Numerical Methods for Integration and Differentiation

- Outline:
  - Motivation
  - Revisiting Taylor series
  - Calculating derivatives numerically
  - Calculating integrals numerically
    - Square and Trapezoid methods
    - Recursive Trapezoid and Romberg Algorithm

Motivation

- Taylor series ... important concept in numerical approximation, used in many algorithms, so need to be familiar with it.
- Same with numerical differentiation, e.g., needed for
  - Optimization algorithms
  - Finding roots of (non-linear) equations
  - Numerical integration of differential equations
- Analytical calculations often result in integrals that cannot be computed analytically
  - Numerical integration schemes

Taylor Series

- Given a smooth function f(x), we can expand it around a point c

$$f(x)=f(c)+f'(c)(x-c)+\frac{1}{2!}f''(c)(x-c)^2+\frac{1}{3!}f'''(x-c)^3+\dots$$

$$=\sum_{k=0}^{\infty}\frac{1}{k!}f^{(k)}(c)(x-c)^k$$

- This is the Taylor series of f at point c. Loosely: “if x is close to c the series converges rapidly and slowly (or not at all) if x is far away from c”
- Convergence:

$$E_{n+1}=f(x)-f_n(x)=\sum_{k=n+1}^{\infty}\frac{f^{(k)}(c)(x-c)^k}{k!}=\frac{f^{(n+1)}(\zeta)(x-c)^{n+1}}{(n+1)!}$$

with ζ some value between x and c

Some familiar examples

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots, \quad |x| < \infty$$

$$\sin(x) = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!} = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots, \quad |x| < \infty$$

$$\cos(x) = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!} = 1 - x - \frac{x^2}{2!} + \frac{x^4}{4!} - \ldots, \quad |x| < \infty$$

$$\frac{1}{1-x} = \sum_{k=0}^{\infty} x^k = 1 + x + x^2 + x^3 + \ldots \quad |x| < 1$$

- Computers calculate many functions like this, e.g.

  $e^x \approx \sum_{k=0}^{N} \frac{x^k}{k!}$ for some large N.

Example

- Calculate e^1 to 6 digit accuracy
- Answer:

$$e = e^1 = 1 + 1 + \frac{1}{2!} + \frac{1}{3!} + \frac{1}{4!} + \frac{1}{5!} + \ldots$$

$$\frac{1}{2!} = 0.5, \frac{1}{3!} = 0.166667, \frac{1}{4!} = 0.041667, \ldots, \frac{1}{9!} = 0.0000027$$

next one gives corrections
<0.000001

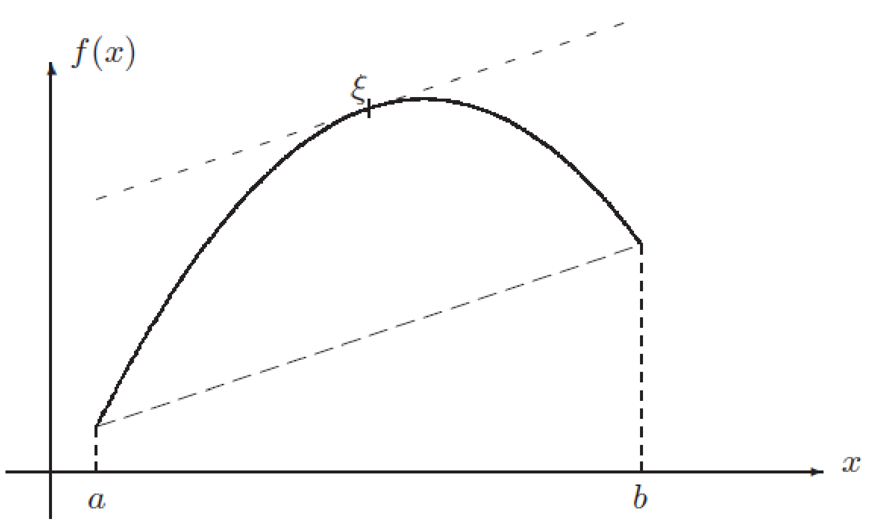
$$\longrightarrow \quad e \approx 1 + 1 + \frac{1}{2!} + \ldots + \frac{1}{9!} = 2.71828$$

