Numerical derivative and quadrature	Numerical derivative 2/16 mmpc4
quadrature = calculating a definite integral	The difference formulas can be derived from the Taylor series.
one dimensional	1st derivative: $f(h) = O(h^{n})$ iff $\exists M > 0$ and
● To fit data by a suitable function → integrate/differentiate this function. Applicable if the data are subject of errors (experimental data). Example: Shomate equation	$\frac{f(x+h)-f(x)}{h} = f'(x) + \frac{h}{2}f''(x) + \frac{h^2}{6}f'''(x) + \cdots + \frac{h}{6} > 0: f(h) \le Mh^n \ \forall \ h \le h_0$ $= f'(x) + \mathcal{O}(h)$
$C_{pm}^{\circ}(T) = A + BT + CT^2 + DT^3 + E/T^2$	$\Rightarrow f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$
 To replace a derivative by a difference, – several points in the neighborhood are needed – the accuracy decreases To replace a quadrature by a sum over selected points in the interval – the accuracy increases 	This is the 1st order formula in $h = \text{error}$ is $\mathcal{O}(h) = \text{error}$ is on the order of h More accurate $f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)$
multidimensional	$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + \mathcal{O}(h^4) $ (1)
partial derivative: repeat in all variables/directions	Bight derivative – if function is known for arguments $> x$
quadrature: up to about 3D–5D, several 1D quadratures nested more dimensions: Monte Carlo, Conroy integration	$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + \mathcal{O}(h^2)$
Numerical derivative II 3/16 mmpc4	Numerical quadrature 4/16 mmpc4
Similarly for the 2nd derivative, the simplest formula: $f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$	Numerical integration in interval $[a, b]$. Assumption: several derivatives exist (are finite) in the interval. If not (e.g., \sqrt{x} in $[0, 1]$), a substitution helps. General formula:
Which step b?	$\int_{a}^{b} f(x) dx = \sum w_i f(x_i), x_i \in [a, b]$
Let $\varepsilon =$ numerical precision: the smallest number > 1 is 1 + ε	Ja Methods:
Typical error of several operations = several ε • 64 bit (double, REAL*8): $\varepsilon = 2^{-52} \doteq 2 \times 10^{-16}$, today's standard (typically 1×10^{-15})	• equidistant arguments (Newton-Cotes): - closed: use $f(a)$, $f(b)$ - open: oply points in (a, b)
• 80 bit (extended, long double, REAL*10): $\varepsilon = 2^{-63} = 1 \times 10^{-19}$	 non-equidistant arguments (Gauss): usually more efficient (if we can calculate the function a calculate is a calculate)
• 32 bit (float, REAL*4): $\varepsilon = 2^{-23} \doteq 1 \times 10^{-7}$	Improper intervals:
(minimum speed gain except GPU)	\bigcirc substitution \rightarrow finite interval
Rule of the thumb: For the best <i>h</i> : rounding error \approx method error.	special methods
rounding error $\propto \epsilon/\hbar$, method error $\propto \hbar^4$, $\Rightarrow \hbar \approx \epsilon^{1/3} = 1 \times 10^{-3}$	lypically an interval is divided into shorter subinterval and a suitable method is used repeatedly
Newton-Cotes formulas 5/16 mmpc4	Gauss quadrature 6/16 mmpc4
Newton-Cotes formulas 5/16 mmpc4 Trapezoidal rule:	Gauss quadrature 6/16 mmpc4 ● Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one)
Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points:	Gauss quadrature 6/16 mmpc4Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4})$
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Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2x more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$	Gauss quadrature 6/16 mmpc4 Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4})$ The four-point formula of the 8th order with a good numerical stability: double Gauss8(double (*f)(double),double a,double b,int n) // int[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals { const double q1=0.430568155797026287612, // sqrt((15+sqrt(120))/140) q2=0.169990521792428132401, // sqrt((15-sqrt(120))/140)
Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2× more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\begin{bmatrix} b & b-a \end{bmatrix} = a \begin{bmatrix} a+b \\ a \end{bmatrix}$	6/16 mmpc46/16 mmpc4Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4})$ The four-point formula of the 8th order with a good numerical stability: double Gauss8(double (rf)(double), double a, double b, int n) // inf[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals { (const double q=0.43068155797026287612, // sqrt((15+sqrt(120))/140) q=0.163990521792428132401, // sqrt((15-sqrt(120))/140) q=0.163990521792428132401, // sqrt(120)/140) may be less stable, double hisher(h-hav, v=h/2-wi); better use 4-8th in
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Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2× more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b) \right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ method	6/16 mmpcd • Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $ \int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4}) • The four-point formula of the 8th order with a good numerical stability: double Gauss8(double (*f)(double),double a,double b,int n) // int[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals { const double q=0.1630668155797026287612, // sqrt((15+sqrt(120))/140) q=0.1630968155797026287612, // sqrt((15-sqrt(120))/140) we0.173927422568726028867; // 1/4-sqrt(5/864) double h=(b-a)/n; double dn=h*q1, h2=h*q2; int i; double sum=0,x; for (i=0; i:q; i++) { x=h*(i+0.5)+a; sum=(f(x-h1)+f(x+h1))*wi+(f(x-h2)+f(x+h2))*w2; } return sum; } return sum; // Interval // Inter$
Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2× more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b) \right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ methodRichardson extrapolation $\frac{7/16}{mmpc4}$	6/16 mmpcd Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4})$ The four-point formula of the 8th order with a good numerical stability: double Gauss8(double (#f)(double),double a, double b, int n) (if (a,b) f(x) dx using 4-point Gauss quadrature with n subintervals (const double q=0.40905021792428132401, // sqrt((15-sqrt(120))/140) q=0.40905021792428132401, // sqrt((15-sqrt(120))/140) q=0.40905021792428132401, // sqrt((15-sqrt(120))/140) q=0.40905021792428132401, // sqrt((5/864) Higher-order methods may be less stable, better use 4-8th in several subintervals for (i=0; i<n; i++)="" li="" return="" sum;<="" x+h+(1+(x-h2)+f(x+h2))+w2;="" x+h+(4-2)+i;="" {="" }=""> </n;> ODE - the initial value problem
Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2× more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b) \right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ methodRichardson extrapolation $\frac{7/16}{mmpc4}$ The error formulas often have the error given by	6/16 mmpcdGauss quadrature6/16 mmpcdTwo-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}} \right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}} \right) \right] + O((b-a)^{4})$ The four-point formula of the 8th order with a good numerical stability: double Gauss8(double (*f)(double),double a,double b,int n) // int[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals { const double q=0-0.40068165797020287612, // sqrt((15-sqrt(120))/140) q=0.16909051792428132401, // sqrt((15-sqrt(120))/140) we0.17392742256072692887; // 1/4-sqrt(5/864) double h=(b-a)/n; double sum=0,x; for (i=0; i:a; i+t) { x=hc(i+0,5)+a; sum==(f(x-h1)+f(x+h1))*wi+(f(x-h2)+f(x+h2))*w2; } return sum; >Higher-order methods may be less stable, better use 4-8th in several subintervals for (i=0; i:a; i+t) { x=hc(i+0,5)+a; sum==(f(x-h1)+f(x+h1))*wi+(f(x-h2)+f(x+h2))*w2; } return sum; >8/16 mmpc4DDE - the initial value problem8/16 mmpc4 $\gamma' = f(x, y), y(x_0) = y_0$ ODE = Ordinary
Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2× more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b) \right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ methodRichardson extrapolation $\frac{7/16}{mmpc4}$ The error formulas often have the error given by $S = S(h) + Ah^{n} + Bh^{n+2} + \cdots n$ is usually even	6/16 mmpcdGauss quadrature6/16 mmpcdTwo-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4})$ The four-point formula of the 8th order with a good numerical stability: double Gaus8(double (#f)(double), double a, double b, int n) // int[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals { const double q=0.40666155797026287612, // sqrt((15+sqrt(120))/140) q=0.10990521792428132401, // sqrt((15-sqrt(120))/140) q=0.10990521792428132401, // sqrt((15-sqrt(120))/140) double +1=her, u2=h/2=V1; double h=1=herq), r; double sum=0,x; for (1=0; icn; i++) { x=het(i+0.5)+a; sum=(f(x=h)+f(x=h))+wi+(f(x=h2)+f(x=h2))+w2; } return sum;Higher-order methods may be less stable, better use 4-8th in several subintervals for (1=0; icn; i++) { x=het(i+0.5)+a; y = f(x, y), y(x_0) = y_08/16 mmpc4 ODE - the initial value problem 8/16 mmpc4 $y' = f(x, y), y(x_0) = y_0$ ODE = Ordinary Differential Equation
Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2× more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b) \right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ methodRichardson extrapolation $f/16$ mmpcdThe error formulas often have the error given by $S = S(h) + Ah^{n} + Bh^{n+2} + \cdots n$ is usually evenGenerally we may have	6/16 mmpcdGauss quadrature6/16 mmpcdTwo-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4})$ The four-point formula of the 8th order with a good numerical stability: double Gauss8(double (*f)(double),double a,double b,int n) // int[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals { const double q=0.16909051792428132401. // sqrt((15-sqrt(120))/140) q=0.16909051792428132401. // sqrt((15-sqrt(120))/140) q=0.169090517924828687; // 1/4-sqrt(5/864) Higher-order methods double h=(b-a)/n; double h=(b-a)/n; double sum=0,x; double sum=0,x; sum==(f(x-h1)+f(x+h1))*wi+(f(x-h2)+f(x+h2))*w2; j return sum;Higher-order methods mpc4 $y' = f(x, y), y(x_0) = y_0$ ODE = Ordinary Differential Equation $y' = f(x, y), y(x_0) = y_0$ ODE = Ordinary Differential Equation y may be a vector (system of ODEs)one higher-order eq. can be transformed to a system of ODEs of the 1st order (but a numerical method tailored to the original ODE may be more efficient)
Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2x more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b) \right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ methodRichardson extrapolation $f/16 mmpc4$ The error formulas often have the error given by $S = S(h) + Ah^{n} + Bh^{n+2} + \cdots$ n is usually evenGenerally we may have $S = S(h) + Ah^{n} + Bh^{n+1} + \cdots$ More accurate result:	6/16 mmpcd Gauss quadrature Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}} \right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}} \right) \right] + O((b-a)^4) The four-point formula of the 8th order with a good numerical stability: double Gauss@(double (#f)(double),double a, double b, int n) // int[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals double (anse@(double (#f)(double),double a, double b, int n) // int[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals double (anse@(double (#f)(double), double a, double b, int n) // int[a,b] f(x) dx using 4-point Gauss quadrature with n subintervals double with example.asymptotic double (ansequadrature with n subintervals (anst double) quere(12-300/31/30) quere(12-300/31/30) quere(12-300/31/30) quere(12-300/31/30) queree double double (ansequadrature with n) viscopic double (ansequadrature with n) // int (a,b) f(x) dx using 4-point Gauss quadrature with n) double with a weree double (ansequadrature with n) double withey a, who have a were as guadrature with n) double with a were as guadrature with n were were as guadrature with n) double withey as guadrature with n) guadrature with n were as guadrature with n) $
