Simple and Composite Rules

Other Approaches

#### 3. Numerical Quadrature

Where analytical abilities end ...

Other Approaches

#### 3.1. Preliminary Remarks

Simple and Composite Rules

## The Integration Problem

 Numerical quadrature denotes numerical computation of a definite integral of the kind

$$I(f) := \int_{\Omega} f(x) dx$$

to a given function  $f: \mathbb{R}^d \supseteq \Omega \to \mathbb{R}$ , the **integrand**, and a given **integration** domain  $\Omega$ .

- In the following, we will deal solely with univariate quadrature, i.e. with the case d=1 of an interval  $\Omega=[a,b]$ . Of course, the big challenge is the higher dimensional case of multivariate quadrature. Especially the high dimensional case of d = 100 (occurring in statistics, physics, and in mathematical finance), or even higher dimensions demands sophisticated numerical methods.
- Use numerical quadrature only: when all other methods fail (e.g., closed) integration using substitution or integration by parts, splitting into sums of integrals between discontinuous points of f, etc.).
- Most methods of numerical quadrature require a sufficient smoothness (differentiability) of the integrand.

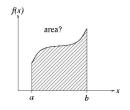
 Almost all rules of quadrature, i.e. instructions for numerical quadrature, can be written as weighted sums of function values (samples):

Other Approaches

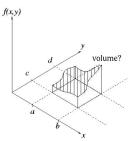
$$I(f) \approx Q(f) := \sum_{i=0}^{n} g_i f(x_i) =: \sum_{i=0}^{n} g_i y_i$$

with weights  $q_i$  and pairwise different nodes  $x_i$ , where  $a \le x_0 < x_1 < \dots < x_{n-1} < x_n \le b$ .

Evaluation of integrand: often expensive! (in particular when f is only given implicitly: e.g., a differential equation may have to be solved every time to be able to evaluate f at a point x) ⇒ interest in rules that allow a high accuracy (a small error of quadrature) with moderate n.



Simple and Composite Rules



## **Exact Integration of a Polynomial Interpolant**

Simple and Composite Rules

 How do we get appropriate rules of quadrature? The standard ansatz is to replace the integrand f by an approximation  $\hat{f}$  that is both easy to construct and easy to integrate which will then be integrated exactly, thus

Other Approaches

$$Q(f) := \int_a^b \tilde{f}(x) dx.$$

• For reasons of simplicity, a **polynomial interpolant** p(x) of f(x) to the nodes  $x_i$  is chosen as approximant  $\tilde{f}$ . In this case, the representation of p(x) via the Lagrange polynomials  $L_i(x)$  of degree n delivers the weights  $g_i$  virtually free of cost:

$$Q(f) := \int_{a}^{b} p(x) dx = \int_{a}^{b} \sum_{i=0}^{n} y_{i} L_{i}(x) dx = \sum_{i=0}^{n} \left( y_{i} \cdot \int_{a}^{b} L_{i}(x) dx \right),$$

with which the weights  $q_i$  are directly defined by

$$g_i := \int_a^b L_i(x) \mathrm{d}x$$

The integrals of Lagrange polynomials can obviously be calculated in advance they do depend on the chosen grid (the nodes) but they do not depend on the integrand f.

 Because of the uniqueness of the interpolation problem (which polynomial interpolant of degree less or equal to n interpolates the n+1 points  $(x_i,1)$ , i = 0, ..., n?), we have

$$\sum_{i=0}^{n} L_i(x) \equiv 1$$

Other Approaches

and therefore also

$$\sum_{i=0}^{n} g_i = \int_a^b \sum_{i=0}^n L_i(x) dx = \int_a^b 1 dx = b - a.$$

 $\Rightarrow$  The sum of the weights is always equal to b-a when a polynomial interpolant is used for quadrature.

#### About the Condition of Numerical Quadrature

Simple and Composite Rules

- How is the problem of numerical quadrature conditioned? Particularly, are there any requirements for the weights  $q_i$  to ensure a good condition?
  - Let's examine small changes  $\delta y_i$  in the input data the nodes  $y_i = f(x_i)$  as well as their effect on the approximate value of the integral.

