MAT 460 Numerical Differential Equations
Spring 2016

Lecture 10

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Topics:

Differentiating (Finite Differences) and Integrating (Quadratur)

Numerical Derivatives (Finite Differences)

Approximation of the first derivative

Definition of the first derivative of a function $f : \mathbb{R} \to \mathbb{R}$:

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

The limit is two-sided, i. e. it can also be negative.

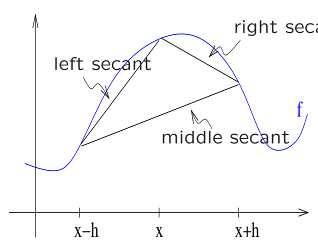
From now on we assume $h > 0$.

Approximation of $f'(x)$ with a difference quotient (secant slope):

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad \text{difference quotient from right,}$$

$$f'(x) \approx \frac{f(x) - f(x-h)}{h} \quad \text{difference quotient from left,}$$

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \quad \text{central difference quotient.}$$



The central difference quotient is the mean value of the difference quotient from the right and the difference quotient from the left.

Question: How accurate are these approximations?

First accuracy tests with polynomials

Straightforward computations show the following.

If $f(x) = 1$ or $f(x) = x$ then

$$\frac{f(x+h) - f(x)}{h} = f'(x) = \frac{f(x) - f(x-h)}{h}.$$

If $f(x) = x^2$ then

$$\frac{f(x+h) - f(x)}{h} \neq f'(x) \neq \frac{f(x) - f(x-h)}{h}.$$

If $f(x) = 1$ or $f(x) = x$ or $f(x) = x^2$ then

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

If $f(x) = x^3$ then

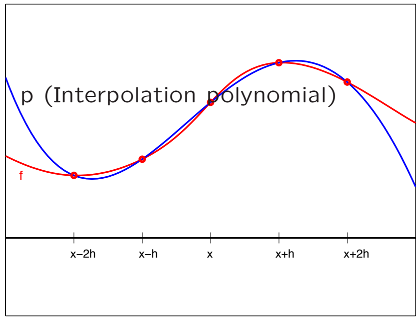
$$\frac{f(x+h) - f(x-h)}{2h} \neq f'(x).$$

With one-sided difference quotients we can compute derivatives for polynomials with degree ≤ 1 exact. With the central difference quotient we can compute derivatives of polynomials with degree ≤ 2 exact.

Approximation formula for the first derivative with 4 (actually 5) nodes:

$$f'(x) \approx \frac{1}{h}\left(\frac{1}{12} f(x-2h) - \frac{2}{3} f(x-h) + \frac{2}{3} f(x+h) - \frac{1}{12} f(x+2h)\right)$$

This formula is exact for all polynomials with degree ≤ 4.



Derivation:

Consider the polynomial p with degree ≤ 4, which interpolates the function f at the nodes $x-2h,\ x-h,\ x,\ x+h,\ x+2h$.

We have $f'(x) \approx p'(x)$.

Lagrange-representation of p:

$$p(t) = f(x-2h)\, L_1(t) + f(x-h)\, L_2(t) + f(x)\, L_3(t) + f(x+h)\, L_4(t) + f(x+2h)\, L_5(t),$$

where $L_1(t), \ldots, L_5(t)$ are the Lagrange-basis polynomials.

Differentiation of p at the position $t = x$ gives

$$p'(x) = f(x-2h)\underbrace{L_1'(x)}_{\frac{1}{12h}} + f(x-h)\underbrace{L_2'(x)}_{-\frac{2}{3h}} + f(x)\underbrace{L_3'(x)}_{0} + f(x+h)\underbrace{L_4'(x)}_{-\frac{2}{3h}} + f(x+2h)\underbrace{L_5'(x)}_{-\frac{1}{12h}}$$