Newton-Cotes formulas5/16 mmpcdTrapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right]h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2x more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2})\right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ methodRichardson extrapolation $7/16$ mmpcdThe error formulas often have the error given by $S = S(h) + Ah^{n} + Bh^{n+2} + \cdots n$ is usually evenGenerally we may have $S = S(h) + Ah^{n} + Bh^{n+1} + \cdots$ More accurate result: $S = \frac{2^n S(h/2) - S(h)}{2^n - 1} + \binom{\mathcal{O}(h^{n+2})}{\mathcal{O}(h^{n+1})}$	6/16 mmpc4Gauss quadrature6/16 mmpc4• Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_a^b f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^4)$ • The four-point formula of the 8th order with a good numerical stability: double Gauss(double (rf)(double).double a.double b.int n) // int(a,b) f(x) dx using 4-point Gauss quadrature with a subintervals { {equivalence(16-a)(16-aq)(10)(140) q2-0.16990621792428132401, // aqrt((15-aqrt(120))/140) web. (172074226877820287712, // aqrt(16-aqrt(120))/140) web. (17207422687782028877; // 1/4-aqrt(5/864) double h=h=hq, h2=hq, i gaus=(16x-h1)+f(x+h1))*w1+(f(x-h2)+f(x+h2))*w2; int i; double sum=0,x; for (1=0, i 4n; i++) { x=h+(i 4, 5)+a; sum==(f(x-h1)+f(x+h1))*w1+(f(x-h2)+f(x+h2))*w2; i=turn sum;B/16 mmpc4ODE - the initial value problemB/16 mmpc4y' = f(x, y), y(x_0) = y_0ODE = Ordinary Differential Equationy' = f(x, y), y(x_0) = y_0ODE = Ordinary Differential Equationy'' = f(x, y), y', subst. $z = y' \Rightarrow z' = f(x, y, z), y' = z$ Runge-Kutta: @ history not needed @ easy change of the step (adaptive) @ qood stability
Newton-Cotes formulas5/16 mmpcdTrapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2× more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b) \right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ methodRichardson extrapolation $7/16$ mmpcdThe error formulas often have the error given by $S = S(h) + Ah^{n} + Bh^{n+2} + \dots n$ is usually evenGenerally we may have $S = S(h) + Ah^{n} + Bh^{n+2} + \dots n$ is usually evenWore accurate result: $S_{2}(h/2)$ $2n-1$ Verame repeat this trick with pair $S_{2}(h/4)$ a $S_{2}(h/2)$, etc.	6/16 mmpc4Gauss quadrature6/16 mmpc4Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_a^b f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^4)$ The four-point formula of the 8th order with a good numerical stability: double Gaum8(double (rf)(double),double a,double b,int n) // int(a,b) f(x) dx using 4-point Gauss quadrature with a subintervals (const double q=0-0.00900521702428132401, // sqrt((15+sqrt(120))/140) q=0-0.109900521702428132401, // sqrt((15+sqrt(120))/140) g=1(x, y), y(x_0) = y_0Higher-order methods double hit=heq1, h2=heq2; may be less stable, double hit=heq1, h2=heq2; may be less stable, double sum=0, x;Moter use 4-8th in several subintervals for (1=0, it=n; it=1) g=1(x, y), y(x_0) = y_0ODE = Ordinary Differential EquationODE - the initial value problem8/16 mmpc4gaue+(f(x-h1)+f(x+h1))*wi+(f(x-h2)+f(x+h2))*w2; > return sum;ODE = ordinary Differential Equationy may be a vector (syste
Newton-Cotes formulas5/16 mmpcdTrapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right] h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2x more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2}) \right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b) \right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x^{2},Example. Verify that the Simpson rule integrates exactly 1, x, x^{2}, x^{3}, but not x^{4}, therefore, it is an $\mathcal{O}(h^{4})$ methodRichardson extrapolation7/16 mmpcdMore accurate result: $S = S(h) + Ah^{n} + Bh^{n+2} + \dots n$ is usually evenGenerally we may have $S = S(h) + Ah^{n} + Bh^{n+1} + \dots$ More accurate result: $S = \frac{2^{n}S(h/2) - S(h)}{2^{n} - 1} + \begin{cases} \mathcal{O}(h^{n+2}) \\ \mathcal{O}(h^{n+1}) \\ \mathcal{O}(h^{n+1}) \end{cases}$ We can repeat this trick with pair $S_{2}(h/2)$ as $S_{2}(h/2)$, etc.Warning, this process fails if the function is not smooth enough (does not have enough derivatives)Example. Show that one step of the Richardson extrapolation of the trapezoidal	6/16 mmpc46/16 mmpc4• Two-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x) dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4})$ • The four-point formula of the 8th order with a good numerical stability: double Gauss@double (*f)(double),double a,double b,int n) (/ int[a,b] f(x) dx using 4-point Gauss quadrature with n agood numerical stability: double = 0.0000000000000000000000000000000000
