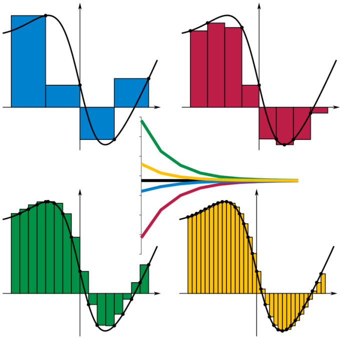
Algorithms and Data Structures

Quadrature
Introduction to Quadrature



Learning goals

- Integration
- Condition of integration
- Discretization

MOTIVATION: INTEGRALS IN STATISTICS

- Expectation of a random variable x with density p that is transformed by a function g:

$$\mathbb{E}_p[g(x)] = \int g(x) \cdot p(x)\, dx$$

- Normalization constant in Bayes' theorem:

$$\overset{\textit{Posterior}}{p(\theta|x)} = \frac{\overset{\textit{Likelihood}}{p(x|\theta)} \cdot \overset{\textit{Prior}}{\pi(\theta)}}{\int p(x|\theta) \cdot \pi(\theta)\, d\theta}$$

The values of the integrals are often not elementary computable and must be calculated numerically on the computer.

INTEGRATION

Goal: Calculation of

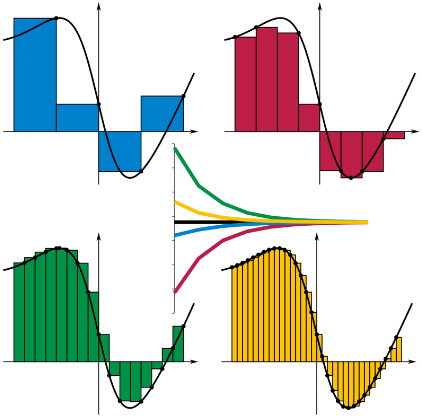
$$I(f) := \int_a^b f(x)dx$$

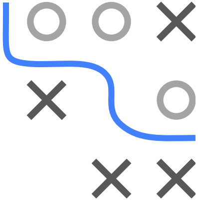
We constrain ourselves to the concept of the **Riemann Integral**, which is defined by **Riemann sums**:

$$S(f) : \; = \; \sum_{k=0}^{n-1} (x_{k+1} - x_k) f(\mathbf{x}_i^{(i)})$$

where $(x_0 = a, x_1, x_2, ..., x_{n-1}, x_n = b)$ is a partition of the interval $[a, b]$ and $\mathbf{x}_i^{(i)} \in [x_i, x_{i+1}]$.

INTEGRATION / 2





https://en.wikipedia.org/wiki/Riemann_sum
Different methods for calculating Riemann sums.
Right (TL), left (BR), minimum (TR) and maximum (BL) method.

INTEGRATION / 3

A function is Riemann-integrable on $[a, b]$, if the Riemann sums approach a fixed number (the value of the integral) as the partitions get finer, so the Riemann integral is the limit of the Riemann sums of a function for any arbitrary partition.

The operator $I(f)$, which assigns the value of the integral to an integrable function, is

- Linear, i.e. $I(\lambda f + \mu g) = \lambda I(f) + \mu I(g)$
- Positive, i.e. $I(f) \geq 0$ for $f(x) \geq 0$ for all $x \in [a, b]$

INTEGRATION / 4

The fundamental theorem of calculus states that the integral (in case of its existence) can be calculated using the indefinite integral

$$I(f) = F(b) - F(a)$$

However, for many interesting functions f there is no elementarily representable integral F and the direct analytical way is not possible.

Examples:

- $f(x) = e^{-\frac{x^2}{2}}$
- Posterior calculations in Bayesian Statistics

NUMERICAL PROBLEM

Given:

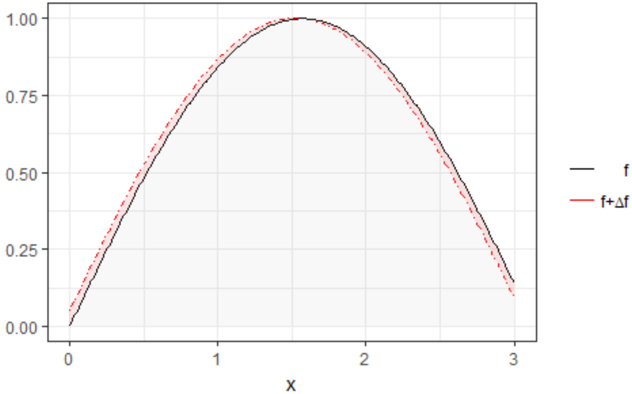
- Function f, can be evaluated anywhere (try to keep the number of evaluations small)
- Interval of integration $[a, b]$
- Error bound $\epsilon > 0$

Searched: $Q(f)$ with $|Q(f) - I(f)| \leq \epsilon \cdot |I(f)|$

$E(f) := |Q(f) - I(f)|$ is referred to as **Quadrature error**.

