Mathematics for Informatics

Introductory Lecture - Optimization (lecture 1 of 12)

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Organization

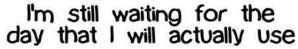
Lecturer:

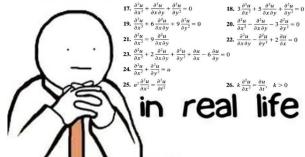
Francesco Dolce (dolcefra@fit.cvut.cz)

Conditions, materials, schedules: https://courses.fit.cvut.cz/NIE-MPI/

see here the conditions to pass the course

Why mathematics?





Why should we learn mathematics?



If someone can take up this position (painlessly), what do you say to yourself?

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If someone can take up this position (painlessly), what do you say to yourself?

Good! I'd like to be agile as she is . . .

OR

Hmm, I didn't need such a daredevil position in my life, I am going to train sitting on a chair instead, that's what I do ...

Understanding

MATHEMATICS

is not about numbers, equations, computations, or algorithms: it is about UNDERSTANDING.

William Paul Thurston

15 Majors that Will Make You Rich (measured by money)

- Petroleum Engineering (\$155,000 after some time)
- Physics (\$101,800)
- Applied Mathematics (\$98,600 "Jobs in this field can be found in nearly every sector.")
- Computer Science (\$97,900)
- Biomedical Engineering (\$97,800)
- Statistics (\$93,800)
- Civil Engineering (\$90,200)
- Mathematics (\$89,900)
- Environmental Engineering (\$88,600)
- Software Engineering (\$87,800)
- Finance (\$87,300)
- Construction Management (\$85,200)
- Biochemistry (\$84,700)
- Geology (\$83,300)
- Management Information Systems (\$82,200)

George Stibitz (Ph.D. in mathematical physics)

He was a Bell Labs researcher known for his work in the 1930s and 1940s on the realization of Boolean logic digital circuits using electromechanical relays as the switching element.



Marian Rejewski, Alan Turing, ... (mathematicians)

Breaking of German codes during WWII.









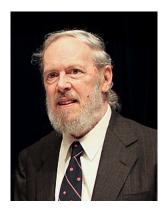
Claude Shannon, (founder of information theory, mathematician)

Shannon is famous for having founded information theory with one landmark paper published in 1948. But he is also credited with founding both digital computer and digital circuit design theory in 1937, when, as a 21year-old master's student at MIT, he wrote a thesis demonstrating that electrical application of Boolean algebra could construct and resolve any logical, numerical relationship.



Dennis RITCHIE, (computer scientist, creator of C programming language)

Ritchie graduated from Harvard University with degrees in physics and applied mathematics.



Linus TORVALDS (developer of the Linux kernel)

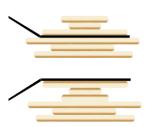
His parents were both journalists. However, he was highly influenced by his maternal grandfather to pursue his career in computers. Since childhood, Linus was brilliant in mathematics. In 1988 he began studing computer science at the University of Helsinki. Linus is from a minority group in Finland and his first language is not Finnish but Swedish. For this reason, his pronunciation of Linux in Swedish were not understood or often taken as an error.



Bill GATES (founder of Microsoft)

In his sophomore year, Gates devised an algorithm for pancake sorting as a solution to one of a series of unsolved problems presented in a combinatorics class by Harry Lewis, one of his professors. Gates' solution held the record as the fastest version for over thirty years; its successor is faster by only 2%. His solution was later formalized in a published paper in collaboration with Harvard computer scientist Christos Papadimitriou.





Larry PAGE and Sergey BRIN (founders of Google)

Larry was in search of a dissertation theme for his PhD in computer science and considered exploring the mathematical properties of the World Wide Web, understanding its link structure as a huge graph.

After graduation at the University of Maryland, Sergey moved to Stanford University to acquire a Ph.D in computer science.

The company was founded while they were both attending Stanford University.



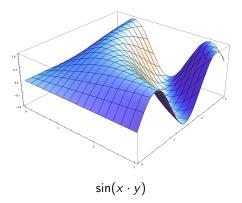


What about us?

What will we be talking about in this course?

Multivariate functions and optimization

- Many problems can be formulated as optimization problems: we maximize/minimize some functions that determines gain/cost/time/distance
- If the function is given analytically, we know how to find the optimum.



General algebra

Notions from general algebra are one of the basic mathematical tools.

