Computational Physics

Numerical Differentiation

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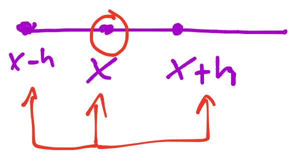
Approximating a Derivative

GOAL: Given a set of tabulated values (x_i, y_i), construct an approximation to the derivative of the function $y(x)$.
RECALL:

$$
\begin{aligned}
\frac{dy}{dx} &= \lim_{h\to 0} \frac{y(x+h) - y(x)}{h} \\
&= \lim_{h\to 0} \frac{y(x) - y(x-h)}{h} \\
&= \lim_{h\to 0} \frac{y(x+h) - y(x-h)}{2\,h}
\end{aligned}
$$



Thus, possible numerical approximation to the derivative are

$$
\begin{aligned}
\frac{dy}{dx} &\approx \frac{y_{i+1} - y_i}{h} \\
&\approx \frac{y_i - y_{i-1}}{h} \\
&\approx \frac{y_{i+1} - y_{i-1}}{2\,h}
\end{aligned}
$$

where $x_{i+1} - x_i = h$

But,

- What is the error we make by using the numerical approximation?
- What is the best choice?
- Which is grid point location where a given numerical approximation applies?
- How to construct more accurate approximations?
- How about higher derivatives?

The tool that we are going to use to answers all of these questions is Taylor series expansions.

$$y(x-x_0) = y_0+(x-x_0)y_0'+\frac{(x-x_0)^2}{2!}y_0''+\frac{(x-x_0)^3}{3!}y_0^{(3)}+\frac{(x-x_0)^4}{4!}y_0^{(4)}+...$$

Approximating the First Order Derivative

GOAL: Find the numerical approximation to the first order derivative of $y(x)$ at x_i using information at the neighboring points $\{x_{i-2}, x_{i-1}, x_i, x_{i+1}, x_{i+2}\}$
From

$$y(x-x_0) = y_0+(x-x_0)y_0'+\frac{(x-x_0)^2}{2!}y_0''+\frac{(x-x_0)^3}{3!}y_0^{(3)}+\frac{(x-x_0)^4}{4!}y_0^{(4)}+...$$

rewrite using $x_{i+1} - x_i = h$

$$\begin{aligned}
y_{i+1} &= y_i + h\,y_i' + \frac{h^2}{2!}y_i'' + \frac{h^3}{3!}y_i^{(3)} + \frac{h^4}{4!}y_i^{(4)} + ... \\
y_{i-1} &= y_i - h\,y_i' + \frac{h^2}{2!}y_i'' - \frac{h^3}{3!}y_i^{(3)} + \frac{h^4}{4!}y_i^{(4)} + ... \\
y_{i+2} &= y_i + (2\,h)\,y_i' + \frac{(2\,h)^2}{2!}y_i'' + \frac{(2\,h)^3}{3!}y_i^{(3)} + \frac{(2\,h)^4}{4!}y_i^{(4)} + ... \\
y_{i-2} &= y_i - (2\,h)\,y_i' + \frac{(2\,h)^2}{2!}y_i'' - \frac{(2\,h)^3}{3!}y_i^{(3)} + \frac{(2\,h)^4}{4!}y_i^{(4)} + ...
\end{aligned}$$

$$x - x_0 = h$$

$$y = y_0 + h y_0' + \frac{h^2}{2!} y_0'' + \frac{h^3}{3!} y_0''' + \cdots$$

$$y_0 \to y_i$$

$$y \to y_{i+1}$$

$$y_{i+1} = y_i + h y_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{6} y_i''' + \cdots$$

$$y_i' = \frac{y_{i+1}}{h} - \frac{y_i}{h} - \frac{h}{2} y_i'' - \frac{h^2}{6} y_i''' - \cdots$$

$$y_i' = \frac{y_{i+1} - y_i}{h} - \frac{h}{2!} y_i'' - \frac{h^2}{3!} y_i''' + \cdots$$

$$y_i' \simeq \frac{y_{i+1} - y_i}{h} + \varepsilon_i + \cdots$$

$\varepsilon_i = -\frac{h}{2!} y_i''$ leading truncation error $\qquad \varepsilon \propto O(h)$ 1st order accurate

