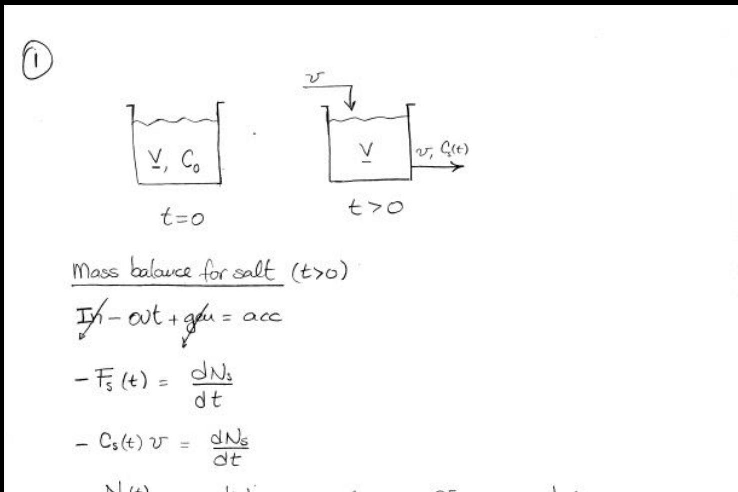
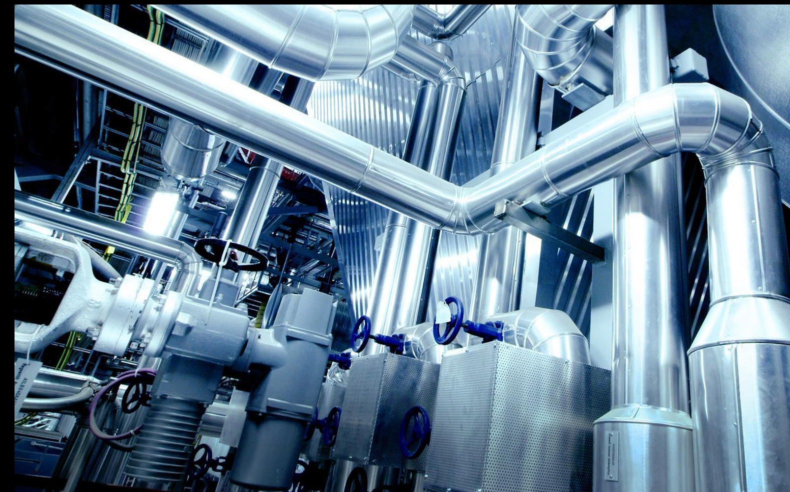


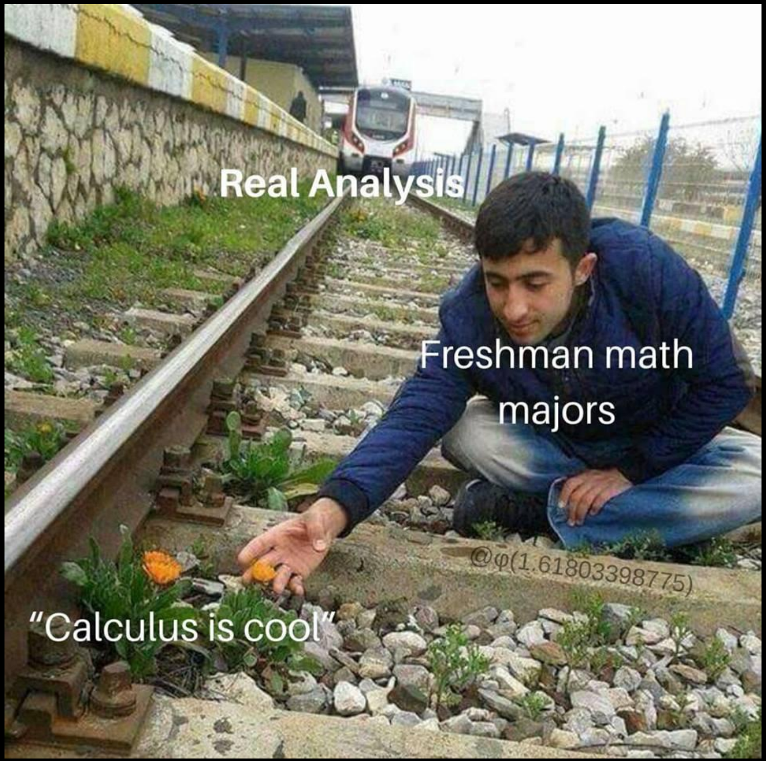


ChE352
Numerical Techniques for Chemical Engineers
Professor Stevenson

Lecture 4

Real Analysis

- Properties of functions and series over the real numbers
- Formalize ideas about calculus
- Vocabulary and notation we'll use for the rest of the course



F&B 1.2: We 💜 Continuous Functions

Sufficient condition for f to be a continuous function:

$$if: \quad \lim_{x \to x_0} f(x) = f(x_0) \quad \forall x \in X$$

$$then: \quad f \text{ is continuous on } X$$

If f is a continuous function of one independent variable on the interval from a to b, we say "*f is in C A B*":

$$f \in C[a,b]$$

Why are continuous functions useful?