Numerical Differentiation

- Want to have a numerical approximation of f'(x), f''(x), etc.
- Reminder: $f'(x)=\lim_{h\to 0}\dfrac{f(x+h)-f(x)}{h}$
- If we set n=0 in Taylor's theorem we have the "Mean-value theorem":

$$f(a)-f(b)=(b-a)f'(\zeta) \longrightarrow f'(\zeta)=\frac{f(b)-f(a)}{b-a}$$

- Can use this to approximate f' if interval (a,b) is small

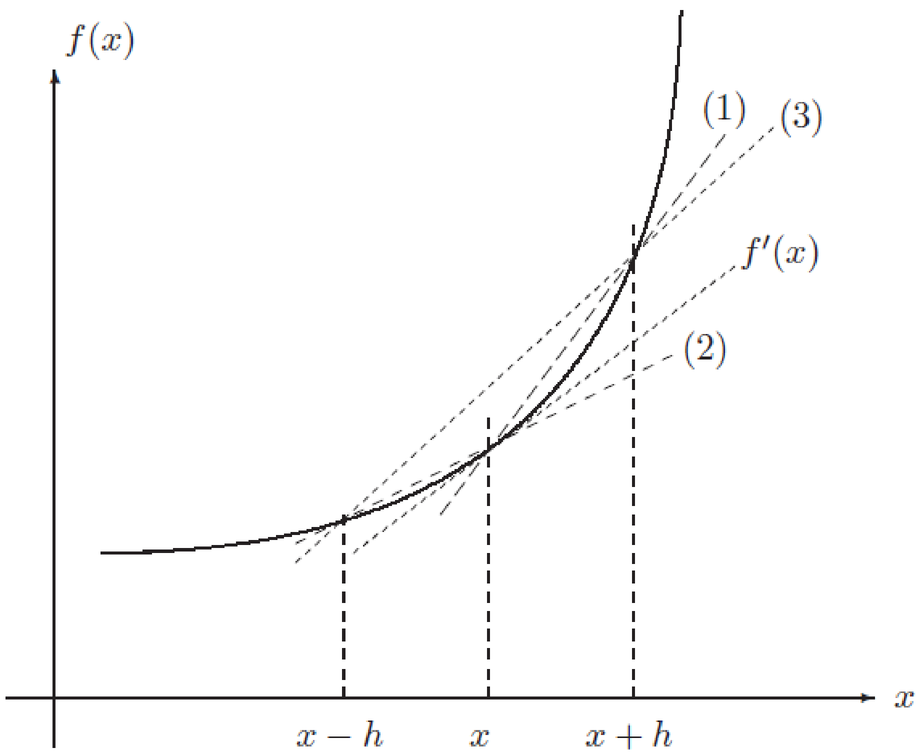


Finite Difference Schemes

$$f'(x) \approx \frac{1}{h}\left(f(x+h) - f(x)\right)$$ → Forward difference (3)

$$f'(x) \approx \frac{1}{h}\left(f(x) - f(x-h)\right)$$ → Backward difference (2)

$$f'(x) \approx \frac{1}{2h}\left(f(x+h) - f(x-h)\right)$$ → Central difference (1)



What about the errors?

- From Taylor:

$$f(x+h)=f(x)+hf'(x)+\frac{1}{2}h^2 f''(x)+\frac{1}{6}h^3 f'''(x)+O(h^4)$$

$$f(x-h)=f(x)-hf'(x)+\frac{1}{2}h^2 f''(x)-\frac{1}{6}h^3 f'''(x)+O(h^4)$$

$$\longrightarrow \frac{1}{h}(f(x+h)-f(x))=f'(x)+\frac{1}{2}hf''(x)+\ldots$$

$$\longrightarrow \frac{1}{h}(f(x)-f(x-h))=f'(x)-\frac{1}{2}hf''(x)+\ldots$$

... both first order in h (error prop. to h)

$$\longrightarrow \frac{1}{2\mathrm{h}}(f(x+h)-f(x-h))=f'(x)+\frac{1}{6}h^2 f'''(x)+\ldots$$

... second order in h (i.e. more accurate)

How to calculate f''?

