Assume:  $\log = \ln$ , 4 d.p.

## Taylor Polynomial

The **Taylor polynomial** of degree n of f, centred at  $x_0$  is defined by

$$P_{n}\left(x\right)=\sum_{k=0}^{n}\frac{f^{\left(k\right)}\left(x_{0}\right)}{k!}\left(x-x_{0}\right)^{k}.$$

Error (Approximating x with  $\tilde{x}$ )

absolute error = 
$$|\tilde{x} - x|$$
  
relative error =  $\frac{|\tilde{x} - x|}{|x|}$ .

## Floating Point Number Systems

 $\mathbb{F}(\beta, k, m, M)$  is a finite subset of the real number system. For  $f \in \mathbb{F}$ :

$$f=\pm \left(d_1 \;.\; d_2 d_3 \ldots d_k\right)_{\beta} \times \beta^e$$

- $\beta \in \mathbb{N}$ : the base
- $d_1.d_2d_3...d_k$ : the significand
- $k \in \mathbb{N}$ : #digits in the significand
- $e \in \mathbb{Z}$ : the exponent,  $m \leq e \leq M$

 $d_i$  are base- $\beta$  digits with  $d_1 \neq 0$  unless f = 0. For  $x \in \mathbb{R}$  and f > 0:

$$f_{\min} = \min_{f \in \mathbb{F}} |f| = \beta^m$$

$$f_{\min} = \max_{f \in \mathbb{F}} |f| = (1 - \beta^{-1})$$

 $f_{\max} = \max_{f = \mathbb{T}} |f| = \left(1 - \beta^{-k}\right) \beta^{M+1}.$ **Underflow**:  $x < f_{\min}$  (replaced by 0). Overflow:  $x > f_{\text{max}}$  (replaced by  $\infty$ ).

For 
$$\mathbb{F}^+ = \{ f \in \mathbb{F} : f > 0 \}$$
:

$$|\mathbb{F}^+| = \left(M-m+1\right)\left(\beta-1\right)\beta^{k-1}.$$
 Representing Real Numbers

If  $x \notin \mathbb{F}$ , x is rounded to the nearest Modified Euler Method representable number with  $fl: \mathbb{R} \to \mathbb{F}$ . To determine fl(x):

- 1. Express x in base- $\beta$ .
- 2. Express x in scientific form.
- 3. Verify that  $m \leq e \leq M$ :
  - if e > M, then  $x = \infty$ .
  - if e < m, then x = 0.
  - else, round to k digits.

$$\frac{\left|fl\left(x\right) - x\right|}{\left|x\right|} \le u = \frac{1}{2}\beta^{1-k}.$$

where u is the **unit roundoff** of  $\mathbb{F}$ . Catastrophic Cancellation

The error when subtracting similar floating point numbers, where at least one is not exactly representable.

### **Taylor Polynomials**

The *n*th degree **Taylor polynomial** of f approximates f for x near  $x_0$ :

$$P_{n}\left(x\right)=\sum_{k=0}^{n}\frac{f^{\left(k\right)}\left(x_{0}\right)}{k!}\left(x-x_{0}\right)^{k}.$$

If f is n+1 times differentiable on [a,b]containing  $x_0$ , then for all  $x \in [a, b]$ , there exists a value  $x_0 < c < x$  such that

$$f\left(x\right) = P_n\left(x\right) + R_n\left(x\right)$$

where

$$R_n(x) = \frac{f^{(n+1)}(c)}{(n+1)!} (x - x_0)^{n+1}$$

is the **remainder (error) term** for  $P_n$ . For distinct increasing  $x_i$  on [a,b] there The maximum value of  $|R_n(x)|$  on [a,b] exists  $c \in [a,b]$  such that bounds the maximum absolute error of the approximation:

$$|f\left(x\right)-P_{n}\left(x\right)|=|R_{n}\left(x\right)|.$$

# **Ordinary Differential Equations**

 $\frac{\mathrm{d}y}{\mathrm{d}t} = f\left(t,\;y\right) \text{ with } y\left(a\right) = \alpha \text{ on } a \leq t \leq b.$  Divide [a,b] into n subintervals of width h = (b-a)/n. Let  $t_i = a + ih$  for i = $0, 1, \dots, n$ . Then  $y_i = y(t_i)$  approximates y at  $t = t_i$ , with  $y_0 = \alpha$ .

