Lecture 8

Automatic Differentiation and Root Finding

CS328 - Numerical Methods for Visual Computing and Machine Learning

Prof. Wenzel Jakob

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

[Wikimedia commons]

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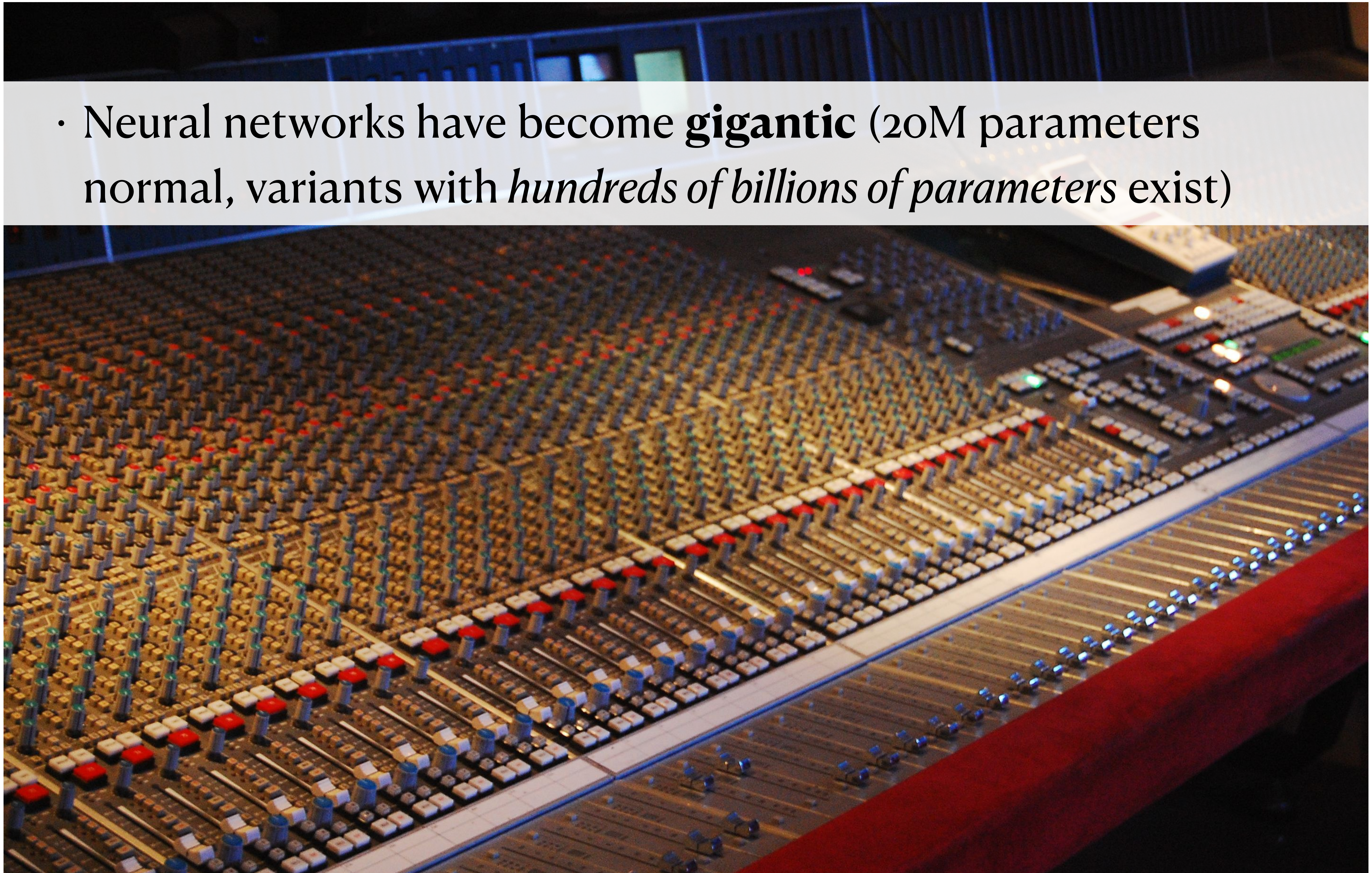