Newton-Cotes formulas5/16 mmpc4Trapezoidal rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + \mathcal{O}((b-a)^{2})$ Several dividing points: $\int_{a}^{b} f(x) dx = \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{f(b)}{2}\right]h + \mathcal{O}(h^{2}), h = \frac{b-a}{n}$ Rectangular rule (open): 2× more accurate than trapezoid $\int_{a}^{b} f(x) dx = (b-a) \left[f(\frac{a+b}{2})\right] + \mathcal{O}((b-a)^{2})$ Simpson's rule: $\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right] + \mathcal{O}((b-a)^{4})$ Order and error: because of linearity, it's enough to verify for 1, x, x ² ,Example. Verify that the Simpson rule integrates exactly 1, x, x ² , x ³ , but not x ⁴ , therefore, it is an $\mathcal{O}(h^{4})$ methodThe error formulas often have the error given by $S = S(h) + Ah^{n} + Bh^{n+2} + \cdots$ n is usually evenGenerally we may have $S = S(h) - Ah^{n} + Bh^{n+1} + \cdots$ More accurate result: $S = \frac{2^{n}S(h/2) - S(h)}{2^{n} - 1} + {\mathcal{O}(h^{n+2}) \\ \mathcal{O}(h^{n+1})}$ We can repeat this trick with pair $S_2(h/4)$ a $S_2(h/2)$, etc.Warning, this process fails if the function is not smooth enough (does not have enough derivatives)Example. Show that one step of the Richardson extrapolation of the trapezoidal rule is equivalent to the Simpson formula	6/16 mmpcdGauss quadrature6/16 mmpcdTwo-point formula of the 4th order has a half error w.r.t. Simpson and needs less ponts (by one) $\int_{a}^{b} f(x)dx = \frac{b-a}{2} \left[f\left(\frac{a+b}{2} - \frac{a-b}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{a-b}{2\sqrt{3}}\right) \right] + O((b-a)^{4})$ The four-point formula of the 8th order with a good numerical stability: double Gauss@double (*f)(double), double a, double b, int n) (// int(a,b) f(c) du using 4-point Gauss quadrature with n aubintervals (const double q=0.109905179202037002037612, // sqrt((15+qqrt(120))/140) q=0.109905179202037002037612, // sqrt((15+qqrt(120))/140) q=0.1099051792020370020377020207612, // sqrt((15+qqrt(120))/140) q=0.1099051792020370020377020207612, // sqrt((15+qqrt(120))/140) q=0.1099051792020370020377020207612, // sqrt((15+qqrt(120))/140) q=0.10990517920203700203770020377020207612, // sqrt((15+qqrt(120))/140) q=0.1099051792020370020370020370020370000370, // sqrt((15+qqrt(120))/140) q=0.1793742204807139020370020370020370020370000370, // sqrt((15+qqrt(120))/140) q=0.179374220480713902037002037700203770203700203770203700203770203700203700020370000370000300, // sqrt(15+qqrt(120))/140) q=0.17937422048071390203700203700203700003700003700003700003000, // sqrt((15+qqrt(120))/140) w=0.17397422048071300, // sqrt((15+qqrt(120))/140) w=0.17397422048071300, // sqrt((15+qqrt(120))/140) w=0.17397422048071300000000000000000000000000000000000

Warm-up: Euler's method 9/16 mmpc4	Runge-Kutta 2nd order (RK2) 10/16 mmpc4
$y' = f(x, y), \ y(x_0) = y_0$ 1 step: $y(x + h) = y(x) + hy' + \mathcal{O}(h^2) = y(x) + hf(x, y) + \mathcal{O}(h^2)$ This method is $\mathcal{O}(h^2)$ locally $\Rightarrow \mathcal{O}(h)$ globally ($\propto 1/h$ steps needed on a finite interval) y' = y	Let's improve Euler – trapezoidal style: $k_{1} := f(x, y)$ $k_{2} := f(x + h, y(x) + hk_{1})$ $y(x + h) := y(x) + \frac{h}{2}(k_{1} + k_{2})$ $x := x + h$ Order derivation is based on: $y'' = df(x, y)/dx = f_{x} + f_{y}y' \Rightarrow$ $y(x + h) = y(x) + \frac{h}{2}(k_{1} + k_{2})$
	$\sum_{k=1}^{O(h^2)} y(x) + \frac{h}{2}(y' + y' + hf_x + hf_yf) = y(x) + hy'(x) + \frac{h^2}{2}y''(x)$ Local error $O(h^3)$ (or better), global error is (at least) $O(h^2)$ Let's improve Euler – rectangular (half-step) style: $k_1 := f(x, y)$ $k_2 := f(x + \frac{h}{2}, y(x) + \frac{h}{2}k_1)$ $y(x + h) := y(x) + hk_2$ $x := x + h$ The same order, smaller error coefficient