FINITE DIFFERENCE

One possibility is then to use

$$y_{i+1} = y_i + h\,y_i' + \frac{h^2}{2!}y_i'' + \frac{h^3}{3!}y_i^{(3)} + \frac{h^4}{4!}y_i^{(4)} + \ldots$$

solving for y_i'

$$y_i' = \frac{y_{i+1} - y_i}{h} - \frac{h}{2!}y_i'' - \frac{h^2}{3!}y_i^{(3)} - \frac{h^3}{4!}y_i^{(4)} + \ldots$$

Notice that at this stage there are no approximations yet since we have kept the infinite sum. It is when we approximate

$$y_i' \approx \frac{y_{i+1} - y_i}{h}$$

when an error is introduced.

Therefore, from

$$y_i' = \frac{y_{i+1} - y_i}{h} - \frac{h}{2!} y_i'' - \frac{h^2}{3!} y_i^{(3)} - \frac{h^3}{4!} y_i^{(4)} + ...$$

we have that

$$\left[\frac{dy}{dx}\right]_i = \left[\frac{\Delta y}{\Delta x}\right]_i + \mathcal{E}_i + \ldots$$

where

$$\left[\frac{\Delta y}{\Delta x}\right]_i = \frac{y_{i+1} - y_i}{h}$$

is the finite difference approximation to y_i' and

$$\mathcal{E}_i = -\frac{h}{2!} y_i''$$

is the leading truncation error. Notice that in this case $\mathcal{E} \propto \mathcal{O}(h)$. That is, the approximation is first order accurate.

$y = y_0 + hy_0' + \frac{h^2}{2!}y_0'' + \frac{h^3}{3!}y_0''' + \frac{h^4}{4!}y_0'''' + \dots$

$y_{i-1} = y_i + hy_i' + h^2/2! \dots$

If we use the point x_{i-1} instead, we get

$$y_i' = \frac{y_i - y_{i-1}}{h} + \frac{h}{2!}y_i'' - \frac{h^2}{3!}y_i^{(3)} + \frac{h^3}{4!}y_i^{(4)} + \dots$$

thus

$$\left[\frac{dy}{dx}\right]_i = \left[\frac{\Delta y}{\Delta x}\right]_i + \mathcal{E}_i + \dots$$

with

$$\left[\frac{\Delta y}{\Delta x}\right]_i = \frac{y_i - y_{i-1}}{h}$$

and

$$\mathcal{E}_i = \frac{h}{2!}y_i''$$

The error again is $\mathcal{E} \propto \mathcal{O}(h)$.

Finally, if we use both the point and x_{i+1} and x_{i-1}, we have from

$$
\begin{aligned}
y_{i+1} &= y_i + h\,y_i' + \frac{h^2}{2!}y_i'' + \frac{h^3}{3!}y_i^{(3)} + \frac{h^4}{4!}y_i^{(4)} + \ldots \\
y_{i-1} &= y_i - h\,y_i' + \frac{h^2}{2!}y_i'' - \frac{h^3}{3!}y_i^{(3)} + \frac{h^4}{4!}y_i^{(4)} + \ldots
\end{aligned}
$$

that

$$y_{i+1} - y_{i-1} = 2\,h\,y_i' + 2\frac{h^3}{3!}y_i^{(3)} + \ldots$$

$$\frac{y_{i+1}-y_{i-1}}{2h} = \left.\frac{dy}{dx}\right|_i$$

thus

$$\left[\frac{dy}{dx}\right]_i = \left[\frac{\Delta y}{\Delta x}\right]_i + \mathcal{E}_i + \ldots$$

with

$$\left[\frac{\Delta y}{\Delta x}\right]_i = \frac{y_{i+1}-y_{i-1}}{2\,h}$$

and

$$\mathcal{E}_i = \frac{h^2}{3!}y_i^{(3)}$$

The error in this case is $\mathcal{E} \propto \mathcal{O}(h^2)$, i.e. second order accurate.