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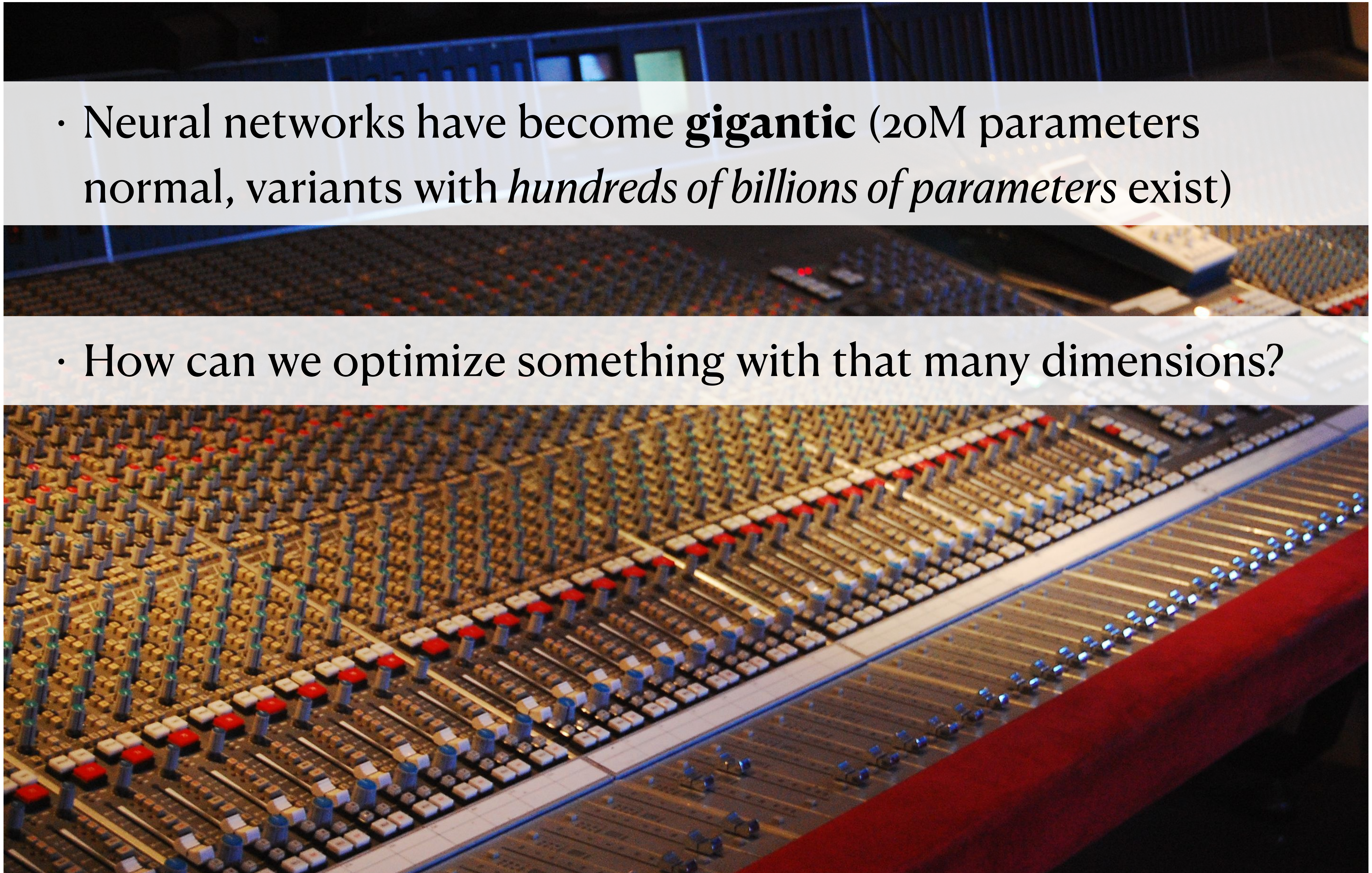
- How can we optimize something with that many dimensions?



