

Review of Splines: Given $n + 1$ distinct points

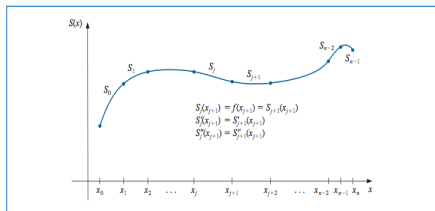
$$(x_0, f(x_0)), (x_1, f(x_1)), \dots, (x_n, f(x_n)),$$

- Find *cubic spline interpolant* $S(x) \in C^2[x_0, x_n]$,

$$S(x) = S_j(x) \stackrel{\text{def}}{=} a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3,$$

for $x \in [x_j, x_{j+1}]$, $0 \leq j \leq n - 1$.

- $S(x_j) = f(x_j)$, $0 \leq j \leq n$.



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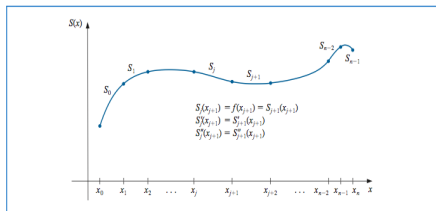
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- $S(x_j) = f(x_j)$, $0 \leq j \leq n$.



- **Fake spine:** $S_n(x) \stackrel{\text{def}}{=} a_n + b_n(x - x_n) + c_n(x - x_n)^2$, for $x \geq x_n$
- **Natural Splines:** $S''_0(x_0) = S''_{n-1}(x_n) = 0$.

Clamped Splines: $S'_0(x_0) = f'(x_0)$, $S'_{n-1}(x_n) = f'(x_n)$

Recall $n + 1$ variables in c with $n - 1$ equations:

$$h_{j-1} c_{j-1} + 2(h_{j-1} + h_j) c_j + h_j c_{j+1} = 3 \left(\frac{a_{j+1} - a_j}{h_j} - \frac{a_j - a_{j-1}}{h_{j-1}} \right), \quad j = 1, \dots, n - 1$$

where for $j = 0, 1, \dots, n - 1$

$$b_j = -\frac{h_j}{3}(2c_j + c_{j+1}) + \frac{a_{j+1} - a_j}{h_j} \cdot (\hat{\ell}_0)$$

$$b_{j+1} = b_j + h_j(c_j + c_{j+1}). \quad (\hat{\ell}_1)$$

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$$\text{Equation for } c_0, c_1: f'(x_0) = S'_0(x_0) = b_0 \stackrel{(\widehat{\ell}_0)}{=} -\frac{h_0}{3}(2c_0 + c_1) + \frac{a_1 - a_0}{h_0}.$$

$$2h_0 c_0 + h_0 c_1 = 3 \left(\frac{a_1 - a_0}{h_0} - f'(x_0) \right).$$

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$$2h_0 c_0 + h_0 c_1 = 3 \left(\frac{a_1 - a_0}{h_0} - f'(x_0) \right).$$

$$\begin{aligned} \text{For } c_{n-1}, c_n: f'(x_n) &= S'_{n-1}(x_n) = b_n \stackrel{(\widehat{\ell}_1)}{=} b_{n-1} + h_{n-1}(c_{n-1} + c_n) \\ &\stackrel{(\widehat{\ell}_0)}{=} -\frac{h_{n-1}}{3}(2c_{n-1} + c_n) + \frac{a_n - a_{n-1}}{h_{n-1}} + h_{n-1}(c_{n-1} + c_n) \end{aligned}$$

$$\text{or: } h_{n-1} c_{n-1} + 2h_{n-1} c_n = 3 \left(f'(x_n) - \frac{a_n - a_{n-1}}{h_{n-1}} \right)$$

Clamped Splines: equations in matrix form

- Equations for $\{c_j\}_{j=0}^n$,

$$\begin{pmatrix} 2h_0 & h_0 & & & & \\ h_0 & 2(h_0 + h_1) & & & & \\ & & \ddots & & & \\ & & & h_{n-2} & 2(h_{n-2} + h_{n-1}) & h_{n-1} \\ & & & & h_{n-1} & 2h_{n-1} \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{n-1} \\ c_n \end{pmatrix} = 3 \begin{pmatrix} \frac{a_1 - a_0}{h_0} - f'(x_0) \\ \frac{a_2 - a_1}{h_1} - \frac{a_1 - a_0}{h_0} \\ \vdots \\ \frac{a_n - a_{n-1}}{h_{n-1}} - \frac{a_{n-1} - a_{n-2}}{h_{n-2}} \\ f'(x_n) - \frac{a_n - a_{n-1}}{h_{n-1}} \end{pmatrix}.$$

- Equations for $\{d_j\}_{j=0}^{n-1}, \{b_j\}_{j=0}^{n-1}$,

$$d_j = \frac{c_{j+1} - c_j}{3h_j}, \quad \text{and} \quad b_j = -\frac{h_j}{3}(2c_j + c_{j+1}) + \frac{a_{j+1} - a_j}{h_j}.$$

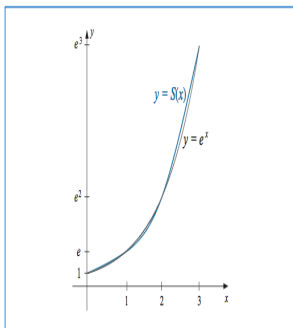
Clamped Splines

```
function Splines = ClampedSplines(x,f,df)
%
% This code implements the clamped splines
%
% Written by Ming Gu for Math 128A, Fall 2008
% Updated by Ming Gu for Math 128A, Spring 2015
%
n = length(x);
h = diff(x(:));
rhs = 3 * diff([df(1);diff(f(:))./h;df(2)]);

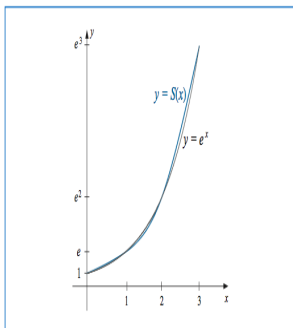
A = diag(h,1)+diag(h,-1)+2*diag([[0;h]+[h;0]]);

%
% compute the c coefficients. This is a simple
% but very slow way to do it.
%
c      = A \ rhs;
d      = (diff(c)./h)/3;
b      = diff(f(:))./h-(h/3).*(2*c(1:n-1)+c(2:n));
Splines.a = f(:);
Splines.b = b;
Splines.c = c;
Splines.d = d;
```

