TUM ModSim, SoSe 2023

Mitschriften basierend auf der Vorlesung von Dr. Hans-Joachim Bungartz

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Introduction

About

Hier sind die wichtigsten Konzepte der ModSim Vorlesung von Dr. Hans-Joachim Bungartz im Sommersemester 2023 zusammengefasst.

Die Mitschriften selbst sind in Markdown geschrieben und werden mithilfe einer GitHub-Action nach jedem Push mithilfe von Pandoc zu einem PDF konvertiert.t

Eine stets aktuelle Version der PDFs kann über modsim_SS23_IN2010_merge.pdf heruntergeladen werden.

Implementation

Außerdem befindet sich eine Implementation von verschiedenen Algorithmen im Ordner `/algorithms` auf GitHub. Diese sind in Python und unter der Verwendung von NumPy geschrieben.

How to Contribute

1. Fork this Repository
2. Commit and push your changes to **your** forked repository
3. Open a Pull Request to this repository
4. Wait until the changes are merged

Contributors

Inhaltsverzeichnis

Focus Analysis / Calculus

Foundations

Functions and their representations

- One-Dimensional
$$f : D \subseteq \mathbb{R}^n \to \mathbb{R}^m, x \mapsto f(x)$$
- Multidimensional
$$f : D \subseteq \mathbb{R} \to \mathbb{R}, x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \mapsto f(x) = \begin{pmatrix} f_1(x_1, \dots, x_n) \\ \vdots \\ f_m(x_1, \dots, x_n) \end{pmatrix}$$

Names for special types of functions

- Curves: $n = 1$ and $m \in \mathbb{N}$
  - plane curves (2D): $n = 1$ and $m = 2$
  - space curves (3D): $n = 1$ and $m = 3$
- Surfaces: $n = 2$ and $m = 3$
- Scalar fields: $n \in \mathbb{N}$ and $m = 1$
- Vector fields: $n = m$

Topology concepts in higher dimensions

There is an analogous concept to open and closed intervals in multi-dimensional spaces.
Given a domain $D \subseteq \mathbb{R}^n$ and its complement $D^c = \mathbb{R}^n \setminus D$

- A point x is called *inner point* if there exists an arbitrarily small ball around this points that fullly lies inside D.
- The set of all inner points of D is called the *interior* of D and is denoted as $\mathring{D}$.
- The domain is called open if $D = \mathring{D}$
- A point $x_0 \in \mathbb{R}^n$ is called *boundary point* if any arbitrarily small ball around this point intersects with both D and its complement D^c
- The set of all boundary points of D is called the *boundary* of D, denoted ∂D
- The set $\bar{D} = D \cup 0\partial D$ is called the *closure* of D

Using these definitions there are multiple attributes assignable to domains.
A domain D is called:

- *closed* if $\partial D \subseteq D$, i.e. $\bar{D} = D$
- *bounded* if $\exists K \in \mathbb{R} : ||x|| < K, \forall x \in D$
- *compact* if it is closed and bounded
- *convex* if all points on a straight line between to points in D are themselves element of D

Continuity

We define continuity in multi-dimensional spaces using converging vector sequences.
A sequence $(x^{(k)})$ converges to the limit x if

$$\lim_{k \to \infty} ||x^{(k)} - x|| = 0$$

Converges of a vector sequence is also equivalent to the convergence of all components.
A vector function is then called continuous at $a \in D$ if for all sequences $(x^{(k)})_{k\in\mathbb{N}_0}$ in D converging to a the corresponding sequence $(f(x^{(k)}))_{k\in\mathbb{N}_0}$ in $\mathbb{R}^m$ converges to $f(a)$ and continuous on D if this holds for all points $a \in D$

Partial Differentiation

Gradient

The Gradient of a function gives the direction of the steepest ascent of the function. It requires that f represents a scalar field.

When applying the limit definition of the derivative to a function in higher dimesions it is not clear from which direction the derivative should be taken.

Using

$$\frac{\partial f}{\partial v}(a) = \lim_{h\to 0} \frac{f(a+hv) - f(a)}{h}$$

we can define the directional derivative of a function $f : \mathbb{R}^n \to \mathbb{R}$ along a vector $v \in \mathbb{R}^n$ at a point $a \in \mathbb{R}^n$.

If we use the coordinate vectors e_i as basis vectors for $\mathbb{R}^n$ we can define the *Gradient* of f at a as

$$\nabla f(a) = \mathrm{grad} f(a) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(a) \\ \vdots \\ \frac{\partial f}{\partial x_n}(a) \end{pmatrix}$$

For continuous functions the directional derivative at the point a along a vector v can be computed as

$$\frac{\partial f}{\partial v}(a) = \langle \nabla f(a), v \rangle$$

Example:

$$f(x, y) = x^2 + y^2 \to \nabla f(a) = \begin{pmatrix} 2x \\ 2y \end{pmatrix}$$

Hessian Matrix

The Hessian matrix of a function $f : \mathbb{R}^n \to \mathbb{R}$ at a point $a \in \mathbb{R}^n$ is the matrix of all second partial derivatives of f at a.