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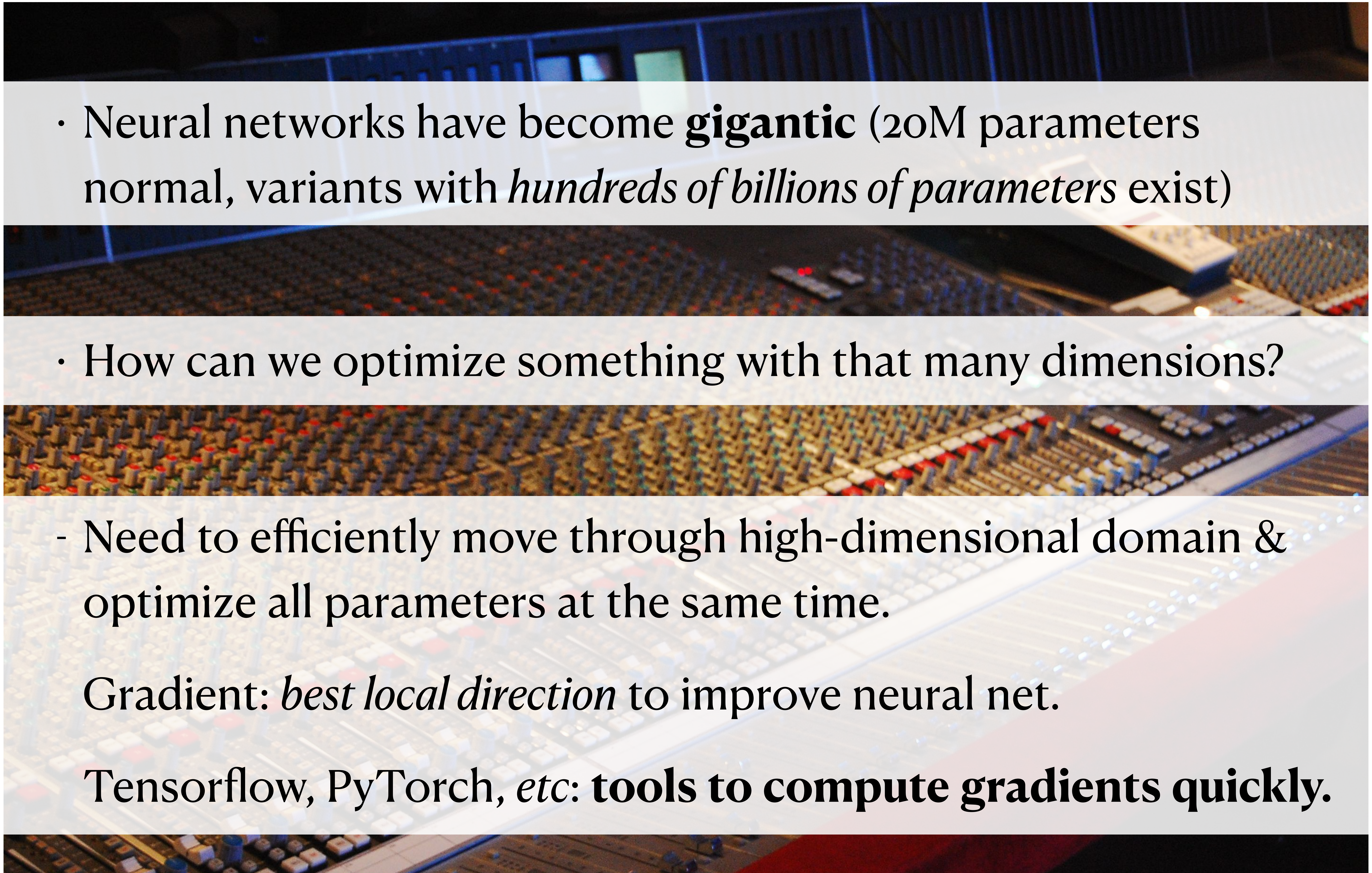

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- Neural networks have become **gigantic** (20M parameters normal, variants with *hundreds of billions of parameters* exist)

- 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.**

How to evaluate gradients?