Other Approaches

- If all input fluctuations are less or equal  $\varepsilon \Rightarrow$  for a change  $\delta Q(f)$  of the approximation value it holds

$$|\delta Q(f)| = \left| \sum_{i=0}^{n} g_i \delta y_i \right| \le \varepsilon \cdot \sum_{i=0}^{n} |g_i|.$$

- If all weights  $g_i$  are positive, then the sum on the right-hand side takes its minimal value b-a and the entire right-hand side is of order of magnitude of  $O(\varepsilon)$ . Thus, in this case, the quadrature problem is **well-conditioned**.
- If, in contrast, negative weights occur, then the sum on the right-hand side of the estimation above might become very big - and with it the upper bound of  $\delta Q(f)$ . In case of **negative weights**, the problem of quadrature can be ill-conditioned



 As we will see in the following section, this demand for positivity of the weights is an exclusion criterion for the integration via the polynomial interpolant in case of big n. As we have already seen at polynomial interpolation, polynomials of high degree are problematic.

#### 3.2. Simple and Composite Rules

## The Rectangle Rule

- In the following, we will introduce some of the most important rules of quadrature.
   We distinguish between simple and composite quadrature rules:
  - A simple rule deals with the whole integration domain [a,b] in one go. For its length, we will use the denotation H:=b-a.

Other Approaches

- A composite rule splits the integration domain into subdomains, applies simple rules there, and forms the total approximation by summing up. This procedure is very similar to the spline interpolation of chapter 2.
- The simplest simple rule is the rectangle rule

$$Q_R(f) := H \cdot f\left(\frac{a+b}{2}\right) = I(p_0),$$

where  $p_0$  denotes the polynomial interpolant of f of degree 0 with the only node  $x_0:=(a+b)/2$ 

- For the **remainder**  $R_R(f) := Q_R(f) - I(f)$ , the relation

$$R_R(f) := -H^3 \cdot \frac{f^{(2)}(\xi)}{24}$$

can be shown for an intermediate point  $\xi \in ]a,b[$ , if f is twice continuously differentiable on ]a,b[.

**Preliminary Remarks** 

- From this relation of the remainder, we first learn that polynomials of degree 0 or 1 are integrated *exactly*. That might surprise at first glance as only a constant interpolant is used. However, in the linear case, the quadrature errors left and right to the centre point of the interval cancel each other.
- Second, we see via the *H*-Terms what has already been clear geometrically: On a small integration interval, the error is asymptotically smaller as well. However, for now, we only examine constant integration domains for the simple rules.

### The Trapezoidal Rule

Simple and Composite Rules

• If we use the linear polynomial interpolant  $p_1$  instead of the constant polynomial interpolant  $p_0$ , we get the **trapezoidal rule**:

$$Q_T(f) := H \cdot \frac{f(a) + f(b)}{2} = I(p_1).$$

- Here, the linear interpolant to the two interval bounds  $x_0 := a$  and  $x_1 := b$  is integrated exactly.
- For the remainder, it can be shown (again without proof)

$$R_T(f) = H^3 \cdot \frac{f^{(2)}(\xi)}{12},$$

where  $\varepsilon$  again identifies an intermediate point in the interior of the integration domain.

- At first glance, the trapezoidal rule might seem hardly helpful: twice as many function evaluations invested, but only a result of comparable quality (integration errors left and right to the centre point of the interval do not cancel each other in case of a quadratic interpolant). Justification of the trapezoidal rule: its superb eligibility as starting point for composite methods.
- The maximal polynomial degree that can be treated exactly by a quadrature rule is called **degree of accuracy** or shortly **accuracy** of the method. Thus, the rectangle rule as well as the trapezoidal rule have accuracy 1.





## **Kepler's Rule and Newton-Cotes Formulas**

Simple and Composite Rules

 You may guess it: Next, we will take the quadratic interpolant p<sub>2</sub> to the three nodes  $x_0 := a$ ,  $x_1 := (a+b)/2$  and  $x_2 := b$  and, with a short calculation, we get Keplers's rule

$$Q_F(f) := H \cdot \frac{f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)}{6} = I(p_2).$$

(By the way, this and more can be admired in the Kepler Museum in Weil der Stadt.)

