m248Week_14_Derivatives_integrals

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1 Math 248 Computers and Numerical Algorithms

2 Hala Nelson

3 Week 14: Numerical Differentiation and Numerical Integration

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4 Numerically Approximating Derivatives of Functions

4.1 Notation: Given an interval $[a, b]$, discretize using $n+1$ equally spaced points, hence the mesh size is $h = \frac{b-a}{n}$. Let f be a continuous function defined on $[a, b]$, and define $f_{i+1} = f(x_i + h), f_{i+2} = f(x_i + 2h), f_{i-1} = f(x_i - h)$, etc.

1. Forward difference approximation of $O(h)$ accuracy for the first derivative (uses 2 points):

$$f'(x_i) \approx \frac{f_{i+1} - f_i}{h}$$

2. Backward difference approximation of $O(h)$ accuracy for the first derivative (uses 2 points):

$$f'(x_i) \approx \frac{f_i - f_{i-1}}{h}$$

3. Central-difference approximations of $O(h^2)$ accuracy for derivatives up to the fourth (uses 2 points, averages forward and backward differences):

$$
\begin{aligned}
f'(x_i) &\approx \frac{f_{i+1} - f_{i-1}}{2h} \\
f''(x_i) &\approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \\
f'''(x_i) &\approx \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2h^3} \\
f^{(4)}(x_i) &\approx \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{h^4}
\end{aligned}
$$

4. Central-difference approximations of $O(h^4)$ accuracy for derivatives up to the fourth:

$$
\begin{aligned}
f'(x_i) &\approx \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} \\
f''(x_i) &\approx \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12h^2} \\
f'''(x_i) &\approx \frac{-f_{i+3} + 8f_{i+2} - 13f_{i+1} + 13f_{i-1} - 8f_{i-2} + f_{i-3}}{8h^3} \\
f^{(4)}(x_i) &\approx \frac{-f_{i+3} + 12f_{i+2} - 39f_{i+1} + 56f_i - 39f_{i-1} + 12f_{i-2} - f_{i-3}}{6h^4}
\end{aligned}
$$

4.2 Error analysis

Use Taylor expansions of $f(x+h)$, $f(x-h)$, $f(x+2h)$, $f(x-2h)$, *etc.* and linear combinations of those to determine both the desired derivative's approximation and the *order* of your method in terms of h.

4.3 Application from Differential Equations

Using finite differences to find a numerical solution for a differential equation (replacing derivatives with linear combinations of discrete function values):

Discretize the one dimensional heat equation

$$u_t = u_{xx}$$

on the interval $[0, 1]$.

5 Exercises

1. **Numerical understanding of the order of a method**. Let $f(x) = \ln(x)$ and consider the following $O(h^2)$ approximation of f'':

$$f''(x_i) \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

a. Calculate the exact value of $f''(1)$.

b. Calculate the error of your approximation for each of $h = 1, h = 0.5, h = 0.25, h = 0.125$ and $h = 0.0625$.

c. Observe the error in part (b) then explain what happens to the error $e(h)$ as you halve h.

d. Deduce that $e(h)$ is indeed $O(h^2)$.

e. Make a *log-log* plot demonstrating the above result.

2. **Application from Differential Equations: Finite differences** Consider the following differential equation:

$$y''(x) = 1, \ \ x \in (0, 1)$$

with boundary conditions $y(0) = -1$ and $y(1) = 0$.

a. Solve the above equation analytically.

b. Solve the above equation numerically using 4 points.

c. Solve the above equation numerically using 8 points.

d. Compare the analytical and numerical results.

e. On the same graph, plot the analytical solution and numerical solutions.

3. **For a particular function, compare the exact derivative with the approximate discrete derivative**. Consider the function

$$f(x) = \ln(1 + x)$$

.

a. Calculate the exact value of $f''(1)$.

b. Approximate $f''(1)$ using the central difference formula

$$f''(x_i) \approx \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12h^2}$$

and $h = 0.01$.

c. What is the order of your approximation in terms of h? Explain the meaning of the order of your method?

4. **Consider the second order differential equation modeling a harmonic oscillator**:

$$y'' + y = 0 \text{ in the domain } x \in (0, \pi/2)$$

with boundary conditions $y(0) = 2$ and $y(\pi/2) = 1$.

a. The exact solution is given by $y(x) = 2\cos(x) + \sin(x)$. Compute $y(0)$, $y(\pi/8)$, $y(\pi/4)$, $y(3\pi/8)$, and $y(\pi/2)$.

b. Discretize the above equation using $y'' \approx \frac{y_{i+1}-2y_i+y_{i-1}}{h^2}$, $y = y_i$ and $h = \pi/8$. Write a linear system of equations representing the discrete differential equation.

c. Solve the above system using numpy.linaglg package.

d. Plot the exact solution and the numerical solution on the same graph.

5. Derive the following three point approximation of the first derivative and prove that it is $O(h^2)$:
$$f'(x_i) \approx \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h}$$

Is this above approximation centered or is it biased (forward or backward)?

6 Numerically Approximating Integrals of Functions

Numerical integration is also called *quadrature*.