Sequences and Convergence

More "numerical" definition of continuity:

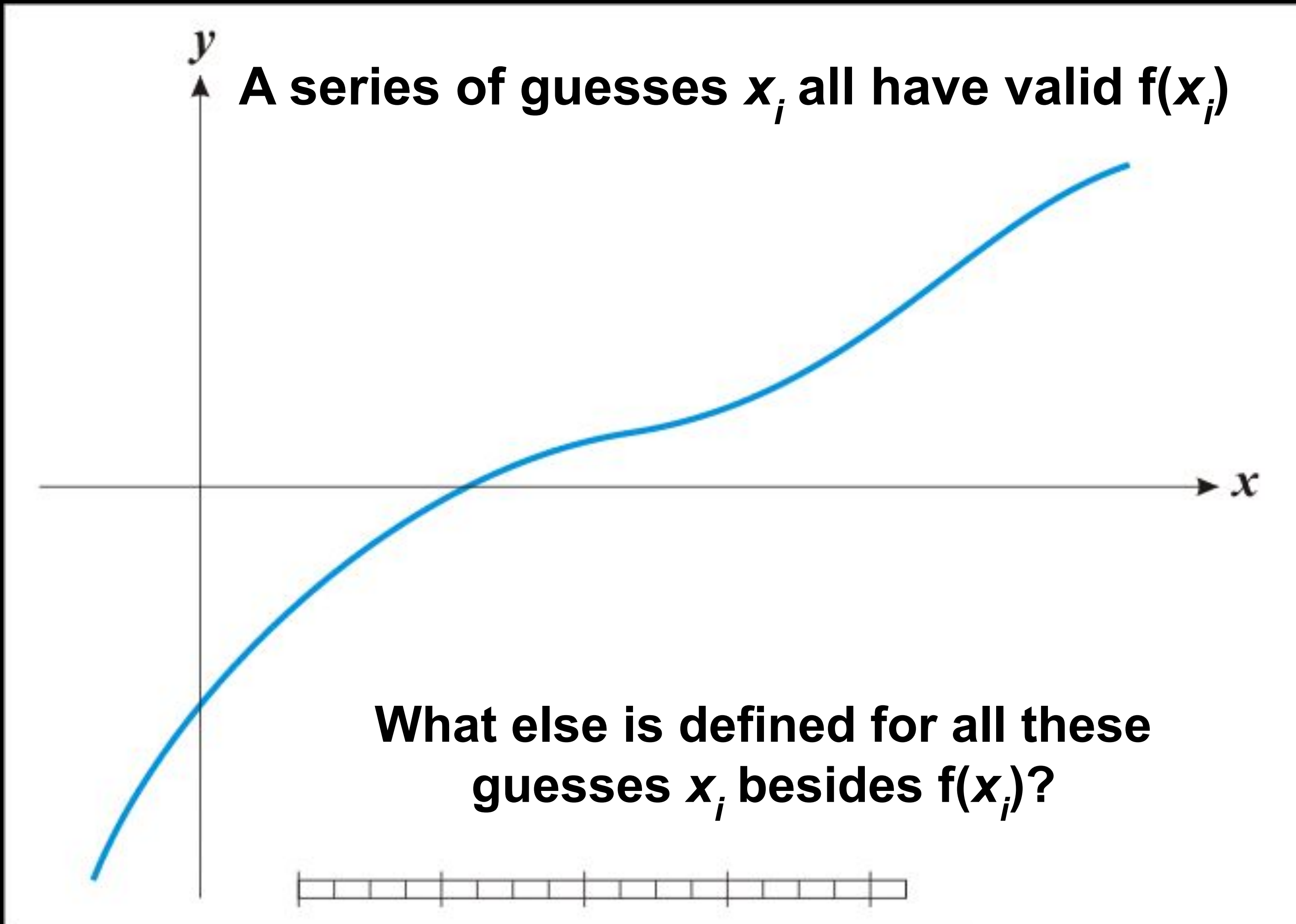
If a function f(x) is continuous, a sequence of trial values x_n such that $x_n \to x_0$ will make f(x_n) approach f(x_0).
This means questions about continuous functions can be solved *iteratively*.

$$\forall f : \mathbb{R} \to \mathbb{R}, \quad X \subset \mathbb{R}$$ ← f is a function taking one real input & giving one real output, and X is also real.

$$if: \quad \{x_n\}_{n=1}^{\infty} \ is\ any\ sequence\ in\ X\ converging\ to\ x_0$$

$$then: \quad \lim_{n\to\infty} f(x_n) = f(x_0)$$

Example: Convergence to a Root



A series of guesses x_i all have valid f(x_i)

What else is defined for all these guesses x_i besides f(x_i)?

