Machine Learning Foundations
Calculus I: Limits & Derivatives

Using Differentiation,
including AutoDiff, in Python to
Optimize Learning Algorithms

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jonkrohn.com/talks

github.com/jonkrohn/ML-foundations

Machine Learning Foundations

Calculus I: Limits & Derivatives

Slides: jonkrohn.com/talks

Code: github.com/jonkrohn/ML-foundations

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The Pomodoro Technique

Rounds of:

- 25 minutes of work
- with 5 minute breaks

Questions best handled at breaks, so save questions until then.

When people ask questions that have already been answered, do me a favor and let them know, politely providing response if appropriate.

Except during breaks, I recommend attending to this lecture only as topics are not discrete: Later material builds on earlier material.

POLL

Where are you?

- The Americas
- Europe / Middle East / Africa
- Asia-Pacific
- Extra-Terrestrial Space

POLL

What are you?

- Developer / Engineer
- Scientist / Analyst / Statistician / Mathematician
- Combination of the Above
- Other

POLL

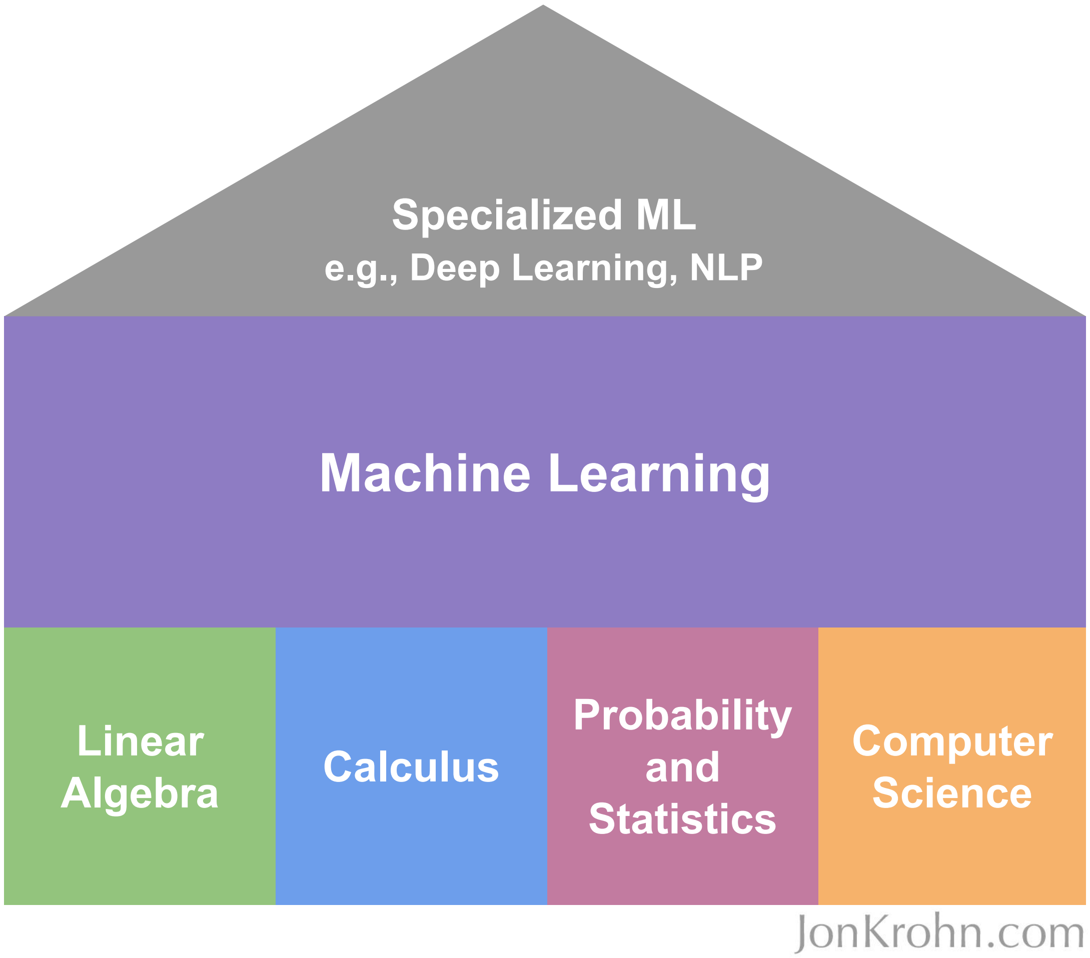
What is your level of familiarity with Calculus?

- Little to no exposure
- Some understanding of the theory
- Deep understanding of the theory
- Deep understanding of the theory and experience applying calculus operations (e.g., differentiation) with code

POLL

What is your level of familiarity with Machine Learning?

- Little to no exposure, or exposure to theory only
- Experience applying machine learning with code
- Experience applying machine learning with code and some understanding of the underlying theory
- Experience applying machine learning with code and strong understanding of the underlying theory


Specialized ML
e.g., Deep Learning, NLP
Machine Learning
Linear Algebra
Calculus
Probability and Statistics
Computer Science
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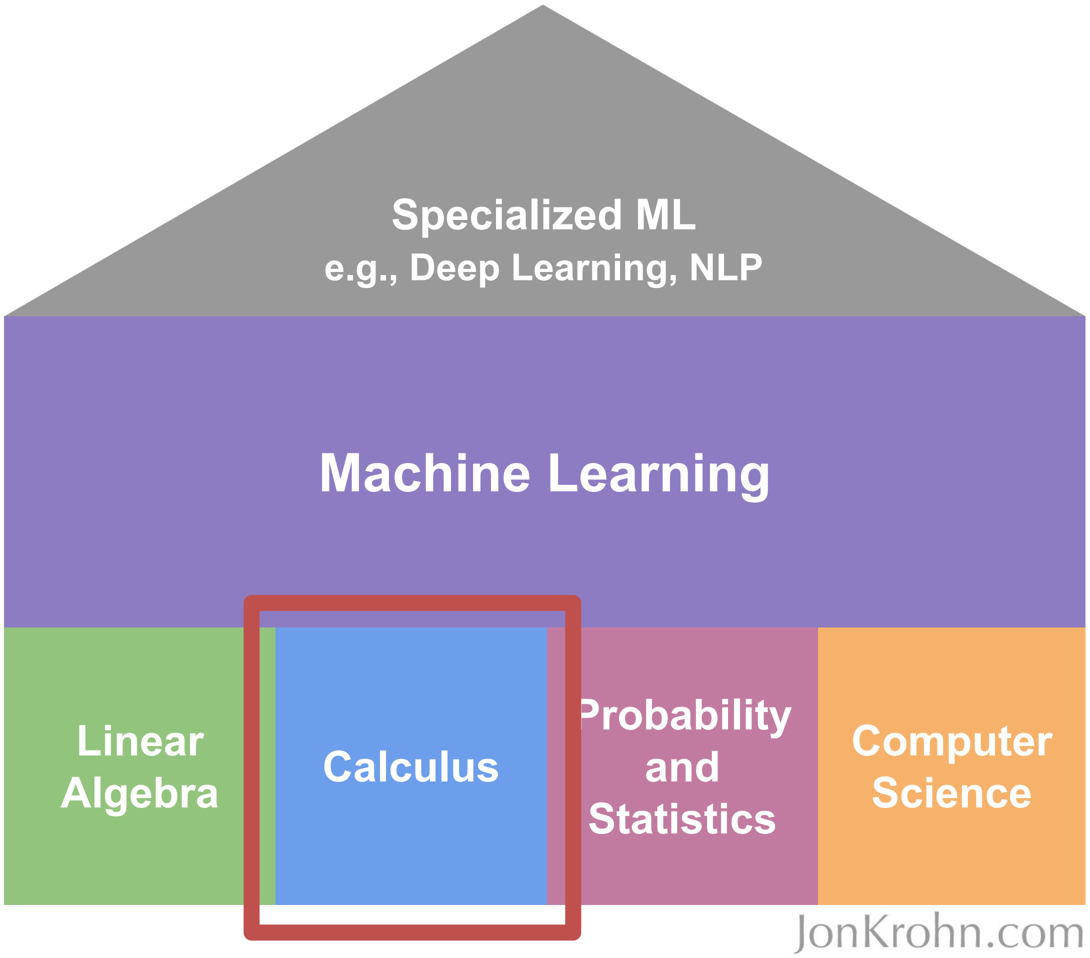
Specialized ML
e.g., Deep Learning, NLP
Machine Learning
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ML Foundations Series

Calculus I **builds upon** and is **foundational for**:

1. Intro to Linear Algebra
2. Linear Algebra II: Matrix Operations
3. **Calculus I: Limits & Derivatives**
4. **Calculus II: Partial Derivatives & Integrals**
5. Probability & Information Theory
6. Intro to Statistics
7. Algorithms & Data Structures
8. **Optimization**

Calculus I: Limits & Derivatives

1. Limits
2. Computing Derivatives with Differentiation
3. Automatic Differentiation

Calculus I: Limits & Derivatives

1. **Limits**
2. Computing Derivatives with Differentiation
3. Automatic Differentiation

Segment 1: Limits

- What Calculus Is
- A Brief History of Calculus
- The Method of Exhaustion
- Calculating Limits

What Calculus Is

- **Mathematical study of continuous change**
- Two branches:
  a. **Differential calculus**: focus of *Calculus I*
  b. **Integral calculus**: a focus of *Calculus II* subject

What Calculus Is

- **Mathematical study of continuous change**
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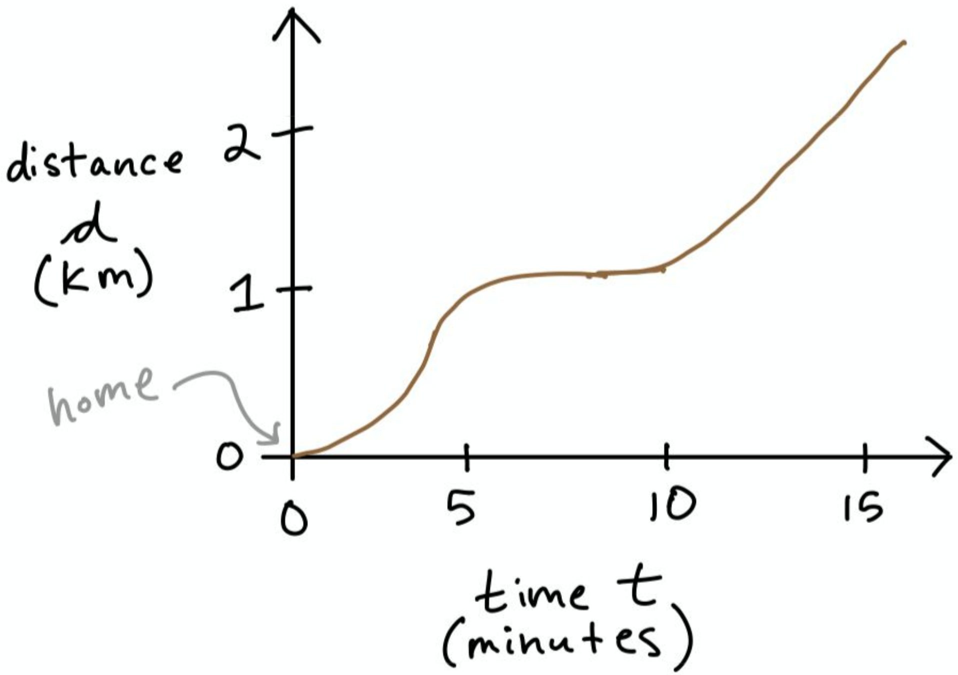
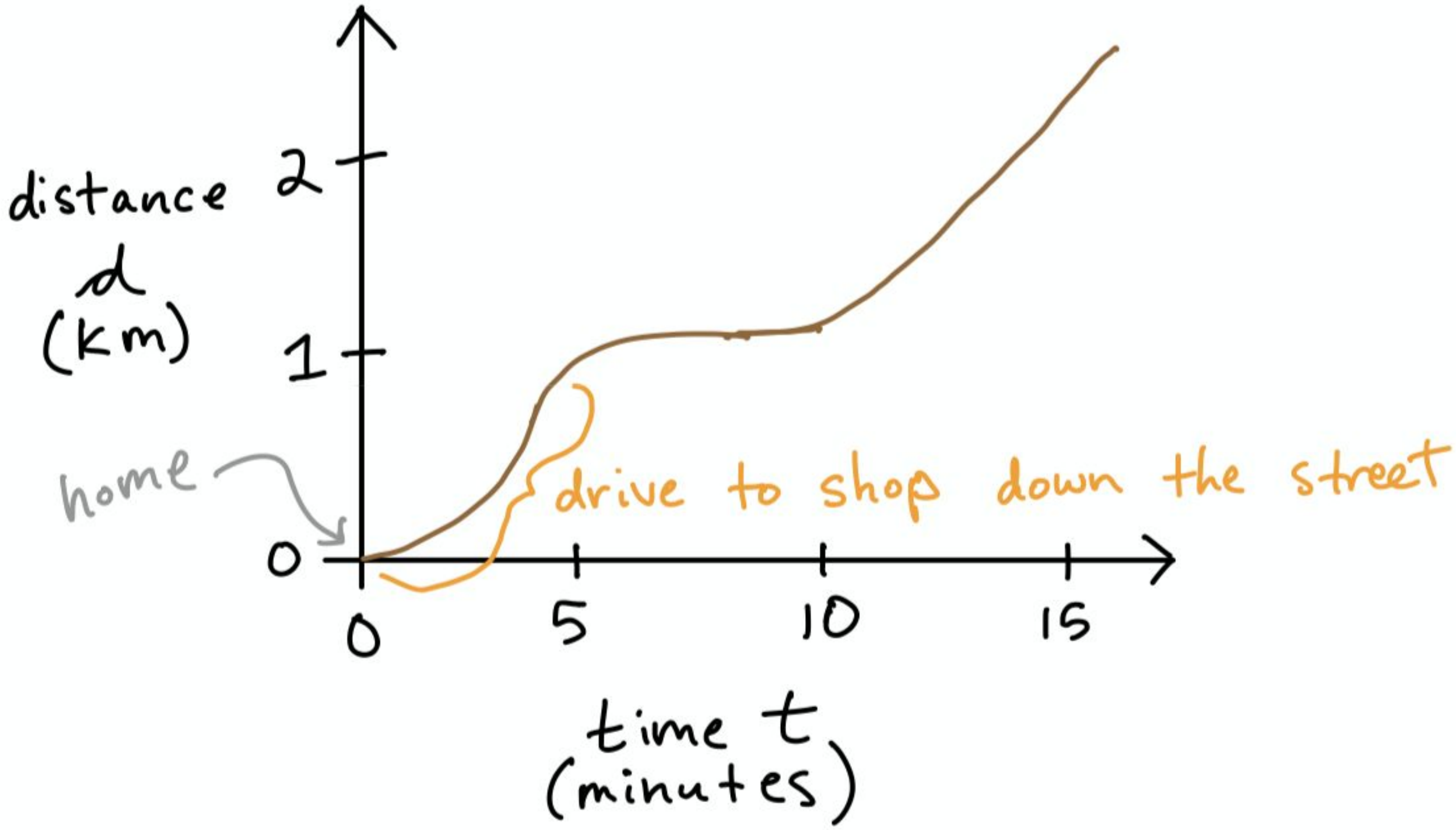
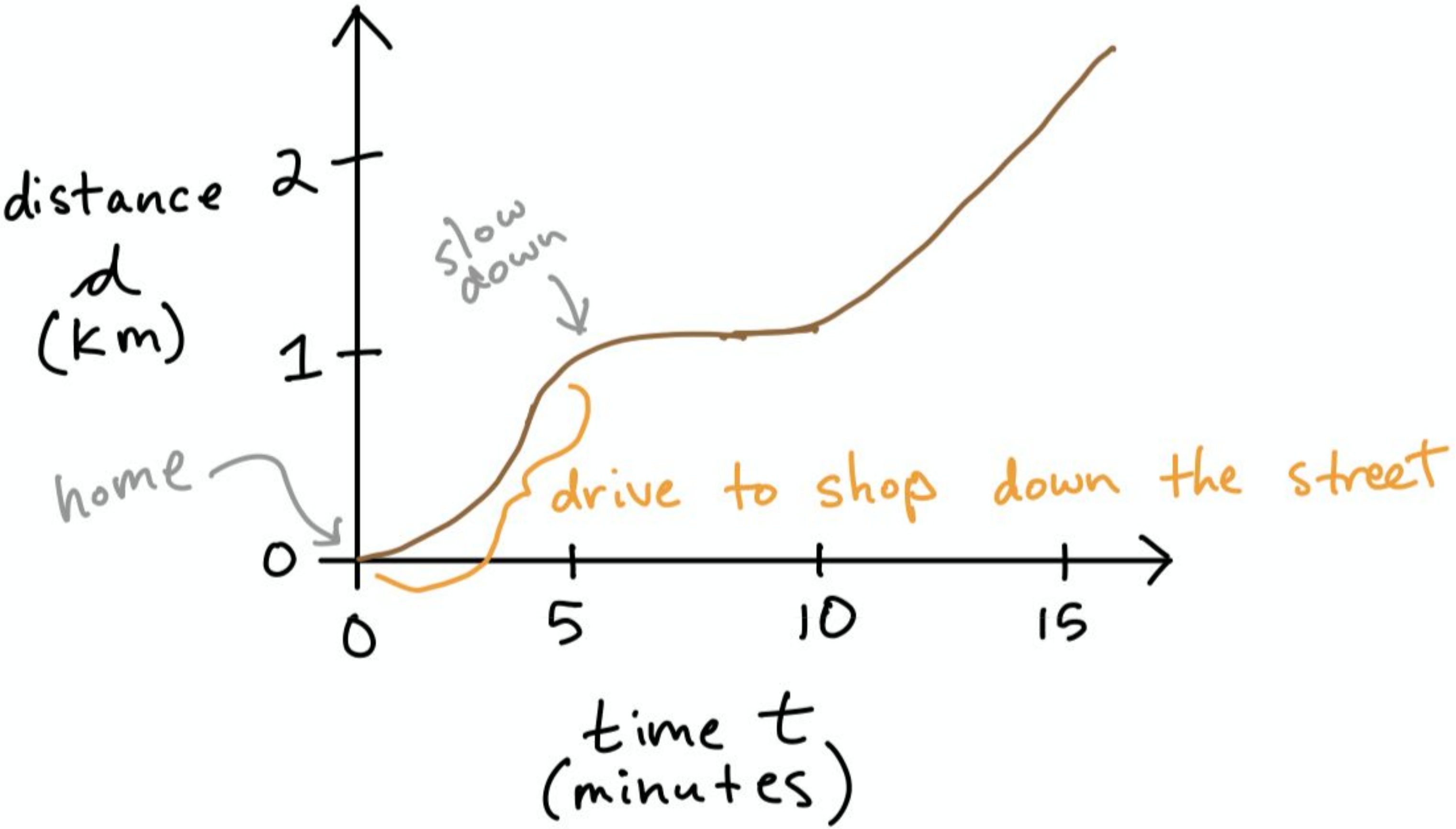
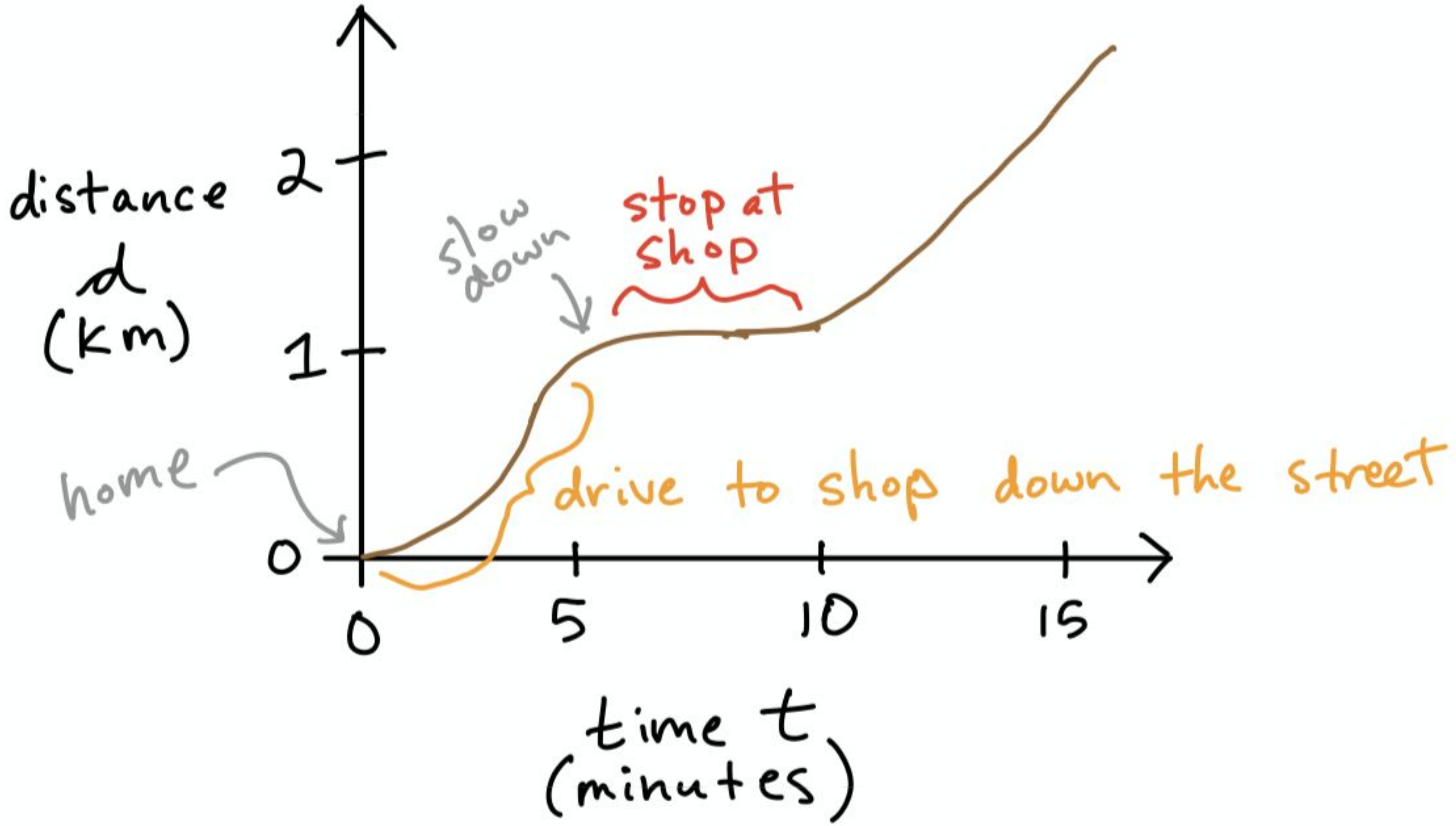
What Differential Calculus Is

