Mathematics for Informatics

Multivariate ptimization
(lecture 5 of 12)

Francesco Dolce

dolcefra@fit.cvut.cz

Czech Technical University in Prague

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Outline

- Examples of single- and multivariate optimization

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- Reminder of univariate optimization

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- Reminder of univariate optimization
- Multivariate optimization:
  - Partial derivative
  - Gradient
  - Tangent plane
  - Hessian (matrix)
  - Minimum, maximum, saddle point

Duration of a text processing program (1 of 6)

Problem

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Problem*: The proportionality constant α is unknown. How would you reasonably estimate its value?*

Duration of a text processing program (2 of 6)

Sketch of a solution:

1. Run the program for several, say n, texts of various lengths and measure the actual running times. This gives us n couples of measurements $(k_1, t_1), (k_2, t_2), \dots, (k_n, t_n)$.

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$$e(\alpha) = (t_1 - \alpha k_1)^2 + (t_2 - \alpha k_2)^2 + \cdots + (t_n - \alpha k_n)^2 = \sum_{i=1}^{n} (t_i - \alpha k_i)^2.$$

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3. In order to find the best approximating proportionality constant α, we find the value of α for which the error $e(\alpha)$ is minimal:

an optimal value of α is a minimum point of the function $e(\alpha)$.

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$$e'(\alpha_0) = 0 \Leftrightarrow \sum_{i=1}^{n} -2k_i(t_i - \alpha_0 k_i) = 0 \Leftrightarrow \sum_{i=1}^{n} k_i t_i = \alpha_0 \sum_{i=1}^{n} k_i^2 \Leftrightarrow \alpha_0 = \frac{\sum_{i=1}^{n} k_i t_i}{\sum_{i=1}^{n} k_i^2}$$

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3. The critical points are our candidates for the points of (local) minimal or maximal values of the function e. To be sure that the value of α we found is a minimum we need the second derivative:

$$e''(\alpha) = \left(\sum_{i=1}^{n} -2k_i(t_i - \alpha k_i)\right)' = \sum_{i=1}^{n} 2k_i^2\,.$$

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Duration of a text processing program (4 of 6)

We know that if $e''(\alpha_0) > 0$ (resp. $e''(\alpha_0) < 0$), then the critical point α_0 is a local strict minimum (resp. strict maximum) point.
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Solution: based on our measurements $(k_1, t_1), (k_2, t_2), \ldots, (k_n, t_n)$, we get the best approximation $t(k) \approx \alpha k$ for

$$\alpha = \alpha_0 = \frac{\sum_{i=1}^{n} k_i t_i}{\sum_{i=1}^{n} k_i^2} .$$

Indeed, this α_0 is the unique (why unique?) global (why global?) minimum point of the approximation error function $e(\alpha)$ since the second derivative

$$e''(\alpha_0) = \sum_{i=1}^{n} 2k_i^2 \quad \text{is positive.}$$

Duration of a text processing program (5 of 6)

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Mathematically*: Denote by $t(k, f)$ the "average" number of seconds needed to process a text of length k, and the frequency of the processor by f. We know that*

$$t(k, f) \approx \alpha k + \beta f \qquad \text{for some } \alpha, \beta \in \mathbb{R}.$$

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Comments

Why "optimization"?

A typical situation in physics, engineering, economy, chemistry, etc. is that you have a function that measures your profit, your loss, the energy of something, etc. The value of such function is given by one or more inputs and the relation between inputs and the resulting value is usually stated as a mathematical formula since all these sciences uses mathematical models to understand and quantify their subject of interest.
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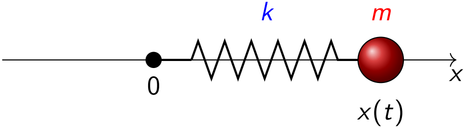
Typically, we want to maximize or minimize such functions (maximize the profit, the energy, minimize the loss, the error) which leads to the problem of finding **optimal** values of the inputs. Therefore the name "optimization".

