Lecture 8

Automatic Differentiation and Root Finding

CS328 - Numerical Methods for Visual Computing and Machine Learning

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EPFL RGL Realistic Graphics Lab

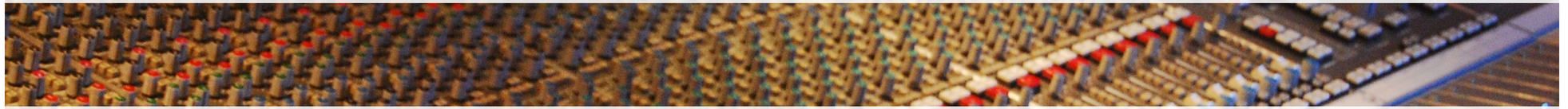
Motivation: training of neural networks

In [27]:
```
for t in range(500):
    # Forward pass: compute predicted y by passing x to the model.
    y_pred = model(x)

    # Compute and print loss.
    loss = loss_fn(y_pred, y)

    # Zero out all gradients
    optimizer.zero_grad()

    # Compute gradient of the loss with respect to model parameters
    loss.backward()

    # Let optimizer update parameters to improve loss fct.
    optimizer.step()
```

Motivation: training of neural networks

- Neural networks have become **gigantic** (20M parameters normal, variants with *hundreds of billions of parameters* exist)

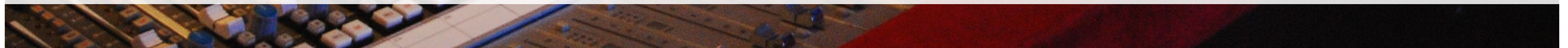
- How can we optimize something with that many dimensions?



- Need to efficiently move through high-dimensional domain & optimize all parameters at the same time.

  Gradient: *best local direction* to improve neural net.

  Tensorflow, PyTorch, *etc*: **tools to compute gradients quickly.**



[Wikimedia commons]

How to evaluate gradients?

Let's review some standaard techniques for evaluating derivatives.

- **Finite Differences**
  - Evaluate function at nearby points to estimate derivative

- **Symbolic (by hand, or with help of software)**
  - Apply all the rules you've learned in MATH-101

- **Automatic differentiation ("AD", "autodiff")**
  - Like "symbolic", but with a few extra tricks!

Finite Differences

Forward difference

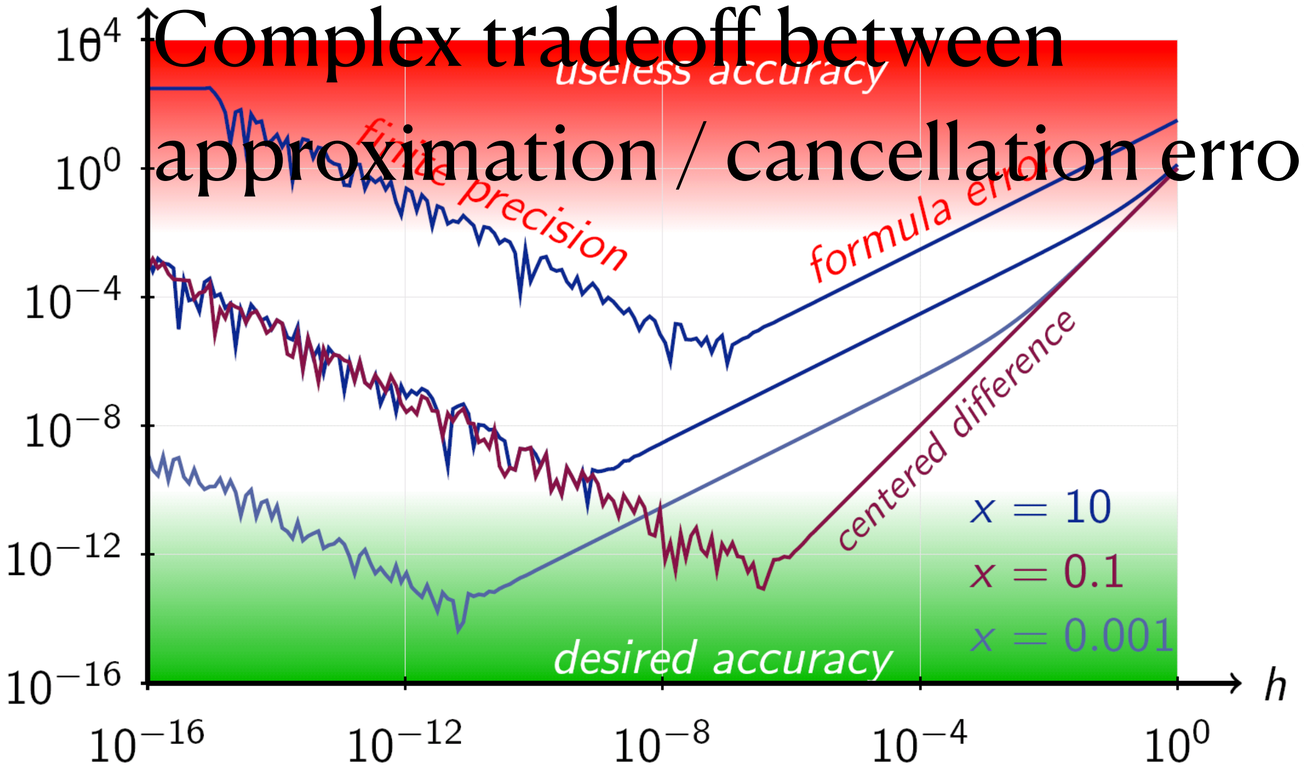
$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Centered difference

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

Main problems:

- (plot shows $f(x) = x^3$, $f'(x) = 3x^2$, $\text{approx}(x) = \ldots$)
- In many dimensions? Must evaluate f at least 1M+1 times
- Complex tradeoff between approximation / cancellation error



Symbolic versus Automatic Derivatives

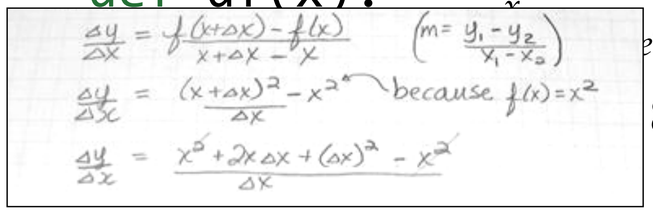
Original calculation:

```
def f(x):
    for i in range(8):
        x = exp(x)
    return x
```

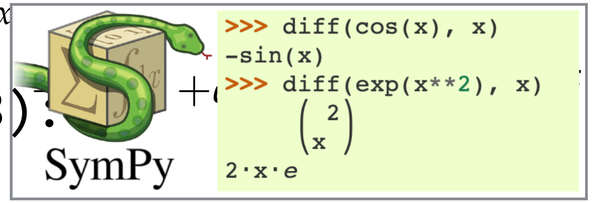
8 exponentials

Symbolic differentiation (forward mode):

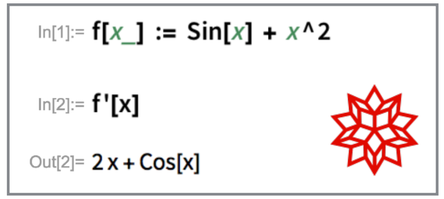
```
def df(x):
    d = 1
    for i in range(8):
        d = d * x
        x = exp(x)
    return d
```



By hand



SymPy

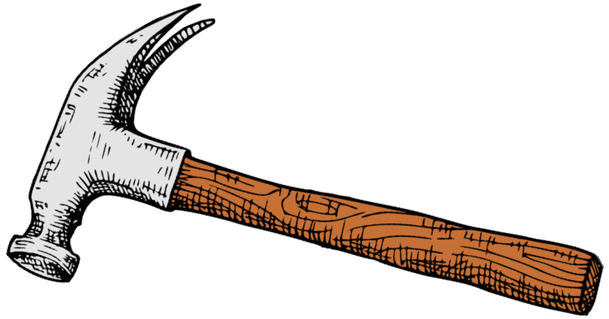


Mathematica

Computer Algebra System (CAS)

37 exponentials (!)

Automatic differentiation



$$f(\mathbf{x}) \xrightarrow{\text{AD}} \frac{\partial}{\partial \mathbf{x}} f(\mathbf{x})$$

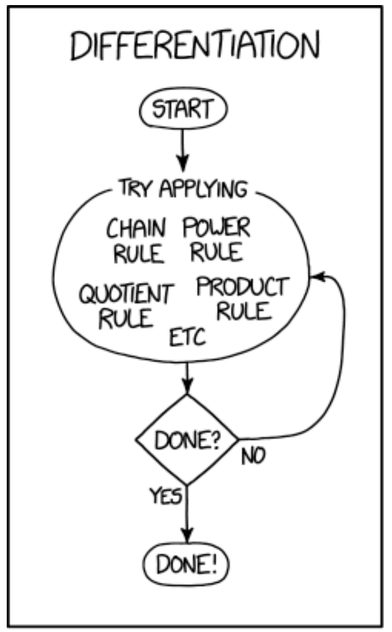
TensorFlow

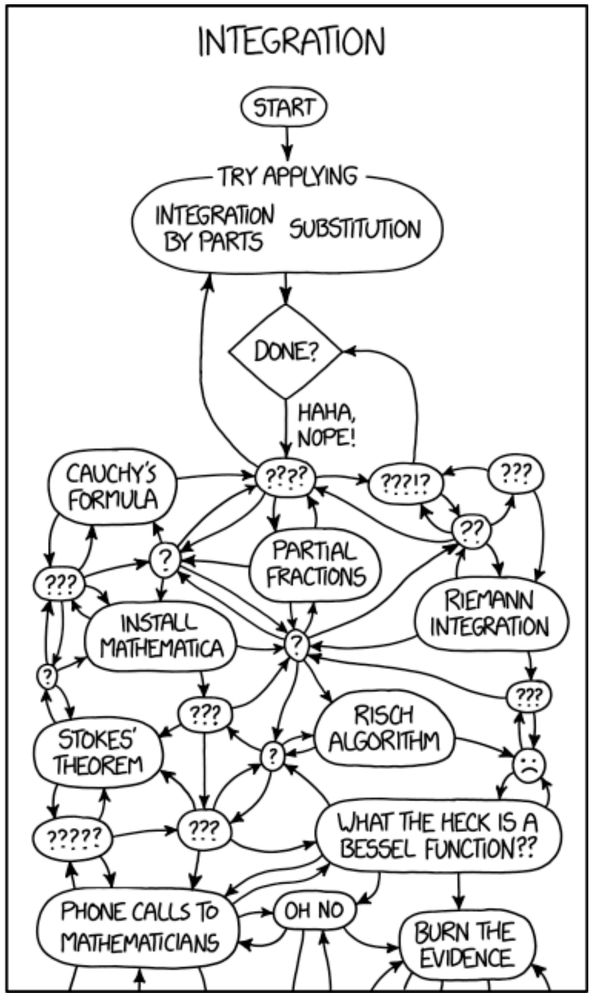
PyTorch

AD Motivation

- Differention is **simple**, really! (at least *locally*)
  - Any program boils down to a sequence of tiny steps (`+`, `-`, `load`, `store`, etc.).
  - If we know how to handle each step, then we can differentiate the entire program!

[xkcd.com]





- AD has two key ingredients:
  - Chain rule
  - Common subexpressions

AD Ingredient 1: The Chain Rule

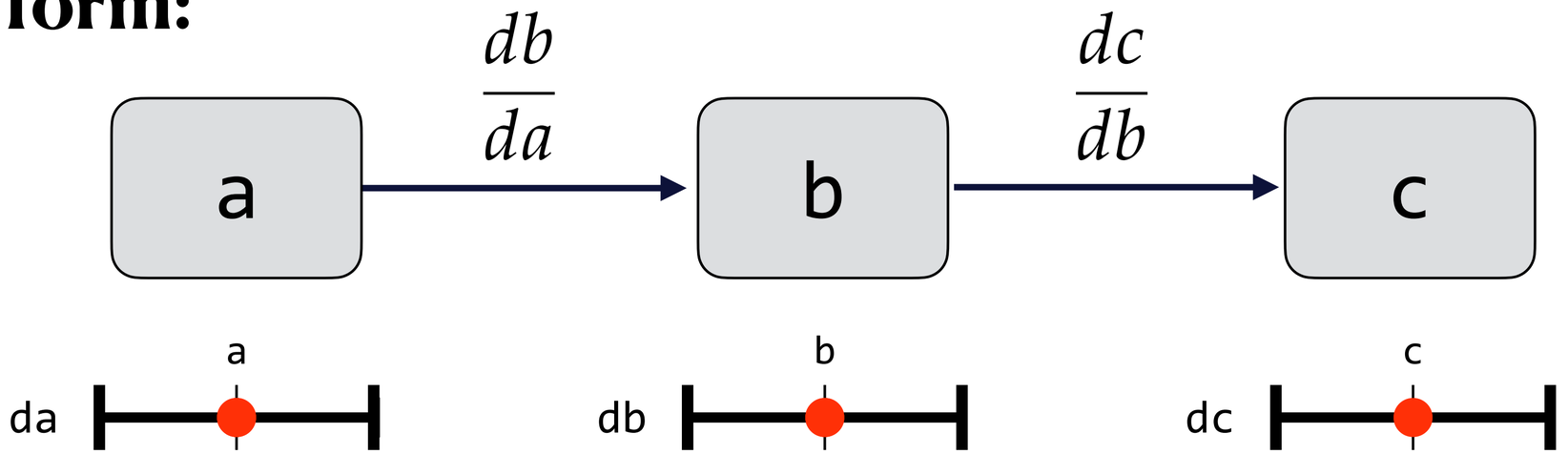
Original calculation:

```
b = f(a)
c = g(b)
```

Chain rule:

$$\frac{dc}{da} = \frac{dc}{db}\frac{db}{da}$$

In graph form:



AD Ingredient 2: Reuse of common subexpressions

Original calculation:

```
b = f(a)
c = g(a)
d = h(b, c)
e = k(d)
```

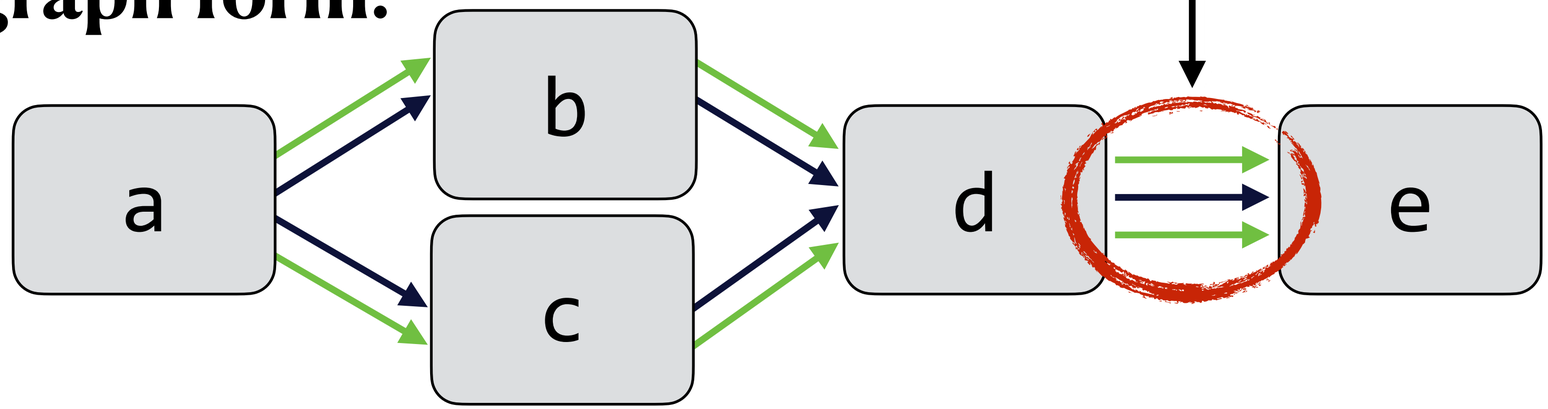
Naïve symbolic derivative:

```
de = dk(h(f(a), g(a))) *
     dh_1(f(a), g(a)) * df(a)
   + dk(h(f(a), g(a))) *
     dh_2(f(a), g(a)) * dg(a)
```

Redundant computation

(as programs grow larger, such unnecessary computation can lead to exponential overheads)

In graph form:



Cheap Gradient Principle

The cost of computing the gradient is nearly the same (typ. $< 5x$) **as that of simply computing the function itself.**

[Griewank 2008]

- Enables fast computation of high-dimensional gradient (crucial for machine learning and many other applications.)