Approximating the Second Order Derivative

From

$$
\begin{aligned}
y_{i+1} &= y_i + h\,y_i' + \frac{h^2}{2!}y_i'' + \frac{h^3}{3!}y_i^{(3)} + \frac{h^4}{4!}y_i^{(4)} + \ldots \\
y_{i-1} &= y_i - h\,y_i' + \frac{h^2}{2!}y_i'' - \frac{h^3}{3!}y_i^{(3)} + \frac{h^4}{4!}y_i^{(4)} + \ldots
\end{aligned}
$$

one has that

$$
y_{i+1} + y_{i-1} = 2\,y_i + 2\frac{h^2}{2!}y_i'' + 2\frac{h^4}{4!}y_i^{(4)} + \ldots
$$

then

$$
\frac{y_{i+1} - 2\,y_i + y_{i-1}}{h^2} = y_i'' + \frac{h^2}{12}y_i^{(4)} + \ldots
$$

$$
y_i'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \frac{h^2}{12}y_i^{(4)} + \ldots
$$

Then

$$\left[\frac{d^2y}{dx^2}\right]_i = \left[\frac{\Delta^2 y}{\Delta x^2}\right]_i + \mathcal{E}_i + \dots$$

where

$$\left[\frac{\Delta^2 y}{\Delta x^2}\right]_i = \frac{y_{i+1} - 2\,y_i + y_{i-1}}{h^2}$$

and

$$\mathcal{E}_i = \frac{h^2}{12} y_i^{(4)}$$

the approximation is second order accurate.

The approximations that we have constructed so far were found with an educated guess. We need a general procedure that does not involve "guessing."

Consider again the first order derivative. Suppose we are looking for a finite difference approximation at the grid point x_i that involves only information at the grid points x_i and x_{i+1}. That is, we are looking for an expression of the form

$$\left[\frac{\Delta y}{\Delta x}\right]_i = a_1\, y_{i+1} + a_0\, y_i$$

such that

$$\left[\frac{dy}{dx}\right]_i = \left[\frac{\Delta y}{\Delta x}\right]_i + \mathcal{E}_i$$

with a_0 and a_1 unknown coefficients to be determined.

Substitute in

$$\left[\frac{\Delta y}{\Delta x}\right]_i = a_1\, y_{i+1} + a_0\, y_i$$

the Taylor expansion of y_{i+1} around x_i. That is,

$$y_{i+1} \quad = \quad y_i + h\, y_i' + \frac{h^2}{2!} y_i'' + \frac{h^3}{3!} y_i^{(3)} + \ldots$$

Then

$$\begin{aligned}
\left[\frac{\Delta y}{\Delta x}\right]_i &= a_1 \left[y_i + h\, y_i' + \frac{h^2}{2!} y_i'' + \frac{h^3}{3!} y_i^{(3)} + \ldots \right] + a_0\, y_i \\
\left[\frac{dy}{dx}\right]_i - \mathcal{E}_i &= (a_1 + a_0) y_i + a_1\, h\, y_i' + a_1 \left[\frac{h^2}{2!} y_i'' + \frac{h^3}{3!} y_i^{(3)} + \ldots \right] \\
y_i' - \mathcal{E}_i &= (a_1 + a_0) y_i + a_1\, h\, y_i' + a_1 \left[\frac{h^2}{2!} y_i'' + \frac{h^3}{3!} y_i^{(3)} + \ldots \right] \\
0 &= (a_1 + a_0) y_i + (a_1\, h - 1) y_i' + \mathcal{E}_i + a_1 \left[\frac{h^2}{2!} y_i'' + \frac{h^3}{3!} y_i^{(3)} + \ldots \right]
\end{aligned}$$

