Chapter 15: Numerical Integration

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Slides for the book
A First Course in Numerical Methods (published by SIAM, 2011)
http://www.ec-securehost.com/SIAM/CS07.html

*Some Slides From Lecture Notes of Peter Arbenz, ETH Zürich

Numerical integration (quadrature)

- The need to integrate arises very frequently in numerical computations. Instance: finite element methods for differential equations use basis functions in the spirit of Chapter 11, in combination with integrals computed over tiny pieces of the computational domain.
- The need to know how to integrate numerically can be more immediate than in the case of differentiation because we often do not know how to integrate even simple-looking functions.
- As opposed to differentiation, which is local in nature, integration is a *global* operation.
- Note that while the derivative of $f(x)$ is typically rougher than f, the integral of $f(x)$ is smoother. Consequently, no special roundoff error difficulties are expected here, unlike in Chapter 14.
- Many-dimensional integration often arises in statistical applications.

Introduction

Let $f(x)$ be a continuous real-valued function of a real variable, defined on a finite interval $a \leq x \leq b$.
We seek to compute the value of the integral,

$$\boxed{\int_a^b f(x)\,dx.}$$

Quadrature means the approximate evaluation of such a definite integral.

Principle idea: Interpolate f by (piecewise) polynomial, then integrate the polynomial.

Introduction (cont.)

The fundamental additive property of definite integrals is the basis for many quadrature formulae. For $a < c < b$ we have

$$\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx$$

In particular, we can subdivide an interval in many subintervals, integrate f in the subintervals, and finally add up these partial integrals to get the overall result.

We can subdivide subintervals that indicate big errors recursively in an adaptive procedure.

Basic rules

Consider only definite integrals; quadrature $\equiv$ numerical integration in one dimension. Seek approximation formulas of the form

$$I_f = \int_a^b f(x)dx \approx \sum_{j=0}^{n} a_j f(x_j).$$

- Derive basic quadrature rules by interpolating the integrand $f(x)$ using Lagrange form and integrating the resulting polynomial.
- The *weights* a_j are then given by

$$a_j = \int_a^b L_j(x)dx, \quad L_j(x) = \prod_{\substack{k=0 \\ k \neq j}}^{n} \frac{(x - x_k)}{(x_j - x_k)}.$$

- These weights are independent of f and can be found in advance!

Newton–Cotes rule

One obvious way to approximate f is by polynomial interpolation and then integrate the polynomial.

Let $a = x_0 < x_1 < x_2 < \cdots < x_n = b$ be equidistant points in $[a, b]$. The Lagrange interpolating polynomial is given by

$$P_n(x) = \sum_{i=0}^{n} L_i(x) f(x_i), \quad L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}, \quad i = 0, \ldots, n.$$

Then

$$\int_a^b f(x)\, dx \approx \int_a^b P_n(x)\, dx = \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)\, dx = \sum_{i=0}^{n} f(x_i) w_i.$$

Clearly, such a method has at least order $n+1$.

Basic quadrature rules

Let $h = b - a$ be the length of the interval. The two simplest quadrature rules are

- midpoint rule

$$M = h\,f\left(\frac{a+b}{2}\right)$$

- trapezoidal rule

$$T = h\frac{f(a)+f(b)}{2}$$

The accuracy of a quadrature rule can be predicted in part by examining its behavior on polynomials.

Order of a quadrature rule is the degree of the lowest degree polynomial that the rule does *not* integrate exactly.

The orders of both midpoint and trapezoidal rule are 2.

Trapezoidal rule again

The trapezoidal rule is the Newton–Cotes rule for $n = 1$:

$$P_1 = f(a)\frac{b-x}{b-a} + f(b)\frac{x-a}{b-a}$$

and (with $x = a + h\xi$)

$$\int_a^b \frac{b-x}{b-a}\,dx = \int_a^b \frac{x-a}{b-a}\,dx = h\int_0^1 \xi\,d\xi = \frac{h}{2}.$$

So,

$$T = \frac{h}{2}(f(a) + f(b)).$$

Simpson's rule

Simpson's rule is the Newton–Cotes rule for $n = 2$: $(x = a + h\xi)$

$$P_2(\xi) = f(a)(1 - 2\xi)(1 - \xi) + f(c)4\xi(1 - \xi) + f(b)\xi(2\xi - 1).$$

$$S = \frac{h}{6}(f(a) + 4f(c) + f(b)), \qquad c = \frac{a+b}{2}.$$

Note that

$$S = \frac{2}{3}M + \frac{1}{3}T.$$

It turns out that Simpson's rule also integrates cubics exactly, but not quartics, so its order is four.