Comments

There is **another very important usage** of the derivative.
Derivatives measure the rate of change of a function. This helps us to describe the behaviour of a **dynamical systems** like a ball on a spring:



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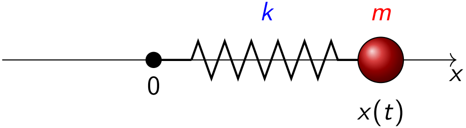

The position of the ball at time t is a function $x(t)$ satisfying the differential equation

$$x''(t) + \omega^2 x(t) = 0\,.$$

The solution of this equation is

$$x(t) = x_0 \cos(\omega t) + \frac{v_0}{\omega} \sin(\omega t), \qquad t \in \mathbb{R},$$

where $x_0 = x(0)$ and v_0 are the position and the speed of the ball at time $t = 0$.
This model is known as harmonic oscillator.

How do we differentiate?

Example

Find the first derivative of $f(x)$, *where*

(a) $f(x) = x^3 + 4x^2 + 6$,

(b) $f(x) = \sin(x^3)$,

(c) $f(x) = e^x \sin x$.

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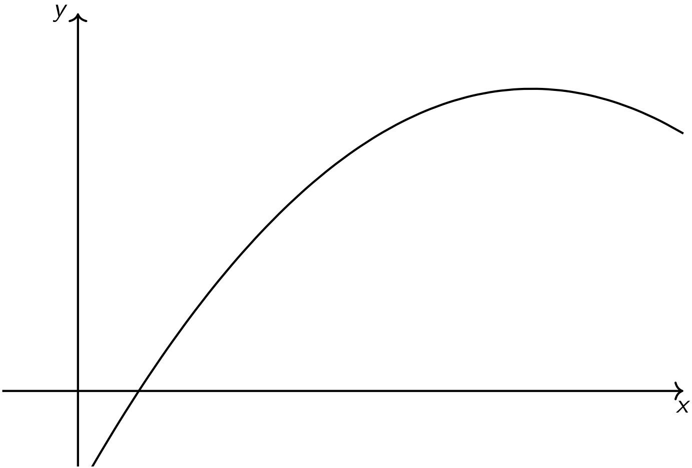
Solutions:

a. $f'(x) = 3x^2 + 8x$,
b. $f'(x) = 3x^2 \cos(x^3)$,
c. $f'(x) = e^x \sin x + e^x \cos x$.

Geometrical meaning of derivative: tangent line (1 of 2)



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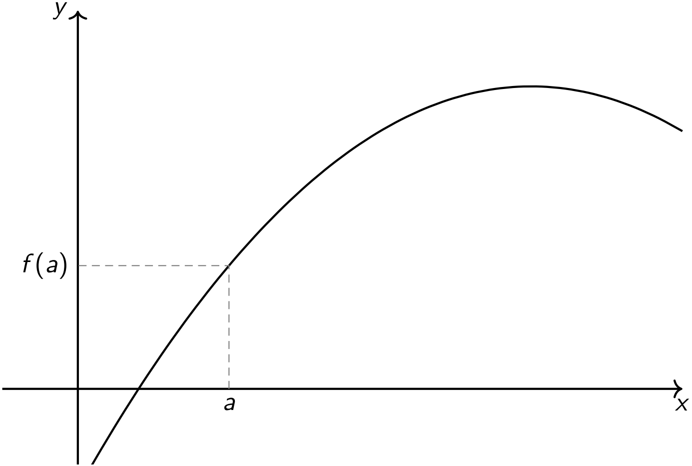

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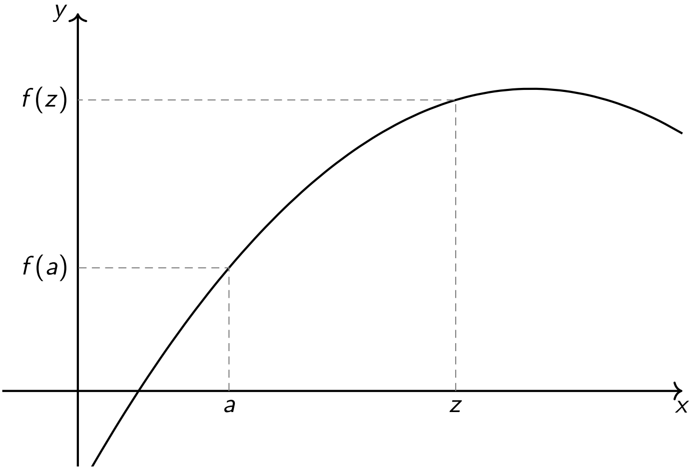