- Here, the remainder fulfils

$$R_F(f) = H^5 \cdot \frac{f^{(4)}(\xi)}{2880}.$$

- If the integrand is four times continuously differentiable, Kepler's rule thus presents a method of order 5 and of accuracy 3.
- The class of quadrature rules that follows from this principle is called Newton-Cotes formulas. Here, it is thus defined

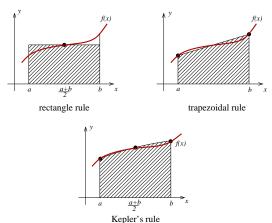
$$Q_{\mathsf{NC}(n)}(f) := I(p_n),$$

where  $p_n$  is the polynomial interpolant of f of the degree n to the n+1equidistant nodes

$$x_i := a + H \cdot \frac{i}{n}, \quad i = 0, ..., n.$$

**Preliminary Remarks** 

- Under the assumption of adequately high differentiability, we obtain with the Newton-Cotes rules for growing n methods of higher order and higher accuracy.
- Attention: For n=8 and  $n\geq 10$  negative weights occur. As hinted before, in those cases, the Newton-Cotes formulas are practically useless.



#### **Clenshaw-Curtis Formulas**

- The problem of negative weights  $g_i$  at higher polynomial degree n does not mean that polynomial interpolants of higher degree cannot serve for purposes of numerical quadrature in principle. One possible remedy is to give up the equidistance of the nodes.
- Exactly this is the principle of the **Clenshaw-Curtis rules**, in which instead of the integration interval [a,b] the semicircle angle  $[0,\pi]$  is uniformly subdivided:

$$x_i := a + H \cdot \frac{1 - \cos\left(\frac{i\pi}{n}\right)}{2}, i = 0, ..., n.$$

- It can be easily demonstrated that the nodes are located more densely at the borders of the integration domain than at its center.
- It can be shown that for this principle of construction of quadrature rules all appearing weights are always positive.
- Therefore, the Clenshaw-Curtis rules also are suited for larger values of n in principle.
- However, those ansatzs only play a little role in practice. Here, composite rules, which we will examine in the following, are more important.

### The Trapezoidal Sum

- The probably most important composite rule is the trapezoidal sum:
  - Firstly, the integration interval [a, b] is divided into n subintervals of length

$$h := \frac{b-a}{n}.$$

- The equidistant junctions  $x_i := a + ih$ , i = 0, ...n, serve as nodes.
- Now the trapezoidal rule is applied to every subinterval  $[x_i, x_{i+1}]$ .
- Finally, the integral values computed this way are summed up to the total integral value:

$$Q_{\mathsf{TS}}(f;h) \; := \; h \cdot \left( \frac{f_0}{2} + f_1 + f_2 + \ldots + f_{n-1} + \frac{f_n}{2} \right) \, ,$$

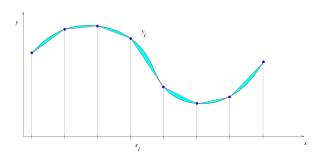
where  $f_i := f(x_i)$ .

For the remainder term of the trapezoidal rule, we have the relation

$$R_{\mathsf{TS}}(f;h) = h^2 \cdot (b-a) \cdot \frac{f^{(2)}(\xi)}{12} = h^2 \cdot H \cdot \frac{f^{(2)}(\xi)}{12} \,,$$

which follows immediately from the remainder formula of the trapezoidal rule by summation of the single remainder terms and multiple application of the intermediate value theorem. **Preliminary Remarks** 

- What does this formula tell us about the remainder term of the trapezoidal sum?
  - Compared to the trapezoidal rule, the accuracy remains 1, whereas the order declines to 2 (one order of magnitude is lost by summation).
  - However, now we have a rule that is easy to implement and with which n can be arbitrarily increased without getting numerical problems.