AD Ingredient 2: Reuse of common subexpressions

Original calculation:

```
b = f(a)
c = g(a)
d = h(b, c)
e = k(d)
```

Naïve symbolic derivative:

```
de = dk(h(f(a), g(a))) *
       dh_1(f(a), g(a)) * df(a)
   + dk(h(f(a), g(a))) *
       dh_2(f(a), g(a)) * dg(a)
```

Optimized:

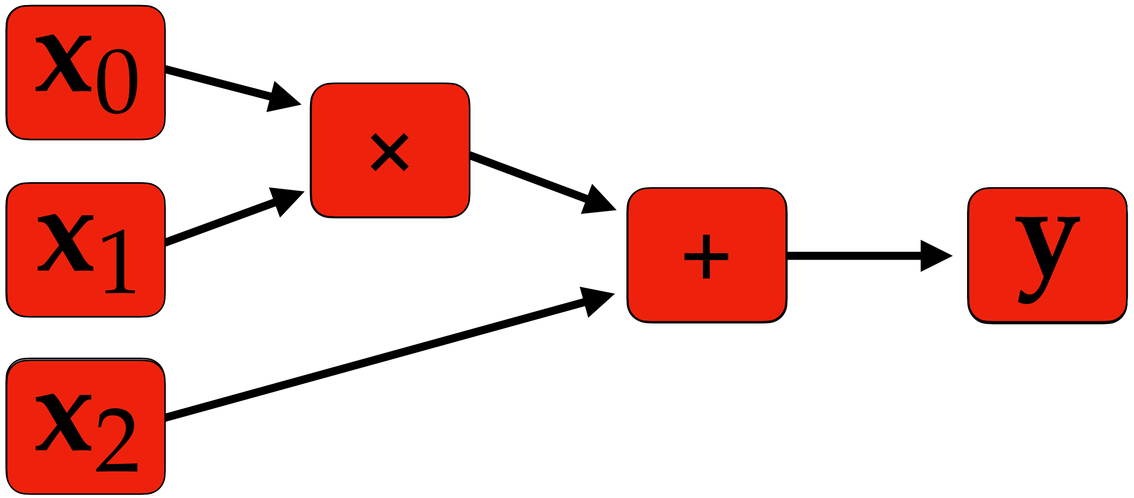
```
b = f(a);          db = df(a);
c = g(a);          dc = dg(a);
d = h(b, c);       dd = dh_1(b, c) * db +
                        dh_2(b, c) * dc;
e = k(d);          de = dk(d) * dd;
```

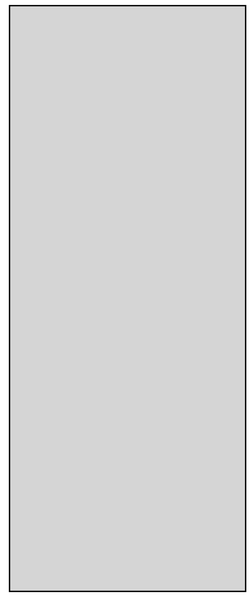
Differentiating a function with respect to an input

Differentiation depends on how variables are *connected*.

This is known as
Forward mode

$$y = x_0 \cdot x_1 + x_2$$





Gradient

Talk is cheap, show me the code!

One possible implementation strategy: *dual numbers*. (we'll discuss 3 today.)

```
class Number:
    def __init__(self, value: float, grad: float):
        self.value = value
        self.grad = grad

    def __add__(self, other: Number):
        return Number(
            value = self.value + other.value,
            grad  = self.grad + other.grad
        )

    def __mul__(self, other: Number):
        return Number(
            value = self.value * other.value,
            grad  = self.grad*other.value + self.value*other.grad
        )
```

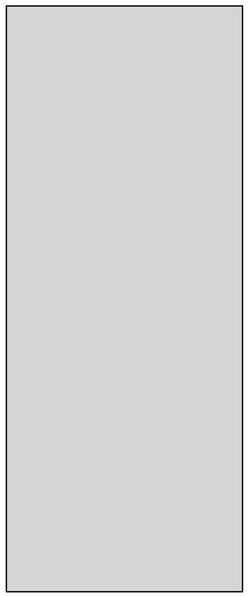
Note: this is *not* the approach used in homework 4, please don't copy code from here.

Demo time

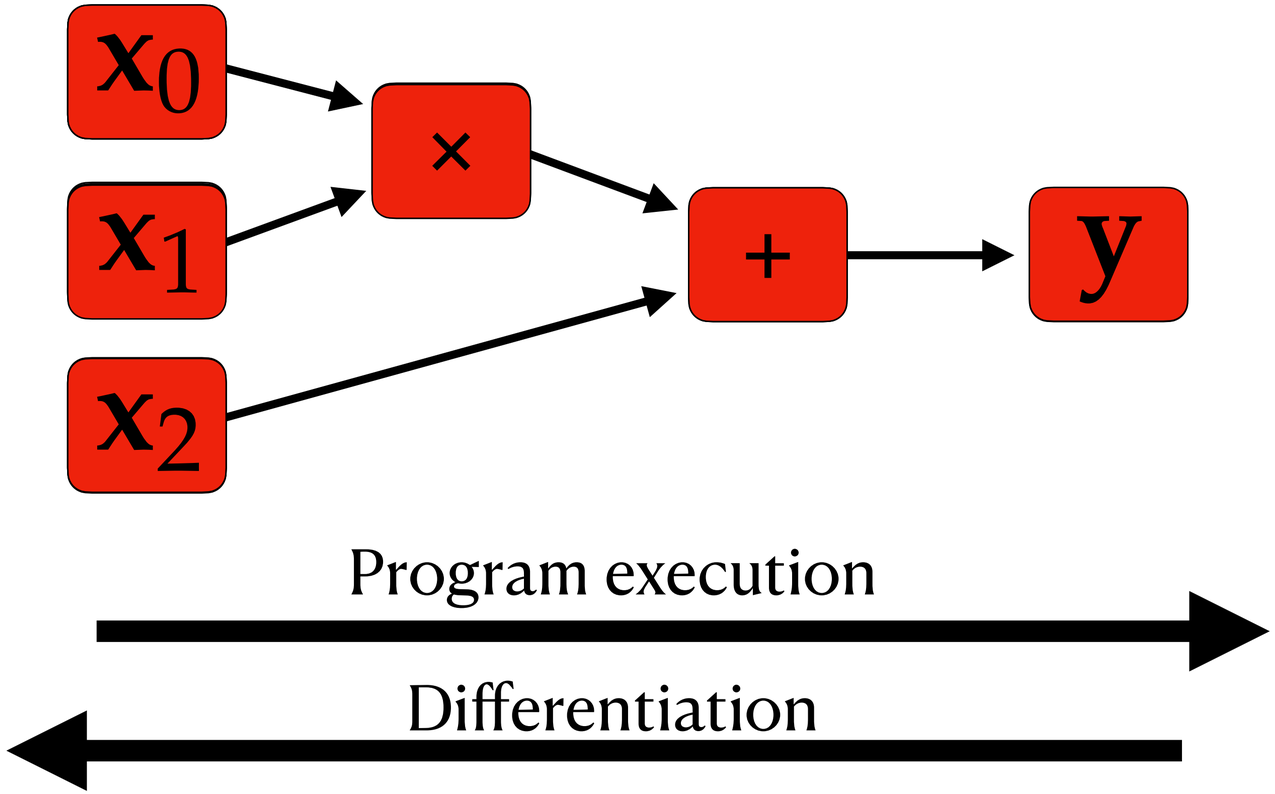
Directionality of differentiation

Reverse mode
aka. backward mode

$$y = x_0 \cdot x_1 + x_2$$



Gradient



The Jacobian of multidimensional functions

Another way to think about forward/reverse mode AD

$$\mathbf{J}_f(\mathbf{x}) = \frac{f(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} \frac{f_1(\mathbf{x})}{\partial \mathbf{x}} \\ \vdots \\ \frac{f_n(\mathbf{x})}{\partial \mathbf{x}} \end{bmatrix} = \begin{bmatrix} \frac{f_1(\mathbf{x})}{\partial x_1} & \cdots & \frac{f_1(\mathbf{x})}{\partial x_m} \\ \vdots & & \\ \frac{f_n(\mathbf{x})}{\partial x_1} & \cdots & \frac{f_n(\mathbf{x})}{\partial x_m} \end{bmatrix}$$

In practice, m and n may be *very large* (> 1 million). **Can't store** a 1M x 1 M entry matrix.

"*Magic*" of AD: can efficiently multiply by that matrix without ever having to build it. Two kinds of matrix-vector products are commonly implemented:

Forward mode: computes $\mathbf{J}_f\,\mathbf{y}$ *Reverse* mode: computes $\mathbf{J}_f^T\,\mathbf{y}$

(for some given input vector $\mathbf{y}$*)*

Strategy 2: AD by recording onto a Tape

Differentiation task

$$\frac{\partial}{\partial \alpha}\left[\alpha \cdot \exp(-\alpha x)\right]$$

```
δa  =
```

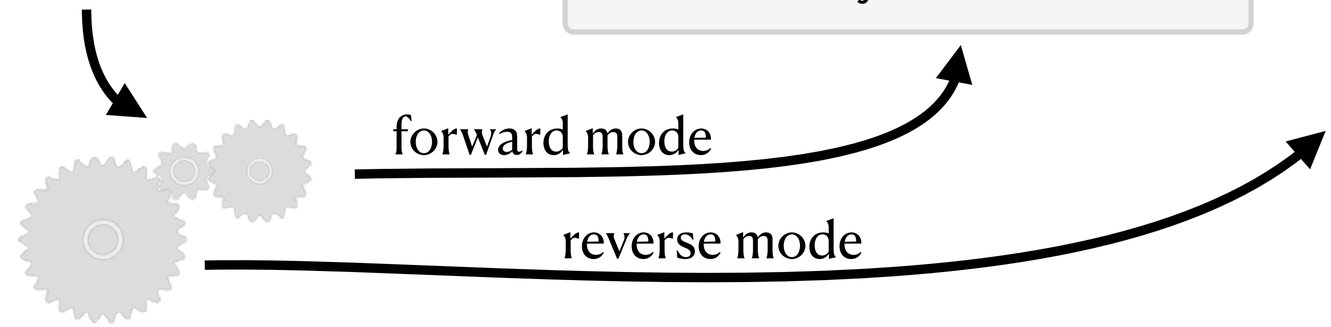
```
δe  = 1
```

Reverse mode

Strategy 3: AD by code transformation

(One can of course also do this by hand, but computer assistance is helpful.)

```python
def pow(x: float, n: int):
    y = 1
    for i in range(n):
        y *= x
    return y
```



AD Compiler

```python
def pow_jvp(x, n, dx):
    y, dy = 1, 0
    for i in range(n):
        dy = x*dy + y*dx
        y *= x
    return dy
```

```python
def pow_vjp(x, n, dy):
    y, dx = 1, 0
    stack = []
    for i in range(n):
        stack.append(y)
        y *= x
    for i in reversed(range(n)):
        y = stack.pop()
        dx += y*dy
        dy *= x
    return dx
```

Technique tree

Forward mode

Use when the function has **few inputs** and **many outputs**, and if you want the derivative wrt. all outputs at once.

Reverse mode

Use when the function has **few outputs** and **many inputs**, and if you want the derivative wrt. all inputs at once.

AD Implementation strategies

Dual numbers

Simple and efficient.

Tape

Simple, but inefficient (memory usage).

Code transformation / by hand

Complicated, ends up being effectively the same as dual numbers.

Dual numbers

Does not make sense for reverse mode.

Tape

What everyone uses in practice.

Code transformation / by hand

Promising but not widely used.

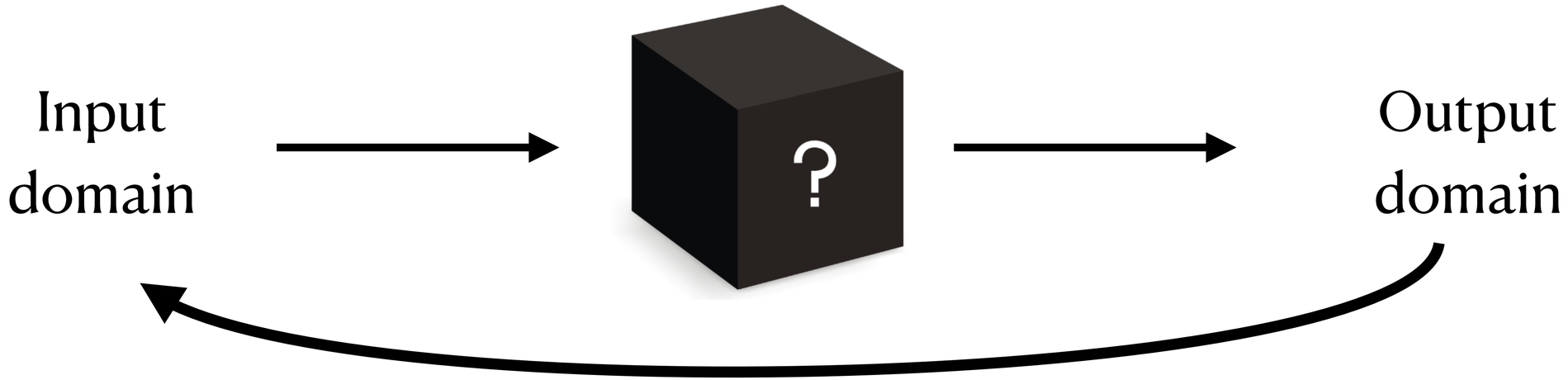
We have gradients.

Now, what?

"Inverse problems"

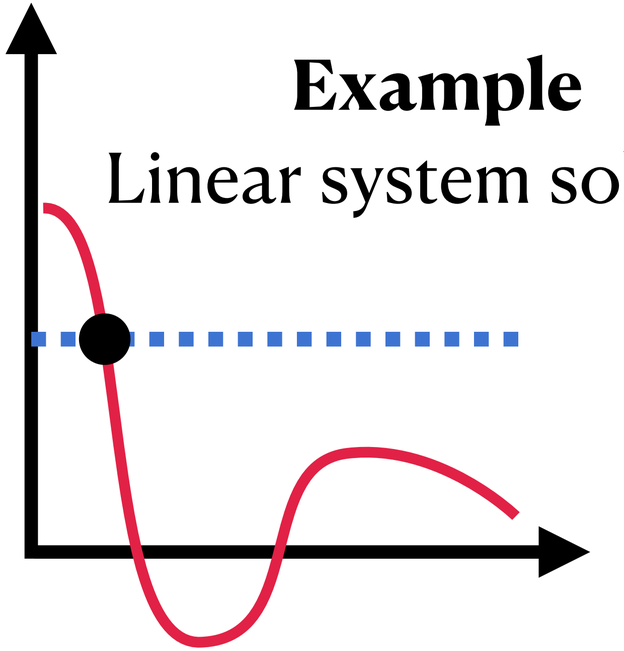
Previously, f was a linear function, which was very useful. But what if it isn't?

$$f(\mathbf{x})$$

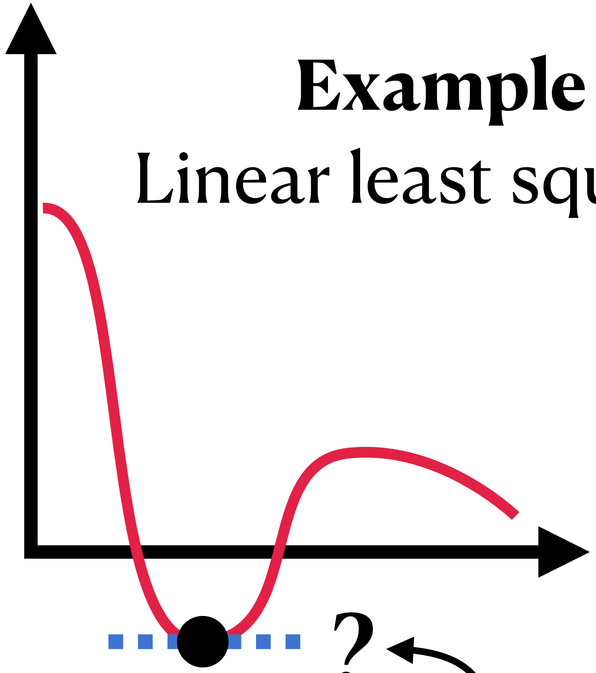


$$f^{-1}(\mathbf{x}) \quad ?$$

Two important kinds of inverse problems



Example
Linear system solving



Example
Linear least squares

?