## Euler's Method (First Order Taylor)

$$\begin{split} y(t) &= P_1(t) + R_1(t) \\ y(t) &= y(t_i) + y'(t_i)(t-t_i) + \mathcal{O}(t^2) \\ y(t_{i+n}) &= y(t_i) + y'(t_i)(t_{i+n} - t_i) + \mathcal{O}(t^2) \\ y(t_{i+n} - t_i + t_i) &= y(t_i) + y'(t_i)(t_{i+n} - t_i) + \mathcal{O}(t^2) \\ y(t_i + h) &= y(t_i) + hy'(t_i) + \mathcal{O}(h^2) \,. \end{split}$$

where the error is proportional to  $h^2$ .

$$y_{i+1} = y_i + hf(t_i, y_i).$$

### Local and Global Error

Assuming the solution was correct at the previous step:

**Local**: error after 1 step —  $\mathcal{O}(h^{p+1})$ . **Global**: error after i steps —  $\mathcal{O}(h^p)$ . The **order** of a method is its global error.

## Second Order Taylor Method

$$y_{i+1} = y_i + h f\left(t_i, \; y_i\right) + \frac{h^2}{2} f'\left(t_i, \; y_i\right).$$

To avoid computing  $f'\left(t,\,y\right)$  use,

$$\begin{split} \frac{f\left(t_{i+1},\,y_{i+1}\right) - f\left(t_{i},\,y_{i}\right)}{h} + \mathcal{O}\left(h\right). \\ y_{i+1} &= y_{i} + \frac{1}{2}\left(k_{1} + k_{2}\right) \\ k_{1} &= hf\left(t_{i},\,y_{i}\right) \\ k_{2} &= hf\left(t_{i} + h,\,y_{i} + k_{1}\right) \end{split}$$

# Runge-Kutta Method (Fourth Order)

$$\begin{split} y_{i+1} &= y_i + \frac{1}{6} \left( k_1 + 2k_2 + 2k_3 + k_4 \right) \\ k_1 &= hf \left( t_i, \ y_i \right) \\ k_2 &= hf \left( t_i + \frac{h}{2}, \ y_i + \frac{k_1}{2} \right) \\ k_3 &= hf \left( t_i + \frac{h}{2}, \ y_i + \frac{k_2}{2} \right) \\ k_4 &= hf \left( t_i + h, \ y_i + k_3 \right) \\ i &= 0, \ 1, \ \dots, \ n-1 \ \text{for all four methods.} \end{split}$$

## Interpolation

$$P_n(x) = a_0 + a_1 x + \dots + a_n x^n.$$

### Lagrange Form

Solve for  $a_i$  then factor  $P_n(x_i)$  for  $y_i$ :

$$P_{n}\left(x\right)=\sum_{i=0}^{n}L_{n,\,i}\left(x\right)y_{i}$$

$$f\left(x\right)=P_{n}\left(x\right)+\frac{f^{\left(n+1\right)}\left(c\right)}{\left(n+1\right)!}\prod_{i=0}^{n}\left(x-x_{i}\right).$$

## Newton's Divided Difference Form

$$\begin{split} P_n\left(x\right) &= a_0 + a_1\left(x - x_0\right) \\ &+ a_2\left(x - x_0\right)\left(x - x_1\right) + \cdots \\ &+ a_n\left(x - x_0\right)\cdots\left(x - x_{n-1}\right) \\ &= \sum_{k=0}^n f\left[x_0, \, x_1, \, \dots, \, x_k\right] \prod_{i=0}^{k-1}\left(x - x_i\right) \\ \text{Solve } P_n\left(x_i\right) &= y_i \text{ for } a_0, \, a_1, \, \dots, \, a_n \text{:} \\ a_0 &= y_0, \quad a_1 &= \frac{y_1 - y_0}{x_1 - x_0} \\ a_2 &= \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{x_2 - x_0} \end{split}$$

## Divided Differences (Simplify $a_i$ )

$$y_{i+1} = y_i + hf\left(t_i, \ y_i\right). \qquad \qquad f\left[x_i\right] = y_i \quad \text{(Zeroth divided difference)}$$
 assuming the solution was correct at the previous step: 
$$\begin{aligned} f\left[x_i, \ x_{i+1}, \ \dots, \ x_{i+k}\right] &= \\ f\left[x_i, \ x_{i+1}, \ \dots, \ x_{i+k}\right] &= \\ f\left[x_{i+1}, \ \dots, \ x_{i+k}\right] - f\left[x_i, \ \dots, \ x_{i+k-1}\right] \\ \hline x_{i+k} - x_i \\ \hline x_{i+k}$$