- Could just calculate the derivative of the first derivative ...
- Better:

$$f(x+h)=f(x)+hf'(x)+\frac{1}{2}h^2 f''(x)+\frac{1}{6}h^3 f'''(x)+\frac{1}{24}h^4 f^{(4)}(x)+\dots$$

$$f(x-h)=f(x)-hf'(x)+\frac{1}{2}h^2 f''(x)-\frac{1}{6}h^3 f'''(x)+\frac{1}{24}h^4 f^{(4)}(x)+\dots$$

$$\longrightarrow \quad f''(x)+\frac{1}{12}h^2 f^{(4)}=\frac{1}{h^2}\left(f(x+h)-2\mathrm{f}(x)+f(x-h)\right)$$

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

... second order in h

Determining Truncation Errors

- Why bother? We have fast computers and can use small values of h, so no problem?
  - Problems with number representations in computers (more later)
  - Often these approximations are iterated in numerical schemes, so errors accumulate fast
- Truncation error calculations might be quite confusing, but idea is simple:
  - Compare finite difference approximation to full Taylor approximation, difference between both gives error terms and order of the method.

Multivariate Taylor

- A few times later in the module we will have to deal with expansions of scalar functions of multiple variables f(x,y,z,...)
- To write this in nice form, introduce multi-indices $\alpha \in N^n, \alpha = (\alpha_{1,.}.., \alpha_n), |\alpha| = \sum_{j=1}^{n} \alpha_j$

$$\alpha! = \alpha_1! \cdot \alpha_2! \cdot \ldots \cdot \alpha_n! \qquad \vec{x}^{\alpha} = x_1^{\alpha_1} \cdot x_2^{\alpha_2} \cdot \ldots \cdot x_n^{\alpha_n}$$

$$D^{\alpha} f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \ldots \partial x_n^{\alpha_n}}$$

- Then:

$$f(\vec{x} + \vec{h}) = \lim_{k \to \infty} \sum_{|\alpha| \leq k} \frac{1}{|\alpha|!} D^{\alpha} f(\vec{x}) \vec{h}^{\alpha}$$

Example

- Taylor

$$f(\vec{x}+\vec{h}) = \lim_{k\to\infty} \sum_{|\alpha|\le k} \frac{1}{|\alpha|!} D^{\alpha} f(\vec{x})\, \vec{h}^{\alpha}$$

- Expand f(x,y) up to second order

$$f(x+h_1, y+h_2) \approx f(x,y) + \partial_x f\, h_1 + \partial_y f\, h_2 + \frac{1}{2!}\partial_x^2 f\, h_1^2 + \partial_x \partial_y h_1 h_2 + \frac{1}{2!}\partial_y^2 h_2^2$$

$\alpha=0$ $\alpha=1$ $\alpha=2$

- Later in the module mostly the linear term will matter ...

Numerical Integration

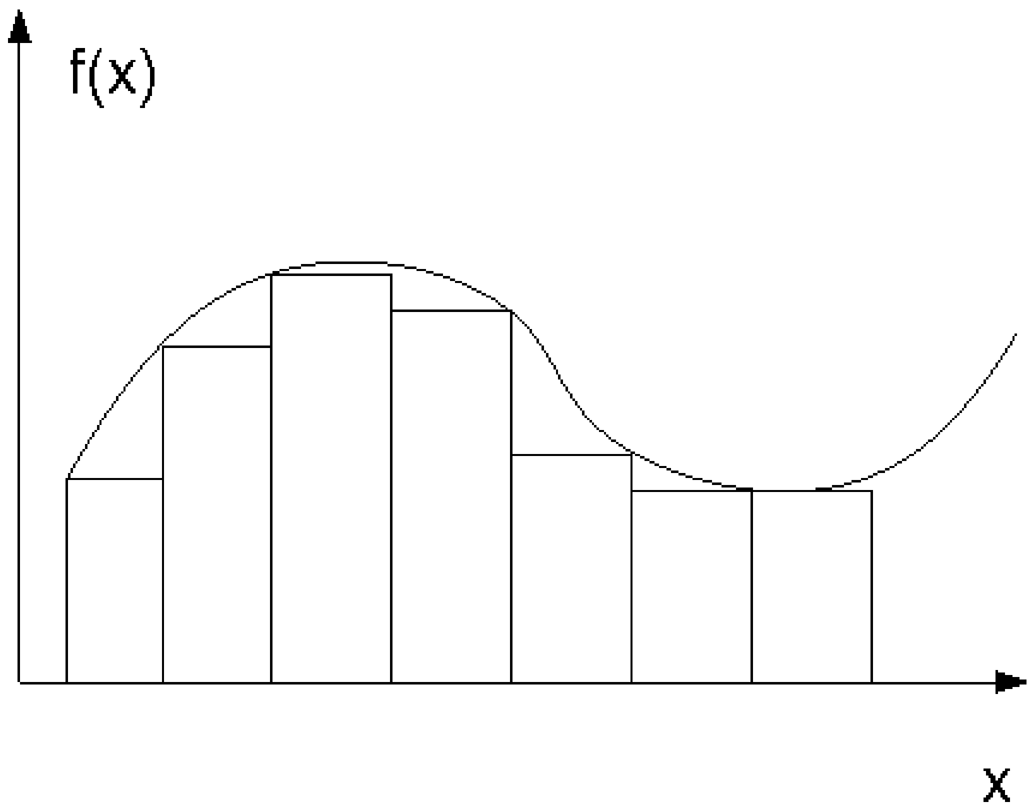
- Given f(x) in the interval [a,b] we want to find an approximation for