# **The Simpson Sum**

- In the same way the trapezoidal sum is a composite quadrature rule on the basis
  of the trapezoidal rule, the Simpson sum is a natural generalization of Kepler's
  rule.
- ullet Starting with the same partition of the integration interval [a,b] as before, now Kepler's rule is applied to every two neighboring subintervals conjointly:

$$Qss(f;h) := \frac{h}{3} \cdot (f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \dots + 2f_{n-2} + 4f_{n-1} + f_n).$$

As remainder term R<sub>SS</sub>(f) we get

$$R_{\rm SS}(f;h) = h^4 \cdot (b-a) \cdot \frac{f^{(4)}(\xi)}{180} = h^4 \cdot H \cdot \frac{f^{(4)}(\xi)}{180} .$$

- Again the order is reduced by 1 to 4 in comparison to the respective simple rule, whereas the accuracy stays unchanged at 3.
- The Simpson sum also offers a simple way to improve the approximation by increasing the number of nodes without getting problems with condition.

## **Example**

Consider a function  $f(x)=x^3$ . The analytical integral in interval [0,1] is  $\frac{1}{4}$ . Now we want to approximate the integral with three nodes, namely  $x_0=0,\,x_1=\frac{1}{2}$  and  $x_2=1$ , and methods as follows.

· Rectangle rule.

$$Q_R = H \cdot f(\frac{a+b}{2}) = 1 \cdot (\frac{1}{2})^3 = \frac{1}{8}$$

Trapezoidal rule.

$$Q_T = H \cdot \frac{f(a) + f(b)}{2} = 1 \cdot \frac{0+1}{2} = \frac{1}{2}$$

Trapezoidal sum.

$$Q_{TS} = h \cdot (\frac{f_0}{2} + f_1 + \frac{f_2}{2}) = \frac{1}{2}(\frac{0}{2} + \frac{1}{8} + \frac{1}{2}) = \frac{5}{16}$$

Kepler's rule.

$$Q_F = H \cdot \frac{f(a) + 4f(\frac{a+b}{2}) + f(b)}{6} = 1 \cdot \frac{0 + \frac{1}{2} + 1}{6} = \frac{1}{4}$$

 Simpson sum. Since in this case we only have two subintervals, the result of Simpson sum is essentially same as the one of Kepler's rule.

Other Approaches

### 3.3. Extrapolation

## Increasing the Order Using Linear Combinations

Simple and Composite Rules

 Once more, we consider Kepler's rule. It is possible to get this formula from the linear combination of three trapezoidal rules (once with step width H and twice with step width H/2):

$$\begin{split} Q_F(f) &= H \cdot \frac{f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)}{6} \\ &= \frac{4}{3} \left(\frac{H}{2} \cdot \frac{f(a) + f\left(\frac{a+b}{2}\right)}{2}\right) + \frac{4}{3} \left(\frac{H}{2} \cdot \frac{f\left(\frac{a+b}{2}\right) + f(b)}{2}\right) \\ &- \frac{1}{3} \left(H \cdot \frac{f(a) + f(b)}{2}\right) \\ &= \frac{4}{3} \frac{H}{2} \left(\frac{f(a)}{2} + f(\frac{a+b}{2}) + \frac{f(b)}{2}\right) - \frac{1}{3} H\left(\frac{f(a)}{2} + \frac{f(b)}{2}\right). \end{split}$$

As the last line shows, this can also be interpreted as a linear combination of two trapezoidal sums.

**Preliminary Remarks** 

- This means: Clever combination of approximation values of *low* approximation order leads to an approximation of *higher* approximation order – without explicitly using the formula of higher order.
- This is a very common principle in numerics that can also be successfully used for other problems than quadrature.
- For the trapezoidal rule this method is less common, but for the trapezoidal sum it is an extremely worthwhile starting point which we will study in the following.

## The Principle of Extrapolation

• The starting point is the **Euler-Maclaurin sum formula** which – to put it simple – delivers an  $h^2$ -series expansion of the trapezoidal sum if f is at least 2m-times continuously differentiable:

$$Q_{\rm TS}(f;h) \; = \; I(f) + \tau_1 h^2 + \ldots + \tau_{m-1} h^{2m-2} + \tau_m(h) \cdot h^{2m} \; , \label{eq:qts}$$

Other Approaches

with a remainder  $\tau_m(h)$  bounded from above for all h (that is the crux of the matter – without this constraint it could always be written like that).

