Calculus and Linear Algebra for Biomedical Engineering

Week 7: Differentiable Functions

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Motivation: Temperature Measurements (yet again)

We have a sequence $y_0, y_1, y_2, \ldots$ of temperature measurements at times $t = 0, 1, 2, \ldots$. (in hours) as before. For the determination of the temperature after 12.7 hours, we suggested to take y_{13}, simply because 13 is the closest point in time for which we have a measurement.

A more sophisticated guess for the temperature is obtained by linear interpolation: We take

$$y_{12.7} \approx y_{12} + 0.7 \cdot (y_{13} - y_{12})$$

The idea is to use information from both neighboring points in time, weighting the contribution of the different points according to their distance.

A mathematical formulation

Again we let $f : [0, M] \to \mathbb{R}$ denote the temperature function.
Measured data:
Measurements $f(t)$ at times $0 = t_0, t_1, t_2, t_3 \ldots, t_N = M \in [0, M]$.

Linear interpolation: Given $s \in [0, M]$, hence s between t_n and t_{n+1}, we define

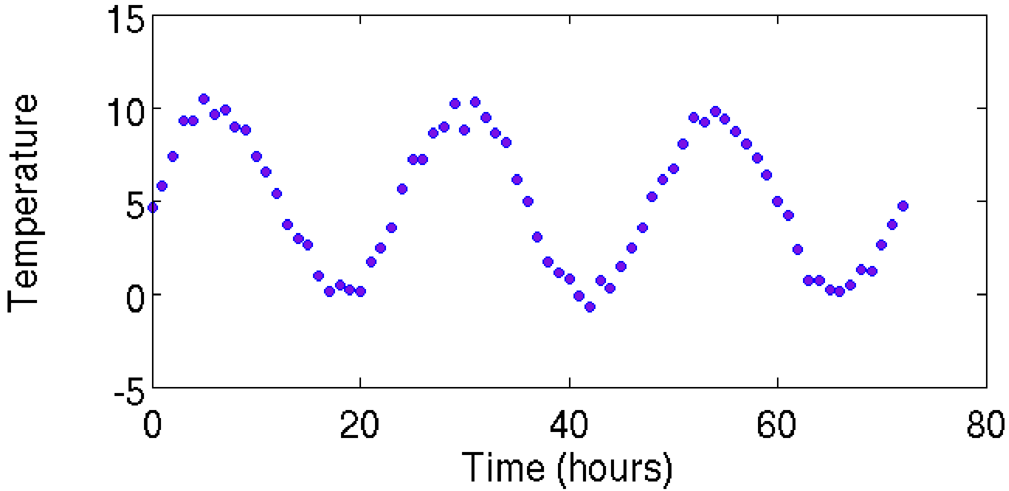
$$g(s) = f(t_n) + \frac{f(t_{n+1}) - f(t_n)}{t_{n+1} - t_n}(s - t_n)$$

Hence the graph of g is obtained by connecting the data points $(t_n, f(t_n))_{n=0,\ldots,N}$ by straight lines.

Question: What do we need to know about f and $t_0, \ldots, t_N$, to estimate the precision of the approximation $f(s) \approx g(s)$, for arbitrary s?

