Computational Physics and Astrophysics

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 high derivatives?

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

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

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

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

we have that

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

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

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

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

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.

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

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

thus

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

with

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

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

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

that

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

thus

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

with

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

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

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

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,

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

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

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

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

FD Approximation	Truncation Error	Convergence
$\frac{y_{i+1}-y_{i-1}}{h}$	$\frac{1}{6}h^2\,y^{(3)}$	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

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
$\frac{-y_{i-2} + 16\,y_{i-1} - 30 y_i + 16 y_{i+1} - y_{i+2}}{12\,h}$	$\frac{-1}{90} h^4\, y^{(6)}$	Forth

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,

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

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

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

Thus, we have then

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

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

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