Derivatives and Differentiability

For a scalar function f(x):

Lagrange Leibniz Newton Euler

$$f'(x) = \frac{df}{dx} = \dot{f}(x) = D_x f(x) = \boxed{\lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}}$$

- If the limit above exists for all x in [a,b], then we say the function f is <u>differentiable</u> over [a,b]
- A function which is differentiable over [a, b] is continuous over [a, b] too (<u>sufficient condition</u>)
- $f'(x_0)$ is the slope of, aka tangent to, f(x) at x_0

We Like Differentiable Functions

- Polynomials have derivatives of all orders (but most of them are zero)
- Sine, cosine, exponential functions have nonzero derivatives of all orders
- Rational (polynomial divided by polynomial) and logarithmic functions have all continuous derivatives too, but careful about their domain
- The sum & difference & product of differentiable & continuous functions is differentiable & continuous, but not always the quotient (division). Why?

$$\boxed{f \ polynomial \rightarrow \quad f \in C^{\infty}\left[a,b\right]}$$

Activity: Taking Derivatives

Find the derivative of the SRK equation of state with respect to the compressibility factor Z:

$$f(Z) = Z^3 - Z^2 + \left(A - B - B^2\right)Z - AB$$

Is f(Z) continuous? Is it differentiable?

Over what domain of Z is f(Z) <u>physically</u> meaningful?

Answer: Taking Derivatives

$$f'(Z) = 3Z^2 - 2Z + A - B - B^2$$

All polynomials are differentiable. f(Z) is physically meaningful for positive real values of Z, because Z is compressibility factor (PV/nRT).

Compare to the standard form of the Soave-Redlich-Kwong equation of state.

$$p = \frac{RT}{V_m - b} - \frac{a}{\sqrt{T}\,V_m\left(V_m + b\right)}$$

Is this differentiable in terms of molar volume V_m?

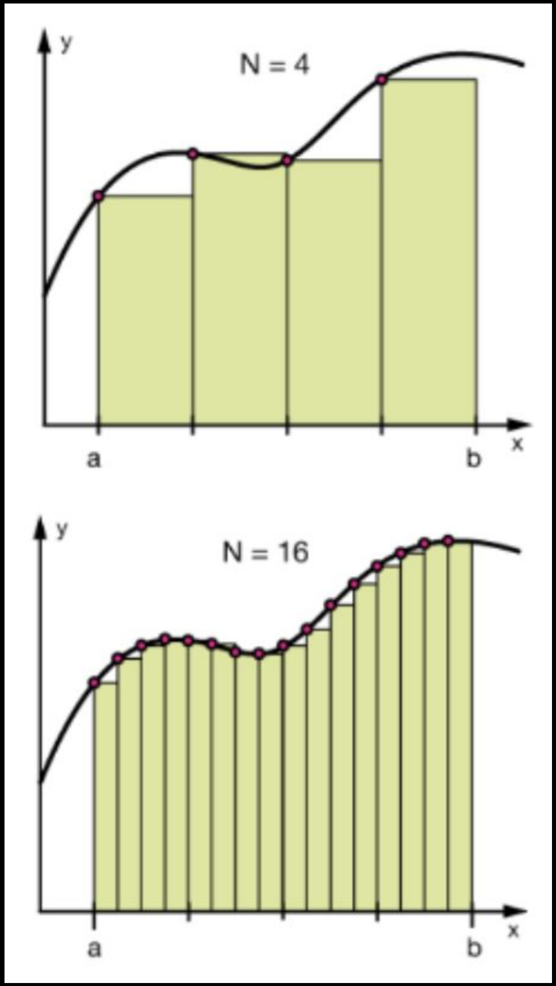
Numerical Definitions of Integrals

$\forall f \; continuous:$

1. $$\int_a^b f(x)\,dx \equiv \lim_{n\to\infty} \frac{b-a}{n} \sum_{i=1}^{n} f(x_i)$$

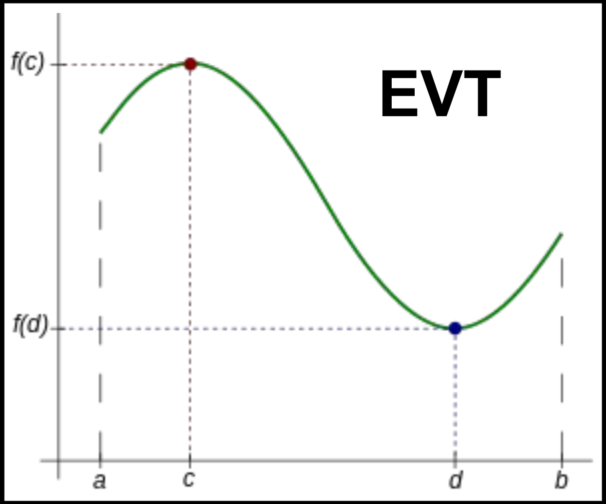
$$x_i \equiv a + \frac{i(b-a)}{n}$$ Discretize x between a and b into n equal slices