Let's review some standaard techniques for evaluating derivatives.

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

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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

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

Finite Differences

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Finite Differences

Example: $f(x) = x^3$

(*plot shows* $f'_{\text{approx}}(x) - 3x^2$)

Forward difference

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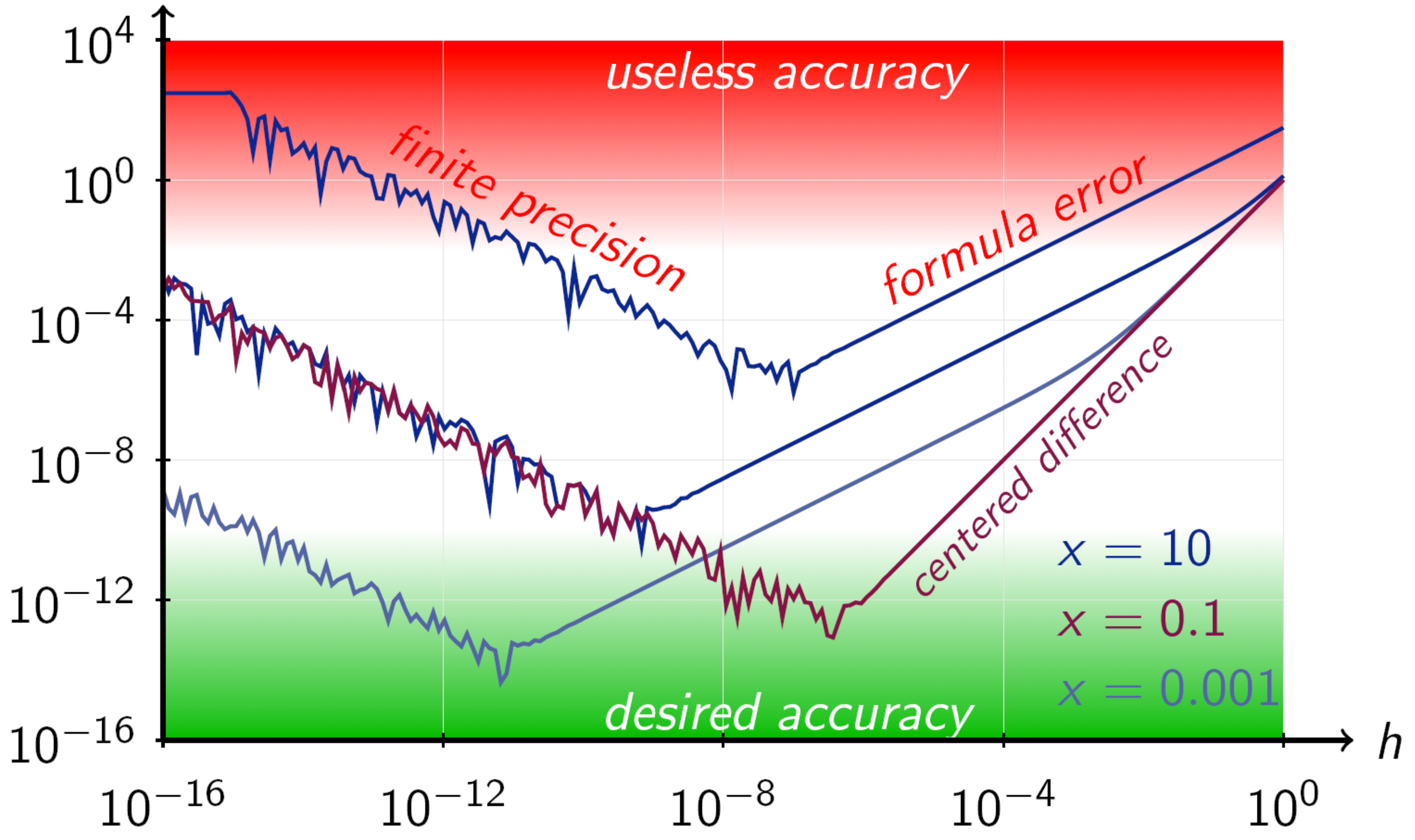

