Calculus I

Essential Terminology for Univariate Scalar Functions

Uwe Naumann

Informatik 12:
Software and Tools for Computational Engineering
RWTH Aachen University
Contents

Objective and Learning Outcomes

Continuity

Intermediate Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Outline

Objective and Learning Outcomes

Continuity

Intermediate Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Objective and Learning Outcomes

Objective

▶ Introduction to essential scalar calculus

Learning Outcomes

▶ You will understand
  ▶ continuity
  ▶ differentiability
  ▶ chain rule of differential calculus
  ▶ partial, total, directional derivative
  ▶ $O(\cdot)$ notation
  ▶ Taylor series.
Outline

Objective and Learning Outcomes

Continuity

Intermediate Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Calculus I

Continuity \((f : \mathbb{R} \rightarrow \mathbb{R})\)

Let \([a, b] \subseteq \mathbb{R}\) be the (open) domain of the univariate scalar function \(f : \mathbb{R} \rightarrow \mathbb{R}\) with image \([c, d] \subseteq \mathbb{R}\).

\(f(x)\) is right-continuous at \(\tilde{x} \in \mathbb{R}\) if

\[
\lim_{\Delta x \to 0, \Delta x > 0} f(\tilde{x} + \Delta x) = f(\tilde{x}) .
\]

\(f\) is left-continuous at \(\tilde{x}\) if

\[
\lim_{\Delta x \to 0, \Delta x > 0} f(\tilde{x} - \Delta x) = f(\tilde{x}) .
\]

\(f\) is continuous at \(\tilde{x}\) if it is both left- and right-continuous at \(\tilde{x}\).

Continuity is a necessary condition for differentiability.
Consider the absolute value function $f(x) = |x|$ at $x = 0$:

The left limit

$$\lim_{{\Delta x \to 0, \Delta x > 0}} f(0 - \Delta x) = f(0) = 0$$

and the right limit

$$\lim_{{\Delta x \to 0, \Delta x > 0}} f(0 + \Delta x) = f(0) = 0$$

are identical proving that $|x|$ is continuous at the origin.

In fact, $|x|$ is continuous throughout its domain $\mathbb{R}$. 
Let $\mathbb{R}$ be the domain of the univariate scalar function $f : \mathbb{R} \to \mathbb{R}$.

The function $f$ is **continuous** at a point $\tilde{x} \in \mathbb{R}$ if

$$\lim_{x \to \tilde{x}} f(x) = f(\tilde{x}).$$

The above implies that for all series $(x_i)_{i=1}^{\infty}$ with

$$\lim_{i \to \infty} x_i = \tilde{x}$$

and $x_i \neq \tilde{x}$ the series $(f(x_i))_{i=1}^{\infty}$ converges to $f(\tilde{x})$.

Continuity in $\mathbb{R}$ requires continuity at all $\tilde{x} \in \mathbb{R}$. 

Outline

Objective and Learning Outcomes

Continuity

Intermedia te Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Intermediate Value Theorem

Let \( y = f(x) \) be continuous within a neighborhood \( x + \Delta x \) of \( x \) taking values \( f(x) \) and \( f(x + \Delta x) \) at the endpoints of the interval. Then \( f \) takes all values between \( f(x) \) and \( f(x + \Delta x) \) over the same interval.

If \( f(x) \) and \( f(x + \Delta x) \) have different signs, then \( f \) has a root within the interval bounded by \( x \) and \( x + \Delta x \), i.e., \( \exists \tilde{x} : f(\tilde{x}) = 0 \).

The simplest possible root finding algorithm follows from iterative / recursive bisection of the interval \( [x, x + \Delta x] \).

Unfortunately, the bisection algorithm converges slowly and does not generalize to higher dimensions. Hence, we are going to investigate superior alternatives.

Note: \( \tilde{x} \) not necessarily unique; \( f \) can take values outside of \( [f(x), f(x + \Delta x)] \).
Bisection

Implementation

```cpp
template<typename T>
T f(const T &x) { ... }

template<typename T>
void solve(T &x, const T &dx) {
    T xu=x+dx;
    while (fabs(x-xu)>1e-7) {
        T xm=(xu+x)/2, ym=f(xm);
        if (ym>0) xu=xm; else if (ym<0) x=xm; else x=xu=xm;
    }
}
```
Outline

Objective and Learning Outcomes

Continuity

Intermediate Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Let $R$ be the domain of the univariate scalar function $f : R \to R$. 