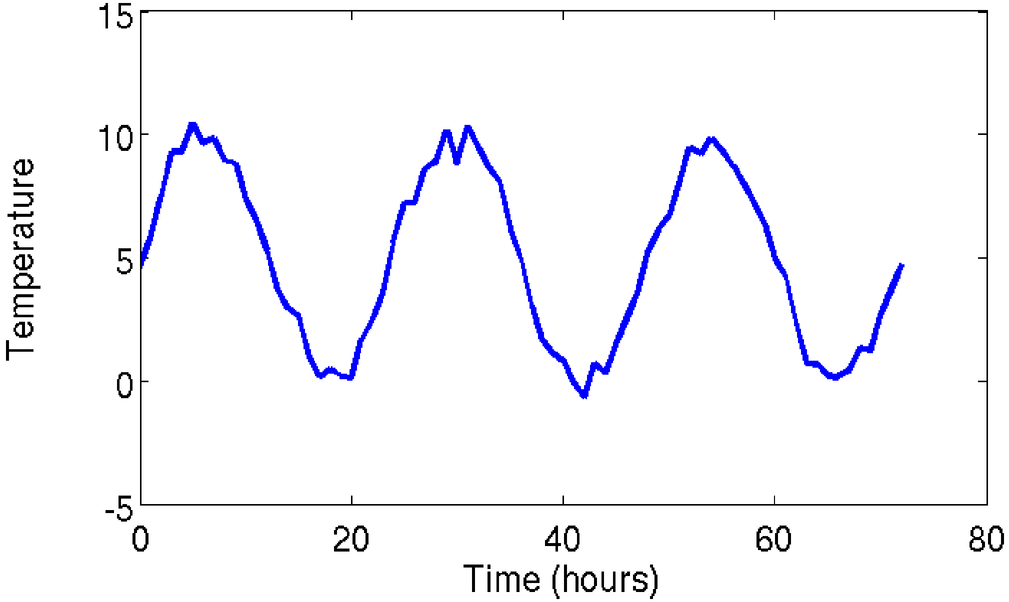
Linear interpolation: An illustration

Scatter plot



Linear interpolation: An illustration

Linear interpolation (often used to visualize discrete data)



Secant and difference quotient

Definition. Let $(a, b) \subset \mathbb{R}$ be an interval, with $x_0 \in (a, b)$ fixed. Let $f : (a, b) \to \mathbb{R}$ be a function.

1. If $x \in (a, b)$, the secant to f through x_0, x is the straight line connecting the points $(x_0, f(x_0))$, and $(x, f(x))$ in the plane.
2. The slope of the secant through x, given as

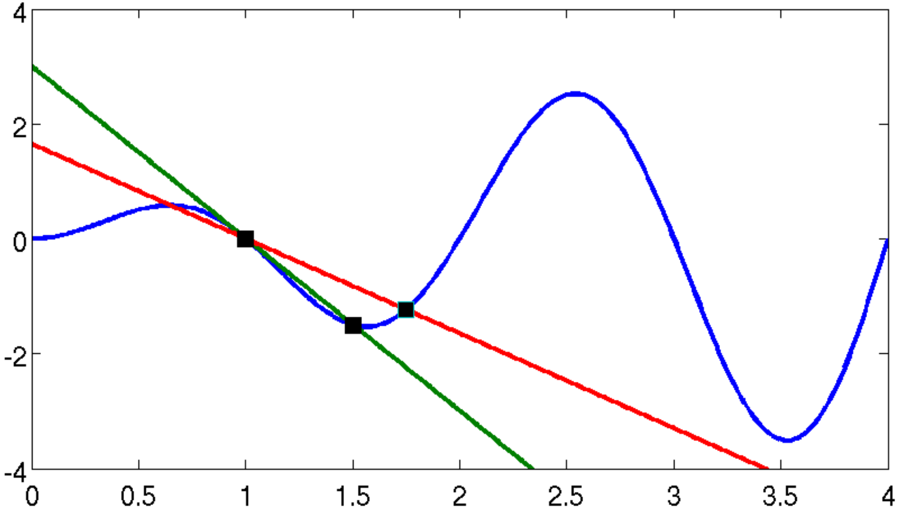
$$\Delta_{f,x_0}(x) = \Delta_f(x) = \frac{f(x) - f(x_0)}{x - x_0}$$

   is called the difference quotient associated to x, x_0.

Examples

Two secants to the function $f(x) = x\sin(\pi x)$ (blue curve) through $x_0 = 1$

Green: $x = 1.5$, Red: $x = 1.75$



Definition of the derivative

Definition. Let $D \subset \mathbb{R}$ and $f : D \longrightarrow \mathbb{R}$, $x_0 \in D$.

(a) f is called differentiable at x_0 if, for some $\delta > 0$, $(x_0-\delta, x_0+\delta) \subset D$, and in addition,

$$\alpha = \lim_{x \to x_0} \Delta_{f,x_0}(x) = \frac{f(x) - f(x_0)}{x - x_0} \tag{1}$$

exists in $\mathbb{R}$.

