MACSI One Day Graduate Course:
Numerical Solution to Differential Equations using Matlab

Part 1: Numerical Differentiation and Finite Difference Methods

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Numerical Differentiation

The problem is: *Given values for a function* f *at points* $x = x_0, x_1, \ldots, x_n$, *find approximations for* $f'(x_i)$ *and* $f''(x_i)$.

Why Bother? After all, unlike, say, numerical integration, differentiation is easy.

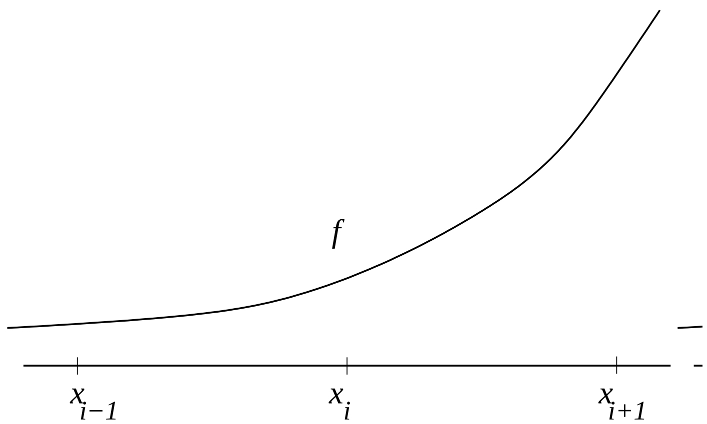
1. Often we don't know f for any x other than the x_i.
2. We might want a simple rule that can be easily programmed.
3. It is a gentle introduction of finite difference methods for boundary value problems.

Numerical Differentiation

Constructing the rules can be done in several ways:

1. Geometrically. Recall, all we are really looking for is the slope of the tangent to $f(x)$ at $x = x_i$.
2. By finding a polynomial that interpolates f and differentiating that.
3. Undetermined coefficients.
4. **Taylor's Theorem**.

Numerical Differentiation Geometry



As suggested by the diagram, one could take

Backward Differencing

$$\frac{df}{dx}(x_i) = f'(x_i) \approx \frac{f_i - f_{i-1}}{x_i - x_{i-1}} =: D^-(f)_i.$$

Forward Differencing

$$f'(x_i) \approx \frac{f_{i+1} - f_i}{x_{i+1} - x_i} =: D^+(f)_i.$$

Since one approach seems to over-estimate $f'(x_i)$, and the other seems to under-estimate it, we could take the average:

Central Differencing

$$f'(x_i) \approx \frac{-f_{i-1} + f_{i+1}}{x_{i+1} - x_{i-1}} =: D^c(f)_i.$$

We are also/primarily interested in approximating

$$\frac{d^2}{dx^2}f(x_i) = f''(x_i).$$

But of course,

$$\frac{d^2}{dx^2}f(x_i) = \frac{d}{dx}\left(\frac{d}{dx}f(x_i)\right) = f''(x_i).$$

so we can use the forward and backward difference operators:

$$f''(x_i) \approx D^+\big(D^-(f)\big)_i.$$

The result is:

2nd Order Central Differencing

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

One may also deduce the rules for D^c and δ^2 above using *undetermined coefficients*: Assume that the rule is of the form

$$a_o f_{i-1} + a_1 f_i + a_{i+1} f_{i+1}$$

and that it will give exactly the right answer for $f(x) \equiv 1$, $f(x) = x$ and $f(x) = x^2$. Then solve for a_0, a_1 and a_2.

This is quite a handy approach if you want to quickly construct a method for estimating derivatives.

The best way to construct differentiation methods — and get error estimates — is to use the celebrated:

Theorem (Taylor's Theorem)

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2}f''(a) + \frac{(x-a)^3}{3!}f'''(a) + \cdots + \frac{(x-a)^n}{n!}f^{(n)}(a) + R_n.$$

where the remainder R_n *is be given by*

$$R_n = \frac{(x-a)^{n+1}}{(n+1)!}f^{(n+1)}(\eta), \qquad \text{for some } \eta \in (a, b).$$

To simplify things, take the points to be equally spaced: $h = x_i - x_{i-1}$.
Suppose we take $a = x_i$ and $x = x_{i-1}$ or $x = x_{i+1}$. Now we can write the truncated Taylor Series:

$$f_{i-1} = f_i - hf'(x_i) + \frac{h^2}{2}f''(\tau),$$

for $\tau \in (x_{i-1}, x_i)$. Rearranging we get

$$f'(x_i) = \frac{1}{h}(f_i - f_{i-1}) + \frac{h}{2}f''(\tau),$$

the backward difference scheme, with an error term.