2. $$\int_a^b f(x)\,dx =$$ Area under the curve of f(x) between a and b



3. The mean of f(x) over [a, b] $= f(c) = \dfrac{1}{b-a}\displaystyle\int_a^b f(x)\,dx$

Extreme Value Theorem

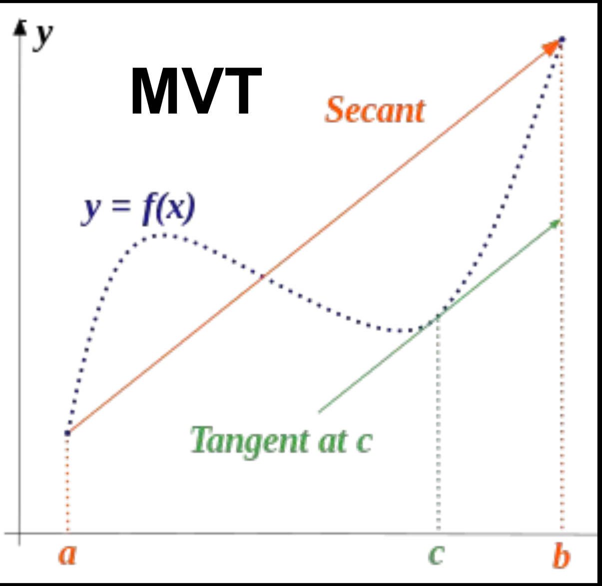


Extreme Value Theorem: if f(x) is continuous on [a, b], there exist points c, d in [a, b] such that f(c) is the maximum of f(x) and f(d) is the minimum.

We build models (like neural networks) from continuous functions partly to take advantage of the Extreme Value Theorem, which shows such functions can be optimized.

Mean Value Theorem

Mean Value Theorem: if f(x) is differentiable on [a, b], point c exists within [a, b] such that f'(c) is exactly the slope of the line between a, f(a) and b, f(b).



Used to define the derivative and integral (Fundamental Theorem of Calculus) and to represent any differentiable function in terms of derivatives (Taylor's Theorem)

Taylor's Theorem

- Estimate f(x) near x_0 using only info at point x_0

Linear approximation

$$P_n(x) = f(x_0) + f'(x_0)(x - x_0)$$

Quadratic

Everything

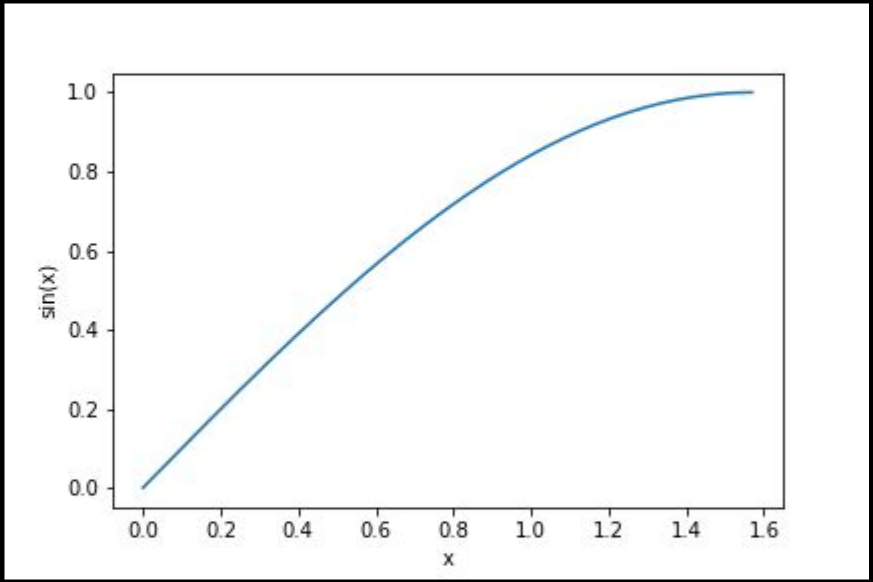
$$+\frac{f''(x_0)}{2!}(x - x_0)^2 + \ldots + \boxed{\frac{f^{(n)}(x_0)}{n!}(x - x_0)^n}$$

$$R_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x - x_0)^{n+1}$$

- $R_n(x)$ is the “remainder”, $\xi(x)$ is a value on $[x_0, x]$

Example: approx sin(x)?

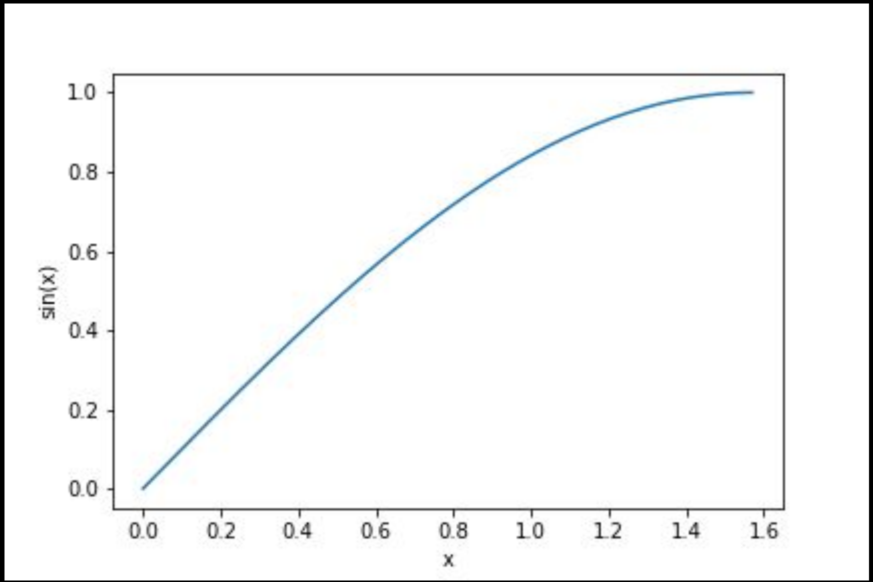
```
import numpy as np
import matplotlib.pyplot as plt
x = np.arange(0, np.pi/2, 0.01)
sin_x = np.sin(x)
plt.plot(x, sin_x)
plt.xlabel('x')
plt.ylabel('sin(x)')
plt.show()
```



What is the first nonzero term of the Taylor Series for sin(x)?