(b) If f is differentiable, the limit α in (1) is called derivative of f at x_0, and denoted by

$$f'(x_0) := \frac{df}{dx}(x_0) := \alpha \, .$$

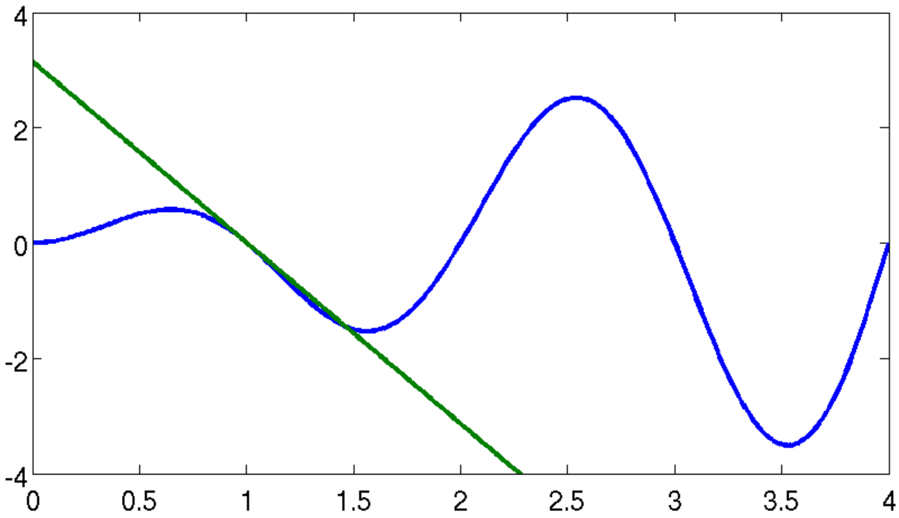
(c) If f is differentiable at all $x_0 \in D$, the function $D \ni x \mapsto f'(x)$ is called derivative function or just derivative of f.

Interpretations of the derivative

- Graphically, the derivative is the slope of the tangent to the graph through $(x_0, f(x_0))$. Alternatively, it can be interpreted as the slope of the graph at x_0.
  The graph of a differentiable function is characterized by the property that it has no sharp corners or bends.
- The common physical interpretation is velocity: If $f(t)$ denotes the distance of an object travelling along a straight line t, the velocity with which the object moves at time t is $f'(t)$, in this context often denoted $\dot{f}(t)$.
- In the modelling of biological or chemical processes, the derivative of a population size or chemical quantity describes its growth rate.

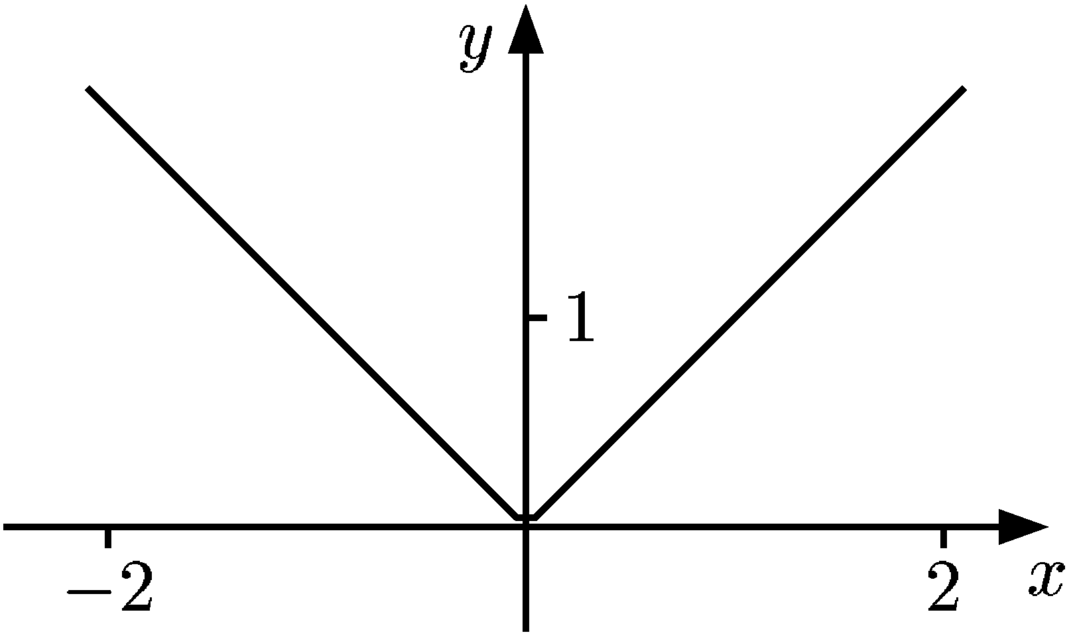
Example

The tangent to the function $f(x) = x\sin(\pi x)$ (blue curve) through $x_0 = 1$



A continuous nondifferentiable function

The function $f(x) = |x|$ is differentiable at $x_0 \neq 0$, but not at $x_0 = 0$.



