NA Slides
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(based on
Numerical Mathematics and
Computing—Cheney/Kincaid)

Taylor Series

- $\Rightarrow$ Definitions and Theorems
- Examples
- Proximity of x to c
- Additional Notes

Taylor Series

- Series definition: If $\exists f^{(k)}(c)$, $k = 0, 1, 2, \cdots$, then:

$$
\begin{aligned}
f(x) &\approx f(c) + f'(c)(x-c) + \frac{f''(c)}{2!}(x-c)^2 + \cdots \\
&= \sum_{k=0}^{\infty} \frac{f^{(k)}(c)}{k!}(x-c)^k
\end{aligned}
$$

- c is a *constant* and much is known about it ($f^{(k)}(c)$)
- x a variable near c, and $f(x)$ is sought
- With $c = 0 \Rightarrow$ Maclaurin series
- What is the error if we stop after n terms?

Key NA questions: What is estimate? What is its error?

Taylor's Theorem

- Theorem: If $f \in C^{(n+1)}([a,b])$ then

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(c)}{k!}(x-c)^k + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-c)^{n+1},$$

where

$$x, c \in [a,b], \;\; \xi(x) \in (x,c) \cup (c,x)$$

- Notes:
    - $\xi = \xi(x)$
    - Error term is just like other terms, with $k := n+1$

ξ-term is "truncation error", due to series termination

Taylor Series—Procedure

- Step-by-step:
  1) Write formula for $f^{(k)}(x)$
  2) Choose c (if not already specified)
  3) Write out summation (and error term)

- Note: sometimes easier to write out a few terms

Taylor Series

- Definitions and Theorems

$\Rightarrow$ Examples

- Proximity of x to c
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Taylor Series: e^x

- $f(x) = e^x$, $|x| < \infty \therefore f^{(k)}(x) = e^x, \forall k$
- Choose $c := 0$
- We have
$$e^x = \sum_{k=0}^{n} \frac{x^k}{k!} + \frac{e^{\xi(x)}}{(n+1)!} x^{n+1}$$
- Error term $\to 0$ as $n \to \infty \therefore$
$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

Taylor Series: $\sin x$

- $f(x) = \sin x$, $|x| < \infty$ $\therefore$ $f^{(k)}(x) = \sin\left(x + \frac{\pi k}{2}\right), \forall k$, $c := 0$

- We have

$$\sin x = \sum_{k=0}^{n} \frac{\sin\left(\frac{\pi k}{2}\right)}{k!} x^k + \frac{\sin\left(\xi(x) + \frac{\pi(n+1)}{2}\right)}{(n+1)!} x^{n+1}$$

- Error term $\to 0$ as $n \to \infty$ $\therefore$ upper limit is ∞

- Even k terms are zero $\therefore$ $\ell = 0, 1, 2, \cdots$, and $k \to 2\ell + 1$

$$\sin x = \sum_{\ell=0}^{\infty} \frac{\sin\left(\frac{\pi(2\ell+1)}{2}\right)}{(2\ell+1)!} x^{2\ell+1} = \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k+1}}{(2k+1)!} = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots$$

Taylor Series: $\cos x$

- $f(x) = \cos x,\ |x| < \infty \mathrel{\therefore} f^{(k)}(x) = \cos\left(x + \frac{\pi k}{2}\right), \forall k,\ c := 0$

- We have

$$\cos x = \sum_{k=0}^{n} \frac{\cos\left(\frac{\pi k}{2}\right)}{k!} x^k + \frac{\cos\left(\xi(x) + \frac{\pi(n+1)}{2}\right)}{(n+1)!} x^{n+1}$$

- Error term $\to 0$ as $n \to \infty \mathrel{\therefore}$ upper limit is ∞

- Odd k terms are zero $\therefore \ell = 0, 1, 2, \cdots,$ and $k \to 2\ell$

$$\cos x = \sum_{\ell=0}^{\infty} \frac{\cos\left(\frac{\pi(2\ell)}{2}\right)}{(2\ell)!} x^{2\ell} = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!} = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots$$

Taylor Series: $(1-x)^{-1}$

- $f(x) = \frac{1}{1-x}$, $|x| < 1 \therefore f^{(k)}(x) = \frac{k!}{(1-x)^{k+1}}, \forall k$, choose $c := 0$
- We have

$$\frac{1}{1-x} = \sum_{k=0}^{n} x^k + \frac{e^{\xi(x)}}{(n+1)!} x^{n+1}$$

- Error term $\to 0$ as $n \to \infty$ *only for* $|x| \le \frac{1}{2}$

$$\frac{1}{1-x} = \sum_{k=0}^{\infty} x^k = 1 + x + x^2 + x^3 + \cdots \quad \left(\text{Zeno: } x = \tfrac{1}{2}, \ldots\right)$$

$\boxed{\text{Need more for the whole range } |x| < 1.}$

Taylor Series: $\ln x$

- $f(x) = \ln x$, $0 < x \leq 2 \therefore f^{(k)}(x) = (-1)^{k-1}\frac{(k-1)!}{x^k}, \forall k > 1$

- Choose $c := 1$

- We have

$$\ln x = \sum_{k=0}^{n} (-1)^{k-1}\frac{(x-1)^k}{k} + (-1)^n \frac{1}{n}\frac{(x-1)^{n+1}}{\xi^{n+1}(x)}$$

- Error term $\to 0$ as $n \to \infty$ *only for* $x \geq 1$

$$\ln x = \sum_{k=0}^{\infty} (-1)^{k-1}\frac{(x-1)^k}{k} = (x-1) - \frac{(x-1)^2}{2} + \frac{(x-1)^3}{3} - \cdots$$

$\boxed{\text{Need more for the whole range } 0 < x \leq 2.}$

Ratio Test and $\ln x$ Revisited

- Theorem: $\left|\frac{a_{n+1}}{a_n}\right| \to (< 1) \Rightarrow$ partial sums converge
- $\ln x$: ratio is $\left|(x-1)\frac{n}{n+1}\right| \therefore$ convergence for $0 < x < 2$
- $x = 2$: $1 - \frac{1}{2} + \frac{1}{3} - \cdots$, which is convergent
- $x = 0$: same series, all same sign $\Rightarrow$ divergent harmonic series
- $\therefore$ we have $0 < x \leq 2$

$(1-x)^{-1}$ Revisited

- Letting $x \to (1-x)$

$$\ln(1-x) = -\left(x + \frac{x^2}{2} + \frac{x^3}{3} + \cdots\right), \quad -1 \le x < 1$$

- $\frac{d}{dx}$: lhs $= \frac{-1}{1-x}$ and rhs $= -\left(1 + x + x^2 + x^3 + \cdots\right)$

- ⚠: no "=" for $x = -1$ as rhs oscillates (note: correct avg value)

- $|x| < 1$ we have (also with ratio test)

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 + \cdots$$

Taylor Series

- Definitions and Theorems
- Examples

$\Rightarrow$ Proximity of x to c

- Additional Notes

Proximity of x to c

Problem: Approximate $\ln 2$

- Solution 1: Taylor $\ln(1+x)$ around 0 with $x=1$

$$\ln 2 = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \frac{1}{6} + \frac{1}{7} - \frac{1}{8} + \cdots$$

- Solution 2: Taylor $\ln\left(\frac{1+x}{1-x}\right)$ around 0 with $x=\frac{1}{3}$

$$\ln 2 = 2\left(3^{-1} + \frac{3^{-3}}{3} + \frac{3^{-5}}{5} + \frac{3^{-7}}{7} + \cdots\right)$$

Proximity of x to c (cont.)

- Approximated values, rounded:
  - Solution 1, first 8 terms: 0.63452
  - Solution 2, first 4 terms: 0.69313

- Actual value, rounded: 0.69315

- $\therefore$ importance of proximity of evaluation and expansion points

$$\boxed{\text{This error is in } \textit{addition} \text{ to the truncation error.}}$$

Taylor Series

- Definitions and Theorems
- Examples
- Proximity of x to c

$\Rightarrow$ Additional Notes

Polynomials and a Second Form

- Polynomials have finite number of non-zero derivatives $\therefore$ Taylor series leads to original polynomial

- Taylor's Theorem, second form ($x =$ *constant* expansion point, $x + h =$ *variable* evaluation point):
  If $f \in C^{(n+1)}([a,b])$ then

$$f(x+h) = \sum_{k=0}^{n} \frac{f^{(k)}(x)}{k!} h^k + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} h^{n+1},$$

$$x, x+h \in [a,b], \;\; \xi(x) \in (x, x+h) \cup (x+h, x)$$

$O()$ Notation and MVT

- "$O()$" notation

$$E_{n+1} = O\left(h^{n+1}\right) \quad \equiv \quad \left|E_{n+1}\right| \leq C|h|^{n+1}.$$

- Mean value theorem (Taylor, $n = 0$): If $f \in C'([a, b])$ then

$$f(b) = f(a) + (b - a)f'(\xi), \;\; \xi \in (a, b)$$

or:

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

Alternating Series Theorem

- Alternating series theorem: If $a_k > 0$, $a_k \geq a_{k-1}$, $\forall k > 1$, and $a_k \to 0$, then

$$\sum_{k=0}^{\infty} (-1)^k a_k \to S \text{ and } |S - S_N| \leq a_{n+1}$$

- Intuitively understood

- Useful for truncation error estimation

Base Representations

$\Rightarrow$ Definitions
- Conversions
- Computer Representation
- Loss of Significant Digits

Number Representation

- Simple representation in one base $\not\Rightarrow$ simple representation in another base, e.g.

$$(0.1)_{10} = (0.0\ 0011\ 0011\ 0011\ \cdots)_2$$

- Base 10:

$$\begin{aligned} 37294 &= 4 + 90 + 200 + 7000 + 30000 \\ &= 4 \times 10^0 + 9 \times 10^1 + 2 \times 10^2 + 7 \times 10^3 + 3 \times 10^4 \end{aligned}$$

in general: $a_n \cdots a_0 = \sum_{k=0}^{n} a_k 10^k$

Fractions and Irrationals

- Base 10 fraction:

$$0.7217 = 7 \times 10^{-1} + 2 \times 10^{-2} + 1 \times 10^{-3} + 7 \times 10^{-4}$$

- In general, for real numbers:

$$a_n \cdots a_0.b_1 \cdots = \sum_{k=0}^{n} a_k 10^k \sum_{k=1}^{\infty} b_k 10^{-k}$$