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

- Main strategy:
  - Cut [a,b] into smaller sub-intervals
  - In each interval i, approximate f(x) by a polynomial p^i
  - Integrate the polynomials analytically and sum up their contributions

First Idea

- Approximate f by a constant for each sub-interval -> $p_i(x) = f(x_i) = f_i$



First Idea

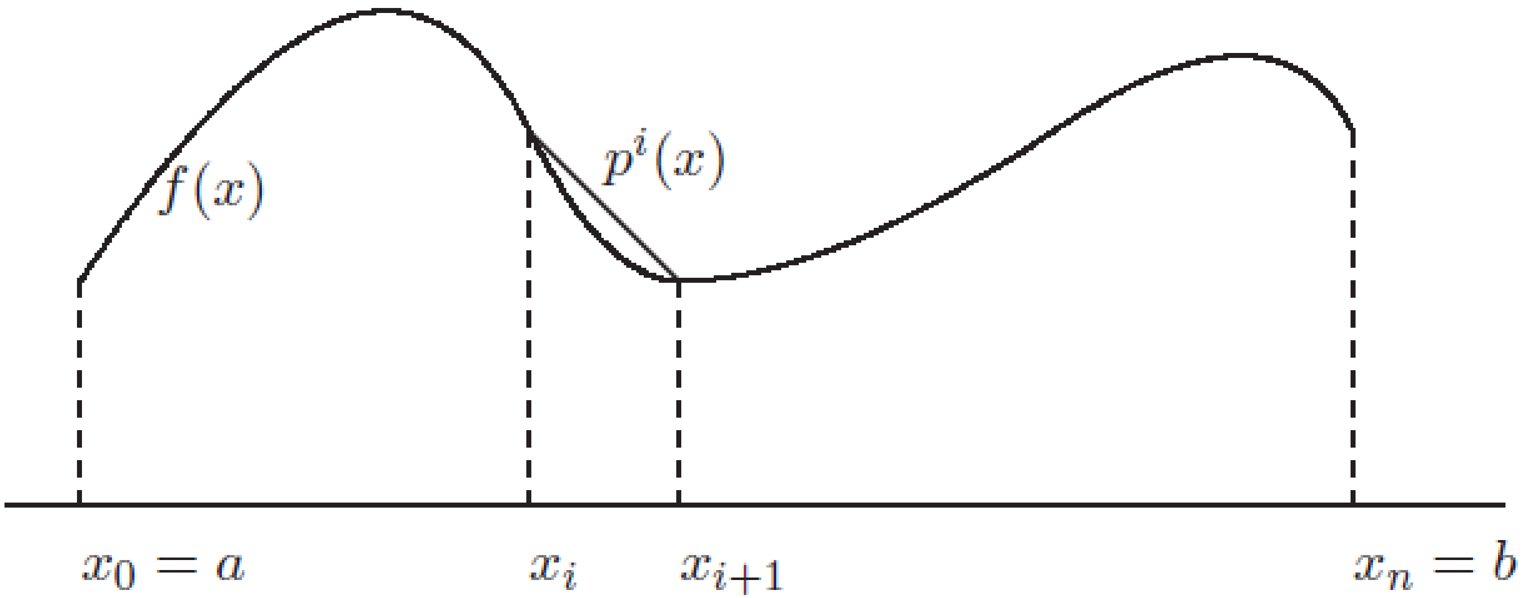
- Each interval $\int_{x_i}^{x_{i+1}} p_i(x)\,dx = \int_{x_i}^{x_{i+1}} f_i\,dx = f_i(x_{i+1} - x_i)$
- Adding and using equidistant intervals