Properties: Continuity, Mean value theorem

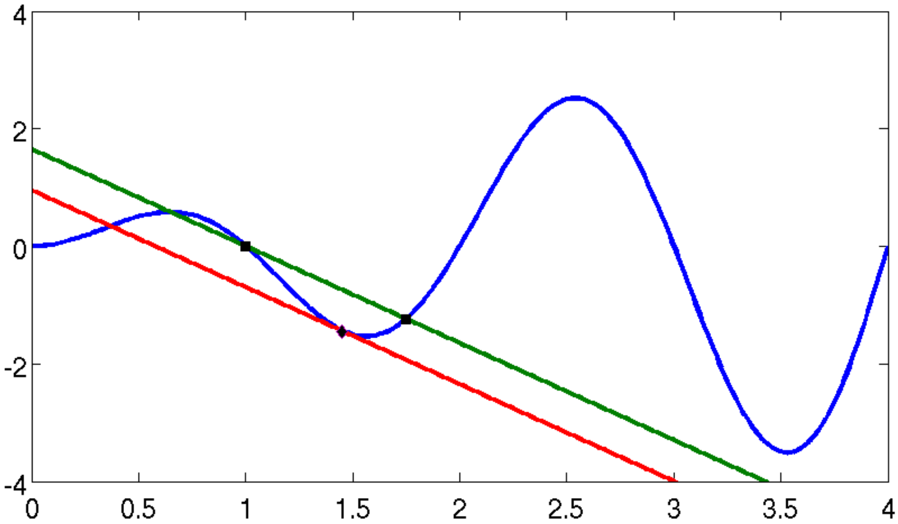
Theorem 1.
Let $f : D \to \mathbb{R}$ be differentiable. Then f is continuous.

Theorem 2. (Mean value theorem)
Let $f : D \to \mathbb{R}$ be continuous on $[x, y]$ and differentiable on (x, y). Then there exists $z \in (x, y)$ such that

$$\frac{f(y) - f(x)}{y - x} = f'(z) \ .$$

Illustration of the mean value theorem

The function $f(x) = x\sin(x)$, $x = 1, y = 1.75$. There exists z between x, y such that the tangent to f at z (red line) is parallel to the secant through $(x, f(x)), (y, f(y))$ (green).



Rules for the computation of derivatives

Theorem 3. Let $f, g : D \to \mathbb{R}$ be differentiable functions.

- Linearity: For all $s, t \in \mathbb{R}$, $sf + tg$ is differentiable on D, wtih $(sf + tg)' = sf' + tg'$.
- Product rule: The function $f \cdot g : D \to \mathbb{R}$, $(f \cdot g)(x) = f(x)g(x)$, is differentiable with $(f \cdot g)' = f' \cdot g + f \cdot g'$.
- Quotient rule: Suppose that $g(x) \neq 0$ for all $x \in D$. Then the map $h(x) = \frac{f(x)}{g(x)}$ is differentiable on D, with

$$h'(x) = \frac{f'(x)g(x) - f(x)g'(x)}{g(x)^2} .$$

- Chain rule: Suppose that $h : E \to \mathbb{R}$ is differentiable on E, with $h(E) \subset D$. Then $g \circ h : E \to \mathbb{E}$ is differentiable on E, with $(g \circ h)(x) = g'(h(x))h'(x)$.

Known classes of differentiable functions

- For $\alpha \in \mathbb{R}$, the function $f(x) = x^\alpha$, is differentiable on $(0, \infty)$ with derivative $f'(x) = \alpha x^{\alpha-1}$. This includes the constant function $f(x) = 1 = x^0$, with derivative $f'(x) = 0$.
- For $s \in \mathbb{R}$, the function $f(x) = x^s$, is differentiable on $\mathbb{R}_0^+$ with derivative $f'(x) = sx^{s-1}$. This includes the constant function $f(x) = 1 = x^0$, with derivative $f'(x) = 0$.
- By the quotient rule, the previous item entails for all $n \in \mathbb{N}$ and $f(x) = x^{-n}$, that $f'(x) = nx^{n-1}$.
- As a consequence, polynomials $f : \mathbb{R} \to \mathbb{R}$ are differentiable.
- Trigonometric functions: $\sin, \cos, \tan$ are differentiable on their domains, with $\sin' = \cos$, $\cos' = -\sin$.

