Finite Differences

Math 131: Numerical Analysis

J.C. Meza

April 2, 2024

Section 1

Finite Differences

Motivation

Computing derivatives numerically arises in many situations in numerical analysis as well as scientific computing. Some of the most common examples include:

- Numerically solving ordinary differential equations (ODEs), partial differential equations (PDEs), nonlinear equations and optimization (e.g. Newton's method).
- Computing derivatives of complicated functions.
- Situations where f is not known explicitly or only as a black box.

The basic tools used for numerical derivatives include one tool that we've been using extensively (Taylor series), and one more recently (polynomial interpolation).

Many Other Examples in Science/Engineering

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f$$ Poisson's Equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$ Heat Equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$ Wave Equation

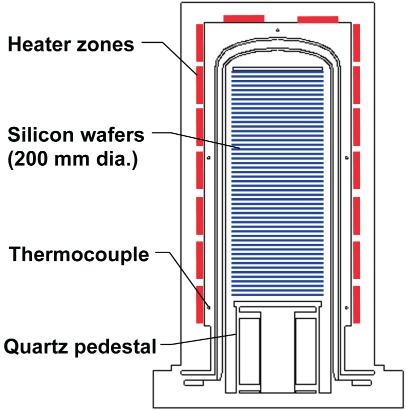
$$\frac{\partial u}{\partial t} = c\frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2}$$ Convection-Diffusion Equation

CVD


Chemical Vapor Deposition
Control
COMPUTATIONAL RESEARCH DIVISION
BERKELEY LAB

Small-batch LPCVD

The design of a small-batch fast-ramp LPCVD furnace can be posed as an optimization problem



- Temperature uniformity across the wafer stack is critical
- Independently controlled heater zones regulate temperature
- Wafers are radiatively heated
- Design parameters:
  - Number of heater zones
  - Size / position of heater zones
  - Pedestal configuration
  - Wafer pitch
  - Insulation thickness
  - Baseplate cooling

Governing Equations

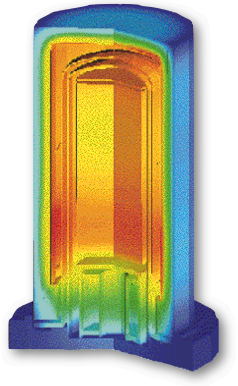
Can cast this problem as heat conduction with radiation losses described by the following equation:

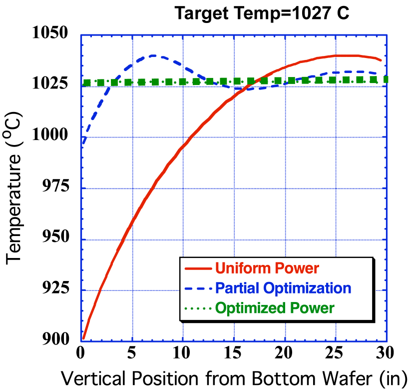
$$\frac{\rho c_P}{k}\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} - \frac{2\sigma\epsilon}{kR}(T^4 - T_{amb}^4)$$

where ρ, c_P, k, ϵ are material constants, R is radius of silicon wafer, σ is the Stefan-Boltzmann constant, T_{amb} is fixed ambient temperature.

Optimized power distribution

Optimized power distribution enhances wafer temperature uniformity for steady-state operation





Simulation of Equipment Design Optimization in Microelectronics Manufacturing, **J.C. Meza, C.H. Tong, C.D. Moen, Proc. 30th Annual Simulation Symposium, Atlanta, GA, April 7-9, 1997.**

C O M P U T A T I O N A L   R E S E A R C H   D I V I S I O N

CVD - Moral of the story

- In theory you have derivatives, but in practice you don't
- Lack of derivatives reduces the choice of numerical methods one can use for optimization
- Accurately computing derivatives trickier than one might think at first glance
- Solution time reduced from a week long job into a 30 minute computation with a solution that was an order of magnitude better

Section 2

First-order Approximations

Taylor Series Approach

Let $f : R^1 \to R^1$ with as many derivatives as we need.

Recall the *Taylor series expansion* for a function

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi), \qquad \xi \in [x, x+h]$$

Rearranging we can write:

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

Forward Difference

This leads to the ***forward difference*** approximation, which can be written as:

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

where we will denote the *truncation error* by

$$-\frac{h}{2} f''(\xi)$$

Notice that the truncation error can be expressed in Big O notation as $O(h)$ and we therefore say that forward differences are an $O(h)$ approximation or that it is ***first order accurate***.

Reminder

Truncation Error is NOT Roundoff Error

The truncation error should not be confused with roundoff error!

Backward Difference

Similarly the ***backward difference*** approximation can be written as

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

with a similar error term. Clearly, backward differences are also first order accurate.

Which one should I use?

- There is no major difference between the two; it mostly comes down to a matter of convenience or preference.
- There are however some situations, where it makes more sense to use one over the other.
  - One recent example is when we had to impose a condition on the cubic spline interpolant and we needed to have the derivative of the first and last spline math the derivative of the function.
  - In that case, we should use the forward difference approximation for the first spline and the backward difference approximation for the last spline.