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} f_i(x_{i+1} - x_i)$$

$$h = \frac{b-a}{n}, x_i = x_0 + (i-1)h \longrightarrow \int_a^b f(x)\,dx \approx h \sum_{i=0}^{n-1} f_i$$

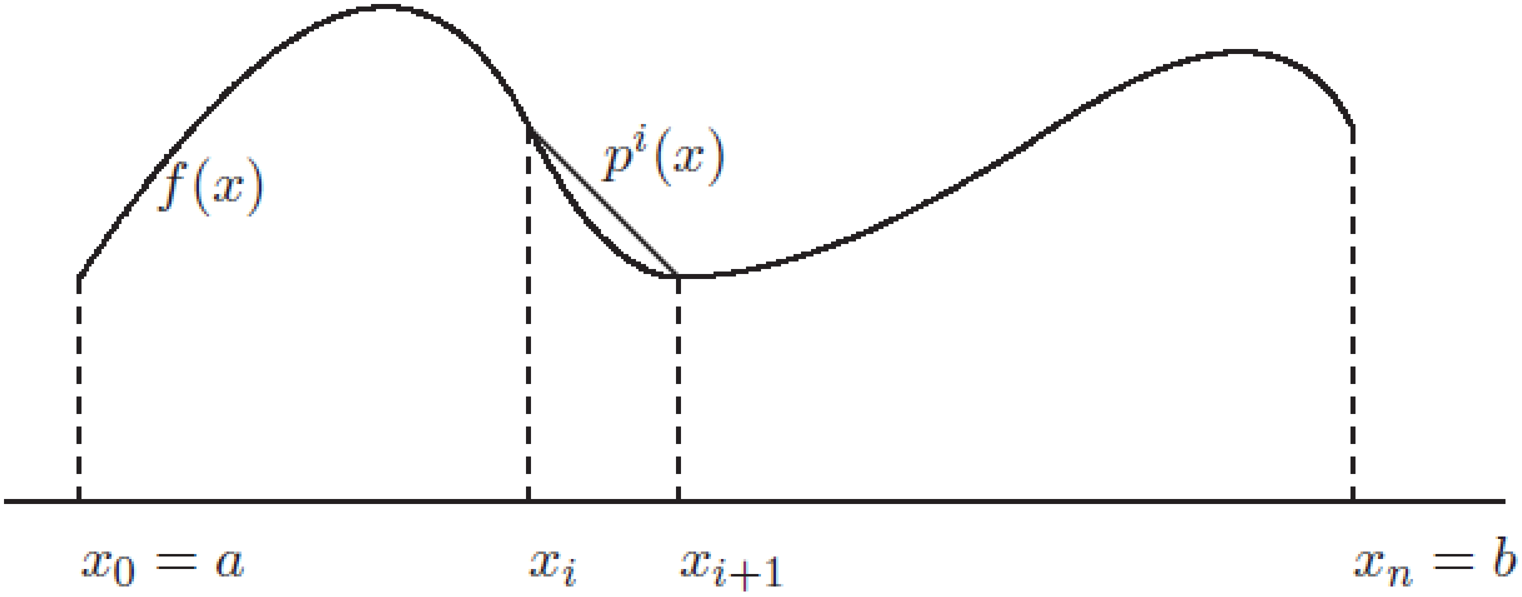
- Error (roughly):
  - Approximation error per for f is ~ h
  - After integration ~ h^2
  - Summing up order 1/h intervals: E~h
  - Maybe we can do better without much more computational effort?

Trapezoid Rule



- On interval $[x_i,x_{i+1}]$ interpolate f(x) by a linear polynomial that connects end points: $f(x_i)=p_i(x_i)$, $f(x_{i+1})=p_i(x_{i+1})$

$$\longrightarrow \quad p_i(x)=f(x_i)+(x-x_i)\frac{f(x_{i+1})-f(x_i)}{x_{i+1}-x_i}$$



- Can now integrate the p(x)'s

$$\int_{x_i}^{x_{i+1}} p_i(x)\,dx = \left[f(x_i)\,x - x_i\,x\,\frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} + x^2/2\,\frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \right]_{x_i}^{x_{i+1}}$$

$$\ldots$$

$$= \frac{1}{2}\left(f(x_{i+1}) + f(x_i)\right)\left(x_{i+1} - x_i\right)$$

which is just the area of the trapezium ...