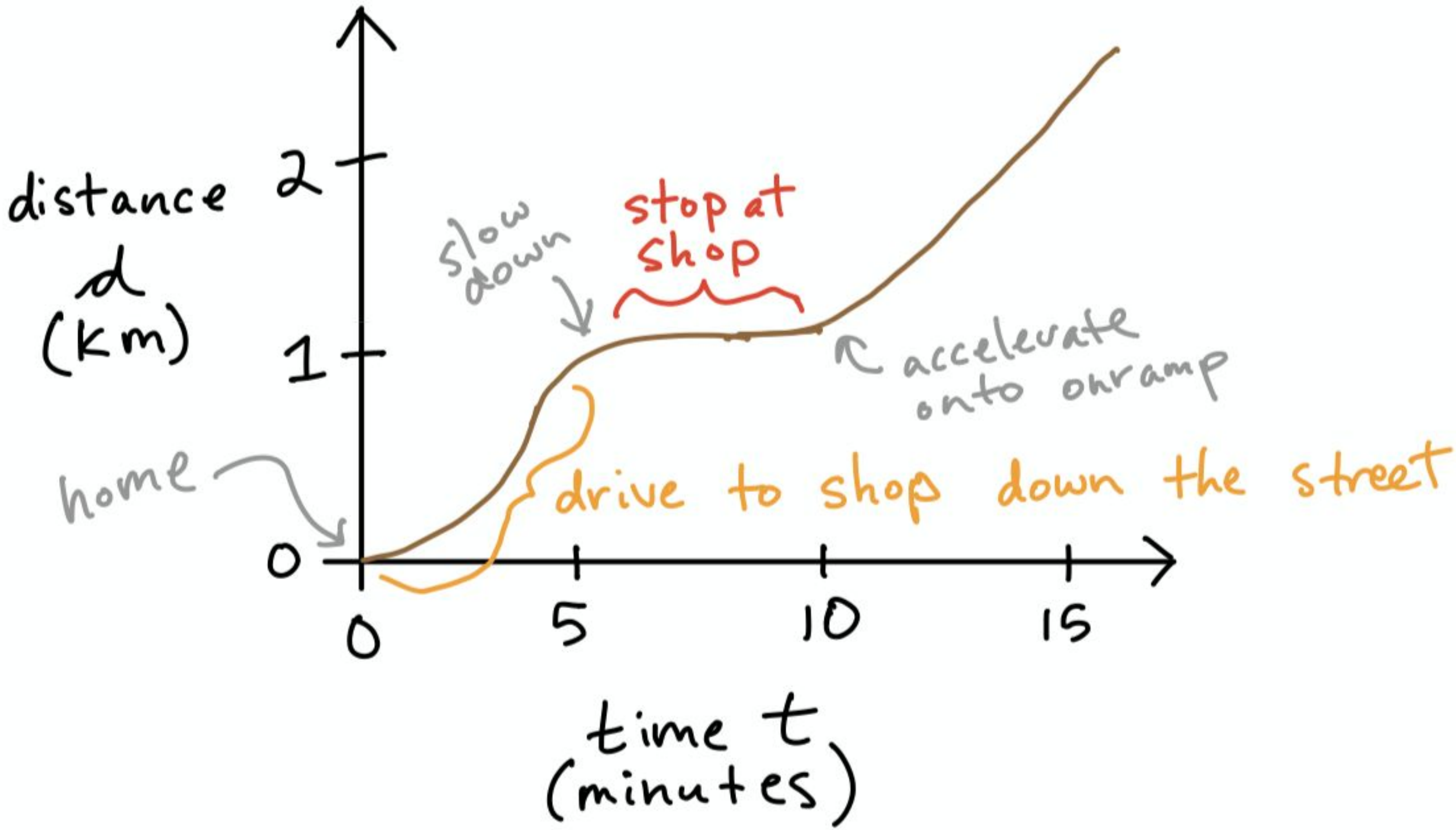
- **Study of rates of change**
- Consider a vehicle traveling some distance d over time t:

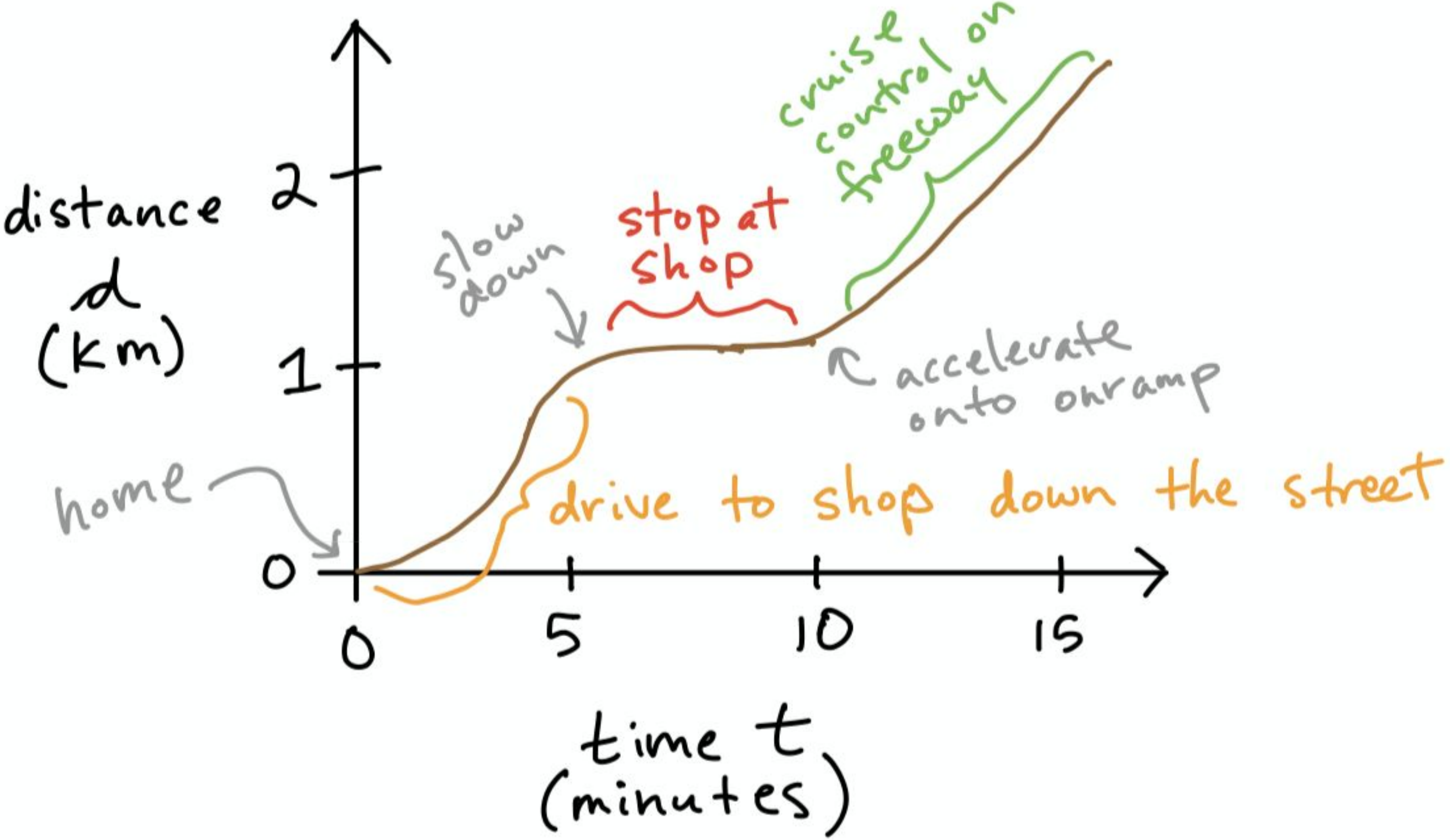


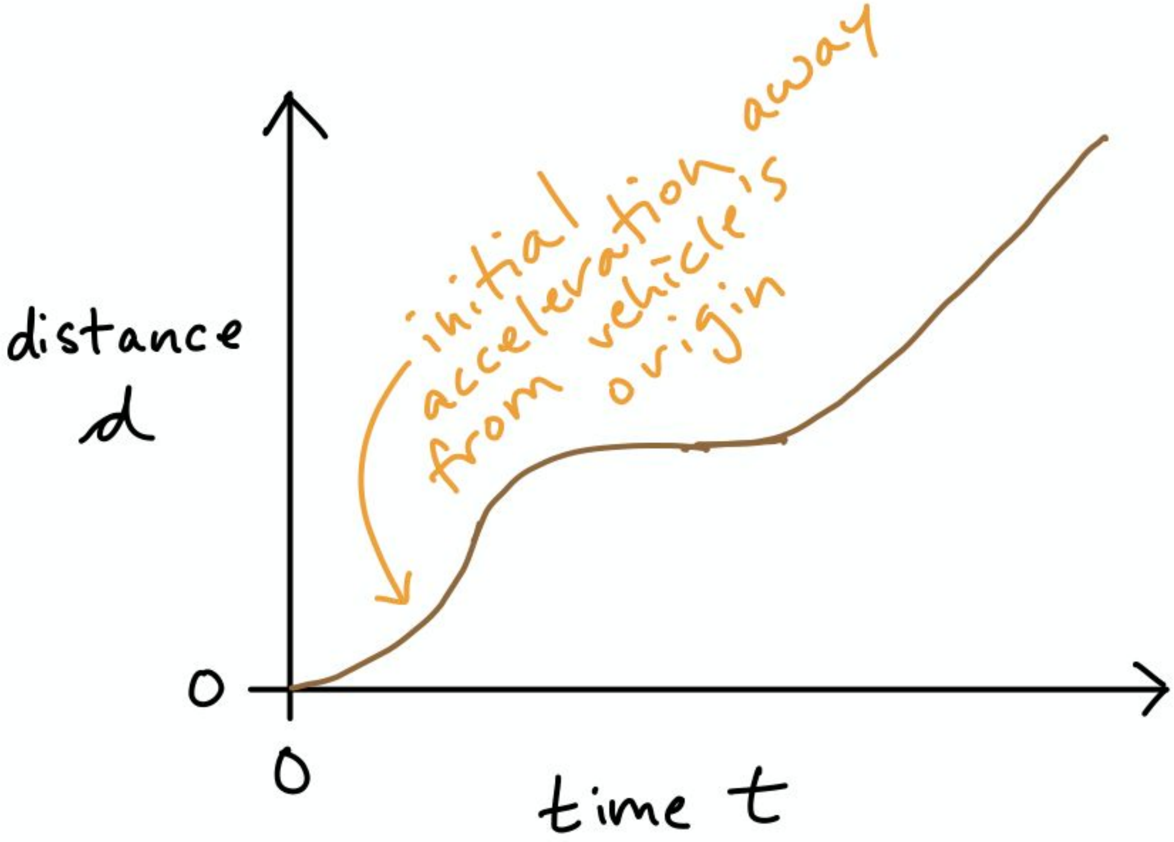

distance
d
(km)
2
1
0
home
drive to shop down the street
0
5
10
15
time t
(minutes)

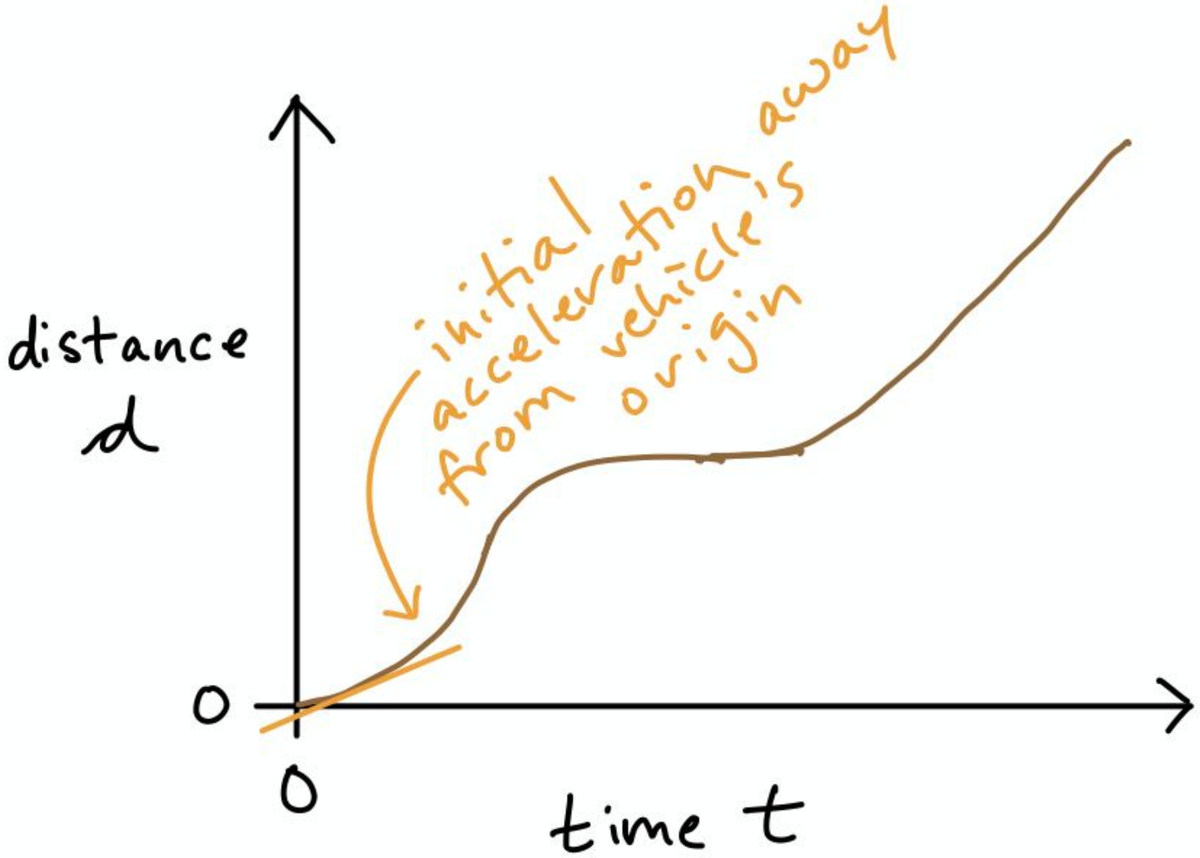

distance
d
(km)
2
1
0
slow down
home
drive to shop down the street
0
5
10
15
time t
(minutes)