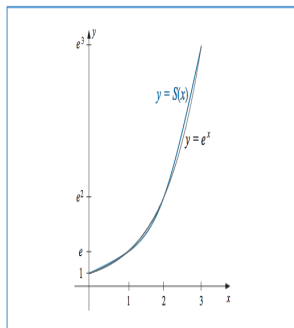
Natural Splines, $f(x) = e^x$,
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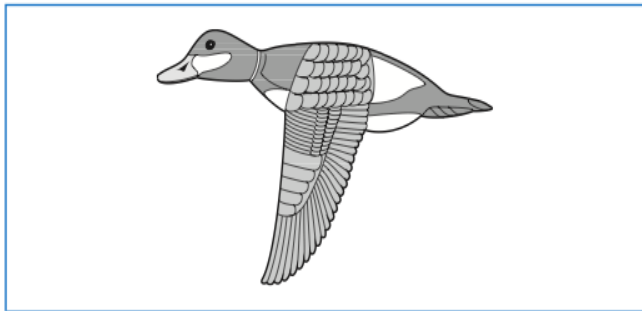


Clamped Splines, $f(x) = e^x$,
 $x_0 = 0, x_1 = 1, x_2 = 2,$
 $x_3 = 3, f'(0) = 1, f'(3) = e^3$



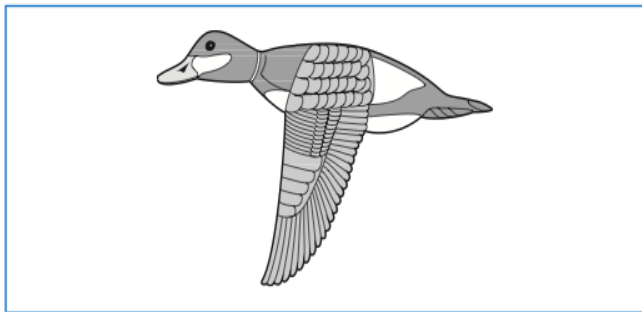
A duck in Splines: to approximate its top profile

- ▶ A duck in flight



A duck in Splines: to approximate its top profile

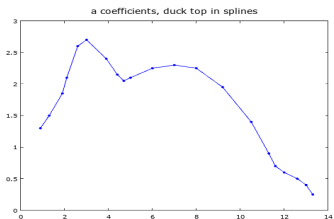
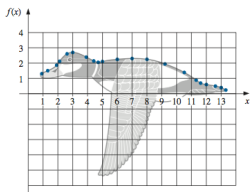
- ▶ A duck in flight



x	0.9	1.3	1.9	2.1	2.6	3.0	3.9	4.4	4.7	5.0	6.0	7.0	8.0	9.2	10.5	11.3	11.6	12.0	12.6	13.0	13.3
$f(x)$	1.3	1.5	1.85	2.1	2.6	2.7	2.4	2.15	2.05	2.1	2.25	2.3	2.25	1.95	1.4	0.9	0.7	0.6	0.5	0.4	0.25

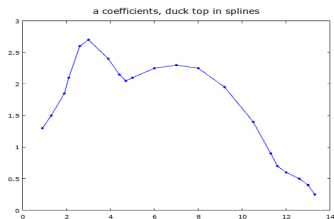
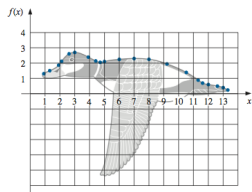
Duck top profile

- Natural Splines, $\{a_k\}$ coefficients

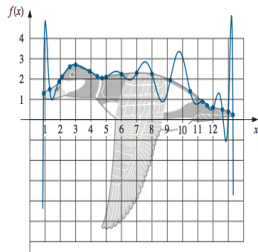


Duck top profile

- Natural Splines, $\{a_k\}$ coefficients



- 20-degree polynomial interpolation



§3.6 Parametric Curve Approximation: $x = x(t)$, $y = y(t)$

- Given $n + 1$ distinct points

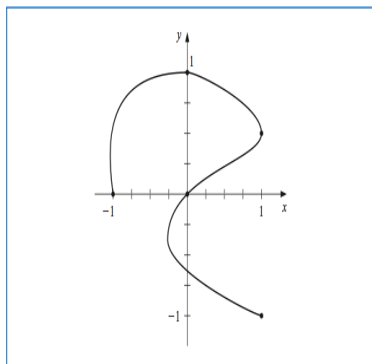
$$(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n),$$

where

$$x_j = x(t_j), \quad y_j = y(t_j), \quad j = 0, 1, \dots, n.$$

- Example

i	0	1	2	3	4
t_i	0	0.25	0.5	0.75	1
x_i	-1	0	1	0	1
y_i	0	1	0.5	0	-1

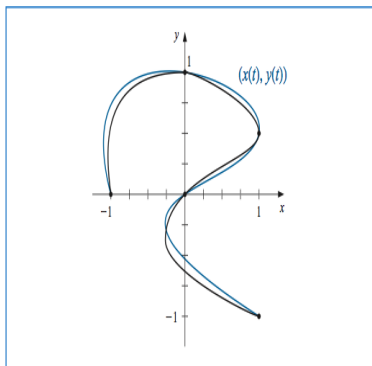


Parametric Curve with Polynomial Interpolation

- 4th degree interpolation on both $x = x(t)$ and $y = y(t)$.

$$x(t) = \left(\left(\left(64t - \frac{352}{3} \right) t + 60 \right) t - \frac{14}{3} \right) t - 1,$$

$$y(t) = \left(\left(\left(-\frac{64}{3}t + 48 \right) t - \frac{116}{3} \right) t + 11 \right) t.$$

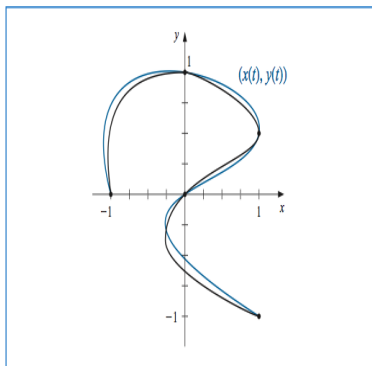


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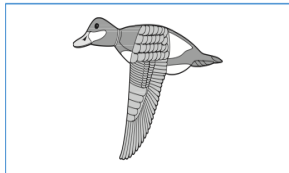
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Would like a better fit

Bezier Curves in Computer Graphics

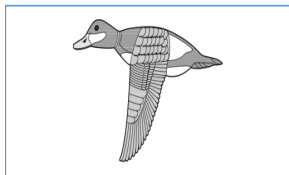
- ▶ **Design:** Piece-wise cubic Hermite polynomials.
- ▶ **Feature:** Each cubic Hermite polynomial is completely determined by function/derivative at endpoints.
- ▶ **Consequence:**, Each portion of the curve can be changed while leaving most of the curve the same.



