Tutorial – Mathematics for Social Scientists

Winter semester 2024/25

Optimization & Multivariate calculus

To do

- weekly recap
- real world applications
- hands on practice
- questions

Chapter 15 | Multivariate Calculus and Optimization

Multidimensional differentiation

→ follows the rules of one-dimensional differentiation ☺

- we are interested in the slope in direction of x, while keeping y fixed – and vice versa
  - same rules, treat every variable as a constant to whose respect we are **not** differentiating!
  - to denote a **partial derivative**, we either use $\frac{\partial}{\partial x}$ or $f_x'(x)$

exampel:

$$f(x,y,z) = 3y^2z^4 - 5xz^2 + 2x^3$$

$$f_x'(x,y,z) = -5z^2 + 6x^2$$
$$f_y'(x,y,z) = 6yz^4$$
$$f_z'(x,y,z) = 12y^2z^3 - 10xz$$

Hands on – partial derivatives

Task: Find the partial derivatives of the following functions!

1) $\frac{\partial}{\partial z} 9x^2 + 3z^2$

2) $\frac{\partial}{\partial z} 8xyz^2 + 10x^2y^2 + 12x^2y + 14x^2z^2$

Hands on – partial derivatives

Solution:

1) $\frac{\partial}{\partial z} 9x^2 + 3z^2 = 6z$

2) $\frac{\partial}{\partial z} 8xyz^2 + 10x^2y^2 + 12x^2y + 14x^2z^2 = 16xyz + 28x^2z$

Gradient

Is a function **partially differentiable**, we can summarize its **(first order) partial derivatives** under the **gradient**

- ALWAYS describes steepest increase/descent!

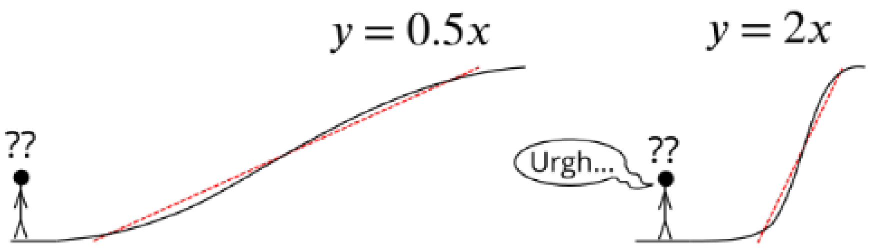
→that's why we are interested in it – optimization

- example: $f(x, y, z) = z \cdot \exp(x^2 + xy)$
  - $f_x(x, y, z) = z \cdot \exp(x^2 + xy) \cdot (2x + y)$
  - $f_y(x, y, z) = z \cdot \exp(x^2 + xy) \cdot x$
  - $f_z(x, y, z) = \exp(x^2 + xy)$
- gradient: $\nabla f(x, y, z) = \begin{pmatrix} z\exp(x^2 + xy)\,(2x + y) \\ z\exp(x^2 + xy)\,x \\ \exp(x^2 + xy) \end{pmatrix}$

Real world applications – Gradient

Which hill would you rather climb?

→ the gradient denotes the direction of steepest increase/decrease!



Two hills

Source: https://undergroundmathematics.org/introducing-calculus/gradients-important-real-world, 28.10.2023

Real world applications – Gradient

Applications of the gradient:

- rate of change of **distance** with respect to **time**
  → velocity
- there is the rate of change of **energy** with respect to **time**
  → power
- the rate of change of **chemical concentrations** with respect to **time**
  → rate of a reaction
- rate of change of **money owing** with respect to **time**
  → compound interest

Source: https://undergroundmathematics.org/introducing-calculus/gradients-important-real-world, 28.10.2023

The Jacobian

Let's do the example from the previous section that we just mentioned. Recall that the function f has components

$$\begin{aligned} f_1(x,y,z) &= 3xy - y^2 z + 2, \\ f_2(x,y,z) &= x^y - xy, \\ f_3(x,y,z) &= z(xz+y) - 2y(e^{x+y}) - 15z, \\ f_4(x,y,z) &= xyz - 1. \end{aligned}$$