Example: approx sin(x) up to $\pi/2$

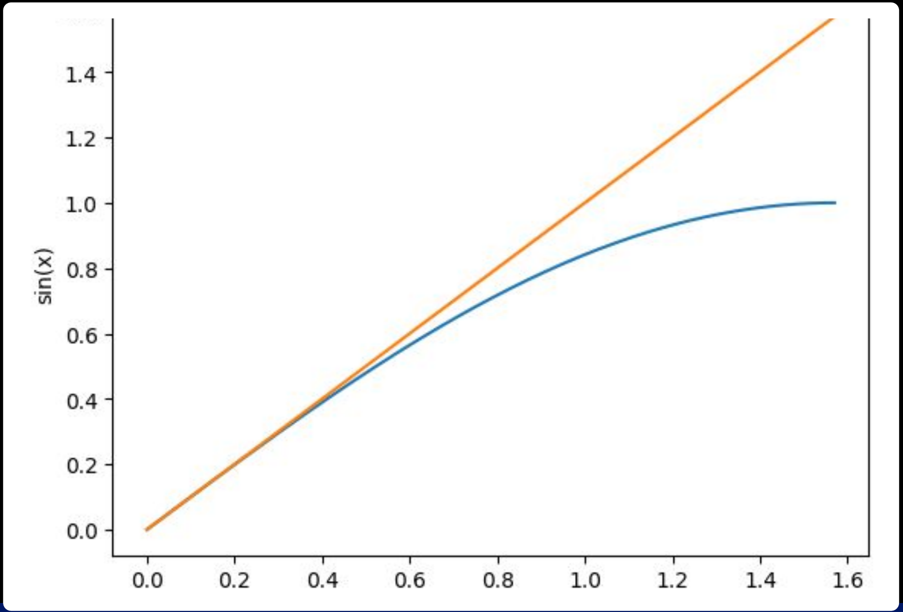
```
import numpy as np
import matplotlib.pyplot as plt
x = np.arange(0, np.pi/2, 0.01)
sin_x = np.sin(x)
plt.plot(x, sin_x)
plt.xlabel('x')
plt.ylabel('sin(x)')
plt.show()
```



Open Colab and plot the first-order (linear) term of the Taylor Series for sin(x)

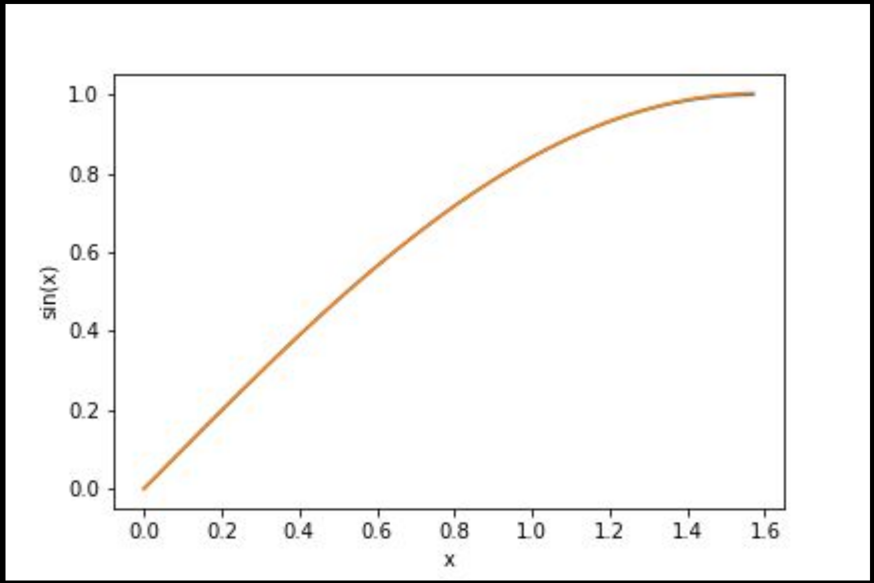
Example: approx sin(x) as x

```
import numpy as np
import matplotlib.pyplot as plt
x = np.arange(0, np.pi/2, 0.01)
sin_x = np.sin(x)
sinish_x = x
plt.plot(x, sin_x)
plt.plot(x, sinish_x)
plt.xlabel('x')
plt.ylabel('sin(x)')
plt.show()
```