Newton–Cotes methods with order up to 8 exist.

Even higher order methods can be computed, but some of their weights w_i get negative which is undesirable for potential round-off.

Midpoint Rule

The trapezoidal and the Simpson rules are instances of **Newton–Cotes** formulas. These are formulas based on polynomial interpolation at equidistant abscissae. If the endpoints a and b are included in the abscissae $x_0, \ldots, x_n$, then the formula is *closed*. Otherwise it is an *open* Newton–Cotes formula. The simplest example of an open formula of this sort is the **midpoint rule**, given by

$$I_f \approx I_{mid} = (b-a) f\left(\frac{a+b}{2}\right),$$

which uses a constant interpolant at the middle of the interval of integration.

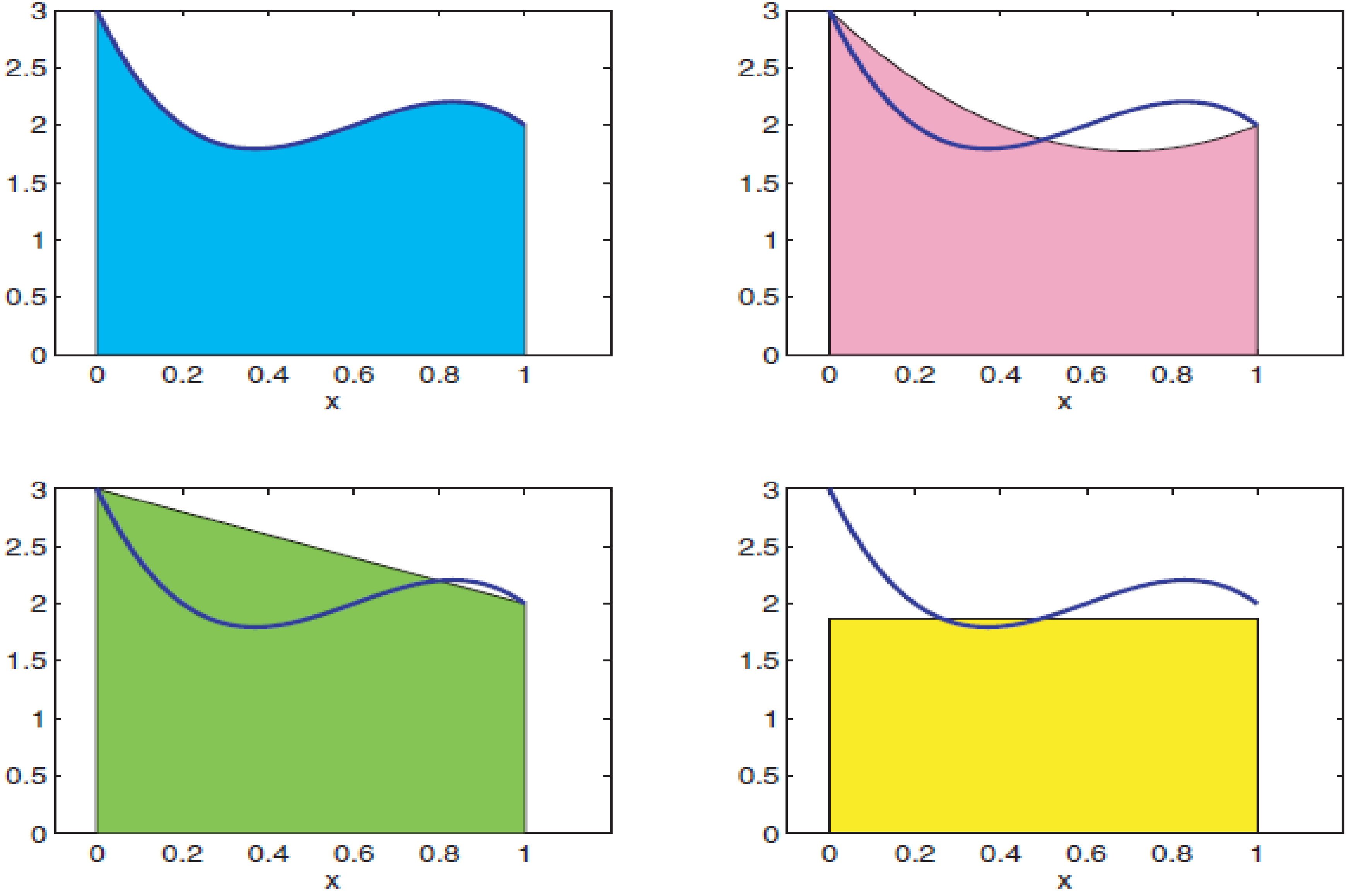


Figure 15.1. *Area under the curve. Top left (cyan): for $f(x)$ that stays nonnegative, I_f equals the area under the function's curve. Bottom left (green): approximation by the trapezoidal rule. Top right (pink): approximation by the Simpson rule. Bottom right (yellow): approximation by the midpoint rule.*