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Main problems:

- 1M dimensions? Must evaluate f at least 1M+1 times
- Complex tradeoff between approximation / cancellation error

Symbolic versus Automatic Derivatives

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def f(x):
    for i in range(8):
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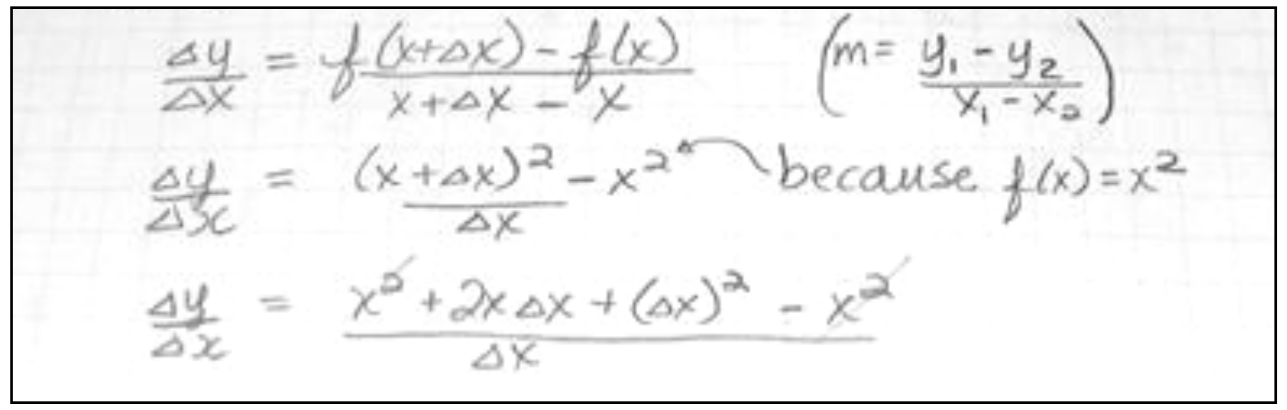

By hand

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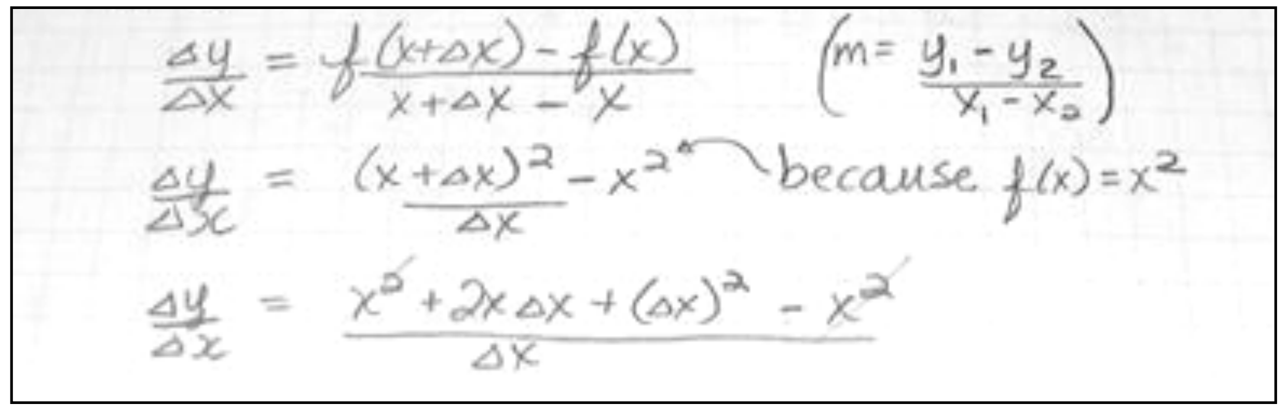