- Note: $\exists$ numbers, i.e., irrationals, such that an infinite number of digits are required, in *any* base, e.g., $e, \pi, \sqrt{2}$

Other Bases

- Base 8, $\nexists$ '8' or '9'

$$(21467)_8 = \cdots = (9015)_{10}$$

$$(0.36207)_8 = 8^{-5}\Big(3 \times 8^4 + \cdots\Big) = \frac{15495}{32768} = (0.47286\ \cdots)_{10}$$

- Base β

$$(a_n \cdots a_0.b_1 \cdots)_\beta = \sum_{k=0}^{n} a_k \beta^k \sum_{k=1}^{\infty} b_k \beta^{-k}.$$

- Base 2: just '0' and '1', or for computers: "off" and "on"

Base Representations

- Definitions

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Conversion: Base 10 $\to$ Base 2

- Basic idea:

$$\begin{aligned} 3781 &= 1 + \underbrace{10}_{(1010)_2}\left(\underbrace{8}_{(1000)_2} + 10(7 + 10(3))\right) = \cdots \\ &= (111\,011\,000\,101)_2 \end{aligned}$$

- Easy for computer, but by hand: $(3781.372)_{10}$

$$\begin{array}{rl} & \text{remainder} \\ 2\overline{)3781} & \\ 2\overline{)1890} & 1 = c_0 \\ 2\overline{)945} & 0 = c_1 \\ \vdots & \end{array} \quad \begin{array}{c} \cdot \\ \downarrow \end{array}$$

$$\begin{array}{ccr} & & 0.372 \\ \cdot & & \underline{2} \\ \downarrow & c_1 = & \boxed{0}.744 \\ & & \underline{2} \\ & c_2 = & \boxed{1}.488 \\ & & \vdots \end{array}$$

Base 8 Shortcut

- Base 2 $\leftrightarrow$ base 8, trivial

$$(551.624)_8 = (101\ \ 101\ \ 001.110\ \ 010\ \ 100)_2$$

- $\approx$ 3 bits for every 1 octal digit
- One digit produced for every step in (hand) conversion
- $\therefore$ base 10 $\rightarrow$ base 8 $\rightarrow$ base 2

Base Representations

- Definitions
- Conversions

$\Rightarrow$ Computer Representation

- Loss of Significant Digits

Computer Representation

- Scientific notation:

$$32.213 \to 0.32213 \times 10^2$$

- In general:

$$x = \pm 0.d_1 d_2 \cdots \times 10^n, \text{ or: } x = \pm r \times 10^n, \ \frac{1}{10} \le r < 1$$

we have sign, “mantissa” r and “exponent” n

- Finite number of mantissa digits, therefore “roundoff” or “truncation” error

Base Representations

- Definitions
- Conversions
- Computer Representation

$\Rightarrow$ Loss of Significant Digits

LSD—Addition

- $(a+b)+c = a+(b+c)$ on the computer?
- Five decimal digits for mantissa

$$1{,}000{,}000. + \underbrace{1. + \cdots + 1.}_{\text{million times}} = 1{,}000{,}000.$$

but

$$\underbrace{1. + \cdots + 1.}_{\text{million times}} + 1{,}000{,}000. = 2{,}000{,}000.$$

$\boxed{\text{Add numbers in size order.}}$

LSD—Subtraction

E.g.: $x - \sin x$ for x's close to zero

$$
\begin{aligned}
x &= \frac{1}{15}\text{(radians)} \\
x &= 0.66666\ \ 66667 \times 10^{-1} \\
\sin x &= 0.66617\ \ 29492 \times 10^{-1} \\
x - \sin x &= 0.00049\ \ 37175 \times 10^{-1} \\
&= 0.49371\ \ 75000 \times 10^{-4}
\end{aligned}
$$

$\boxed{\text{Avoid subtraction of close numbers.}}$

LSD Avoidance for Subtraction

- $\sqrt{x^2+1}-1$ for $x \approx 0 \rightarrow \frac{x^2}{\sqrt{x^2+1}+1}$
- $x - \sin x$ for $x \approx 0 \rightarrow$ use Taylor series
- $e^x - e^{-2x}$ for $x \approx 0 \rightarrow$ use Taylor series twice and add common powers
- $\cos^2 x - \sin^2 x$ for $x \approx \frac{\pi}{4} \rightarrow \cos 2x$
- $\ln x - 1$ for $x \approx e \rightarrow \ln \frac{x}{e}$

Nonlinear Equations

- $\Rightarrow$ Motivation
- Bisection Method
- Newton's Method
- Secant Method
- Summary

Motivation

- BVP: dipping of suspended power cable. What is λ?

$$\lambda \cosh \frac{50}{\lambda} = \lambda + 10$$

- (Some) simple equations $\Rightarrow$ solve analytically

$$\begin{aligned} 6x^2 - 7x + 2 &= 0 \\ (3x-2)(2x-1) &= 0 \\ x &= \frac{2}{3}, \frac{1}{2}, \end{aligned} \qquad \begin{aligned} \cos 3x - \cos 7x &= 0 \\ 2 \sin 5x \sin 2x &= 0 \\ x &= \frac{n\pi}{5}, \frac{n\pi}{2}, \quad n \in \mathbb{Z} \end{aligned}$$

Motivation (cont.)

- In general, we cannot exploit the function, e.g.:

$$2^{x^2} - 10x + 1$$

and

$$\cosh\left(\sqrt{x^2+1} - e^x\right) + \log|\sin x|$$

$\boxed{\text{Need a general, function-independent algorithm.}}$

Nonlinear Equations

- Motivation
- $\Rightarrow$ Bisection Method
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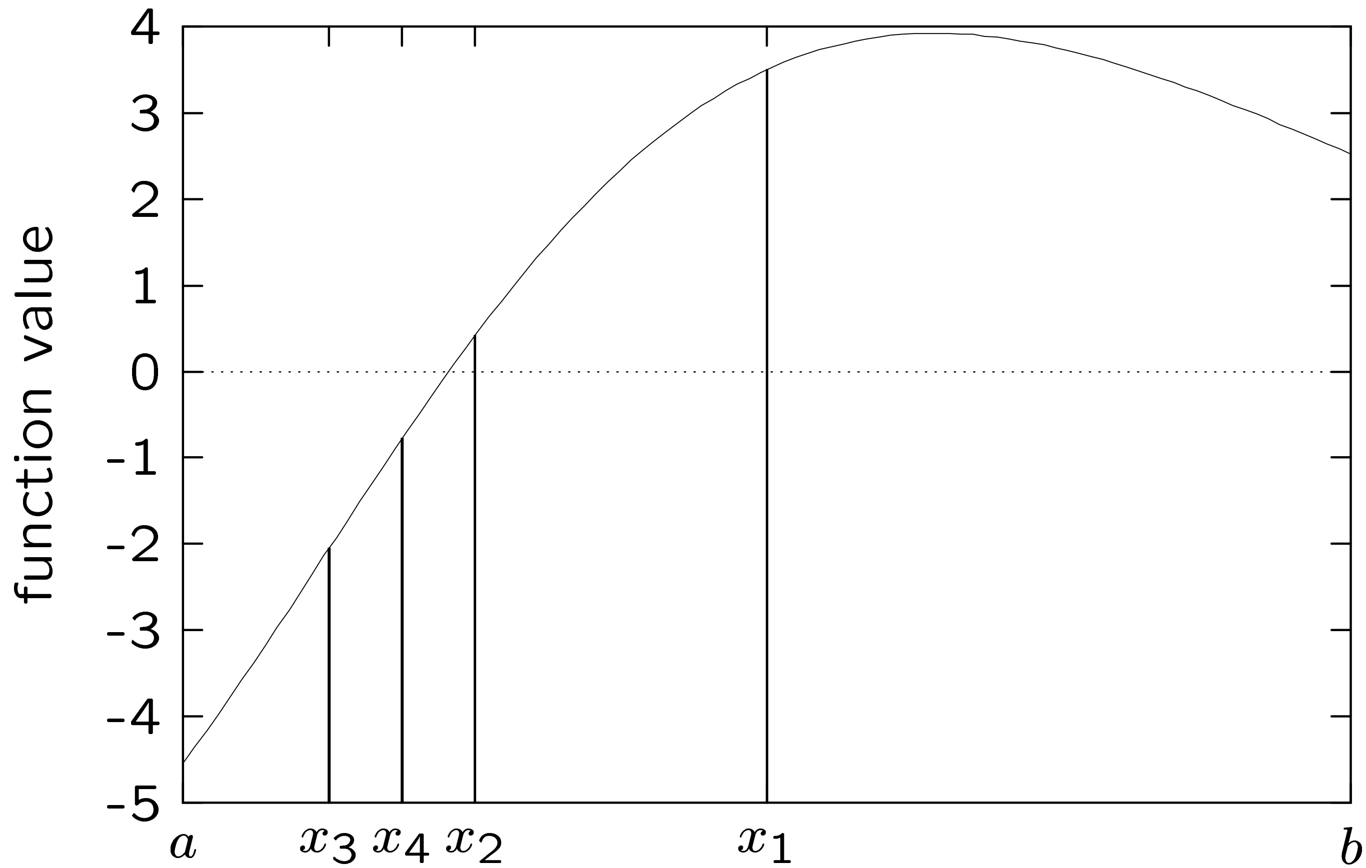
Bisection Method—Example



$\boxed{\text{Intuitive, like guessing a number} \in [1, 100].}$

Restriction and Error Estimate

- Need function to slice x-axis
- $\therefore$ start with two point a and $b \ni f(a)f(b) < 0$
- After n steps, guess midpoint of current range
- Error: $\frac{b-a}{2^{n+1}}$ (think of $n = 0, 1, 2$)

$$\boxed{\text{Question: Given tolerance, what is } n\text{? } \ldots}$$

Convergence Rate

- Given tolerance τ (e.g., 10^{-6}), how many steps are needed?
- Error from before: $\epsilon \leq \frac{b-a}{2^{n+1}} < \tau \times 2$, log (any base)

$$\log{(b-a)} - n\log 2 < \log 2\tau$$

or

$$n > \frac{\log{(b-a)} - \log 2\tau}{\log 2}$$

$\boxed{\text{Rate is independent of function.}}$

Convergence Rate (cont.)

