# 12.010 Computational Methods of Scientific Programming

Lecture 10: Code re-visits

# Summary

- **Issues from notebooks that students want to look at?**
- Re-examine codes; clean-up and add documentation
- polyarea
  - Check the sign of area (code seemed to depend on int versus float)
  - Crossing line issue: Algorithm to test
  - Adding image and graphical selection of areas
- OS check in my.style creation
- Improvements to integrators and ODE solvers

# OS check

- One notebook used unix ! echo construction to create my.style.  This works on unix and macosx but not windows
- Check OS:
  import sys
  sys.platform
- Returns darwin for mac, linux2 for my Ubuntu system?

# Revisit tick marks

- Update to last cell in Lec09_graphics.ipynb to change ticks with ax.tick_params

# Revisit polyarea.ipynb

- Issue with test of concave/convex with integers and floats
- Graphical interface to get values into program: Use image to background of figure.
- Axis to np.append in polyarea: Current works but could be improved
- Crossing line code?

# Derivatives revisit

- Looked at derivative for function evaluated at discrete set of point $x_0$, $x_1$, … separated by distance, h.
  - Forward/backward deriv (one sided)
    - $f'(x_j) \approx 1/h[\ f(x_{j+1})-f(x_j)\ ]$
  - Centered deriv
    - $f'(x_j) \approx 1/2h[\ f(x_{j-1})-f(x_{j+1})\ ]$
  - Centered was more accurate than forward
- There are other formula that increase accuracy, starting from Taylor series

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \ldots$$

# Derivatives revisit

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \dots$$ ➔

(1) $f(x_{j-2}) \approx f(x_j) - f'(x_j)2h + \frac{1}{2}f''(x_j)4h^2 - \frac{1}{6}f'''(x_j)8h^3 + \frac{1}{24}f''''(x_j)16h^4 - \frac{1}{120}f'''''(x_j)32h^5 + \dots$

(2) $f(x_{j-1}) \approx f(x_j) - f'(x_j)h + \frac{1}{2}f''(x_j)h^2 - \frac{1}{6}f'''(x_j)h^3 + \frac{1}{24}f''''(x_j)h^4 - \frac{1}{120}f'''''(x_j)h^5 + \dots$

(3) $f(x_{j-1}) \approx f(x_j) + f'(x_j)h + \frac{1}{2}f''(x_j)h^2 + \frac{1}{6}f'''(x_j)h^3 + \frac{1}{24}f''''(x_j)h^4 + \frac{1}{120}f'''''(x_j)h^5 + \dots$

(4) $f(x_{j+2}) \approx f(x_j) + f'(x_j)2h + \frac{1}{2}f''(x_j)4h^2 + \frac{1}{6}f'''(x_j)8h^3 + \frac{1}{24}f''''(x_j)16h^4 + \frac{1}{120}f'''''(x_j)32h^5 + \dots$

$$x_j = x_0 + h(j-1)$$

# Derivatives revisit

(1) $f(x_{j-2}) \approx f(x_j) - f'(x_j)2h + \frac{1}{2}f''(x_j)4h^2 - \frac{1}{6}f'''(x_j)8h^3 + \frac{1}{24}f''''(x_j)16h^4 - \frac{1}{120}f'''''(x_j)32h^5 + \ldots$

(2) $f(x_{j-1}) \approx f(x_j) - f'(x_j)h + \frac{1}{2}f''(x_j)h^2 - \frac{1}{6}f'''(x_j)h^3 + \frac{1}{24}f''''(x_j)h^4 - \frac{1}{120}f'''''(x_j)h^5 + \ldots$

(3) $f(x_{j-1}) \approx f(x_j) + f'(x_j)h + \frac{1}{2}f''(x_j)h^2 + \frac{1}{6}f'''(x_j)h^3 + \frac{1}{24}f''''(x_j)h^4 + \frac{1}{120}f'''''(x_j)h^5 + \ldots$

(4) $f(x_{j+2}) \approx f(x_j) + f'(x_j)2h + \frac{1}{2}f''(x_j)4h^2 + \frac{1}{6}f'''(x_j)8h^3 + \frac{1}{24}f''''(x_j)16h^4 + \frac{1}{120}f'''''(x_j)32h^5 + \ldots$