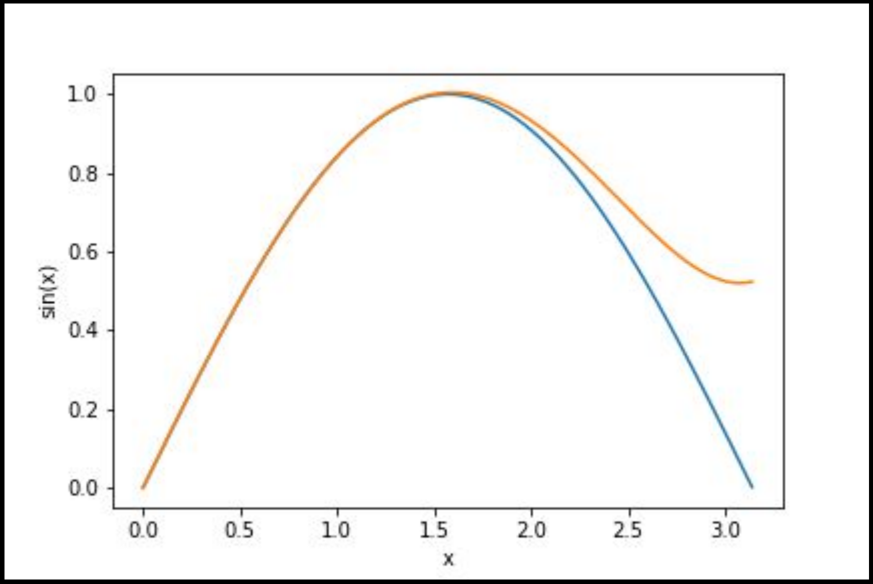
Example: approx sin(x) better

```
import numpy as np
import matplotlib.pyplot as plt
x = np.arange(0, np.pi/2, 0.01)
sin_x = np.sin(x)
sinish_x = x - x**3/(3*2) + x**5/(5*4*3*2)
plt.plot(x, sin_x)
plt.plot(x, sinish_x)
plt.xlabel('x')
plt.ylabel('sin(x)')
plt.show()
```



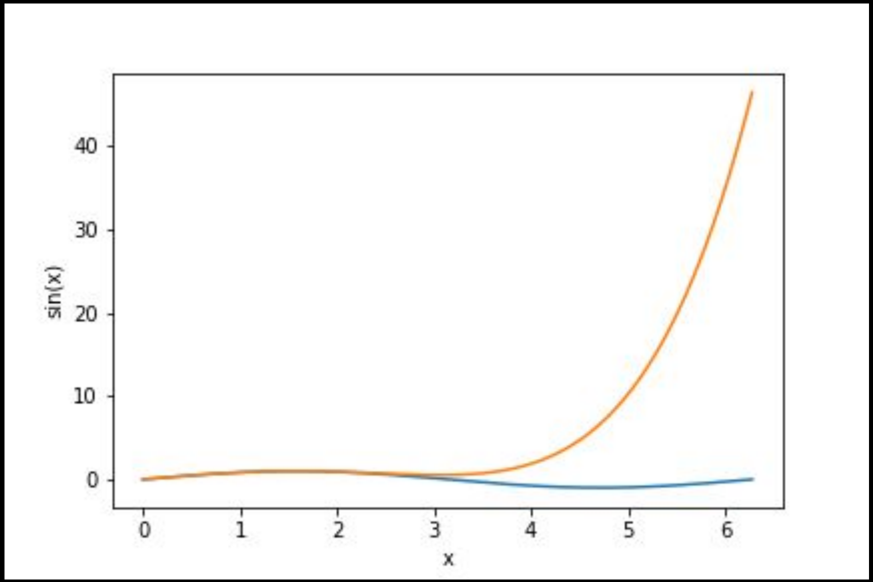
Example: approx sin(x) up to π

```
import numpy as np
import matplotlib.pyplot as plt
x = np.arange(0, np.pi, 0.01)
sin_x = np.sin(x)
sinish_x = x - x**3/(3*2) + x**5/(5*4*3*2)
plt.plot(x, sin_x)
plt.plot(x, sinish_x)
plt.xlabel('x')
plt.ylabel('sin(x)')
plt.show()
```



Example: approx sin(x) up to 2π

```
import numpy as np
import matplotlib.pyplot as plt
x = np.arange(0, np.pi*2, 0.01)
sin_x = np.sin(x)
sinish_x = x - x**3/(3*2) + x**5/(5*4*3*2)
plt.plot(x, sin_x)
plt.plot(x, sinish_x)
plt.xlabel('x')
plt.ylabel('sin(x)')
plt.show()
```

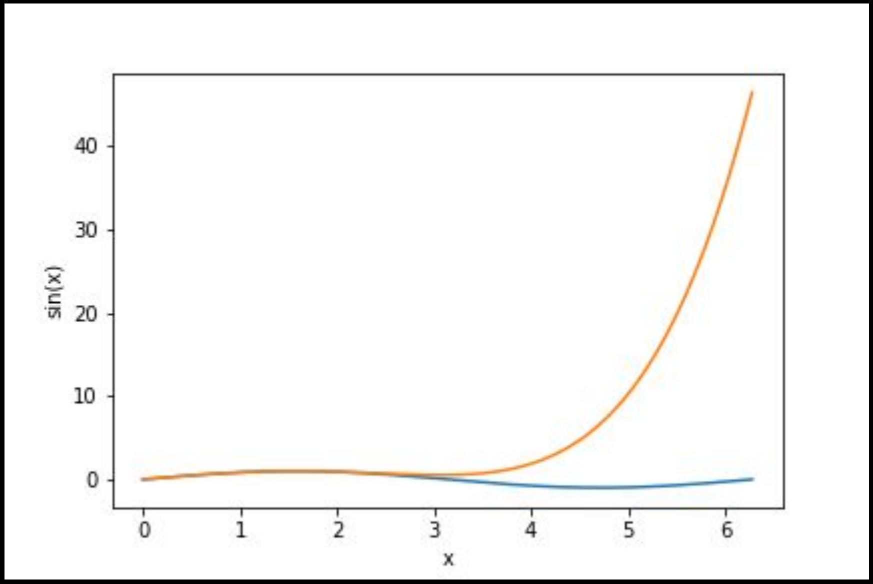


Taylor series error

- Like any infinite series approximation, Taylor series suffer from:
  - Truncation error
  - Round-off error
- Using lots of terms will decrease truncation error, but increase round-off error
- Best to keep (x - a) small