1. Fundamental theorem of calculus.
2. Riemann Integral:
$$\int_a^b f(x)dx = \lim_{\max(\Delta x_i)\to 0} \sum_{i=0}^{n} f(x_i^*)\Delta x_i$$
3. Equal subintervals: Divide $[a, b]$ into n equal subintervals of length $h = \frac{b-a}{n}$ each. The partition is then $a = x_0 < x_1 < \cdots < x_n = b$, where $x_i = x_0 + ih$. The following quadratures depend on the choice of the representative point x_i^* in each subinterval:

- Left (approx. f by constants):
$$\int_a^b f(x)dx \approx (f(x_0) + f(x_1) + \cdots + f(x_{n-1})).h$$
This method is $O(h)$
$$E_L \leq \frac{b-a}{2} M_1 h$$
where M_1 bounds $|f'|$.
- Right (approx. f by constants):
$$\int_a^b f(x)dx \approx (f(x_1) + f(x_2) + \cdots + f(x_n)).h$$
This method is $O(h)$
$$E_R \leq \frac{b-a}{2} M_1 h$$
where M_1 bounds $|f'|$.
- Midpoint (approx. f by constants):
$$\int_a^b f(x)dx \approx \left(f\left(\frac{x_0+x_1}{2}\right) + f\left(\frac{x_1+x_2}{2}\right) + \cdots + f\left(\frac{x_{n-1}+x_n}{2}\right)\right).h$$
This method is $O(h^2)$
$$E_M \leq \frac{b-a}{24} M_2 h^2$$
where M_2 bounds $|f''|$.

- (Weighted quadrature) Trapezoidal rule (approx. f by deg 1 polyn.'s):

$$\int_a^b f(x)dx \approx (f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n)).\frac{h}{2}$$

  This method is $O(h^2)$

$$E_T \leq \frac{b-a}{12} M_2 h^2$$

  where M_2 bounds $|f''|$.

- (Weighted quadrature) Simpson's rule (approx. f on two subintervals- three interpolating points- by deg 2 polyn.'s):

$$\int_a^b f(x)dx \approx (f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)+\cdots+2f(x_{n-2})+4f(x_{n-1})+f(x_n)).\frac{h}{3}$$

  This requires an even number of subintervals. This method is $O(h^4)$

$$E_S \leq \frac{b-a}{180} M_4 h^4$$

  where M_4 bounds $|f^{(4)}|$. Note that this rule integrates polynomials of degrees 1, 2 and 3 exactly since the fourth derivative of these is zero, making the error $E_S = 0$.

4. Error analysis: This link has a good summary and examples of Error Theorems `http://math.cmu.edu/~mittal/Recitation_notes.pdf`.

Proofs of error theorems: Good link: `https://pdfs.semanticscholar.org/80df/a6fc1262412f3d050e340f06ea7800c5317d.pdf`

7 Exercises (Numerically Approximating Integrals)

1. (Programming) Write a program that numerically computes the integral of a continuous function over an interval $[a, b]$ using Left rule, Right rule, Trapezoidal rule, and Simpson's rule.

2. Consider the following integral:

$$\int_0^\infty e^{-x^2} dx$$

a. Estimate numerically (show all your work) using trapezoidal rule, $b = 5$ and $n = 5$ subintervals.

b. Give an upper bound for the error using trapezoidal rule with the above information.

c. The above integral can be solved analytically and the exact answer is $\frac{\sqrt{\pi}}{2}$. What is the exact error incurred when using the trapezoidal rule?

d. How big should n be in order to get an error less than 10^{-10}?

e. Verify your answers using the numerical integration program.

3. Consider the integral $\int_1^2 \frac{1}{x} dx$.

a. Find the analytical (exact) value of this integral.

b. Consider a partition of $[1, 2]$ using only two subintervals.

c. Draw a graph illustrating how Simpson's rule works.

d. Use the information from Week on interpolating polynomials to find $P_2(x)$ that interpolates the three points involved in Simpson's rule.

e. Approximate $\int_1^2 \frac{1}{x}dx$ by $\int_1^2 P_2(x)dx$ and calculate the error.

4. How many subintervals would you need to approximate $\int_1^2 \frac{1}{x}dx$ up to 10^{-6} using

a. Trapezoidal rule.

b. Simpson's rule.

8 Recall from Linear Algebra: Solving systems of equations using Gaussian elimination

1. Gaussian elimination (by hand and program) for dense and tridiagonal matrices.
2. Pivoting (by hand and program).
3. Backward substitution (by hand and program).
4. Solving tridiagonal systems using Gaussian elimination (important for differential equations applications). **Important idea here:** Exploiting the simple structure of the matrix and the many zeros for more efficient storage on the computer and less computationally expensive code (than those algorithms for more dense matrices, like Gaussian elimination).

8.1 Examples

1. **Tridiagonal system** Solve the following system by hand:

$$\begin{cases} 3x - y = 2 \\ -x + 3y - z = 1 \\ -y + 3z - w = 1 \\ -z + 3w = 2 \end{cases}$$

2. **Dense system** Solve the following system by hand:

$$\begin{cases} a + 2b + 4c = 23 \\ a + b + c = 7 \\ 4a + 2b + c = 2 \end{cases}$$

3. (Programming) Use your code that solves the above systems to check your answer.

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