For the central difference scheme, write:

$$f_{i+1} = f_i + hf'(x_i) + \frac{h^2}{2}f''(x_i) + \frac{h^3}{6}f'''(\tau_1), \quad \text{for } \tau_1 \in (x_i, x_{i+1}),$$
$$f_{i-1} = f_i - hf'(x_i) + \frac{h^2}{2}f''(x_i) - \frac{h^3}{6}f'''(\tau_2), \quad \text{for } \tau_2 \in (x_{i-1}, x_i).$$

Now subtract the 2nd equation from the 1st and divide by $2h$ to get the central difference operator $D^c(f)_i$,
To complete the error terms, just observe that, if $f'''(x)$ is continuous on $[x_{i-1}, x_{i+1}]$, then there must be a point $\tau \in [x_{i-1}, x_{i+1}]$ such that $f'''(\tau) = (f'''(\tau_1) + f'''(\tau_2))/2$.

To get the second-order difference operator $\delta^2(f)_i$, just extend the formulae above by one more term

$$f_{i+1} = f_i + hf'(x_i) + \frac{h^2}{2}f''(x_i) + \frac{h^3}{6}f'''(x_i) + \frac{h^4}{24}f^{(iv)}(\tau_1),$$
$$f_{i-1} = f_i - hf'(x_i) + \frac{h^2}{2}f''(x_i) - \frac{h^3}{6}f'''(x_i) + \frac{h^4}{24}f^{(iv)}(\tau_2),$$

add them and divide by h^2:

$$\begin{aligned} f''(x_i) &= \delta^2 f_i + \frac{h^2}{12}f^{(iv)}(\tau) \\ &= \frac{1}{h^2}(f_{i-1} - 2f_i + f_{i+1}) + \frac{h^2}{12}f^{(iv)}(\tau) \end{aligned}$$

for some $\tau \in (x_{i-1}, x_{i+1}$.

Our differential equation is

$$-u''(x) + r(x)u(x) = f(x) \quad \text{for } 0 < x < 1.$$
$$u(0) = \alpha, u(1) = \beta.$$

Idea:

- Choose a number $N \geqslant 2$ of points in your mesh:

  $0 = x_0 < x_1 < \cdots < x_{n-1} < x_n = 1$, where $x_k - x_{k-1} = h = \dfrac{1}{N}$.
- Replace the 2nd derivative in the equation with the 2nd order difference formula that we found earlier.

$$u''(x_i) \approx \delta^2 u_i = \frac{1}{h^2}(u_{i-1} - 2u_i + u_{i+1}).$$

- Solve the resulting system of linear equations to get an approximation for the solution to the DE *at the mesh points*.

Finite Difference Method

Let u_k be the approximation for $u(x_k)$. Then:

$$u_0 = A$$

$$-\frac{1}{h^2}(u_{k-1} - 2u_k + u_{k+1}) + r_k u_k = f_k$$

$$u_N = B$$

where r_k and f_k are short-hand for $r(x_k)$ and $f(x_k)$.

This is just the linear system of equations:

$$\mathbf{A}\mathbf{u} = \mathbf{f}$$

where $\mathbf{u}$ and $\mathbf{v}$ are vectors:

$$\mathbf{u} = \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_n \end{pmatrix} \quad \mathbf{f} = \begin{pmatrix} \alpha \\ f_1 \\ f_2 \\ f_3 \\ \vdots \\ \beta \end{pmatrix}.$$

And A is the matrix

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \dots & 0 \\ -1/h^2 & 2/h^2 + r_1 & -1/h^2 & 0 & 0 & \dots & 0 \\ 0 & -1/h^2 & 2/h^2 + r_2 & -1/h^2 & 0 & \dots & 0 \\ 0 & 0 & -1/h^2 & 2/h^2 + r_2 & -1/h^2 & \dots & 0 \\ \vdots & & & & & \ddots & \\ 0 & 0 & 0 & 0 & 0 & \dots & 1 \end{pmatrix}$$

This is a *tridiagonal* linear system of equations: it is easily solved.