For any Taylor series of order n, if we know that the (n+1)th derivative $f^{(n+1)}(x) \leq M$, we know that the truncation error is bounded by:

$$|E_n(x)| \leq \frac{M|x-a|^{(n+1)}}{(n+1)!}$$



Exercise: error bounds

For our 5th-order Taylor approximation of sin(x), $x - x^3/6 + x^5/120$, find a bound x_b such that truncation error $|E_5(x_b)| \leq 0.01$

For any Taylor series of order n, if we know that the (n+1)th derivative $f^{(n+1)}(x) \leq M$, we know that the truncation error is bounded by:

$$|E_n(x)| \leq \frac{M|x-a|^{(n+1)}}{(n+1)!}$$

Hardest part is finding a bound M on the (n+1)th derivative of our true function f. Sometimes impossible, sometimes easy.

What is M in this case?

Exercise: error bounds

For our 5th-order Taylor approximation of sin(x), $x - x^3/6 + x^5/120$, find a bound x_b such that truncation error $|E_5(x_b)| \leq 0.01$

For any Taylor series of order n, if we know that the (n+1)th derivative $f^{(n+1)}(x) \leq M$, we know that the truncation error is bounded by:

$$|E_n(x)| \leq \frac{M|x-a|^{(n+1)}}{(n+1)!}$$

$$\downarrow$$

$$0.01 \leq \frac{(x_b - 0)^6}{6!}$$

$$\downarrow$$

$$0.01(6!) = (x_b)^6$$

$$\downarrow$$

$$|x_b| = 1.39$$

Answer: max of *all* derivatives of sine & cosine is 1. Here, a = 0 (this Taylor series is centered at zero). Plug in $x = x_b$ and solve.

Exercise: error bounds

For our 5th-order Taylor approximation of sin(x), $x - x^3/6 + x^5/120$, find a bound x_b such that truncation error $|E_5(x_b)| \leq 0.01$

For any Taylor series of order n, if we know that the (n+1)th derivative $f^{(n+1)}(x) \leq M$, we know that the truncation error is bounded by:

$$|E_n(x)| \leq \frac{M|x-a|^{(n+1)}}{(n+1)!}$$

$$\downarrow$$

$$0.01 \leq \frac{(x_b - 0)^6}{6!}$$

$$\downarrow$$

$$0.01(6!) = (x_b)^6$$

$$\downarrow$$

$$|x_b| = 1.39$$

Does this still work if we use n = 6? Why?

Test the answer in Python

```
x = 1.39  # 5th-order bound xb
sinish_x = x - x**3/(3*2) + x**5/(5*4*3*2)
sin_x = np.sin(x)
print(f'True error = {sinish_x - sin_x:.4f}')
```

Open Colab and try this!

Test the answer in Python

```
x = 1.39  # 5th-order bound xb
sinish_x = x - x**3/(3*2) + x**5/(5*4*3*2)
sin_x = np.sin(x)
print(f'True error = {sinish_x - sin_x:.4f}')
```

```
True error = 0.0019
```

(Well below our bound of 0.01)

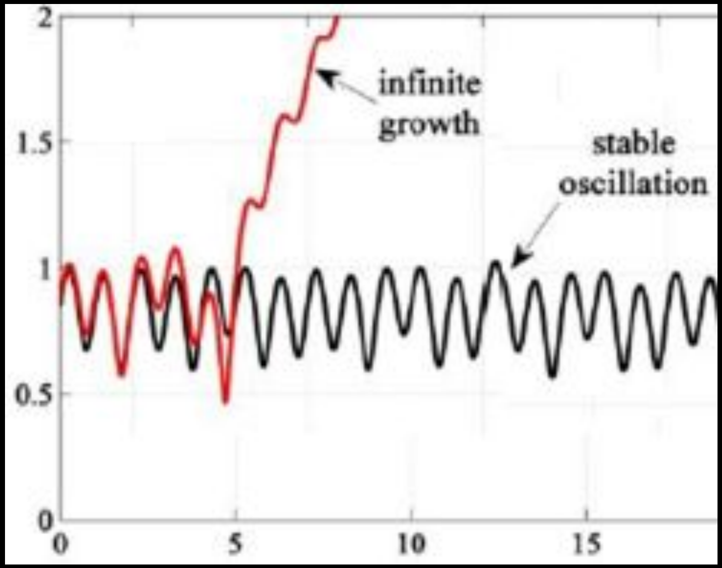
Test the answer in Python

```
x = 1.75  # 6th-order bound xb
sinish_x = x - x**3/(3*2) + x**5/(5*4*3*2)
sin_x = np.sin(x)
print(f'True error = {sinish_x - sin_x:.4f}')
```

```
True error = 0.0096
```

(Right below our bound of 0.01)

Stability



- How can you tell if an approximation is **stable**?
- Try **small** perturbations in input ("small" depends on the problem at hand)
- If the output changes **significantly** (as defined by the problem at hand), you have **instability**

Exercise: stability bounds

```
sinish_x = x - x**3/(3*2) + x**5/(5*4*3*2)
```

$$\textbf{sinish}(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!}$$

We can still find stability bounds for **sinish**(x) even if we don't know any bound M on the derivatives of the true function sin(x).