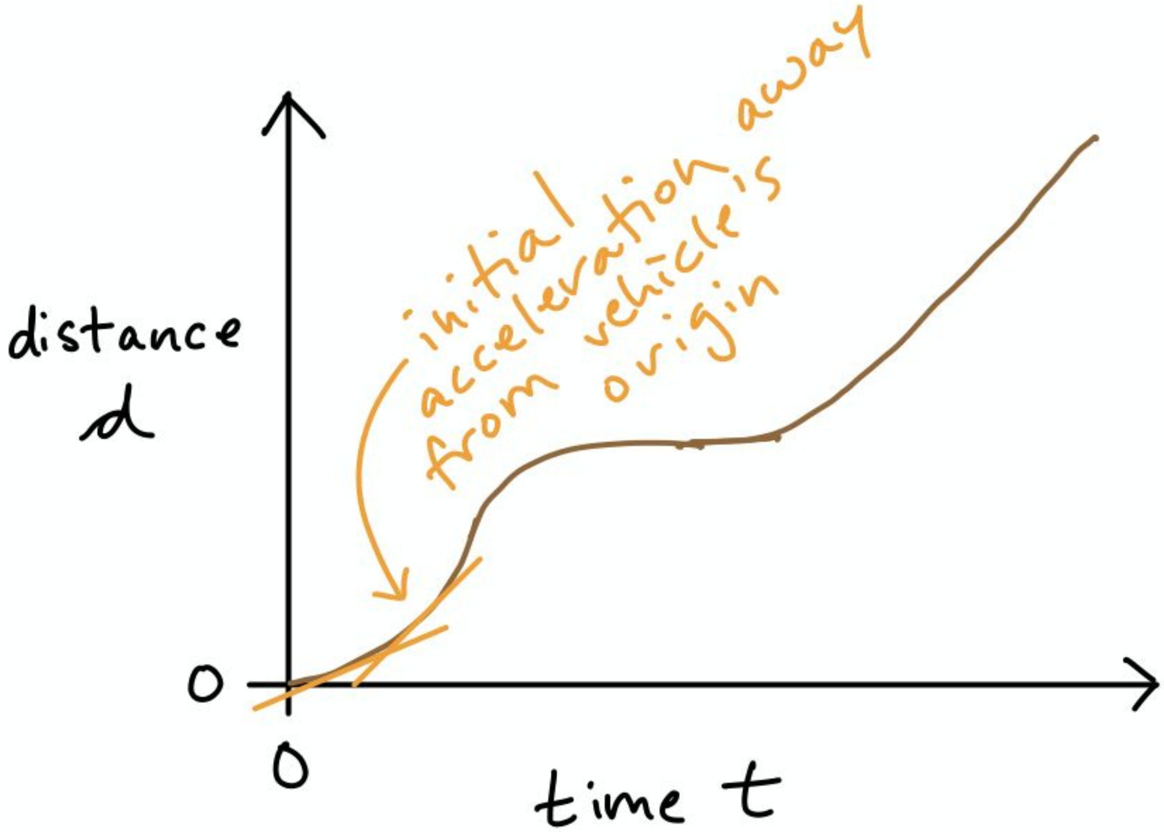

distance
d
(km)
2
1
0
slow down
stop at shop
home
drive to shop down the street
0
5
10
15
time t
(minutes)


distance
d
(km)
2
1
0
slow down
stop at shop
accelerate onto onramp
home
drive to shop down the street
0
5
10
15
time t
(minutes)

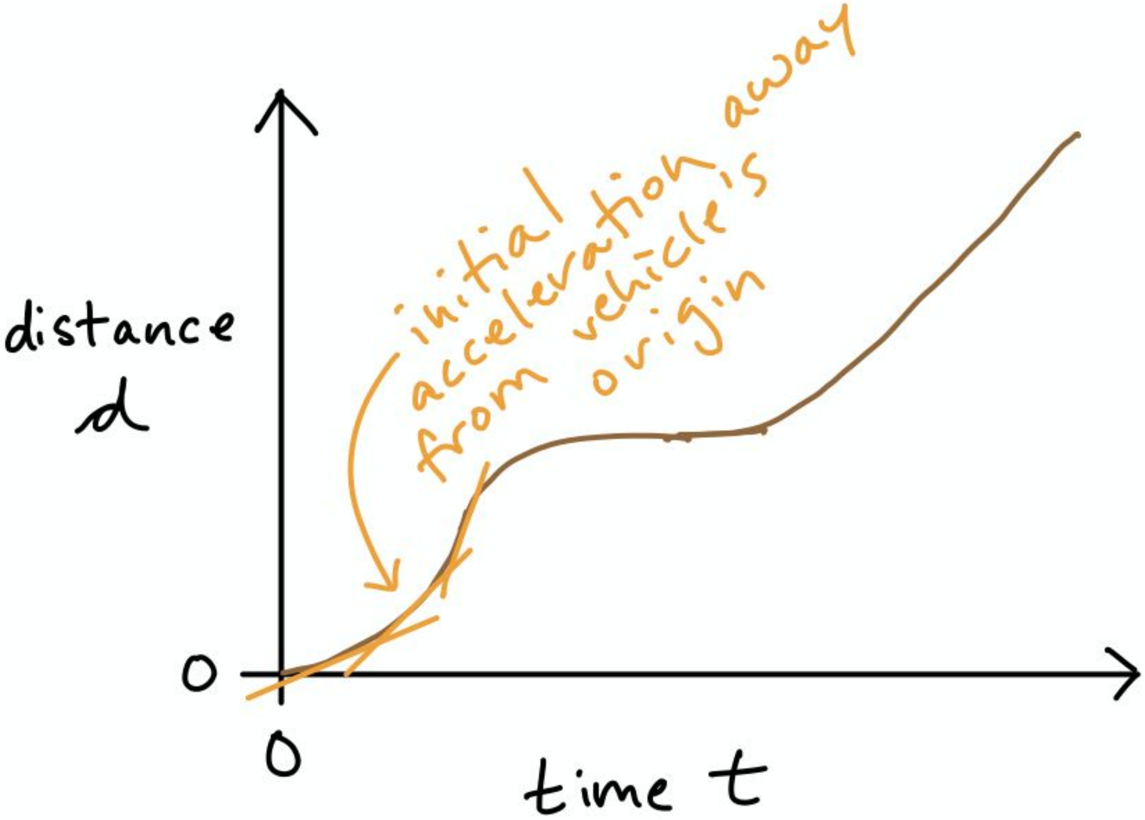

distance
d
(km)
2
1
0
0
5
10
15
time t
(minutes)
home
drive to shop down the street
slow down
stop at shop
accelerate onto onramp
cruise control on freeway