Since

$$0 = (a_1 + a_0)y_i + (a_1\,h - 1)y_i' + \mathcal{E}_i + a_1\left[\frac{h^2}{2!}y_i'' + \frac{h^3}{3!}y_i^{(3)} + ...\right]$$

is valid for an arbitrary function $y(x)$, then the only way this expression is satisfied if

$$\begin{aligned} 0 &= a_1 + a_0 \\ 0 &= a_1\,h - 1 \\ 0 &= \mathcal{E}_i + a_1\left[\frac{h^2}{2!}y_i'' + \frac{h^3}{3!}y_i^{(3)} + ...\right] \end{aligned}$$

which yields

$$\begin{aligned} a_0 &= -1/h \\ a_1 &= 1/h \\ \mathcal{E}_i &= -\frac{h}{2!}y_i'' + \ldots \end{aligned}$$

which is the results we derived before

$$\left[\frac{\Delta y}{\Delta x}\right]_i = \frac{y_{i+1} + y_i}{h}$$

Finite Difference Approximations: First Derivative

$y' =$

FD Approximation	Truncation Error	Convergence
$\frac{y_{i+1}-y_{i-1}}{2h}$	$\frac{1}{6}h^2\,y^{(3)}$	Second
$\frac{y_{i+1}-y_i}{h}$	$-\frac{1}{2}h\,y^{(2)}$	First
$\frac{y_i-y_{i-1}}{h}$	$\frac{1}{2}h\,y^{(2)}$	First
$\frac{-3\,y_i+4\,y_{i+1}-y_{i+2}}{2\,h}$	$\frac{1}{3}h^2\,y^{(3)}$	Second
$\frac{y_{i-2}-8\,y_{i-1}+8y_{i+1}-y_{i+2}}{12\,h}$	$\frac{1}{30}h^4\,y^{(5)}$	Forth

Finite Difference Approximations: Second Derivative

y''

FD Approximation	Truncation Error	Convergence
$\frac{y_{i+1}-2\,y_i+y_{i-1}}{h^2}$	$\frac{1}{12}h^2\,y^{(4)}$	Second
$\frac{y_i-2\,y_{i+1}+y_{i+2}}{h^2}$	$h\,y^{(3)}$	First
$\frac{-y_{i-2}+16\,y_{i-1}-30y_i+16y_{i+1}-y_{i+2}}{12\,h^2}$	$\frac{-1}{90}h^4\,y^{(6)}$	Forth

Discretization

* solve a continuum system approximately using discretization

* continuum function might depend on t, $0 \leq t \leq t_{max}$
  ∞ # of t's

* discrete function will be defined finite # of times
  t^n, $n = 1, 2, \cdots, n$ $\therefore$ finite # of t's

* Reduce ∞ DOF to finite because computational
  → resources are finite

* Replace differential equations with algebraic eqn.
  → can then solve them computationally

* We will focus on finite differencing (not finite element, spectral)

* $$\underbrace{\frac{df(x)}{dx} \equiv f'(x)}_{\text{continuum}} = \lim_{h \to 0} \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{FDA}} \qquad h = \Delta x$$

Steps for Solving DE using FDA

1. formulate precise + complete mathematical description
   - * specify independent variables $t, x, \ldots$
   - * specify domain in terms of those variables