- Base 2 (i.e., bits of accuracy)

$$n > \log_2 (b - a) - 1 - \log_2 \tau$$

i.e., number of steps is a constant plus one step per bit

- Convergence rate: linear, i.e., $C \in [0, 1)$

$$\left| x_{n+1} - x \right| \leq C |x_n - x|, \;\; n \geq 1, \text{ and}$$

$$\left| x_{n+1} - x \right| \leq C^n |x_1 - x|.$$

$\boxed{\text{Okay, but restrictive and slow.}}$

Nonlinear Equations

- Motivation
- Bisection Method

$\Rightarrow$ Newton's Method

- Secant Method
- Summary

Newton's Method—Definition

- Approximate $f(x)$ near x_0 by (note: $f(x_0) = \ell(x_0)$)

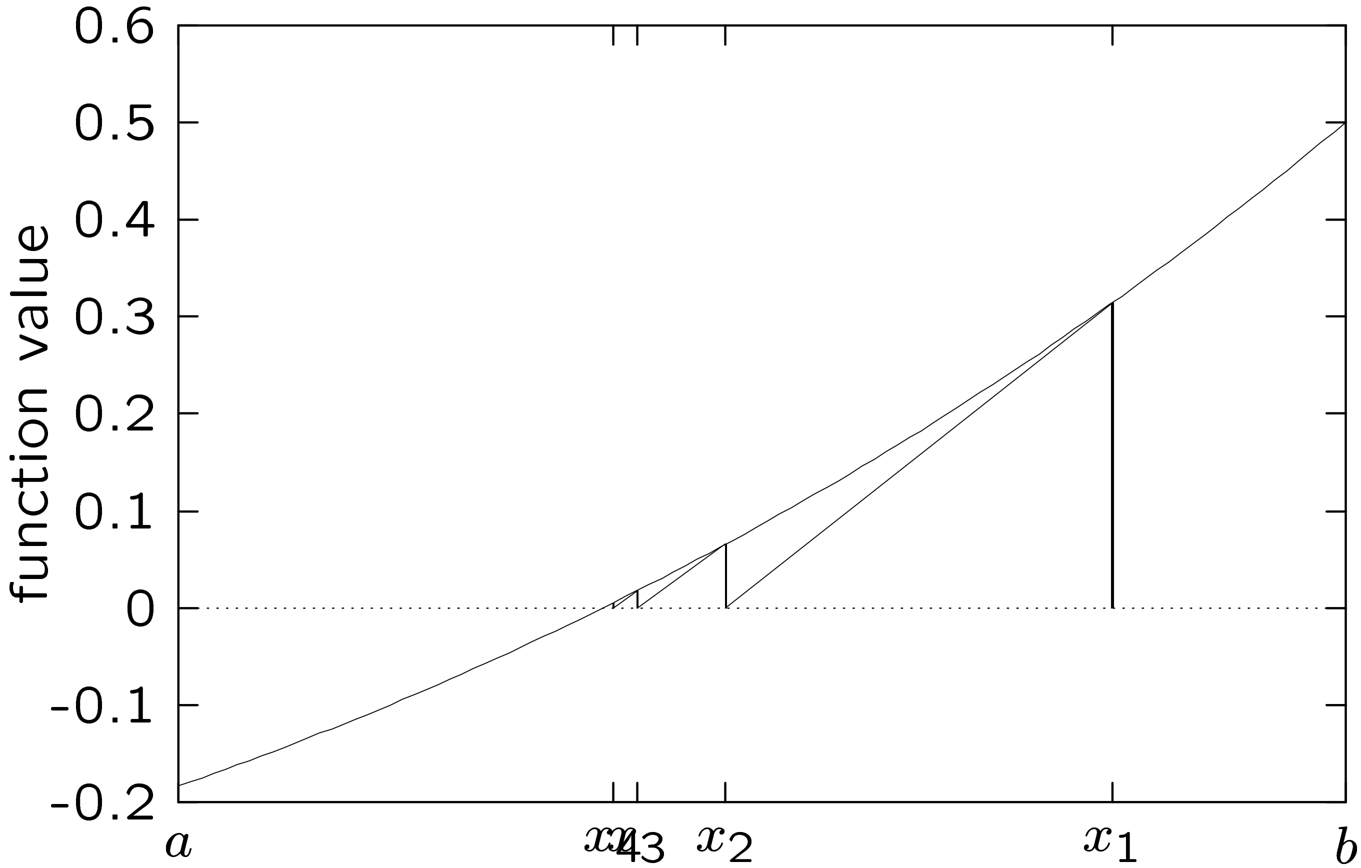
$$f(x) \approx f'(x_0)(x - x_0) + f(x_0) \equiv \ell(x)$$

- Want $\ell(\widehat{x}) = 0 \Rightarrow \widehat{x} = x_0 - \frac{f(x_0)}{f'(x_0)}$, $\therefore x_1 := \widehat{x}$, $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}, \cdots$

- Alternatively (Taylor's): have x_0, for what h is $f\left(\underbrace{x_0 + h}_{\equiv x_1}\right) = 0$?

- $f(x_0 + h) \approx f(x_0) + hf'(x_0)$ or $h = -\frac{f(x_0)}{f'(x_0)}$

Newton's Method—Example



Convergence Rate

- Theorem: With the following three comditions:

  $^{1)}f(r) = 0$, $^{2)}f'(r) \neq 0$, $^{3)}f \in C^2\Big[B\Big(r, \widehat{\delta}\Big)\Big] \Rightarrow$

  $\exists \delta \ni \forall x_0 \in B(r, \delta)$ and $\forall n$ we have $\Big|x_{n+1} - r\Big| \leq C(\delta)|x_n - r|^2$

- English: With enough continuity and proximity $\Rightarrow$
  quadratic convergence!

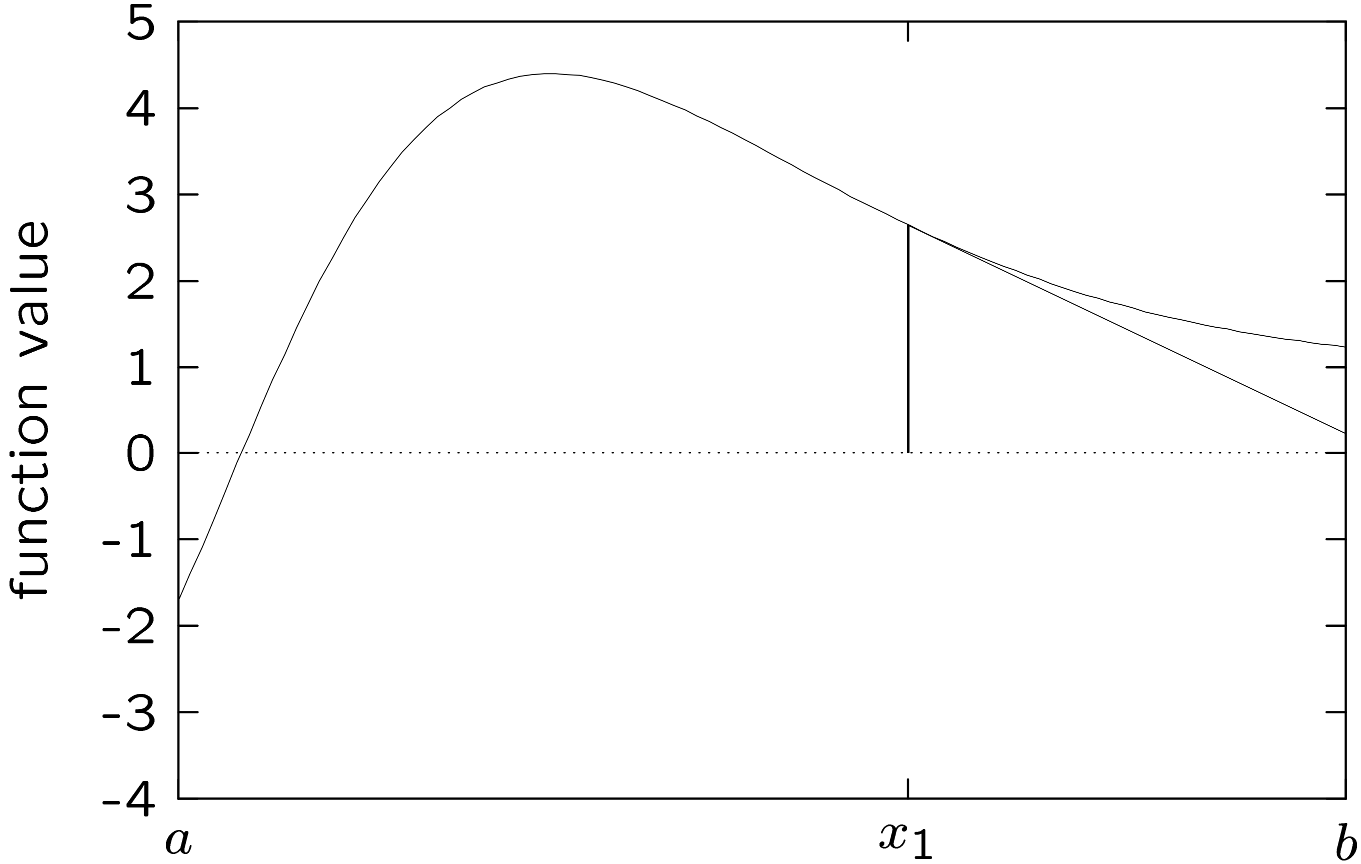
$\boxed{\text{Newton's method can be very fast.}}$