Then the Jacobian matrix J is

$$J = \begin{pmatrix} 3y & 3x - 2yz & -y^2 \\ yx^{y-1} - y & \ln(x)x^y - x & 0 \\ z^2 - 2y(e^{x+y}) & z - 2(e^{x+y}) - 2y(e^{x+y}) & 2xz + y - 15 \\ yz & xz & xy \end{pmatrix}.$$

$$f(x_1, x_2, \dots, x_n) = (f_1, f_2, \dots, f_m)$$

$$J_f = \begin{pmatrix} \dfrac{\partial f_1}{\partial x_1} & \dfrac{\partial f_1}{\partial x_2} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \dfrac{\partial f_2}{\partial x_1} & \dfrac{\partial f_2}{\partial x_2} & \cdots & \dfrac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \dfrac{\partial f_m}{\partial x_2} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{pmatrix}$$

The Hessian – Hesse matrix

The **Hessian** or **Hesse matrix** is a quadratic matrix that represents the **second derivatives** of a multivariate function in calculus

$$H_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 x_2} \\ \frac{\partial^2 f}{\partial x_2 x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

- The entry of row i and column j is: $\left(H_f\right)_{i,j} = \frac{\partial^2 f}{\partial x_i x_j}$
- **Note**: the Hesse matrix of f is the transpose of the Jacobian of f's gradient!

$$H\big(f(x)\big) = J\big(\nabla f(x)\big)^T$$

Hesse matrix – Computation

Example: Find H for $f(x, y) = \ln(2x) + 3xy^2$

Algorithm:

1) find first order partial derivatives
2) find second order partial derivatives
3) arrange based on row and column order

$$H_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 x_2} \\ \frac{\partial^2 f}{\partial x_2 x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

$$\left(H_f\right)_{i,j} = \frac{\partial^2 f}{\partial x_i x_j}$$

Hesse matrix – Computation

1) find first order partial derivatives of:

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

$$f_x(x, y) = \frac{2}{2x} + 3y^2 = \frac{1}{x} + 3y^2$$

$$f_y(x, y) = 6xy$$

2) find Second order partial derivatives

$$f_{xx}(x, y) = \frac{-1}{x^2}$$

$$f_{yy}(x, y) = 6x$$

$$f_{xy}(x, y) = 6y$$

$$f_{yx}(x, y) = 6y$$

Hesse matrix – Computation

Example: Find H for $f(x,y) = \ln(2x) + 3xy^2$

3) arrange based on row and column order

$$H_f = \begin{bmatrix} f_{xx}(x,y) = \frac{-1}{x^2} & f_{xy}(x,y) = 6y \\ f_{yx}(x,y) = 6y & f_{yy}(x,y) = 6x \end{bmatrix}$$

→ Do you notice something?

Hesse matrix – Computation

Example: Find H for $f(x,y) = \ln(2x) + 3xy^2$

3) arrange based on row and column order

$$H_f = \begin{bmatrix} f_{xx}(x,y) = \dfrac{-1}{x^2} & f_{xy}(x,y) = 6y \\ f_{yx}(x,y) = 6y & f_{yy}(x,y) = 6x \end{bmatrix}$$

→ The second order partial derivatives are the same!

Satz von Schwarz

- **Note**: For second order derivatives, the 'order of differentiation' across different variables **does NOT** matter

$$H_f = \begin{bmatrix} f_{xx}(x,y) = \frac{-1}{x^2} & f_{xy}(x,y) = 6y \\ f_{yx}(x,y) = 6y & f_{yy}(x,y) = 6x \end{bmatrix}$$

- we can differentiate by x first and by y second – and vice versa

→ this will make your lives easier ☺

Logarithms… a reminder!

How do we **differentiate logarithms**?

$$f(x) = \ln(some\ x) \rightarrow f'(x) = \frac{inner\ derivative\ of\ some\ x}{some\ x}$$

How do we find **higher order derivatives**?

$$x^n(t) = \frac{(-1)^{n-1}(n-1)!}{t^n}$$

Hands on – Hesse matrix

Task: Find the Hesse matrix for the following functions!

1) $f(x, y) = 5x^2y^3 - \ln(3x)$
2) $f(x, y) = 12 - 3x^2 - 6x - y^2 + 12y$

Hands on – Hesse matrix – Solution

- $f(x,y) = 5x^2y^3 - \ln(3x)$
  - $f_x(x,y) = 10y^3x - \frac{1}{x}$
  - $f_y(x,y) = 15x^2y^2$

- $H = \begin{bmatrix} \frac{1}{x^2} + 10y^3 & 30xy^2 \\ 30xy^2 & 30x^2y \end{bmatrix}$

- $f(x,y) = 12 - 3x^2 - 6x - y^2 + 12y$
  - $f_x(x,y) = -6x - 6$
  - $f_y(x,y) = -2y + 12$

- $H = \begin{bmatrix} -6 & 0 \\ 0 & -2 \end{bmatrix}$

Definiteness

NOTE: we can use definiteness to assess whether a critical points is a minimum, a maximum or a saddle!