1/(12h) { 8 x [ (2) – (3) ] – [ (4) – (1) ] } ➔

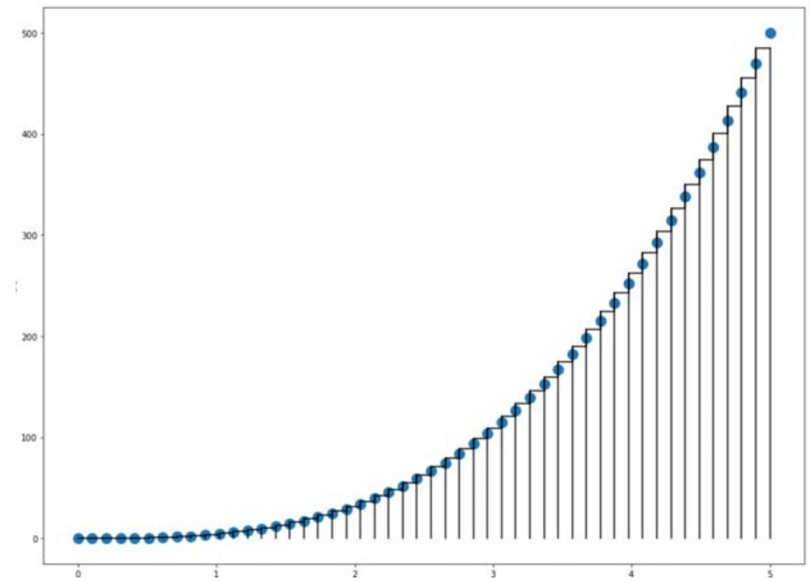
$$f'(x_j) \approx \frac{f(x_{j-2}) - 8f(x_{j-1}) + 8f(x_{j+1}) + f(x_{j+2})}{12h} + \ldots$$

# Derivatives revisit

- Work through – Lec11-accurate-deriv.ipynb
  - Add comments together to explain!

# Integration revisit

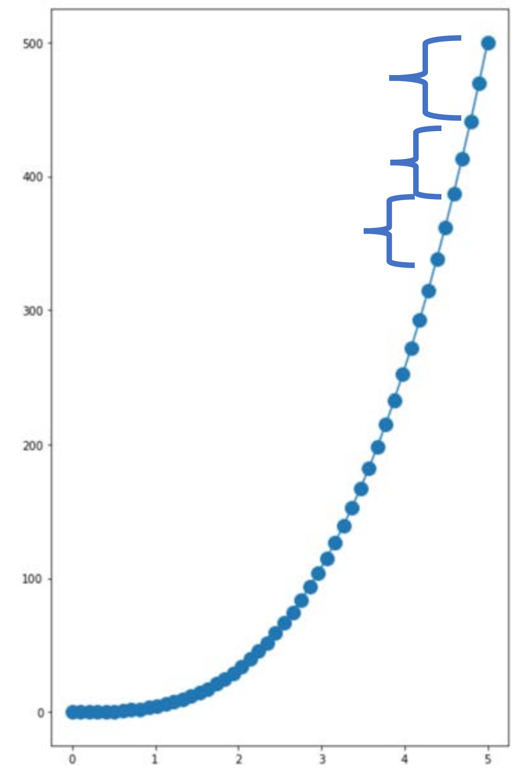
- We looked at trapezoidal method for integration in Lec05-integration.ipynb




- More accurate approach
  - Simpsons – fits quadratic

# Integration revisit

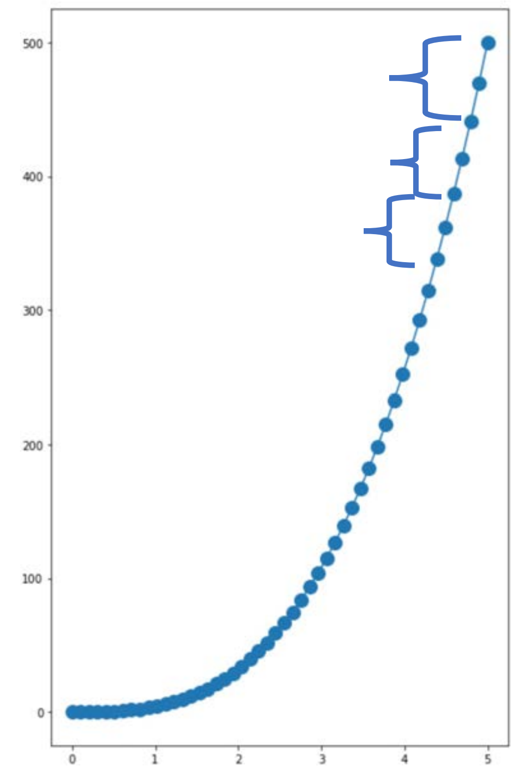
- Simpsons rule
  - Fit quadratic curves to successive subintervals, each spanning 3-points.
  - Requires an even number of sub-intervals.
    - e.g. figure shows 3 successive sets of 3-points
    - Covers 6 sub-intervals
    - Simpson
      - Fit separate quadratic ($ax^2+bx+c$) to each set of 3-points
      - Derive a simple formula for the area under each quadratic