Error in basic rules

- The error satisfies

$$E(f) = \int_a^b f(x)dx - \sum_{j=0}^{n} a_j f(x_j)$$
$$= \int_a^b f[x_0, x_1, \ldots, x_n, x](x - x_0)(x - x_1) \cdots (x - x_n)dx.$$

- To estimate this further can be delicate. Results:

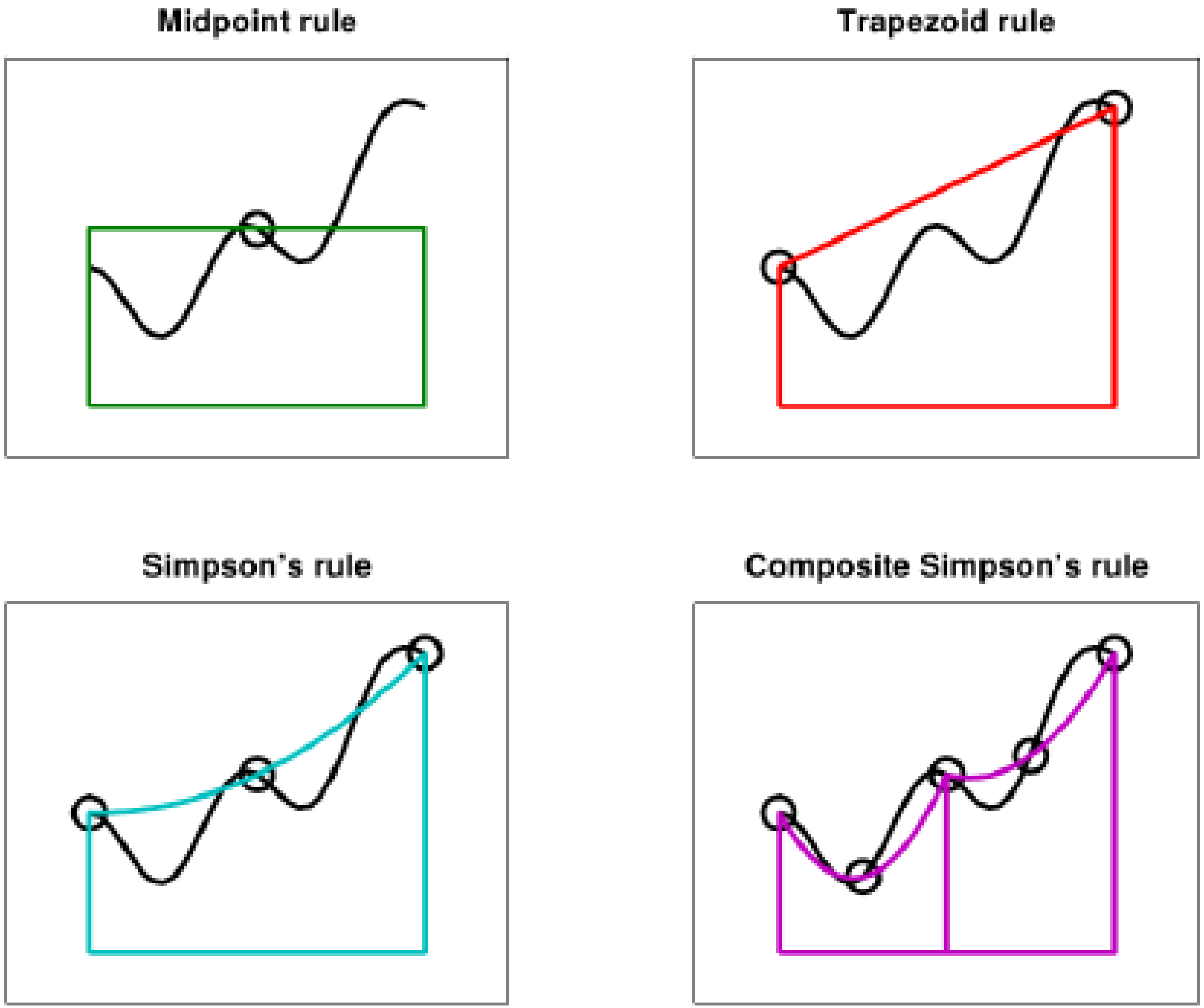
Method	Formula	Error
Midpoint	$(b-a)f(\frac{a+b}{2})$	$\frac{f''(\xi_1)}{24}(b-a)^3$
Trapezoidal	$\frac{b-a}{2}[f(a)+f(b)]$	$-\frac{f''(\xi_2)}{12}(b-a)^3$
Simpson	$\frac{b-a}{6}[f(a)+4f(\frac{b+a}{2})+f(b)]$	$-\frac{f''''(\xi_3)}{90}(\frac{b-a}{2})^5$