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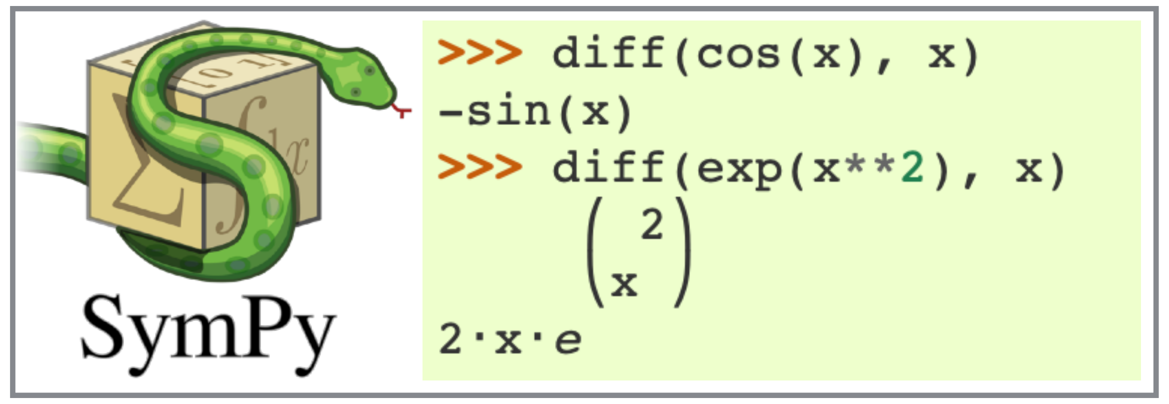

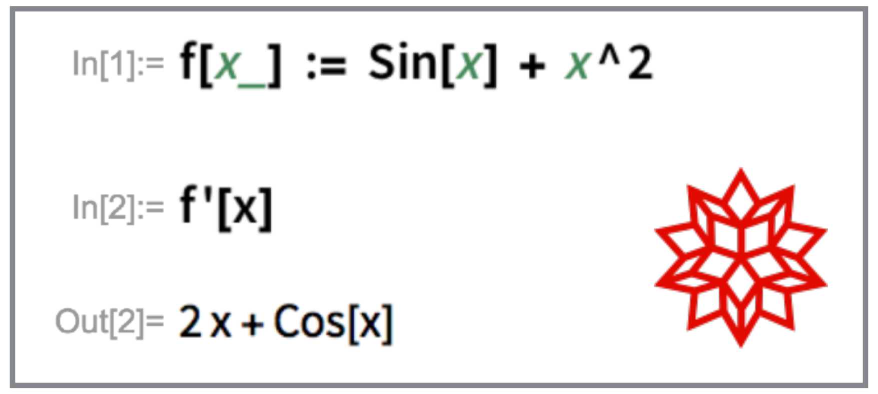

SymPy Mathematica

Computer Algebra System (CAS)

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37 exponentials (!)