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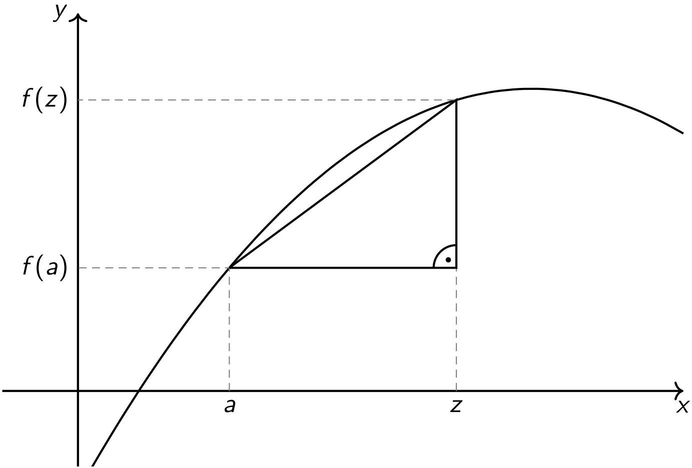

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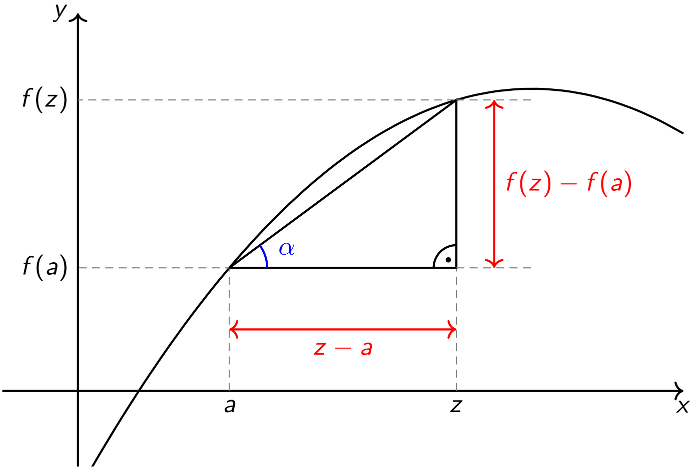

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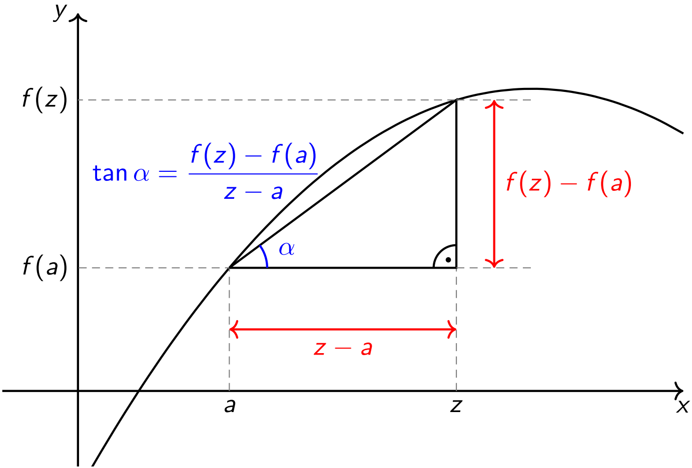