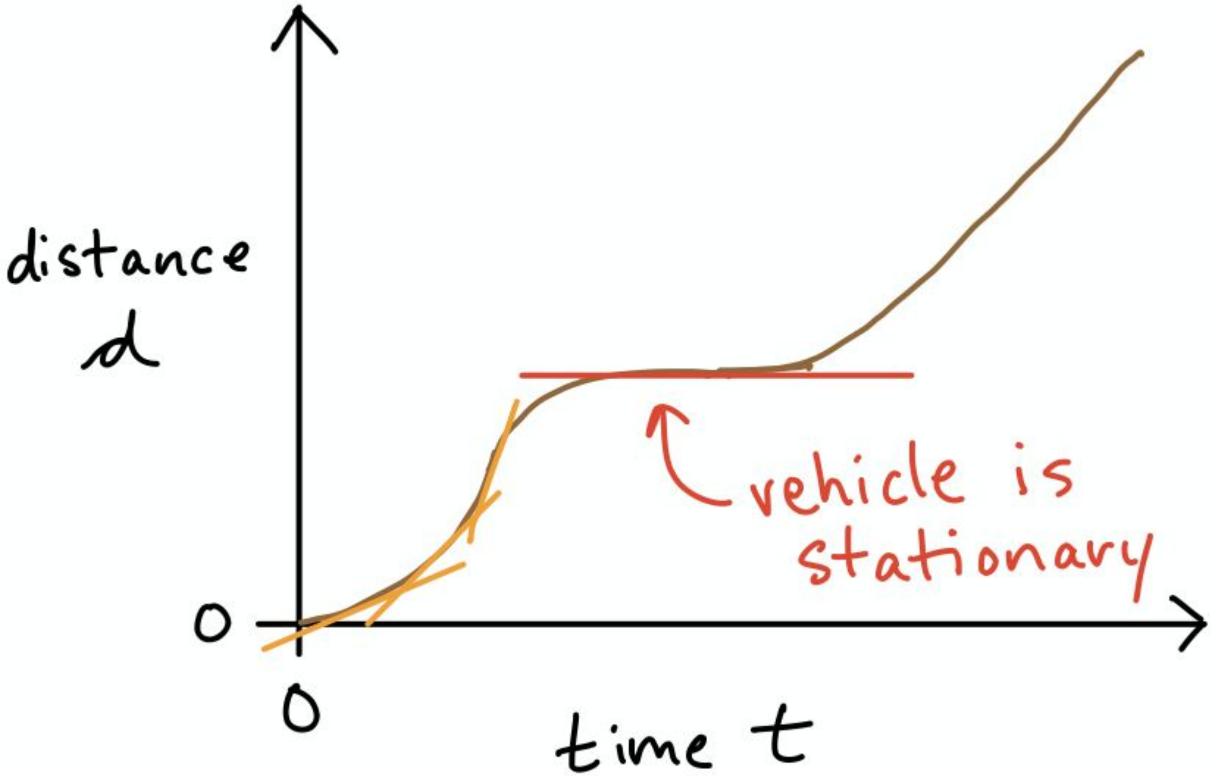

initial acceleration away from vehicle's origin
distance
d
0
0
time t

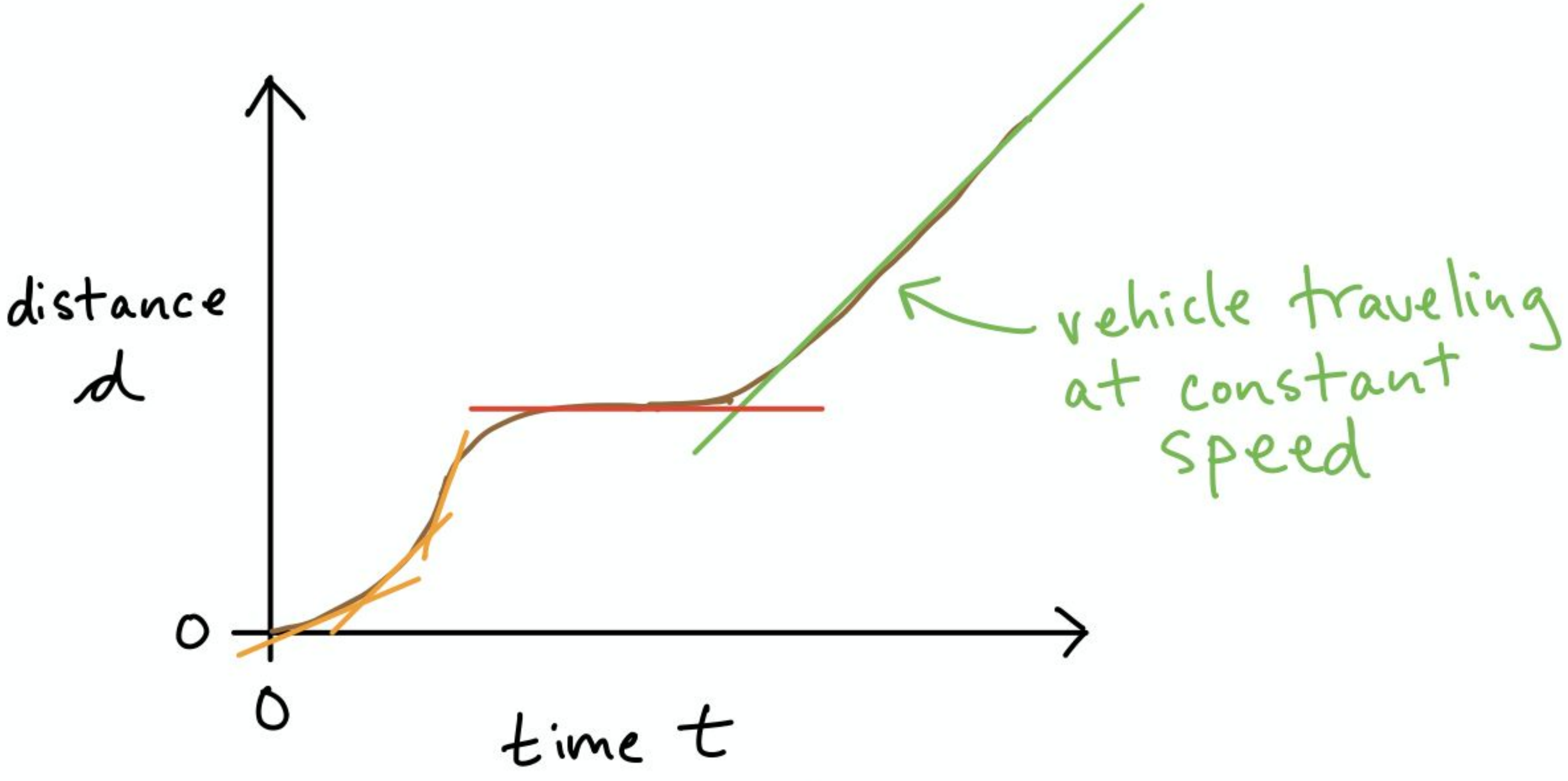

initial acceleration away from vehicle's origin
distance
d
0
0
time t

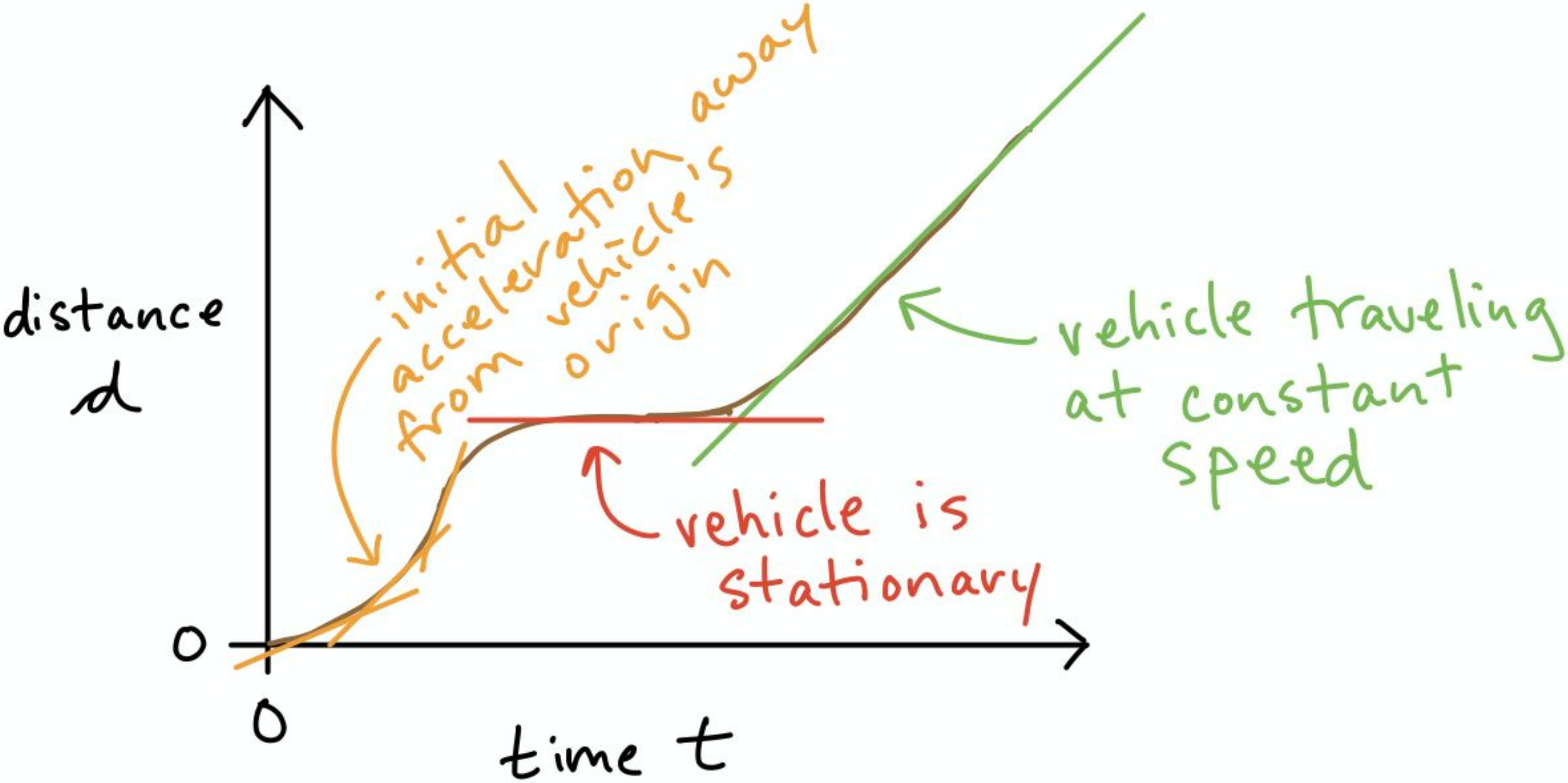


distance
d
0
0
time t
initial acceleration away from vehicle's origin

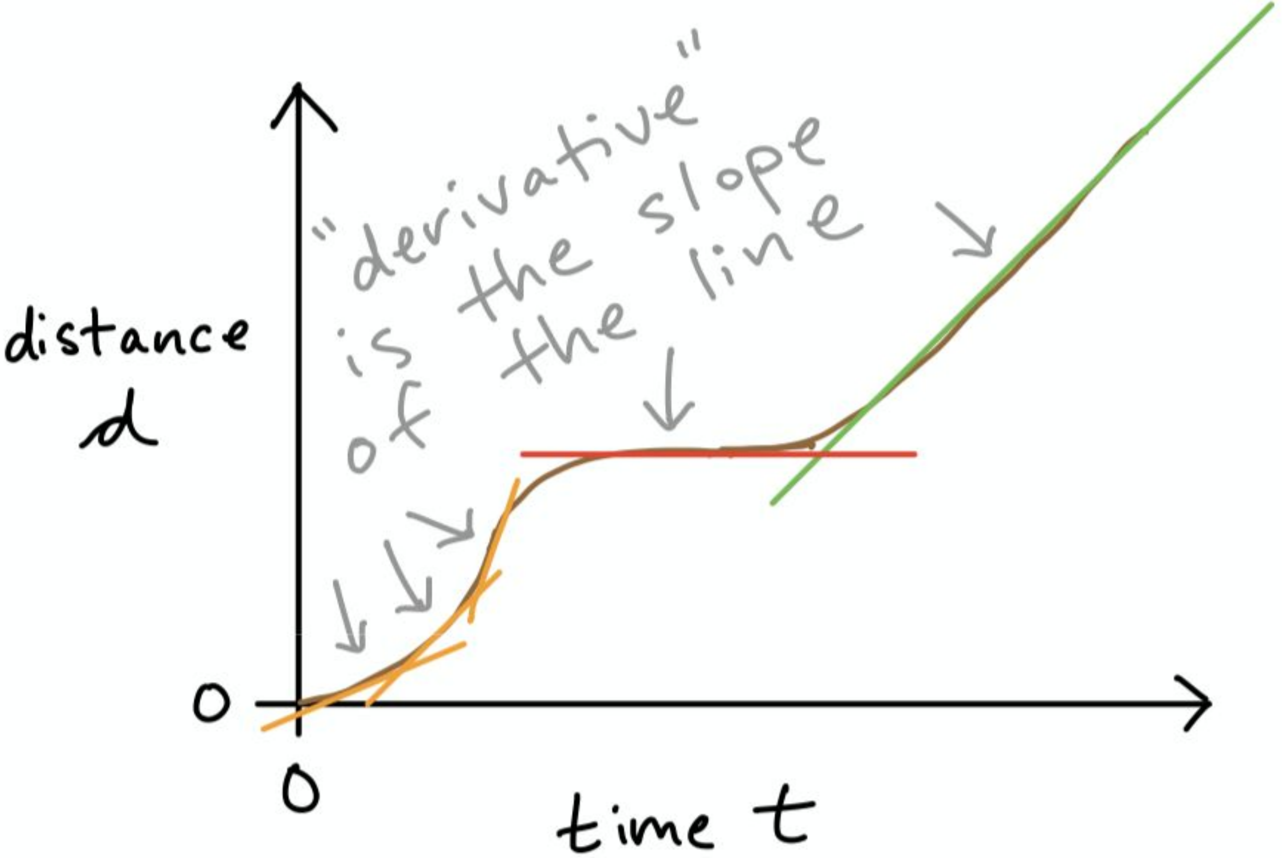

distance
d
0
0
time t
initial acceleration away from vehicle's origin

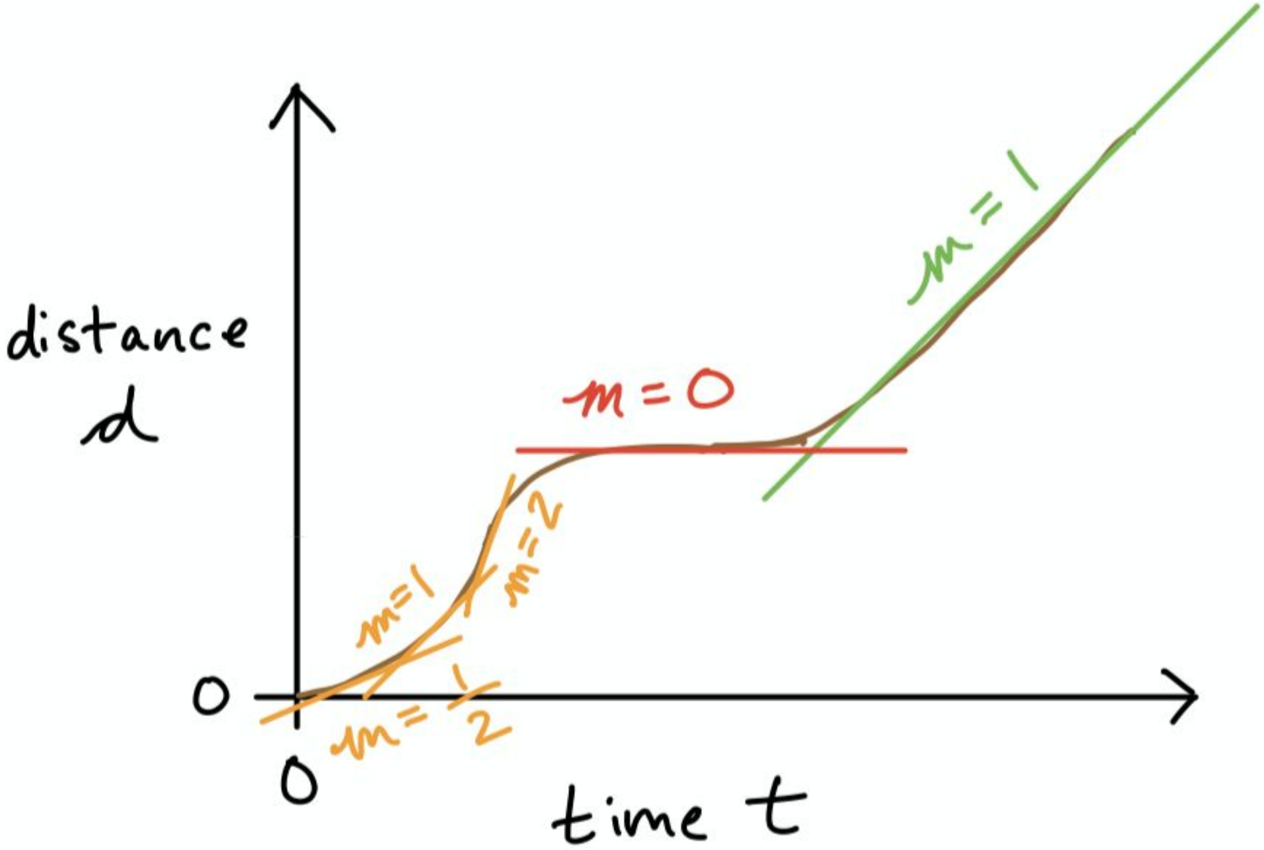

distance
d
0
0
time t
vehicle is stationary


distance
d
0
0
time t
vehicle traveling
at constant
speed

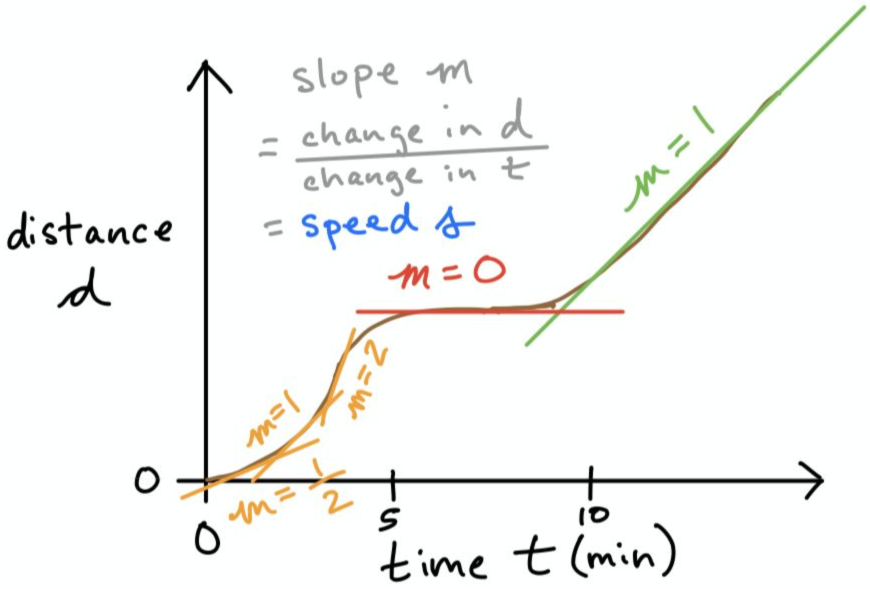


initial acceleration away from vehicle's origin
distance
d
0
0
time t
vehicle is stationary
vehicle traveling at constant speed

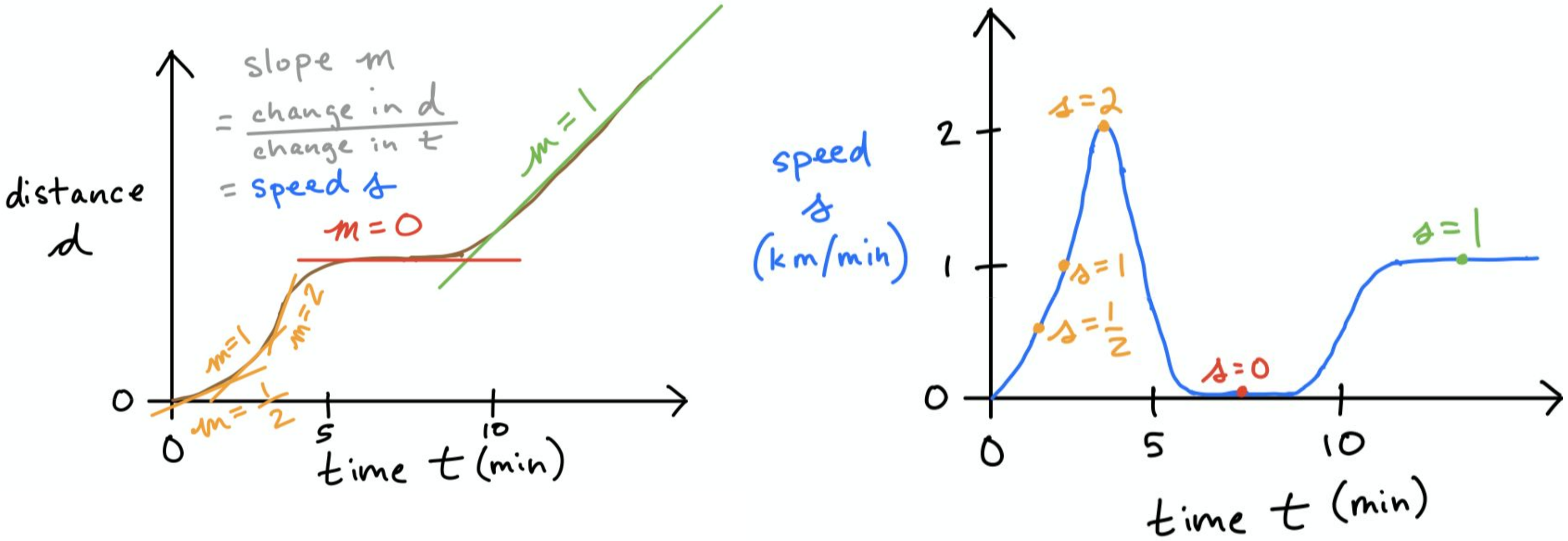

"derivative" is the slope of the line
distance d
time t
0
0

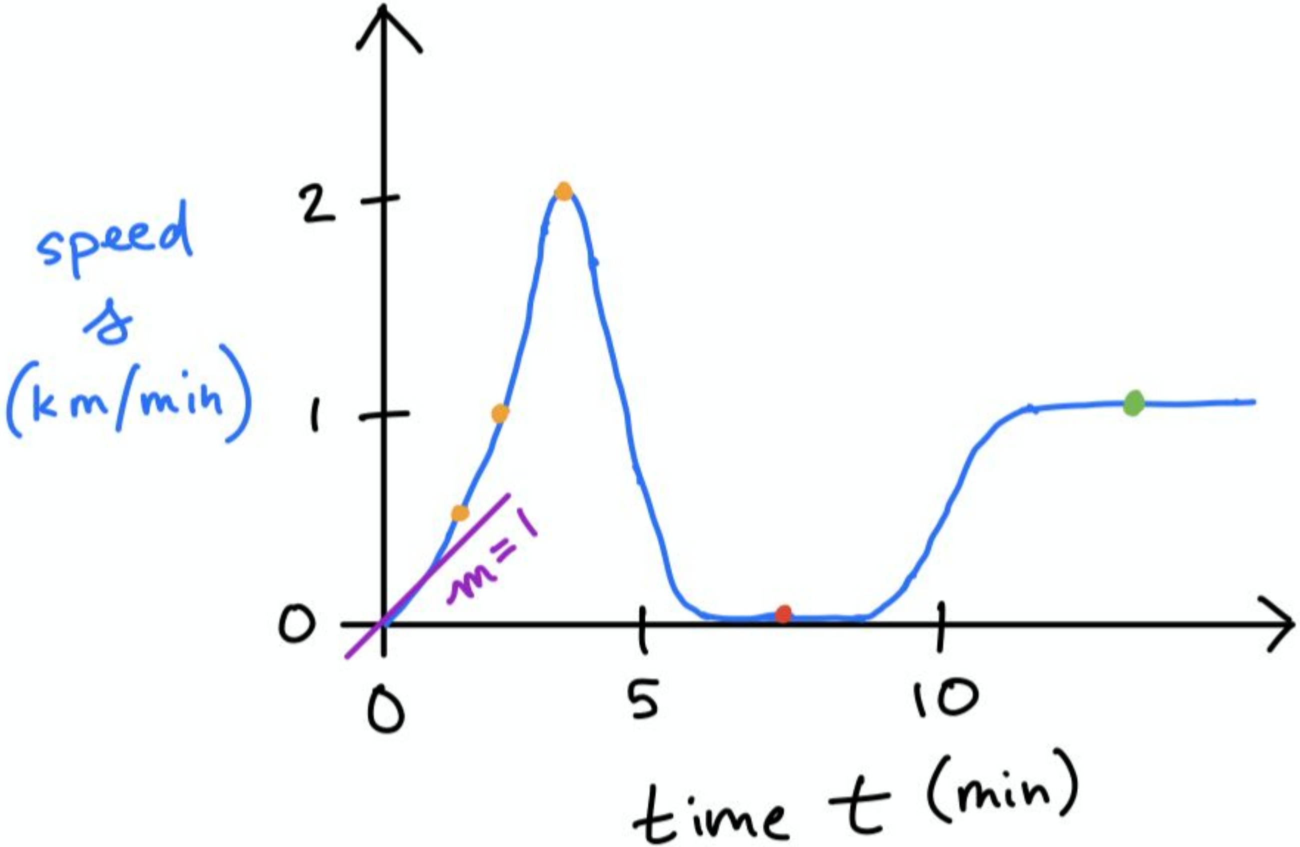


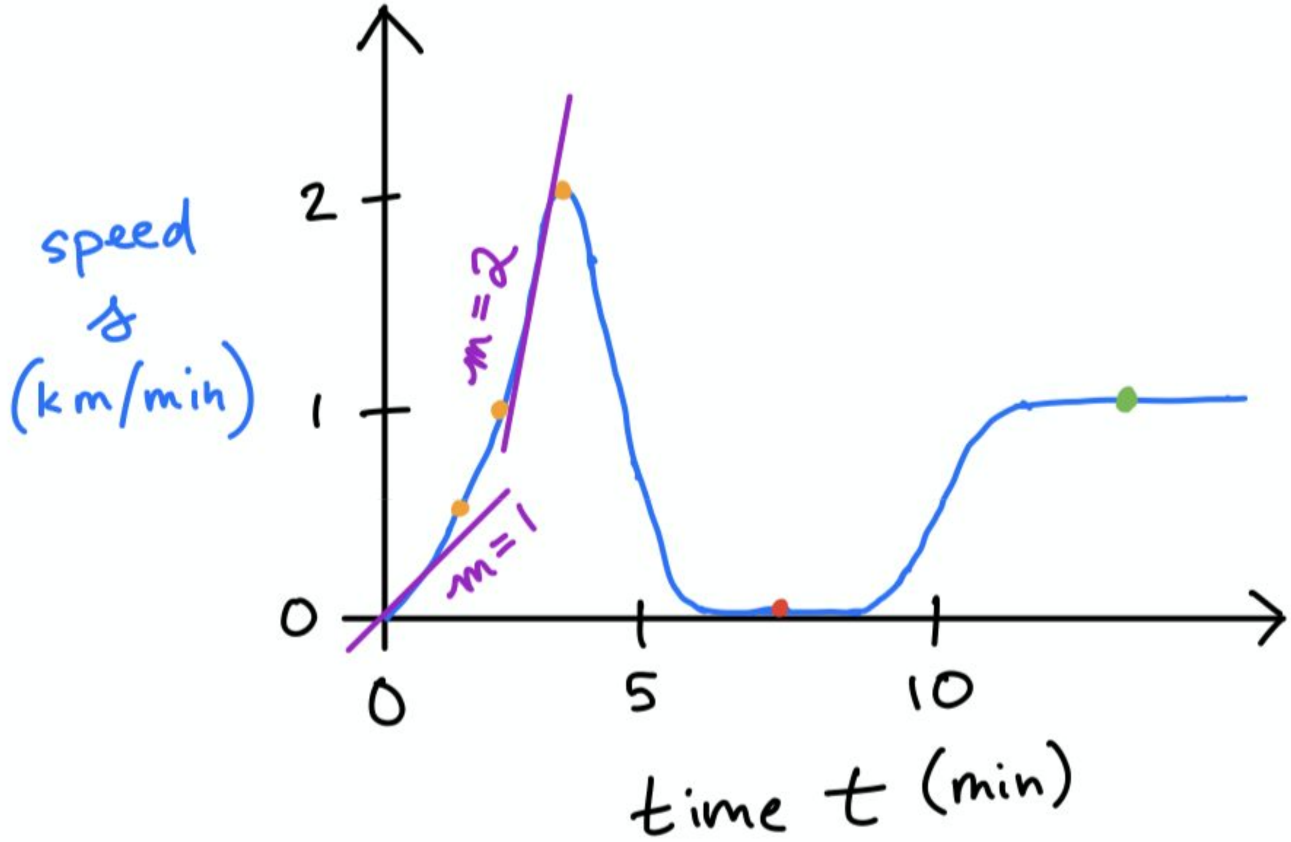
distance
d
time t
0
0
m = 0
m = 1
m=1
m=2
m = 1/2