minimum Y value unknown, so this isn't exactly the same as root finding

Conversion:
normal equations

problems can often be converted

Root finding ⟷ Optimization

Root finding

Let's start with a simple 1D problem

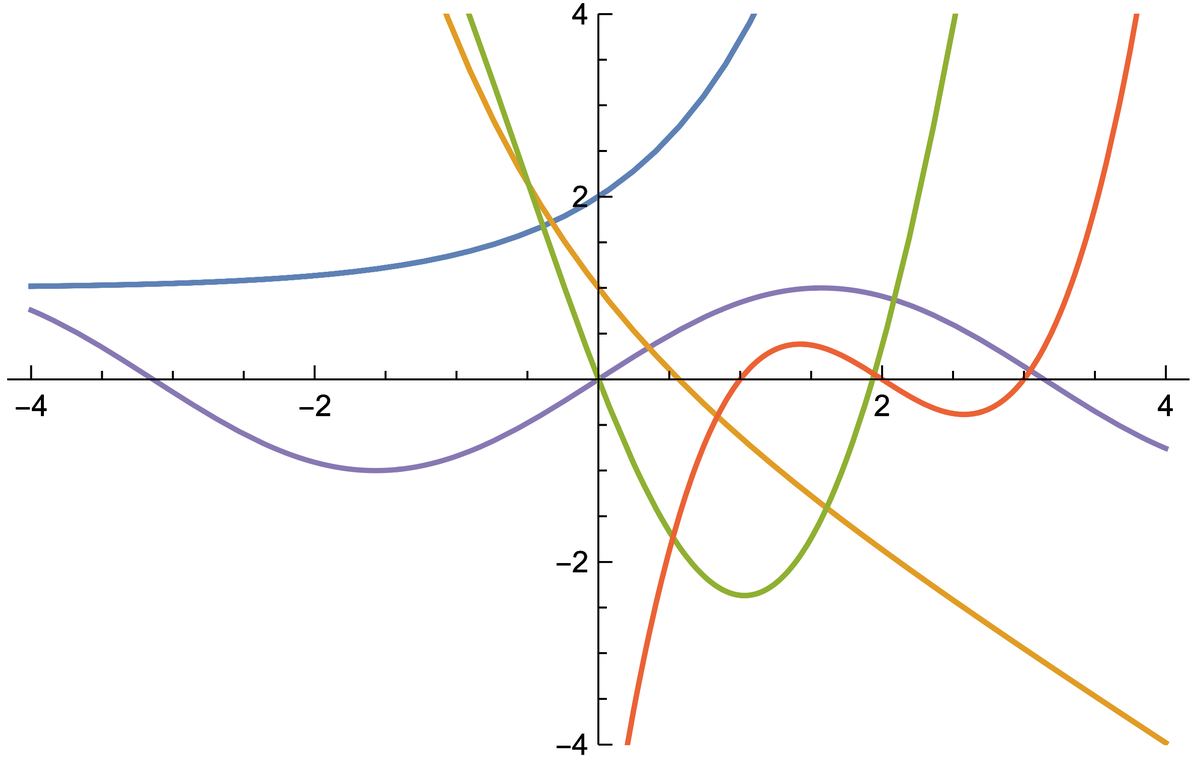
$$f : \mathbb{R} \to \mathbb{R}$$

Find x so that $f(x) = 0$.

How many solutions?

Linear systems have 0, 1, or ∞ solutions. Anything possible in the nonlinear case

- A few examples from [Heath 2002]:
  - $\exp(x) + 1 = 0$
  - $\exp(-x) - x = 0$
  - $x^2 - 4\sin(x) = 0$
  - $x^3 - 6x^2 + 11x - 6 = 0$
  - $\sin(x) = 0$



"Evil functions"

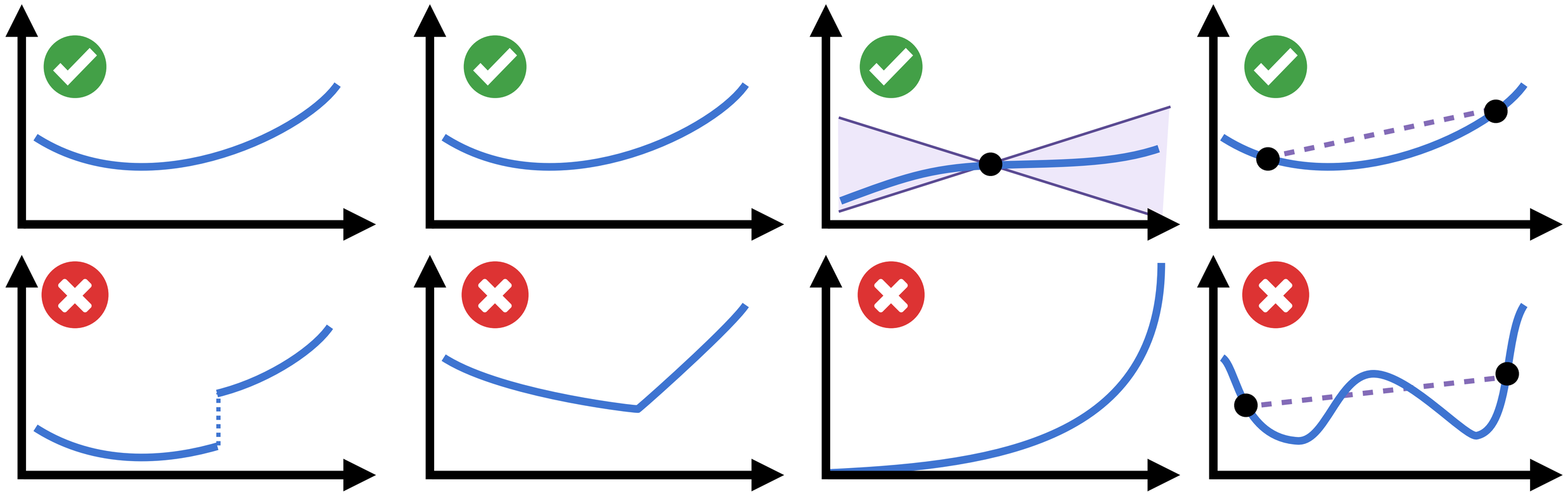
All sorts of things could be lurking inside. How are we expected to deal with such functions?

$$f_1(x) := \begin{cases} 1, & x \in \mathbb{Q} \\ -1, & x \in \mathbb{R} \setminus \mathbb{Q} \end{cases}$$

$$f_2(x) := \begin{cases} 1, & x \neq 0.13525634 \\ 0, & x = 0.13525634 \end{cases}$$

Common assumptions

Must assume *something*. This determines how the solution algorithm will work.



Continuity | **Differentiability** | ***Lipschitz* continuity** | **Convexity**

Actually: kinks usually OK, we mainly need the ability to *evaluate* derivatives.

Mostly used for optimization.

A model problem

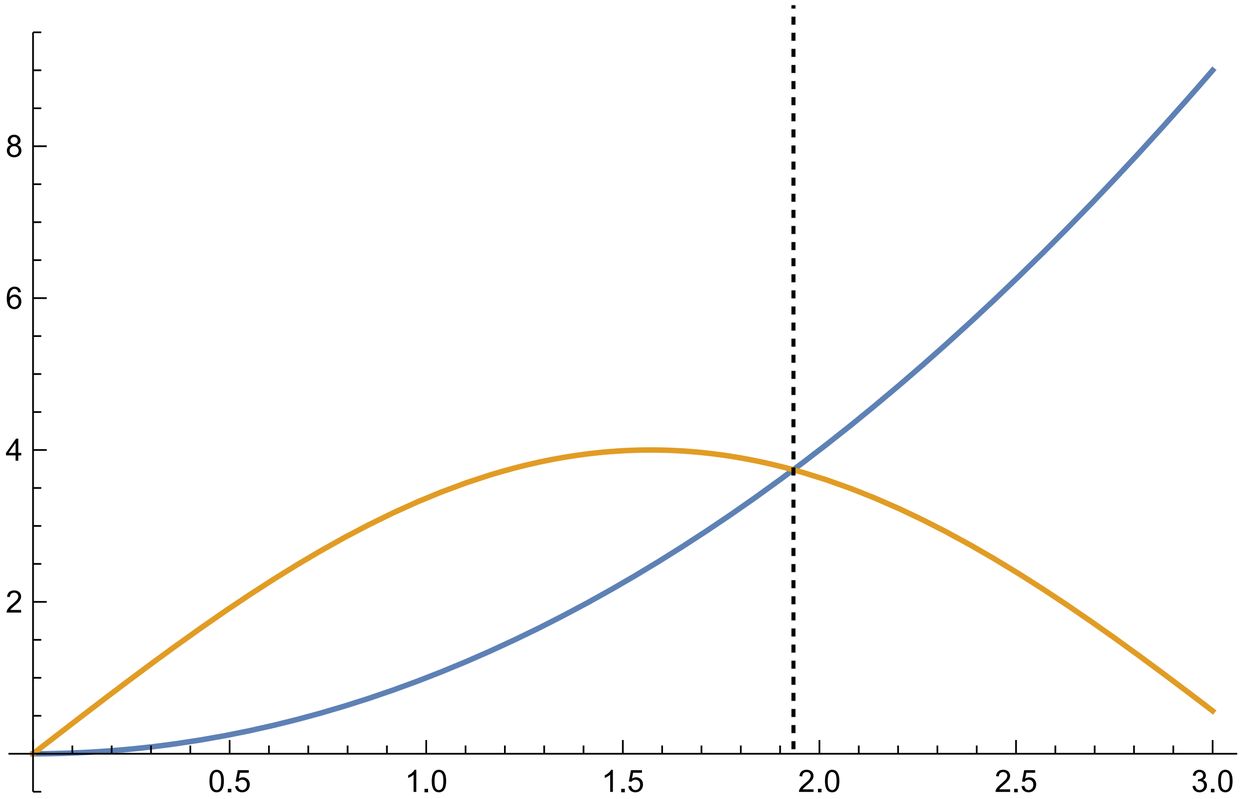
Mathematica:

```
In[1]:= Solve[x^2 == 4 Sin[x], x]
```

Solve: This system cannot be solved with the methods available to Solve.

$$x^2 = 4 \sin x$$

Solution is not analytic!

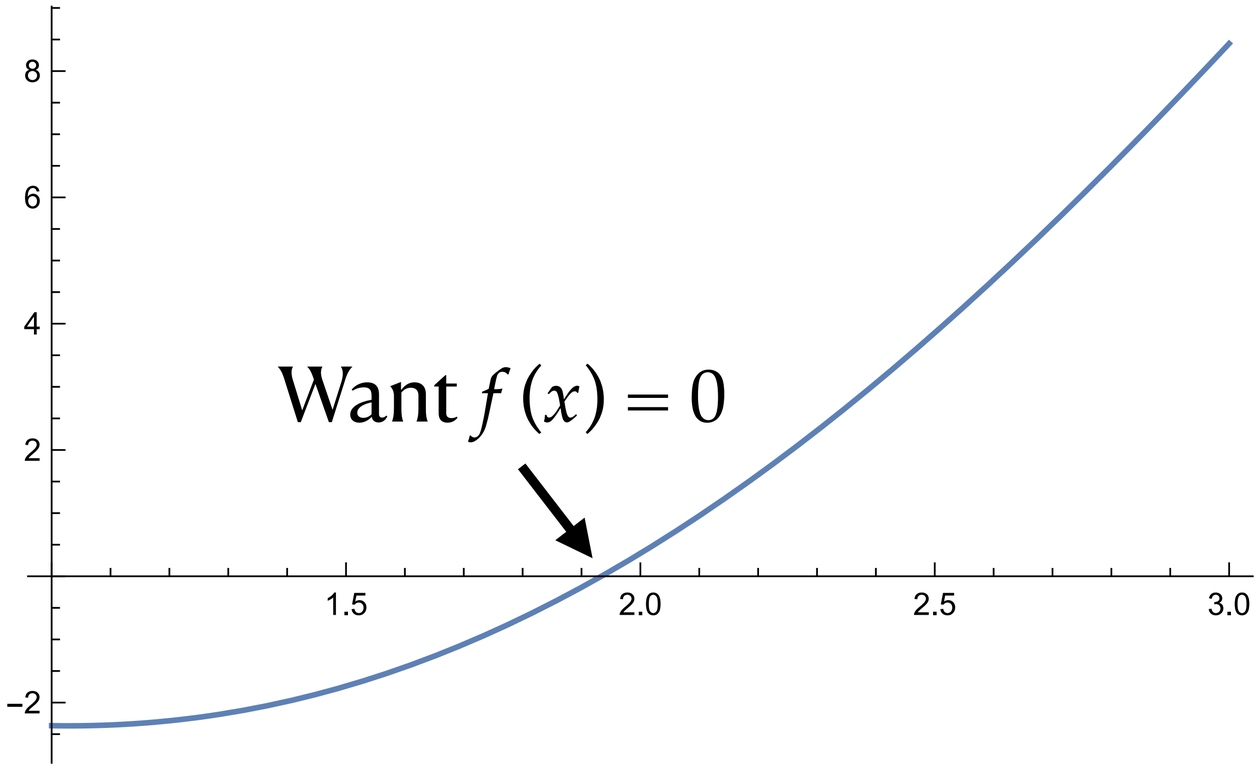


A model problem

Can more or less read off solution from graph, *how difficult can it be?*

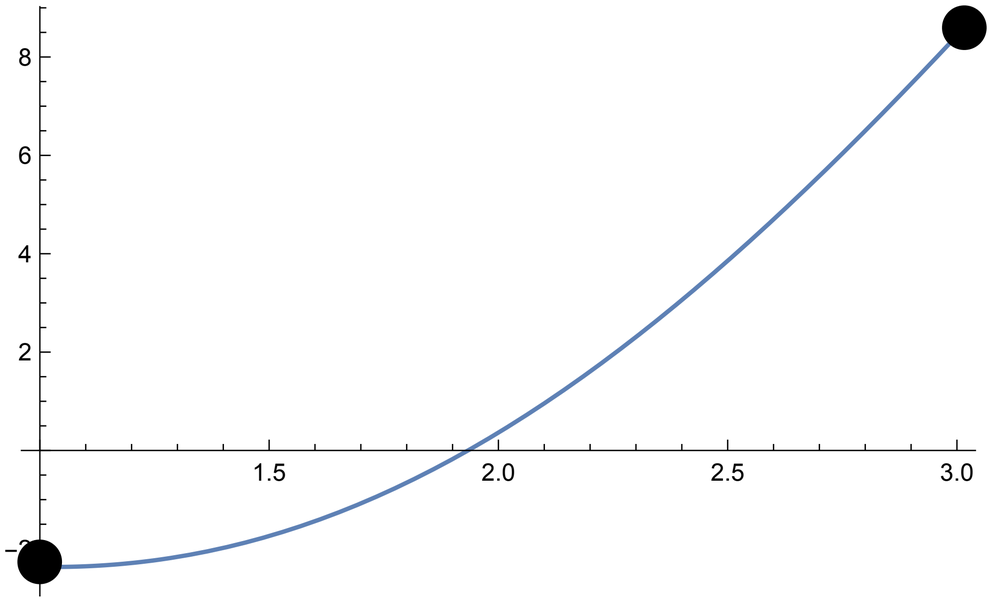
$$f(x) := x^2 - 4\sin x$$

*Plot required thousands of function evaluations, each one is potentially **very expensive** (evaluating $f(x)$ once: test a new drug compound on patients, build a rocket and collect a sample on Mars.)*



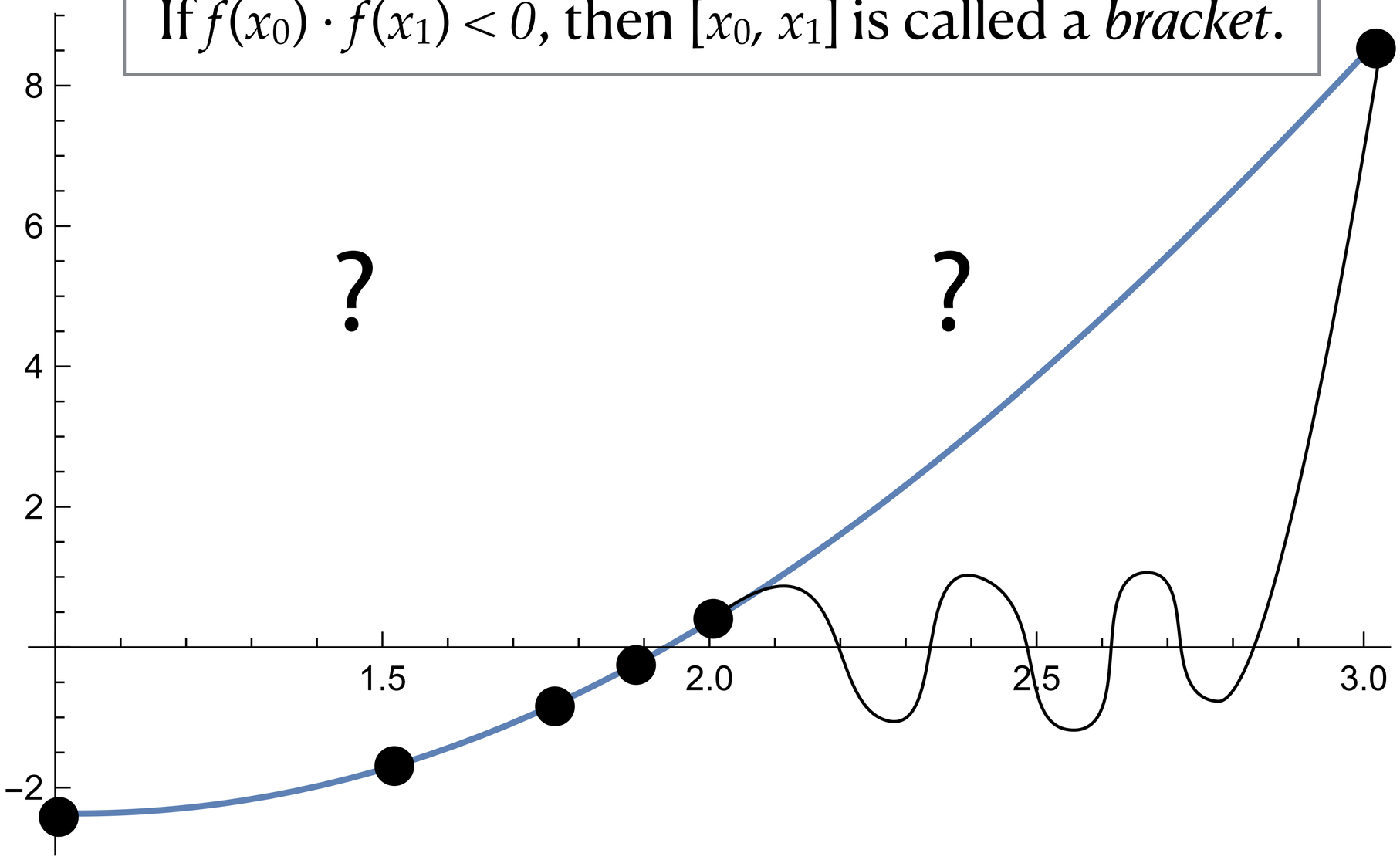
Intermediate Value Theorem

If f is continuous and $f(x_0) = y_0$, $f(x_1) = y_1$,
then $f(x)$ on (x_0, x_1) must pass through
<u>every</u> value between y_0 and y_1.