Vector spaces

For vector space V over real/complex numbers holds:

- $\langle \vec{v}, \vec{v} \rangle > 0$ → positive definite
- $\langle \vec{v}, \vec{v} \rangle < 0$ → negative definite
- $\langle \vec{v}, \vec{v} \rangle \geq 0$ → positive semidefinite
- $\langle \vec{v}, \vec{v} \rangle \leq 0$ → negative semidefinite

Matrices

- For quadratic symmetrical matrix A with eigenvalues λ holds:
  - $\lambda > 0$ → positive definite
  - $\lambda < 0$ → negative definite
  - $\lambda \geq 0$ → positive semidefinite
  - $\lambda \leq 0$ → negative semidefinite
  - indefinite → both positive and negative eigenvalues

Optimization (wo. constraints)

Algorithm:

1) find $\nabla f(x)$
2) set $\nabla f(x^*) = 0$ and solve for all x^*
   → stationary points
3) find Hesse matrix H for $f(x)$
4) for each stationary point x^*, substitute x^* into H
   → assess definiteness
5) compare local maxima and minima to find global extreme points

- if H is negative definite:
  → local maximum
- if H is negative definite:
  → local minimum
- if H is indefinite:
  → saddle point
- if H is semidefinite:
  → inconclusive… use e.g. eigenvalues

Optimization (wo. constraints)

Example: Find the extreme points of $f(x, y) = x^2 - 3xy + y$

1) find $\nabla f(x, y)$

- $f_x(x, y) = 2x - 3y$
- $f_y(x, y) = -3x + 1$

$\rightarrow \nabla f(x, y) = \begin{pmatrix} 2x - 3y \\ -3x + 1 \end{pmatrix}$

2) set $\nabla f(x^*) = 0$ and solve for all x^*

- $2x - 3y = 0 \rightarrow 2\left(\frac{1}{3}\right) - 3y = 0 \rightarrow y = \frac{2}{9}$
- $-3x + 1 = 0 \rightarrow x = \frac{1}{3}$

Optimization (wo. constraints)

Example: Find the extreme points of $f(x,y) = x^2 - 3xy + y$

3) find Hesse matrix $\boldsymbol{H}$ for $\boldsymbol{f(x)}$

- $f_{xx}(x,y) = 2$
- $f_{yy}(x,y) = 0$
- $f_{xy}(x,y) = -3$
- $f_{yx}(x,y) = -3$

$$\rightarrow H = \begin{pmatrix} 2 & -3 \\ -3 & 0 \end{pmatrix}$$

4) substitute $\boldsymbol{x^*}$ into $\boldsymbol{H}$

- no variables left in H
- H consists of both positive and negative values → indefinite→ saddle point at $f(\frac{1}{3} | \frac{2}{9})$

Hands on – Optimization (wo. constraints)

Task: Find the extrema of the following functions!

1) $f(x, y) = 12 - 3x^2 - 6x - y^2 + 12y$

2) $f(x, y) = x^2y - 4y + \ln(x)$

Hands on – Optimization (wo. constraints)

Solution: Find the extrema of the following functions!

1) $f(x, y) = 12 - 3x^2 - 6x - y^2 + 12y$

→ Maximum at (-1, 6)

2) $f(x, y) = x^2y - 4y + \ln(x)$

→ Saddle at (-2, -1/8) and Saddle at (2, -1/8)

Solution – Extrema $\mathrm{f}(\mathrm{x}, \mathrm{y}) = 12 - 3x^2 - 6x - y^2 + 12y$