Example: Computing a derivative

We are given the function $f(x) = (x^4 + x^2)^{1/2} = (g_1 \circ (g_2 + g_3))(x)$, where

- $g_1(t) = t^{1/2}$, with $g_1'(t) = \frac{t^{-1/2}}{2} = \frac{1}{2\sqrt{t}}$;
- $g_2(t) = x^2$, with $g_2'(t) = 2x$;
- $g_3(t) = x^4$, with $g_3'(t) = 4x^3$.

Applying the chain rule gives

$$f'(x) = g_1'(g_2(x) + g_3(x)) \cdot (g_2'(x) + g_3'(x)) \ ,$$

and plugging in the derivatives, we obtain

$$f'(x) = \underbrace{\frac{1}{2\sqrt{x^4 + x^2)}}}_{g_1'(g_2(x) + g_3(x)))} (\underbrace{2x}_{g_2'(x)} + \underbrace{4x^3}_{g_3'(x)}) = \frac{x + 2x^3}{\sqrt{x^4 + x^2}}$$

Example: Computing a derivative

We are given the function $f(x) = \sqrt{\sin(x^2)} = (g_1 \circ g_2 \circ g_3)(x)$, where

- $g_1(t) = t^{1/2}$, with $g_1'(t) = \frac{t^{-1/2}}{2} = \frac{1}{2\sqrt{t}}$;
- $g_2(t) = \sin(t)$, with $g_2'(t) = \cos(t)$;
- $g_3(t) = t^2$, with $g_3'(t) = 2t$.

Applying the chain rule twice gives

$$f'(x) = g_1'(g_2(g_3(x))) \cdot (g_2 \circ g_3)'(x) = g_1'(g_2(g_3(x))) \cdot g_2'(g_3(x)) \cdot g_3'(x) \ ,$$

and plugging in the derivatives, we obtain

$$f'(x) = \underbrace{\frac{1}{2\sqrt{\sin(x^2)}}}_{g_1'(g_2(g_3(x)))} \ \underbrace{\cos(x^2)}_{g_2'(g_3(x))} \ \underbrace{2x}_{g_3'(x)} = \frac{x\cos(x^2)}{\sqrt{\sin(x^2)}}$$

Higher order derivatives

Definition. Let $D \subset \mathbb{R}$ and $f : D \to \mathbb{R}$ be a differentiable function.

- If f' is differentiable on D, we call the derivative of f' second derivative of f, denoted by

$$f^{(2)} := f'' := \frac{d^2 f}{dx^2} := \frac{df'}{dx} \ .$$

  The function f is then called twice differentiable.

- More generally, if f is n-time differentiable (with $n \in \mathbb{N}$), such that its nth derivative $f^{(n)}$ is differentiable again, the $n+1$st derivative of f is defined as

$$f^{(n+1)} := \frac{d^{n+1} f}{dx^{n+1}} := \frac{df^{(n)}}{dx} \ .$$

  f is then called $n+1$ times differentiable.
  We use f''', f'''' etc. for the third, fourth etc. derivative .
  If all derivatives exist, f is called infinitely differentiable.

Examples

- The function $f(x) = x^n$ has derivative $f'(x) = nx^{n-1}$. Repeated differentiation gives

$$f^{(k)}(x) = \begin{cases} n \cdot (n-1) \cdot \ldots \cdot (n-k+1)x^{n-k} & k \leq n \\ 0 & k > n \end{cases} .$$

In particular, f is infinitely differentiable. As a consequence, polynomials are infinitely differentiable.

- The function $f(x) = \sin(x)$ is infinitely differentiable: $f'(x) = \cos(x)$, $f''(x) = -\sin(x) = -f(x)$. Hence we can differentiate $\sin$ infinitely many times.

- The function

$$f(x) = \begin{cases} x^2 & x \geq 0 \\ 0 & x < 0 \end{cases}$$

is differentiable, but not twice differentiable on $\mathbb{R}$: f' is not differentiable at 0.

Taylor's theorem

Theorem. (Taylor)
Let $D \subset \mathbb{R}$ and $f : D \to \mathbb{R}$ be $n+1$ times differentiable. Let $x_0, y \in D$ be such that all points between x_0, y are in D. Then there exists z between (x_0, y) such that

$$\begin{aligned} f(y) &= \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(y-x)^k + \frac{f^{(n+1)}(z)}{(n+1)!}(y-x_0)^{n+1} \\ &= f(x_0) + f'(x)(y-x_0) + \frac{f''(x_0)}{2}(y-x_0)^2 + \ldots + \frac{f^{(n)}(x_0)}{n!}(y-x_0)^n \\ &\quad + \frac{f^{(n+1)}(z)}{(n+1)!}(y-x_0)^{n+1} \;, \end{aligned}$$

where we used $n! = 1 \cdot 2 \cdot \ldots \cdot n$.