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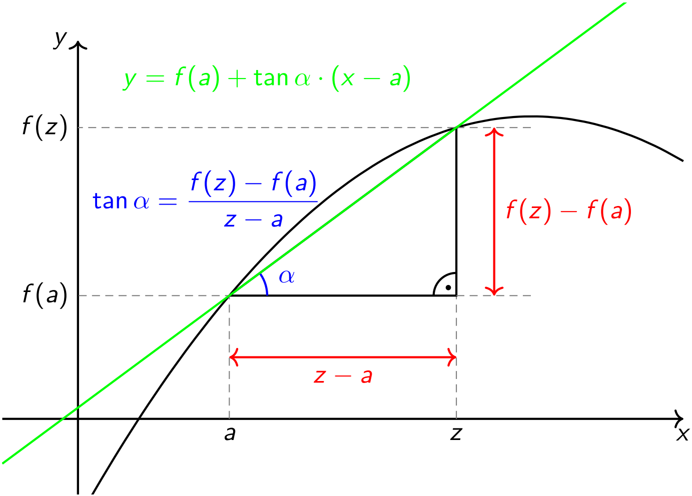

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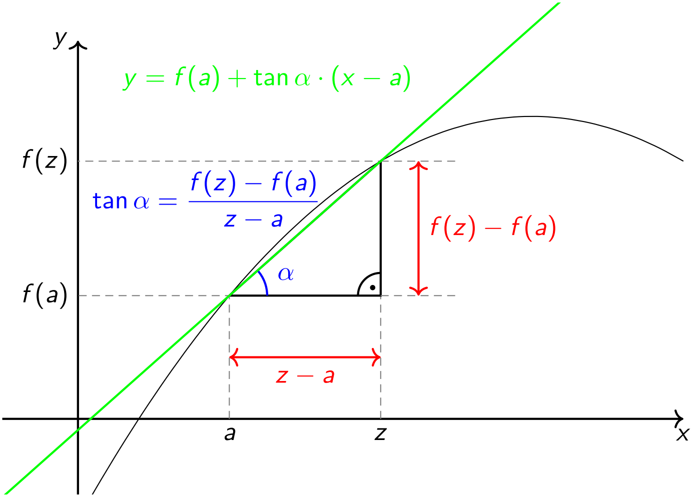

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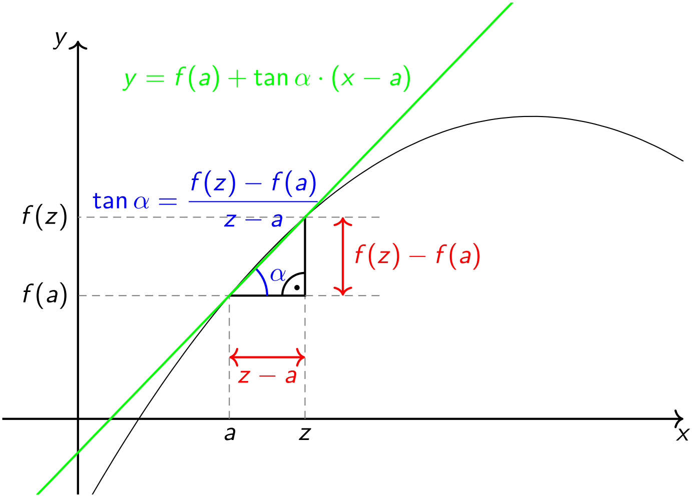

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- The tangent line at the point x_0 satisfies the equation

$$y = f'(x_0)(x - x_0) + f(x_0).$$

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With this geometrical explanation it is easy to see that the following statements are true:

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Example

Find all critical points of

$$f(x) = \frac{x^3}{3} + 2x^2 + 3x + 6\,.$$

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- An illustrative example of function with positive second derivative is $f(x) = x^2$.

Second derivative as a criterion for extremal values

Again, if we understand the geometrical meaning of the second derivative, we can easily see that the following statements are true:

Theorem

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

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Question: what can happen if $f''(x_0) = 0$?

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The goal of this and the next lecture is to understand what happens when we have more than 1 variable. We shall build a similar cookbook for such functions.

Graph of multivariate functions (1 of 2)

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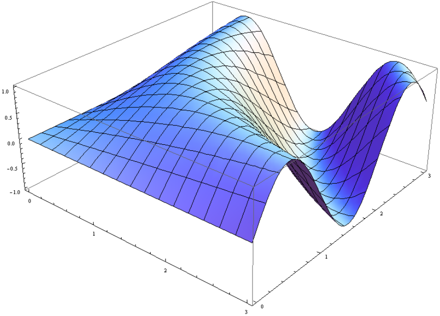
What if the function depends on more variables? For instance: $f(x, y)$.