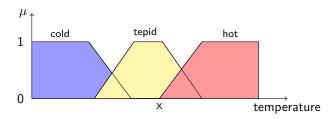
	1	2	3	4	5	6	7	8	9	10	11	12
1	1	2	3	4	5	6	7	8	9	10	11	12
2	2	4	6	8	10	12	1	3	5	7	9	11
3	3	6	9	12	2	5	8	11	1	4	7	10
4	4	8	12	3	7	11	2	6	10	1	5	9
5	5	10	2	7	12	4	9	1	6	11	3	8
6	6	12	5	11	4	10	3	9	2	8	1	7
7	7	1	8	2	9	3	10	4	11	5	12	6
8	8	3	11	6	1	9	4	12	7	2	10	5
9	9	5	1	10	6	2	11	7	3	12	8	4
10	10	7	4	1	11	8	5	2	12	9	6	3
11	11	9	7	5	3	1	12	10	8	6	4	2
12	12	11	10	9	8	7	6	5	4	3	2	1

Cayley table of the group \mathbb{Z}_{13}^{\times}

Besides a general introduction, we will focus on finite groups and fields, which form the basis for cryptography, hash functions, etc.

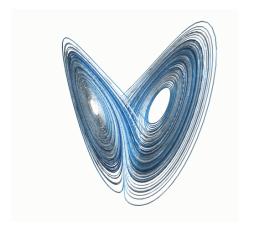
Fuzzy Logic

Describe systems by properties which are not evaluated by values beyond just true or false.



Numerical mathematics

Continuous mathematics using the computer, stability of numerical algorithms \dots



Where shall we start?

• Examples of single- and multivariate optimization

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- Examples of single- and multivariate optimization
- Reminder of univariate optimization

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

Problem

Imagine the following situation: You have created a program that processes a text input by a user. You know, from theoretical analysis of the source code and algorithms used within the program, that it is impossible to determine the exact time needed to process a text of length k. However, you know that it is approximately proportional to the length of the text.

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

Sketch of a solution:

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

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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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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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Find the critical points, i.e., the points α_0 where $e'(\alpha_0)$ is zero or does not exist:

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

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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:

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

continues ...

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. If $e''(\alpha_0) = 0$, then α is neither of these two cases (maybe an inflexion point?).

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Solution: based on our measurements $(k_1, t_1), (k_2, t_2), \dots, (k_n, t_n)$, 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

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

Problem (slight modification)

Imagine the following situation: You have created a program that processes a text input by a user. You know, from theoretical analysis of the source code and algorithms used within the program, that it is impossible to determine precisely the time needed to process a text of length k. However, you know that it is approximately proportional to the length of the text and to the frequency of the processor.

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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

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Sketch of solution:

• Run the program for several, say n, texts of various lengths on computers with different frequencies and measure the actual running times. This gives us n triplets of measurements $(k_1, t_1, f_1), (k_2, t_2, f_2), \ldots, (k_n, t_n, f_n)$.

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In order to find the best approximating constants α and β , we find values of α and β for which the error $e(\alpha, \beta)$ is minimal: an optimal value of α and β is the "two-dimensional" minimum point of $e(\alpha, \beta)$.

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.

An example of such function is our function $e(\alpha, \beta)$ that measures the approximation error.

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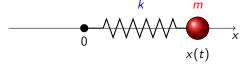
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Typically, we want to maximize or minimize such functions (maximize the profit, the energy, minimize the loss, the error) which leads to the problem of finding **optimal** values of the inputs. Therefore the name "optimization".

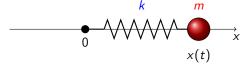
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Derivatives measure the rate of change of a function. This helps us to describe the behaviour of a **dynamical systems** like a ball on a spring:



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

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

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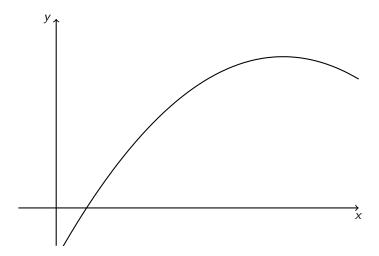
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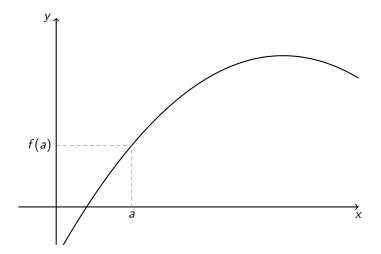
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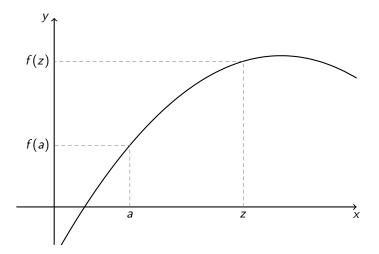
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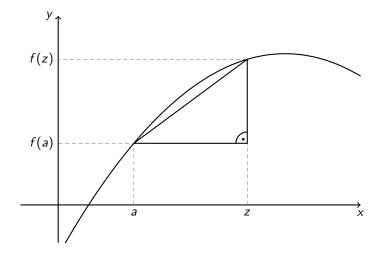
Solutions:

