Calculus I

Essential Terminology for Univariate Scalar Functions

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Informatik 12:
Software and Tools for Computational Engineering

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Contents

Outline

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

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

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

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

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

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

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 $\tilde{x} = 0$:

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 $\boldsymbol{R}$.

Let R be the domain of the univariate scalar function $f : R \rightarrow R$.

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

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

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

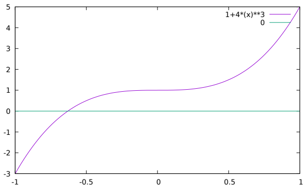
$$\lim_{i \to \infty} x_i = \tilde{x}$$

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

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

Outline

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 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 $[f(x), f(x + \Delta x)]$

```
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

Let R be the domain of the univariate scalar function $f : R \to R$.

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

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

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

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

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

$$\lambda^+ = \lambda^- \equiv \frac{df}{dx}(\tilde{x}) \quad .$$

Consider the absolute value function $f(x) = |x|$ at $\tilde{x} = 0$.

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

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

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

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

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

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

$$\lim_{\Delta x \rightarrow 0} \frac{r}{|\Delta x|} = 0 \quad .$$

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

$$f' = f'(x) = \frac{df}{dx}(x) : \boldsymbol{R} \rightarrow \boldsymbol{R}$$

is called the [first] derivative of f.

Outline

Let $y = f(x) : \boldsymbol{R} \to \boldsymbol{R}$ (or open subdomains in $\boldsymbol{R}$) be such that

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

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

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 $\tilde{x} \in \boldsymbol{R}$ 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,

$$\exists C > 0 \in \boldsymbol{R} : |f(x)| \leq C \cdot |g(x)|$$

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,

$$f(x) = O(x) \quad \Rightarrow \quad f(x) = O(x^2) \quad \Rightarrow \quad f(x) = O(x^3) \quad \ldots$$

we state the lowest upper bound.

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

Outline

Let $f : \mathbf{R} \to \mathbf{R}$ be n-times continuously differentiable.

Given the value of $f(x)$ at some point $\tilde{x} \in \mathbf{R}$ 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

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

Example

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

$$f(x+\Delta x) = 1.1^3 = 1^3 + 3\cdot 1^2 \cdot 0.1 + 6 \cdot 1 \cdot 0.1^2 + 6 \cdot 0.1^3 = 1.331$$
$$\approx_{O(\Delta x^3)} 1^3 + 3\cdot 1^2 \cdot 0.1 + 6 \cdot 1 \cdot 0.1^2 = 1.33$$
$$\approx_{O(\Delta x^2)} 1^3 + 3\cdot 1^2 \cdot 0.1 = 1.3$$
$$\approx_{O(\Delta x^1)} 1^3 = 1$$

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

$$f(x+\Delta x) = sin(1.1) = 0.891207\ldots$$
$$\approx_{O(\Delta x^4)} \sin(1) + \cos(1)\cdot 0.1 - \sin(1)\cdot 0.1^2 - \cos(1)\cdot 0.1^3 = \underline{0.8912}04\ldots$$
$$\approx_{O(\Delta x^3)} \sin(1) + \cos(1)\cdot 0.1 - \sin(1)\cdot 0.1^2 = \underline{0.8912}94\ldots$$
$$\approx_{O(\Delta x^2)} \sin(1) + \cos(1)\cdot 0.1 = \underline{0.89}5501\ldots$$
$$\approx_{O(\Delta x^1)} \sin(1) = \underline{0.8}41471\ldots$$

Outline

A function $f : \boldsymbol{R} \rightarrow \boldsymbol{R}$ is called linear if

- $f(a+b) = f(a) + f(b)$
- $f(\alpha \cdot a) = \alpha \cdot f(a)$

for all $a, b, \alpha \in \boldsymbol{R}$.

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

$$f(a+b) = p \cdot (a+b) = p \cdot a + p \cdot b = f(a) + f(b)$$
$$f(\alpha \cdot a) = p \cdot \alpha \cdot a = \alpha \cdot p \cdot a = \alpha \cdot f(a)$$

Functions of the form $f(x) = p \cdot x + q$ with constant $p, q \in \boldsymbol{R}$ 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 $f : \boldsymbol{R} \rightarrow \boldsymbol{R}$ 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 $x \in [(a, b) \subseteq]\boldsymbol{R}$, e.g, $f(x) = 42$ is constant over $\boldsymbol{R}$.

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

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

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

etc.

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A function $f : \mathbb{R} \to \mathbb{R}$ 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

  $$\forall x \in (a, b) : f'(x)\ [<]\ \leq 0 \, .$$

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ 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 $f : \mathbb{R} \rightarrow \mathbb{R}$ 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 $\mathbb{R}$.

Let $f : \boldsymbol{R} \rightarrow \boldsymbol{R}$ be continuous over $[a, b] \subset \boldsymbol{R}$.

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 $f : \boldsymbol{R} \rightarrow \boldsymbol{R}$ be twice differentiable over $[a, b] \subset \boldsymbol{R}$. 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 $\boldsymbol{R}$; $f(x) = \cos(x)$ is strictly concave over $(-\frac{\pi}{2}, \frac{\pi}{2})$; $f(x) = 42 \cdot x$ is (not strictly) concave over $\boldsymbol{R}$.

Outline

Summary

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

Next Steps

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