## Newton's Forward Difference Form

Equally spaced abscissas:  $h = x_{i+1} - x_i$ . Forward Difference Operator

$$\begin{split} \overline{\Delta y_i &= y_{i+1} - y_i, \quad \Delta^{k+1} y_i = \Delta \left( \Delta^k y_i \right)} \\ \Delta^2 y_i &= y_{i+2} - 2 y_{i+1} + y_i \\ \Delta^3 y_i &= y_{i+3} - 3 y_{i+2} + 3 y_{i+1} - y_i \\ f\left[ x_0, \, x_1, \, \dots, \, x_k \right] &= \frac{\Delta^k y_0}{k! b^k} \end{split}$$

Substitute  $x=x_0+sh$   $(x_i=x_0+ih),$  with  $s=\frac{x-x_0}{h}$  into the divided difference

$$P_{n}\left(x\right)=\sum_{k=0}^{n}\frac{\Delta^{k}y_{0}}{k!}\prod_{i=0}^{k-1}\left(s-i\right)$$

## Difference Tables

$$\begin{array}{ccc} x_i & y_i \\ \div & f[x_i] & f[x_i, x_i+1] & f[x_i, x_{i+1}, x_{i+2}] \\ \Delta & y_i & \Delta y_i & \Delta^2 y_i \end{array}$$

# Root Finding (f(x) = 0)

## Intermediate Value Theorem

For continuous f on [a,b] with  $f(a) \leq$  $k \leq f(b), \exists c_1 \in [a,b] : f(c_1) = k.$ If f(a) f(b) < 0 (f(a) and f(b) haveopposite signs),  $\exists c_2 \in [a, b] : f(c_2) = 0$ .

## **Bisection Method**

- 1. Find [a, b] such that f(a) f(b) < 0.
- 2. For  $p = \frac{a+b}{2}$ , evaluate f(p).
  - If f(p) = 0, then p is a root of f.
  - If f(a) f(p) < 0, then p becomes the new b and the root lies in [a, p].
  - If f(p) f(b) < 0, then p becomes

## 3. Go to step 2.

### **Fixed-Point Iteration**

Rewrite f(x) = 0 as x = q(x). Solve by finding a fixed-point p s.t. q(p) = p.

$$x_{n+1}=g\left( x_{n}\right) \quad \left( n\geq 0\right) .$$

Find the root of the tangent line at each Approximate  $f'(x_n)$  with the secant iterate  $x_n$  using the first degree Taylor between  $x_{n-1}$  and  $x_n$ : polynomial and solving for x:

$$f(x) \approx f(x_n) + f'(x_n) (x - x_n) \stackrel{\text{set}}{=} 0$$

$$x=x_{n+1}=x_{n}-\frac{f\left(x_{n}\right)}{f'\left(x\right)}\quad\left(n\geq0\right)$$

polynomial and solving for 
$$x$$
: 
$$f\left(x\right) \approx f\left(x_{n}\right) + f'\left(x_{n}\right)\left(x - x_{n}\right) \stackrel{\text{set}}{=} 0$$
 
$$f\left(x_{n}\right) = 0$$
 with two initial values for  $n \geq 1$ .

A convergent  $\{x_n\}$  satisfies (for large n)  $|x_{n+1} - p| \approx \lambda |x_n - p|^r$ 

# Fixed-point iteration (r = 1)

 $\overline{p}$  is a fixed-point and  $0 < \lambda < 1$ .

# Newton's method (r=2)

p is a root and  $\lambda > 0$ .

Secant method  $(r = \frac{1+\sqrt{5}}{2} \approx 1.618)$ 

 $\overline{p}$  is a root and  $\lambda > 0$ .

