Math 385 Notes

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Finite Differences and Finite Difference Method

We know that, given a real-valued function f differentiable at x_0, the derivative at this point x_0 is given by $f'(x_0) = \lim_{x \to x_0} \frac{f(x)-f(x_0)}{x-x_0}$. Finite differences are useful because the researcher often knows values of a function without specifically knowing the actual function itself. Moreover, using finite differences the researcher can infer approximate values of the derivative of an unknown function as well.

FINITE DIFFERENCES

Finite differences, the discrete form of the derivative, is the entry point into numerical processes to approximate the solution of a differential equation.We now present several finite difference formulae used to numerically approximate first and second derivatives of a function.

Let f be a real-valued function defined on $[a, b]$. Let $\Delta x = x_{i+1} - x_i = \frac{b-a}{n}$ and consider the partition $a = x_0 < x_1 < x_2 < \ldots < x_n = b$.

Suppose then that f is at least three times differentiable, so that we may write the Taylor expansion for f at x_i and evaluated at x_{i+1}. Then we have:

$$\text{(I)}\ f(x_{i+1}) = f(x_i + \Delta x) = f(x_i) + f'(x_i)\,\Delta x + \frac{f''(x_i)\,(\Delta x)^2}{2} + \frac{f^{(3)}(x_i)\,(\Delta x)^3}{6} + O\left((\Delta x)^4\right)$$

$$\text{(II)}\ f(x_{i-1}) = f(x_i - \Delta x) = f(x_i) - f'(x_i)\,\Delta x + \frac{f''(x_i)\,(\Delta x)^2}{2} - \frac{f^{(3)}(x_i)\,(\Delta x)^3}{6} + O\left((\Delta x)^4\right)$$

where $O\left((\Delta x)^4\right)$ is the remainder of the Taylor expansion of order-3 for our function, which is of the form $C(\Delta x)^4$, for C a constant. In particular, this term converges to 0 as $(\Delta x)^4$ goes to zero.

▸ Forward Difference (aka Forward Euler)

Using equation (I) , if we substract $f(x_i)$ from both sides and divide by Δx, we get

(III) $$\underbrace{\frac{f(x_{i+1})-f(x_i)}{\Delta x}}_{\text{Forward Difference}} = f'(x_i) + \frac{f''(x_i)\,\Delta x}{2} + \frac{f^{(3)}(x_i)\,(\Delta x)^2}{6} + O(\Delta x)^3 \approx f'(x_i) + O(\Delta x)$$

The expression on the left hand side of (III) is called the forward difference of f at x_i. The right hand side of this equation ensures us that the foward difference converges to $f'(x_i)$ with order Δx, i.e. Forward Euler converges to $f'(x_i)$ as Δx goes to zero.

▸ Backward Difference (aka Backward Euler)

Using equation (II), if we substract $f(x_i)$ from both sides and divide by Δx, we get

$$\frac{f(x_{i-1})-f(x_i)}{\Delta x} = -f'(x_i) + \frac{f''(x_i)\,\Delta x}{2} - \frac{f^{(3)}(x_i)\,(\Delta x)^2}{6} + O(\Delta x)^3 \cong -f'(x_i) + O(\Delta x)$$

Multiplying by -1, we can rewrite the equation as

(IV) $$\underbrace{\frac{f(x_i)-f(x_{i-1})}{\Delta x}}_{\text{Backward Difference}} = f'(x_i) - \frac{f''(x_i)\,\Delta x}{2} + \frac{f^{(3)}(x_i)\,(\Delta x)^2}{6} + O(\Delta x)^3 \approx f'(x_i) + O(\Delta x)$$

The left hand side of equation (IV) also approximates the derivative of f at x_i. We call this expression the backward difference. Again this value converges to $f'(x_i)$ with order Δx, i.e. Backward Euler converges to $f'(x_i)$ as Δx goes to zero .

Thus Backward and Forward Euler have the same order of convergence.

▸ Central Difference

Now we average the two Euler methods, i.e. we add (III) and (IV) and divide by 2:

(V) $$\underbrace{\frac{f(x_{i+1})-f(x_{i-1})}{2\,\Delta x}}_{\text{Centered Difference}} = f'(x_i) + \frac{f^{(3)}(x_i)\,(\Delta x)^2}{6} + O(\Delta x)^3 \approx f'(x_i) + O\big((\Delta x)^2\big)$$

The left hand side of (V) is called the centered difference of f at x_i. This expression converges to $f'(x_i)$ with order $(\Delta x)^2$,i.e. it converges faster than the Euler methods. Thus we may conclude that the centered difference yields a better approximation of the derivative than either the forward or backward differences.