     $0 \le t \le t_{max}$

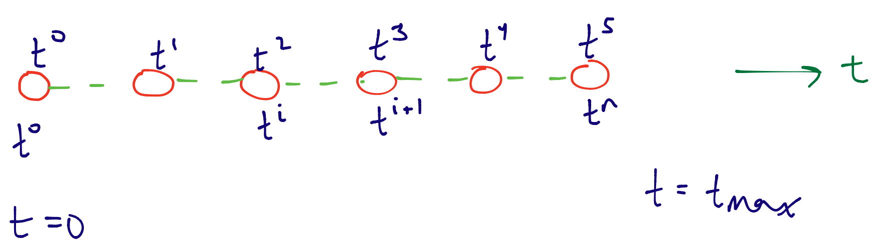
     $0 \le L \le 100$
   - * write down dependent variable $y(x), f(x) \ldots$
   - * write down equations
   - * specify boundary conditions

DO THIS NOW FOR $f(x) = \sin(x)$

what b.c. make sense?

* exp. single particle Newton's 2nd Law

$$m a(t) = m \frac{d^2 x(t)}{dt^2} = F_{applied}(t)$$

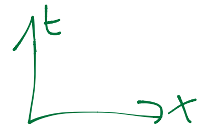


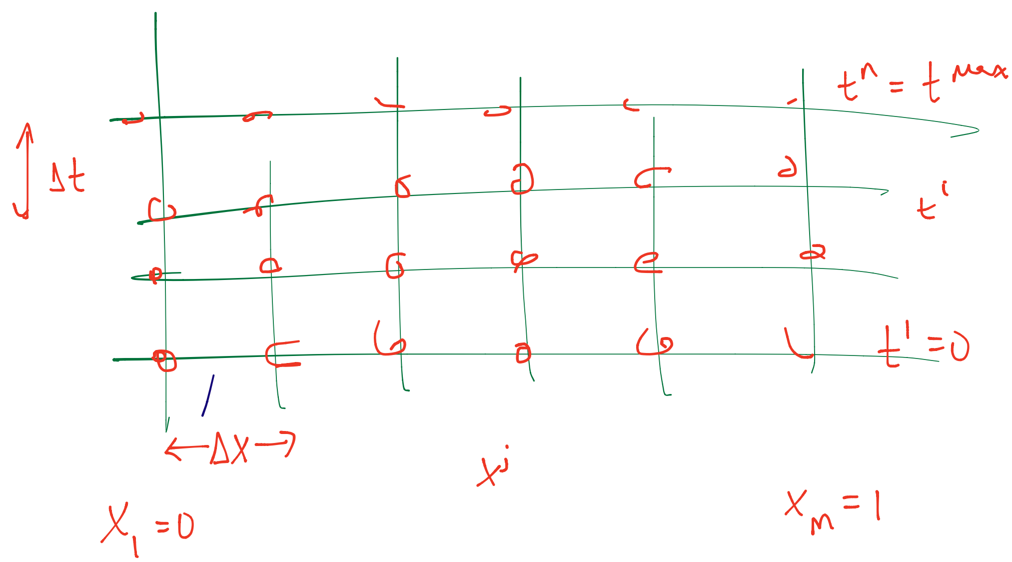
Uniform mesh $t^{i+1} = t^i + \Delta t = t^i + h$

particles located at $x^i = x(t^i)$

EOM determine $x^i \to x^{i+1} \to \ldots$

FDA mesh





2. Define grid, assume uniform, $\Delta t, \Delta x, \ldots$
   mesh spaces control accuracy of FDA
   assume $h \to 0 \to$ continuum solution
   i.e. converge

3. replace derivatives w/ FDA

4. Solve this new set of algebraic eqns.

5. convergence test + error analysis

repeat using everything the same BUT h

is it converging?

errors behaving as predicted?