### Numerical Differentiation

Forward  $(h = x - x_0, c \in [x_0, x_0 + h])$ 

$$f'\left(x_{0}\right)=\frac{f\left(x_{0}+h\right)-f\left(x_{0}\right)}{h}-\frac{h}{2}f''\left(c\right)$$

Backward  $(-h = x - x_0, c \in [x_0 - h, x_0])$ 

$$f'\left(x_{0}\right)=\frac{f\left(x_{0}\right)-f\left(x_{0}-h\right)}{h}+\frac{h}{2}f''\left(c\right)$$

## Central Difference (Second Order)

Derive using 
$$\begin{split} f\left(x_{0}+h\right)-f\left(x_{0}-h\right) &:\\ f'\left(x_{0}\right)=\frac{f\left(x_{0}+h\right)-f\left(x_{0}-h\right)}{2h}\\ &-\frac{h^{2}}{a}f^{(3)}\left(c\right) \end{split}$$

Derive using  $f(x_0 + h) + f(x_0 - h)$ :

$$\begin{split} f''\left(x_{0}\right) &= -\frac{h^{2}}{12}f^{(4)}\left(c\right) \\ &+ \frac{f\left(x_{0}+h\right) - 2f\left(x_{0}\right) + f\left(x_{0}-h\right)}{h^{2}} \end{split}$$

 $+\frac{f\left(x_{0}+h\right)-2f\left(x_{0}\right)+f\left(x_{0}-h\right)}{h^{2}}$   $f^{(4)}\left(c\right)=\frac{f^{(4)}\left(c_{1}\right)+f^{(4)}\left(c_{2}\right)}{2}\text{ and }c\in\left[c_{1},c_{2}\right],$ with  $c_1 \in [x_0 - h, x_0]$  and  $c_2 \in [x_0, x_0 + h]$ .

## Brouwer's Fixed-Point Theorem

For g continuous on [a,b], and LU Decomposition (A = LU  $\Longrightarrow$  Lz = b, Ux = z) differentiable (a,b),with  $g(x) \in [a,b] : \forall x \in [a,b], \text{ let a}$ positive constant k < 1 exist such that LU = $|g'(x)| \leq k \ \forall x \in (a,b)$ . Then, g has a unique fixed-point p in [a,b], and  $x_{n+1} = g(x_n)$  will converge to p for all  $x_0$  in [a,b].

## Convergence of Rootfinding Methods Numerical Integration (Quadrature)

$$I = \int_{a}^{b} f\left(x\right) \mathrm{d}x \approx \sum_{i=0}^{n} w_{i} f\left(x_{i}\right)$$

for weights  $w_i$  and abscissas  $x_i$ .

Divide [a,b] into n subintervals of width h=(b-a)/n. Let  $x_i=a+ih$  for i = 0, 1, ..., n, so that  $x_0 = a$  and  $x_n = b$ .

## Trapezoidal Rule (Second Order)

Approximate f(x) over each subinterval  $[x_{i-1}, x_i]$  with a degree 1 interpolant:

$$P_{1,\,i}\left(x\right) = y_{i-1} + s\Delta y_{i-1} = y_{i-1} + s\left(y_i - y_{i-1}\right)$$

and integrate w.r.t. s:  $x = x_{i-1} + sh$ , dx = h ds, with limits  $s \in [0, 1]$ :

$$\int_{x_{i-1}}^{x_i} f\left(x\right) \mathrm{d}x \approx \int_0^1 P_{1,\,i}\left(x\right) h \, \mathrm{d}s = \frac{h}{2} \left(y_{i-1} + y_i\right) \quad \left(i = 1, 2, \ldots, n\right).$$

$$\begin{split} I &= \sum_{i=1}^{n} \int_{x_{i-1}}^{x_{i}} f\left(x\right) \mathrm{d}x \approx \sum_{i=1}^{n} \frac{h}{2} \left[ f\left(x_{i-1}\right) + f\left(x_{i}\right) \right] \\ &= \frac{h}{2} \left[ f\left(x_{0}\right) + 2 \sum_{i=1}^{n-1} f\left(x_{i}\right) + f\left(x_{n}\right) \right] - \frac{\left(b-a\right)h^{2}}{12} f''\left(c\right) \end{split}$$