Convergence Rate Example

$f(x) = x^3 - 2x^2 + x - 3, \;\; x_0 = 4$

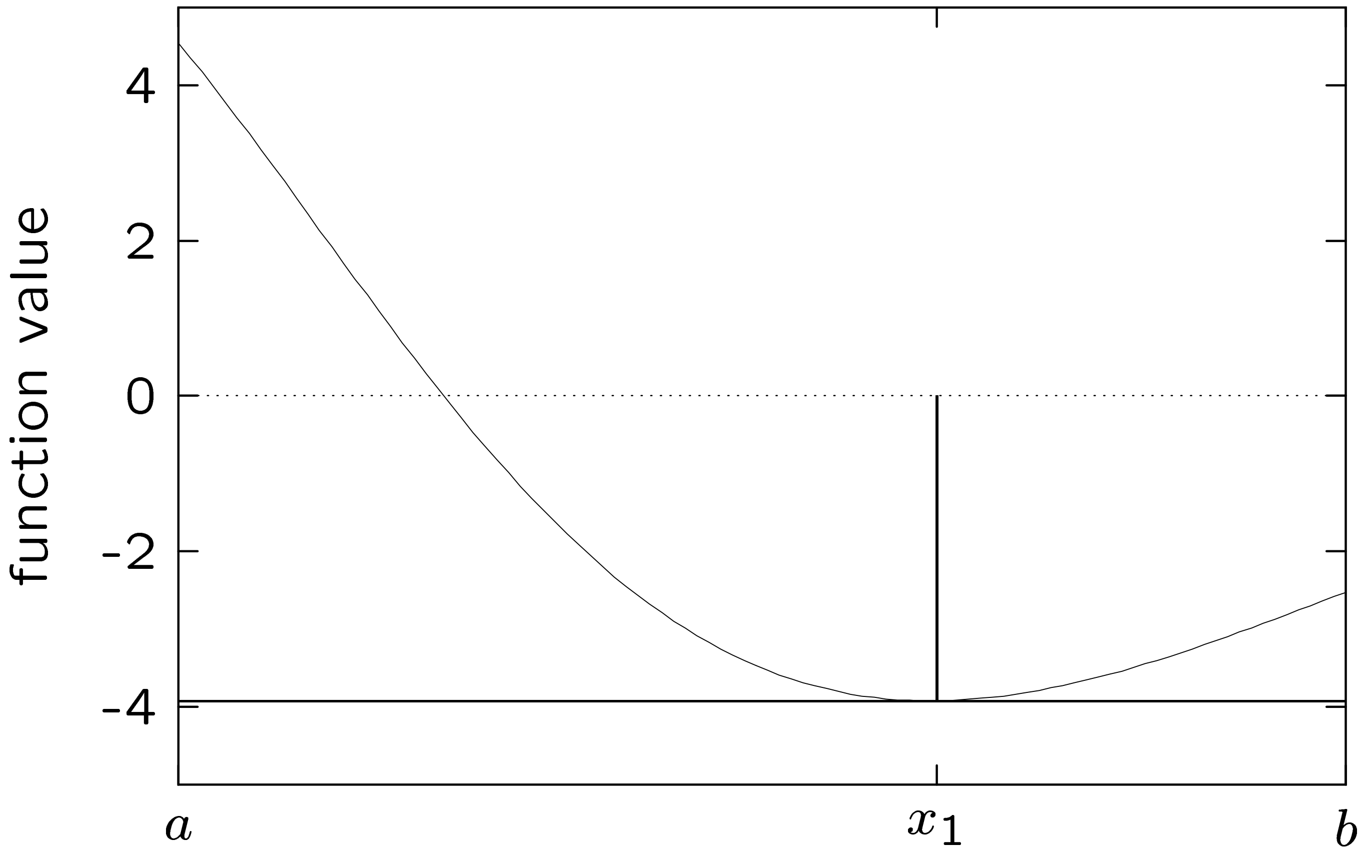
n	x_n	$f(x_n)$
0	4	33
1	3	9
2	2.4375	2.036865234375
3	2.21303271631511	0.256363385061418
4	2.17555493872149	0.00646336148881306
5	2.17456010066645	$4.47906804996122e-06$
6	2.17455941029331	$2.15717547991101e-12$

Sample Newton Failure #1



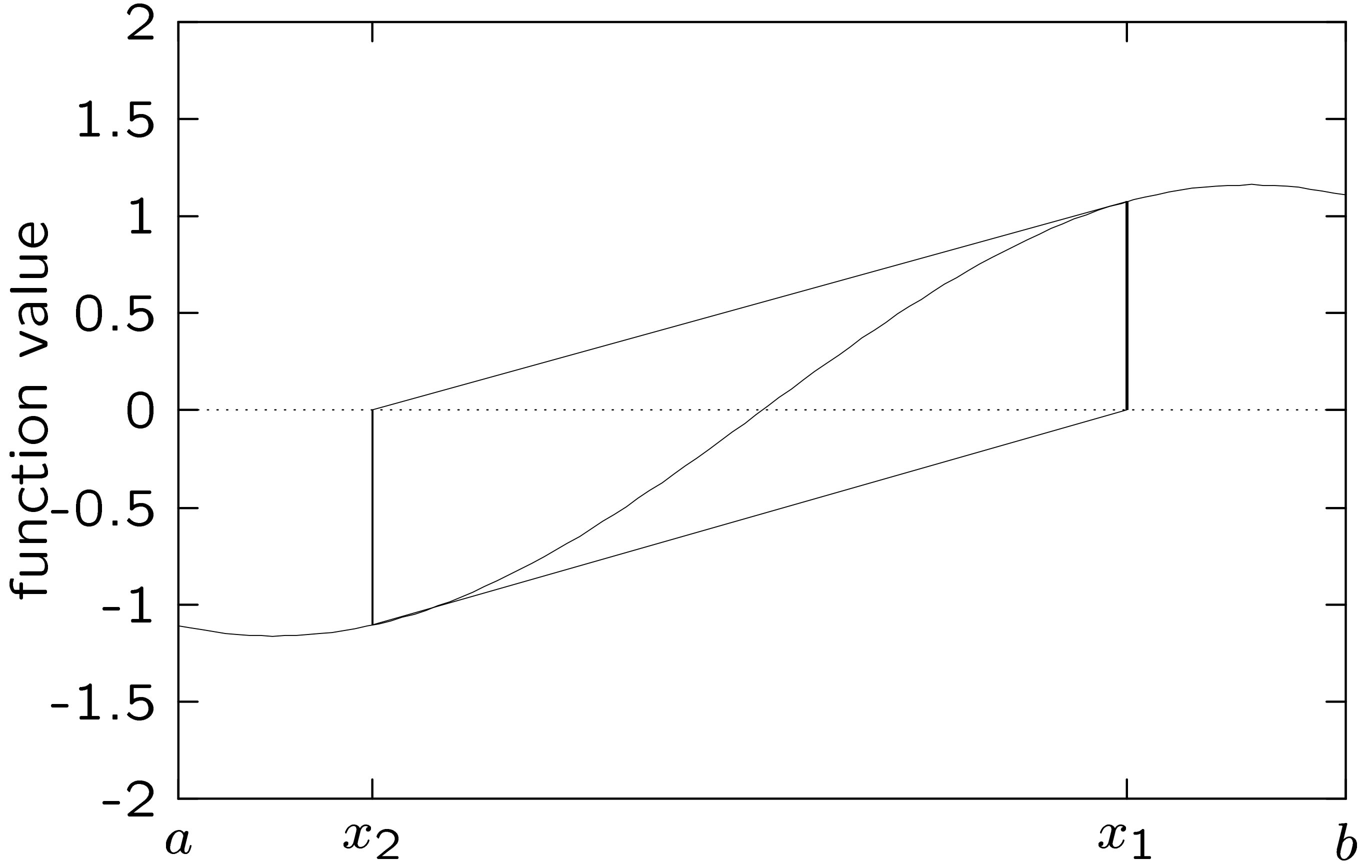
$$\boxed{\text{Runaway process}}$$

Sample Newton Failure #2



Division by zero derivative—recall theorem condition

Sample Newton Failure #3



$\boxed{\text{Loop-d-loop}}$

- Motivation
- Bisection Method
- Newton's Method

$\Rightarrow$ Secant Method

- Summary

Secant Method—Definition

- Motivation: avoid derivatives
- Taylor (or derivative): $f'(x_n) = \frac{f(x_n)-f(x_{n-1})}{x_n - x_{n-1}}$
- $\therefore x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n)-f(x_{n-1})}$
- Bisection requirements comparison:
  - $\boxed{\surd}$ 2 previous points
  - $\boxed{\times}$ $f(a)f(b) < 0$
- Superlinear convergence: $\left|x_{n+1} - r\right| \leq C|x_n - r|^{1.618\cdots}$

Nonlinear Equations

- Motivation
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- Secant Method

$\Rightarrow$ Summary

Root Finding—Summary

Performance and requirements:

	speedy	# pts.	$f(a)f(b) < 0$	$f \in C'$	nbhd(r)
bisection	$\times$	2	$\surd$	$\times$	$\times$
Newton	$\surd$	1	$\times$	$\surd$	$\surd$
secant	$\cancel{\surd}$	2	$\times$	$\times$	$\surd$

Interpolation and Approximation

- ⇒ Motivation
- Polynomial Interpolation
- Numerical Differentiation
- Additional Notes

Motivation

- $\{(x_i, y_i) | i = 0, \cdots, n\}$, ($x_i$ distinct), want simple (e.g., polynomial) $p(x) \ni y_i = p(x_i), i = 0, \cdots, n \quad \equiv$ "interpolation"

- Assume data includes errors, relax equality but still close, ..., least squares

- Replace complicated $f(x)$ with simple $p(x) \approx f(x)$, ..., splines

$$\boxed{\text{Use } p(x) \text{ for } f(x_{\text{new}}),\ \int f(x)\,dx,\ \ldots.}$$

Interpolation and Approximation

- Motivation
- ⇒ Polynomial Interpolation
- Numerical Differentiation
- Additional Notes

Polynomial Interpolation

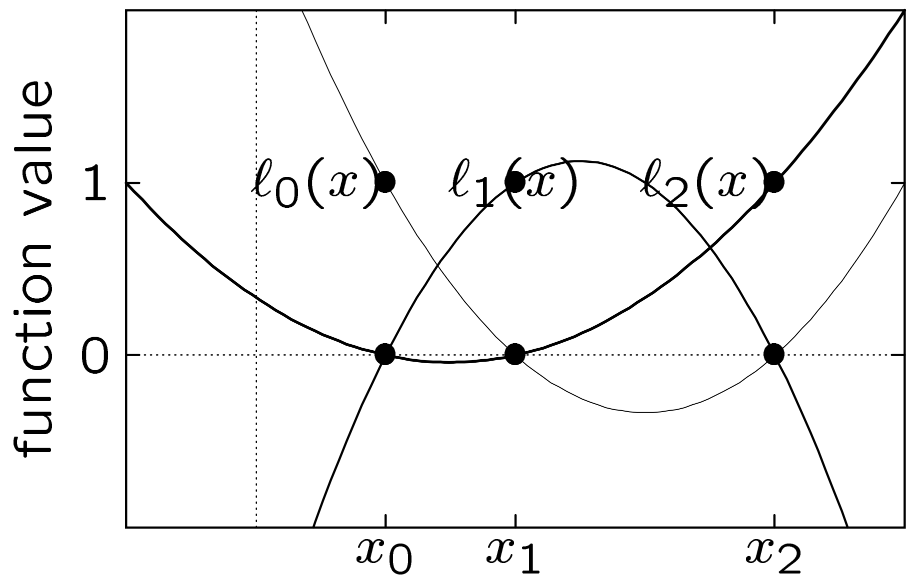
- $n = 0$: $p(x) = y_0$
- $n = 1$: $p(x) = y_0 + g(x)(y_1 - y_0)$, $g(x) \in P_1$, and
  $g(x) = \begin{cases} 0, & x = x_0, \\ 1, & x = x_1 \end{cases}$ $\therefore g(x) = \frac{x - x_0}{x_1 - x_0}$
- $n = 2$: more complicated, ...