- **Idea**: Compute approximation values  $T(h_i)$  for the sought integral I(f) using the trapezoidal sum, namely for the different step widths  $h_i$ .
- For the choice of the (sensibly converging to zero) sequence of step width  $h_i$ , i=1,2,3,..., there are two important alternatives:
  - successive bisection:  $h_i := \frac{b-a}{n_i}, \ n_i := 2^i,$
  - slow accretion:  $h_i:=\frac{b-a}{n_i},\ n_i:=2,3,4,6,8,12,...$

Other Approaches

### The Principle of Extrapolation (2)

• Now, write the expansions for the chosen  $h_i$  one below the other:

$$T(h_1) = I(f) + \tau_1 h_1^2 + \dots + \tau_{m-1} h_1^{2m-2} + \tau_m(h_1) \cdot h_1^{2m}$$

$$T(h_2) = I(f) + \tau_1 h_2^2 + \dots + \tau_{m-1} h_2^{2m-2} + \tau_m(h_2) \cdot h_2^{2m}$$

$$T(h_3) = I(f) + \tau_1 h_3^2 + \dots + \tau_{m-1} h_3^{2m-2} + \tau_m(h_3) \cdot h_3^{2m}$$

$$\dots = \dots$$

Note that the left hand sides (the computed trapezoidal sum values) are known whereas I(f) as well as all  $\tau_i$  are not known and are only given formally. Above, everything unknown is marked red.

 Now it is clear how we have to proceed: Combine pairs of rows such that the respective leading term of order in  $h^2$  is eliminated – and, hey presto, we have approximations that are two orders better.

## The Principle of Extrapolation (3)

**Preliminary Remarks** 

- Romberg had a different perception for this idea of Richardson and attained a more efficient calculation scheme:
  - Due to the Euler-Maclaurin sum formula, it is natural to consider T as a function of  $h^2$ , to approximate it by a polynomial p of degree m-1 that interpolates T in the nodes  $(h_i^2, T(h_i)), i = 1, ..., m$ , and to use p(0) as approximation for  $I(f) = T(h \to 0)$ .
  - As the sought "intermediate point" h = 0 here is located outside of the interval of nodes  $h_i$ , we speak of **extrapolation** instead of interpolation.
  - The technical realization of the computation of p(0) is done best with Neville's scheme (see section 2.2).
  - From this results the following algorithm, the **Romberg quadrature**:

```
for i:=1 to m do
  chose n[i]; h[i] := (b-a)/n[i];
  T[i]:=trapezoidal sum of step width h[i]
  for k:=i-1 downto 1 do
    T[k] := T[k+1] + (T[k+1] - T[k]) / (h[k] * *2/h[i] * *2-1)
  od:
od;
p(0) := T[1];
```

(Verify this algorithm with the help of Neville's algorithm!)

## **Short Analysis of Extrapolation**

Simple and Composite Rules

- Accuracy of extrapolation:
  - The attractiveness of the quadrature via extrapolation lies in its significantly higher approximation quality compared to the trapezoidal rule. For the error of quadrature, it can be shown that

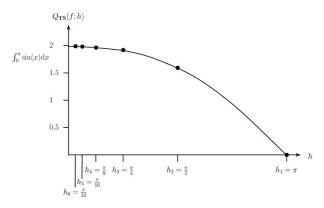
$$|p(0) - I(f)| = O(h_1^2 \cdot h_2^2 \cdot \dots \cdot h_m^2),$$

Other Approaches

if f is 2m-times continuously differentiable and p denotes the interpolating polynomial with  $p(h_i^2) = T(h_i), i = 1, ..., m$ .

- A calculation example for several values of m may illustrate the meaning of "significant" in this context!
- The price for better approximation is higher differentiability of the integrand f that has to be presumed. Therefore, extrapolation is to be used whenever very smooth functions have to be integrated. However, for functions with kinks etc., it does not help.
- This also is a very typical situation for numerics. Not only performance and speed are of importance but also universality (the so-called robustness): How big is the class of functions to which a method can be applied?





h	$h_1$	$h_2$	$h_3$	$h_4$	$h_5$	$h_6$
$Q_{TS}(f;h)$	0	1.571	1.896	1.974	1.993	1.998
error	2	0.429	0.104	$2.6 \cdot 10^{-2}$	$7 \cdot 10^{-3}$	$2 \cdot 10^{-3}$

For comparison:

Romberg quadrature for  $h_6$  delivers the error  $=2\cdot 10^{-9}$  (smaller by a factor of  $10^{-6}$  to the error of the trapezoidal sum for  $h_6$ !).