$f(x,y) = 12 - 3x^2 - 6x - y^2 + 12y$

1) find gradient $\nabla f(x,y)$

$f_x(x,y) = -6x - 6$

$f_y(x,y) = -2y + 12$

$$\nabla f(x,y) = \begin{pmatrix} -6x - 6 \\ -2y + 12 \end{pmatrix}$$

2) set $\nabla f(x,y)$ equal to 0

$-6x - 6 = 0 \rightarrow -6x = 6 \rightarrow x = -1$

$-2y + 12 = 0 \rightarrow y = 6$

3) find Hessian

$$H = \begin{pmatrix} -6 & 0 \\ 0 & -2 \end{pmatrix}$$

4) evaluate Hessian

- no variables left!
- negative values only

↳ maximum at $f(-1|6)$

Solution – Extrema $\mathrm{f}(\mathrm{x},\mathrm{y}) = x^2y - 4y + \ln(x)$

1) find $\nabla f(x,y)$

$$f_x(x,y) = 2xy + \frac{1}{x}$$
$$f_y(x,y) = x^2 - 4$$
$$\nabla f(x,y) = \begin{pmatrix} 2xy + \frac{1}{x} \\ x^2 - 4 \end{pmatrix}$$

2) set $\nabla f(x,y)$ equal to 0

$$2xy + \frac{1}{x} = 0 \quad \begin{cases} 2 \cdot 2y + \frac{1}{2} = 4y = -\frac{1}{2} \to y = -0.125 = -\frac{1}{8} \\ 2 \cdot (-2)y - \frac{1}{2} = -4y = \frac{1}{2} \to y = -\frac{1}{8} \end{cases}$$

$$x^2 - 4 = 0 \to x^2 = 4 \Rightarrow x_1 = 2, \quad x_2 = (-2)$$

3) find Hessian!

$$H = \begin{pmatrix} 2y - \frac{1}{x^2} & 2x \\ 2x & 0 \end{pmatrix}$$

4) plug in critical points & evaluate!

$x = -2,\ y = -\frac{1}{8}$:

$$H = \begin{pmatrix} -\frac{2}{8} - \frac{1}{4} & -4 \\ -4 & 0 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -4 \\ -4 & 0 \end{pmatrix}$$

→ all values are negative but note that $x = (-2)$ and $\ln(-2)$ is not defined!

→ to be sure, we shall find the Eigenvalues!

$$\det\left(\begin{pmatrix} -\frac{1}{2} & -4 \\ -4 & 0 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right)$$

$$= -\frac{\lambda(-1 - 2\lambda)}{2} - 16$$

$$\left.\begin{aligned} \lambda_1 &= \frac{-1 + \sqrt{257}}{4} = 3.7578 \\ \lambda_2 &= \frac{-1 - \sqrt{257}}{4} = -4.2578 \end{aligned}\right\} \text{both positive \& negative}$$

↳ indefinite!

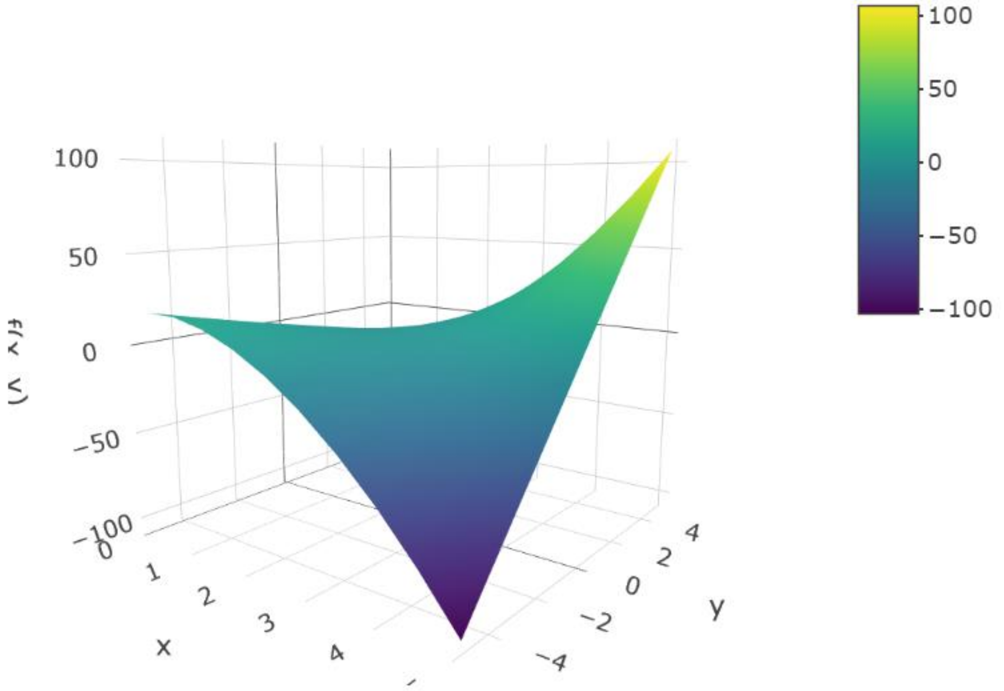
Solution – Extrema $\mathrm{f}(\mathrm{x}, \mathrm{y}) = x^2 y - 4y + \ln(x)$