As duck flies, parametric curve can effectively evolve.

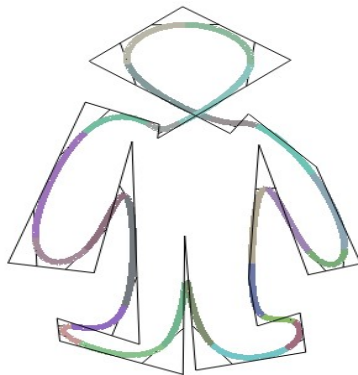
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▶ Bezier Curves with GUIDE POINTS



https://www.youtube.com/watch?v=TeXajQ62yZ8&ab_channel=corex

Parametric Curves: Piece-wise cubic Hermite polynomials

- ▶ **Given (I):** $n + 1$ data points $(x(t_0), y(t_0)), \dots, (x(t_n), y(t_n))$.
- ▶ **Given (II):** $n + 1$ derivatives $\frac{dy}{dx} \Big|_{t=t_i}, 0 \leq i \leq n$.

- ▶ **Find:** $2 \times n$ pieces of cubic Hermite polynomials:

$$x = x_i(t), \quad y = y_i(t), \quad \text{for } i \in [t_i, t_{i+1}], \quad 0 \leq i \leq n,$$

such that

$$\begin{pmatrix} x_i(t_i) \\ y_i(t_i) \end{pmatrix} = \begin{pmatrix} x(t_i) \\ y(t_i) \end{pmatrix}, \quad \begin{pmatrix} x_i(t_{i+1}) \\ y_i(t_{i+1}) \end{pmatrix} = \begin{pmatrix} x(t_{i+1}) \\ y(t_{i+1}) \end{pmatrix},$$
$$\frac{dy}{dx} \Big|_{t=t_i} = \frac{y'_i(t_i)}{x'_i(t_i)}, \quad \text{and} \quad \frac{dy}{dx} \Big|_{t=t_{i+1}} = \frac{y'_i(t_{i+1})}{x'_i(t_{i+1})}$$

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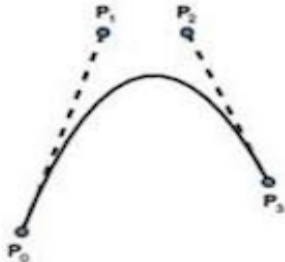
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- ▶ 8 parameters in $x_i(t), y_i(t)$
- ▶ only 6 given conditions for each i
- ▶ use guidepoints

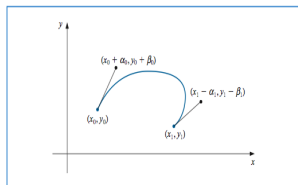


Cubic Bézier Curve

Guidepoints guide slopes (for $[t_i, t_{i+1}] = [0, 1]$)

- Unique cubic Hermite polynomials $x(t), y(t)$ with

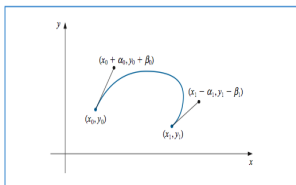
$$\begin{pmatrix} x(0) \\ y(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, \quad \begin{pmatrix} x(1) \\ y(1) \end{pmatrix} = \begin{pmatrix} x_1 \\ y_1 \end{pmatrix},$$
$$\begin{pmatrix} x'(0) \\ y'(0) \end{pmatrix} = \begin{pmatrix} \alpha_0 \\ \beta_0 \end{pmatrix}, \quad \begin{pmatrix} x'(1) \\ y'(1) \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix}$$



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- Guidepoints

$$(x_0 + \alpha_0, y_0 + \beta_0) \text{ and } (x_1 - \alpha_1, y_1 - \beta_1)$$

- Guidepoints guide slopes

$$\frac{dy}{dx} \Big|_{t=0} = \frac{\beta_0}{\alpha_0}, \quad \text{and} \quad \frac{dy}{dx} \Big|_{t=1} = \frac{\beta_1}{\alpha_1}.$$

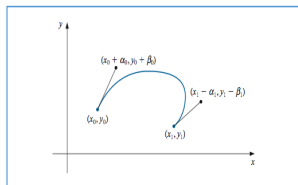
- two degrees of freedom in guidepoints

$$\beta_0 = \alpha_0 \left(\frac{dy}{dx} \Big|_{t=0} \right), \quad \text{and} \quad \beta_1 = \alpha_1 \left(\frac{dy}{dx} \Big|_{t=1} \right)$$

Guidepoints guide slopes (for $[t_i, t_{i+1}] = [0, 1]$)

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- Guidepoints

$$(x_0 + \alpha_0, y_0 + \beta_0) \text{ and } (x_1 - \alpha_1, y_1 - \beta_1)$$

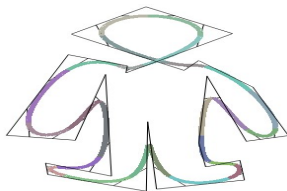
- Guidepoints guide slopes

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- choice of guidepoints changes curve shapes



```
function [bx,by] = Bezier(x,y,alpha,beta,alpha,beta)

n = length(x);

bx = zeros(n-1,4);

by = zeros(n-1,4);

bx=[x(1:n-1),alpha(1:n-1),x(2:n)-x(1:n-1)-alpha(1:n-1),
2*(x(2:n)-x(1:n-1))-(alpha(1:n-1)+alpha(2:n))];

by=[y(1:n-1),beta(1:n-1),y(2:n)-y(1:n-1)-beta(1:n-1),
2*(y(2:n)-y(1:n-1))-(beta(1:n-1)+beta(2:n))];
```

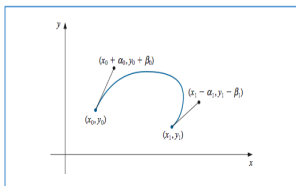

Guidepoints guide slopes: example

- Unique cubic Hermite polynomials $x(t)$, $y(t)$ with

$$\begin{pmatrix} x(0) \\ y(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} x(1) \\ y(1) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

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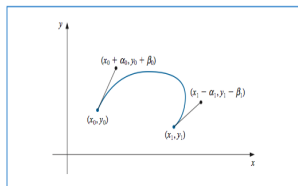
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- Guidepoints guide slopes

$$\frac{dy}{dx} \Big|_{t=0} = \frac{\beta_0}{\alpha_0} = 1, \quad \text{and} \quad \frac{dy}{dx} \Big|_{t=1} = \frac{\beta_1}{\alpha_1} = -1.$$