Use of continuity in our model problem

If $f(x_0) \cdot f(x_1) < 0$, then $[x_0, x_1]$ is called a *bracket*.



Bisection search

function *"bracket"* *stopping criterion thresholds*

```
def bisect(f, l, r, eps1, eps2):
    while True:
        m = l + (r - l) / 2

        if np.abs(f(m)) < eps1 or np.abs(l - r) < eps2:
            return m

        if f(l) * f(m) < 0:
            r = m
        else
            l = m
```

Does not use function values!

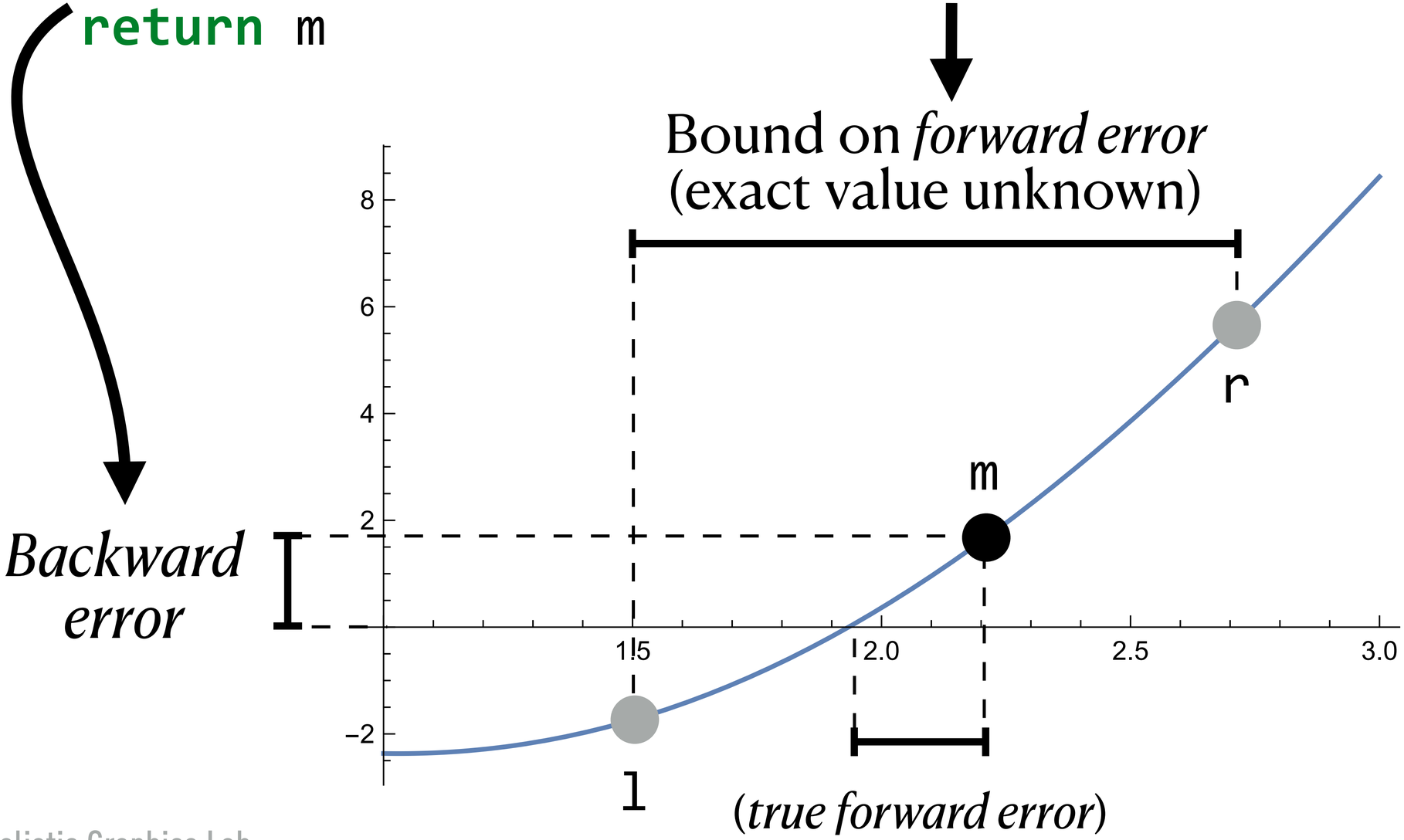
(only their sign is relevant)

Is this code optimal?

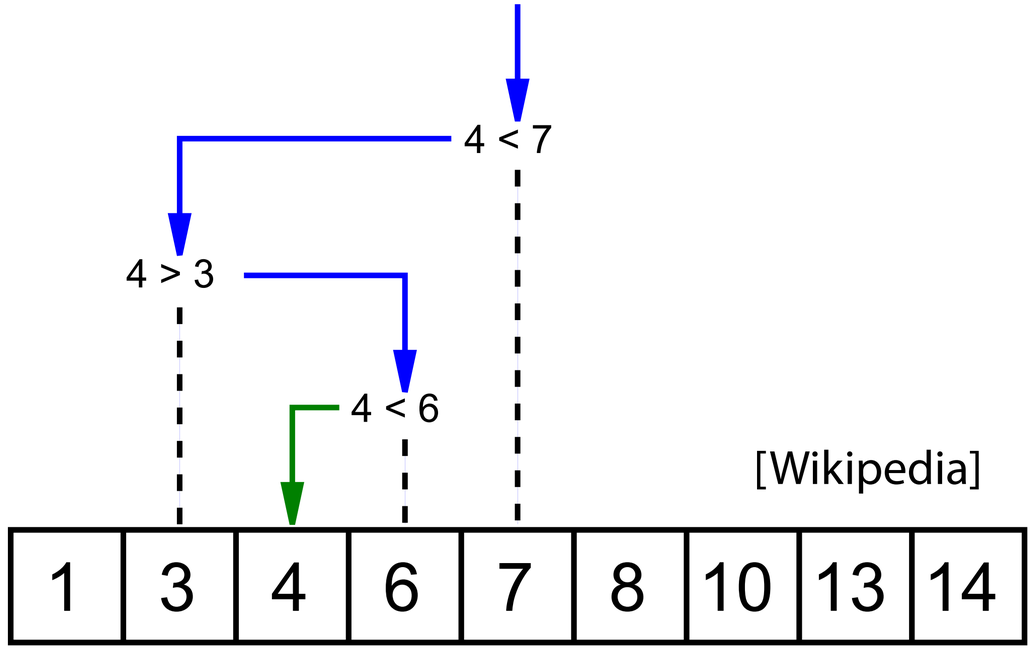
No, it could be implemented with ~1/3 the number of *f*-evaluations.

Stopping criteria for nonlinear methods

```
if np.abs(f(m)) < eps₁ or np.abs(l - r) < eps₂:
    return m
```



Does this seem at all familiar?



Binary search for 4 in sorted list.

Complexity of (discrete) algorithm: $O(\log n)$

Can we find an analogy of "*complexity*" for root finding?

Order and rate of convergence

Suppose that we can find numbers o and r so that

$$\lim_{k \to \infty} \frac{E_{k+1}}{E_k^o} = r.$$

where E_k is the error after iteration k, then:

- o is called the **order of convergence**, which tells us how quickly the algorithm convergences.
  - $o = 1$: linear convergence, $o = 2$: quadratic convergence, etc.
- r is called the **rate of convergence**. It distinguishes convergence speed of algorithms with the same order.

Convergence order and rate of bisection

Error bound (before 1st iteration) : $r - l$

Error bound (after 1st iteration) : $(r - l) / 2$

Generally: $E_{k+1} = \frac{1}{2} E_k \Leftrightarrow \frac{E_{k+1}}{E_k^1} = \frac{1}{2}$

In other words: **order** of convergence = 1 (*linear*)
rate of convergence = 1 / 2

A method with a **linear order of convergence** gains a fixed number of accurate digits per iteration (depending on **rate**). Here:

- 1 base-2 digit every iteration. 1 base-10 digit every $\frac{\log 10}{\log 2} \approx 3$ iterations.

Convergence speed of bisection

Let's apply bisection to the root-finding example function with

$$f(x) := x^2 - 4\sin x$$

Here, *l* and *r* denote the bracket; the solution lies in between.

l	$f(l)$	r	$f(r)$
1.000000	−2.365884	3.000000	8.435520
1.000000	−2.365884	2.000000	0.362810
1.500000	−1.739980	2.000000	0.362810
1.750000	−0.873444	2.000000	0.362810
1.875000	−0.300718	2.000000	0.362810
1.875000	−0.300718	1.937500	0.019849
1.906250	−0.143255	1.937500	0.019849
1.921875	−0.062406	1.937500	0.019849
1.929688	−0.021454	1.937500	0.019849

l	$f(l)$	r	$f(r)$
1.933594	−0.000846	1.937500	0.019849
1.933594	−0.000846	1.935547	0.009491
1.933594	−0.000846	1.934570	0.004320
1.933594	−0.000846	1.934082	0.001736

[Heath]

Midpoint = **1.933**838

True solution = 1.9337537628..

(13 iterations for ~4 digits)

Newton's method

- Based on first-order Taylor expansion:

$$f(x+h) \approx f(x) + f'(x)h$$

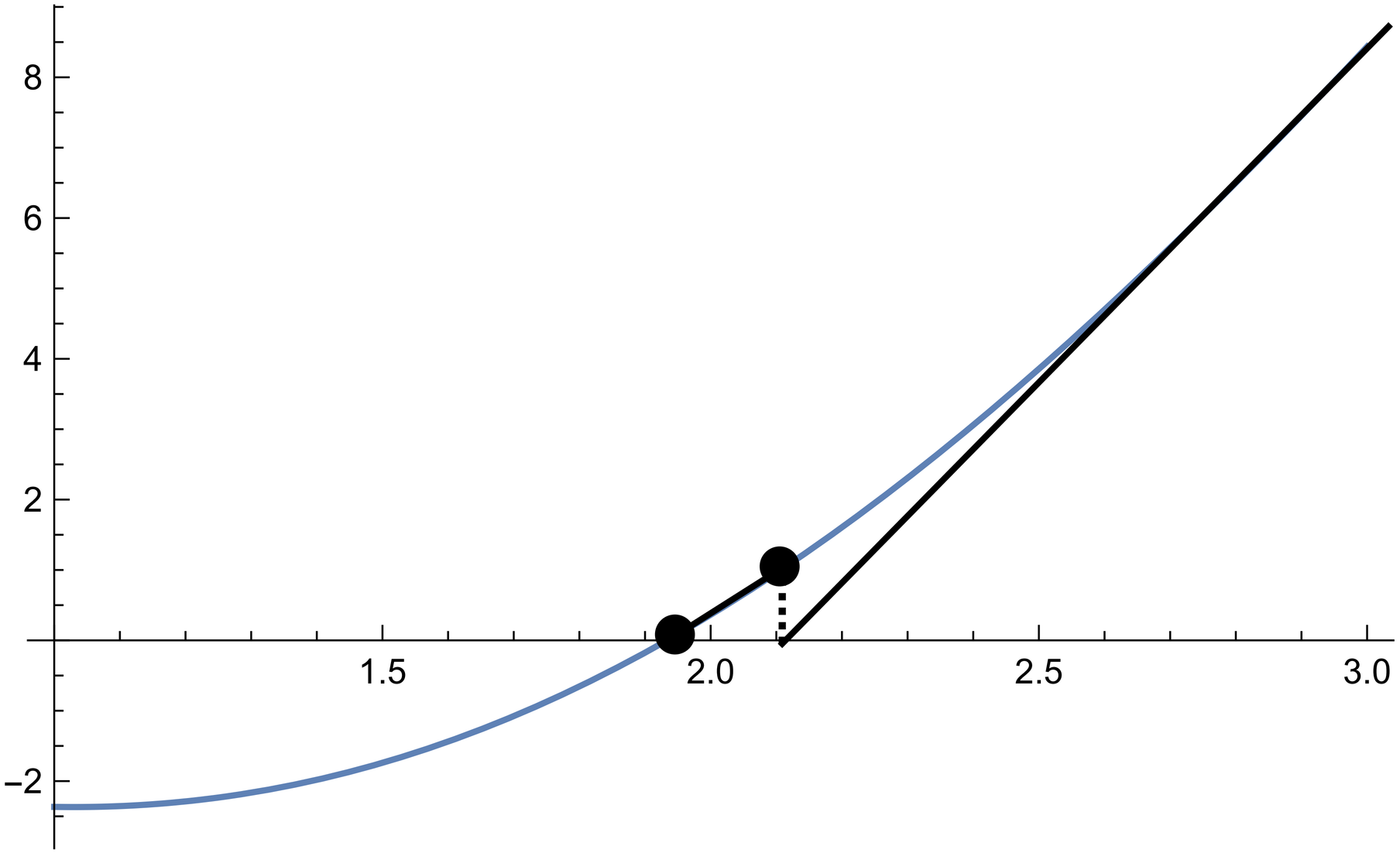
- Let's set this approximation to zero and solve for h.

$$f(x+h) = 0 \Leftrightarrow h = -\frac{f(x)}{f'(x)}$$

- Move to that position, and repeat..

$$x_k = x_{k-1} - \frac{f(x_{k-1})}{f'(x_{k-1})}$$

Visualization of Newton's method



Convergence of Newton's method

x	$f(x) := x^2 - 4\sin x$	$f'(x) := 2x - 4\cos x$	h
3.000000	8.435520	9.959970	−0.846942
2.153058	1.294772	6.505771	−0.199019
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(5 iterations for ~7 digits)

[Heath]

The method has a quadratic order of convergence, meaning that the number of valid digits approximately **doubles** per iteration.