Finite difference formulas for higher order derivatives

$$f''(x) \approx \frac{f(x-h) - 2\,f(x) + f(x+h)}{h^2},$$

$$f'''(x) \approx \frac{-f(x-h) + 3\,f(x) - 3\,f(x+h) + f(x+2h)}{h^3}$$

$$f^{(4)}(x) \approx \frac{f(x-2h) - 4\,f(x-h) + 6\,f(x) - 4\,f(x+h) + f(x+2h)}{h^4}$$

$$f^{(5)}(x) \approx \frac{-f(x-2h) + 5\,f(x-h) - 10\,f(x) + 10\,f(x+h) - 5\,f(x+2h) + f(x+3h)}{h^5}$$

Nodes:

1. The coefficients in these formulas are binomial coefficients (with alternating signs).
2. The formula for $f^{(n)}(x)$ is exact for all polynomials with degree $\leq n$.
3. These formulas can be derived by differentiation interpolation polynomials or directly from the generalized mean value theorem

$$f[x_1,\ x_2 \ldots x_{n+1}] = \frac{f^{(n)}(\xi)}{n!} \approx \frac{f^{(n)}(x)}{n!},$$

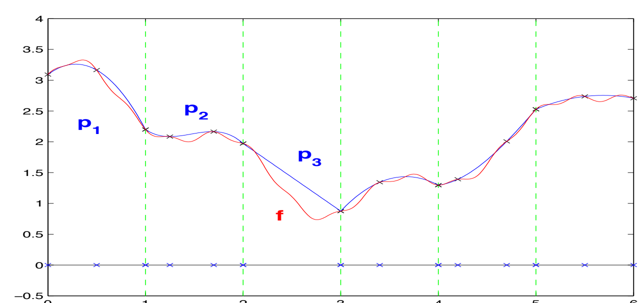
by substituting $x + k\,h$ for the x_j.

Numerical Integration (Quadratur)

Problem: How to numerically evaluate the definite integral $\int_a^b f(x)\,dx$, of a function f, whose anti-derivative we cannot find in any text book?

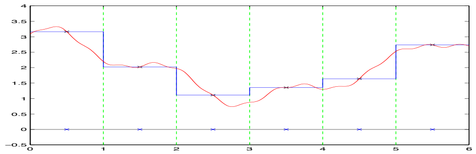
First Idea: Integrals of polynomials are easy to compute. We divide the interval $[a,b]$ in sub-intervals $[x_j, x_{j+1}]$ and approximate the integral of f in each sub-interval by the integral of a polynomial p_j, which interpolates f:

$$\int_a^b f(x)\,dx = \sum_{j=1}^{n} \int_{x_j}^{x_j+1} f(x)\,dx \approx \sum_{j=1}^{n} \int_{x_j}^{x_j+1} p_j(x)\,dx.$$

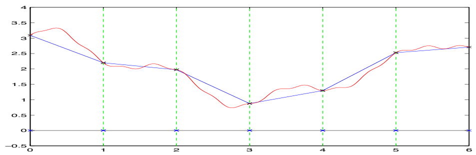


Simple cases

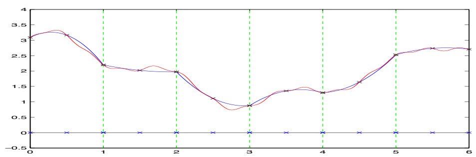
One node per interval, interpolation polynomials are constant functions.



Nodes only at the endpoints of the interval, linear interpolation, **trapezoidal rule**



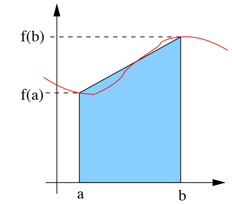
Three nodes (left-,right-,midpoint) per interval, interpolation with parabolas, **Simpson rule (Kepler's barrel rule)**.