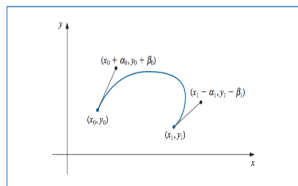
Guidepoints guide slopes: example

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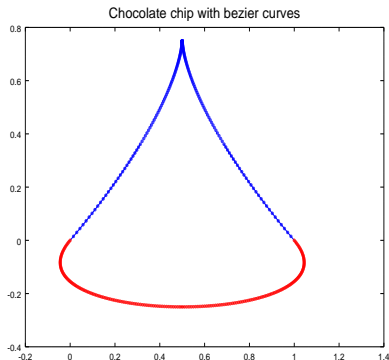
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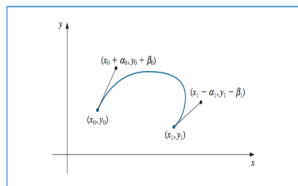
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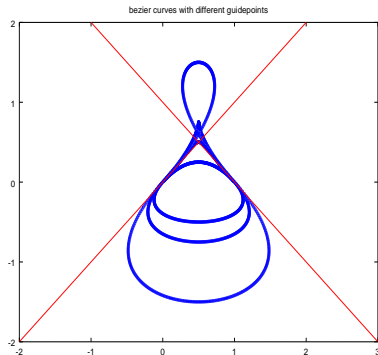
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Parametric Curves: Summary of approaches

- ▶ **Given (I):** $n + 1$ data points $(x(t_0), y(t_0)), \dots, (x(t_n), y(t_n))$.
- ▶ **Given (II):** $n + 1$ derivatives $\frac{dy}{dx} \big|_{t=t_i}, 0 \leq i \leq n$.

Approaches

- ▶ Polynomial interpolations with $n + 1$ data points $(x(t_0)), \dots, (x(t_n))$ and $(y(t_0)), \dots, (y(t_n))$, respectively.
(likely to be unreliable)
- ▶ Splines approximations with $n + 1$ data points $(x(t_0)), \dots, (x(t_n))$ and $(y(t_0)), \dots, (y(t_n))$, respectively.
(more reliable and more computational cost)
- ▶ Bezier curves with Hermite polynomials
(more reliable and less computational cost)

Neural Networks have changed the story

curve fitting

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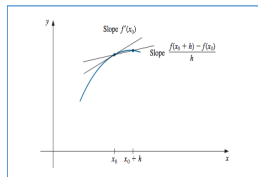
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§4.1 Numerical Differentiation

Derivative of given function $f(x)$ at x_0

$$\begin{aligned} f'(x_0) &= \lim_{h \rightarrow 0} \frac{f(x_0 + h) - f(x_0)}{h} \\ &\approx \frac{f(x_0 + h) - f(x_0)}{h}, \quad |h| \text{ tiny} \end{aligned}$$

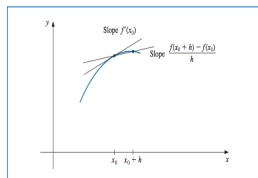


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By Taylor expansion, there is a ξ between x_0 and $x_0 + h$,

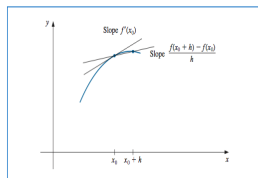
$$f(x_0 + h) = f(x_0) + h f'(x_0) + \frac{1}{2} h^2 f''(\xi),$$

$$\text{therefore } f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{1}{2} h f''(\xi)$$

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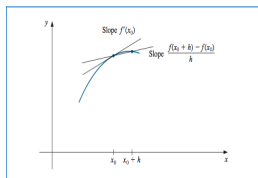
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- ▶ **forward-difference formula** for $h > 0$,
- ▶ **backward-difference formula** for $h < 0$.

Numerical Differentiation, example

Example: Use the forward-difference formula to approximate the derivative of $f(x) = \ln(x)$ at $x_0 = 1.8$, using $h = 0.1, 0.05, 0.01$.

Because $f''(\xi) = -1/\xi^2$ for $\xi \in [x_0, x_0 + h] \subset [1.8, 1.9]$, it follows that the approximation error

$$\frac{1}{2} |h f''(\xi)| \leq \frac{1}{2} \left| \frac{h}{1.8^2} \right|.$$

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h	$f(1.8 + h)$	$\frac{f(1.8 + h) - f(1.8)}{h}$	$\frac{ h }{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.05	0.61518564	0.5479795	0.0077160
0.01	0.59332685	0.5540180	0.0015432

Numerical Differentiation, via polynomial interpolation

Suppose that $\{x_0, x_1, \dots, x_n\}$ are $n + 1$ distinct numbers,

$$f(x) = \left(\sum_{j=0}^n f(x_j) L_j(x) \right) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^n (x - x_i), \quad L_j(x) = \prod_{i \neq j} \frac{(x - x_i)}{(x_j - x_i)},$$

for some $\xi(x)$.

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for some $\xi(x)$. So

$$\begin{aligned} f'(x) = & \left(\sum_{j=0}^n f(x_j) L'_j(x) \right) + \left(\frac{f^{(n+1)}(\xi(x))}{(n+1)!} \right) \frac{d}{dx} \left(\prod_{i=0}^n (x - x_i) \right) \\ & + \frac{d}{dx} \left(\frac{f^{(n+1)}(\xi(x))}{(n+1)!} \right) \left(\prod_{i=0}^n (x - x_i) \right). \end{aligned}$$

Last term messy, but $= 0$ for $x = x_k, k = 0, 1, \dots, n$

Numerical Differentiation, via polynomial interpolation

$$\begin{aligned}f'(x_k) &= \left(\sum_{j=0}^n f(x_j) L'_j(x_k) \right) + \left(\frac{f^{(n+1)}(\xi(x_k))}{(n+1)!} \right) \left(\prod_{i \neq k} (x_k - x_i) \right) \\ &\approx \sum_{j=0}^n f(x_j) L'_j(x_k).\end{aligned}$$

$(n+1)$ -point formula, works (in theory) for any nodal choices.

2-point formulas ($n = 1$), $j = 0, 1$

$$\begin{aligned} L_0(x) &= \frac{x - x_1}{x_0 - x_1}, & L'_0(x) &= \frac{1}{x_0 - x_1}, \\ L_1(x) &= \frac{x - x_0}{x_1 - x_0}, & L'_1(x) &= \frac{1}{x_1 - x_0} = -L'_0(x) \end{aligned}$$

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$$\text{So } f'(x_0) \approx f(x_0) L'_0(x_0) + f(x_1) L'_1(x_0) = \frac{f(x_1) - f(x_0)}{x_1 - x_0},$$

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$$\text{where } L'_j(x_k) = \begin{cases} \frac{1}{x_j - x_k} \prod_{i \neq j, k} \frac{(x_k - x_i)}{(x_j - x_i)}, & \text{for } k \neq j, \\ \sum_{i \neq j} \frac{1}{x_j - x_i} & \text{for } k = j. \end{cases}$$

$(n+1)$ -point formula, works for any nodal choices.