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def f(x):
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    return x
```

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Automatic differentiation (forward mode):

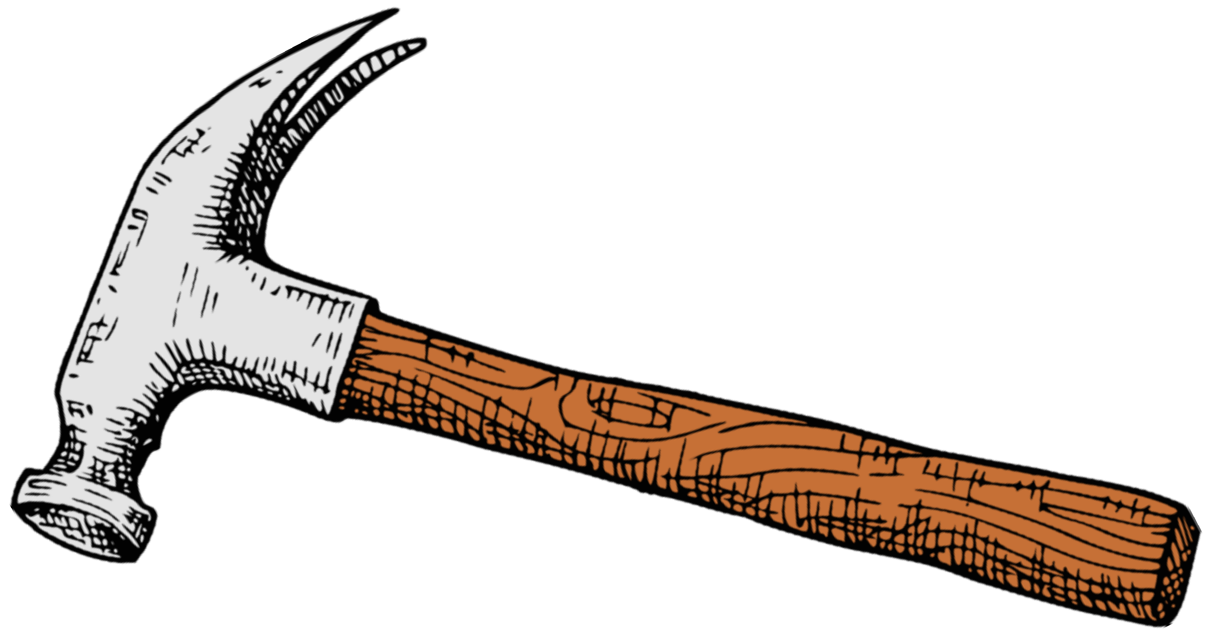
```
def df(x):
    d = 1
    for i in range(8):
        x = exp(x)
        d = d * x
    return d
```

8 exponentials

Automatic differentiation

