§5.2 Finite Difference Approximations

- Given the function $y = f(x)$, determine $f'(x_k)$, for a specified $x_{k;}$ use forward and backward Taylor Series expansions of $f(x)$ about x:

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

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

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

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

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Finite Difference Approximations

- Suppose we need sums and differences of those expansions:

$$f(x+h)+f(x-h)=2f(x)+h^2f''(x)+\frac{h^4}{12}f^{iv}(x)+\cdots$$

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

$$f(x+2h)+f(x-2h)=2f(x)+4h^2f''(x)+\frac{4h^4}{3}f^{iv}(x)+\cdots$$

$$f(x+2h)-f(x-2h)=4hf'(x)+\frac{8h^3}{3}f'''(x)+\cdots$$

even derivatives

odd derivatives

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Finite Difference Approximations

- First Central Difference Approximations (**FCDA**):

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

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

Truncation error behaves like h^2

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Finite Difference Approximations

- Now, let's approximate higher-order derivatives:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \frac{h^2}{12} f^{iv}(x) + \cdots$$

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

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

$$f^{iv}(x) = \frac{f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h)}{h^4} + O(h^2)$$

Finite Difference Approximations

- CDA Table of Coefficients

	$f(x\text{-}2h)$	$f(x\text{-}h)$	$f(x)$	$f(x+h)$	$f(x+2h)$
$2hf'(x)$		-1	0	1	
$h^2f''(x)$		1	-2	1	
$2h^3f'''(x)$	-1	2	0	-2	1
$h^4f^{iv}(x)$	1	-4	6	-4	1

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Finite Difference Approximations

- First Non-central Difference Approximations (when you cannot evaluate *f(x)* on both sides of *x*):

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(x) - \frac{h^2}{6} f'''(x) - \frac{h^3}{4!} f^{iv}(x) - \cdots$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

First Forward Diff. Approx. (FFDA)

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

First Backward Diff. Approx. (FBDA)

(Truncation error behaves like h not h^2)

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Finite Difference Approximations

- We can also derive the following for $f''(x)$:

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

- Let's look at the tables of coefficients for **FFDA** and **FBDA** – notice the similarities (on next slide).

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Finite Difference Approximations

- FFDA Table of Coefficients

	$f(x)$	$f(x+h)$	$f(x+2h)$	$f(x+3h)$	$f(x+4h)$
$hf'(x)$	-1	1			
$h^2f''(x)$	1	-2	1		
$h^3f'''(x)$	-1	3	-3	1	
$h^4f^{iv}(x)$	1	-4	6	-4	1

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Finite Difference Approximations

- FBDA Table of Coefficients

	$f(x-4h)$	$f(x-3h)$	$f(x-2h)$	$f(x-h)$	$f(x)$
$hf'(x)$				-1	1
$h^2f''(x)$			1	-2	1
$h^3f'''(x)$		-1	3	-3	1
$h^4f^{iv}(x)$	1	-4	6	-4	1

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Finite Difference Approximations

- How can we produce non-central diff. formulas with truncation errors of $O(h^2)$ rather than $O(h)$?

Can show that

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

and solving for $f'(x)$ yields

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

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Second Forward Diff. Approximation (SFFDA)

Finite Difference Approximations

- SFFDA Table of Coefficients

	$f(x)$	$f(x+h)$	$f(x+2h)$	$f(x+3h)$	$f(x+4h)$	$f(x+5h)$
$2hf'(x)$	-3	4	-1			
$h^2f''(x)$	2	-5	4	-1		
$2h^3f'''(x)$	-5	18	-24	14	-3	
$h^4f^{iv}(x)$	3	-14	26	-24	11	-2

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Finite Difference Approximations

- A similar table for **SBFDA** (Second Backward Finite Difference Approximation) is shown on p. 187 of the textbook.
- Notice that the sums of coefficients in these tables (when you traverse any row) is always **zero.**
- When h is taken to be very small, the values of $f(x)$, $f(x \pm h)$, $f(x \pm 2h)$,… become almost equal so taking linear combinations of them can produce cancellation errors (**loss of significant figures**); if h is too large, the truncation error can grow!

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Finite Difference Approximations

- Precautions: use double-precision (64-bit arithmetic) and formulas with $O(h^2)$ truncation errors.

- **Example**: Problem 6 on p. 196 of textbook, use F.D. approximation of $O(h^2)$ to compute $f'(2.36)$ and $f''(2.36)$.

x	2.36	2.37	2.38	2.39
$f(x)$	0.85866	0.86289	0.86710	0.87129

Do we need to know what $f(x)$ is?

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Finite Difference Approximations

x	2.36	2.37	2.38	2.39
$f(x)$	0.85866	0.86289	0.86710	0.87129

$$f'(x) \approx \frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

$$f''(x) \approx \frac{-f(x+3h)+4f(x+2h)-5f(x+h)+2f(x)}{h^2}$$

Show $f'(2.36) = 0.424$ and $f''(2.36) = -0.200$; what is h?

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§5.3 Richardson Extrapolation

- Can we **boost** the accuracy of finite difference approximations?
- Suppose we approximate the quantity G via $G=g(h)+E(h)$, and suppose the error $E(h)$ has the form $E(h)=ch^p$ (c, p are constants).
- Let h_1 so that $G=g(h_1)+ch_1^p$, then repeat the approx. with $h=h_2$ so that $G=g(h_2)+ch_2^p$.