Trapezoid (3)

- Adding up all intervals

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} \frac{1}{2}\left(f(x_{i+1}) + f(x_i)\right)\left(x_{i+1} - x_i\right)$$

- Using equidistant intervals

$$h = \frac{b-a}{n},\ x_i = x_0 + (i-1)h$$

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} \frac{h}{2}\left(f(x_{i+1}) + f(x_i)\right)$$

$$\int_a^b f(x)\,dx \approx h\left[\frac{1}{2} f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2} f(x_n)\right] := T(f;h)$$

Error Estimate

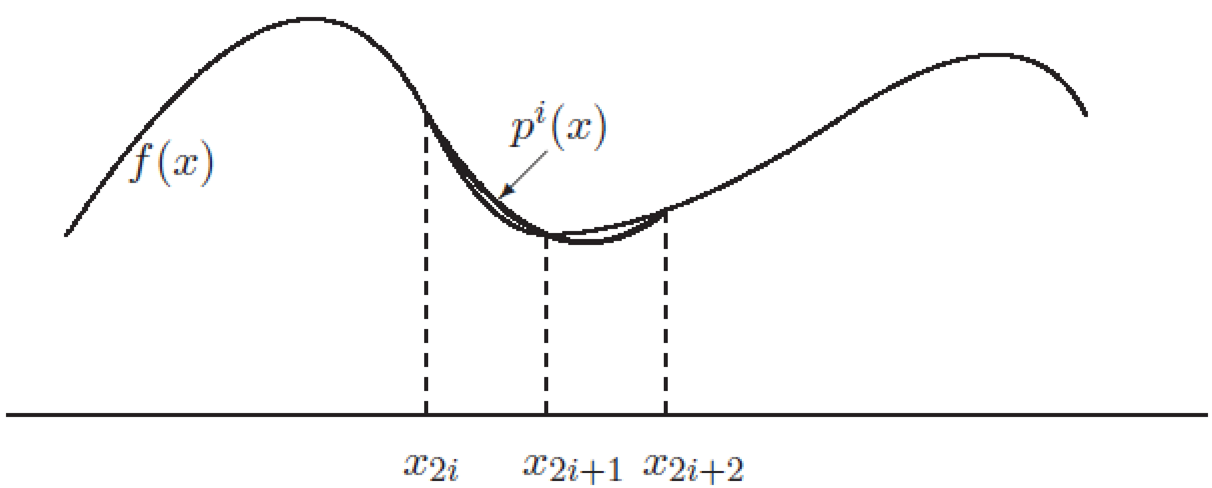
- Only approximate functions over the intervals, hence there is an systematic truncation error

$$E(f;h)=I(f)-T(f;h)=\sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}}[f(x)-p^i(x)]$$
$$=\sum_{i=0}^{n-1}E_i(f;h)$$

- Error from linear approximation of f per interval $\propto h^2$
- Integration -> $E_i \propto h^3$
- Summing up order of 1/h E's -> $E \propto h^2$

Simpson's Rule

- So far, approximated f by
  - A constant -> E~h
  - A linear function -> E~h^2
  - Maybe try a quadratic function -> Simpson's rule



Simpson's Rule (2)

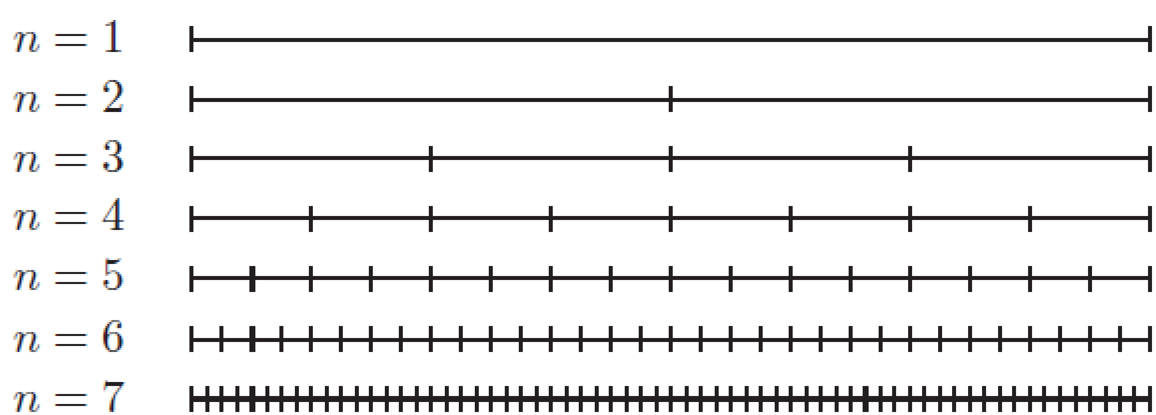
- Won't go into any technical details about this, but for equidistant intervals one has