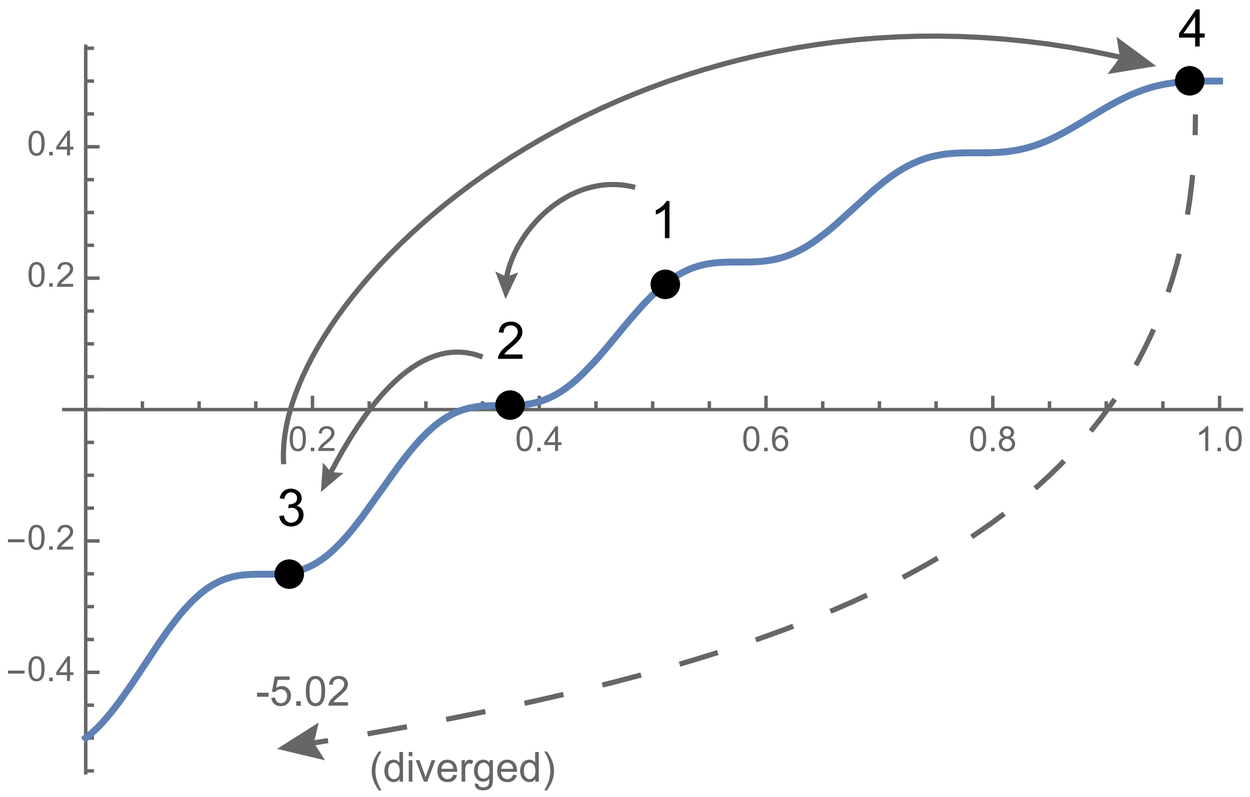
1D Root Finding: Pros/Cons

Property	Bisection	Newton's method
Speed	😞 Slow	😊 Extremely fast (only a few iterations once we're sufficiently close to root)
Reliability	😊 Always works	😞 Divergence, multiple roots, …
Requirements	😐 Continuity, bracket	😐 Derivative

Can combine both: Newton-Bisection

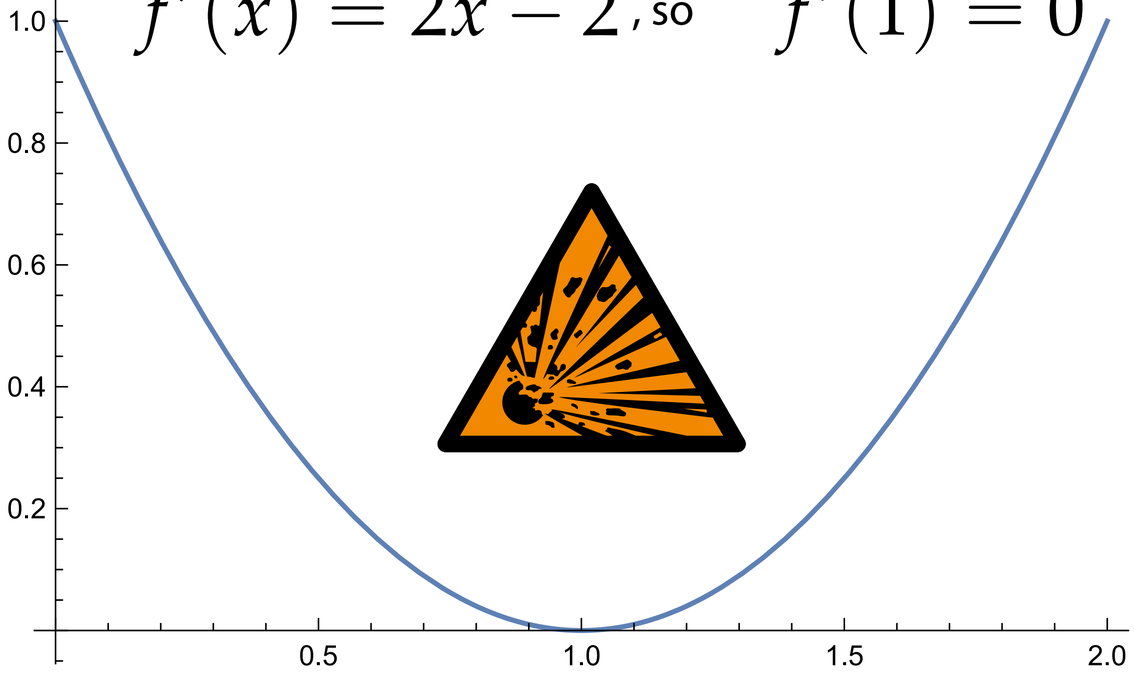
Speed	Reliability	Requirements
😊 Extremely fast	😊 Always works	😬 Continuity, bracket, derivatives

Failure cases of Newton's Method



$$f(x) = (x-1)^2$$

$$f'(x) = 2x - 2\text{, so} \quad f'(1) = 0$$



In theory: division by zero at $x = 1$.

In practice: slow convergence.

N dimensions

Multivariate root finding

$$f : \mathbb{R}^n \rightarrow \mathbb{R}^n$$

Find $\mathbf{x}$ so that $f(\mathbf{x}) = \mathbf{0}$.

High dimensional spaces

- Derivative are crucial especially in **higher dimensions**.
  - In 1-D, can move in two directions
  - in N-D can move in 2^N "diagonal" directions alone. That's just *too many* to check.
  - The gradient points into the direction of ascent and maps the behavior of the function locally.
  - Foundation of all breakthroughts in ML in the last years. You *cannot* train a neural network without gradients.

MidJourney: A sign post with many different hikes in Switzerland.

Newton's method for root finding in N dimensions

This algorithm trivially genaralizes

1D case: $f(x+h) \approx f(x) + f'(x)h = 0$

$$x_k = x_{k-1} - \frac{f(x_{k-1})}{f'(x_{k-1})}$$

N-D case: $\mathbf{f}(\mathbf{x}+\mathbf{h}) \approx \mathbf{f}(\mathbf{x}_{k-1}) + \nabla\mathbf{f}(\mathbf{x}_{k-1})\mathbf{h} = 0$

$$\mathbf{x}_k = \mathbf{x}_{k-1} - \left[\nabla\mathbf{f}(\mathbf{x}_{k-1})\right]^{-1}\mathbf{f}(\mathbf{x}_{k-1})$$

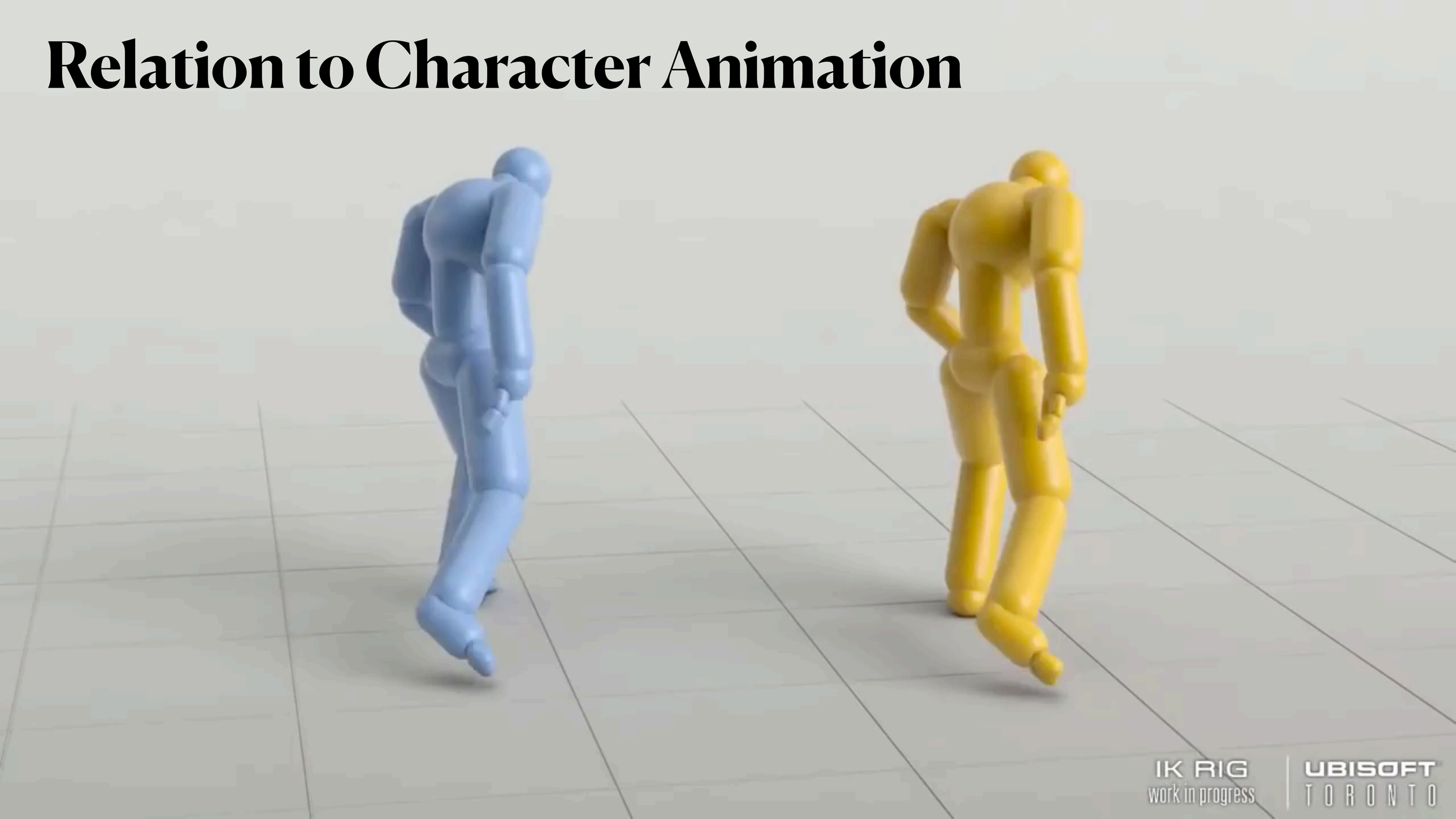
Newton's method for root finding in N dimensions

$$\mathbf{x}_k = \mathbf{x}_{k-1} - \left[\nabla \mathbf{f}(\mathbf{x}_{k-1})\right]^{-1} \mathbf{f}(\mathbf{x}_{k-1})$$

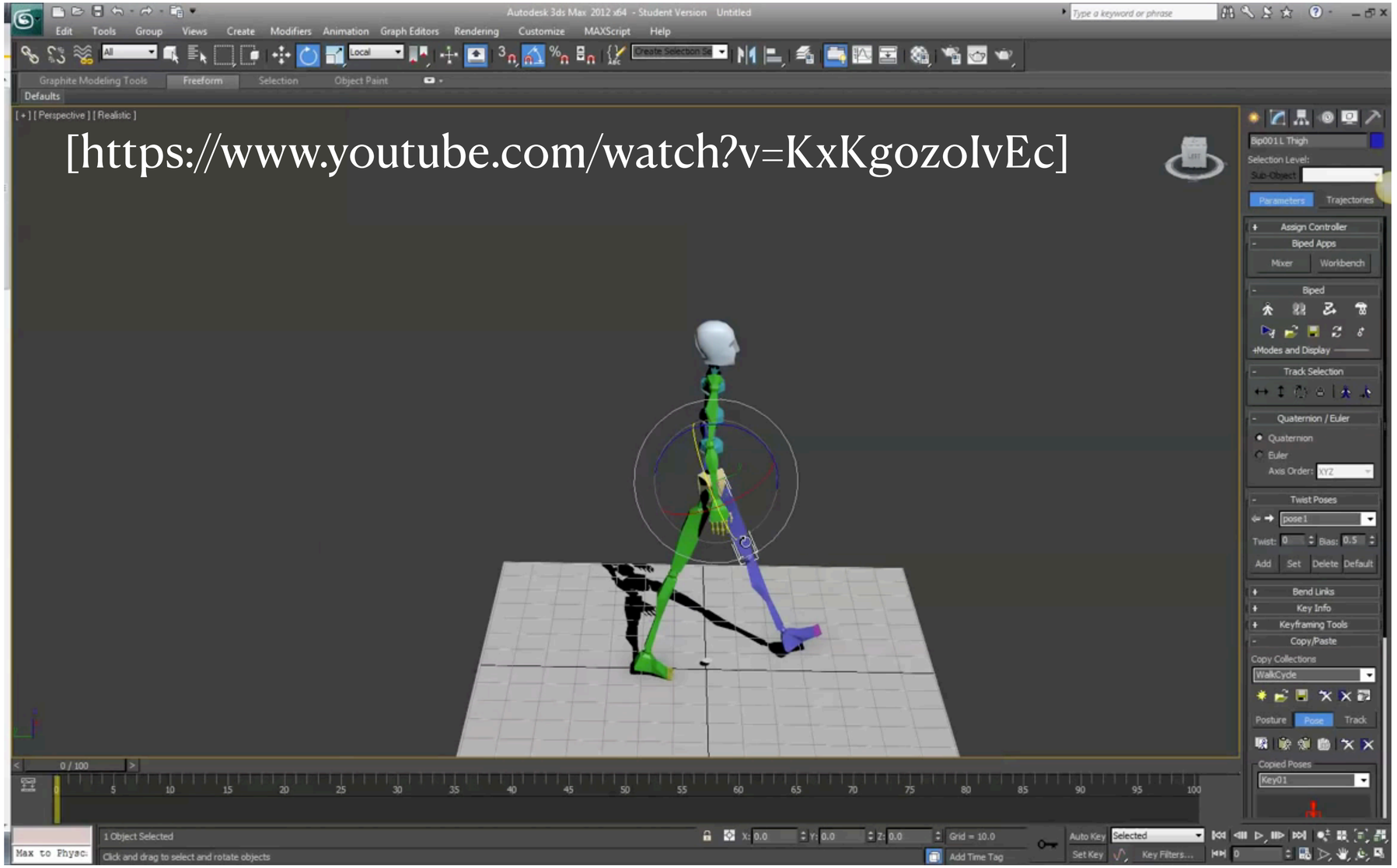
Advantages and disadvantages:

- Rapid quadratic convergence, but may diverge..
- No simple+safe hybrid method (e.g. Newton-Bisection) in N-D.
- Need to compute Jacobian & solve linear system:
  requires $O(n^3)$ operations *per iteration!!*
  - Linear system solve could fail (ill-conditioned/singular. More dimensions in which things can go wrong..)
  - Assumes input and output spaces have matching dimension.