3-point formulas ($n = 2$), equi-spaced nodes

Choose $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, with $h \neq 0$.

$$\begin{aligned}f'(x_0) &= \frac{1}{2h} (-3f(x_0) + 4f(x_1) - f(x_2)) + \frac{h^2}{3} f^{(3)}(\xi_0) \\&= \frac{1}{2h} (-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)) + \frac{h^2}{3} f^{(3)}(\xi_0)\end{aligned}$$

$$f'(x_0 + h) = \frac{1}{2h} (-f(x_0) + f(x_0 + 2h)) - \frac{h^2}{6} f^{(3)}(\xi_1)$$

$$f'(x_0 + 2h) = \frac{1}{2h} (f(x_0) - 4f(x_0 + h) + 3f(x_0 + 2h)) + \frac{h^2}{3} f^{(3)}(\xi_2)$$

Second order derivatives, equi-spaced points

$$\begin{aligned}f(x_0 + h) &= f(x_0) + f'(x_0) h + \frac{1}{2} f''(x_0) h^2 + \frac{1}{6} f'''(x_0) h^3 \\&\quad + \frac{1}{24} f^{(4)}(\xi_+) h^4,\end{aligned}$$

$$\begin{aligned}f(x_0 - h) &= f(x_0) - f'(x_0) h + \frac{1}{2} f''(x_0) h^2 - \frac{1}{6} f'''(x_0) h^3 \\&\quad + \frac{1}{24} f^{(4)}(\xi_-) h^4.\end{aligned}$$

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Adding up, terms with difference signs cancel,

$$\begin{aligned}f(x_0 + h) + f(x_0 - h) &= 2f(x_0) + f''(x_0) h^2 + \frac{h^4}{24} \left(f^{(4)}(\xi_+) + f^{(4)}(\xi_-) \right) \\&= 2f(x_0) + f''(x_0) h^2 + \frac{2h^4}{24} f^{(4)}(\xi).\end{aligned}$$

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Therefore

$$f''(x_0) = \frac{f(x_0 + h) + f(x_0 - h) - 2f(x_0)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi).$$

Round-Off Error Instability: example

Three-point midpoint formula

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi).$$

- ▶ every computation incurs round-off error.
- ▶ division by $2h$ magnifies round-off error
- ▶ assume round-off error model

$$f(x_0 + h) = \widehat{f}(x_0 + h) + e(x_0 + h)$$

$$f(x_0 - h) = \widehat{f}(x_0 - h) + e(x_0 - h)$$

for $|e(x_0 + h)| \leq \epsilon$, $|e(x_0 - h)| \leq \epsilon$

- ▶ no other round-off errors

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It follows

$$\begin{aligned}f'(x_0) - \frac{\widehat{f}(x_0 + h) - \widehat{f}(x_0 - h)}{2h} &= \frac{e(x_0 + h) - e(x_0 - h)}{2h} - \frac{h^2}{6}f^{(3)}(\xi) \\ \left| f'(x_0) - \frac{\widehat{f}(x_0 + h) - \widehat{f}(x_0 - h)}{2h} \right| &\leq \left| \frac{e(x_0 + h) - e(x_0 - h)}{2h} \right| + \frac{h^2}{6}|f^{(3)}(\xi)|\end{aligned}$$

Round-Off Error Instability: example

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- ▶ assume an upper bound: $|f^{(3)}(\xi)| \leq M$

$$\left| f'(x_0) - \frac{\widehat{f}(x_0 + h) - \widehat{f}(x_0 - h)}{2h} \right| \leq \frac{\epsilon}{h} + \frac{M h^2}{6} \stackrel{\text{def}}{=} e(h).$$

Round-Off Error Instability: example

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- ▶ $e(h)$ too big as $h \rightarrow 0^+$

Round-Off Error Instability: optimal h choice

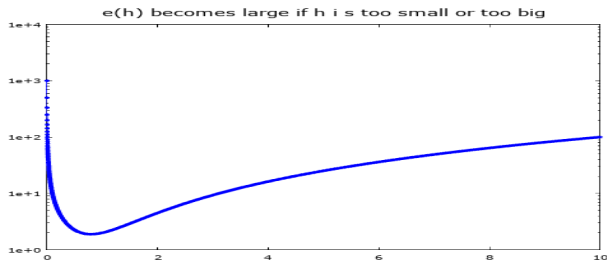
$$e(h) = \frac{\epsilon}{h} + \frac{M h^2}{6}$$

is smallest at

$$h_{\min} = \left(\frac{3\epsilon}{M} \right)^{\frac{1}{3}} = O\left(\epsilon^{\frac{1}{3}}\right),$$

with

$$e(h_{\min}) = \frac{1}{2} (9 M \epsilon^2)^{\frac{1}{3}} = O\left(\epsilon^{\frac{2}{3}}\right).$$



§4.2 Richardson's Extrapolation

- ▶ **Given (I):** A formula $N_1(h)$ that approximates an unknown constant M for any $h \neq 0$.

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- ▶ **Given (II):** Truncation error satisfies power series for $h \neq 0$

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots = O(h), \quad (1)$$

with (unknown) constants K_1, K_2, K_3, \dots .

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$$\left(\text{EXAMPLE: } f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h} \right)$$

- ▶ **Given (II):** Truncation error satisfies power series for $h \neq 0$

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \dots = O(h), \quad (1)$$

with (unknown) constants K_1, K_2, K_3, \dots .

$$\left(f'(x_0) - \frac{f(x_0+h) - f(x_0)}{h} = -\frac{1}{2} h f''(x_0) - \dots - \frac{1}{n!} h^{n-1} f^{(n)}(x_0) - \dots \right)$$

Goal: Generate higher order approximations

- ▶ **Key:** Equation (1) works for *any* $h \neq 0$, including $\frac{h}{2}$.

Extrapolation, Step I

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \dots, \quad (1)$$

$$M - N_1\left(\frac{h}{2}\right) = K_1\left(\frac{h}{2}\right) + K_2\left(\frac{h}{2}\right)^2 + K_3\left(\frac{h}{2}\right)^3 + \dots. \quad (2)$$

(2) $\times 2$ - (1):

$$\begin{aligned} M - N_2(h) &= -\frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \dots - (1 - 2^{-(t-1)})K_t h^t - \dots, \\ &\stackrel{\text{def}}{=} \hat{K}_2 h^2 + \hat{K}_3 h^3 + \dots \hat{K}_t h^t + \dots = O(h^2), \end{aligned} \quad (3)$$

$$\text{where } N_2(h) = N_1\left(\frac{h}{2}\right) + \left(N_1\left(\frac{h}{2}\right) - N_1(h)\right).$$

Equation (3) again power series, but now 2nd order.