Lagrange Polynomials

- $\ell_i(x) \in P_n$, $\ell_i\left(x_j\right) = \delta_{ij}$, $i = 0, \cdots, n$

- $\delta_{ij} = \begin{cases} 0, & i \neq j, \\ 1, & i = j \end{cases}$

- E.g., $n = 2$:



Lagrange Polynomials (cont.)

- We have

$$\begin{aligned}
\ell_0(x) &= \frac{x-x_1}{x_0-x_1}\cdot\frac{x-x_2}{x_0-x_2}, \quad y_0\ell_0\big(x_j\big)=y_0\delta_{0j} &= \begin{cases} 0, & j\neq 0, \\ y_0, & j=0 \end{cases}\\
\ell_1(x) &= \frac{x-x_0}{x_1-x_0}\cdot\frac{x-x_2}{x_1-x_2}, \quad y_1\ell_1\big(x_j\big)=y_1\delta_{1j} &= \begin{cases} 0, & j\neq 1, \\ y_1, & j=1 \end{cases}\\
\ell_2(x) &= \frac{x-x_0}{x_2-x_0}\cdot\frac{x-x_1}{x_2-x_1}, \quad y_2\ell_2\big(x_j\big)=y_2\delta_{2j} &= \begin{cases} 0, & j\neq 2, \\ y_2, & j=2 \end{cases}
\end{aligned}$$

- $\therefore\ \exists! p(x)\in P_2$, with $p\big(x_j\big)=y_j$, $j=0,1,2$: $p(x)=\sum_{i=0}^{2} y_i\ell_i(x)$

- In general: $\ell_i(x) = \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}, \quad i=0,\cdots,n$

Error of Polynomial Interpolation

- $\{(x_i, f(x_i)) | i = 0, \cdots, n\}$, $|f(x) - p(x)| = ?$
- Runge function: $f_R(x) = \left(1 + x^2\right)^{-1}, x \in [-5, 5]$ and *uniform* mesh:

$$\lim_{n \to \infty} \max_{-5 \le x \le 5} |f_R(x) - p_n(x)| = \infty$$

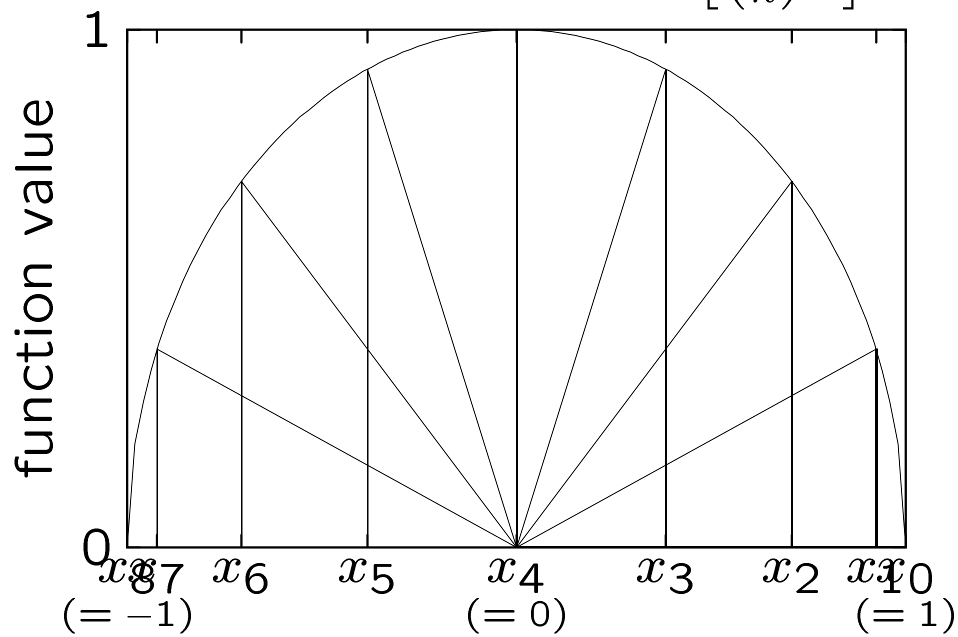
⚠: high oscillations.

Error of PI (cont.) and Cheb. Pts.

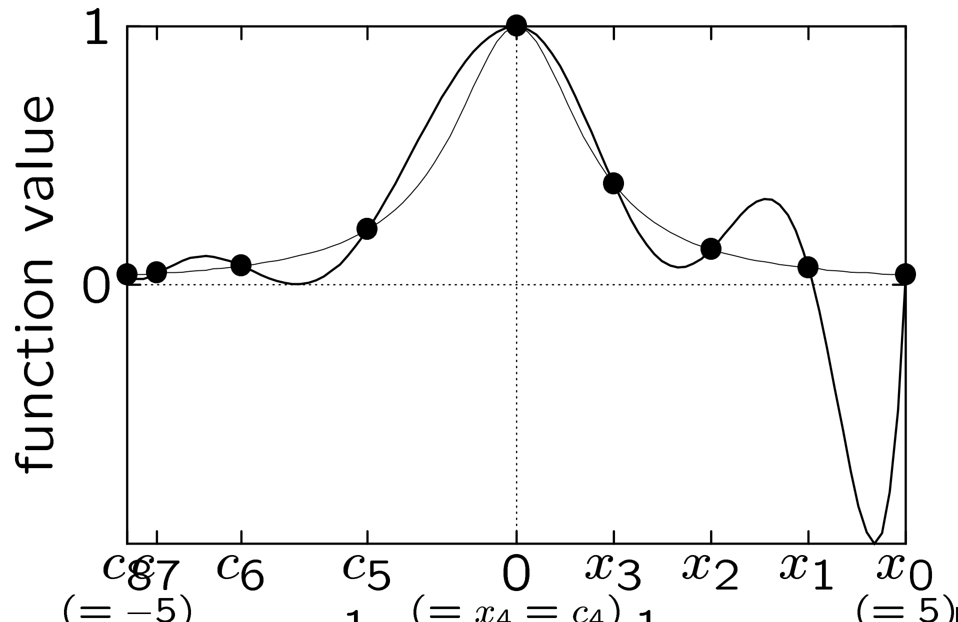
- Theorem: $\ldots$, $f \in C^{(n+1)}([a,b])$, $\forall x \in [a,b]$, $\exists \xi \in (a,b) \ni$

$$f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) \prod_{i=0}^{n} (x - x_i)$$

- Chebyshev points on $[-1,1]$: $x_i = \cos\left[\left(\frac{i}{n}\right)\pi\right]$, $i = 0, \cdots, n$



Error of PI (cont.) and Cheb. Pts.



- In general on $[a,b]$: $x_i = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)\cos\left[\left(\frac{i}{n}\right)\pi\right]$, $i = 0, \cdots, n$

- Points concentrated at edges

$$\boxed{\text{Cheb. pts.: same method, change pts. to minimize } \prod.}$$

Interpolation and Approximation

- Motivation
- Polynomial Interpolation

$\Rightarrow$ Numerical Differentiation

- Additional Notes

Numerical Differentiation

- $f'(x) \approx \frac{f(x+h)-f(x)}{h}$
- Error = ?
- Taylor: $f(x+h) = f(x) + hf'(x) + h^2\frac{f''(\xi)}{2}$
- $\therefore f'(x) = \frac{f(x+h)-f(x)}{h} - \frac{1}{2}hf''(\xi)$
- I.e., truncation error: $O(h)$

$\boxed{\text{Can we do better?}}$

Numerical Differentiation—Take Two

- Taylor:

$$f(x \pm h) =$$
$$\frac{f(x) \pm hf'(x) + h^2\frac{f''(x)}{2!} \pm h^3\frac{f'''(x)}{3!} + h^4\frac{f^{(4)}(x)}{4!} \pm h^5\frac{f^{(5)}(x)}{5!} + \cdots}{f(x+h) - f(x-h) = 2hf'(x) + 2h^3\frac{f'''(x)}{3!} + 2h^5\frac{f^{(5)}(x)}{5!} + \cdots}$$

- $\therefore$

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

We gained $O(h)$ to $O\left(h^2\right)$. However, ...

Richardson Extrapolation—Take Three

- We have

$$f'(x) = \underbrace{\frac{f(x+h) - f(x-h)}{2h}}_{\equiv \phi(h)} + a_2 h^2 + a_4 h^4 + a_6 h^6 + \cdots$$

- Halving the stepsize, $\therefore$

$$\begin{aligned} \phi(h) &= f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \cdots \\ \phi\left(\frac{h}{2}\right) &= f'(x) - a_2 \left(\frac{h}{2}\right)^2 - a_4 \left(\frac{h}{2}\right)^4 - a_6 \left(\frac{h}{2}\right)^6 - \cdots \\ \phi(h) - 4\phi\left(\frac{h}{2}\right) &= -3f'(x) - \frac{3}{4} a_4 h^4 - \frac{15}{16} a_6 h^6 - \cdots \end{aligned}$$

$\boxed{\textit{Q}\text{: So what? }\textit{A}\text{: The } h^2 \text{ term disappeared!}}$

Richardson—Take Three (cont.)