# Integration revisit

- Simpsons rule
  - If we have three points $x_0$ $x_1$ $x_2$ (where $x_1$=0.5($x_0$ +$x_2$ ) ) then we can fit a quadratic such that

$$\int_{x_0}^{x_2} f(x)dx \approx \int_{x_0}^{x_2} (Ax^2 + Bx + c)dx$$



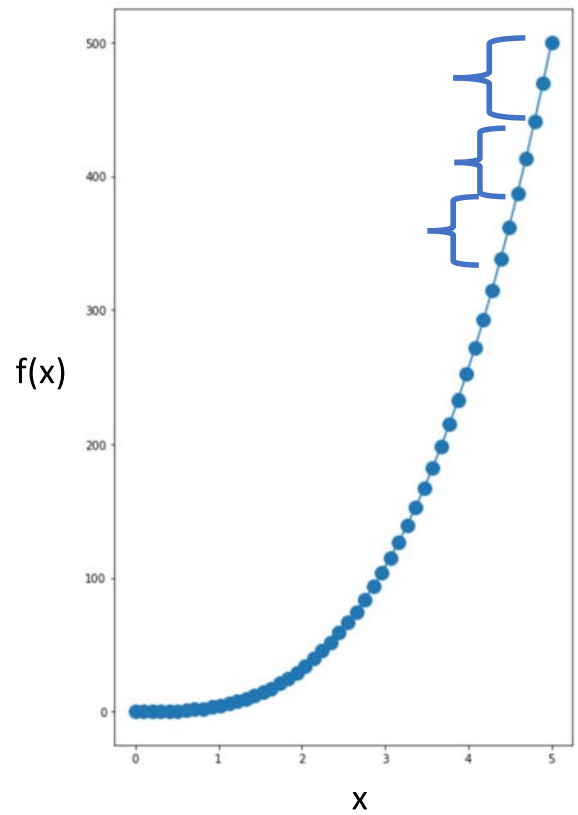
# Integration revisit

- Simpsons rule
  - Analytically we have

$\int_{x_0}^{x_2}(Ax^2+Bx+c)dx = \frac{A}{3}(x_2^3-x_0^3)+\frac{B}{2}(x_2^2-x_0^2)+ +$
C$(x_2^2-x_0^2)$

if $x_1=0.5(x_0+x_2)$ i.e $x_1$ is local mid-point between $x_0$ $x_2$ then can show this is same as

$$\frac{\Delta x}{3}(f(x_2)+4f(x_1)+f(x_0))$$



# Integration revisit

## Derivation (from https://math.libretexts.org ! )

$$= \frac{A}{3}(x_2^3 - x_0^3) + \frac{B}{2}(x_2^2 - x_0^2) + C(x_2 - x_0)$$

$$= \frac{A}{3}(x_2 - x_0)(x_2^2 + x_2x_0 + x_0^2) + \frac{B}{2}(x_2 - x_0)(x_2 + x_0) + C(x_2 - x_0)$$

Factor out $\frac{x_2 - x_0}{6}$.

$$= \frac{x_2 - x_0}{6}\left(2A(x_2^2 + x_2x_0 + x_0^2) + 3B(x_2 + x_0) + 6C\right)$$

Rearrange the terms. Note: $\Delta x = \frac{x_2 - x_0}{2}$

$$= \frac{\Delta x}{3}\left((Ax_2^2 + Bx_2 + C) + (Ax_0^2 + Bx_0 + C) + A(x_2^2 + 2x_2x_0 + x_0^2) + 2B(x_2 + x_0) + 4C\right)$$

Factor and substitute:

$f(x_2) = Ax_2^2 + Bx_2 + C$ and $f(x_0) = Ax_0^2 +$

$$= \frac{\Delta x}{3}\left(f(x_2) + f(x_0) + A(x_2 + x_0)^2 + 2B(x_2 + x_0) + 4C\right)$$

Substitute $x_2 + x_0 = 2x_1$.

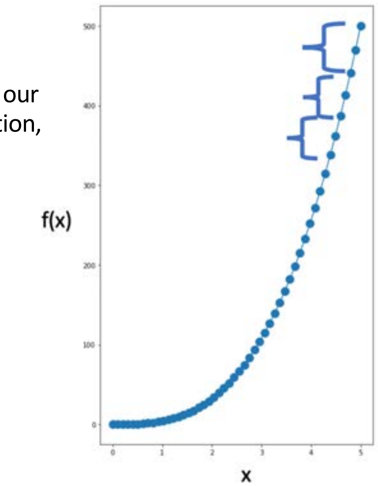
Note: $x_1 = \frac{x_2 + x_0}{2}$, the midpoint.

$$= \frac{\Delta x}{3}\left(f(x_2) + f(x_0) + A(2x_1)^2 + 2B(2x_1) + 4C\right)$$

Expand and substitute $f(x_1) = Ax_1^2 + Bx_1 + C$.

$$= \frac{\Delta x}{3}\left(f(x_2) + 4f(x_1) + f(x_0)\right).$$



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(also Keplersche Fassregel, 100 years before!)

# Integration revisit

Try Lec11-accurate-integral.ipynb