Numerical Calculus

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1 Semiconductor Concepts

Solving the Poisson's equation
Calculation of the carrier density
Calculation of the current
Calculation of the SS
Calculation of Gate current

2 Expansion of a function

Consider a that we are given a set of data points (y_i, x_i) or a function, so we can expand the particular function in the vicinity of x_i as

$$f_{i+1} = f_i + f_i' h + f_i'' \frac{h^2}{2!} + \cdots \quad (1)$$

or we can also write the Taylor's series at point x_{i-1}

$$f_{i-1} = f_i - f_i' h + f_i'' \frac{h^2}{2!} + \cdots \quad (2)$$

3 Differentiation

Based on the above expression we can calculate the derivative as

$$f_i' = \frac{f_{i+1} - f_i}{h} + O(h) \quad (3)$$

Using similar arguments we can extend our derivative calculations to higher order terms

$$f_i' = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} + O(h^2) \quad (4)$$

Another form using the second Taylor's series we can write

$$f_i' = \frac{f_i - f_{i-1}}{h} + O(h) \quad (5)$$

The first form of the derivative is called as the forward difference form while the second one is called as the backward difference. We can also write the derivative as

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2) \quad (6)$$

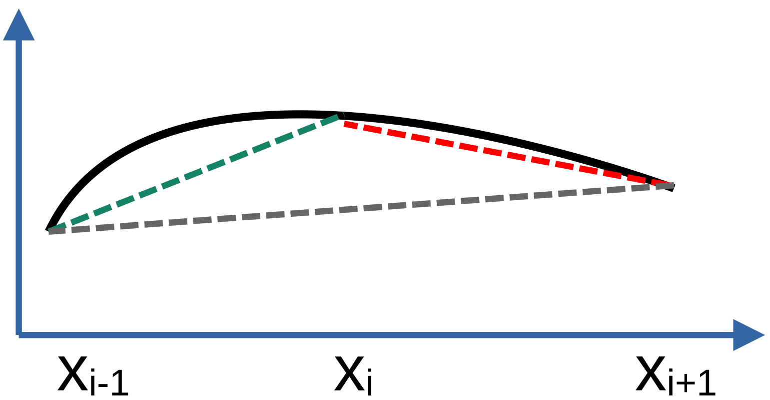

Figure 1: Green: Backward derivative; Red: Forward Difference; Grey: Central Difference

Another more accurate derivative form would be

$$f_i' = \frac{f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}}{12h} + O(h^4) \tag{7}$$

Can you guess the how the above form is derived ? by writing the Taylor's series expansion at further points and relating it to f_i

What about the second order derivative

$$f_i'' = \frac{f_{1+1} - 2f_i + f_{i-1}}{h^2} + O(h^2) \tag{8}$$

A sort a cool derivation for this is as follows.

$$f_i'' = \frac{f_{i+0.5}' - f_{i-0.5}'}{h} \tag{9}$$

$$f_i'' = \frac{f_{i+1} - f_i - f_i + f_{i-1}}{h^2} \tag{10}$$

Note that in the above equations we have assumed that the spacing between the data is the same. However, practically this rarely the case. Even in the simulations you will quickly realize that there are regions where the electric field is changing very rapidly and at other places the fields are almost zero. In such cases it is important to have a non-uniform mesh. In this case the error may not be the same as in the case of the equal spacing. For example in the case of f_i'' the error is of the order h^2 but in the case of the non-equal spacing the error would be of the order h

Another way to deal with unequally spaced data is to fit a polynomial (Lagrange interpolation) to it and then calculate the derivative.

$$f_i' = f_{i-1}\frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f_i\frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})} + f_{i+1}\frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_i)(x_{i+1} - x_{i-1})} \tag{11}$$

3.1 Differentiating Noisy data

Derivatives as we know are very sensitive to the data quality. If there is a noise then it will adversely affect the derivative calculations. The derivative process is very sensitive and noise will render it unstable. In this case it is important that we use our curve fitting machinery to fit the data first to a polynomial and then differentiate it. If we know the underlying relationship then in that case we will form the basis of our curve fitting function. The polynomial or the appropriate underlying functional form can come from the our understanding of the physics.

3.2 Differentiating unequally spaced data

One of the ways that we can do is to fit the curve with a polynomial (recall that in the curve fitting/interpolation part we never restricted the spacing)

However, it more preferable to differentiate an unequally spaced data points we just have to rederive all the formulae from the Taylor's series again but now the only the fact that is important is that we need not have $(x_{i+1} - x_i = x_i - x_{i-1})$.

3.3 How does it work in the real world

We can use the Taylor's series to get to higher order formulae for the derivatives, but at the points that are closer to the boundary, we will require the values of the variables that are outside the boundary. Hence we can reduce the h and work with lower order/ less accurate differentiation formulae.