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

Example:

$$f(x, y) = x^2 + y^2 \to H_f(a) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

Jacobian Matrix

The Jacobian matrix of a function $f : \mathbb{R}^n \to \mathbb{R}^m$ at a point $a \in \mathbb{R}^n$ is the matrix of all partial derivatives of f at a.

In contrast to the Gradient the Jacobian matrix works for vector fields. It gives an analogue to the gradient for vector fields.

$$Df(a) = J_f(a) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(a) & \frac{\partial f_1}{\partial x_2}(a) & \dots & \frac{\partial f_1}{\partial x_n}(a) \\ \frac{\partial f_2}{\partial x_1}(a) & \frac{\partial f_2}{\partial x_2}(a) & \dots & \frac{\partial f_2}{\partial x_n}(a) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(a) & \frac{\partial f_m}{\partial x_2}(a) & \dots & \frac{\partial f_m}{\partial x_n}(a) \end{pmatrix} = \begin{pmatrix} \nabla f_1(a)^T \\ \nabla f_2(a)^T \\ \dots \\ \nabla f_m(a)^T \end{pmatrix}$$

Example:

$$f(x,y) = \begin{pmatrix} x^2 + y \\ x^2 + y^2 \end{pmatrix} \to J_f(a) = \begin{pmatrix} 2x & 1 \\ 2x & 2y \end{pmatrix}$$

Calculation rules for the Jacobian

- Addition rule: $J(f+g) = J_f + J_g$
- Homogeneous rule: $J(cf) = cJ_f$
- Product rule: $J(f^T \cdot g) = f(x)^T J_g(x) + g(x)^T J_f(x)$

Laplace Operator

The Laplace operator is a second order partial derivative operator. It is defined on Scalar fields and is used to compute the rate of change of a scalar field.

$$\Delta f = \nabla^2 f = \sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2}$$

Example:

$$f(x,y) = x^2 + y^2 \to \Delta f(a) = 2 + 2 = 4$$

Divergence

The Divergence of a vector field is the rate of shrinkage or expansion around a point. It is defined as the sum of the partial derivatives of the components of the vector field.

$$\text{div} f = \sum_{i=1}^{n} \frac{\partial f_i}{\partial x_i} = \nabla \cdot f$$

Example:

$$f(x,y) = \begin{pmatrix} x^2 \\ y^2 \end{pmatrix} \to \text{div} f(a) = \frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} = 2x + 2y$$

Curl / Rotation

The Curl of a vector field is the rate of rotation around a point. It is defined as the cross product of the partial derivatives of the components of the vector field.

$$\text{rot} f = \nabla \times f = \begin{pmatrix} \frac{\partial f_3}{\partial x_2} - \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_1}{\partial x_3} - \frac{\partial f_3}{\partial x_1} \\ \frac{\partial f_2}{\partial x_1} - \frac{\partial f_1}{\partial x_2} \end{pmatrix}$$

Example:

$$f(x,y,z) = \begin{pmatrix} x^2 y \\ y^2 x \\ yz \end{pmatrix} \to \text{rot} f(a) = \begin{pmatrix} z \\ 0 \\ y^2 - x^2 \end{pmatrix}$$

Taylor Expansion

It is also possible to approximate functions of multiple variables by Taylor expansions, by using the analog for higher order derivatives for functions of multiple variables.

Coordinate Transformations

A bijection between two coordinate systems is called a coordinate transformation. It is a function $\phi : \mathbb{R}^n \to \mathbb{R}^m$ that maps points in one coordinate system to points in another coordinate system and vice versa.

Jacobian Matrix of a Coordinate Transformation

The Jacobian matrix of this transformation is called *coordinate transformation matrix* and is defined as the matrix of all partial derivatives of the coordinate transformation.

Its determinant is called the *Jacobian determinant*.

Example:

We define the Transformation ϕ from polar coordinates to cartesian coordinates as follows:

$$\begin{aligned} \phi(r,\phi) &= \begin{pmatrix} r\cos\phi \\ r\sin\phi \end{pmatrix} := \begin{pmatrix} x \\ y \end{pmatrix} \\ \implies J_\phi(r,\phi) &= \begin{pmatrix} \cos\phi & -r\sin\phi \\ \sin\phi & r\cos\phi \end{pmatrix} \\ \implies \det J_\phi(r,\phi) &= r \end{aligned}$$

Roots and Optima

Newton's Method