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Richardson Extrapolation

- Using both right-hand-sides for *G* and eliminating the constant *c* yields:

Richardson Extrapolation Formula (REF)

$$G = \frac{\left(\frac{h_1}{h_2}\right)^p g(h_2) - g(h_1)}{\left(\frac{h_1}{h_2}\right)^p - 1}.$$

Common to use $h_2 = h_1/2$ so that formula becomes:

$$G = \frac{2^p g\left(\frac{h_1}{2}\right) - g(h_1)}{2^p - 1}.$$

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Richardson Extrapolation Example

- **Example**: suppose we want to approximate $f''(1)$ for $f(x)=e^{-x}$, given $g(h)=g(0.64)=0.380610$ and $g(h/2) = g(0.32)=0.371035.$

  Estimates obtained from central finite diff. approx. to $f''(1)$.

  The truncation error in the central diff. approx. is $E(h)=O(h^2)=c_1h^2+c_2h^4+c_3h^6+\ldots$

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Richardson Extrapolation Example

- If we approximate $f''(1)$ using REF with h_1=0.64 and p=2, i.e.,

$$f''(1) = \frac{2^2 g(0.32) - g(0.64)}{2^2 - 1} = 0.367843$$

One can show that the $O(h^2)$ term in $E(h)$ will be eliminated so that $E(h)=O(h^4)$.

How well was the approximation improved by REF?

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Richardson Extrapolation Example

$$f''(1) = \frac{2^2 g(0.32) - g(0.64)}{2^2 - 1} = 0.367843$$

0.36787944	Exact value
0.367843	REF
0.380610	g(0.64)
0.371035	g(0.32)

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Richardson Extrapolation Example

- Example 5.2 (p.190 in textbook)

x	0	0.1	0.2	0.3	0.4
$f(x)$	0.000	0.0819	0.1341	0.1646	0.1797

Compute $f'(0)$ as accurately as possible using REF with two forward diff. approx. of O(h^2) to $f'(0)$. Let h_1=0.2 and h_2=0.1 and recall CFFDA of O(h^2):

$$f'(x) \approx \frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}.$$

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Richardson Extrapolation Example

- Example 5.2 (p.190 in textbook)

x	0	0.1	0.2	0.3	0.4
$f(x)$	0.000	0.0819	0.1341	0.1646	0.1797

$$g(h_1) = \frac{-f(0.4) + 4f(0.2) - 3f(0)}{2(0.2)} = 0.8918$$

$$g(h_2) = \frac{-f(0.2) + 4f(0.1) - 3f(0)}{2(0.1)} = 0.9675$$

Choose p=2 for REF to remove h^2 term in error.

$O(h^4)$ accurate

$$f'(0) \approx G = \frac{2^2 g(0.1) - g(0.2)}{2^2 - 1} = 0.9927$$

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§5.4 Derivatives by Interpolation

- Can approximate the derivative of *f(x)* by the derivative of an interpolant.
- Helpful when data points are **not evenly-spaced** (i.e., *h* is not constant).
- Assume *f(x)* is fit with a polynomial of degree *n* having the form:

$$P_{n-1}(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n .$$

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(use $n+1$ data points and keep $n < 6$ to avoid spurious oscillations)

Derivatives by Interpolation

- Important: for evenly-spaced data points, poly. interpolation and finite diff. approximations produce **identical** results.

- Could use a least-squares fit to determine the a_i's, but the costs of solving a linear system of equations (probably with pivoting) is too high; what about using a cubic spline?

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Derivatives by Interpolation

- Compute the second derivatives (K_i) as done earlier for all knots, then take derivatives of cubic spline functions $f_{i,i+1}(x)$:

$$f'_{i,i+1}(x) = \frac{K_i}{6}\left[\frac{3(x-x_{i+1})^2}{x_i - x_{i+1}} - (x_i - x_{i+1})\right]$$

$$- \frac{K_{i+1}}{6}\left[\frac{3(x-x_i)^2}{x_i - x_{i+1}} - (x_i - x_{i+1})\right] + \frac{y_i - y_{i+1}}{x_i - x_{i+1}}$$

Quadratic function

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Derivatives by Interpolation

- And similar for $f''_{i,i+1}(x)$ we would have:

Linear function

$$f''_{i,i+1}(x) = K_i \frac{x - x_{i+1}}{x_i - x_{i+1}} - K_{i+1} \frac{x - x_i}{x_i - x_{i+1}}.$$

- Next Python-based assignment will be based Problems 12 and 13 from Problem Set 5.1 on pp. 196-197.
  Hints:

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Derivatives by Interpolation

- **<u>Example 5.4</u>**: on pp. 192-193 of textbook; given the data points below compute $f'(2)$ and $f''(2)$ using a quadratic interpolant of the form $P_2(x)=a_0+a_1x+a_2x^2$ and then using a natural cubic splines. Compare the results.

x	1.5	1.9	2.1	2.4	2.6	3.1
$f(x)$	1.0628	1.3961	1.5432	1.7349	1.8423	2.0397

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Derivatives by Interpolation

- **Example 5.5**: on pp. 194-195 of textbook; given the **noisy data** points below compute $f'(0)$ and $f'(1)$ using the best poly. fit (try degrees 2,3,4 and see which one yields the smallest std. dev. error).

x	0	0.2	0.4	0.6	0.8	1.0	1.2	1.4
$f(x)$	1.9934	2.1465	2.2129	2.1790	2.0683	1.9448	1.7655	1.5891

Upshot: typically get rough approximations to derivatives when the data is noisy!

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