CONDITION OF INTEGRATION

Question: How much does the value of the integral change if we integrate a slightly transformed function $f + \Delta f$ instead of f?



CONDITION OF INTEGRATION / 2

The relative condition is defined by the condition number κ, i.e. the smallest $\kappa \geq 0$, so that

$$\frac{|I(f) - I(f + \Delta f)|}{|I(f)|} \leq \kappa \frac{\|\Delta f\|_\infty}{\|f\|_\infty}$$

It holds:

$$\begin{aligned}
|I(f) - I(f + \Delta f)| &\overset{\text{linearity}}{=} |I(f) - I(f) - I(\Delta f)| \\
&= \left| \int_a^b \Delta f(x) dx \right| \leq \int_a^b |\Delta f(x)| dx \\
&\leq (b - a) \max_{x \in [a,b]} |\Delta f(x)| \\
&= (b - a) \|\Delta f\|_\infty
\end{aligned}$$

$$\frac{|I(f) - I(f + \Delta f)|}{|I(f)|} = \frac{|I(\Delta f)|}{|I(f)|} \leq (b - a) \frac{\|\Delta f\|_\infty}{|I(f)|} = (b - a) \frac{\|f\|_\infty}{|I(f)|} \frac{\|\Delta f\|_\infty}{\|f\|_\infty}$$

CONDITION OF INTEGRATION / 3

The condition number for the integration is therefore limited by

$$\kappa = (b - a)\frac{\|f\|_\infty}{|I(f)|}$$

In general, quadrature - in contrast to numerical differentiation - is well conditioned. However, the upper bound for the condition is large if

- The function allows for large function values (large $\|f\|_\infty = \max_x f(x)$)
- The absolute value of the integral is very small

If the problem is ill-conditioned, the result should be critically questioned (regardless of the stability of the algorithm).

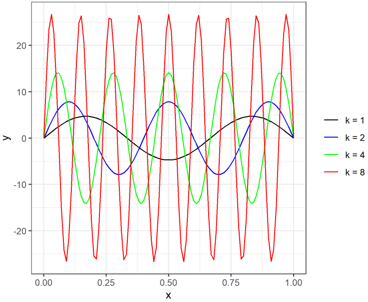
CONDITION OF INTEGRATION / 4

Example:

Oscillating functions: $f_k(x) = \frac{(2k+1)\pi}{2}\sin((2k+1)\pi x)$

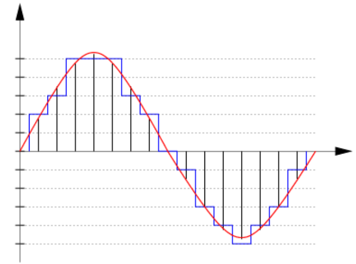
The following holds: $I(f_k) = \int_0^1 f_k(x)dx = 1$ and $\|f_k\|_\infty = \frac{(2k+1)\pi}{2}$ and hence

$$\kappa = \frac{(2k+1)\pi}{2} \to \infty \quad \text{for } k \to \infty$$



DISCRETIZATION

Discretization is a central concept of numerical mathematics and the basis of many quadrature formulas. A continuous object (e.g. a function) is divided into *n* "parts" to allow numerical evaluation and implementation.



Discretization of a continuous function.

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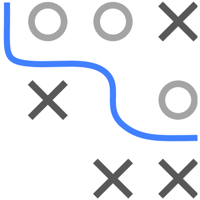
ERROR ANALYSIS: DISCRETIZATION ERROR



Let x_n be the numerical solution for the discretized object and x^* the exact solution.

Due to the discretization an error is made, the so-called **truncation error**

$$|x_n - x^*|$$

Of course, this error should disappear for $n \to \infty$, the number of grid points in a discretization.

When using discretization, we are interested in how quickly the truncation error disappears.

CONVERGENCE RATES FOR DISCRETIZATION

Definition:
The solution of the discretized problem x_n converges with **order p** towards the solution of the continuous problem x^* if there are constants $M > 0$ and $n_0 \in \mathbb{N}$, such that

$$|x_n - x^*| \leq M \cdot n^{-p} \quad \text{for all } n > n_0$$

or equivalently

$$|x_n - x^*| \in \mathcal{O}(n^{-p})$$

For $p = 1$ we speak of **linear** convergence, for $p = 2$ of **quadratic** convergence.