- Divide by 3 and write $f'(x)$

$$\begin{aligned} f'(x) &= \frac{4}{3}\phi\left(\frac{h}{2}\right) - \frac{1}{3}\phi(h) - \frac{1}{4}a_4h^4 - \frac{5}{16}a_6h^6 - \cdots \\ &= \phi\left(\frac{h}{2}\right) + \underbrace{\frac{1}{3}\left[\phi\left(\frac{h}{2}\right) - \phi(h)\right]}_{\equiv(*)} + O\left(h^4\right) \end{aligned}$$

- $(*)$ only uses old and current information

$$\boxed{\text{We gained } O\left(h^2\right) \text{ to } O\left(h^4\right)\text{!!}}$$

Interpolation and Approximation

- Motivation
- Polynomial Interpolation
- Numerical Differentiation

$\Rightarrow$ Additional Notes

Additional Notes

- Three $f'(x)$ formulae used additional points $\Rightarrow$
  vs. Taylor, more derivatives in *same* point

- Similar for $f''(x)$:

$$f(x \pm h) = f(x) \pm hf'(x) + h^2 \frac{f''(x)}{2!} \pm h^3 \frac{f'''(x)}{3!} + h^4 \frac{f^{(4)}(x)}{4!} \pm h^5 \frac{f^{(5)}(x)}{5!} + \cdots$$

- Adding:

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + O\left(h^4\right)$$

or:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O\left(h^2\right)$$

Numerical Quadrature

- $\Rightarrow$ Introduction
- Riemann Integration
- Composite Trapezoid Rule
- Composite Simpson's Rule
- Guassian Quadrature

Numerical Quadrature—Motivation

- Analytical solutions—rare:

$$\int_0^{\frac{\pi}{2}} \sin x \, dx = -\cos x|_0^{\frac{\pi}{2}} = -(0-1) = 1$$

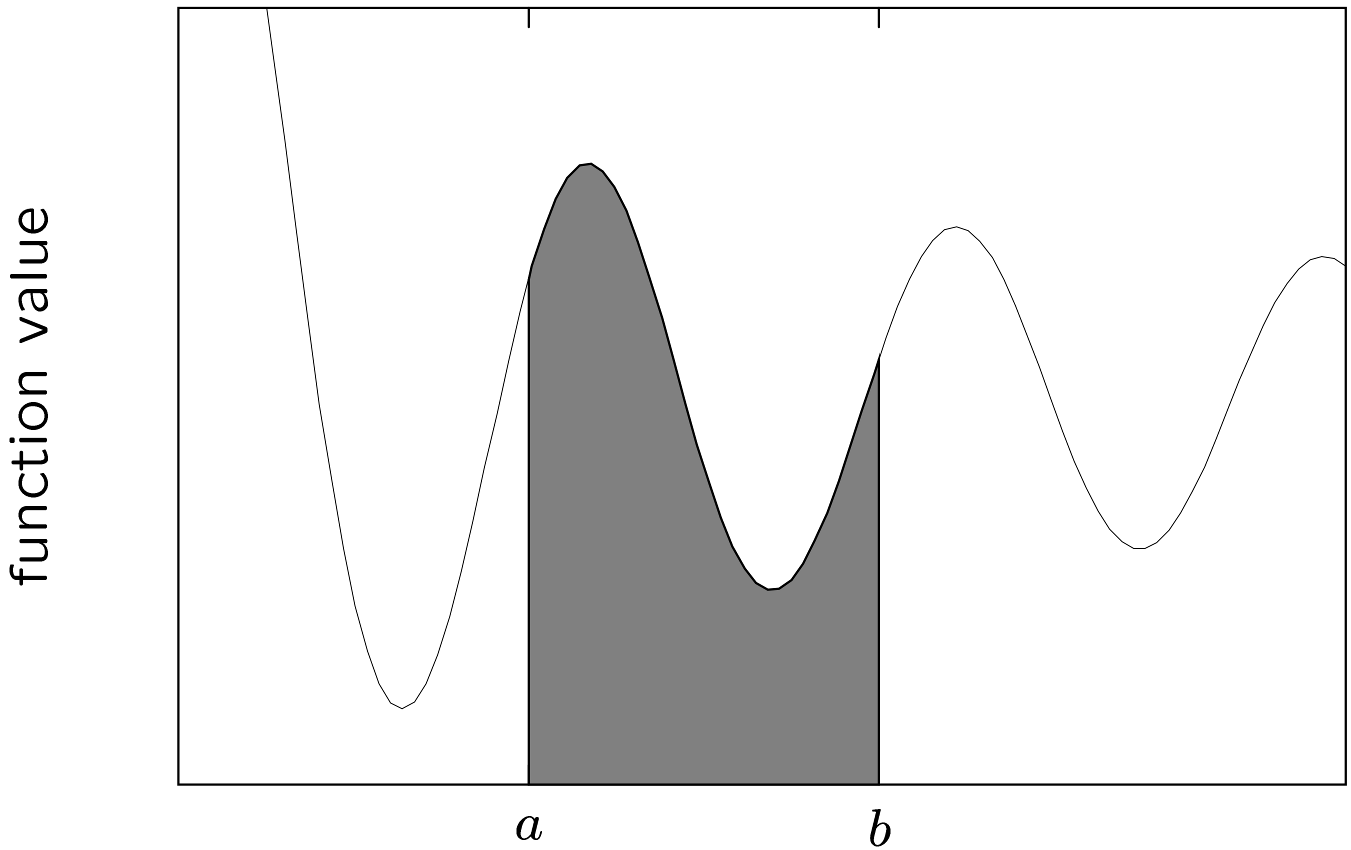
- In general:

$$\int_0^{\frac{\pi}{2}} \left[1 - a^2 \sin^2 \theta\right]^{\frac{1}{3}} d\theta$$

$\boxed{\text{Need general numerical technique.}}$

Numerical Quadrature—Interpretation

- $f(x) \geq 0$ on $[a, b]$ bounded $\Rightarrow \int_a^b f(x)\,dx$ is area under $f(x)$



Definitions

- Mesh: $P \equiv \{a = x_0 < x_1 < \cdots < x_n = b\}$, n intervals ($n+1$ points)

- Infima and suprema:

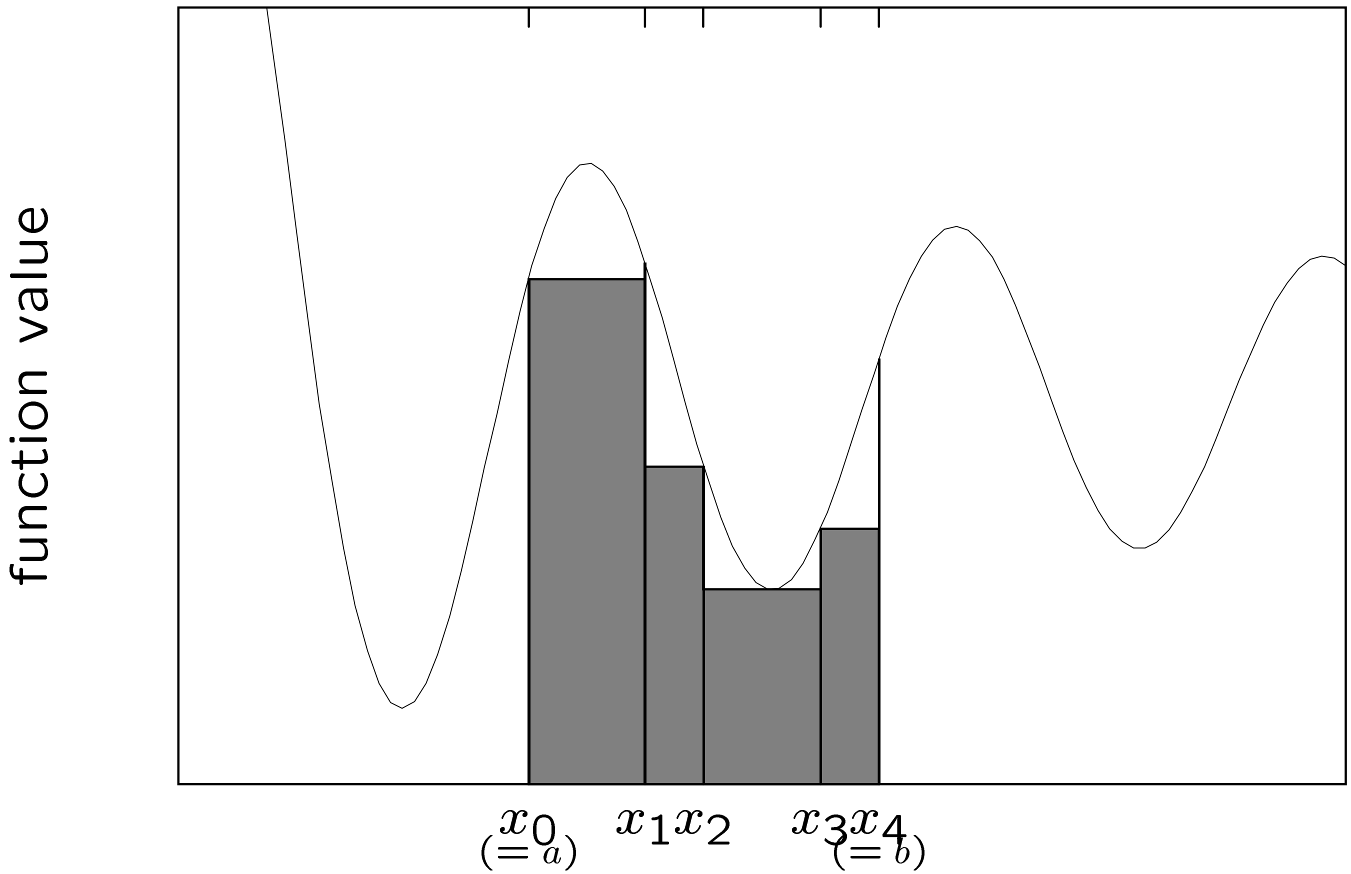
$$
\begin{aligned}
m_i &\equiv \inf\left\{f(x) : x_i \le x \le x_{i+1}\right\} \\
M_i &\equiv \sup\left\{f(x) : x_i \le x \le x_{i+1}\right\}
\end{aligned}
$$

- Lower and upper sums:

$$
\begin{aligned}
L(f;P) &\equiv \sum_{i=0}^{n-1} m_i\left(x_{i+1} - x_i\right) \\
U(f;P) &\equiv \sum_{i=0}^{n-1} M_i\left(x_{i+1} - x_i\right)
\end{aligned}
$$