- These are all Newton-Cotes formulas: Trapezoidal and Simpson are *closed*, midpoint is *open*.

Composite Rules

- Applying a quadrature rule to $\int_a^b f(x)\,dx$ may not yield an approximation with the desired accuracy.
- To increase the accuracy, one can partition the interval $[a, b]$ into subintervals and apply the quadrature rule to each subinterval.
- The resulting formula is known as a composite rule.

Composite Rules (cont.)



Composite methods

- The basic rules are good for small intervals. So, use them on subintervals.
- Similar to piecewise polynomial interpolation, but easier because no need here to worry about global smoothness.
- $$\int_a^b f(x)dx = \sum_{i=1}^{r} \int_{t_{i-1}}^{t_i} f(x)dx, \quad \text{e.g. } t_i = a + ih.$$
- If error in basic rule is $E(f) = \tilde{K}(b-a)^{q+1}$ then error in composite method is

$$E(f) = K(b-a)h^q.$$

Composite trapezoidal rule

Let $[a, b]$ be partitioned into n equidistant subintervals (x_i, x_{i+1}) of length $h = x_{i+1} - x_i = (b-a)/n$.

Then we apply the trapezoidal rule to each subinterval to obtain the *composite trapezoidal rule*

$$\boxed{T(h) = h\left(\tfrac{1}{2}y_0 + y_1 + \cdots + y_{n-1} + \tfrac{1}{2}y_n\right), \qquad y_i = f(x_i).}$$

The error of the composite trapezoidal rule is

$$\left| \int_a^b f(x)dx - T(h) \right| = \frac{(b-a)h^2}{12} |f''(\xi)|, \quad \xi \in [a, b].$$

Composite trapezoidal rule (cont.)

Let's assume we have computed $T(h)$. How do we compute $T(h/2)$?

$$
\begin{aligned}
T(h/2) &= \frac{h}{2}\left(\frac{1}{2}y_0 + y_1 + \cdots + y_{2n-1} + \frac{1}{2}y_{2n}\right) \\
&= \frac{h}{2}\left(\frac{1}{2}y_0 + y_2 + \cdots + y_{2n-2} + \frac{1}{2}y_{2n}\right) \\
&\quad + \frac{h}{2}(y_1 + y_3 + \cdots + y_{2n-1}) \\
&= \frac{1}{2}T(h) + \frac{h}{2}(y_1 + y_3 + \cdots + y_{2n-1})
\end{aligned}
$$