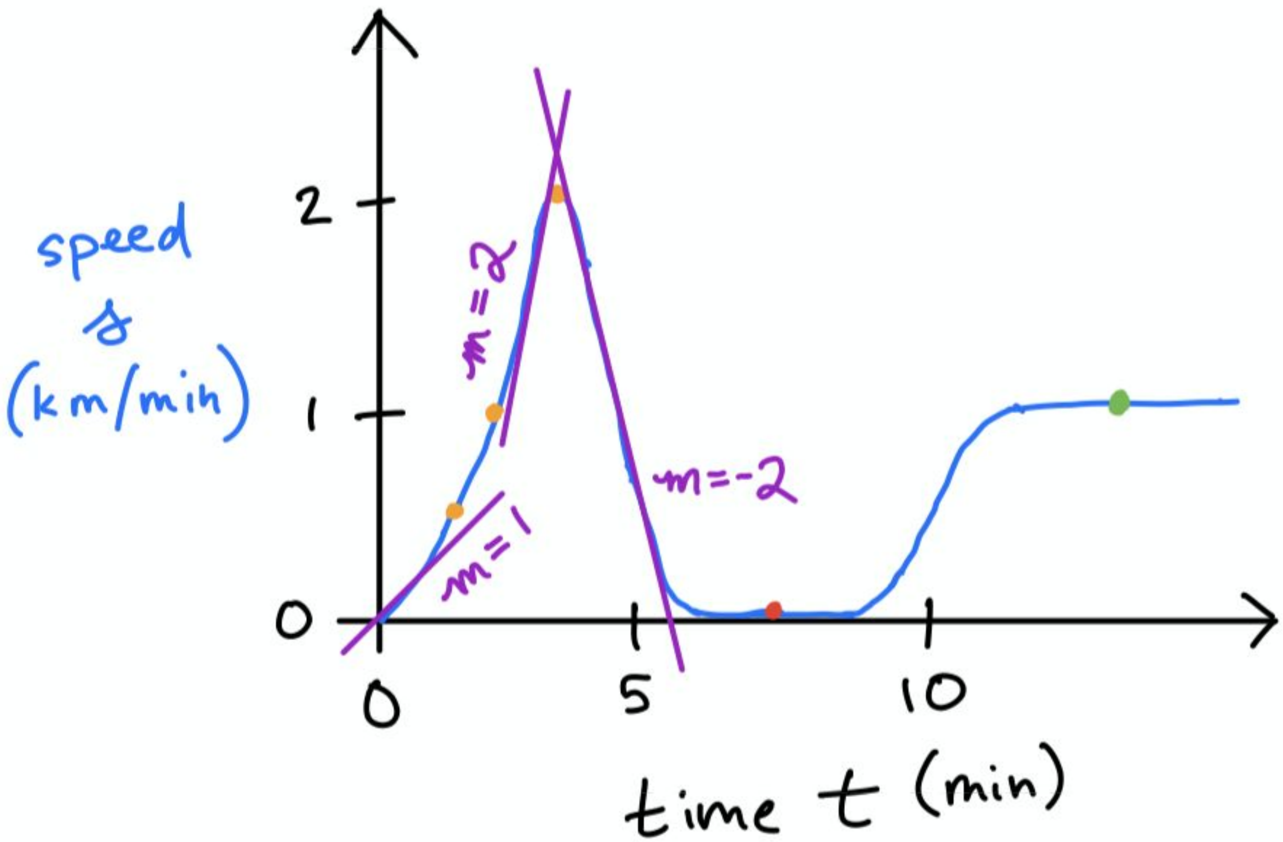


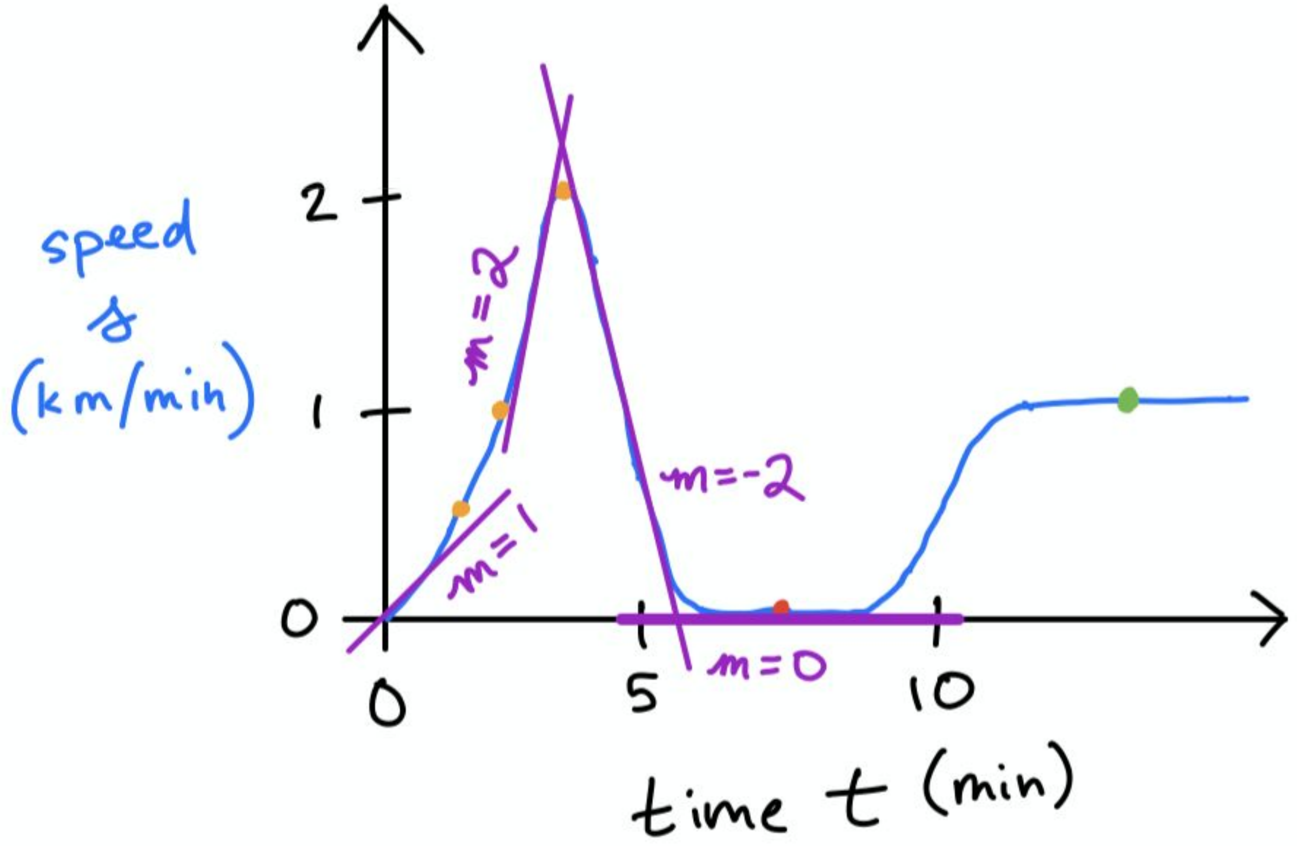
slope m
= change in d / change in t
= speed s
distance
d
0
m = 0
m = 1
m = 1
m = 2
m = 1/2
0
5
10
time t (min)

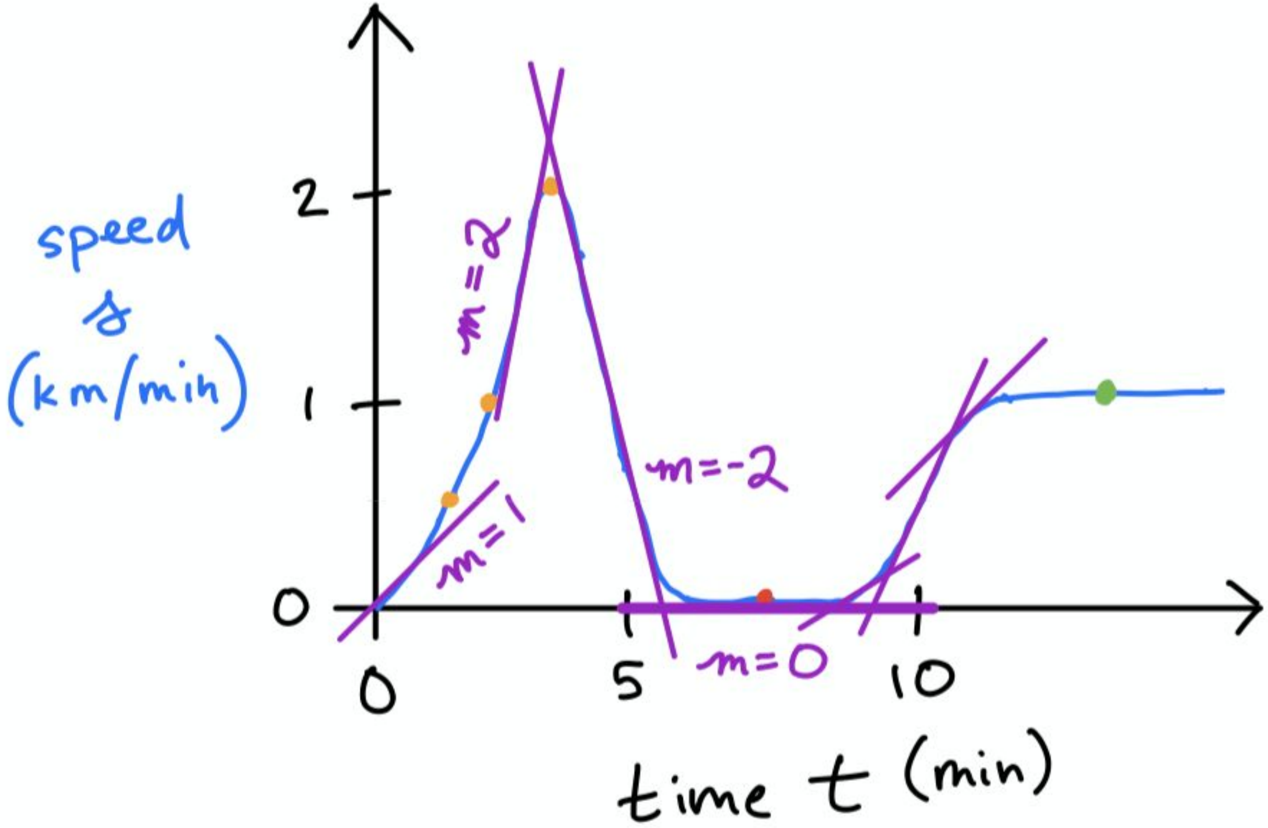

slope m
= change in d / change in t
= speed s
distance d
m = 0
m = 1
m = 2
m = 1
m = 1/2
0
0
5
10
time t (min)
speed s (km/min)
s = 2
s = 1
s = 1/2
s = 0
s = 1
2
1
0
0
5
10
time t (min)


speed
y
(km/min)
2
1
0
m=1
0
5
10
time t (min)

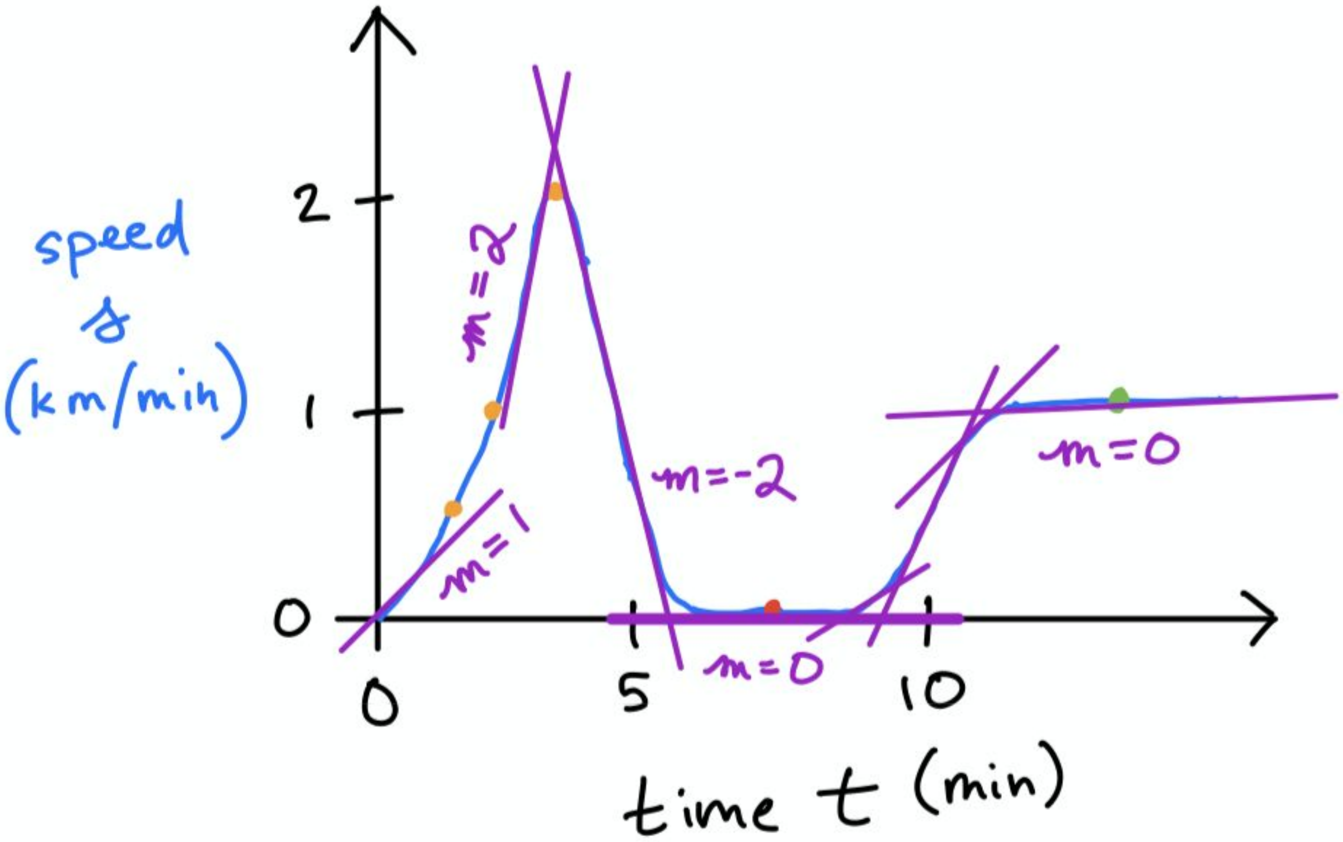

speed
y
(km/min)
2
1
0
m=2
m=1
0
5
10
time t (min)

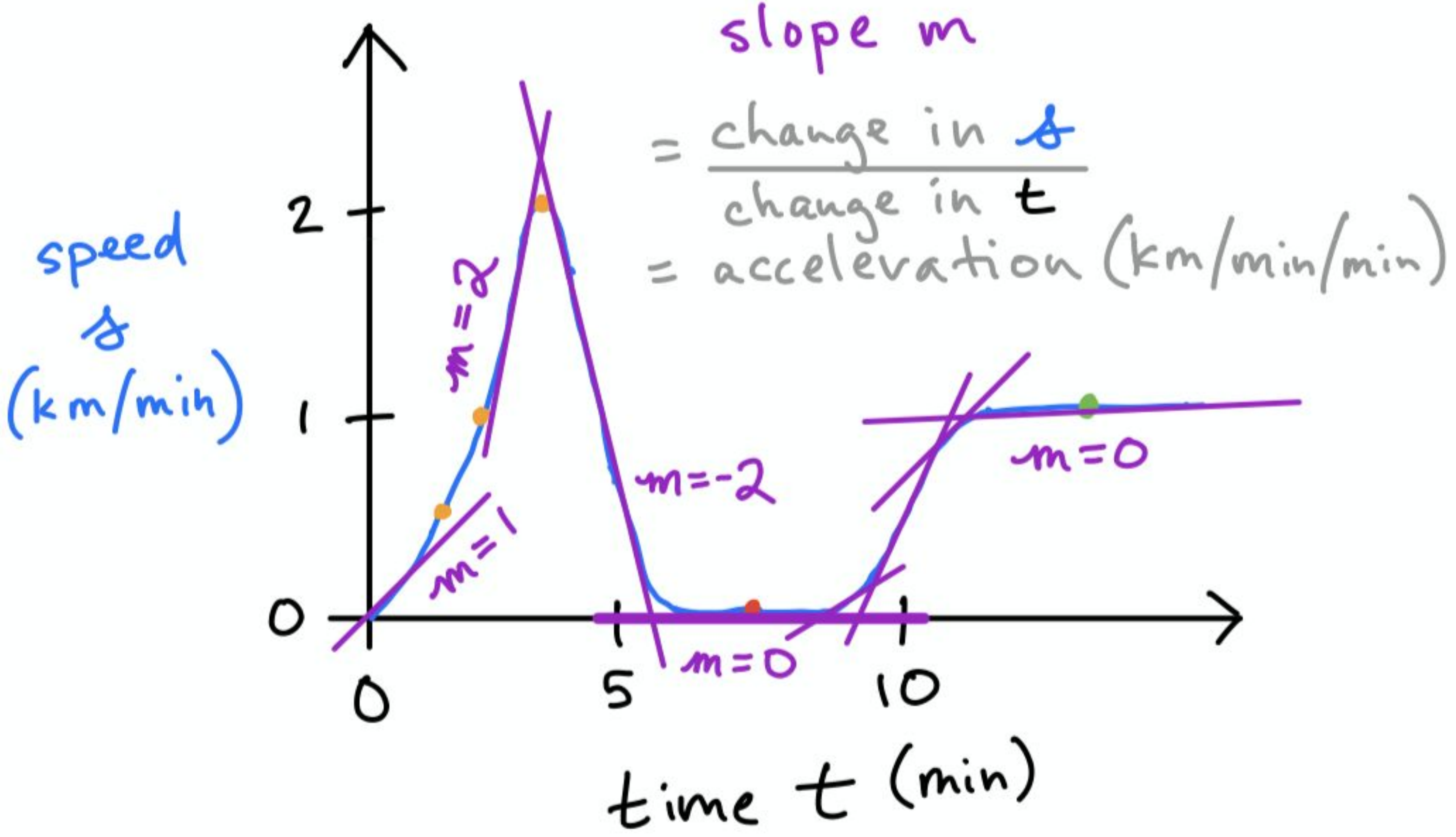

speed
y
(km/min)
2
1
0
m=2
m=1
m=-2
0
5
10
time t (min)


speed
s
(km/min)
2
1
0
m=2
m=1
m=-2
m=0
0
5
10
time t (min)



speed
y
(km/min)
2
1
0
0
5
10
m=2
m=-2
m=1
m=0
time t (min)


speed
y
(km/min)
2
1
0
m=2
m=-2
m=1
m=0
m=0
0
5
10
time t (min)

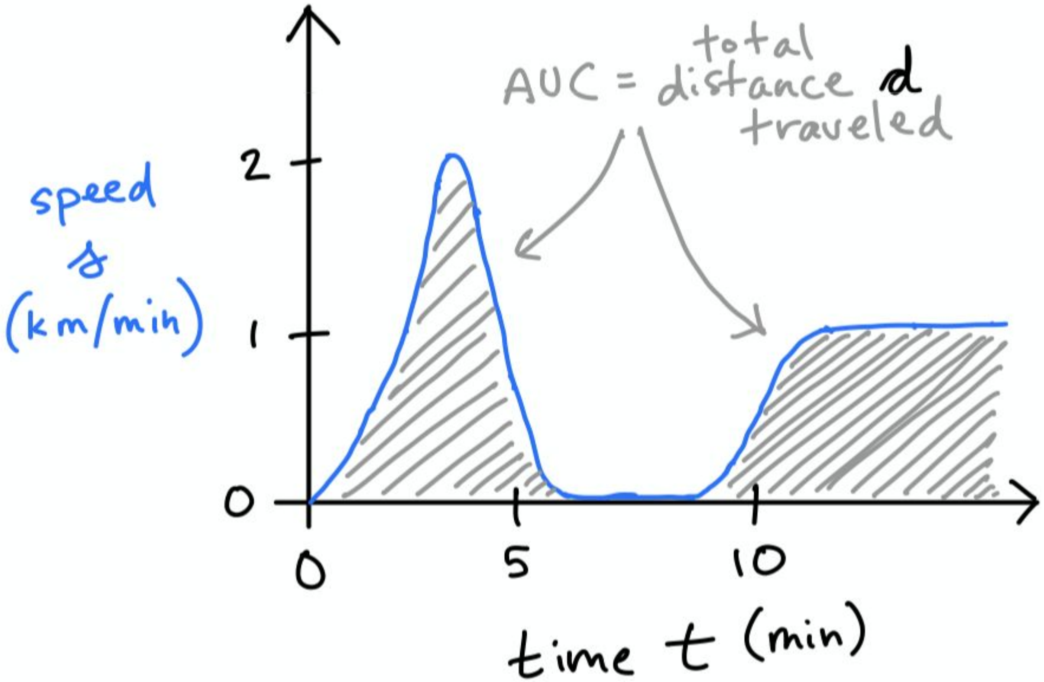

slope m
= change in s / change in t
= acceleration (km/min/min)
speed
s
(km/min)
2
1
0
m=2
m=-2
m=1
m=0
m=0
m=0
0
5
10
time t (min)

What Calculus Is

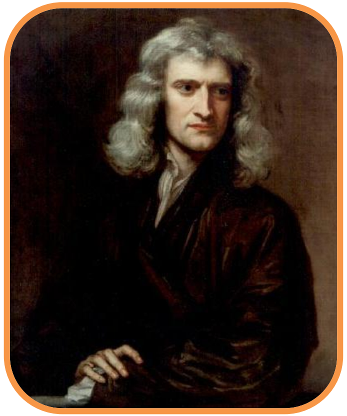
- **Mathematical study of continuous change**
- Two branches:
  a. **Differential calculus**: focus of *Calculus I*
  b. **Integral calculus**: a focus of *Calculus II* subject

What Integral Calculus Is

- **Study of areas under curves**
- Facilitates the inverse of differential calculus:



A Brief History of Calculus

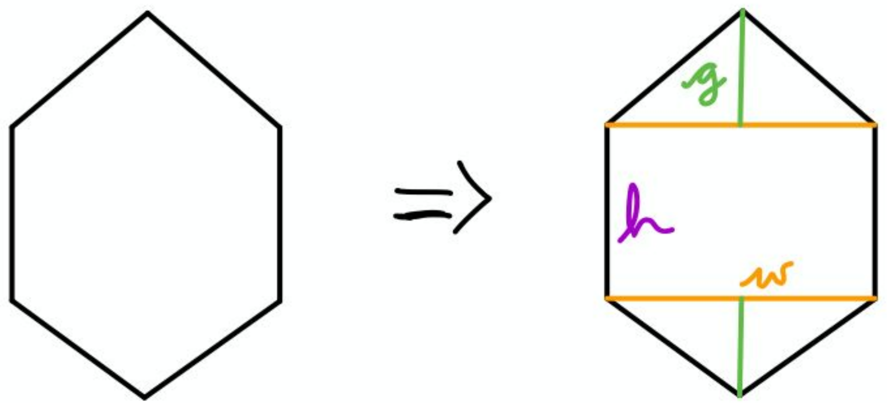


- ~1800 BCE: Egyptian papyrus with area calculations
- "Method of exhaustion" *(covered next)* developed by:
  - Greeks Eudoxus (~400 BCE) and Archimedes (~250 BCE)
  - Independently by Chinese Liu Hui (~250 CE)
- Arab al-Haytham (11th c. CE) used integrals to calculate volumes
- Indians (14th c.) had differentiation-like methods
- 17th c.: **Gottfried Leibniz** (Germany) & **Isaac Newton** (England)
  - Independently developed modern calculus
  - Incl. higher-order differentiation and integration
  - Incl. rules like "product rule" & "chain rule" *(in Calc I)*
  - Leibniz named it and devised notation (*we mostly use his!*)
  - Newton applied it first to physics, e.g.:
    - Laws of motion
    - Gravity

Images from public domain

The Method of Exhaustion

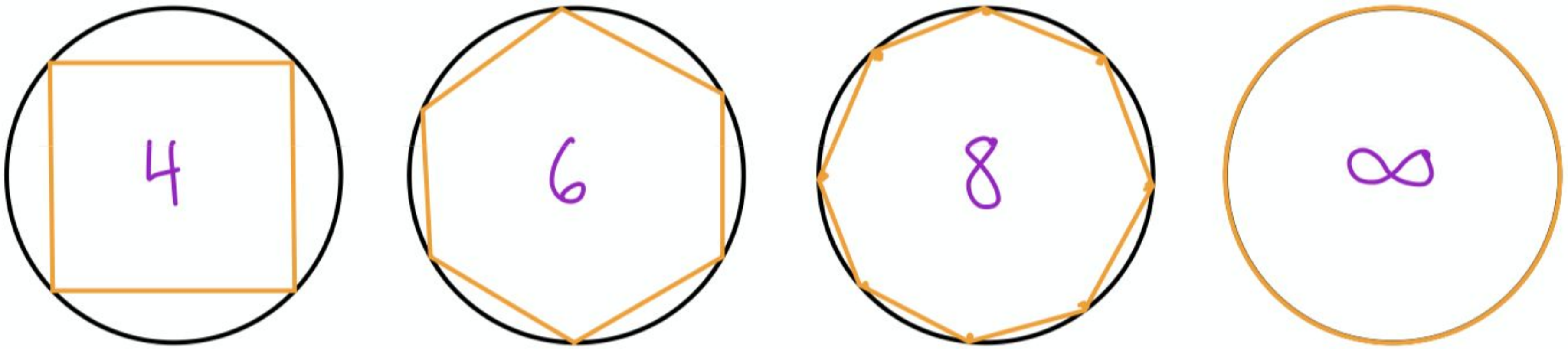
- **Polygon**: shape with multiple straight sides (3+; typically 5+)
  - Greeks learned to find area by filling with triangles



$$\text{area} = \frac{1}{2}(gw) + hw + \frac{1}{2}(gw)$$

The Method of Exhaustion

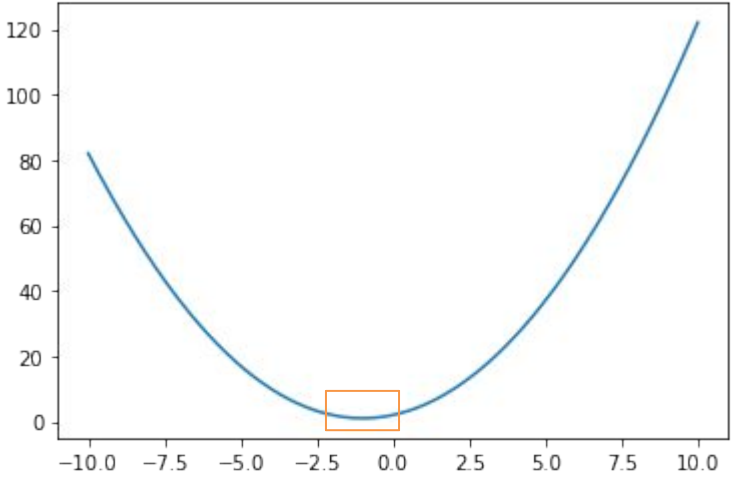
...the **Method of Exhaustion** builds on this to find area of curved shapes:

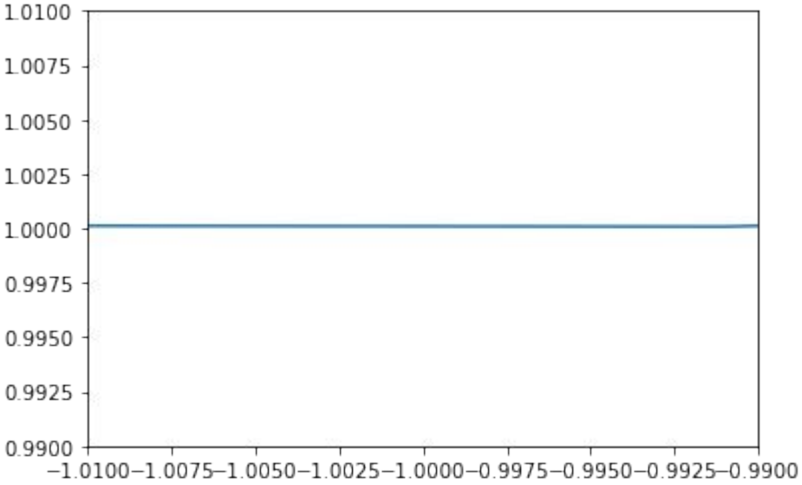


- Integral calculus is directly based on this method.
- Calculus in general relies on the idea of approaching infinity.
  - Leibniz gave field the name "calculus of the infinitesimals"

Calculus of the Infinitesimals

As integral accuracy improves as we approach an infinite-sided polygon, so too does differential accuracy improve as we approach a curve infinitely closely:



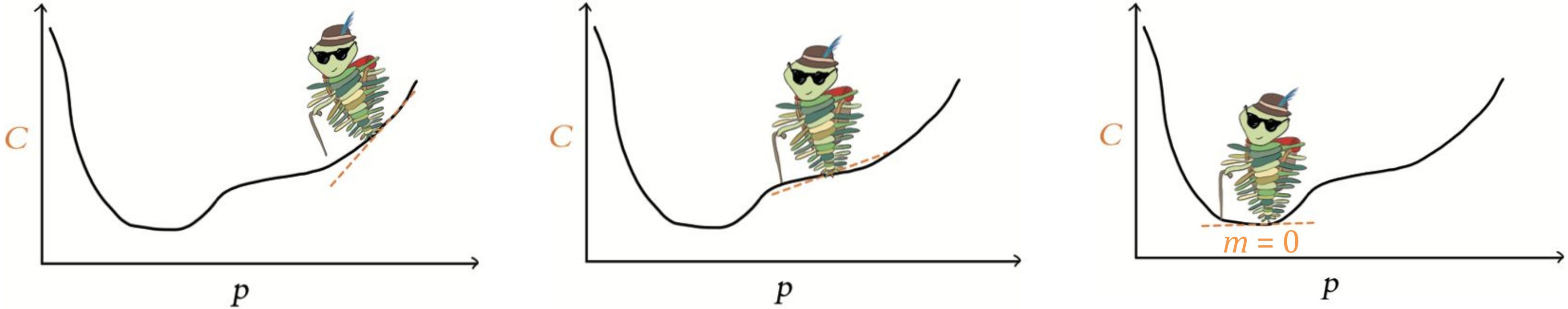


Hands-on code demo

Modern Calculus Applications

Differentials: optimize by finding minima and maxima of curves

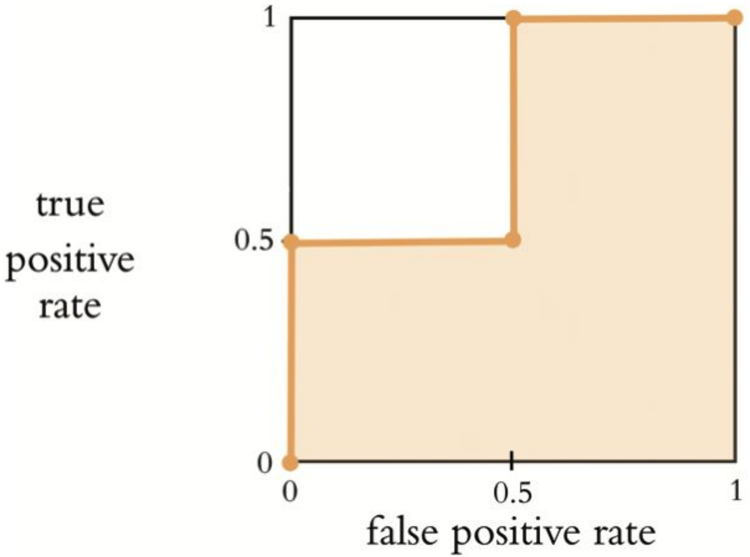
- Used, e.g., in engineering (max strength) and finance (min cost)
- Widely used in machine learning, incl. deep learning
    - **Gradient descent** to minimize cost (see `jonkrohn.com/deepTF1`)
    - Gradient ascent to maximize reward (see `jonkrohn.com/DQN`)
- Higher-order derivatives used in "fancy" optimizers *(Optimization)*



Modern Calculus Applications

Integrals: find area under the curve

- **Receiver operating characteristic** *(Calc II)*
- Probability theory's "expectation" of random variable is widely used in machine learning, incl. deep learning *(Prob. & Info. Thy.)*



Limits

Trivially easy to calculate for a continuous function, e.g.:

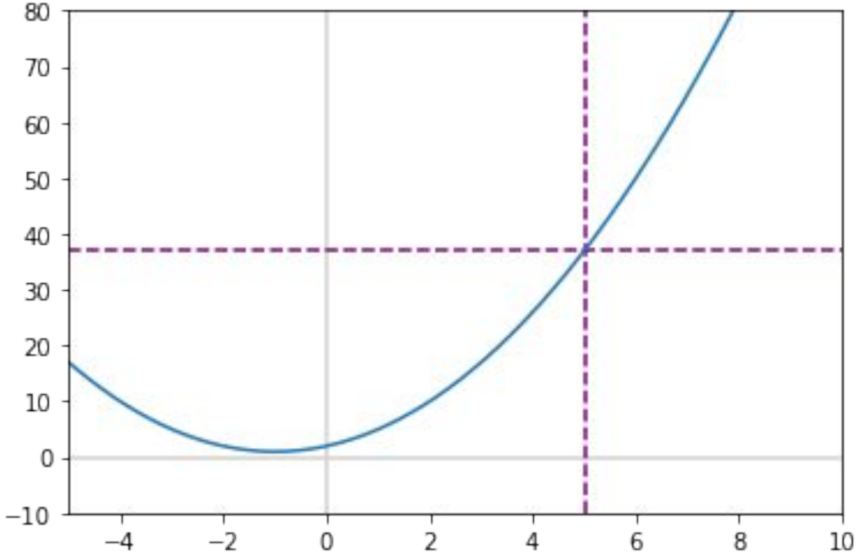
What is the limit as x approaches 5 in the expression $x^2 + 2x + 2$?

$$\lim_{x \to 5} (x^2 + 2x + 2)$$

$$= 5^2 + 2 \cdot 5 + 2$$

$$= 25 + 10 + 2$$

$$= 37$$

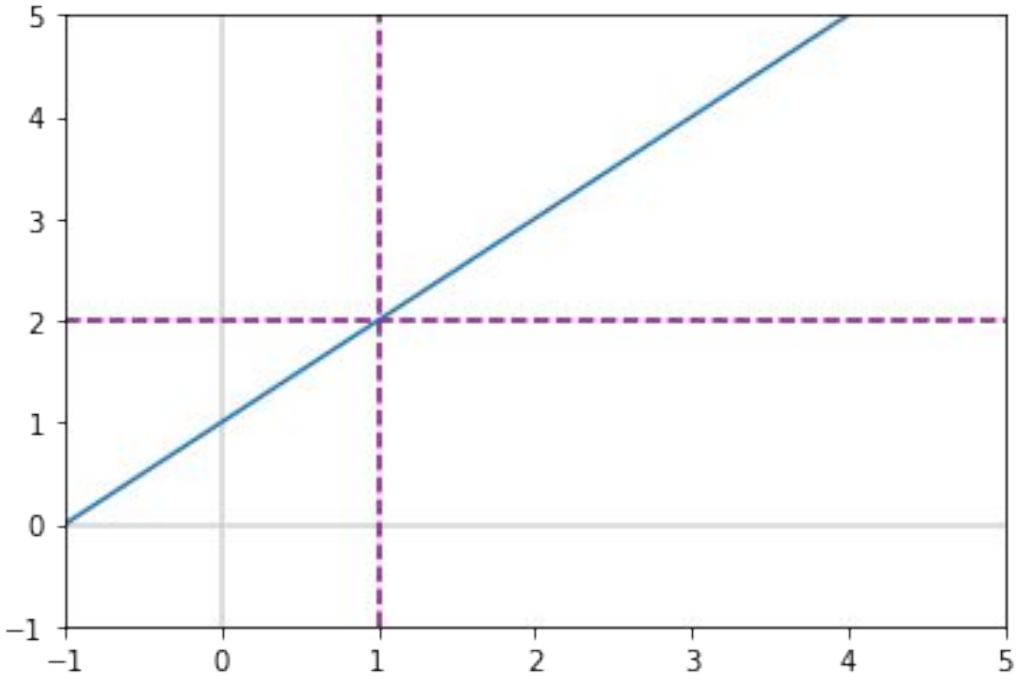


Limits

However, some functions are not continuous:

$$\lim_{x \to 1} \frac{x^2 - 1}{x - 1}$$

Hands-on code demo



Limits

In some cases, we can solve the limit through algebra, e.g., factoring:

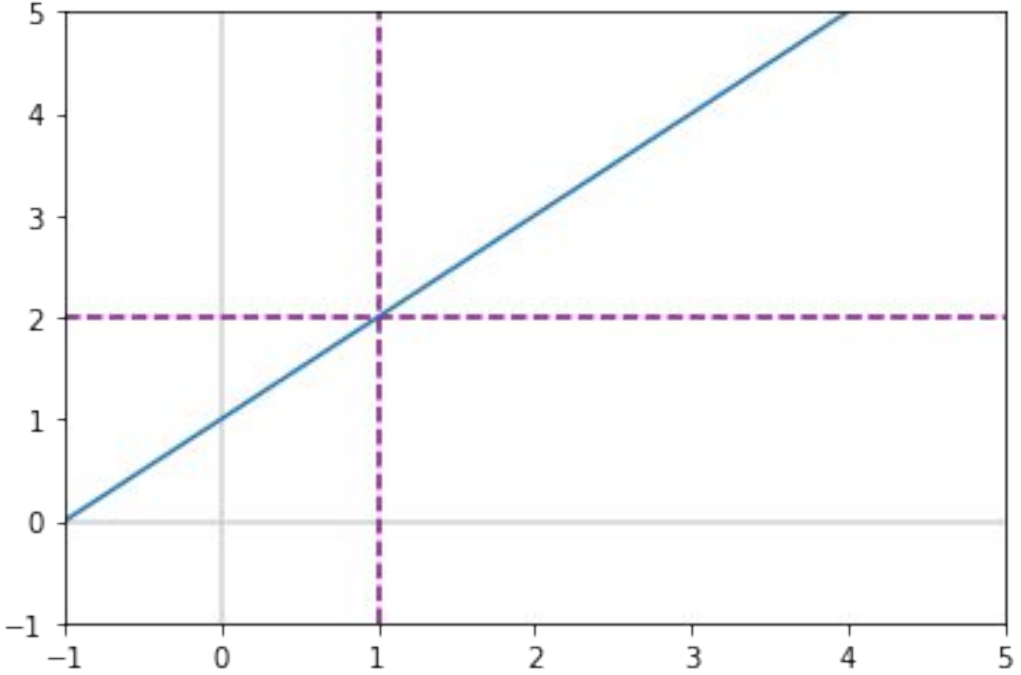
$$\lim_{x \to 1} \frac{x^2 - 1}{x - 1}$$

$$= \lim_{x \to 1} \frac{(x-1)(x+1)}{(x-1)}$$

$$= \lim_{x \to 1} \frac{\cancel{(x-1)}(x+1)}{\cancel{(x-1)}}$$

$$= \lim_{x \to 1} (x+1)$$

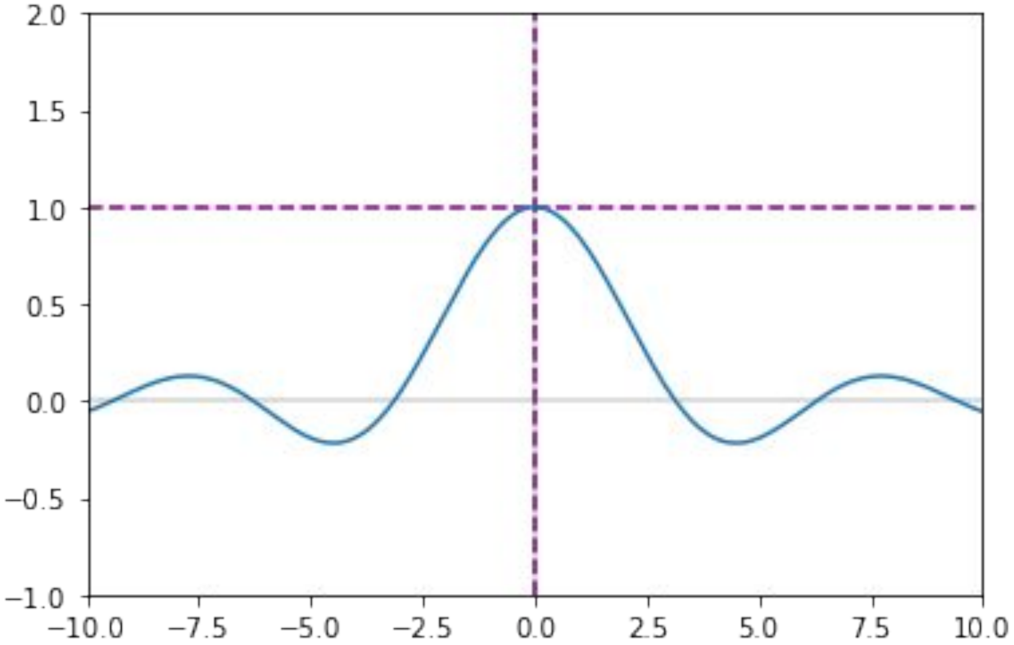
$$= 1 + 1$$



Limits

In other cases, we can't use algebra, but approaching the limit still works:

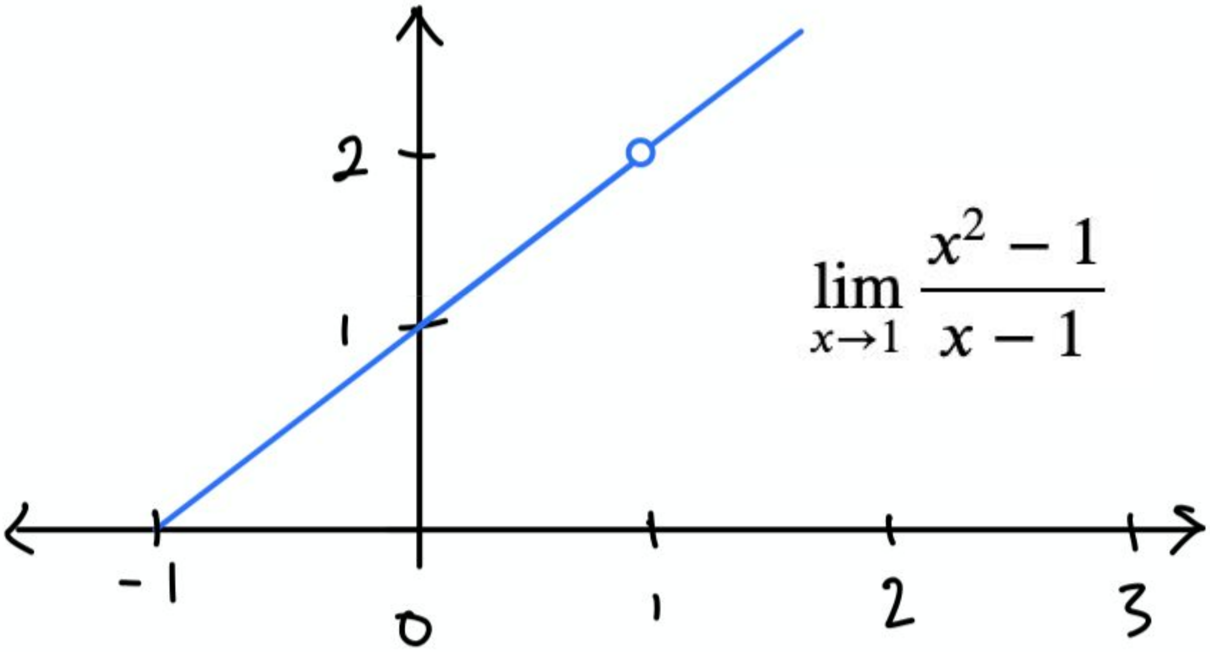
$$\lim_{x \to 0} \frac{\sin x}{x}$$



Hands-on code demo

Limits

Technically, charts should illustrate undefined points, e.g.:

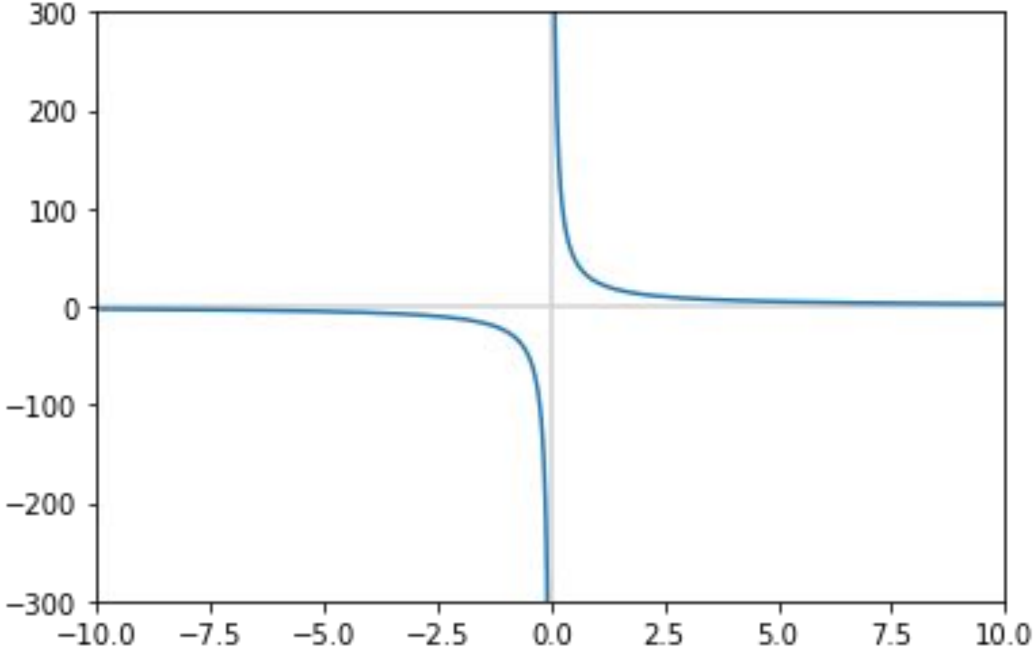


$$\lim_{x \to 1} \frac{x^2 - 1}{x - 1}$$

Limits

Finally, it is common for limits to approach infinity:

$$\lim_{x \to \infty} \frac{25}{x}$$



Hands-on code demo

Solutions

① $\lim_{x \to 0} \frac{x^2-1}{x-1}$

$= \frac{0^2-1}{0-1}$

$= \frac{-1}{-1}$

$= 1$

② $\lim_{x \to -5} \frac{x^2-25}{x+5}$

$= \lim_{x \to -5} \frac{\cancel{(x+5)}(x-5)}{\cancel{x+5}}$

$= \lim_{x \to -5} x-5$

$= -5-5 = -10$

Solutions

3

$$\lim_{x \to 4} \frac{x^2 - 2x - 8}{x - 4}$$

$$= \lim_{x \to 4} \frac{\cancel{(x-4)}(x+2)}{\cancel{x-4}}$$

$$= \lim_{x \to 4} x + 2$$

$$= 4 + 2 = 6$$

Solutions

4. 0

5. $\lim_{x \to 0^+} f(x) = \infty$ (right-handed limit)

$\lim_{x \to 0^-} f(x) = -\infty$ (left-handed limit)

Calculus I: Limits & Derivatives

1. Limits
2. **Computing Derivatives with Differentiation**
3. Automatic Differentiation

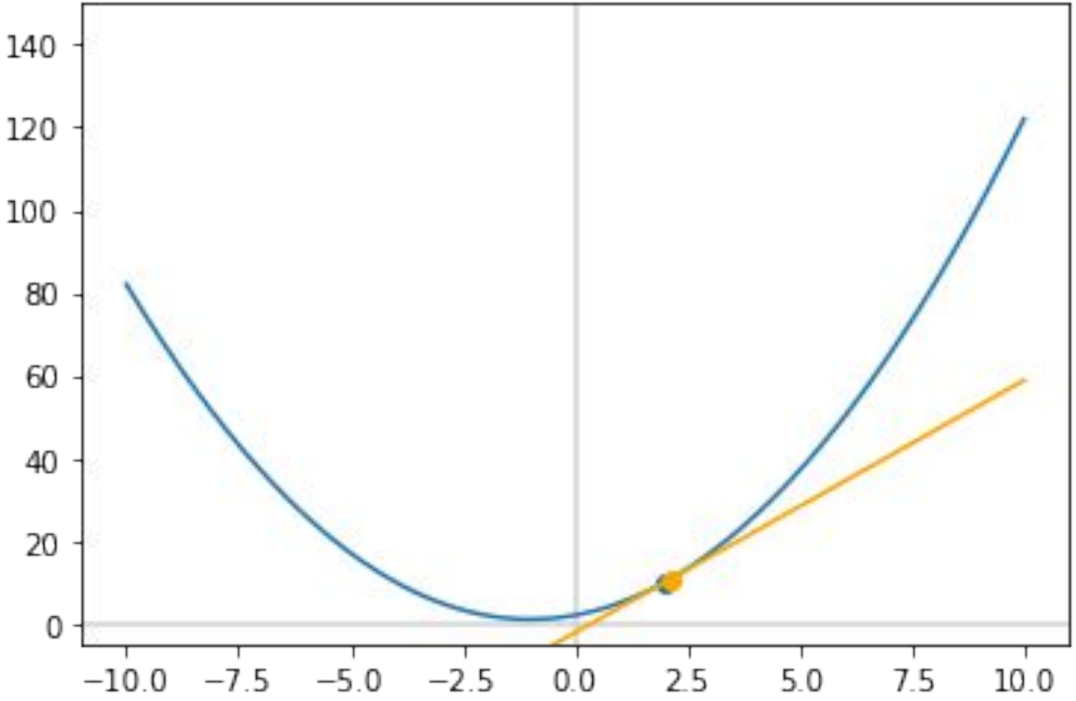
Segment 2: Derivatives & Differentiation

- The Delta Method
- The Differentiation Equation
- Differentiation Notation
- The Power Rule
- The Constant Multiple Rule
- The Sum Rule
- The Product Rule
- The Quotient Rule
- The Chain Rule

The Delta Method

Hands-on code demo

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$



Derivative Notation

$$y = f(x)$$

differentiation operator:					$\frac{d}{dx}$	D_x
first derivative of y w.r.t. x:	$\dot{y}$	y'	$f'(x)$	$\frac{dy}{dx}$	$\frac{d}{dx}f(x)$	$D_x f$
second derivative of y w.r.t. x:	$\ddot{y}$	y''	$f''(x)$	$\frac{d^2y}{dx^2}$	$\frac{d^2}{dx^2}f(x)$	$D_x^2 f$

Derivative of a Constant

Assuming c is constant: $\frac{d}{dx} c = 0$

The Power Rule

$$\frac{d}{dx} x^n = n x^{n-1}$$

The Constant Multiple Rule

$$\frac{d}{dx}(cy) = c\frac{d}{dx}(y) = c\frac{dy}{dx}$$

The Constant Multiple Rule *Simplified*

$$y = 2x^4$$

$$\frac{dy}{dx} = 2(4x^3) = 8x^3$$

The Sum Rule

$$\frac{d(y+w)}{dx} = \frac{dy}{dx} + \frac{dw}{dx}$$

Exercises

1. Differentiate $y = -5x^3$
2. Differentiate $y = 2x^2 + 2x + 2$
3. Differentiate $y = 10x^5 - 6x^3 - x - 1$
4. Use paper and pencil (i.e., the derivative rules) to find the slope of $y = x^2 + 2x + 2$ where $x = 2$
5. Repeat Exercise 4 but where $x = -1$

Solutions

① Differentiate $y = -5x^3$

$$\frac{dy}{dx} = -5(3x^2) = -15x^2$$

② Differentiate $y = 2x^2 + 2x + 2$

$$\frac{dy}{dx} = 2(2x^1) + 2(1x^0) + 0$$
$$= 2(2x) + 2(1)$$
$$= 4x + 2$$

Solutions

③ Differentiate $y = 10x^5 - 6x^3 - x - 1$

$$\frac{dy}{dx} = 10(5x^4) - 6(3x^2) - 1x^0 - 0$$

$$= 50x^4 - 18x^2 - 1$$

Solutions

(4) Using paper & pencil, find the slope of the curve $y = x^2 + 2x + 2$ where $x = 2$ as well as where $x = -1$

$$\frac{dy}{dx} = 2x + 2$$

$$\therefore m_1 = 2(2) + 2 = 4 + 2 = 6$$

$$m_2 = 2(-1) + 2 = -2 + 2 = 0$$

The Product Rule

$$\frac{d(wz)}{dx} = w\frac{dz}{dx} + z\frac{dw}{dx}$$

Useful:

- During calculations involving several rules
- Whenever product is incalculable pre-diff.

The Quotient (i.e., Fraction) Rule

$$\frac{d}{dx}\left(\frac{w}{z}\right) = \frac{z\frac{dw}{dx} - w\frac{dz}{dx}}{z^2}$$

The Chain Rule

- Many applications within ML
  - Gradient descent in general
  - Critical for backpropagation algo used to train neural nets
- Based on *nested functions* (a.k.a. *composite functions*):
  - Let's say $y = (5x + 25)^3$
  - We can let $u = 5x + 25$
  - In that case, $y = u^3$
  - y is a function of u, and u is a function of x
- *Chain rule* is easy way to find derivative of nested function:

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$$

The Chain Rule

$$y = (2x^2 + 8)^2$$

$$y = u^2$$

$$\frac{dy}{du} = 2u$$

$$= 2(2x^2 + 8)$$

$$= 4x^2 + 16$$

$$u = 2x^2 + 8$$

$$\frac{du}{dx} = 4x$$

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$$

$$= (4x^2 + 16)(4x)$$

$$= 16x^3 + 64x$$

Exercises

1. Use the product rule to find $f'(x)$ where $y = (2x^2 + 6x)(2x^3 + 5x^2)$
2. Use the quotient rule to find y' where $y = 6x^2/(2 - x)$
3. Differentiate $y = (3x + 1)^2$
4. Find y' where $y = (x^2 + 5x)^6$
5. Differentiate $f(x) = 1/((\mathrm{x}^4 + 1)^5 + 7)$

Solutions

1.

$$\frac{d(wz)}{dx} = w\frac{dz}{dx} + z\frac{dw}{dx}$$

$$y = (2x^2 + 6x)(2x^3 + 5x^2)$$

$$w = 2x^2 + 6x \qquad z = 2x^3 + 5x^2$$

$$\frac{dw}{dx} = 4x + 6 \qquad \frac{dz}{dx} = 6x^2 + 10x$$

$$\frac{d(wz)}{dx} = w\frac{dz}{dx} + z\frac{dw}{dx}$$

$$= (2x^2 + 6x)(6x^2 + 10x) + (2x^3 + 5x^2)(4x + 6)$$

$$= 12x^4 + 20x^3 + 36x^3 + 60x^2 + 8x^4 + 12x^3 + 20x^3 + 30x^2$$

$$= 20x^4 + 88x^3 + 90x^2$$

Solutions

2.

$$\frac{d}{dx}\left(\frac{w}{z}\right) = \frac{z\frac{dw}{dx} - w\frac{dz}{dx}}{z^2}$$

$$y = \frac{6x^2}{2-x} \qquad w = 6x^2 \qquad z = 2-x$$

$$\frac{dw}{dx} = 12x \qquad \frac{dz}{dx} = -1$$

$$y' = \frac{d}{dx}\left(\frac{w}{z}\right) = \frac{(2-x)(12x) - (6x^2)(-1)}{(2-x)^2}$$

$$= \frac{24x - 12x^2 + 6x^2}{(2-x)^2}$$

$$= \frac{24x - 6x^2}{(2-x)^2}$$

Solutions

3.

$$y = (3x+1)^2$$

$$y = u^2$$

$$\frac{dy}{du} = 2u$$
$$= 2(3x+1)$$
$$= 6x+2$$

$$u = 3x+1$$

$$\frac{du}{dx} = 3$$

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$$
$$= (6x+2)(3) = 18x+6$$

Solutions

4.

$$y = (x^2 + 5x)^6$$

$$y = u^6$$

$$\frac{dy}{du} = 6u^5$$

$$= 6(x^2 + 5x)^5$$

$$u = x^2 + 5x$$

$$\frac{du}{dx} = 2x + 5$$

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$$

$$= \left(6(x^2 + 5x)^5\right)(2x + 5)$$

Solutions

5.

$$y = \frac{1}{(x^4+1)^5+7}$$

$$y = \frac{1}{u} = u^{-1}$$

$$\frac{dy}{du} = (-1)u^{-1-1}$$

$$= -u^{-2}$$

$$= -(t^5+7)^{-2}$$

$$= -((x^4+1)^5+7)^{-2}$$

$$u = t^5 + 7$$

$$\frac{du}{dt} = 5t^4$$

$$= 5(x^4+1)^4$$

$$t = x^4 + 1$$

$$\frac{dt}{dx} = 4x^3$$

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dt}\frac{dt}{dx}$$

$$= \left(-((x^4+1)^5+7)^{-2}\right)\left(5(x^4+1)^4\right)\left(4x^3\right)$$

Power Rule on a Function Chain

$$\frac{d}{dx} u^n = n u^{n-1} \frac{du}{dx}$$

Exercise

Repeat questions 4 and 5 using the power rule.

Calculus I: Limits & Derivatives

1. Limits
2. Computing Derivatives with Differentiation
3. **Automatic Differentiation**

Segment 3: Automatic Differentiation

- Autodiff with PyTorch
- Autodiff with TensorFlow
- Machine Learning via Differentiation
- Cost (or Loss) Functions
- The Future: Differentiable Programming

Automatic Differentiation

- A.K.A.:
  - Autodiff
  - Autograd
  - Computational diff.
  - Reverse mode diff.
  - Algorithmic diff.
- Distinct from classical methods:
  - Numerical diff. (delta method; introduces rounding errors)
  - Symbolic diff. (algebraic rules; computationally inefficient)
- Relative to classical methods, better handles:
  - Functions with many inputs (common in ML)
  - Higher-order derivatives

Automatic Differentiation

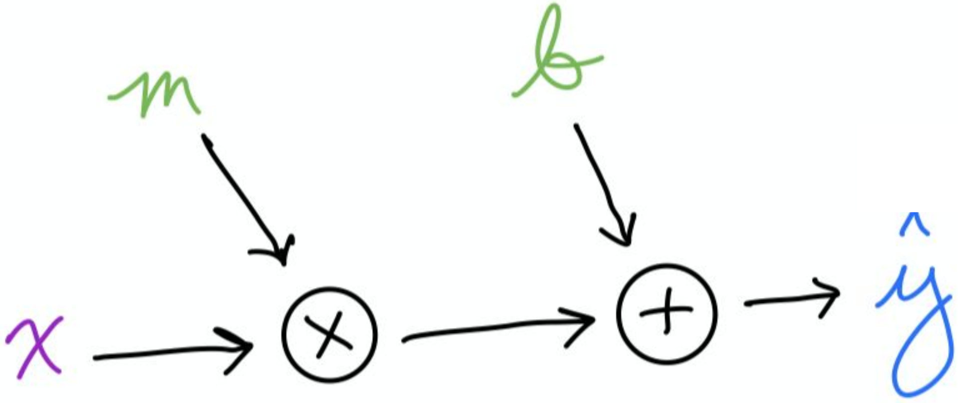
- Application of chain rule (typically *partial* derivative) to sequence (forward pass) of arithmetic operations
- Whereas chain rule by hand typically begins at most-nested function, autodiff proceeds from outermost function inward
- Small constant factor more compute than forward pass (at most)

$$\frac{dy}{dx} = \frac{dy}{du} \frac{du}{dx}$$

Hands-on code demo

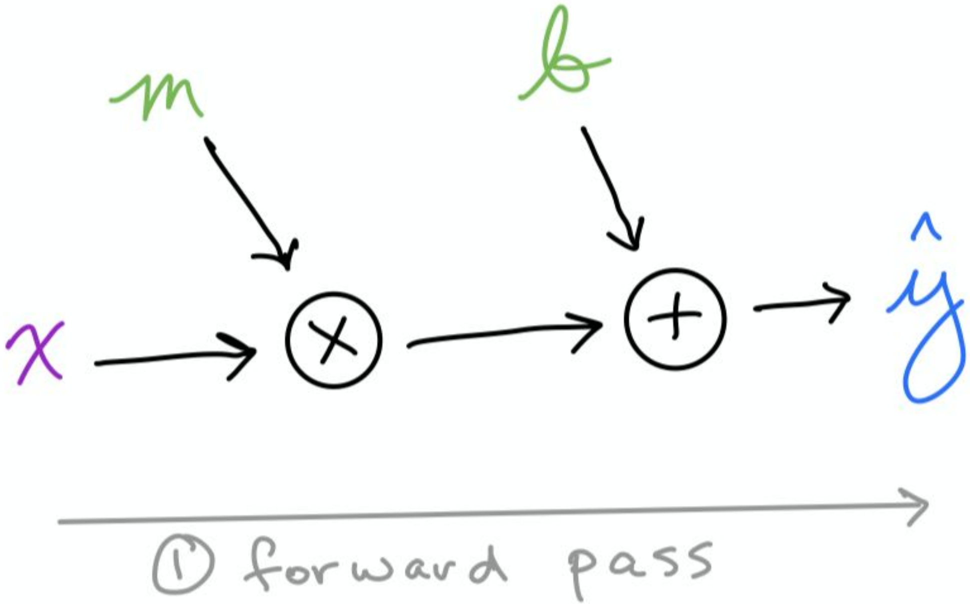
Fitting a Line with Machine Learning

- Line equation $y = mx + b$ as *directed acyclic graph* (DAG)
- Nodes are input, output, parameters, or operations
- Directed edges ("arrows") are tensors (N.B.: non-operation nodes can be tensors too)