Relation to Character Animation

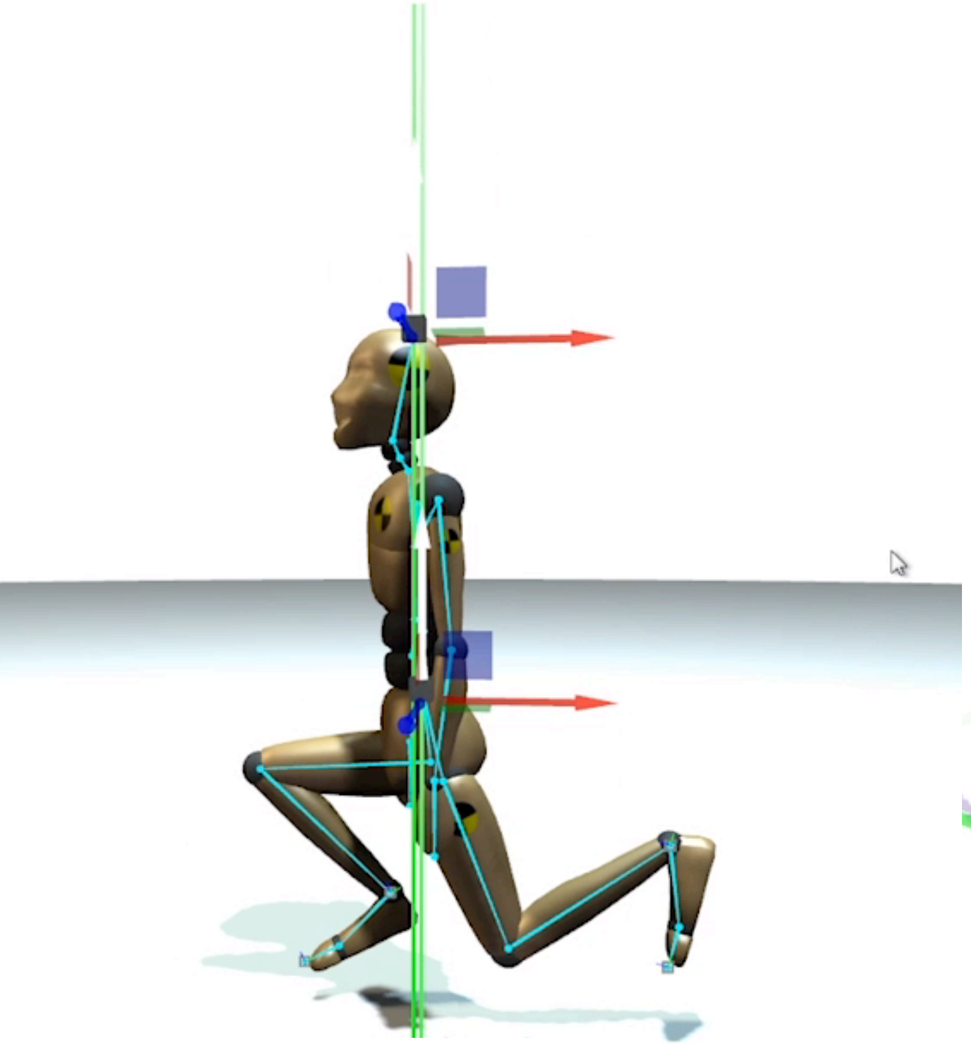


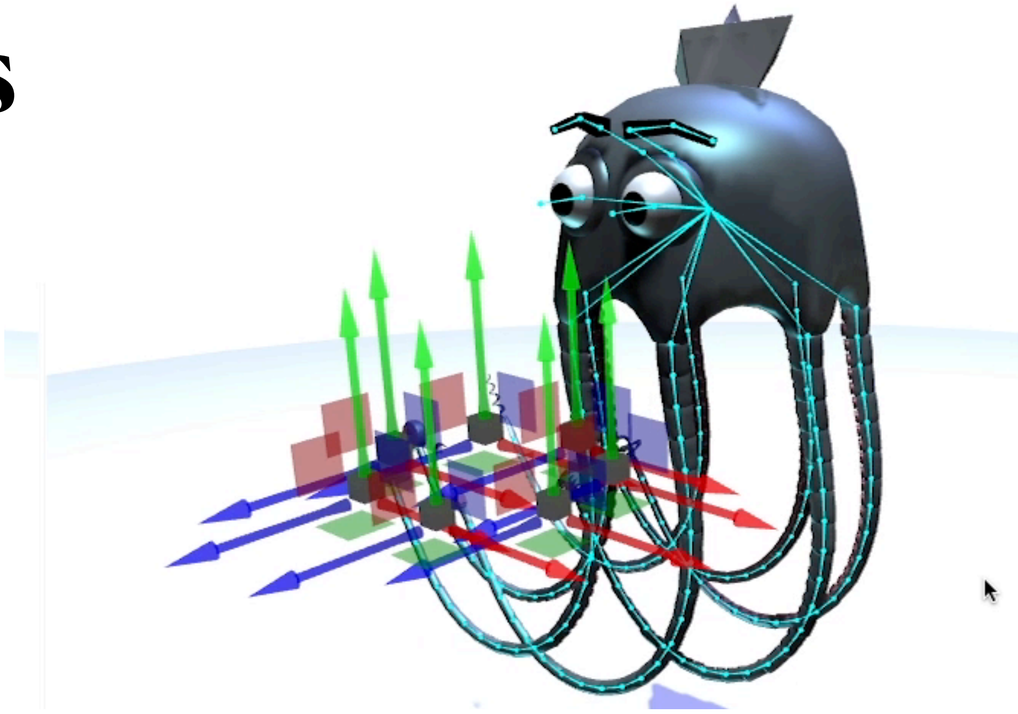
Connection to Character Animation



Inverse Kinematics

[Harish et al. 2016, EPFL]



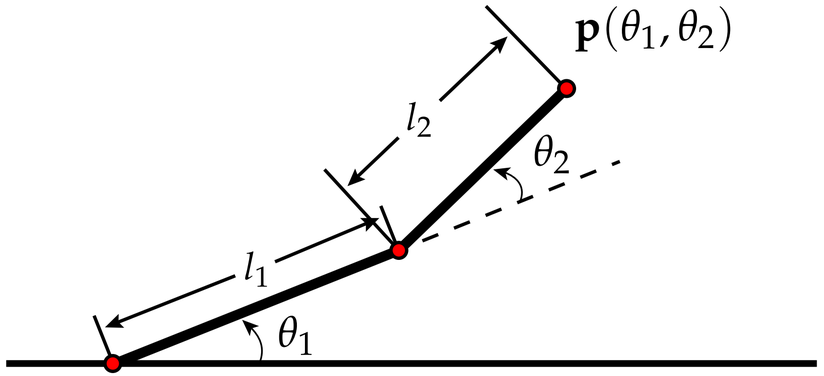


Inverse Kinematics via Newton's method

n unknowns

$$\mathbf{p}(\theta_1, \theta_2, \theta_3, \ldots, \theta_n) = \mathbf{p}_{\text{target}}$$

2 equations



Idea: solve with Newton's method

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} - [\nabla \mathbf{p}(\boldsymbol{\theta}_{k-1})]^{-1} \mathbf{p}(\boldsymbol{\theta}_{k-1})$$

Idea 2: solve with Newton's method + pseudoinverse

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} - [\nabla \mathbf{p}(\boldsymbol{\theta}_{k-1})]^{+} \mathbf{p}(\boldsymbol{\theta}_{k-1})$$

Root finding

Let's start with a simple 1D problem

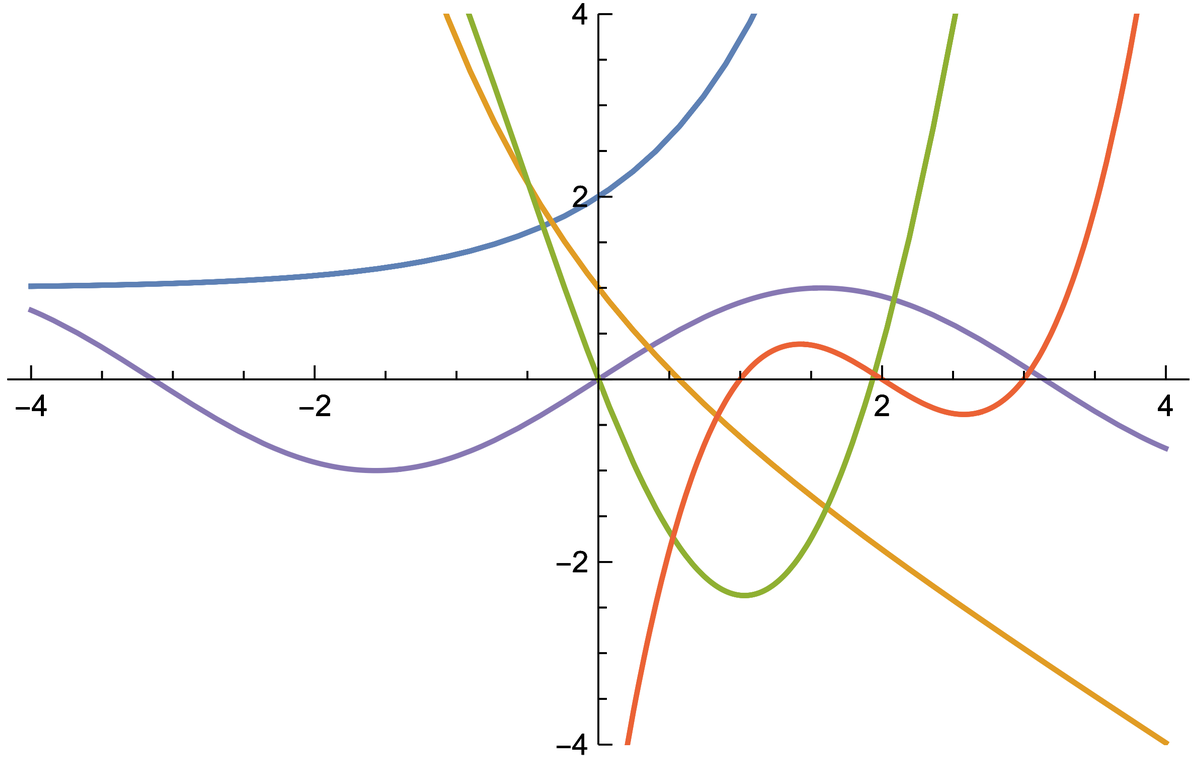
$$f : \mathbb{R} \rightarrow \mathbb{R}$$

Find x so that $f(x) = 0$.

How many solutions?

Linear systems have 0, 1, or ∞ solutions. Anything possible in the nonlinear case

- A few examples from [Heath 2002]:
  - $\exp(x) + 1 = 0$
  - $\exp(-x) - x = 0$
  - $x^2 - 4\sin(x) = 0$
  - $x^3 - 6x^2 + 11x - 6 = 0$
  - $\sin(x) = 0$



"Evil functions"

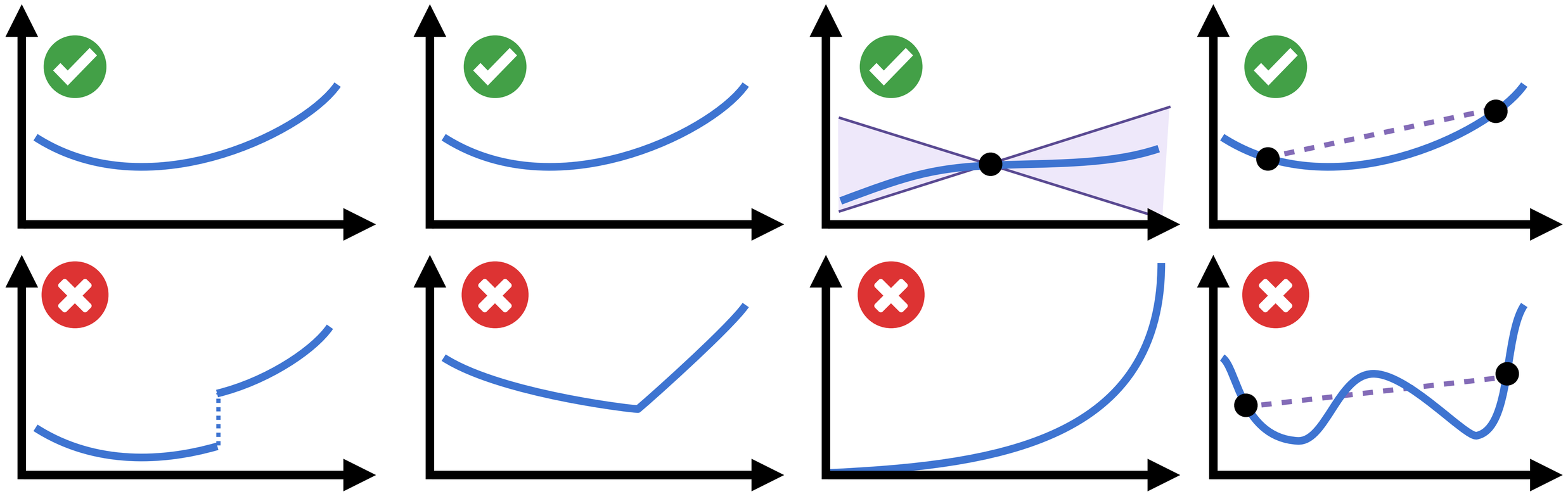
All sorts of things could be lurking inside. How are we expected to deal with such functions?

$$f_1(x) := \begin{cases} 1, & x \in \mathbb{Q} \\ -1, & x \in \mathbb{R} \setminus \mathbb{Q} \end{cases}$$

$$f_2(x) := \begin{cases} 1, & x \neq 0.13525634 \\ 0, & x = 0.13525634 \end{cases}$$

Common assumptions

Must assume *something*. This determines how the solution algorithm will work.



Continuity | **Differentiability** | ***Lipschitz* continuity** | **Convexity**

Actually: kinks usually OK, we mainly need the ability to *evaluate* derivatives.

Mostly used for optimization.

A model problem

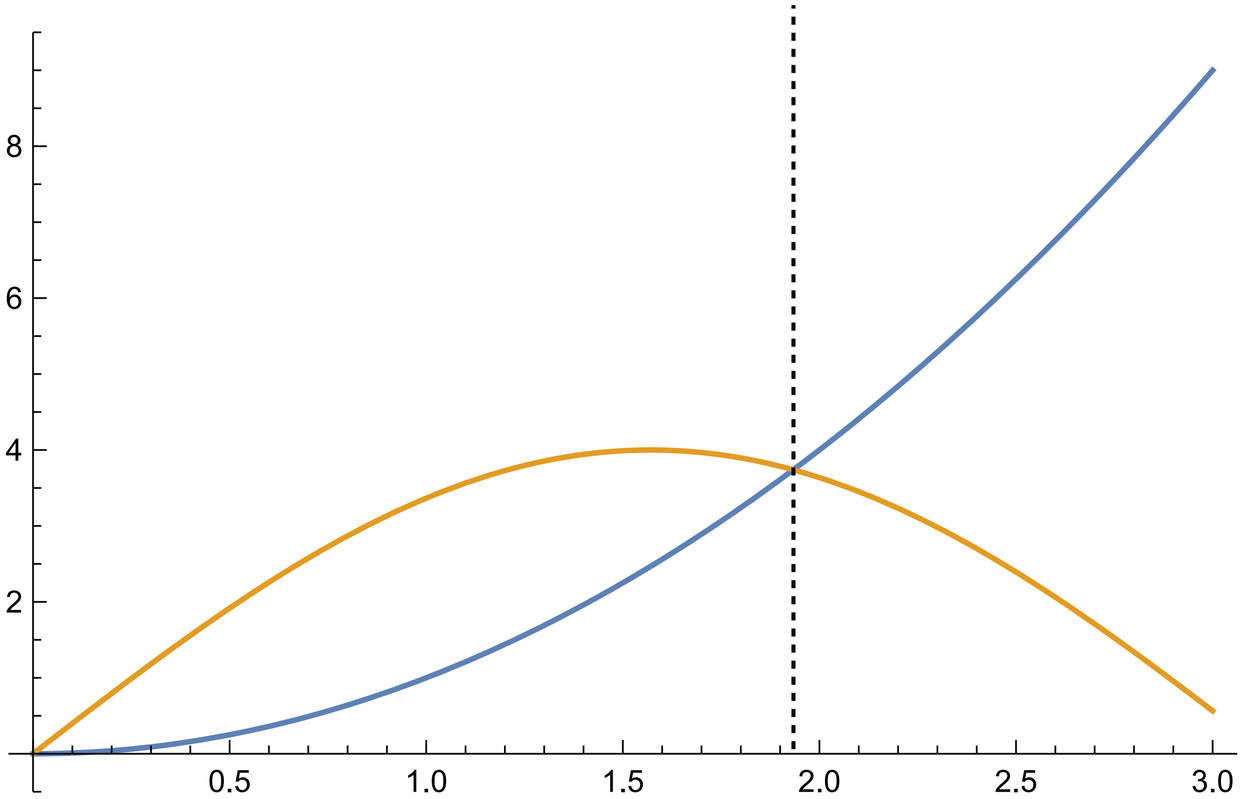
Mathematica:

```
In[1]:= Solve[x^2 == 4 Sin[x], x]
```

Solve: This system cannot be solved with the methods available to Solve.

$$x^2 = 4 \sin x$$

Solution is not analytic!