Taylor polynomial

Definition. If f is $n+1$ times differentiable, the polynomial

$$T_{n,x_0}(y) = f(x_0) + f'(x)(y - x_0) + \frac{f''(x_0)}{2}(y - x_0)^2 + \ldots + \frac{f^{(n)}(x_0)}{n!}(y - x_0)^n$$

is called Taylor polynomial of f of degree n. The difference

$$R_{n,x_0}(y) = f(x) - T_{n,x_0}(y) = \frac{f^{(n+1)}(z)}{(n+1)!}(y - x_0)^{n+1}$$

is called the remainder term.

Interpretation of the Taylor polynomial

By Taylor's theorem,

$$f(y) - T_{n,x_0}(y) = \frac{f^{(n+1)}(z)}{(n+1)!}(y - x_0)^{n+1} \; .$$

As $f^{(n+1)}$ is continuous, there exists $M > 0$ such that $f^{(n+1)}(z) \leq M$ for all z between y, x_0, and thus

$$|f(y) - T_{n,x_0}(y)| \leq \frac{M}{(n+1)!}|y - x_0|^n < \frac{M}{(n+1)!}\epsilon^n$$

if $|y - z_0| < 0$. The right-hand side goes to zero as $\epsilon \to 0$.

Note: The speed with which $\epsilon^n \to 0$ for $\epsilon \to 0$ increases with n.

Hence, T_{n,x_0} is a polynomial approximation of f near x_0. The quality of approximation increases as $n \to \infty$.

Back to the initial example

Measured data:
Measurements $f(t)$ at times $0 = t_0, t_1, t_2, t_3 \ldots, t_N = M \in [0, M]$.

Linear interpolation: Given $s \in [0, M]$, hence s between t_n and t_{n+1}, we define

$$g(s) = f(t_n) + \frac{f(t_{n+1}) - f(t_n)}{t_{n+1} - t_n}(s - t_n)$$

Wanted: An estimate for $|f(s) - g(s)|$.

Estimating the approximation error

We assume f to be twice differentiable on $[0, M]$. In particular, $|f''(z)| \leq K$, for all $z \in [0, M]$, with K a suitable constant.

Using the mean value theorem, we obtain

$$g(s) = f(t_n) + f'(z)(s - t_n) \ ,$$

for z between s and t_n.

Moreover, using Taylor approximation of degree one,

$$f(s) = f(t_n) + f'(t_n)(s - t_n) + \frac{f''(y)}{2}(s - t_n)^2 \ ,$$

with y between s and t_n. Hence,

$$f(s) - g(s) = (f'(t_n) - f'(z))(s - t_n) + \frac{f''(y)}{2}(s - t_n)^2 \ . \tag{2}$$

Estimating the approximation error

Applying the mean value theorem to f', we obtain

$$f'(t_n) - f'(z) = f''(r)(t_n - z)$$

with r between t_n and z.

In particular: Assume that $t_{n+1} - t_n = \delta$. Then $|s - t_n| < \delta$, and if z is between s and t_n, also $|t_n - z| < \delta$, and thus

$$\begin{aligned} |f(s) - g(s)| &\leq |(f'(t_n) - f'(z))(s - t_n)| + |\frac{f''(y)}{2}(s - t_n)^2| \\ &\leq (|f''(r)| + |f''(y)|)\delta^2 \\ &\leq 2K\delta^2 \ . \end{aligned}$$

Conclusions

Positive conclusion: As the distance δ of neighboring measurement points decreases, the approximation error can be estimated by a quadratic function of δ.
($\leadsto$ Rule of thumb: Doubling the number of measurements results in dividing the approximation error by four.)

Drawback: If we don't know f, how do we estimate the constant K?

Summary

- Important definitions: Secant, difference quotient, derivative of a function
- Properties of differentiable functions: Continuity, Mean value theorem
- Known classes of differentiable functions: Polynomials, trigonometric functions, powers, roots
- Computational rules for derivatives: Linearity, product rule, chain rule
- Higher derivatives, Taylor's theorem