Extrapolation, Step II

$$M - N_2(h) = \hat{K}_2 h^2 + \hat{K}_3 h^3 + \cdots \hat{K}_t h^t + \cdots, \quad (3)$$

$$M - N_2\left(\frac{h}{2}\right) = \hat{K}_2 \left(\frac{h}{2}\right)^2 + \hat{K}_3 \left(\frac{h}{2}\right)^3 + \cdots. \quad (4)$$

$$\frac{(4) \times 2^2 - (3)}{2^2 - 1}:$$

$$M - N_3(h) = -\frac{\hat{K}_3}{6} h^3 - \cdots - \frac{1 - 2^{-(t-2)}}{3} \hat{K}_t h^t - \cdots, \quad (5)$$

$$\text{where } N_3(h) \stackrel{\text{def}}{=} N_2\left(\frac{h}{2}\right) + \frac{N_2\left(\frac{h}{2}\right) - N_2(h)}{3}.$$

Equation (5) is one more power series, but 3rd order.

Extrapolation, Step III

- Assume

$$M - N_j(h) = \hat{K}_j h^j + \hat{K}_{j+1} h^{j+1} + \dots \hat{K}_t h^t + \dots ,$$

- replace h by $h/2$:

$$M - N_j\left(\frac{h}{2}\right) = \hat{K}_j \left(\frac{h}{2}\right)^j + \hat{K}_{j+1} \left(\frac{h}{2}\right)^{j+1} + \dots \hat{K}_t \left(\frac{h}{2}\right)^t + \dots .$$

$$\frac{\text{second equation} \times 2^j - \text{first equation}}{2^j - 1}:$$

$$M - N_{j+1}(h) = -\frac{\hat{K}_{j+1}}{2(2^j - 1)} h^{j+1} - \dots = O(h^{j+1}),$$

$$\text{where } N_{j+1}(h) \stackrel{\text{def}}{=} N_j\left(\frac{h}{2}\right) + \frac{N_j\left(\frac{h}{2}\right) - N_j(h)}{2^j - 1}.$$

Richardson's Extrapolation Table

$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^4)$
$N_1(h) \searrow$ \rightarrow			
$N_1(\frac{h}{2}) \searrow$ \rightarrow	$N_2(h) \searrow$ \rightarrow		
$N_1(\frac{h}{4}) \searrow$ \rightarrow	$N_2(\frac{h}{2}) \searrow$ \rightarrow	$N_3(h) \searrow$ \rightarrow	
$N_1(\frac{h}{8}) \rightarrow$	$N_2(\frac{h}{4}) \rightarrow$	$N_3(\frac{h}{2}) \rightarrow$	$N_4(h)$

Richardson's Extrapolation: even power series

- ▶ **Given (I):** A formula $N_1(h)$ that approximates an unknown constant M for any $h \neq 0$.
- ▶ **Given (II):** Truncation error satisfies even power series

$$M - N_1(h) = K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots = O(h^2), \quad (1)$$

with (unknown) constants K_1, K_2, K_3, \dots .

Goal: Generate higher order approximations

- ▶ **Key:** Equation (1) works for *any* h , including $\frac{h}{2}$.

Even power extrapolation, Step I

$$M - N_1(h) = K_1 h^2 + K_2 h^4 + K_3 h^6 + \dots, \quad (1)$$

$$M - N_1\left(\frac{h}{2}\right) = K_1\left(\frac{h}{2}\right)^2 + K_2\left(\frac{h}{2}\right)^4 + K_3\left(\frac{h}{2}\right)^6 + \dots. \quad (2)$$

$$\frac{(2) \times 2^2 - (1)}{2^2 - 1}:$$

$$\begin{aligned} M - N_2(h) &= -\frac{K_2}{4} h^4 - \frac{5K_3}{16} h^6 - \dots - \frac{1 - 2^{-2(t-1)}}{3} K_t h^{2t} - \dots, \\ &\stackrel{\text{def}}{=} \hat{K}_2 h^4 + \hat{K}_3 h^6 + \dots \hat{K}_t h^{2t} + \dots = O(h^4), \end{aligned} \quad (3)$$

$$\text{where } N_2(h) = N_1\left(\frac{h}{2}\right) + \frac{N_1\left(\frac{h}{2}\right) - N_1(h)}{3}.$$

Equation (3) again even power series, but now 4th order.

Even extrapolation, Step II

$$M - N_2(h) = \hat{K}_2 h^4 + \hat{K}_3 h^6 + \dots \hat{K}_t h^{2t} + \dots, \quad (3)$$

$$M - N_2\left(\frac{h}{2}\right) = \hat{K}_2 \left(\frac{h}{2}\right)^4 + \hat{K}_3 \left(\frac{h}{2}\right)^6 + \dots. \quad (4)$$

$$\frac{(4) \times 2^4 - (3)}{2^4 - 1}:$$

$$M - N_3(h) = -\frac{\hat{K}_3}{20} h^6 - \dots - \frac{1 - 2^{-2(t-2)}}{15} \hat{K}_t h^{2t} - \dots,$$

$$\text{where } N_3(h) \stackrel{\text{def}}{=} N_2\left(\frac{h}{2}\right) + \frac{N_2\left(\frac{h}{2}\right) - N_2(h)}{15}.$$

One more even power series, but now 6-th order.

Even extrapolation, Step III

- Assume

$$M - N_j(h) = \hat{K}_j h^{2j} + \hat{K}_{j+1} h^{2(j+1)} + \dots \hat{K}_t h^{2t} + \dots ,$$

- replace h by $h/2$:

$$M - N_j\left(\frac{h}{2}\right) = \hat{K}_j \left(\frac{h}{2}\right)^{2j} + \hat{K}_{j+1} \left(\frac{h}{2}\right)^{2(j+1)} + \dots \hat{K}_t \left(\frac{h}{2}\right)^{2t} + \dots .$$

$$\frac{\text{second equation} \times 4^j - \text{first equation}}{4^j - 1}:$$

$$M - N_{j+1}(h) = -\frac{3\hat{K}_{j+1}}{4(4^j - 1)} h^{2(j+1)} - \dots = O\left(h^{2(j+1)}\right),$$

$$\text{where } N_{j+1}(h) \stackrel{\text{def}}{=} N_j\left(\frac{h}{2}\right) + \frac{N_j\left(\frac{h}{2}\right) - N_j(h)}{4^j - 1}.$$