CODE

take 1^{st} and 2^{nd} derivative of $\sin(x)$; prove you get the correct answer

Richardson Extrapolation

Consider the case of the center finite difference approximation to the second derivative. That is, $y_i'' = D_2(h)_i + \mathcal{E}_i(h)$ where

$$D_2(h)_i = \frac{y_{i+1} - 2\,y_i + y_{i-1}}{h^2}$$

and

$$\begin{aligned}\mathcal{E}(h) &= \frac{1}{12} h^2 y^{(4)} + \mathcal{O}(h^4) + \mathcal{O}(h^6) + \mathcal{O}(h^8)\ldots \\ &= C_2 h^2 + C_4 h^4 + C_6 h^6 + \ldots\end{aligned}$$

Evaluate the derivative approximation with h and $h/2$; that is,

$$\begin{aligned} y'' &= D_2(h) + C_2 h^2 + C_4 h^4 + \ldots \\ y'' &= D_2(h/2) + C_2 \left(\frac{h}{2}\right)^2 + C_4 \left(\frac{h}{2}\right)^4 + \ldots \end{aligned}$$

Multiply the second equation by 4 and subtract the first equation.

$$\begin{aligned} 3\,y'' &= 4\,D_2(h/2) - D_2(h) + 4\,C_4 \left(\frac{h}{2}\right)^4 - C_4 h^4 + \ldots \\ y'' &= \frac{1}{3}\left[4\,D_2(h/2) - D_2(h)\right] - \frac{3}{4} C_4 h^4 + \ldots \end{aligned}$$

Thus, we have then

$$y'' = D_4(h) + \bar{C}_4 h^4 + \bar{C}_6 h^6 + \ldots$$

where now the approximation is given by (notice is 4th order)

$$D_4(h) = \frac{1}{3}\left[4\,D_2(h/2) - D_2(h)\right]$$

Richardson Extrapolation

Consider the case of the center finite difference approximation to the second derivative. That is, $y_i'' = D_2(h)_i + \mathcal{E}_i(h)$ where

$$D_2(h)_i = \frac{y_{i+1} - 2\,y_i + y_{i-1}}{h^2}$$

and

$$\begin{aligned}\mathcal{E}(h) &= \frac{1}{12}h^2 y^{(4)} + \mathcal{O}(h^4) + \mathcal{O}(h^6) + \mathcal{O}(h^8)\ldots \\ &= C_2 h^2 + C_4 h^4 + C_6 h^6 + \ldots\end{aligned}$$

$$4y'' = 4D_2\left(\frac{h}{2}\right) + \frac{4C_2h^2}{4} + C_4\left(\frac{h}{2}\right)^4$$

$$\underline{-y'' = -D_2(h) - C_2h^2 - C_4h^4}$$

$$3y'' = 4D_2\left(\frac{h}{2}\right) - D_2(h) + 4C_4\left(\frac{h}{2}\right)^4 - C_4h^4 + \cdots$$

$$y'' = \frac{1}{3}\left[4D_2\left(\frac{h}{2}\right) - D_2(h)\right] - \frac{3}{4}C_4h^4 + \cdots$$ improved!

but $D_2(h) = \dfrac{y_{i+1} - 2y_i + y_{i-1}}{h^2}$

$$y'' = \frac{1}{3}\left[16\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} - \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}\right] - \frac{3}{4}C_4h^4$$

Using your code, implement
forward
backward
center differencing y'

$u(x) = \sin \pi x$
$u'(x) = \pi \cos \pi x$ > smooth ∴ can predict truncation error using Taylor series

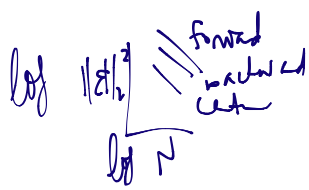
$-1 \le x \le 1$ $\Delta x = \frac{2}{N}$; $x_i = i\Delta x - 1$, $i = 0, \dots, N$

$\varepsilon_i = \tilde{u}'(x_i) - u(x_i)$
FDA - analytical derivatives

measure how ε changes as $N \uparrow$

rms $\|\varepsilon\|_2 = \Delta x \left(\sum_{i=0}^{N} \varepsilon_i^2 \right)^{1/2}$

$\|\varepsilon\|_\infty = \max_{0 \le i \le N} (\varepsilon_i)$ $N = 1024$



compute slope

compare to order