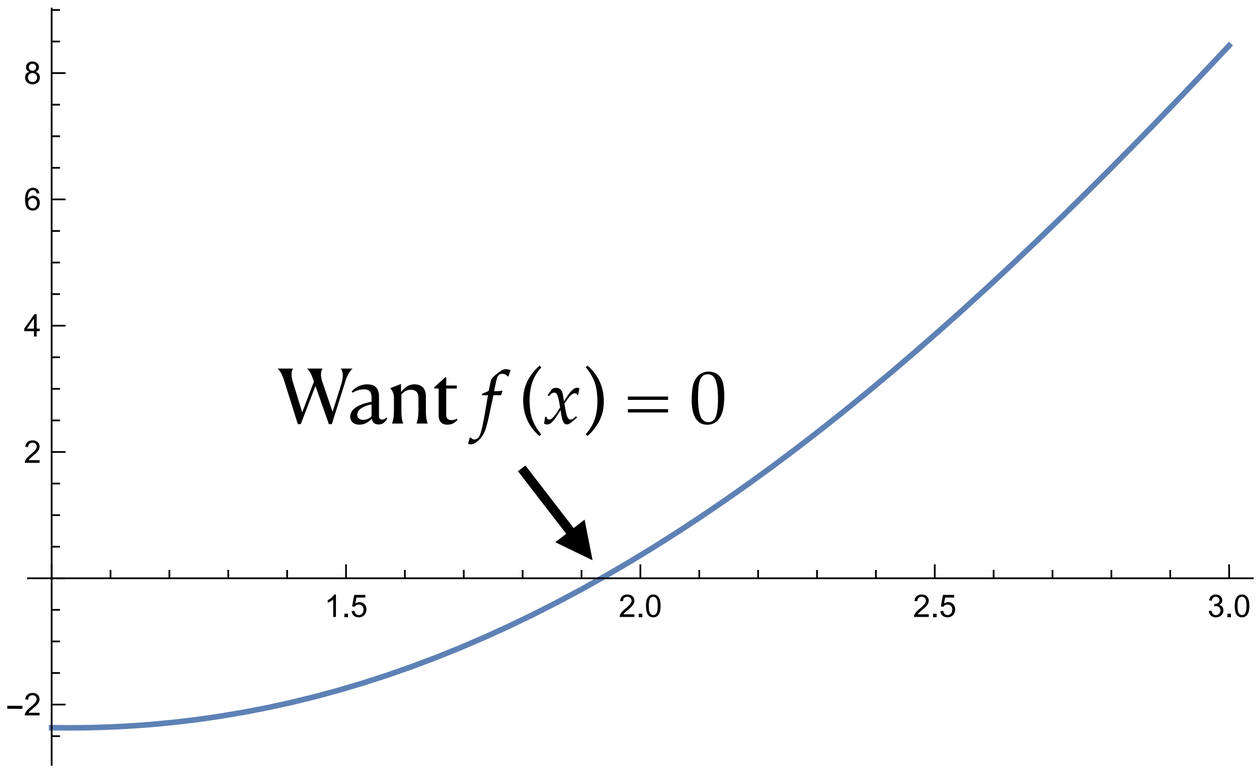


A model problem

Can more or less read off solution from graph, *how difficult can it be?*

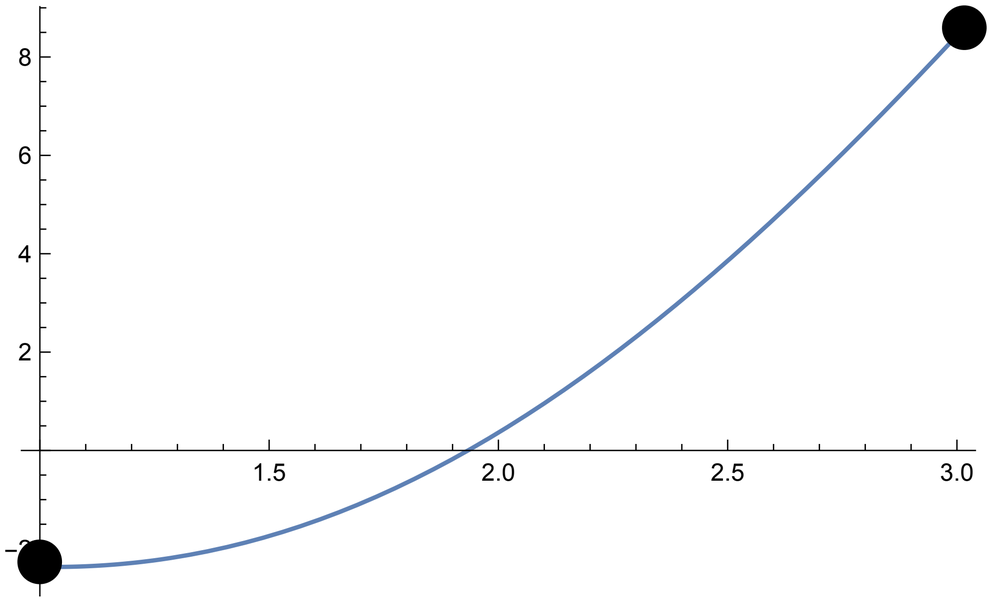
$$f(x) := x^2 - 4\sin x$$

*Plot required thousands of function evaluations, each one is potentially **very expensive** (evaluating $f(x)$ once: test a new drug compound on patients, build a rocket and collect a sample on Mars.)*



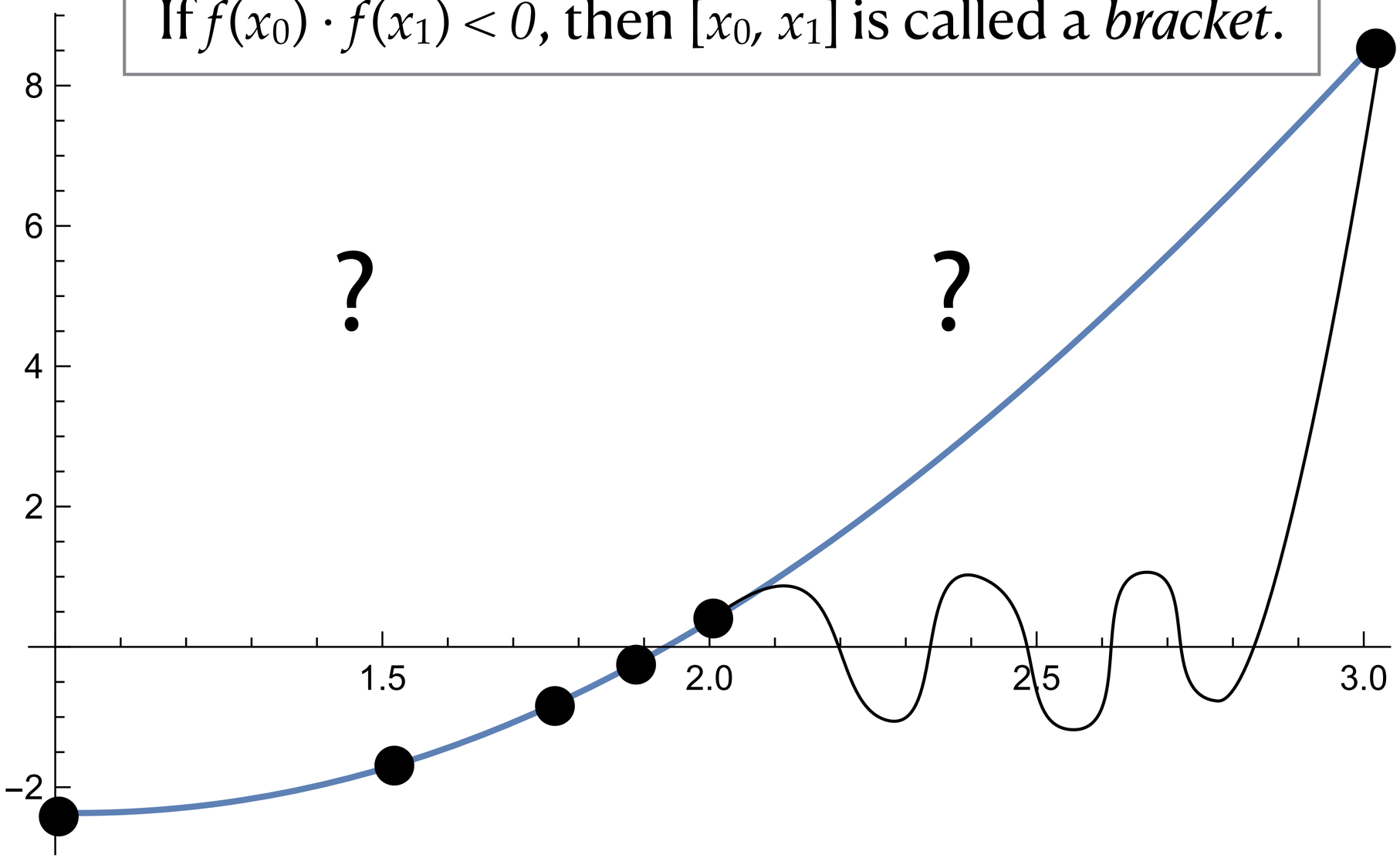
Intermediate Value Theorem

If f is continuous and $f(x_0) = y_0$, $f(x_1) = y_1$,
then $f(x)$ on (x_0, x_1) must pass through
<u>every</u> value between y_0 and y_1.



Use of continuity in our model problem

If $f(x_0) \cdot f(x_1) < 0$, then $[x_0, x_1]$ is called a *bracket*.



Bisection search

function *"bracket"* *stopping criterion thresholds*

```
def bisect(f, l, r, eps1, eps2):
    while True:
        m = l + (r - l) / 2

        if np.abs(f(m)) < eps1 or np.abs(l - r) < eps2:
            return m

        if f(l) * f(m) < 0:
            r = m
        else
            l = m
```

Does not use function values!

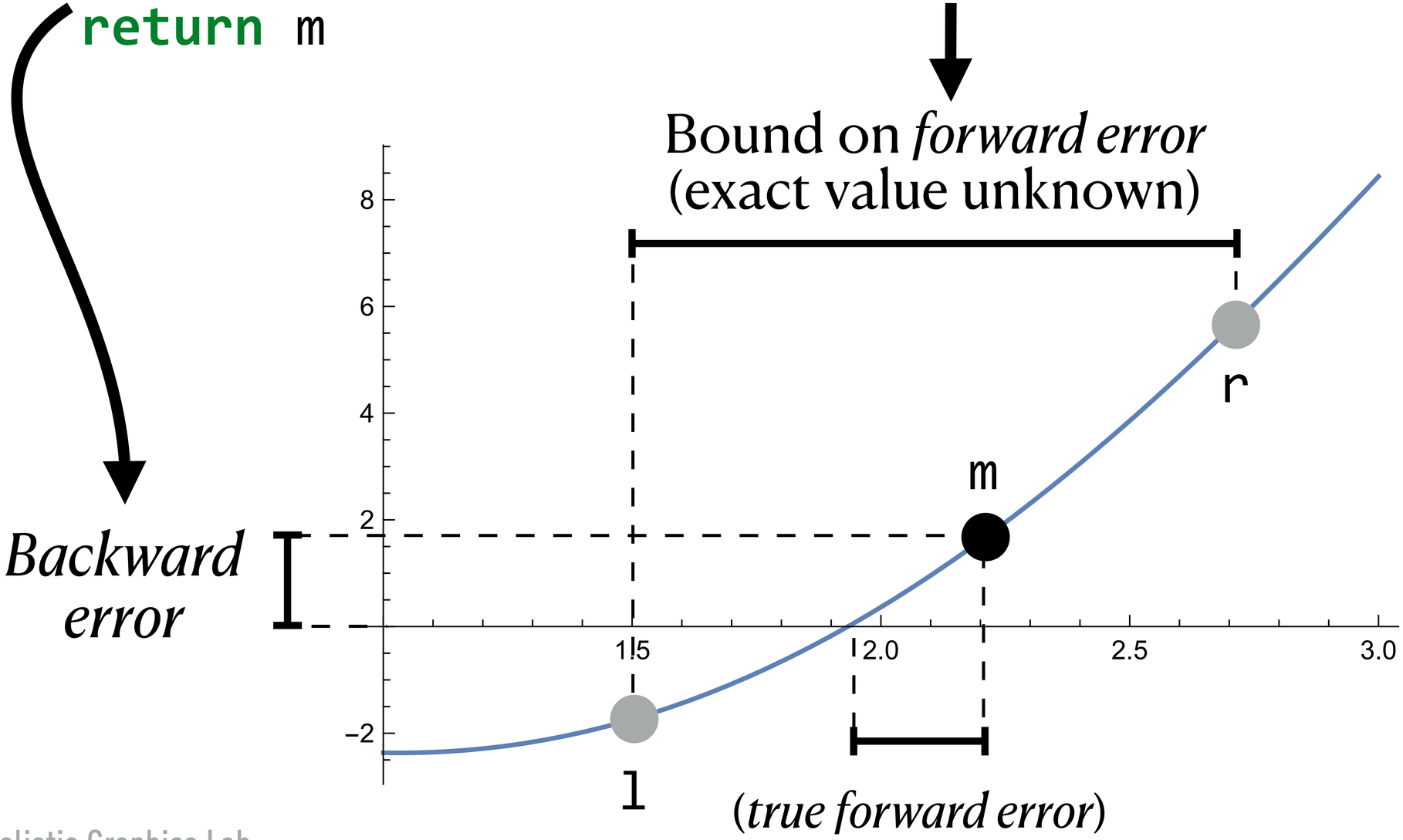
(only their sign is relevant)

Is this code optimal?

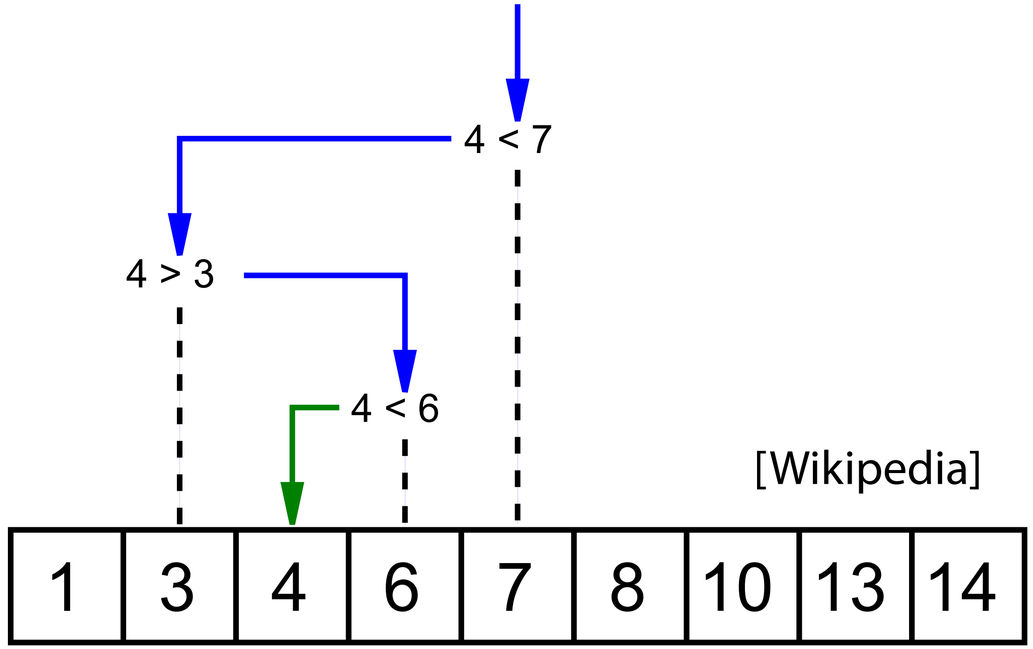
No, it could be implemented with ~1/3 the number of *f*-evaluations.

Stopping criteria for nonlinear methods

```
if np.abs(f(m)) < eps₁ or np.abs(l - r) < eps₂:
    return m
```



Does this seem at all familiar?



Binary search for 4 in sorted list.

Complexity of (discrete) algorithm: $O(\log n)$

Can we find an analogy of "*complexity*" for root finding?

Order and rate of convergence

Suppose that we can find numbers o and r so that

$$\lim_{k \to \infty} \frac{E_{k+1}}{E_k^o} = r.$$

where E_k is the error after iteration k, then:

- o is called the **order of convergence**, which tells us how quickly the algorithm convergences.
  - $o = 1$: linear convergence, $o = 2$: quadratic convergence, etc.
- r is called the **rate of convergence**. It distinguishes convergence speed of algorithms with the same order.

Convergence order and rate of bisection

Error bound (before 1st iteration) : $r - l$

Error bound (after 1st iteration) : $(r - l) / 2$

Generally: $E_{k+1} = \frac{1}{2} E_k \Leftrightarrow \frac{E_{k+1}}{E_k^1} = \frac{1}{2}$

In other words: **order** of convergence = 1 (*linear*)
rate of convergence = 1 / 2

A method with a **linear order of convergence** gains a fixed number of accurate digits per iteration (depending on **rate**). Here:

- 1 base-2 digit every iteration. 1 base-10 digit every $\frac{\log 10}{\log 2} \approx 3$ iterations.