$f(x)$ is right-differentiable at $\bar{x} \in R$ if the limit 

$$
\lambda^+ = \lim_{\Delta x \to 0} \frac{f(\bar{x} + \Delta x) - f(\bar{x})}{\Delta x}
$$

exists (is finite). $f$ is left-differentiable at $\bar{x}$ if 

$$
\lambda^- = \lim_{\Delta x \to 0} \frac{f(\bar{x}) - f(\bar{x} - \Delta x)}{\Delta x}
$$

exists (is finite). $f$ is differentiable at $\bar{x}$ if it is both left- and right-differentiable and 

$$
\lambda^+ = \lambda^- \equiv dx(\bar{x})
$$
Consider the absolute value function $f(x) = |x|$ at $x = 0$.

The left limit is derived from the backward difference

$$
\lim_{\Delta x \to 0, \Delta x > 0} \frac{f(0) - f(0 - \Delta x)}{\Delta x} = \lim_{\Delta x \to 0, \Delta x > 0} \frac{0 - \Delta x}{\Delta x} = -1
$$

while a forward difference is used to get the right limit

$$
\lim_{\Delta x \to 0, \Delta x > 0} \frac{f(0 + \Delta x) - f(0)}{\Delta x} = \lim_{\Delta x \to 0, \Delta x > 0} \frac{\Delta x}{\Delta x} = 1.
$$

The limits are distinct proving that $|x|$ is not differentiable at the origin. However, $|x|$ is differentiable everywhere else within its domain $\mathbb{R}$. 
Differentiability

Alternative Formulation \((f : \mathbb{R} \rightarrow \mathbb{R})\)

Let \(\mathbb{R}\) be the domain of the univariate scalar function \(f : \mathbb{R} \rightarrow \mathbb{R}\). The function \(f\) is differentiable at point \(\tilde{x} \in \mathbb{R}\) if there is a scalar \(f' \in \mathbb{R}\) such that

\[
f(\tilde{x} + \Delta x) = f(\tilde{x}) + f' \cdot \Delta x + r
\]

with asymptotically vanishing remainder \(r = r(\tilde{x}, \Delta x) \in \mathbb{R}\), that is,

\[
\lim_{\Delta x \to 0} \frac{r}{|\Delta x|} = 0.
\]

Differentiability in \(\mathbb{R}\) requires differentiability at all \(\tilde{x} \in \mathbb{R}\) (and similarly for non-scalar cases). The function

\[
f' = f'(x) = \frac{df}{dx}(x) : \mathbb{R} \rightarrow \mathbb{R}
\]

is called the [first] derivative of \(f\).
Outline

Objective and Learning Outcomes

Continuity

Intermediate Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Let $y = f(x) : \mathbb{R} \to \mathbb{R}$ (or open subdomains in $\mathbb{R}$) be such that

$$y = f(x) = f_2(f_1(x)) = f_2(z)$$

with (continuously) differentiable $f_1, f_2 : \mathbb{R} \to \mathbb{R}$.

Then $f$ is (continuously) differentiable and

$$\frac{df}{dx} (\tilde{x}) = \frac{df_2}{dx} (\tilde{z}) = \frac{df_2}{dz} (\tilde{z}) \cdot \frac{df_1}{dx} (\tilde{x})$$

for all $\tilde{x} \in \mathbb{R}$ and $\tilde{z} = f_1(\tilde{x})$. 
Given two functions \( f(x) \) and \( g(x) \) the notation

\[ f = O(g) \]

implies that \( f \) grows up to a constant factor as \( g \), that is,

\[ \exists C > 0 \in \mathbb{R} : |f(x)| \leq C \cdot |g(x)| \]

for all \( x \) within the shared domains of \( f \) and \( g \).

E.g, \( f(x) = O(x^2) \) implies that \( f(x) \) does not grow faster than \( C \cdot x^2 \) for some constant \( C > 0 \).

Although,

\[ f(x) = O(x) \, \Rightarrow \, f(x) = O(x^2) \, \Rightarrow \, f(x) = O(x^3) \, \ldots \]

we state the lowest upper bound.