Example: Forward Difference

Computation of forward difference for $\exp(x), x = 1$

Table 1: Forward Difference for exp(x), x = 1

h	fprime	F.D	err (F.D)
0.100000	2.718282	2.858842	0.1405601
0.050000	2.718282	2.787386	0.0691040
0.025000	2.718282	2.752545	0.0342635
0.012500	2.718282	2.735342	0.0170603
0.006250	2.718282	2.726794	0.0085124
0.003125	2.718282	2.722534	0.0042517

Exercise

Compute the forward difference of

$$f(x) = \tan(x), x = \pi/4$$

for

$$h = 0.1, 0.05, 0.025, 0.125, 0.00625, 0.003125$$

Solution

Table 2: Forward/Backward Difference for tan(x), x = pi/4

h	fprime	F.D	B.D	err (F.D)	err (B.D)
0.100000	2	2.230489	1.823712	0.2304888	0.1762881
0.050000	2	2.107112	1.906275	0.1071118	0.0937249
0.025000	2	2.051721	1.951616	0.0517205	0.0483838
0.012500	2	2.025423	1.975410	0.0254233	0.0245897
0.006250	2	2.012605	1.987603	0.0126050	0.0123966
0.003125	2	2.006276	1.993776	0.0062761	0.0062241

Section 3

Central Differences

Central Differences

Consider the Taylor series at $x + h$ and $x - h$

$$
\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(\xi_1(x)) \\
f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(\xi_2(x))
\end{aligned}
\tag{1}
$$

for some $\xi_1 \in [x, x+h], \xi_2 \in [x-h, x]$.

(cont.)

Subtracting the second equation from the first gives us:

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{6}[f'''(\xi_1(x)) + f'''(\xi_2(x))]$$

and solving for f' we get:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} \cdot \frac{1}{2}[f'''(\xi_1(x)) + f'''(\xi_2(x))]$$

(cont.)

The last term that includes the third derivative at two different points can be replaced by using the Intermediate Value Theorem to yield:

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

Equation 2 is called the central (or centered) difference approximation.

Example: Central vs. F.D.

Compare central vs. forward differences for $f(x) = \tan(x), x = \pi/4$

Table 3: Forward v. Central Difference for tan(x), x = pi/4

h	F.D	err (F.D)	C.D	err (C.D.)
0.100000	2.230489	0.2304888	2.027100	0.0271004
0.050000	2.107112	0.1071118	2.006693	0.0066934
0.025000	2.051721	0.0517205	2.001668	0.0016683
0.012500	2.025423	0.0254233	2.000417	0.0004168
0.006250	2.012605	0.0126050	2.000104	0.0001042
0.003125	2.006276	0.0062761	2.000026	0.0000260

Section 4

Higher Order

Practical Tips

- It is not too difficult to generate other (higher-order) formulats using similar techniques.
- One must remember that we need to balance accuracy with the additional work needed and to be aware of any special conditions or structure available
- For example the case of specifying derivative conditions for cubic splines at the end points, discussed earlier in this section.

Section 5

Second Derivatives

Second Derivative Formulas

Using similar techniques as for the centered difference formulas we can develop approximations for the second derivative of a function.

Consider once again the Taylor series for a function about a point:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_1(x))$$
$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_2(x))$$

(cont.)

Here, as we want to have a formula for the second derivative, our goal is to get rid of the other terms, and in particular the first derivative. Hence, let's add the two equations:

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{24}\left[f^{(4)}(\xi_1(x)) + f^{(4)}(\xi_2(x))\right]$$

(cont.)

Solving for f'' we get:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^4}{24}\left[f^{(4)}(\xi_1(x)) + f^{(4)}(\xi_2(x))\right]$$

Now using the same trick we used before by appealing to the IVT, we have the following formula for numerically computing the second derivative.

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

This approximation is clearly $O(h^2)$ and we say that it is a ***second order approximation.***

Example: Second derivatives

Second Derivatives using finite differences

Table 4: Second Derivate for exp(x), x = 1

h	f(x)	f2prime	err
0.10000	2.718282	2.720548	0.0022660
0.05000	2.718282	2.718848	0.0005664
0.02500	2.718282	2.718423	0.0001416
0.01250	2.718282	2.718317	0.0000354
0.00625	2.718282	2.718291	0.0000088

Section 6

Summary

Summary

- Introduced concept of numerical differentiation
- Presented 3 formulas for first derivatives: two of which are first order approximation and one that is second order
- Presented a formula for second derivatives

Section 7

Supplementary Materials

Review - Big O Notation

Remember that we denote a quantity x as $O(h)$ if it is at most proportional to h, for example Ch for some constant C. One way to think of it as

$$\lim_{h \to 0} \frac{O(h)}{h} = C < \infty$$

Notice that according to our definition, both forward and backward difference formulas have truncation error that is $O(h)$.

Question

- What is the order of

$$\frac{h}{2}f''(x) + \frac{h^2}{3}f'''(x)?$$

- Just need to take a look at the lowest power of h. If the power of h is 1, we say that it is *first order.* If the power of h is 2, we say that it is *second order,* and so on.

Tip

All other things being equal, we want as high a power of* h *for our error term as we can achieve!*

Proof for Central Differences Formula

The last term that includes the third derivative at two different points can be replaced by using the Intermediate Value Theorem:

Intermediate Value Theorem

Suppose that *(i)* f is continuous on the closed finite interval $[a, b]$ and *(ii)* $f(a) < c < f(b)$. Then there exists some point $x \in [a, b]$ such that $f(x) = c$.

(cont.)

Notice that, since the average value must lie in between the value at the two end points a straightforward application of the IVT says:

$$\frac{1}{2}[f'''(\xi_1(x)) + f'''(\xi_2(x))] = f'''(\xi), \quad \xi \in [x-h, x+h]$$

Substituting for the f''' terms yields:

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

Equation 2 is called the central (or centered) difference approximation.