Composite trapezoidal method

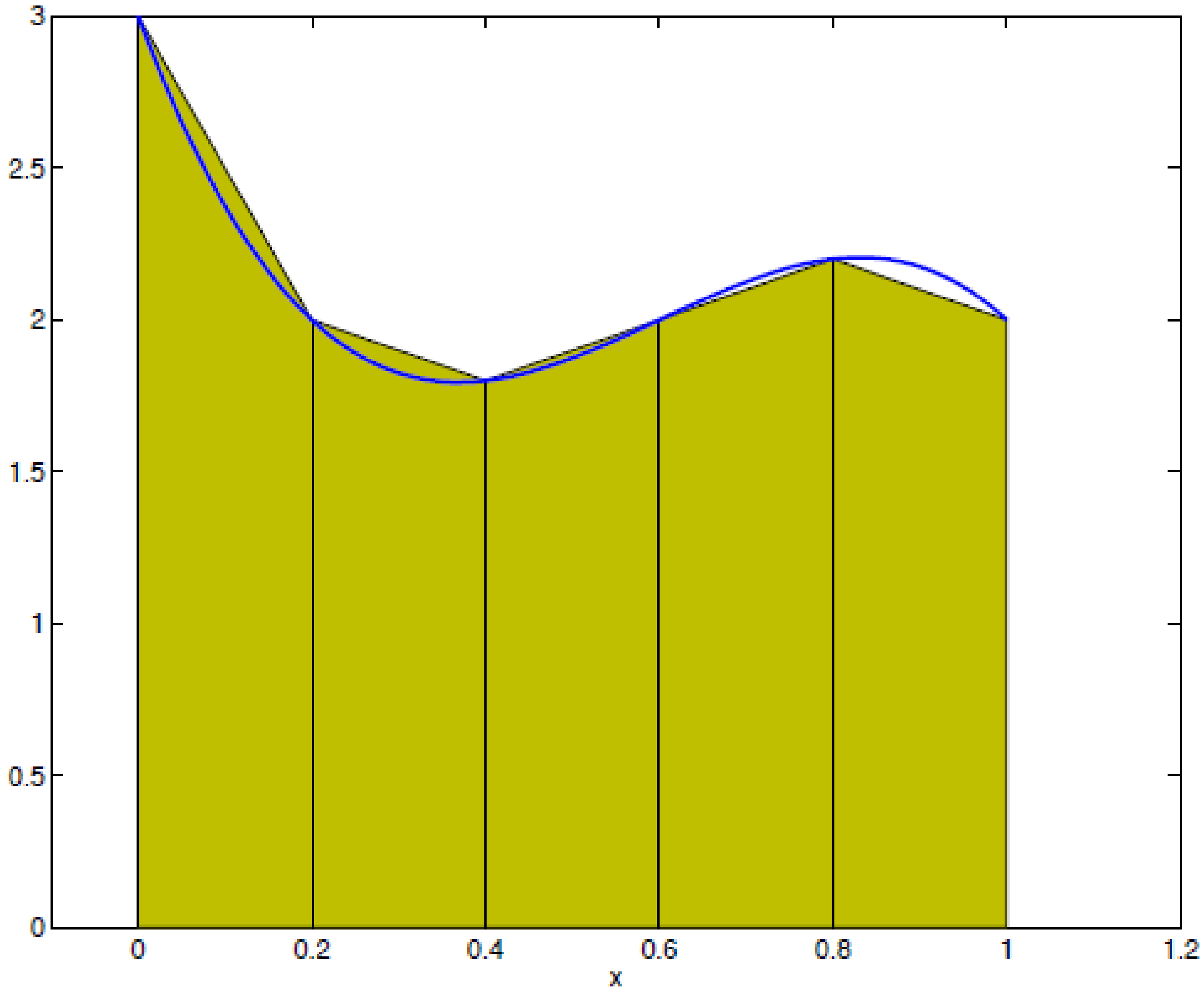
- Composite method

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(a) + 2f(t_1) + 2f(t_2) + \cdots + 2f(t_{r-1}) + f(b)].$$

- Error estimate

$$E(f) = \sum_{i=1}^{r} \left(-\frac{f''(\eta_i)}{12} h^3 \right) = -\frac{f''(\eta)}{12}(b-a)h^2.$$

Composite trapezoidal



r=5

i=0,1,...,5

Composite Simpson method

- Composite method (for convenience, pose basic rule on subinterval of length $2h$):

$$\int_{t_{2k-2}}^{t_{2k}} f(x)dx \approx \frac{2h}{6}[f(t_{2k-2}) + 4f(t_{2k-1}) + f(t_{2k})].$$

  Then sum up contributions (using even r), obtaining the famous formula

$$\int_a^b f(x)dx \quad \approx \quad \frac{h}{3}[f(a) + 2\sum_{k=1}^{r/2-1} f(t_{2k}) + 4\sum_{k=1}^{r/2} f(t_{2k-1}) + f(b)].$$