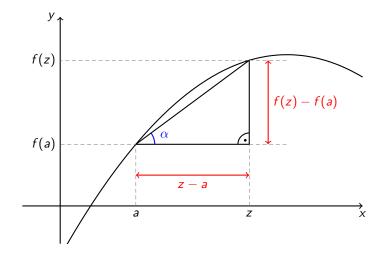
- $f'(x) = 3x^2 + 8x,$
- $f'(x) = 3x^2 \cos(x^3),$
- $f'(x) = e^x \sin x + e^x \cos x.$

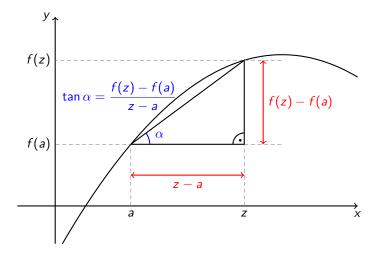


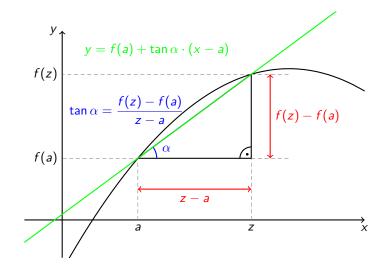


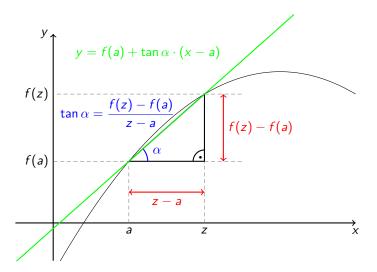


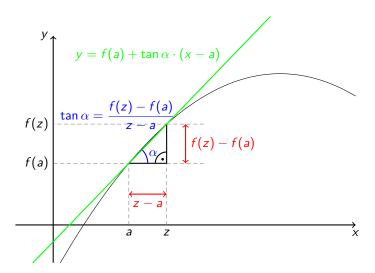












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- The slope of the tangent line to f(x) at the point x_0 equals the first derivative evaluated at x_0 : $f'(x_0)$.
- The tangent line at the point x_0 satisfies the equation

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

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.

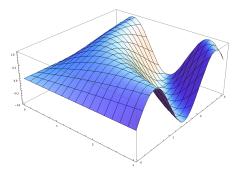
Graph of multivariate functions (1 of 2)

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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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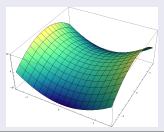
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Example

How does the graph of $f(x, y) = x^2 - y^2$ look like?



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.

Partial derivative – definition

The derivative of a (single variate) function f(x) is the following limit (if it exists):

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The partial derivative of $f(x_1, x_2, ..., x_n)$ with respect to x_i at the point $(x_1, x_2, ..., x_n)$ is defined by (if the limit below exists)

$$\frac{\partial f}{\partial x_{i}}(x_{1}, x_{2}, \dots, x_{i-1}, x_{i}, x_{i+1}, \dots, x_{n}) =
= \lim_{\delta \to 0} \frac{f(x_{1}, x_{2}, \dots, x_{i-1}, x_{i} + \delta, x_{i+1}, \dots, x_{n}) - f(x_{1}, x_{2}, \dots, x_{n})}{\delta}.$$

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

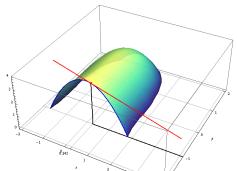
Partial derivative – definition

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

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

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 $f(x_1, x_2, ..., x_n)$ we define second partial derivatives

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

in particular, for i = j we have

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

Partial derivatives - exercises

Example

Find partial derivatives with respect to all variables

- $f(x,y) = xy + e^x \cos y,$
- $f(x,y) = x^2y^3 + x^3y^4 e^{xy^2}$
- $f(x, y, z) = \sin(xy/z).$

Example

Find all second partial derivatives of the functions

- $f(x, y) = x^2 + xy^2 + 3x^3y$
- $f(x, y, z) = e^{xz} + y \cos x,$
- $f(x, y, z) = z \cos(xy) + x \sin(yz).$

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

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