4 Integration

4.1 Necessity of numerical integration

Many practically relevant integrations cannot be evaluated analytically. In many other cases the process of performing analytical integration is too difficult.

4.2 Introduction

Let us say I want to find the perimeter of a circle but we dont know the value of pi. How can we do it? The answer to it is by converting the circle into a polygon and calculating the length of the sides of the triangle. In the same vein, we can compute the integration as well which is nothing but an area under the curve. What we essentially have to do is divide the curve into small segments and assume that the value of the function in each segment is constant/flat. Now we can compute the integration by calculating the area under each segment. This reminds us of divide and conquer approach.

4.3 Integrating Methods

Depending on the accuracy required, a number of methods already exist in the literature. Of these we will consider some of them that I have used at some point in my research career and these are by no means an exhaustive list

4.3.1 Naive method

The most simplest one is to assume that the value of the function in the segment $(x_i,\ x_{i+1})$ is equal to f_i or f_{i+1}.

$$I = \int_a^b f(x)dx = \Sigma_{i=1}^{N-1} \int_i^{i+1} f(x)dx \approx \Sigma_{i=1}^{N-1} f_i h \approx \Sigma_{i=1}^{N-1} f_{i+1} h \tag{12}$$

Note that here the summation runs over the segments.

4.3.2 Trapezoidal method

In the previous method it is obvious to see that the h required for getting sufficiently accurate results would be very small. Can we make some approximation that might help us. The answer is obvious. We can take an average value of the f in the interval. This would result in

$$I = \int_a^b f(x)dx = \Sigma_{i=1}^{N-1} \int_i^{i+1} f(x)dx \approx \Sigma_{i=1}^{N-1} \frac{f_i + f_{i+1}}{2} f_i h + O(h^2) \tag{13}$$

$$I = (b-a)\left(\frac{f_1 + 2\sum_{i=2}^{N-1} f_i + f_N}{2(N-1)}\right) \tag{14}$$

Geometrically the segment represents a trapezium unlike the rectangle in the previous method. By taking an average we are implicitly making an assumption that the function varies linearly in the segment (x_i, x_{i+1})

Does this bring back any memory ? We are essentially interpolating the function f(x) in the interval $(x_i x_{i+1})$. Please convince yourselves of this particular fact.

4.3.3 Simpson's 1/3 method

How can we go to higher order of approximation. Simple use higher order polynomial to fit the function. If we assume that the function is linear then we just require 2 data points to fit the function but if we assume that the function is quadratic (parabola) the we will naturally require 3 data points (x_{i+1}, y_{i+1}), (x_i, y_i), (x_{i-1}, y_{i-1}). We can write the Lagrange interpolating function as

$$p(x) = \frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} y_{i-1} + \frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})} y_i + \frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)} y_{i+1} + O(h^3). \tag{15}$$

Since this is a polynomial we can now integrate it between the (x_{i-1}, x_{i+1}) This results in the following function

$$\begin{aligned} I &= h\frac{f_1 + 4f_2 + f_3}{3} + h\frac{f_3 + 4f_4 + f_5}{3} + \cdots + h\frac{f_{N-2} + 4f_{N-1} + f_N}{3} \\ &= (b-a)\frac{f_1 + 4\sum_{k=2,4,}^{N-1} f_k + 2\sum_{j=1,3,}^{N-2} f_j + f_N}{3(N-1)} \end{aligned}$$

Can you guys see any problems with this method. It requires even number of elements or segments. Now if we know the analytical function we can simply discretize it in the even number of segments. But in practical cases this may not be possible. So we can divide the discretized domain into N-2 segments and 1 segment where in we can apply simple trapezoidal rule. **Can you improve it further ?**

4.4 Monte Carlo Method

Using the basic calculus, it is can be shown that the integration can be written in the form of

$$I = \int_a^b f(x)dx = (b-a) f_{avg}$$

In order to compute f_{avg}, we can generate uniformly distributed random numbers between x= a and x= b compute the average as

$$f_{avg} = \frac{1}{K}\sum_{i=1}^{K} f(x_i)$$

where K is the number of random sampling points. Obviously as the number of the random samples increases the accuracy of the integration increases.

For well behaved integrands and 1D integrations, the standard method like Trapezoidal and Simpson's schemes function perfectly well and are better than the Monte Carlo schemes. However for ill-behaved integrands and for the case of the multidimensional integrations, Monte Carlo based integration schemes perfrom better than the conventional integration methods.

4.5 Integration of Noisy Data

In this first part of this topic we discussed the differentiation and saw that small deviations/noises can really cause havoc on the correct values of differentiation. Because of this we had to introduce an a curve to fit the underlying data and then differentiate it. This was because we were interested in the difference and then divided it with a small quantity (h). This particular process magnified the noise in the data. But unlike this, in the integration we are averaging the data (this is clear in the trapezoidal rule)