▸ Second Central Difference

If we substract (IV) from (III), and then divide by Δx, we get

(VI) $$\underbrace{\frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2}}_{\text{Second Centered Difference}} \approx f''(x_i) + O\left((\Delta x)^2\right)$$

The term on the left hand side of (VI) approximates the second derivative of f at x_i and it is called the second centered difference of f at x_i. Again, the second central difference converges to $f''(x_i)$ with order $(\Delta x)^2$.

** For videos explaining all of the above methods visit the following link:
`http://mathforcollege.com/nm/nbm/com/02dif/index.html` **

Notice that when defining the finite differences we used a uniform partition along the x-axis. Generally speaking, finite differences perform best when the partition is uniform. With the aid of more advanced techniques researchers however do achieve good results with non-uniform partitions. For our purposes here, we will restrict attention to the uniform case. In addition there are many other forms of finite differences which are used in particular circumstances.

FDM : APPROXIMATION OF THE ONE – D HEAT EQUATION

We now show how finite differences may be used to approximate the solution of a differential equation. The treatment of the finite difference method (FDM) given here is by no means exhaustive. It will serve to only convince the reader that finite differences are useful.
Consider the following commonly occurring setting. Suppose an unknown function is defined on an interval of the x-axis and a time interval, $u = u(x, t)$, $u : [a, b] \times [0, 1] \longrightarrow \mathbb{R}$ and satisfies the following differential equation:

(VII) $$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$ **(One-D Heat Equation)**

This equation is called the one dimensional heat equation, as it represents the flow of heat across a thin rod. However, this equation also arises in settings which have nothing to do with heat flow, although for now we focus on the heat flow setting. In this context, the values $u = u(x, t)$ represent temperatures at the location x and time t.

We will use a method called FTCS (Forward-Time Centered-Space). If we partition the intervals $x \in [a,\ b]$ and $t \in [0,\ 1]$ in a uniform manner, and write $u_i^n = u(x_i,\ t_n)$, then we can recast equation (VII) in finite difference form using the forward difference (III) for time (with respect to t) and the second centered difference (VI) for space (with respect to x).
Then we have

(VIII) $$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^n - 2\,u_i^n + u_{i-1}^n}{(\Delta x)^2}$$

This equation can be rearranged as

(IX) $$u_i^{n+1} = \lambda\, u_{i-1}^n + (1 - 2\,\lambda)\, u_i^n + \lambda\, u_{i+1}^n$$

where $\lambda = \alpha \frac{\Delta t}{(\Delta x)^2}$.**Note:** This term λ is related to stability (it is often called the amplification factor for stability). If $\lambda > 1$, the system is considered unstable.**

Notice that equation (IX) states that the temperature at a location on the next time step is a linear combination of the prior temperature at that location and at the nearest neighbors. Hence, if we knew values for u at $t = 0$, then we could use equation (IX) to calculate values at $t = t_1$. Then by repeating the process (looping!) we can get values for each successive time step.

But before doing this we need to ensure that the problem has a unique solution. If this is the case we say that we have a 'well posed problem', which means that the underlying physics of the problem is deterministic. To achieve a deterministic problem it is necessary that we know the temperature at the boundaries. In particular we must have prior knowledge of u_o^n and u_{k+1}^n for each time step. For simplicity we suppose that the boundary temperatures are time independent. We set $u_o^n = \tau_o$ and $u_{k+1}^n = \tau_{k+1}$ and rewrite equations (VIII) and (IX) as

(X) $$u_1^{n+1} - \lambda\tau_o = (1 - 2\,\lambda)\, u_1^n + \lambda\, u_2^n \qquad \text{(left boundary)}$$
$$u_k^{n+1} - \lambda\tau_{k+1} = (1 - 2\,\lambda)\, u_k^n + \lambda\, u_{k-1}^n \qquad \text{(right boundary)}$$