Richardson's Even Extrapolation Table

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
$N_1(h) \searrow$ \rightarrow			
$N_1(\frac{h}{2}) \searrow$ \rightarrow	$N_2(h) \searrow$ \rightarrow		
$N_1(\frac{h}{4}) \searrow$ \rightarrow	$N_2(\frac{h}{2}) \searrow$ \rightarrow	$N_3(h) \searrow$ \rightarrow	
$N_1(\frac{h}{8}) \rightarrow$	$N_2(\frac{h}{4}) \rightarrow$	$N_3(\frac{h}{2}) \rightarrow$	$N_4(h)$

Even extrapolation, example

Consider Taylor expansion for a given function $f(x)$ with $h > 0$:

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \dots + \frac{1}{n!}f^{(n)}(x)h^n + \dots,$$

$$f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 + \dots + \frac{1}{n!}f^{(n)}(x)(-h)^n + \dots.$$

Take the difference:

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \dots + \frac{1}{(2t+1)!}f^{(2t+1)}(x)h^{2t} + \dots.$$

This is an even power series with 2nd order approximation

$$f'(x), \approx N_1(h) \stackrel{\text{def}}{=} \frac{f(x+h) - f(x-h)}{2h}.$$

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4th order approximation

$$\begin{aligned} f'(x) &\approx N_1(h) + \frac{N_1(h) - N_1(2h)}{3} \\ &= \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h}. \end{aligned}$$

Even extrapolation, example

Approximate $f'(2.0)$ with central difference $N_1(0.1)$ and extrapolation $N_2(0.1)$ for $f(x) = xe^x$.

Solution: $f'(x) = (1+x)e^x$, therefore $f'(2.0) = 3e^2 \approx 22.167$.



$$N_1(0.1) = \frac{f(2.1) - f(1.9)}{2 \times 0.1} \approx 22.229.$$



$$N_1(0.2) = \frac{f(2.2) - f(1.8)}{2 \times 0.2} \approx 22.414.$$

$$N_2(0.2) = N_1(h) + \frac{N_1(h) - N_1(2h)}{3} \approx 22.167.$$

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- ▶ covers material up to and include §4.2 (six questions total)
 - ▶ one question each from chapters 1 and 4
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- ▶ You can skip the exam, but this is NOT encouraged
 - ▶ Final worth 50 (as opposed to 30) points if you do skip.
 - ▶ If you submit the exam, it WILL count.



Sample exam problem

- ▶ How many multiplications and additions are required to determine a sum of the form

$$S \stackrel{\text{def}}{=} \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j \quad (1)$$

- ▶ Modify the sum in part (1) to an equivalent form that reduces the number of computations.

Sample exam problem

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$$S \stackrel{\text{def}}{=} \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j \quad (1)$$

- ▶ Modify the sum in part (1) to an equivalent form that reduces the number of computations.

SOLUTION:

- ▶ it takes $m n$ multiplications and $m n$ additions in (1).
- ▶ Rewrite

$$S \stackrel{\text{def}}{=} \left(\sum_{i=1}^n \alpha_i \right) \left(\sum_{j=1}^m \beta_j \right)$$

it takes 1 multiplication and $m + n$ additions.

Sample exam problem

The following two methods are proposed to compute $7^{1/5}$.
Discuss their orders of convergence, assuming $p_0 = 1$.

1. $p_{n+1} = p_n - \frac{p_n^5 - 7}{5p_n^4}$

2. $p_{n+1} = p_n - \frac{p_n^5 - 7}{100}$

Sample exam problem

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2. $p_{n+1} = p_n - \frac{p_n^5 - 7}{100}$

SOLUTION:

1. Newton's method, quadratic convergence.
2. fixed point iteration, linear convergence.

Sample exam problem

A quadratic spline interpolating function S defined with the nodes $x_0 < x_1 < x_2$ is such that S is a quadratic polynomial on each of the intervals $[x_0, x_1]$ and $[x_1, x_2]$, respectively. Assume that $S(x) \in C^2[x_0, x_2]$. Show that S must be a quadratic polynomial on the entire interval $[x_0, x_2]$.

Sample exam problem

A quadratic spline interpolating function S defined with the nodes $x_0 < x_1 < x_2$ is such that S is a quadratic polynomial on each of the intervals $[x_0, x_1]$ and $[x_1, x_2]$, respectively. Assume that $S(x) \in C^2[x_0, x_2]$. Show that S must be a quadratic polynomial on the entire interval $[x_0, x_2]$.

SOLUTION: Parameterize S as

$$S(x) = \begin{cases} a_0 + b_0 (x - x_1) + c_0 (x - x_1)^2, & \text{if } x \in [x_0, x_1], \\ a_1 + b_1 (x - x_1) + c_1 (x - x_1)^2, & \text{if } x \in [x_1, x_2]. \end{cases}$$

The condition that $S(x) \in C^2[x_0, x_2]$ implies that

$$S(x) \Big|_{x=x_1^-} = S(x) \Big|_{x=x_1^+}, \quad S(x)' \Big|_{x=x_1^-} = S(x)' \Big|_{x=x_1^+}, \quad S(x)'' \Big|_{x=x_1^-} = S(x)'' \Big|_{x=x_1^+}$$

This leads to

$$a_0 = a_1, \quad b_0 = b_1, \quad c_0 = c_1$$

§4.3 Numerical Integration: general idea

- ▶ **Goal:** Numerical method /quadrature for approximating $\int_a^b f(x)dx$.

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- ▶ **Goal:** Numerical method / quadrature for approximating $\int_a^b f(x)dx$.
- ▶ **Approach:** Replacing $f(x)$ by a polynomial.
 - ▶ **Choose:** $n + 1$ points $a \leq x_0 < x_1 < \dots < x_n \leq b$.
 - ▶ **Interpolation:**

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{j=0}^n (x - x_j), \quad P(x) = \sum_{j=0}^n f(x_j) L_j(x).$$

- ▶ **Approximate Integration:**

$$\begin{aligned} \int_a^b f(x)dx &= \left(\int_a^b P(x)dx \right) + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi(x)) \prod_{j=0}^n (x - x_j) dx \\ &= \left(\sum_{j=0}^n a_j f(x_j) \right) + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi(x)) \prod_{j=0}^n (x - x_j) dx \\ &\approx \sum_{j=0}^n a_j f(x_j), \end{aligned}$$

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The Trapezoidal Rule: $n = 1$, $x_0 = a$, $x_1 = b$, $h = b - a$.