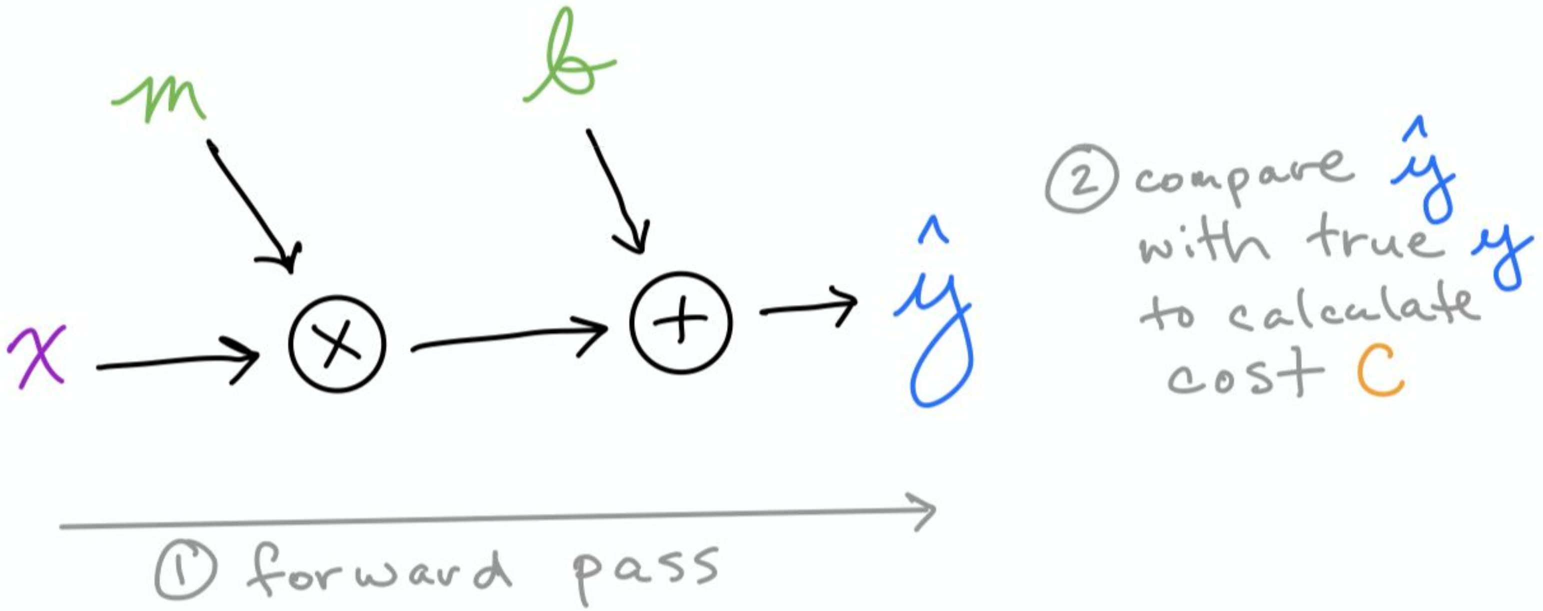


Hands-on code demo: `regression-in-pytorch.ipynb`

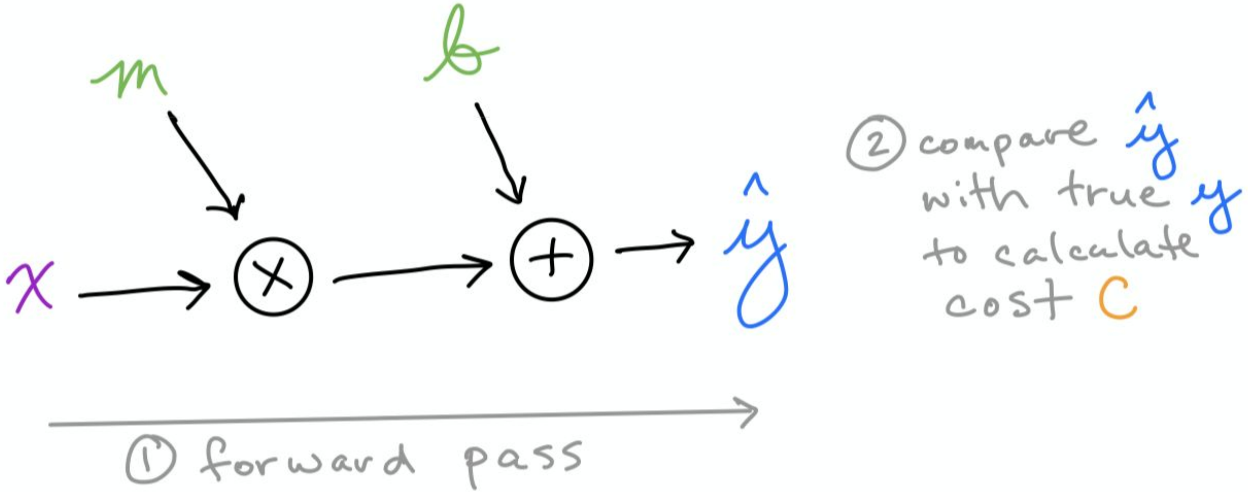
Machine Learning



Machine Learning



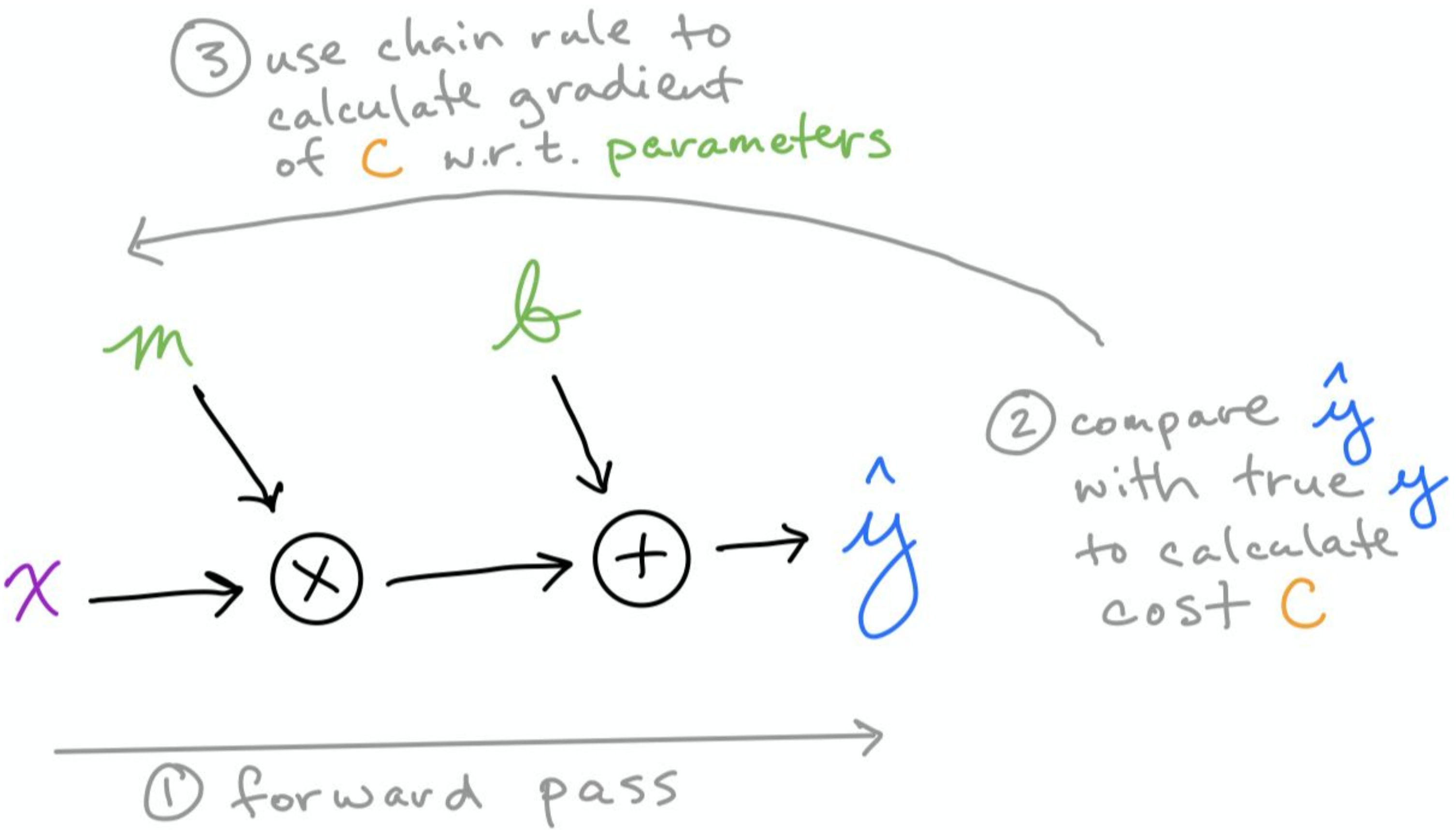
The Chain Rule’s Necessity



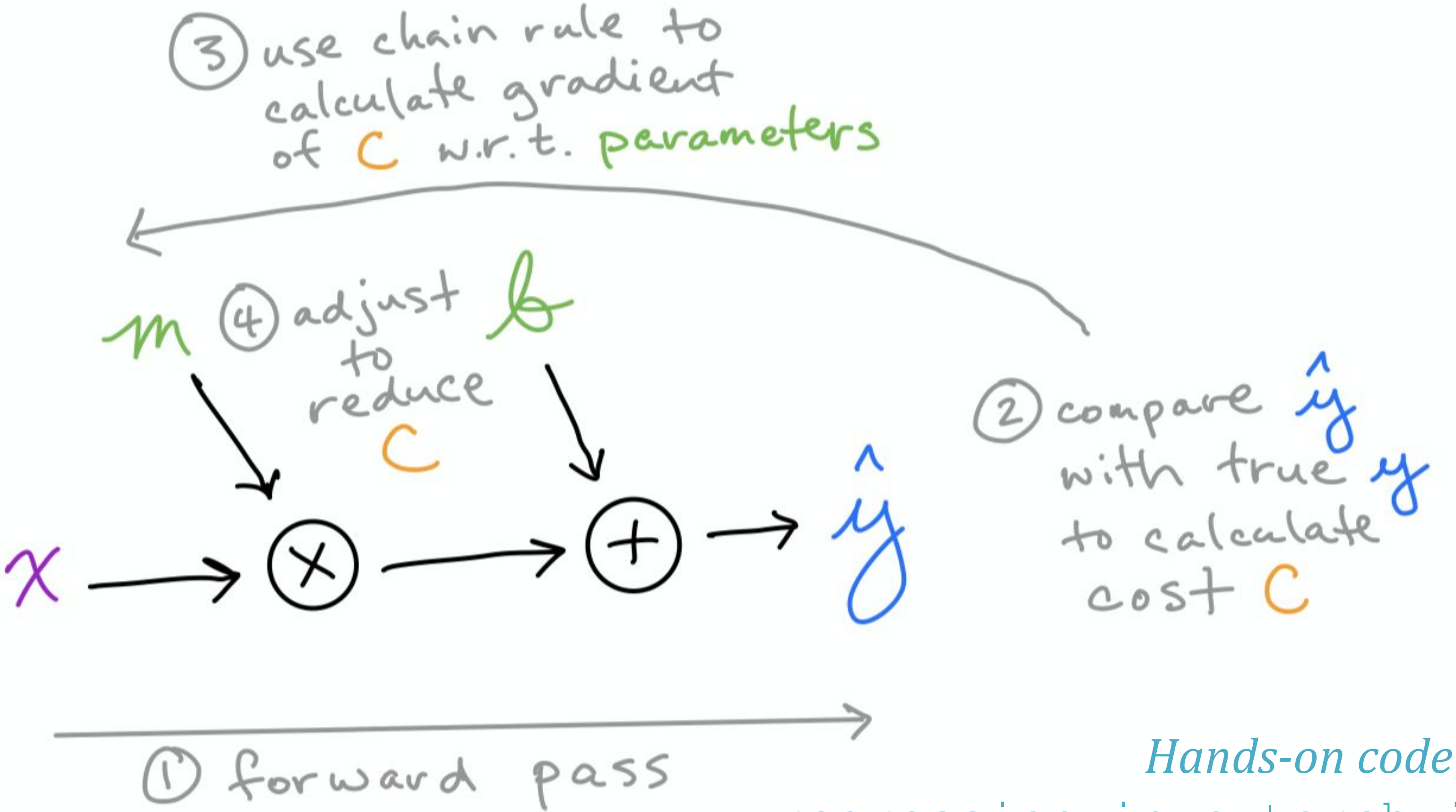
$$\hat{y} = f(x, m, b) \qquad C = g(\hat{y}, y)$$

$$C = g(f(x, m, b), y)$$

Machine Learning



Machine Learning



Hands-on code demo:
`regression-in-pytorch.ipynb`

Exercises

1. Use PyTorch (or TensorFlow, if you like) to find the slope of $y = x^2 + 2x + 2$ where $x = 2$.

2. Use the *Regression in PyTorch* notebook to simulate a new linear relationship between y and x, and then fit the parameters m and b.

3. Read about how *differential programming*, wherein computer programs can be differentiated, could be common soon (perhaps thanks to *quantum* ML; see `pennylane.ai`).

Next Subject: *Calculus II*

- Partial derivatives
  - Required for autodiff from regressions to deep neural nets
- Integrals
  - Calculate area under a curve, e.g., for ROC AUC metric

POLL *with Multiple Answers Possible*

What follow-up topics interest you most?

- Linear Algebra
- More Calculus
- Probability / Statistics
- Computer Science (e.g., algorithms, data structures)
- Machine Learning Basics
- Advanced Machine Learning, incl. Deep Learning
- Something Else

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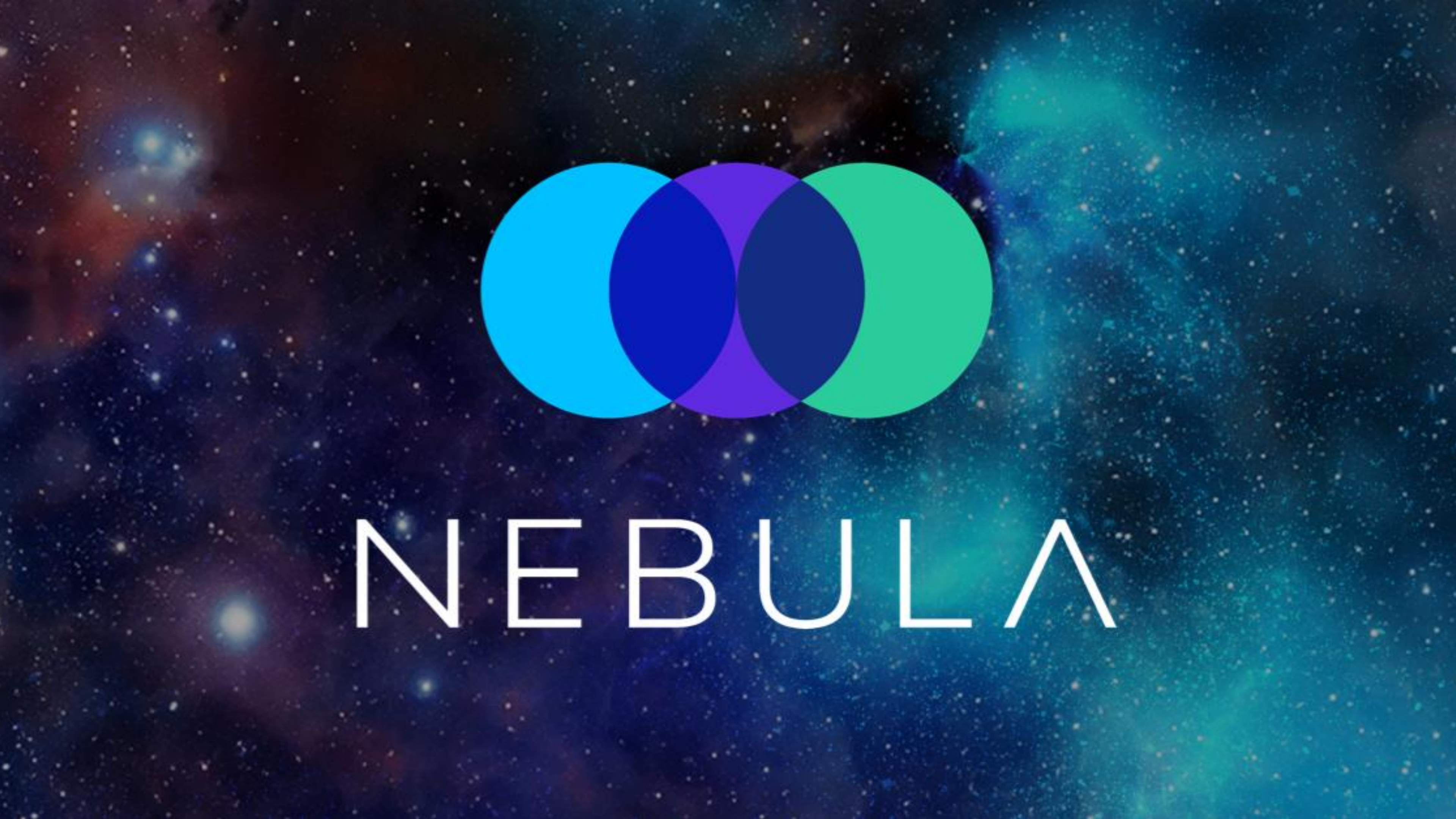
NEBULA

PLACEHOLDER
FOR:

5-Minute Timer

PLACEHOLDER
FOR:

10-Minute Timer

PLACEHOLDER
FOR:

15-Minute Timer