Now we recast equations (IX) and (X) in matrix format. In particular we show the derivation of the values at the $(n+1)^{\text{th}}$ time step from the n^{th} time step :

$$\underbrace{\begin{pmatrix} 1-2\lambda & \lambda & 0 & . & 0 & 0 \\ \lambda & 1-2\lambda & \lambda & . & 0 & 0 \\ 0 & \lambda & 1-2\lambda & . & \lambda & 0 \\ . & . & . & . & . & . \\ 0 & 0 & \lambda & . & 1-2\lambda & \lambda \\ 0 & 0 & 0 & . & \lambda & 1-2\lambda \end{pmatrix}}_{\text{FTCS tridiagonal matrix}} \begin{pmatrix} u_1^n \\ u_2^n \\ . \\ . \\ u_k^n \end{pmatrix} = \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ . \\ . \\ u_k^{n+1} \end{pmatrix} \underbrace{-\lambda \begin{pmatrix} \tau_o \\ \tau_1 \\ . \\ . \\ \tau_{k+1} \end{pmatrix}}_{\text{We will ignore this term for our purpose}}$$

We can also use a method called BTCS (Backward-Time Centered Space). In this procedure we use the same technique as we did on FTCS but this time we recast equation (VII) in finite difference form using the backward difference (IV) for time (with respect to t) and the second centered difference (VI) for space (with respect to x). Then we have :

(XI) $u_i^{n-1} = (1+2\lambda)\, u_i^n - \lambda\, u_{i+1}^n - \lambda\, u_{i-1}^n$

Then we look the again at the temperature at the boundaries. Making the same assumptions as in the previous case, we set $u_o^n = \tau_o$ and $u_{k+1}^n = \tau_{k+1}$ and after some algebraic manipulation we end up getting the following equation in matrix form :

$$\underbrace{\begin{pmatrix} 1+2\lambda & -\lambda & 0 & . & 0 & 0 \\ -\lambda & 1+2\lambda & -\lambda & . & 0 & 0 \\ 0 & -\lambda & 1+2\lambda & . & -\lambda & 0 \\ . & . & . & . & . & . \\ 0 & 0 & -\lambda & . & 1+2\lambda & -\lambda \\ 0 & 0 & 0 & . & -\lambda & 1+2\lambda \end{pmatrix}}_{\text{BTCS tridiagonal matrix}} \begin{pmatrix} u_1^n \\ u_2^n \\ . \\ . \\ u_k^n \end{pmatrix} = \begin{pmatrix} u_1^{n-1} \\ u_2^{n-1} \\ . \\ . \\ u_k^{n-1} \end{pmatrix} \underbrace{-\lambda \begin{pmatrix} \tau_o \\ \tau_1 \\ . \\ . \\ \tau_{k+1} \end{pmatrix}}_{\text{We will ignore this term for our purpose}}$$

▸ Crank-Nicholson

We begin by adding explicit and implicit equations together and dividing by 2:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^{n+1} - 2\,u_i^{n+1} + u_{i-1}^{n+1}}{2\,\Delta x^2} + \alpha \frac{u_{i+1}^n - 2\,u_i^n + u_{i-1}^n}{2\,\Delta x^2}.$$

Next, add and subtract a fictitious state $u_i^{n+(1/2)}$ on the left hand side:

$$\frac{u_i^{n+1} - u_i^{n+(1/2)}}{\Delta t} + \frac{u_i^{n+(1/2)} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^{n+1} - 2\,u_i^{n+1} + u_{i-1}^{n+1}}{2\,\Delta x^2} + \alpha \frac{u_{i+1}^n - 2\,u_i^n + u_{i-1}^n}{2\,\Delta x^2}.$$

Now divide this into two separate processes:

$$\frac{u_i^{n+(1/2)} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{2\Delta x^2},$$

$$\frac{u_i^{n+1} - u_i^{n+(1/2)}}{\Delta t} = \alpha \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{2\Delta x^2}.$$

This yields a two-step time process. The first step from u^n to $u^{n+(1/2)}$ is implicit while the second bit from $u^{n+(1/2)}$ to u^{n+1} is explicit. We already know that both tri-diagonal matrices for explicit and implicit are symmetric. In this case the entries are half the value computed for explicit and implicit.

Note:

‣ We call BTCS an implicit method because it requires a LinearSolve (we know the u_j^{n-1} and need to solve for the u_j^n).

LinearSolve makes implicit methods more computational expensive than explicit methods.

‣ We call FTCS an explicit method. Instead of using LinearSolve we simply use matrix multiplication (we know the u_j^n and need to solve for the u_j^{n+1}), which is less computationally expensive than LinearSolve.

Error associated with these methods:

Implicit methods tend to undershoot actual values whereas explicit methods overestimate. Crank-Nicholson outperforms both of these methods.

Definition: An FDM is said to be consistent if the rendering is "meaningful", i.e. the solution converges to Δx as $\Delta t \to 0$.

• Lax-Richtmeyer Theorem:

If the finite difference method (FDM) is consistent, then it is stable iff it is convergent.