Mathematics for Informatics

Multivariate optimization (lecture 2 of 12)

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

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

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Example

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

Gradient of a function

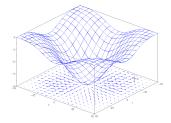
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Geometrical meaning: the gradient points is the direction of the greatest rate of increase of the function. Its magnitude equals the rate of increase.



Gradient and the directional derivative

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

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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.*, $\nabla f(a_1, a_2, \ldots, a_n) \cdot \vec{v}$.

Tangent plane

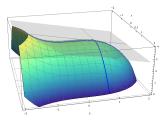
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$$z = \frac{\partial f}{\partial x}(x_0, y_0) \cdot (x - x_0) + \frac{\partial f}{\partial y}(x_0, y_0) \cdot (y - y_0) + f(x_0, y_0).$$

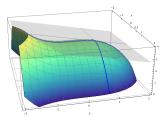


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Example

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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

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

Critical points - more variables

For an *n*-variable function $f(x_1, x_2, ..., x_n)$ the situation is analogous: The critical points of $f(x_1, x_2, ..., x_n)$ 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

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

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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

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

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We get

$$\nabla f(x_1, x_2, x_3) = (x_3 + 2x_1, -1 + x_3 + 2x_2, x_1 + x_2 + 6x_3)$$

which always exists.

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$$\nabla f(x_1, x_2, x_3) = (x_3 + 2x_1, -1 + x_3 + 2x_2, x_1 + x_2 + 6x_3)$$

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''(x₀) > 0, then the function is convex at x₀, and x₀ is a point of a minimum.
- If f''(x₀) < 0, then the function is concave at x₀, and x₀ 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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- If $f''(x_0) = 0$, then x_0 may be a minimum, maximum, inflection point, ...

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 $f(x_1, x_2, ..., x_n)$ we define the Hessian matrix as

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

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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() positively definite if for all non-zero vectors $\mathbf{a} \in \mathbb{R}^n$ it holds that $\mathbf{a}A\mathbf{a}^T > 0$;

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- 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

- (a) if $\nabla^2 f(b)$ is positively definite, then b is a point of local minimum;
- (a) if $\nabla^2 f(b)$ is negatively definite, then b is a point of local maximum;
- () 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:

Hessian

- 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.

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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.