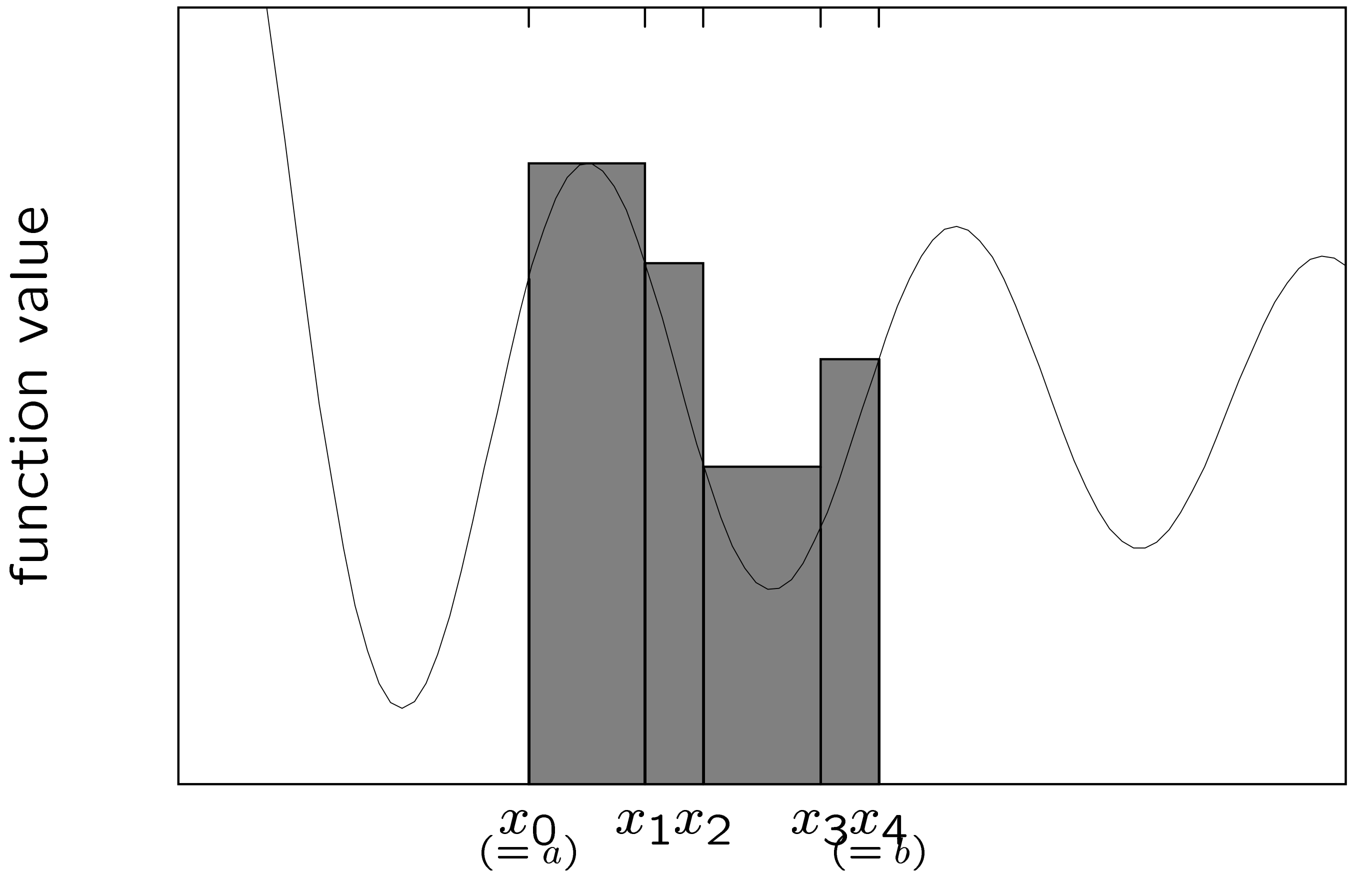
- For example, ...

Lower Sum—Interpretation



Clearly a lower bound of integral estimate, and . . .

Upper Sum—Interpretation



... an upper bound. What is the error?

Lower and Upper Sums—Example

- $f(x) = x^2$, $[a,b] = [0,1]$ and $P = \left\{0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\right\}$
- $\ldots$, $L = \frac{7}{32}$, $U = \frac{15}{32}$
- Split the difference: estimate $\frac{11}{32}$ (actual $\frac{1}{3}$)

$$\boxed{\text{Naive approach and low } n\text{, still error of } \tfrac{1}{96}.\ (!)}$$

Numerical Quadrature—Rethinking

- Perhaps lower and upper sums are enough?
  - ∗ Error seems small
  - ∗ Work seems small as well
- Do they converge to integral as $n \to \infty$?

$\boxed{\text{Proceed in theoretical and practical directions.}}$

Numerical Quadrature

- Introduction

$\Rightarrow$ Riemann Integration

- Composite Trapezoid Rule
- Composite Simpson's Rule
- Guassian Quadrature

Riemann Integrability

- $f \in C^0([a,b])$, $[a,b]$ bdd $\Rightarrow f$ is Riemann integrable
- Counter example: Dirichlet function $d(x) \equiv \begin{cases} 0, & x \text{ rational}, \\ 1, & x \text{ irrational} \end{cases}$

  $\Rightarrow L = 0, \;\; U = b - a$
- When integrable, and max interval in $P \to 0$:

$$\lim_{n\to\infty} L(f;P) = \int_a^b f(x)\,dx = \lim_{n\to\infty} U(f;P)$$

Challenge: Estimate n

- Restrictions for example:
  - $*$ Monotone functions
  - $*$ Uniform partition
- Challenge:
  - $*$ $\int_0^\pi e^{\cos x}\, dx$
  - $*$ error $< \frac{1}{2} \times 10^{-3}$
  - $*$ using L and U
  - $*$ $n = ?$

Estimate n—Solution

- $f(x) = e^{\cos x} \searrow$ on $[0, pi]$ $\therefore m_i = f\left(x_{i+1}\right)$ and $M_i = f(x_i)$
- $\therefore L(f;P) = h \sum_{i=0}^{n-1} f\left(x_{i+1}\right)$ and $U(f;P) = h \sum_{i=0}^{n-1} f(x_i)$
- Want $\frac{1}{2}(U - L) < \frac{1}{2} \times 10^{-3}$ or $\frac{\pi}{n}\left(e^1 - e^{-1}\right) < \times 10^{-3}$
- $\ldots$ $n \geq 7385$ (!!)
- Note: 2 $f(x)$ evaluations for $(U - L)$, but > 7000 for either one

$\boxed{\text{We need something better.}}$

Numerical Quadrature

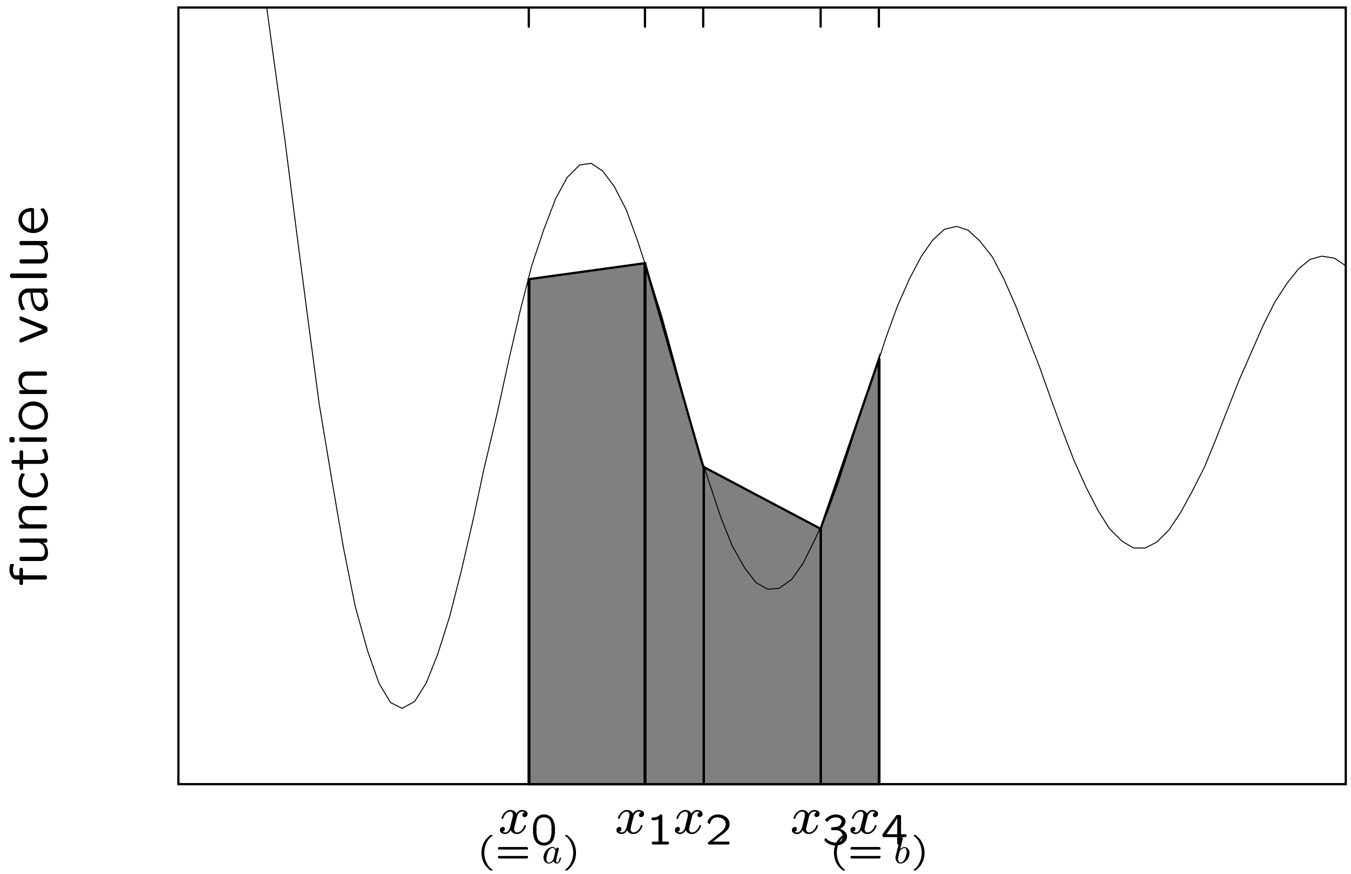
- Introduction
- Riemann Integration
- $\Rightarrow$ Composite Trapezoid Rule
- Composite Simpson's Rule
- Guassian Quadrature

Composite Trapezoid Rule (CTR)