### 3.4. Other Approaches

#### Monte-Carlo Quadrature

Simple and Composite Rules

- We have only discussed the one-dimensional case here. Of course, more interesting is the multivariate case of integrands with several variables. Here, the curse of dimensionality leads to a fast increase of the number of nodes and thereby also of the computational costs and memory requirements: A product approach of a rule with n points in one dimension already requires  $n^2$  in two and  $n^d$  in d space dimensions.
- Nowadays, totally different methods than the examined ones are used for large values of d, for example Monte-Carlo methods as well as quasi Monte-Carlo methods (also called minimal discrepancy methods).
- Monte-Carlo methods are of stochastic nature.
- We examine a simple two-dimensional example:
  - Let  $\chi_A(x,y)$  and  $\chi_B(x,y)$  be the characteristic functions to the circle  $A:=\{(x,y): x^2+y^2\leq 1\}$  and to the rectangle  $B:=[-1,1]^2$ , respectively (with value 1, if inside, and with value 0, if outside, respectively). The integral of  $\chi_A(x,y)$  is sought, hence, de facto the circle constant  $\pi$ .
  - Our random experiment: Choose a point  $(x_i, y_i) \in B$  randomly (uniform distribution!).





- Our random variables  $Z_i$ :  $Z_i = \chi_A(x_i, y_i)$ .
- Then, the law of large numbers states that, with increasing  $n, \frac{1}{n} \cdot \sum_{i=1}^n Z_i$  converges to  $\pi/4$  in the sense of probability (i. e. not for "sure"!).
- The whole thing defined as a problem of quadrature:

$$\pi \ = \ \int_{B} \chi_{A}(x,y) \mathrm{d}(x,y) \ = \ 4 \cdot \int_{\mathbb{R}^{2}} \frac{1}{4} \cdot \chi_{B}(x,y) \cdot \chi_{A}(x,y) \mathrm{d}(x,y)$$
$$= \ 4 \cdot E(\chi_{A}((X,Y))) \ \approx \ 4 \cdot \frac{1}{n} \cdot \sum_{i=1}^{n} \chi_{A}(x_{i},y_{i}) \ = \ \frac{4}{n} \cdot \sum_{i=1}^{n} Z_{i} \, .$$

Note that the function  $\frac{1}{4} \cdot \chi_B(x,y)$  here plays the role of the probability density.

#### Gaussian Quadrature

Simple and Composite Rules

 By means of the Clenshaw-Curtis rules we already saw in section 3.2 that it might be of advantage to leave the equidistant distribution. That's exactly what we want to do now in a systematic way.

Other Approaches

• For reasons of simplicity we examine the integration interval [-1, 1]. Then the standard ansatz is

$$I(f) = \int_{-1}^{+1} f(x) dx \approx \sum_{i=1}^{n} g_i f(x_i)$$

with nodes  $x_i$  and weights  $q_i$ , where now the  $x_i$  are also free parameters of the method which can be used to fulfill additional requirements.

• The idea of the Gaussian quadrature is to place the nodes in a way that polynomials of a degree as big as possible are integrated exactly – the highest possible accuracy degree is aimed at:

$$I(p) = \int_{-1}^{1} p(x) dx \stackrel{!}{=} \sum_{i=1}^{n} g_{i} p(x_{i})$$

for all  $p \in \mathbb{P}_k$  with k as big as possible. At this, we keep in the back of our minds the series expansion for f, of which as many leading terms as possible are supposed to be integrated exactly (high orders of error for decreasing interval width).

• With the Gaussian quadrature the (maximum possible) degree of accuracy 2n-1is obtained.