Trapezoidal rule

Area of only one trapezoid in the interval $[a, b]$:

$$T = (b-a)\frac{f(a)+f(b)}{2} \approx \int_a^b f(x)\,dx. \qquad (*)$$

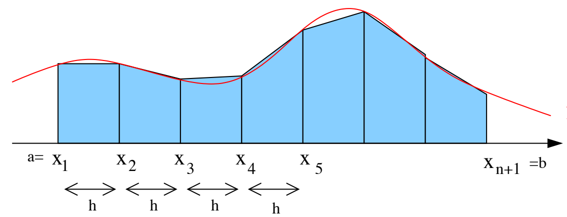


Sum of trapezoids if interval consists of sub-intervals with equidistant length $[x_j, x_{j+1}]$, $x_j = a + (j-1)h,\ h = (b-a)/n$:

$$\int_a^b f(x)\,dx \approx T(h) = \sum_{j=1}^{n} h\,\frac{f(x_{j+1}) + f(x_j)}{2} = h\left(\frac{1}{2}(f(a)+f(b)) + \sum_{j=2}^{n} f(x_j)\right) \qquad (**).$$

Nodes:

1. Let $x_1 = a,\ x_{n+1} = b$.
2. Formula $(**)$ is sometimes called **trapezoidal sum rule**.



Error of numerical integration with trapezoidal rule

We have

$$\int_a^b f(x)\,dx = \underbrace{h\,\frac{f(a)+f(b)}{2}}_{T} - \underbrace{\frac{h^3}{12} f''(\xi)}_{error}, \qquad h := b-a$$

for a point $\xi \in [a, b]$.

Proof: Let $p(x) = f(a)\,\frac{x-b}{a-b} + f(b)\,\frac{x-a}{b-a} = f(a) + \frac{f(b)-f(a)}{b-a}(x-a)$ be the linear interpolation polynomial. In the last lecture we showed that

$$f(x) = p(x) + f[a,b,x]\,(x-a)(x-b) \qquad \textit{and} \qquad f[a,b,x] = \frac{f''(\xi)}{2} \quad \text{for any } \xi \in [a,b]. \quad (*)$$

We get

$$\begin{aligned}
\int_a^b f(x)\,dx &= \int_a^b (p(x) + f[a,b,x]\,(x-a)(x-b)\,)\,dx \\
&= \int_a^b p(x)\,dx + \int_a^b f[a,b,x]\,(x-a)(x-b)\,dx \\
&= h\,\frac{f(a)+f(b)}{2} + \int_a^b f[a,b,x]\,\underbrace{(x-a)(x-b)}_{\le 0}\,dx \\
&= h\,\frac{f(a)+f(b)}{2} + f[a,b,\tilde{x}]\underbrace{\int_a^b (x-a)(x-b)\,dx}_{-(b-a)^3/6},\ \tilde{x} \in [a,b] \text{ (mean value theorem)} \\
&= T - f''(\xi)\,h^3/12 \qquad \text{for a } \xi \in [a,b] \quad \text{(with } (*))
\end{aligned}$$

Error of numerical integration error with trapezoidal sum formula

Let $h = (b-a)/n$ and

$$T(h) = h\left(\frac{1}{2}(f(a)+f(b)) + \sum_{j=1}^{n-1} f(a + j\,h)\right)$$

Then we have for a $\xi \in [a, b]$:

$$\int_a^b f(x)\,dx = T(h) - \frac{(b-a)\,h^2}{12} f''(\xi)$$

Proof: In the lecture.

Note: The convergence of the trapezoidal sum formula is of one order lower than the convergence of the standard trapezoidal rule.

Reason: the errors in each step sum up.

(Simpson rule) Kepler's barrel rule for one interval

Let p be the interpolation polynomial (parabola) to the nodes $a, b, (a+b)/2$.
The Lagrange-representation of p is

$$p(x) = f(a)\underbrace{\frac{(x-\frac{a+b}{2})(x-b)}{(a-\frac{a+b}{2})(a-b)}}_{L_1(x)} + f\left(\frac{a+b}{2}\right)\underbrace{\frac{(x-a)(x-b)}{(\frac{a+b}{2}-a)(\frac{a+b}{2}-b)}}_{L_2(x)} + f(b)\underbrace{\frac{(x-a)(x-\frac{a+b}{2})}{(a-b)(b-\frac{a+b}{2})}}_{L_3(x)}.$$