► **Linear Interpolation:**

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)}f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)}f(x_1),$$
$$f(x) = P_1(x) + \frac{1}{2}f''(\xi(x))(x - x_0)(x - x_1).$$

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► **Quadrature:**

$$\begin{aligned} \int_a^b P_1(x) dx &= \int_a^b \left(\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right) dx \\ &= \frac{1}{2} \left(\frac{(x - x_1)^2}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{(x_1 - x_0)} f(x_1) \right)_{x_0}^{x_1} = \frac{h}{2} (f(x_0) + f(x_1)). \end{aligned}$$

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► **Linear Interpolation:**

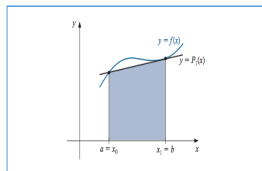
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► **Quadrature:**

$$\begin{aligned}\int_a^b P_1(x)dx &= \int_a^b \left(\frac{(x - x_1)}{(x_0 - x_1)}f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)}f(x_1) \right) dx \\ &= \frac{1}{2} \left(\frac{(x - x_1)^2}{(x_0 - x_1)}f(x_0) + \frac{(x - x_0)^2}{(x_1 - x_0)}f(x_1) \right) \Big|_{x_0}^{x_1} = \frac{h}{2} (f(x_0) + f(x_1)).\end{aligned}$$

$$\begin{aligned}\text{error} &= \int_a^b \frac{1}{2}f''(\xi(x))(x - x_0)(x - x_1)dx \\ &= \frac{f''(\xi)}{2} \int_a^b (x - x_0)(x - x_1)dx \\ &= -\frac{f''(\xi)}{12}(b - a)^3\end{aligned}$$



Simpson's Rule: $n = 2$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

► **Quadratic Interpolation:**

$$P_2(x_j) = f(x_j), \quad j = 0, 1, 2.$$

$$\begin{aligned} P_2(x) = & \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_1)(x - x_0)}{(x_2 - x_1)(x_2 - x_0)} f(x_2) \\ & + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1). \end{aligned}$$

► **Interpolation error:**

$$f(x) = P_2(x) + \frac{1}{3!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)(x - x_2).$$

► **Simpson's Rule and error:**

$$\int_a^b f(x) dx = \int_a^b P_2(x) dx + \int_a^b \left(\frac{1}{3!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)(x - x_2) \right) dx$$

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$$f(x) = P_2(x) + \frac{1}{3!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)(x - x_2).$$

► **Simpson's Rule and error:**

$$\begin{aligned} \int_a^b f(x) dx &= \int_a^b P_2(x) dx + \int_a^b \left(\frac{1}{3!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)(x - x_2) \right) dx \\ &\approx \int_a^b P_2(x) dx = \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2)) \end{aligned}$$

Simpson's Rule: $n = 2$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

► Quadrature Rule

$$\int_a^b f(x) dx \approx \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2))$$

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$$\int_a^b f(x) dx \approx \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2))$$

► Quadrature Error:

$$\frac{1}{3!} \int_a^b f^{(3)}(\xi(x))(x - x_0)(x - x_1)(x - x_2) dx$$

maybe

$$\frac{f^{(3)}(\xi)}{6} \int_a^b (x - x_0)(x - x_1)(x - x_2) dx$$

???

0.

Simpson's Rule: $n = 2$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

► Quadrature Rule

$$\int_a^b f(x) dx \approx \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2))$$

► Quadrature Error:

$$\begin{aligned} & \frac{1}{3!} \int_a^b f^{(3)}(\xi(x))(x-x_0)(x-x_1)(x-x_2) dx \\ \underline{\underline{\text{maybe}}} & \quad \frac{f^{(3)}(\xi)}{6} \int_a^b (x-x_0)(x-x_1)(x-x_2) dx \\ \underline{\underline{???}} & \quad 0. \end{aligned}$$

Error estimate wrong. Need approach better than in book.

Simpson's Rule: $n = 3$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

► **Cubic Interpolation** with double node in x_1 :

$$P_3(x_j) = f(x_j), \quad j = 0, 1, 2; \quad P'_3(x_1) = f'(x_1).$$

$$\begin{aligned} P_3(x) = & \frac{(x - x_1)^2(x - x_2)}{(x_0 - x_1)^2(x_0 - x_2)} f(x_0) + \frac{(x - x_1)^2(x - x_0)}{(x_2 - x_1)^2(x_2 - x_0)} f(x_2) \\ & + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \left(1 - \frac{(x - x_1)(2x_1 - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} \right) f(x_1) \\ & + \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f'(x_1). \end{aligned}$$

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► **Interpolation error:**

$$f(x) = P_3(x) + \frac{1}{4!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)^2(x - x_2)$$

Simpson's Rule: $n = 3$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

► **Quadrature Rule**

$$\begin{aligned}\int_a^b P_3(x) dx &= f(x_0) \int_a^b \frac{(x-x_1)^2(x-x_2)}{(x_0-x_1)^2(x_0-x_2)} dx + f(x_2) \int_a^b \frac{(x-x_1)^2(x-x_0)}{(x_2-x_1)^2(x_2-x_0)} dx \\ &\quad + f(x_1) \int_a^b \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \left(1 - \frac{(x-x_1)(2x_1-x_0-x_2)}{(x_1-x_0)(x_1-x_2)} \right) dx \\ &\quad + f'(x_1) \int_a^b \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_1-x_0)(x_1-x_2)} dx\end{aligned}$$

Simpson's Rule: $n = 3$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

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Stroke of luck: $f'(x_1)$ does not end up in quadrature

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$$\begin{aligned} \text{Quadrature Error} &= \frac{1}{4!} \int_a^b f^{(4)}(\xi(x)) (x-x_0)(x-x_1)^2(x-x_2) dx \\ &= \frac{f^{(4)}(\xi)}{4!} \int_a^b (x-x_0)(x-x_1)^2(x-x_2) dx = -\frac{f^{(4)}(\xi)}{90} h^5 \end{aligned}$$

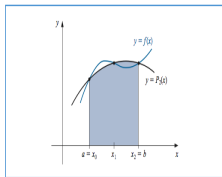
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$$\int_a^b f(x) dx = \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2)) - \frac{f^{(4)}(\xi)}{90} h^5.$$



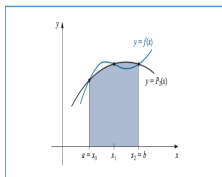
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Book wrong: $f'(x_1) \neq P'(x_1)$



Correct plot: $f'(x_1) = P'(x_1)$

Example: approximate $\int_0^2 f(x)dx$: Simpson wins

	(a)	(b)	(c)	(d)	(e)	(f)
$f(x)$	x^2	x^4	$(x+1)^{-1}$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
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DoP = 1 for Trapezoidal Rule, **DoP** = 3 for Simpson.