\( \Omega(\cdot) \) notation covers the corresponding highest lower bound.
Outline

Objective and Learning Outcomes

Continuity

Intermediate Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Let $f : \mathbb{R} \to \mathbb{R}$ be $n$-times continuously differentiable.

Given the value of $f(x)$ at some point $\tilde{x} \in \mathbb{R}$ the function value $f(\tilde{x} + \Delta x)$ at a neighboring point can be approximated by a Taylor series as

$$f(\tilde{x} + \Delta x) \approx O(\Delta x^n) \ f(\tilde{x}) + \sum_{k=1}^{n-1} \frac{1}{k!} \cdot \frac{d^k f}{dx^k}(\tilde{x}) \cdot \Delta x^k.$$

Throughout this course we assume convergence of the Taylor series for $k \to \infty$ to the true value of $f(\tilde{x} + \Delta x)$ within all subdomains of interest, which is not the case for arbitrary functions.

For $n = 4$ we get

$$f(\tilde{x} + \Delta x) = f(\tilde{x}) + f'(\tilde{x}) \cdot \Delta x + \frac{1}{2} \cdot f''(\tilde{x}) \cdot \Delta x^2 + \frac{1}{6} \cdot f'''(\tilde{x}) \cdot \Delta x^3 + O(|\Delta x|^4).$$
Taylor Series

Example

Consider \( y = f(x) = x^3 \) at \( x + \Delta x \) for \( x = 1 \) and \( \Delta x = 0.1 \).

\[
f(x + \Delta x) = 1.1^3 = 1^3 + 3 \cdot 1^2 \cdot 0.1 + 6 \cdot 1 \cdot 0.1^2 + 6 \cdot 0.1^3 = 1.331 \\
\approx O(\Delta x^3) \quad 1^3 + 3 \cdot 1^2 \cdot 0.1 + 6 \cdot 1 \cdot 0.1^2 = 1.33 \\
\approx O(\Delta x^2) \quad 1^3 + 3 \cdot 1^2 \cdot 0.1 = 1.3 \\
\approx O(\Delta x^1) \quad 1^3 = 1
\]

Consider \( y = f(x) = \sin(x) \) at \( x + \Delta x \) for \( x = 1 \) and \( \Delta x = 0.1 \).

\[
f(x + \Delta x) = \sin(1.1) = 0.891207 \ldots \\
\approx O(\Delta x^4) \quad \sin(1) + \cos(1) \cdot 0.1 - \sin(1) \cdot 0.1^2 - \cos(1) \cdot 0.1^3 = 0.891204 \ldots \\
\approx O(\Delta x^3) \quad \sin(1) + \cos(1) \cdot 0.1 - \sin(1) \cdot 0.1^2 = 0.891294 \ldots \\
\approx O(\Delta x^2) \quad \sin(1) + \cos(1) \cdot 0.1 = 0.895501 \ldots \\
\approx O(\Delta x^1) \quad \sin(1) = 0.841471 \ldots
\]
Outline

Objective and Learning Outcomes

Continuity

Intermediate Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Further Essential Terminology

Linearity \((f : \mathbb{R} \rightarrow \mathbb{R})\)

A function \(f : \mathbb{R} \rightarrow \mathbb{R}\) is called **linear** if

\[
\begin{align*}
\triangleright f(a + b) &= f(a) + f(b) \\
\triangleright f(\alpha \cdot a) &= \alpha \cdot f(a)
\end{align*}
\]

for all \(a, b, \alpha \in \mathbb{R}\).

Example: \(f(x) = p \cdot x\) with constant \(p \in \mathbb{R}\) is linear.

\[
\begin{align*}
f(a + b) &= p \cdot (a + b) = p \cdot a + p \cdot b = f(a) + f(b) \\
f(\alpha \cdot a) &= p \cdot \alpha \cdot a = \alpha \cdot p \cdot a = \alpha \cdot f(a)
\end{align*}
\]

Functions of the form \(f(x) = p \cdot x + q\) with constant \(p, q \in \mathbb{R}\) are called **affine**. Linear functions are affine with \(q = 0\).

Roots of affine functions are defined by **linear equations** \(f(x) = p \cdot x + q = 0\).
Let $f : R \rightarrow R$ be **analytic** (infinitely often differentiable), e.g., $x^2, e^x, \sin(x), \ldots$

$f$ is **constant** [over $(a, b)$] if its derivatives vanish identically for all $x \in [(a, b) \subseteq]R$, e.g., $f(x) = 42$ is constant over $R$.