We compute:

$$\int_a^b L_1(x)\,dx \;=\; \int_a^b L_3(x)\,dx \;=\; \frac{b-a}{6}, \qquad \int_a^b L_2(x)\,dx = \frac{4(b-a)}{6}.$$

This implies

$$\begin{aligned} S := \int_a^b p(x)\,dx \;&=\; f(a)\int_a^b L_1(x)\,dx + f\left(\frac{a+b}{2}\right)\int_a^b L_2(x)\,dx + f(b)\int_a^b L_3(x)\,dx \\ &=\; \frac{b-a}{6}\left(f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right) \end{aligned}$$

Error of numerical integration with the Simpson rule: If $f:[a,b]\to\mathbb{R}$ is 4-times continuous differentiable, then we have for a $\xi\in[a,b]$:

$$\int_a^b f(x)\,dx = S - \frac{f^{(4)}(\xi)}{2880}h^5, \qquad h = b-a$$

Simpson sum rule

For the Simpson sum rule we divide the integration interval
into intervals of length h and apply the Simpson rule in each sub-interval:
Let $h=(b-a)/n$, $x_j = a+(j-1)h$, $j=1,\dots,n+1$, in particular $x_1=a$, $x_{n+1}=b$.
Then

$$\begin{aligned} \int_a^b f(x)\,dx \;&=\; \sum_{j=1}^{n}\int_{x_j}^{x_{j+1}} f(x)\,dx \\ &\approx\; \sum_{j=1}^{n}\frac{h}{6}\big(f(x_j) + 4\,f(\frac{x_j+x_{j+1}}{2}) + f(x_{j+1})\big) \\ &=\; \frac{h}{6}\Big(f(x_1) + 4\,f(\frac{x_1+x_2}{2}) + 2\,f(x_2) + 4\,f(\frac{x_2+x_3}{2}) + 2\,f(x_3) + \dots \\ &\qquad \dots + 2\,f(x_n) + 4\,f(\frac{x_n+x_{n+1}}{2}) + f(x_{n+1})\Big). \end{aligned}$$

Construction of Quadrature formulas

We construct Quadrature formulas as follows: Chose a finite sequence τ_j with

$$0 \le \tau_1 < \tau_2 < \dots < \tau_n \le 1.$$

Set $x_j = a + \tau_j\,h$, with $h = b-a$. The interpolation polynomial p of degree $\le n-1$
with the nodes x_j to the function $f:[a,b]\to\mathbb{R}$ is

$$p(x) = f(x_1)\,L_1(x) + f(x_2)\,L_2(x) + \dots + f(x_r)\,L_r(x).$$

with the Lagrange-basis polynomials: $L_k(x_j) = \delta_{k,j}$.
From this we get the approximation

$$\int_a^b f(x)\,dx \;\approx\; Q(f) \;:=\; \int_a^b p(x)\,dx \;=\; h\,(\gamma_1\,f(x_1) + \gamma_2\,f(x_2) + \dots + \gamma_n\,f(x_n))$$

with the weights

$$\gamma_j := \frac{1}{h}\int_a^b L_j(x)\,dx$$

Straightforward computation shows that the weights depend only on the sequence τ_j and
not on the position of the interval $[a,b]$.

If we choose the τ_j to be equidistant, the resulting quadrature formulas are called **Newton-Cotes-formulas**. When additionally $\tau_1 = 0$ and $\tau_n = 1$ (also $x_1 = a$ and $x_n = b$) then the corresponding Newton-Cotes-formulas are called **closed**.