## Simpson's Rule (Fourth Order

Approximate  $f\left(x\right)$  over each subinterval  $\left[x_{2i-2},x_{2i}\right]$  with a degree 2 interpolant:

$$P_{2,i}\left(x\right) = y_{2i-2} + s\Delta y_{2i-2} + \frac{s\left(s-1\right)}{2}\Delta^{2}y_{2i-2}$$

$$f^{(3)}\left(c\right) = \frac{f^{(3)}(c_{1}) + f^{(3)}(c_{2})}{2} \text{ and } c \in [c_{1}, c_{2}], \qquad = y_{2i-2} + s\left(y_{2i} - y_{2i-1}\right) + \frac{s\left(s-1\right)}{2}\left(y_{2i} - 2y_{2i-1} + y_{2i-2}\right)$$
with  $c_{1} \in [x_{0} - h, x_{0}] \text{ and } c_{2} \in [x_{0}, x_{0} + h]. \text{ and integrate w.r.t. } s: \ x = x_{2i-2} + sh, \ dx = h \ ds, \ \text{with limits } s \in [0, 2]:$ 
Second Derivative (Third Order)
$$\int_{x_{2i}}^{x_{2i}} f(x) dx \approx \int_{x_{2i}}^{2} P_{2i}(x) h \ ds = \frac{h}{2}\left(y_{2i} + 4y_{2i-1} + y_{2i-2}\right) \left(y_{2i} - 2y_{2i-1} + y_{2i-2}\right)$$

$$\int_{x_{2i-2}}^{x_{2i}} f\left(x\right) \mathrm{d}x \approx \int_{0}^{2} P_{2,\,i}\left(x\right) h \, \mathrm{d}s = \frac{h}{3} \left(y_{2i-2} + 4y_{2i-1} + y_{2i}\right) \quad \left(i = 1, 2, \ldots, n/2\right).$$

$$\begin{split} I &= \sum_{i=2}^{n/2} \int_{x_{2i-2}}^{x_{2i}} f\left(x\right) \mathrm{d}x \approx \sum_{i=2}^{n/2} \frac{h}{3} \left[ f\left(x_{2i-2}\right) + 4f\left(x_{2i-1}\right) + f\left(x_{2i}\right) \right] \\ &= \frac{h}{3} \left[ f\left(x_{0}\right) + 4\sum_{i=1}^{n/2} f\left(x_{2i-1}\right) + 2\sum_{i=1}^{n/2-1} f\left(x_{2i}\right) + f\left(x_{n}\right) \right] - \frac{(b-a)\,h^4}{180} f^{(4)}\left(c\right) \end{split}$$

Linear Systems (Ax = b)

$$\begin{split} \mathbf{LU} &= \begin{bmatrix} 1 & 0 & 0 \\ \frac{a_{21}}{u_{11}} & 1 & 0 \\ \frac{a_{31}}{u_{11}} & \frac{a_{32} - \ell_{31} u_{12}}{u_{22}} & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} - \ell_{21} u_{12} & a_{23} - \ell_{21} u_{13} \\ 0 & 0 & a_{33} - \ell_{31} u_{13} - \ell_{32} u_{23} \end{bmatrix} \\ &= \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ \ell_{21} u_{11} & \ell_{21} u_{12} + u_{22} & \ell_{21} u_{13} + u_{23} \\ \ell_{31} u_{11} & \ell_{31} u_{12} + \ell_{32} u_{22} & \ell_{31} u_{13} + \ell_{32} u_{23} + u_{33} \end{bmatrix} \end{split}$$

Symmetric Positive Definite:  $x^{\top} Ax > 0 : \forall x \in \mathbb{R}^n$ .

Cholesky Decomposition (A =  $\mathrm{LL}^ op \implies \mathrm{L}z = b, \ \mathrm{L}^ op x = z$ )

$$\begin{split} \mathbf{L} &= \begin{bmatrix} \sqrt{a_{11}} & 0 & 0 \\ \frac{a_{21}}{\ell_{11}} & \sqrt{a_{22} - \ell_{21}^2} & 0 \\ \frac{a_{31}}{\ell_{11}} & \frac{a_{32} - \ell_{21} \ell_{31}}{\ell_{22}} & \sqrt{a_{33} - \ell_{31}^2 - \ell_{32}^2} \end{bmatrix} \\ \mathbf{L} \mathbf{L}^\top &= \begin{bmatrix} \ell_{11}^2 & \ell_{11} \ell_{21} & \ell_{11} \ell_{31} \\ \ell_{11} \ell_{21} & \ell_{21}^2 + \ell_{22}^2 & \ell_{21} \ell_{31} + \ell_{22} \ell_{32} \\ \ell_{11} \ell_{31} & \ell_{21} \ell_{31} + \ell_{22} \ell_{32} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 \end{bmatrix} \end{split}$$