We only need the change in the *known* function **sinish**(x) with respect to small changes in x.

Exercise: stability bounds

```
sinish_x = x - x**3/(3*2) + x**5/(5*4*3*2)
```

$$\mathbf{sinish}(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!}$$

Find bounds x_b such that, within these bounds, a given change in x always produces an equal or smaller change in **sinish**(x):

$$\left.\frac{\partial \mathbf{sinish}(x)}{\partial x}\right|_{x_b} \leq 1$$

Exercise: stability bounds

$$\mathbf{sinish}(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!}$$

$$\left.\frac{\partial \mathbf{sinish}(x)}{\partial x}\right|_{x_b} \leq 1$$

$$\frac{\partial \mathbf{sinish}(x)}{\partial x} = \boxed{?}$$

Exercise: stability bounds

$$\boxed{\begin{gathered}\mathbf{sinish}(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} \\ \left.\frac{\partial\,\mathbf{sinish}(x)}{\partial x}\right|_{x_b} \leq 1\end{gathered}}$$

$$\frac{\partial\,\mathbf{sinish}(x)}{\partial x} = 1 - \frac{3x^2}{3!} + \frac{5x^4}{5!}$$

Exercise: stability bounds

$$\mathbf{sinish}(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!}$$

$$\left.\frac{\partial\mathbf{sinish}(x)}{\partial x}\right|_{x_b} \leq 1$$

$$\frac{\partial\mathbf{sinish}(x)}{\partial x} = 1 - \frac{3x^2}{3!} + \frac{5x^4}{5!}$$

$$1 - \frac{x_b^2}{2!} + \frac{x_b^4}{4!} \leq 1$$

Substitute x_b for x and the bound 1 for d**sinish**(x)/dx

Exercise: stability bounds

$$-\frac{x_b^2}{2!}+\frac{x_b^4}{4!}\le 0$$

$$\frac{x_b^4}{4!}\le\frac{x_b^2}{2!}$$

→ Safe to divide by $x_b{}^2$ since it is always positive. →

$$\frac{x_b^2}{4!}\le\frac{1}{2}$$

Within these bounds, the approximation is stable, but is it accurate?

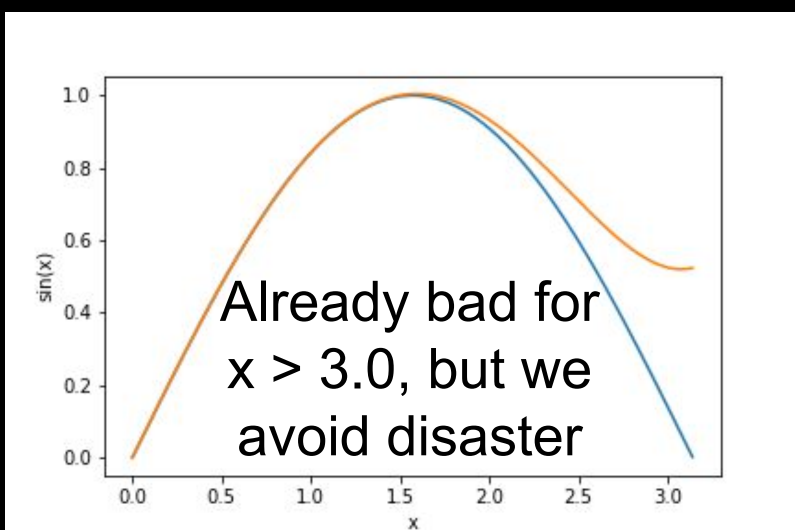
$$x_b^2\le 12$$

$$x_b\le\sqrt{12}\quad(\sim 3.46)$$

Exercise: stability bounds

$$-\frac{x_b^2}{2!} + \frac{x_b^4}{4!} \leq 0$$

$$\frac{x_b^4}{4!} \leq \frac{x_b^2}{2!}$$ → Safe to divide by x_b^2 since it is always positive. → $$\frac{x_b^2}{4!} \leq \frac{1}{2}$$



$$x_b^2 \leq 12$$

$$x_b \leq \sqrt{12} \quad (\sim 3.46)$$

Summary and Problems

- Open Python Numerical Methods, go to 18.4: Summary and Problems
- Do problems 2, 4, & 5. For reference:

$$P_n(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \ldots + \boxed{\frac{f^{(n)}(x_0)}{n!}(x - x_0)^n}$$

Definition of a Taylor series

All reading for next week: writing fast code (PNM 8.1-8.3), root finding (PNM 19.1-19.5), convergence (F&B 1.4)