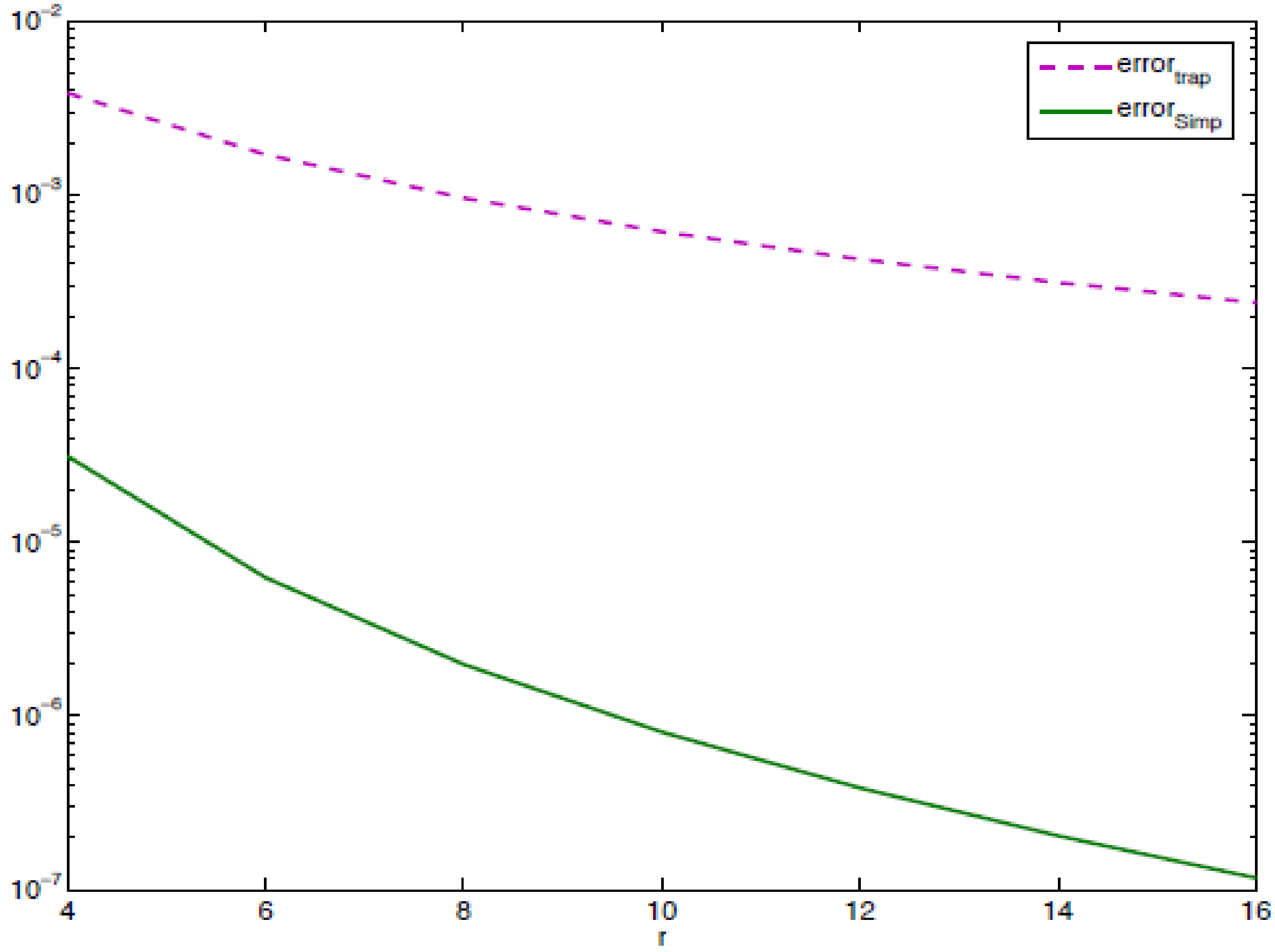
  Error estimate

$$E(f) = -\frac{f''''(\zeta)}{180}(b-a)h^4.$$

Example: errors for trapezoidal and Simpson

Integrate $I = \int_0^1 e^{-x^2} dx$.
Plot errors for $h = 1/r$: evidently the 4th order Simpson is much more accurate.

h=(b-a)/r



Composite trapezoidal, midpoint and Simpson methods

With $rh = b - a$, r a positive integer (must be even in the Simpson case), we have the **formulas**

$$\begin{aligned}
\int_a^b f(x)dx &\approx \frac{h}{2}[f(a) + 2\sum_{i=1}^{r-1} f(a+ih) + f(b)], \quad \text{trapezoidal} \\
&\approx \frac{h}{3}[f(a) + 2\sum_{k=1}^{r/2-1} f(t_{2k}) + 4\sum_{k=1}^{r/2} f(t_{2k-1}) + f(b)], \quad \text{Simpson} \\
&\approx h\sum_{i=1}^{r} f(a + (i-1/2)h), \quad \text{midpoint.}
\end{aligned}$$