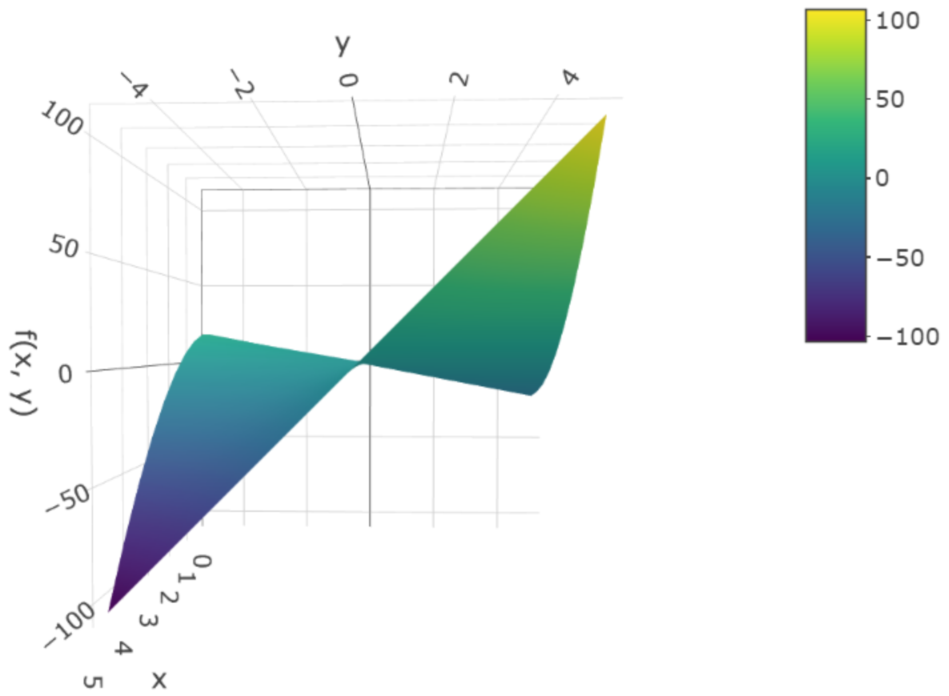
$x = 2, y = -\frac{1}{8}$

$$H = \begin{pmatrix} -\frac{2}{8} - \frac{1}{4} & 4 \\ 4 & 6 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & 4 \\ 4 & 0 \end{pmatrix} \Rightarrow \underline{\text{indefinite!}}$$

$\Rightarrow$ f(x, y) has two saddle points at f$(-2, -\frac{1}{8})$ and f$(2, -\frac{1}{8})$

$f(x, y) = x^2y - 4y + \ln(x)$ plotted in R using Plotly





Multidimensional integration

Intuition:

- **univariate** integrals give the area under the curve
- **bivariate** integrals give the volume under the surface
- … is also pretty much the same as one-dimensional integration
  → at least given the problems we will solve in this class

- let’s visualize ☺
  - https://matheistkeinarschloch.de/mehrdimensionale-integration/

Sentence of Fubini

- if one of the two integrals exists and is defined, the other integral exists as well…

$$\int_a^b \int_c^d |f(x,y)|\, dx\, dy = \int_c^d \int_a^b |f(x,y)|\, dy\, dx$$

- when may we switch integrals around?
  - when f is non-negative over the area of integration
  - when f is not complicated … e.g. a polynomial, exponentials, sin(x), cos(x),…

Multidimensional integration

Example:

$$\begin{aligned}\int_0^1 \int_0^3 6x + 4xy + 2y^2 + 2dy\, dx &= \int_0^1 (\int_0^3 6x + 4xy + 2y^2 + 2dy)\, dx \\ &= \int_0^1 [6xy + 2xy^2 + \frac{2}{3}xy^3 + 2y]_{y=0}^3\, dx \\ &= \int_0^1 18x + 18x + 18 + 6\, dx \\ &= [18x^2 + 24x]_{x=0}^1 = 42\end{aligned}$$

Time for your questions

- Any questions during the week?
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