- Each area: $\frac{1}{2}\Big(x_{i+1} - x_i\Big)\Big[f(x_i) + f\Big(x_{i+1}\Big)\Big]$
- Rule: $T(f;P) \equiv \frac{1}{2}\sum_{i=0}^{n-1}\Big(x_{i+1} - x_i\Big)\Big[f(x_i) + f\Big(x_{i+1}\Big)\Big]$
- Note: for monotone functions (any mesh): $T = (U + L)/2$

$\boxed{\text{What does this look like?}}$

CTR—Interpretation



$\boxed{\textit{Almost} \text{ always better than } L \text{ or } U. \text{ (When not?)}}$

Uniform Mesh and Error

- Constant stepsize h

$$T(f;P) \equiv h\left\{\sum_{i=0}^{n-1} f(x_i) + \frac{1}{2}[f(x_0) + f(x_n)]\right\}$$

- Theorem: $f \in C^2([a,b]) \rightarrow \exists \xi \in (a,b) \ni$

$$\int_a^b f(x)\,dx - T(f;P) = -\frac{1}{12}(b-a)h^2 f''(\xi) = O\left(h^2\right)$$

- Note: leads to Romberg algorithm (built on Richardson extrapolation)

$\boxed{\text{How many steps does } T(f;P) \text{ require?}}$

$e^{\cos x}$ Revisited

- Challenge: $\int_0^\pi e^{\cos x}\,dx$, error $< \frac{1}{2} \times 10^{-3}$, using T, $n = ?$
- $f(x) = e^{\cos x} \Rightarrow f'(x) = -e^{\cos x}\sin x \ \ldots \ |f''(x)| \leq e$ on $[0, \pi]$
- $\therefore$ $|\text{error}| < \frac{1}{12}\pi(\pi/n)^2 e < \frac{1}{2} \times 10^{-3}$
- $\ldots \ n \geq 119$
- Recall: monotonic $\therefore$ identical to $(L + U)/2$, *but* L and U used loose error bounds

$$\boxed{\text{Better estimate of } \textit{error} \therefore \text{ better estimate of } n}$$

Another CTR Example

- Challenge: $\int_0^1 e^{-x^2}\,dx$, error $< \frac{1}{2} \times 10^{-4}$, $n = ?$
- $f(x) = e^{-x^2}$, $\Rightarrow$ $f'(x) = -2xe^{-x^2}$ and $f''(x) = \left(4x^2 - 2\right)e^{-x^2}$
- $\therefore\ |f''(x)| \le 2$ on $[0, 1]$
- $\Rightarrow |\text{error}| \le \frac{1}{6}h^2 \le \frac{1}{2} \times 10^{-4}$
- We have: $n^2 \ge \frac{1}{3} \times 10^4$ or $n \ge 58$ subintervals

$\boxed{\text{How can we do better?}}$

Numerical Quadrature

- Introduction
- Riemann Integration
- Composite Trapezoid Rule
- $\Rightarrow$ Composite Simpson's Rule
- Guassian Quadrature

CTR on Two Intervals

- $n = 2$ (i.e., 3 points):

$$\begin{aligned} T(f) &= \frac{b-a}{2}\left\{ f\left(\frac{a+b}{2}\right) + \frac{1}{2}[f(a)+f(b)] \right\} \\ &= \frac{b-a}{4}\left[f(a) + 2f\left(\frac{a+b}{2}\right) + f(b) \right] \end{aligned}$$

  with error $= O\left(\left(\frac{b-a}{2}\right)^2\right)$

- Note: trapezoid rule is integral of linear interpolant on each interval

$$p_1(x) = \frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b)$$

- $\int_a^b p_1(x)\,dx$ calculation ...

Trapezoid Rule as $\int$Interpolant

(Note: this is intuitive.)

$$
\begin{aligned}
\int_a^b p_1(x)\,dx &= \frac{f(a)}{a-b}\int_a^b (x-b)\,dx + \frac{f(b)}{b-a}\int_a^b (x-a)\,dx \\
&= \frac{f(a)}{a-b}\left[\frac{b^2-a^2}{2} - b(b-a)\right] + \frac{f(b)}{b-a}\left[\frac{b^2-a^2}{2} - a(b-a)\right] \\
&= -f(a)\left[\frac{a+b}{2} - b\right] + f(b)\left[\frac{a+b}{2} - a\right] \\
&= -f(a)\left(\frac{a-b}{2}\right) + f(b)\left(\frac{b-a}{2}\right) \\
&= \frac{b-a}{2}(f(a)+f(b))
\end{aligned}
$$

$$\boxed{\text{CTR is integral of composite linear interpolant.}}$$

Simpson's Rule Over Two Intervals

- Motivation: use $p_2(x)$ over the two intervals
- Similar analysis actually loses $O(h)$, but ... $\exists \xi \in (a,b) \ni$

$$\int_a^b f(x)\,dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\xi)$$

- Similar to CTR, but weights midpoint more
- Note: for each method, denominator $= \sum$ coefficients

$\boxed{\text{Each method multiplies width by weighted average of height.}}$

Composite Simpson's Rule (CSR)

- For n even intervals, $h = \frac{b-a}{n}$, $\exists \xi \in (a,b) \ni$

$$\int_a^b f(x)\,dx = \frac{h}{3}\Bigg\{[f(a)+f(b)] + 4\sum_{i=1}^{n/2} \underbrace{f[a+(2i-1)h]}_{\text{interval midpoints}} + 2\sum_{i=1}^{(n-2)/2} \underbrace{f(a+2ih)}_{\text{internal interval boundaries}}\Bigg\} - \frac{b-a}{180} h^4 f^{(4)}(\xi)$$

- Note: denominator $= \sum$ coefficients $= 3n$ (but $2n+1$ function evaluations)

- Another accuracy angle: error $= 0\ \forall f \in P_3$

$$\boxed{\text{Can we do better than } P_3\text{?}}$$

Integration Introspection

- Simpson beat CTR (for $n = 2$) because heavier weighted midpoint

- But CSR similarly suffers at interval boundaries (weight $=$ 2 vs. 4)

- All composite rules
  - ∗ patch together local calculations
  - ∗ $\therefore$ will suffer from this

- What about higher degree interpolation?

- Also: we are choosing
  - ∗ calculation nodes
  - ∗ weights

Numerical Quadrature

- Introduction
- Riemann Integration
- Composite Trapezoid Rule
- Composite Simpson's Rule

$\Rightarrow$ Guassian Quadrature

Interpolatory Quadrature

- $x_i, \ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \dfrac{x - x_j}{x_i - x_j}, \; i = 0, \cdots, n, \; p(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x)$

- If $f(x) \approx p(x) \Rightarrow$ hopefully $\int_a^b f(x)\,dx \approx \int_a^b p(x)\,dx$

- $\int_a^b p(x)\,dx = \int_a^b \sum_{i=0}^{n} f(x_i)\ell_i(x)\,dx = \sum_{i=0}^{n} f(x_i) \underbrace{\int_a^b \ell_i(x)\,dx}_{\equiv A_i}$

- $A_i = A_i\Big(a, b; \{x_j\}_{j=0}^{n}\Big)$, but $A_i \neq A_i(f)$!

$$\boxed{\text{(Endpoints, nodes)} \Rightarrow A_i \Rightarrow \int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i).}$$

Interp. Quad.—Error Analysis

- $\forall f \in P_n \Rightarrow f(x) = p(x)$, and $\therefore$
  $\forall f \in P_n \Rightarrow \int_a^b f(x)\,dx = \sum_{i=0}^{n} A_i f(x_i)$, i.e., error $= 0$
- $n + 1$ weights determined by nodes x_i (and a and b)
- True for *any* choice of $n + 1$ nodes x_i
- What if we choose $n + 1$ *specific* nodes (with weights, total: $2(n + 1)$ choices)?

$$\boxed{\text{Can we get error} = 0 \ \forall f \in P_{2n+1}?}$$

Gaussian Quadrature (GQ)—Theorem

- Let
  - $q(x) \in P_{n+1} \ni \int_a^b x^k q(x)\, dx = 0, \;\; k = 0, \cdots, n$
    i.e., $q(x) \perp$ all polynomials of lower degree
  - $x_i, i = 0, \cdots, n, \ni q(x_i) = 0$
    i.e., x_i are zeros of $q(x)$

- Then $\forall f \in P_{2n+1}$

$$\int_a^b f(x)\, dx = \sum_{i=0}^{n} A_i f(x_i)$$

$$\boxed{\text{We jumped from } P_n \text{ to } P_{2n+1}!}$$

Gaussian Quadrature—Proof

- Let $f \in P_{2n+1}$, and divide by $q \ni f = pq + r \therefore p, r \in P_n$
- We have

$$\begin{aligned}
\int_a^b f(x)\,dx &= \int_a^b p(x)q(x)\,dx + \int_a^b r(x)\,dx && \text{(division above)} \\
&= \int_a^b r(x)\,dx && (\perp' \text{ity of } q(x)) \\
&= \sum_{i=0}^{n} A_i r(x_i) && (r \in P_n) \\
&= \sum_{i=0}^{n} A_i [f(x_i) - p(x_i)q(x_i)] && \text{(division above)} \\
&= \sum_{i=0}^{n} A_i f(x_i) && (x_i \text{ are zeros of } q(x))
\end{aligned}$$

■

GQ—Additional Notes

- Example $q_n(x)$: Legendre Polynomials: for $[a,b]=[-1,1]$ and $q_n(1)=1$ ($\exists$ a 3-term recurrence formula)

$$q_0(x)=1,\;\; q_1(x)=x,\;\; q_2(x)=\frac{3}{2}x^2-\frac{1}{2},\;\; q_3(x)=\frac{5}{2}x^3-\frac{3}{2}x,\cdots$$

- Gaussian nodes $\in (a,b) \Rightarrow$

  good if $f(a)=\infty$ and/or $f(b)=\infty$ (e.g., $\displaystyle\int_0^1 \frac{1}{\sqrt{x}}\,dx$)

- More general: with weight function $w(x)$ in
  - $*$ original integral
  - $*$ $q(x)$ orthogonality
  - $*$ weights A_i

Numerical Quadrature—Summary

(n intervals)

	# func. evals	node placement	error $= 0\ \forall P_{\square}$
CTR	$n+1$	uniform	1
CSR	$2n+1$	uniform	3
interp.	$n+1$	any (distinct)	n
GQ	$n+1$	zeros of $q(x)$	$2n+1$