$f$ is (at most) **affine** if its second and higher derivatives vanish identically for all $x \in R$, e.g., $f(x) = 42 \cdot x - 24$ is affine over $R$ while $f(x) = 42 \cdot x$ is linear.

$f$ is (at most) **quadratic** if its third and higher derivatives vanish identically for all $x \in R$, e.g., $f(x) = 42 \cdot x^2 - 24 \cdot x + 1$ is quadratic over $R$.

$f$ is (at most) **cubic** if its fourth and higher derivatives vanish identically for all $x \in R$, e.g., $f(x) = 42 \cdot x^3 - 24$ is cubic over $R$.

etc.
Further Essential Terminology

Monotonicity ($f : \mathbb{R} \rightarrow \mathbb{R}$)

A function $f : \mathbb{R} \rightarrow \mathbb{R}$ is

- [strictly] monotonically increasing over $(a, b) \subseteq \mathbb{R}$ if

  \[ \forall x_0, x_1 \in (a, b) : x_0 < x_1 \Rightarrow f(x_0)[<] \leq f(x_1) \]

  or, equivalently, if $f$ is differentiable over $(a, b)$, then

  \[ \forall x \in (a, b) : f'(x) [>] \geq 0 . \]

- [strictly] monotonically decreasing over $(a, b)$ if

  \[ \forall x_0, x_1 \in (a, b) : x_0 < x_1 \Rightarrow f(x_0)[>] \geq f(x_1) \]

  or, equivalently, if $f$ is differentiable over $(a, b)$, then

  \[ \forall x \in (a, b) : f'(x) [<] \leq 0 . \]
Further Essential Terminology
Convexity \((f : \mathbb{R} \to \mathbb{R})\)

Let \(f : \mathbb{R} \to \mathbb{R}\) be continuous over \([a, b] \subset \mathbb{R}\). Then \(f\) is [strictly] convex if

\[
\forall x_0, x_1 \in [a, b] : f \left( \frac{x_0 + x_1}{2} \right) \leq \frac{f(x_0) + f(x_1)}{2}
\]

(points of all secants above the graph of \(f\))

Let \(f : \mathbb{R} \to \mathbb{R}\) be twice differentiable over \([a, b] \subset \mathbb{R}\). Then \(f\) is [strictly] convex if \(f''(x) \geq 0\) for all \(x \in [a, b]\).

Examples: \(f(x) = x^2\) and \(f(x) = e^x\) are strictly convex over \(\mathbb{R}\); \(f(x) = \sin(x)\) is strictly convex over \((\pi, 2 \cdot \pi)\); \(f(x) = 42 \cdot x\) is (not strictly) convex over \(\mathbb{R}\).
Further Essential Terminology

Concavity \((f : \mathbb{R} \rightarrow \mathbb{R})\)

Let \(f : \mathbb{R} \rightarrow \mathbb{R}\) be continuous over \([a, b] \subset \mathbb{R}\).

\(f\) is [strictly] concave if

\[
\forall x_0, x_1 \in [a, b]: f\left(\frac{x_0 + x_1}{2}\right) \geq \frac{f(x_0) + f(x_1)}{2}
\]

(points of all secants below the graph of \(f\))

Let \(f : \mathbb{R} \rightarrow \mathbb{R}\) be twice differentiable over \([a, b] \subset \mathbb{R}\). Then \(f\) is [strictly] concave if \(f''(x) \leq 0\) for all \(x \in [a, b]\).

Examples: \(f(x) = -x^2\) and \(f(x) = -e^x\) are strictly concave over \(\mathbb{R}\);
\(f(x) = \cos(x)\) is strictly concave over \((-\frac{\pi}{2}, \frac{\pi}{2})\); \(f(x) = 42 \cdot x\) is (not strictly) concave over \(\mathbb{R}\).
Outline

Objective and Learning Outcomes

Continuity

Intermediate Value Theorem and Bisection

Differentiability

Chain Rule

Taylor Series

Further Essential Terminology

Summary and Next Steps
Summary

- Introduction of essential calculus
- Roots of nonlinear equations by bisection

Next Steps

- Play with bisection code
- Continue the course to find out more ...