$

which, using the standard procedure for a system of linear equations, gives us the only solution $\left(\frac{1}{20}, \frac{11}{20}, \frac{-1}{10}\right)$.

Type of a critical point (1 of 4)

In the one dimensional case, we can use the second derivative to decide the type of the critical point.

Theorem

Let x_0 be a critical point of a function $f(x)$ such that $f'(x_0) = 0$ and $f''(x_0)$ exists.

- *If $f''(x_0) > 0$, then the function is convex at x_0, and x_0 is a point of a minimum.*
- *If $f''(x_0) < 0$, then the function is concave at x_0, and x_0 is a point of a maximum.*
- *If $f''(x_0) = 0$, then x_0 may be a minimum, maximum, inflection point, ...*

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Do we have something similar for more variables? What is the second derivative?

Type of a critical point (2 of 4)

The analogue of the second derivative is the following.

Definition

For a function $f(x_1, x_2, \ldots, x_n)$ we define the Hessian matrix as

$$\nabla^2 f(x_1, x_2, \ldots, x_n) = \begin{pmatrix} \dfrac{\partial^2 f}{\partial x_1^2}(x_1, \ldots, x_n) & \cdots & \dfrac{\partial^2 f}{\partial x_1 \partial x_n}(x_1, \ldots, x_n) \\ \vdots & \ddots & \vdots \\ \dfrac{\partial^2 f}{\partial x_n \partial x_1}(x_1, \ldots, x_n) & \cdots & \dfrac{\partial^2 f}{\partial x_n^2}(x_1, \ldots, x_n) \end{pmatrix}$$

assuming that all the derivatives exist.

Type of a critical point (3 of 4)

We would like to construct rules like "If $f''(x_0) > 0$, then the critical point x_0 is the point of minimum".

But to say that the matrix is "positive" is problematic ... Let us use a different notion.

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5. *indefinite otherwise.*

Type of a critical point (4 of 4)

Theorem

If $f : \mathbb{R}^n \to \mathbb{R}$ has all second partial derivative continuous at a critical point $b \in \mathbb{R}^n$, then

(i) *if $\nabla^2 f(b)$ is positively definite, then b is a point of local minimum;*

(ii) *if $\nabla^2 f(b)$ is negatively definite, then b is a point of local maximum;*

(iii) *if $\nabla^2 f(b)$ is indefinite, then b is a saddle point.*

Sylvester's criterion on definiteness

For an $n \times n$ dimensional **symmetric** matrix A we define the principal minors:

- M_1 is the upper left 1-by-1 corner of A,
- M_2 is the upper left 2-by-2 corner of A,
- ...
- M_n is the upper left n-by-n corner of A.

Theorem

Let $A \in \mathbb{R}^{n,n}$ be a symmetric matrix.

- *A is positively definite if and only if the determinants of all principal minors are positive.*
- *A is negatively definite if and only if the determinant of M_i is negative for odd i and positive for even i.*

Example

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Find all minima and maxima of the function

$$f(x, y) = \frac{3x^4 - 4x^3 - 12x^2 + 18}{12(1 + 4y^2)}.$$

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Solution: The critical points are $(-1,0)$, $(0,0)$ and $(2,0)$; they are a saddle point, a point of maximum and a point of minimum, respectively.