Graph of a two-variable function $\sin(x \cdot y)$: the set of points $(x, y, \sin(x \cdot y))$.

Graph of multivariate functions (2 of 2)

- To depict a graph of a two-variable function we need a third axis (typically z-axis) and a 3-dimensional figure. Such graph is in general some surface.
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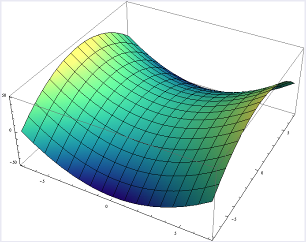

Partial derivative – introduction

Given the function $f(x, y) = x^2 + xy + y^2$.

- If we fix the value of the variable y to 3, we obtain a univariate function $f(x) = x^2 + 3x + 9$ having its derivative equal to $2x + 3$.

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- In general $\frac{\partial f}{\partial x}(x, y)$ and $\frac{\partial f}{\partial y}(x, y)$ are two-variate functions.

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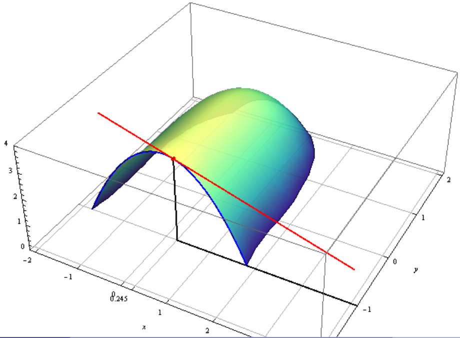
Since the definition is similar, even the geometrical meaning is analogous.

Partial derivative – definition

The partial derivatives of $f(x, y)$ can be in short denoted by

$$f_x(x, y) = \frac{\partial f}{\partial x}(x, y) \quad \text{and} \quad f_y(x, y) = \frac{\partial f}{\partial y}(x, y).$$

The number $f_x(x, y)$ for given values of x and y is again the slope of a tangent line, but a surface has infinitely many tangent lines in all possible directions at any point, so which one is this one?
It is the only tangent line which is parallel to the x-axis.



Second partial derivatives

Definition

For a function $f(x_1, x_2, \ldots, x_n)$ *we define second partial derivatives*

$$f_{x_j x_i}(x_1, x_2, \ldots, x_n) = \frac{\partial^2 f}{\partial x_j \partial x_i}(x_1, x_2, \ldots, x_n) = \frac{\partial}{\partial x_j}\left(\frac{\partial f}{\partial x_i}(x_1, x_2, \ldots, x_n)\right),$$

in particular, for $i = j$ *we have*

$$f_{x_i x_i}(x_1, x_2, \ldots, x_n) = \frac{\partial^2 f}{\partial x_i^2}(x_1, x_2, \ldots, x_n) = \frac{\partial}{\partial x_i}\left(\frac{\partial f}{\partial x_i}(x_1, x_2, \ldots, x_n)\right).$$

Partial derivatives – exercises

Example

Find partial derivatives with respect to all variables

(a) $f(x, y) = xy + e^x \cos y$,

(b) $f(x, y) = x^2y^3 + x^3y^4 - e^{xy^2}$,

(c) $f(x, y, z) = \sin(xy/z)$.

Example

Find all second partial derivatives of the functions

(a) $f(x, y) = x^2 + xy^2 + 3x^3y$,

(b) $f(x, y, z) = e^{xz} + y \cos x$,

(c) $f(x, y, z) = z \cos(xy) + x \sin(yz)$.

Equality of mixed partial derivatives

The fact that the mixed partial derivatives are equal is not a coincidence:

Theorem

If a function $f(x, y)$ has continuous second partial derivatives, then the mixed second derivatives are equal, i.e.,

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This theorem is not true in general, a counterexample is the function

$$f(x,y) = \begin{cases} 0 & \text{at point } (0,0) \\ \dfrac{xy(x^2-y^2)}{x^2+y^2} & \text{otherwise.} \end{cases}$$