Runge-Kutta 4th order (RK4)	Predictor-corrector – intro
Popular method of the 4th order (local error $\mathcal{O}(h^5)$): $k_1 := f(x, y)$ $k_2 := f(x + \frac{h}{2}, y(x) + \frac{h}{2}k_1)$ $k_3 := f(x + \frac{h}{2}, y(x) + \frac{h}{2}k_2)$ $k_4 := f(x + h, y(x) + hk_3)$ $y(x + h) := y(x) + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$ x := x + h	 We know a history = values (and/or derivatives, i.e., rhs). predictor: we predict y^P(x + h): using rhs (usually more stable and more accurate) without evaluating the rhs (Gear methods - polynomial extrapolation) [optional modificator] corrector: we calculate the corrected y^C(x + h): rhs calculated once rhs calculated twice, three times, rhs calculated iteratively until some precision limit is reached Problem - stability: the single-step errors propagate to further steps. The method must guarantee that the errors do not cumulate and do not explode (exponentially/exponential oscillations) If the coefficients of a method are large with alternating sigs, the method will likely be unstable
Predictor-corrector – 3rd order example	3rd order example – stability
Let's first rewrite RK2 to the predictor-corrector form: $y^{P}(x + h) = y(x) + hf(x, y(x)) + \mathcal{O}(h^{2})$ $y^{C}(x + h) = y(x) + \frac{h}{2}[f(x, y(x)) + f(x + h, y^{P}(x + h))] + \mathcal{O}(h^{3})$ the 2nd step is $\mathcal{O}(h^{3})$ because it is trapezoid, and the error in $y^{P}(x + h)$ is $h\mathcal{O}(h^{2})$. Let's try to improve both steps. Predictor: $y^{P}(x + h) = y(x) + \frac{h}{2}[3f(x) - f(x - h)] + \mathcal{O}(h^{3})$ where $f(x) \equiv f(x, y(x))$ and $f(x - h) \equiv f(x - h, y(x - h))$ (from the previous step). We shall look for the corrector in the form: $y^{C}(x + h) = y(x) + h[af(x - h) + bf(x) + cf(x + h, y^{P}(x + h))]$ The test function method using equation $y = y'$ (see matenum4.mw) \Rightarrow $y^{C}(x + h) = y(x) + \frac{h}{12}[-f(x - h) + 8f(x) + 5f(x + h, y^{P}(x + h)] + \mathcal{O}(h^{4})$ = this is a 3rd order method (locally $\mathcal{O}(h^{4})$)	The method is $\mathcal{O}(h^4)$ locally, so we can write (neglecting $\mathcal{O}(h^5)$): $y(x-ih) = y^{\text{exact}}(x-ih) + \epsilon_i h^4$ Let's use the test equation $y' = y$ with $y(0) = 1$ (the solution is $y = e^x$). Using Maple: $\epsilon_{i+1} = \epsilon_i - 13/144$ • any error of $y(x-h)$, $y(x-2h)$ does not propagate (with precision up to h^4) • an error $\propto h^4$ is generated in one step
Milne method mmpc4	Stability + mpc4
Corrector = Simpson formula. $y^{P}(x + h) = y(x - 3h) + \frac{4h}{3}[2f(x) - f(x - h) + 2f(x - 2h)]$ $y^{C}(x + h) = y(x - h) + \frac{h}{3}[f(x - h) + 4f(x) + f(x + h, y^{P}(x + h)]$ Local error = $\mathcal{O}(h^{5})$. Let $y(ih)$ be subject to error $\epsilon_{i}h^{5}$. The error propagates as follows (see matenum4.mw using $y' = y$):	A typical equation for error propagation in predictor-corrector methods is (in h^n , where n is the local order) $\epsilon_{i+1} := a_c + a_0 \epsilon_i + a_1 \epsilon_{i-1} \cdots a_n \epsilon_{i-n}$ This is a linear difference equation . A general solution is: $\epsilon_i = \sum_{x} b_x x^i + b_c$ where the sum is over all roots of the so called characteristic polynomial :
$e_{t+1} - \overline{90} + e_{t-1}$	$x^{n+1} = c_0 x^n + \dots + c_n x^0$
 <i>ϵ_{i+1}</i> := 1/90 + <i>ϵ_i</i> would be OK, a constant error cannot be removed in principle (unless the order increases) example of an unstable method: <i>ϵ_{i+1}</i> := 4/3<i>ϵ_i</i> + 1/90 example of a stable method: <i>ϵ_{i+1}</i> := 3/4<i>ϵ_i</i> + 1/90 the Milne method method is at the edge of stability (a sort of very particular problem) 	(In case of multiple roots the basis is { x^i , i x^i }, similarly as for systems of homo- geneous linear differential equations.) The errors should not exponentially grow, thus $ x < 1$ must be satisfied. Example of a difference equation Fibonacci sequence: $F_0 = 0$, $F_1 = 1$, $F_n = F_{n-1} + F_{n-2}$ for $n > 1$