$$I \approx S(f;h) = \frac{h}{3} \sum_{i=0}^{n-1} \left[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2}) \right]$$

- One can show that Simpson's rule is 4th order, i.e. $E \propto h^4$

Recursive Trapezoid

- A way to control truncation error without unnecessary computations
- Divide [a,b] into 2^n sub-intervals and evaluate Trapezoid rule for $h_n = 2^{-n}(b-a)$ and $h_{n+1} = h_n/2$



- Apply Trapezoid rule

Recursive Trapezoid (2)

- For h_n: $T(f;h_n)=h_n\left[\frac{f(a)+f(b)}{2}+\sum_{i=1}^{2^n-1} f(a+ih_n)\right]$
- For h_{n+1}: $T(f;h_{n+1})=h_{n+1}\left[\frac{f(a)+f(b)}{2}+\sum_{i=1}^{2^{n+1}-1} f(a+ih_{n+1})\right]$
- One can show ...

$$T(f;h_{n+1})=\frac{1}{2}T(f;h_n)+h_{n+1}\sum_{j=0}^{2^n-1} f(a+(2j+1)h_{n+1})$$

- Advantages
  - Keep computation at level n. If not accurate enough -> add another level
  - Don't need to re-evaluate at points we have already evaluated before

Romberg Method

- Idea:
  - Say we have calculated T(f;h), T(f;h/2), T(f;h/4), ...
  - Combine these numbers to get better approximation?
- One can show that

$$E(f;h) = I(f) - T(f;h) = a_2 h^2 + a_4 h^4 + a_6 h^6 + \dots \quad (1)$$

only depends on even powers of h

$$\rightarrow E(f;h/2) = I(f) - T(f;h/2) = a_2 (h/2)^2 + a_4 (h/2)^4 + a_6 (h/2)^6 + \dots$$

(2)

Romberg (2)

- Re-arranging for I yields:

$$I(f)=T(f;h)+a_2h^2+a_4h^4+a_6h^6+\ldots \qquad (1')$$

$$I(f)=T(f;h/2)+a_2(h/2)^2+a_4(h/2)^4+a_6(h/2)^6+\ldots \qquad (2')$$

- Multiplying (2') by 4 and subtracting (1'):

$$3I(f)=4T(f;h/2)-T(f;h)+a'_4h^4+\ldots$$

$$I(f)=\underbrace{4/3T(f;h/2)-T(f;h)}_{U(h)}+a''_4h^4+\ldots$$

- U(h) is fourth order accuracy!
- This is called **Richardson extrapolation**

Romberg (3)

- Obviously, we can continue with this idea:

$$I(f) = U(h) + a''_4 h^4 + a''_6 h^6 + \ldots \qquad (3)$$

$$I(f) = U(h/2) + a''_4 (h/2)^4 + a''_6 (h/2)^6 + \ldots \qquad (4)$$

- To cancel the fourth order term we multiply (4) by 2^4 and subtract (3)

$$V(h) = \frac{2^4 U(h/2) - U(h)}{2^4 - 1} = U(h/2) + \frac{U(h/2) - U(h)}{2^4 - 1}$$

and $I(f) = V(h) + a'''_6 h^6 + \ldots$

- And so on ... yields the Romberg Algorithm

Romberg Algorithm

- Set H=b-a and define

$$R(0,0)=T(f;H)$$

$$R(1,0)=T(f;H/2)$$

$$\ldots$$

$$R(1,0)=T(f;H/2^n)$$

(e.g. calculated by recursive Trapezoid)

- Then:

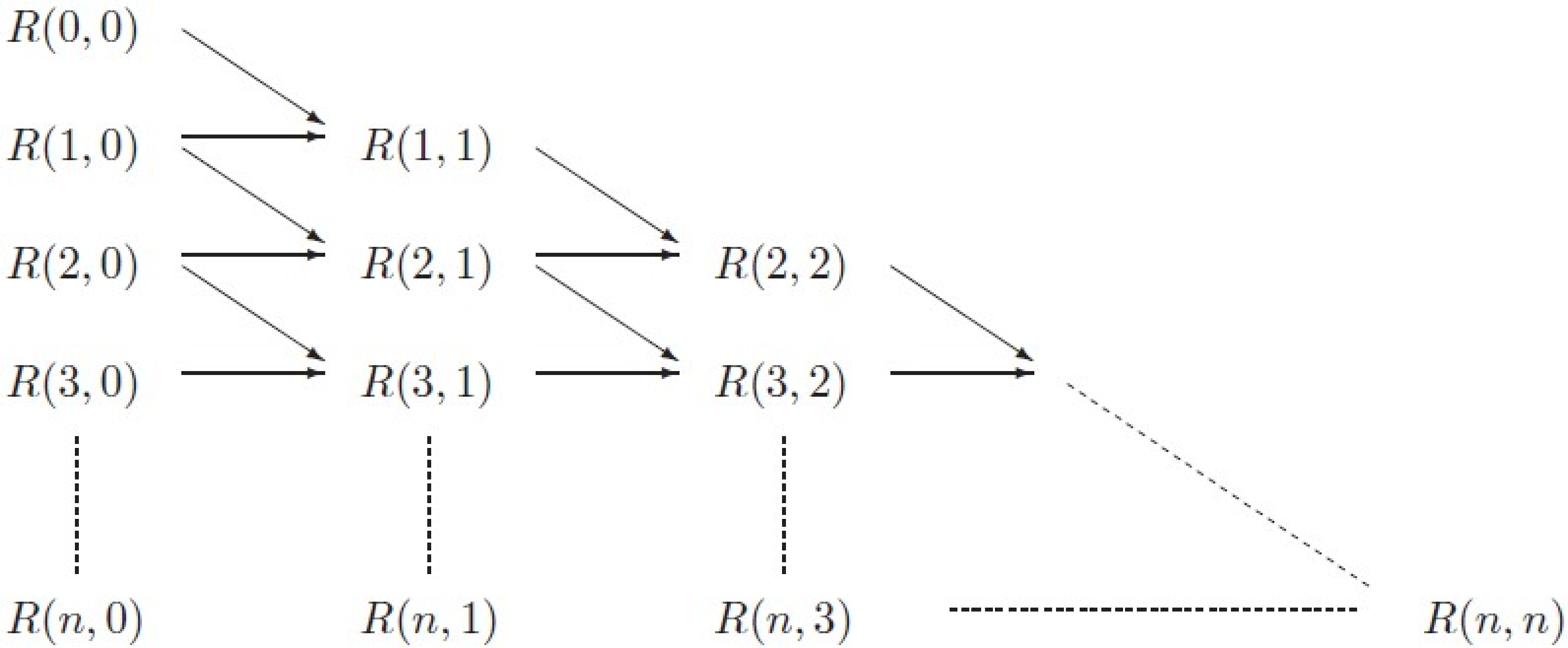
$$R(n,m)=R(n,m-1)+\frac{R(n,m-1)-R(n-1,m-1)}{2^{2\mathrm{m}}-1}$$

- and

$$I(f)=R(m,m)+O(h^{2(m+1)})$$

Romberg Triangle

- Recursive calculation of the R(n,m)'s ...



More Ideas ...

- “Mesh” should be finer when f changes a lot
  - -> adaptive methods
- Gaussian quadrature:
  - All methods somehow approximate integrals via
    $$\int_a^b f(x)\,dx \approx A_0 f(x_0) + A_1 f(x_1) + \ldots + A_n f(x_n)$$
  - Squares $x_0 = a,\ A_0 = 1$
  - Trapezoid $x_0 = a,\ x_1 = b,\ A_0 = A_1 = 1$
  - Could also optimize the xi and Ai to improve precision
  - Gaussian quadrature does this tuning these parametes to get integrals for polynomials of order m right

Summary

- What is important to remember:
  - Taylor series and how to use them to estimate truncation errors
  - The idea of numerical differentiation
  - The idea of basic schemes for numerical integration, say Trapezoid
  - More advanced stuff is nice to remember but can be looked up when needed