# Simple and Composite Rules The Nodes of the Gaussian Quadrature

- We skip the derivation and come right to business:
  - There is exactly one set of nodes  $x_i$ , i = 1, ..., n, with which the degree of accuracy 2n-1 is achievable, and those are the pairwise different roots of the Legendre polynomials

$$\omega_n(x) := \frac{n!}{(2n)!} D^n ((x^2 - 1)^n).$$

Other Approaches

At the boundaries, they are located more densely than in the interior of the integration interval.

- There is exactly one set of weights  $q_i$  with which the degree of accuracy 2n-1 is achievable, namely

$$g_i := \int_{-1}^{+1} L_i(x) \, \mathrm{d}x$$

with Lagrange polynomials  $L_i \in \mathbb{P}_{n-1}$  that were already introduced in the last chapter.

- The necessity of this requirement is clear: The  $L_i$  have to be integrated exactly as polynomials of degree n-1 by the Gaussian quadrature, in the weighted sum all summands except  $g_i L_i(x_i) = g_i$  disappear due to its definition.

- As the  $L_i^2(x) \in \mathbb{P}_{2n-2}$  are also still integrated exactly, furthermore, it follows that all weights are positive. This underlines the advantages of the Gaussian quadrature.
- The roots of the Legendre polynomials are tabled for common values of n in respective books.

Other Approaches

#### **Archimedes' Quadrature**

Simple and Composite Rules

- A very old but nevertheless convincing approach for the numerical quadrature primarily when considered from the algorithmic point of view – comes from Archimedes.
- This is an ancestor of the algorithmic paradigm divide et impera omnipresent in computer science.
- **Problem**: Compute the area (the integral) between the function  $f(x) := 1 x^2$  and the segment of the x-axis between -1 and 1 (numerically the lucky Archimedes did not yet know about calculus and integration).
- Idea:
  - Choose a triangle with vertices  $(-1,0),\,(0,1),$  and (1,0) as a first approximation.
  - The difference area consists of two parabola segments of half width, on which this method is now applied to.
  - Continue recursively, until the partial areas stay under a threshold  $\varepsilon$  or until a maximum depth is reached.
  - The sum of all partial areas is an approximation for the value of the integral –
    in the concrete example with the geometric series even the formula for the
    exact value 4/3.

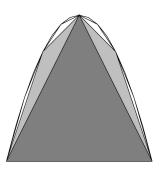




#### Advantages:

**Preliminary Remarks** 

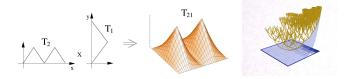
- The method is simple.
- The method is hierarchically incremental: The first big triangles are also used within a finer resolution. Applying other methods, everything calculated beforehand becomes obsolete when refining (which was a disaster for people without calculator such as Archimedes).
- The method offers direct access to the adaptive refinement: By the areas of the individual triangles, it can be controlled where it should be further refined and where it should not.



### **Archimedes in Multiple Dimensions**

Simple and Composite Rules

- Archimedes' quadrature can be easily generalized to the case of multiple space dimensions:
  - The higher dimensional space with is dealt with dimensionwise (tensor product ansatz, for the first time demonstrated by Cavalieri).
  - In 2D, the volume is filled with pagoda instead of triangles, in the general d-dimensional case with according equivalents.
  - Here as well, a hierarchical basis underlies the base of the pagoda gets smaller and smaller.
  - By omitting "dispensable" nodes (pagoda with smaller contribution to the volume), very efficient quadrature techniques (so-called sparse grids) result here - especially for the nasty high dimensional case.



### 3.5. Applications of Quadrature

## Numerical Quadrature in Computer Science

Simple and Composite Rules

- In computer graphics, radiosity methods are used to render global lighting as realistic as possible. For this purpose, at every point the incoming and the outgoing light is summed up over all possible directions, i.e. it is integrated.
- In visualization, at volume rendering, integration occurs, i.e. when rendering 3D data (e.g. of imaging in medical science), to find suitable color values for the individual pixels (cumulated and weighted values from the interior of the object along a ray, e.g. to show something specific and to hide other things).
- In numerical simulation, finite elements methods are a standard method to solve partial differential equations numerically. At this class of methods, so-called ansatz functions have to be integrated over simple structured elements.
- Everywhere in image processing when smoothing or blurring, integrals are also involved. Especially, every averaging process of continuous data stands for an integration process.