Closed Newton-Cotes-formulas (equidistant nodes)

n	weights γ_j	name	error	accuracy
2	$\frac{1}{2}\ \frac{1}{2}$	Trapezoidal rule	$-\frac{h^3}{12}f''(\xi)$	1
3	$\frac{1}{6}\ \frac{2}{3}\ \frac{1}{6}$	Simpson-rule (Kepl. barrel rule)	$-\frac{h^5}{2880}f^{(4)}(\xi)$	3
4	$\frac{1}{8}\ \frac{3}{8}\ \frac{3}{8}\ \frac{1}{8}$	Newtons 3/8-rule	$-\frac{3\,h^5}{19440}f^{(4)}(\xi)$	3
5	$\frac{7}{90}\ \frac{32}{90}\ \frac{12}{90}\ \frac{32}{90}\ \frac{7}{90}$	Milne-rule	$-\frac{h^7}{1935360}f^{(6)}(\xi)$	5
6	$\frac{19}{288}\ \frac{75}{288}\ \frac{50}{288}\ \frac{50}{288}\ \frac{75}{288}\ \frac{19}{288}$	6-point-rule	$-\frac{275\,h^7}{12096*5^7}f^{(6)}(\xi)$	5
7	$\frac{41}{840}\ \frac{216}{840}\ \frac{27}{840}\ \frac{272}{840}\ \frac{27}{840}\ \frac{216}{840}\ \frac{41}{840}$	Weddle-rule	$-\frac{9\,h^9}{1400*6^9}f^{(8)}(\xi)$	7

For the degree of accuracy see next slide.

Maximal degree of accuracy for the Gauss-Legendre-Quadrature

A quadrature formula

$$\int_a^b f(x)\,dx \approx h\,(\gamma_1 f(x_1) + \gamma_2 f(x_2) + \ldots + \gamma_n f(x_n)) \qquad (*)$$

with weights γ_j and nodes $x_j \in [a, b]$ is called accurate with degree m, when in $(*)$ equality holds for all polynomials f with degree $\le m$, and when additionally a polynomial f with degree $m + 1$ exist, such that both sides of $(*)$ are not equal.

With n equidistant nodes we get degree of accuracy $n-1$ when n is even, and degree of accuracy n, when n is odd.

We get maximal degree of accuracy $2n - 1$ with the following choice of nodes

$$x_j = \frac{a+b}{2} + \frac{h}{2}\tau_{nj}, \qquad j = 1, \ldots, n, \qquad h = b - a$$

where $\tau_{n1}, \ldots, \tau_{nn}$ are the zeros of the n-th Legendre-polynomials p_n:

$$p_n(x) = \frac{1}{2^n\,n!}\frac{d^n}{dx^n}[(x^2-1)^n].$$

The corresponding quadrature formulas are called **Gauß-Legendre-formulas**.
For $n = 2$ we get $\tau_{21} = -1/\sqrt{3}$, $\tau_{22} = 1/\sqrt{3}$, $\gamma_1 = \gamma_2 = 1/2$. So

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left(f\left(\frac{a+b}{2} - \frac{h}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{h}{2\sqrt{3}}\right)\right).$$

Gauss-Legendre-quadrature with 2 nodes versus Trapezoidal rule

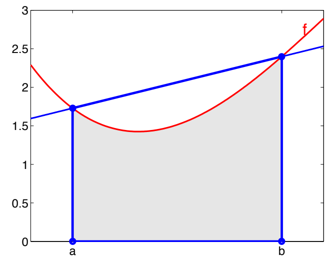
Trapezoidal rule:

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\,(f(a) + f(b)), \qquad h = b - a$$

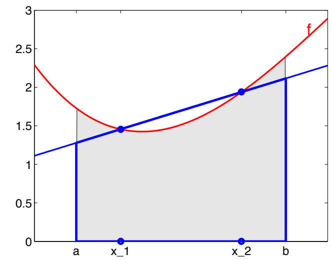
Gauss-Legendre-quadrature with 2 nodes:

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\,(f(x_1) + f(x_2)), \qquad x_j = \frac{a+b}{2} + (-1)^j\frac{h}{2\sqrt{3}}$$

Trapezoidal rule:



Gauss-Legendre:



The Gauss-Legendre-quadrature formula is exact for polynomials with degree ≤ 3.