Convergence speed of bisection

Let's apply bisection to the root-finding example function with

$$f(x) := x^2 - 4\sin x$$

Here, *l* and *r* denote the bracket; the solution lies in between.

l	$f(l)$	r	$f(r)$
1.000000	−2.365884	3.000000	8.435520
1.000000	−2.365884	2.000000	0.362810
1.500000	−1.739980	2.000000	0.362810
1.750000	−0.873444	2.000000	0.362810
1.875000	−0.300718	2.000000	0.362810
1.875000	−0.300718	1.937500	0.019849
1.906250	−0.143255	1.937500	0.019849
1.921875	−0.062406	1.937500	0.019849
1.929688	−0.021454	1.937500	0.019849

l	$f(l)$	r	$f(r)$
1.933594	−0.000846	1.937500	0.019849
1.933594	−0.000846	1.935547	0.009491
1.933594	−0.000846	1.934570	0.004320
1.933594	−0.000846	1.934082	0.001736

[Heath]

Midpoint = **1.933**838

True solution = 1.9337537628..

(13 iterations for ~4 digits)

Newton's method

- Based on first-order Taylor expansion:

$$f(x+h) \approx f(x) + f'(x)h$$

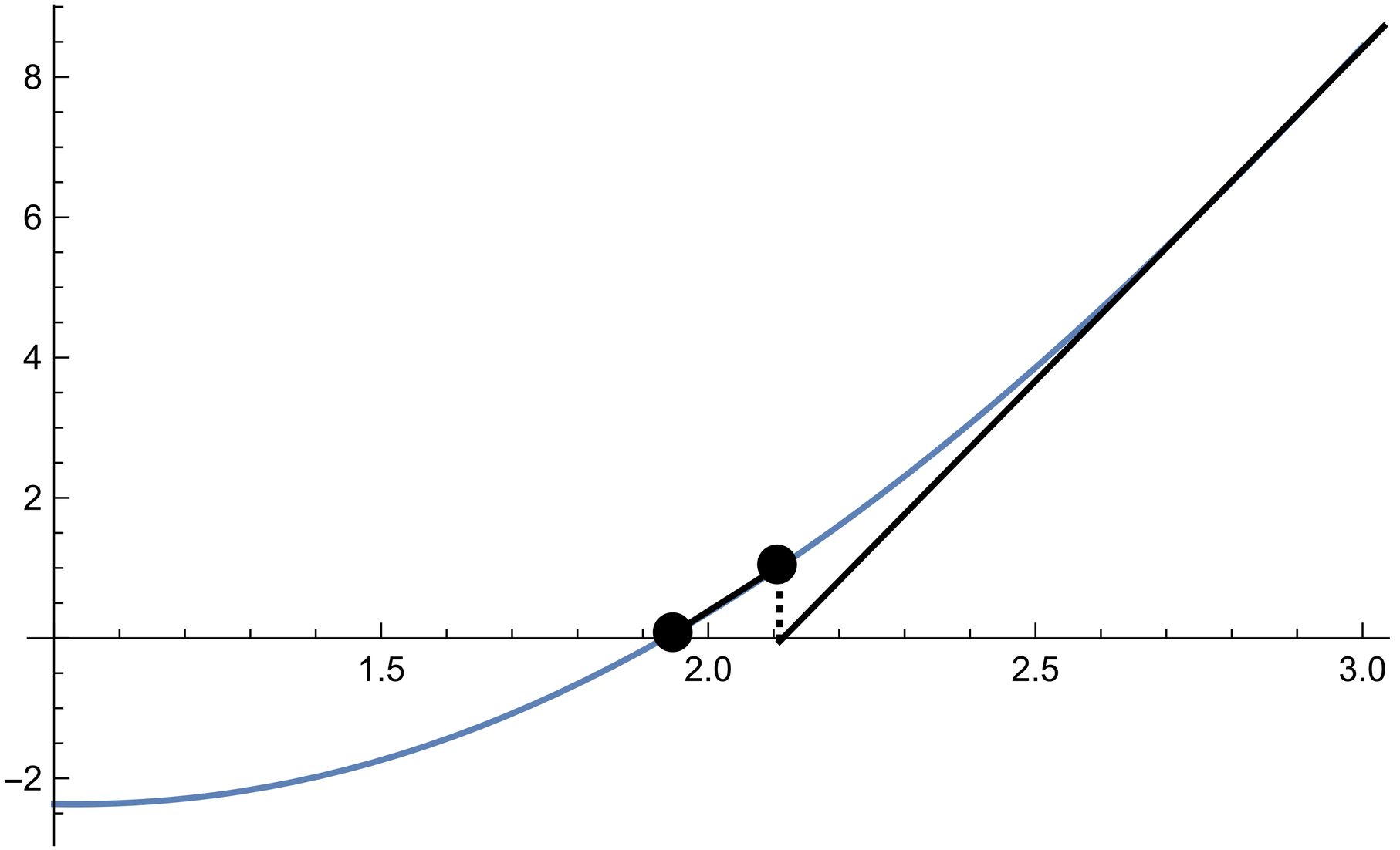
- Let's set this approximation to zero and solve for h.

$$f(x+h) = 0 \Leftrightarrow h = -\frac{f(x)}{f'(x)}$$

- Move to that position, and repeat..

$$x_k = x_{k-1} - \frac{f(x_{k-1})}{f'(x_{k-1})}$$

Visualization of Newton's method



Convergence of Newton's method

x	$f(x) := x^2 - 4\sin x$	$f'(x) := 2x - 4\cos x$	h
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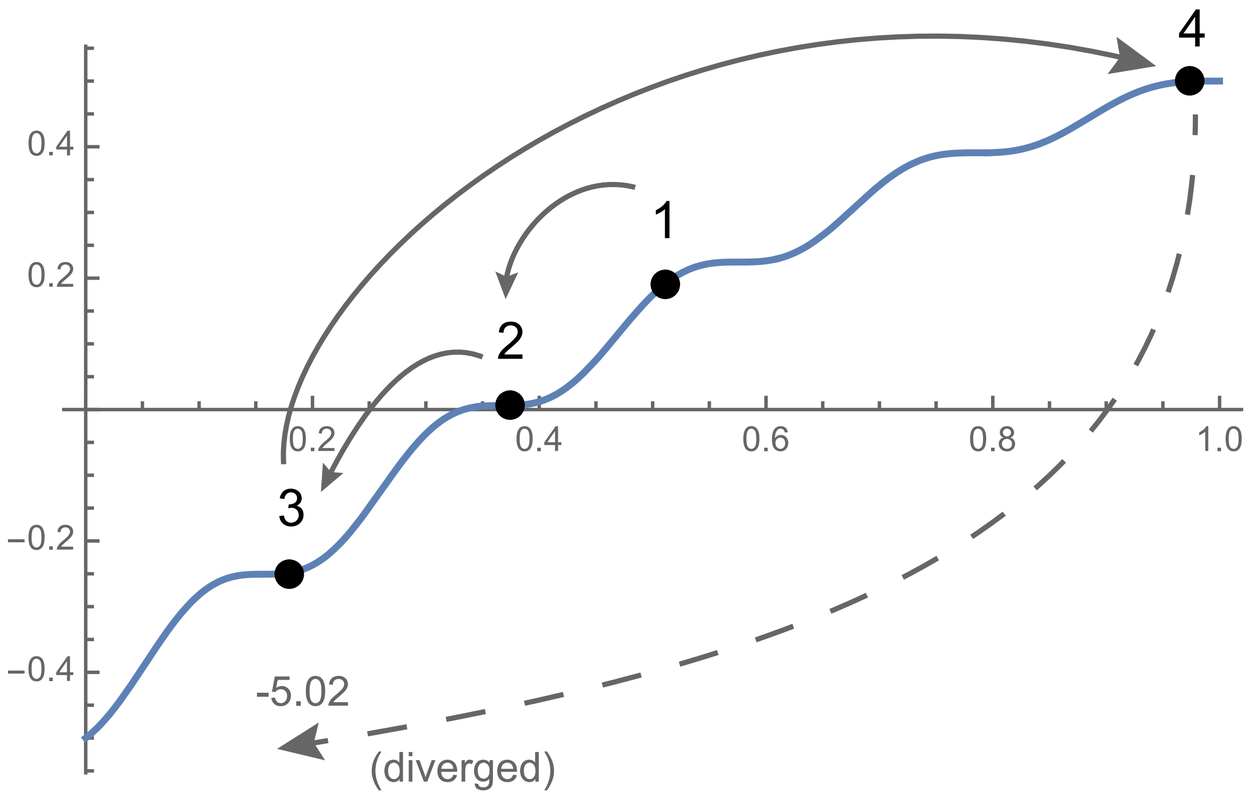
Failure cases of Newton's Method



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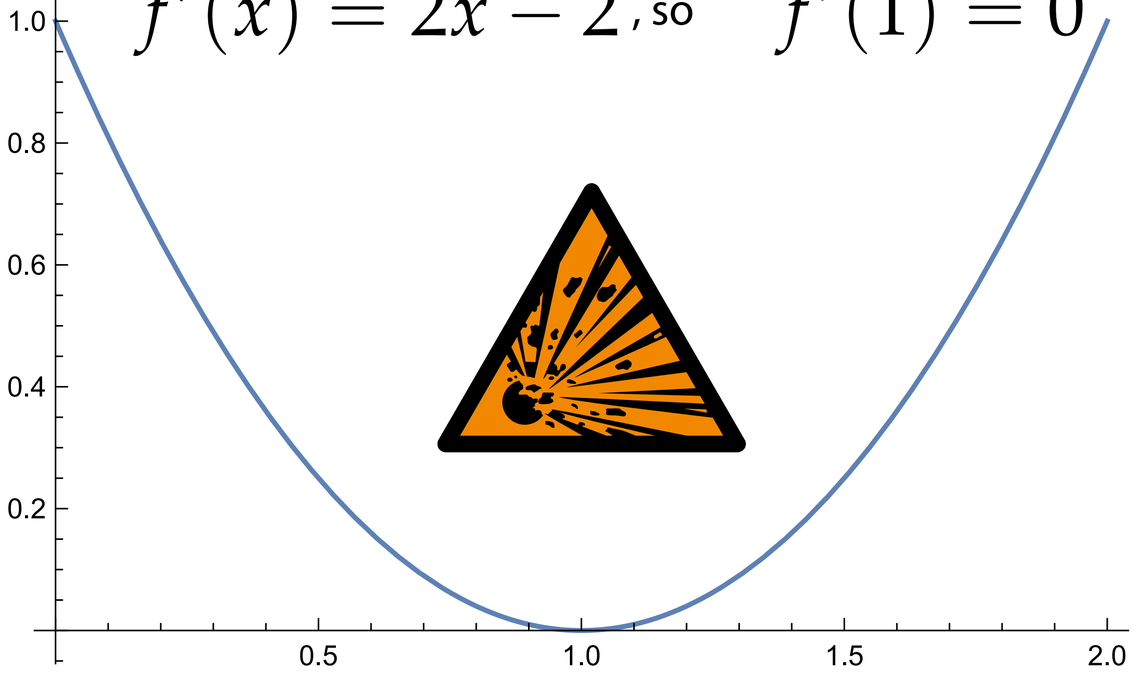

In theory: division by zero at $x = 1$.

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N dimensions

Multivariate root finding

$$f : \mathbb{R}^n \rightarrow \mathbb{R}^n$$

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Newton's method for root finding in N dimensions

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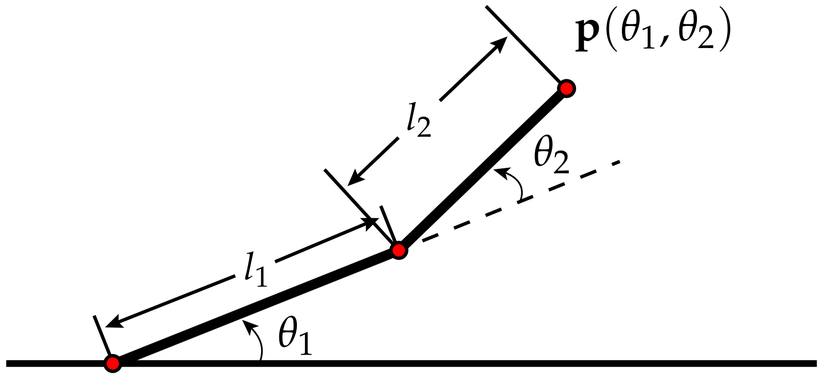
  - Assumes input and output spaces have matching dimension.

HW3: Inverse Kinematics via Newton's method

n unknowns

$$\mathbf{p}(\theta_1, \theta_2, \theta_3, \ldots, \theta_n) = \mathbf{p}_{\text{target}}$$

2 equations



Idea: solve with Newton's method

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} - [\nabla \mathbf{p}(\boldsymbol{\theta}_{k-1})]^{-1} \mathbf{p}(\boldsymbol{\theta}_{k-1})$$

Idea 2: solve with Newton's method + pseudoinverse

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} - [\nabla \mathbf{p}(\boldsymbol{\theta}_{k-1})]^{+} \mathbf{p}(\boldsymbol{\theta}_{k-1})$$

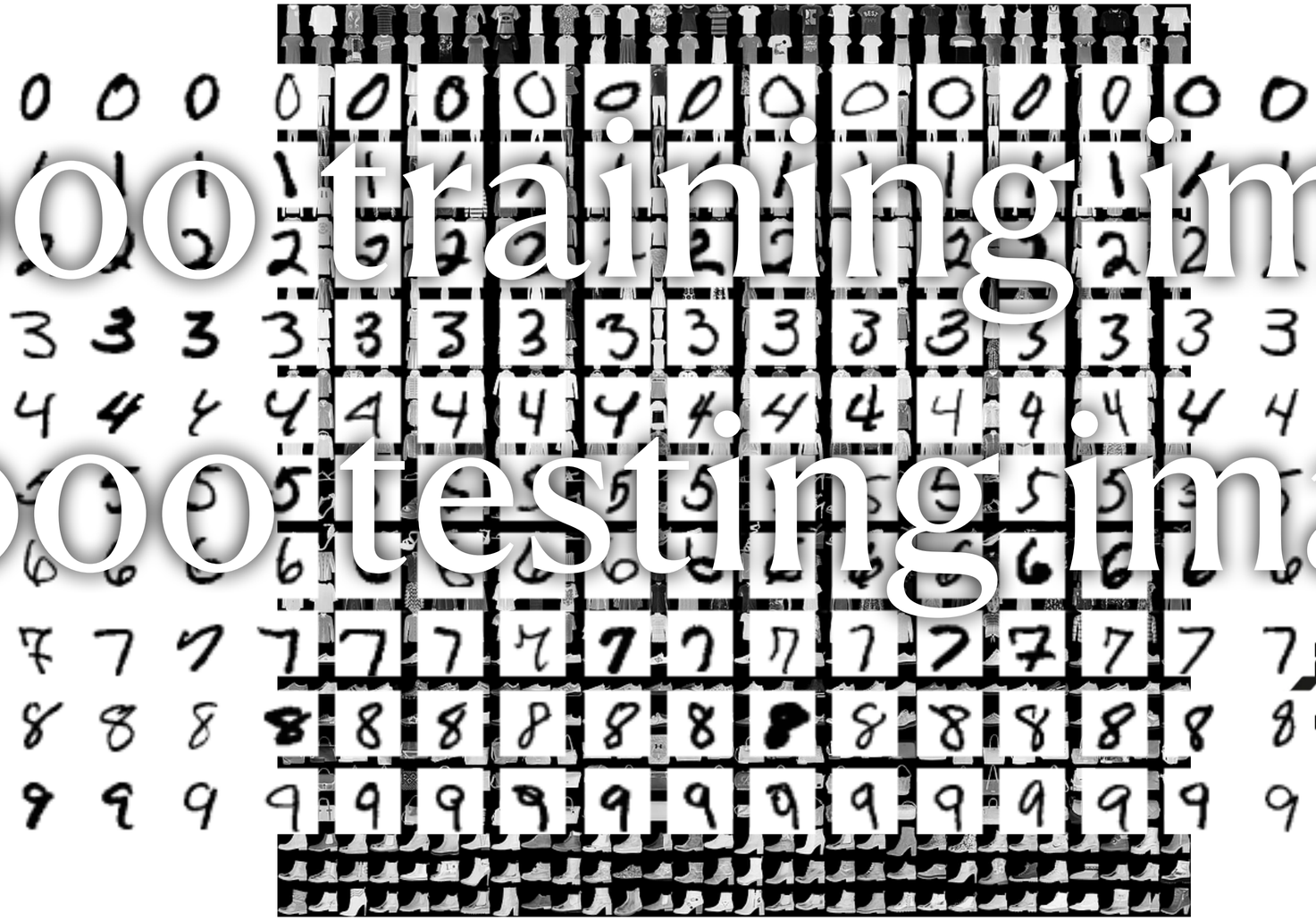
HW4: MyTorch

- Gradient-based optimization framework.
- A simple neural network with 3 layers (discussed next lecture)
- Reaches ~85% accuracy on Fashion-MNIST
- All built by yourself using only NumPy!

MyTorch

A benchmark problem

"MNIST" and "Fashion-MNIST"



60'000 training images

10'000 testing images

zalando