Reason: the grey areas above and the white area below the trapezoidal line are equal.
Proof sketch on the next slide.

Proof sketch for accuracy of Gauss-Legendre-quadrature formula with 2 nodes

Let

$$p(x) = (x - x_1)(x - x_2), \qquad x_j = \frac{a+b}{2} + (-1)^j\frac{h}{2\sqrt{3}}, \qquad h = b - a$$

Prove the following by computation:

(1) $\int_a^b q(x)p(x)\,dx = 0$ for all linear polynomials $q(x) = \alpha_1 x + \beta_1$.

(2) $\int_a^b r(x)\,dx = \frac{h}{2}(r(x_1) + r(x_2))$ for all linear polynomials $r(x) = \alpha_2 x + \beta_2$.

Now let f be a polynomial with degree ≤ 3.
Then we have for suitable linear polynomials q, r (polynomial division with p)

$$f(x) = q(x)\,p(x) + r(x).$$

Because $p(x_1) = p(x_2) = 0$ er we have $f(x_1) = r(x_1)$ and $f(x_2) = r(x_2)$.
Together with (1) and (2) this gives

$$\int_a^b f(x)\,dx = \int_a^b (q(x)\,p(x) + r(x))\,dx = \int_a^b r(x)\,dx = \frac{h}{2}(r(x_1) + r(x_2)) = \frac{h}{2}(f(x_1) + f(x_2))$$

Gauss-Legendre-quadrature formulas with 3 nodes (degree of accuracy 5):

$$\int_a^b f(x)\,dx \approx \frac{h}{18}\left(5\,f\left(\frac{a+b}{2} - \sqrt{\frac{3}{5}}\frac{h}{2}\right) + 8\,f\left(\frac{a+b}{2}\right) + 5\,f\left(\frac{a+b}{2} + \sqrt{\frac{3}{5}}\frac{h}{2}\right)\right)$$

$$h = b - a$$

For comparison we consider again the **Simpson-rule (degree of accuracy 3)**:

$$\int_a^b f(x)\,dx \approx \frac{h}{6}\left(f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right)$$

Quadrature functions in Matlab: `integral(f,a,b)`, `quad(f,a,b)` etc.

Idea of the Romberg-method

Consider again the trapezoidal sum rule: Summing the trapezoids when dividing the interval $[a,b]$ into intervals of same length $[a+jh,\ a+(j+1)h]$, $h=(b-a)/n$ gives:

$$\int_a^b f(x)\,dx \;\approx\; T(h) = h\left(\frac{1}{2}(f(a)+f(b)) + \sum_{j=1}^{n} f(a+j\,h)\right) \qquad (*).$$

This method is simple, but requires small step size h to get reasonable accuracy. On the other hand the step size cannot be made too small, then the rounding errors would sum up in the summation. A better method is the **extrapolation method of Romberg**.
It is based on the following theorem (difficult to prove): To every $(2m+1)$-time continuous differentiable function $f:[a,b]\to\mathbb{R}$ constants τ_j exist, such that

$$T(h) = \underbrace{\tau_0 + \tau_2\,h^2 + \tau_4\,h^4 + \ldots + \tau_{2m}\,h^{2m}}_{q(h^2)} + \mathcal{O}(h^{2m+2}), \qquad \text{where } \tau_0 = \int_a^b f(x)\,dx$$

Then after computing a trapezoidal sum with $m+1$ small steps h_j we have approximately

$$q(h_j^2) \approx T(h_j).$$

With this we can approximate the polynomial q. We use an interpolation polynomial p with degree m, satisfying

$$p(h_j^2) = T(h_j)$$

Then we get

$$\int_a^b f(x)\,dx = \tau_0 = q(0) \approx p(0).$$

Using Aitken's Lemma (more precise: with the so called Neville-Aitken-Algorithm) the $p(0)$ can be determined without having to compute the coefficients of p.