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

Automatic differentiation



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

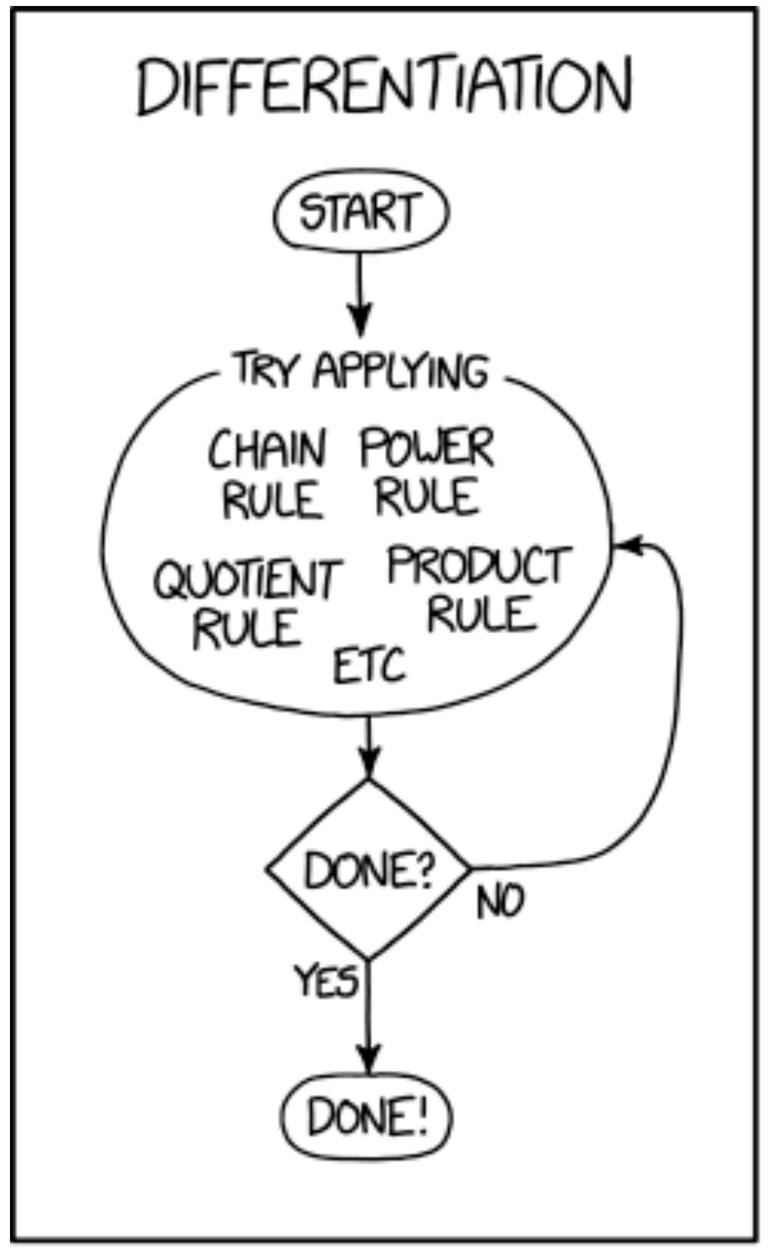
TensorFlow

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]



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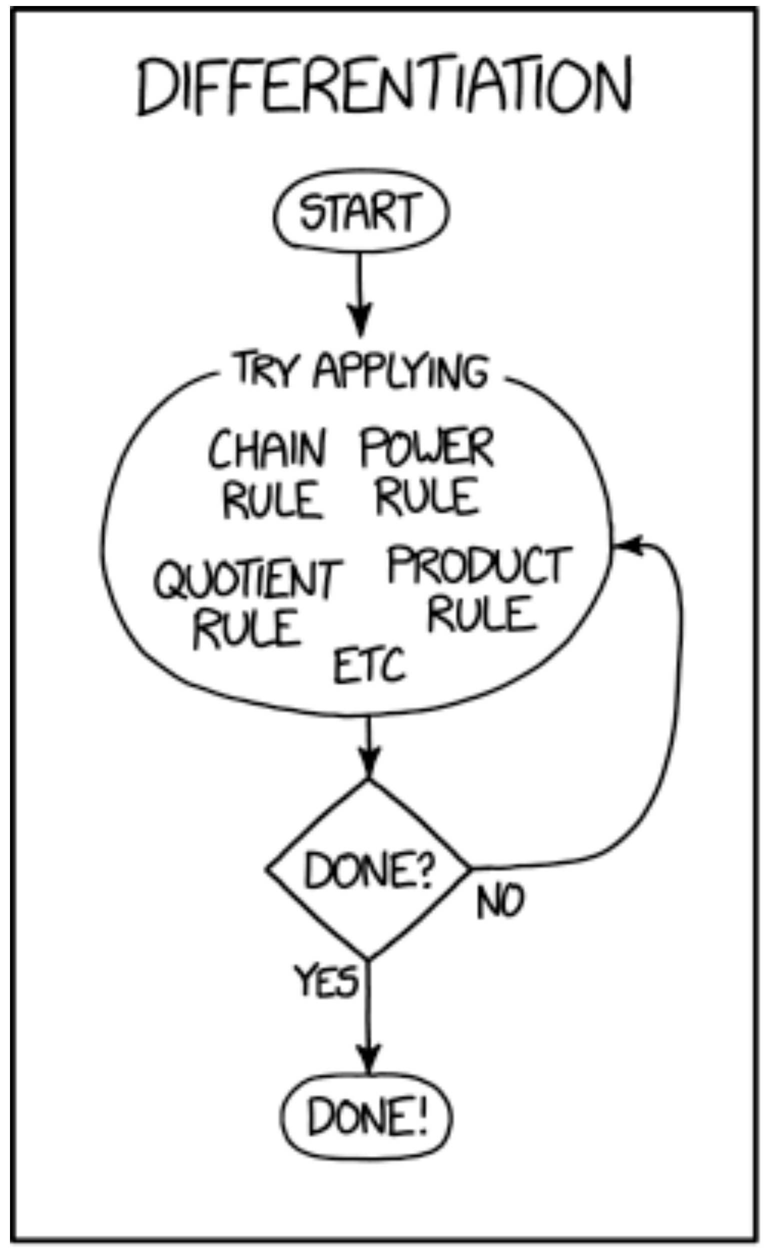

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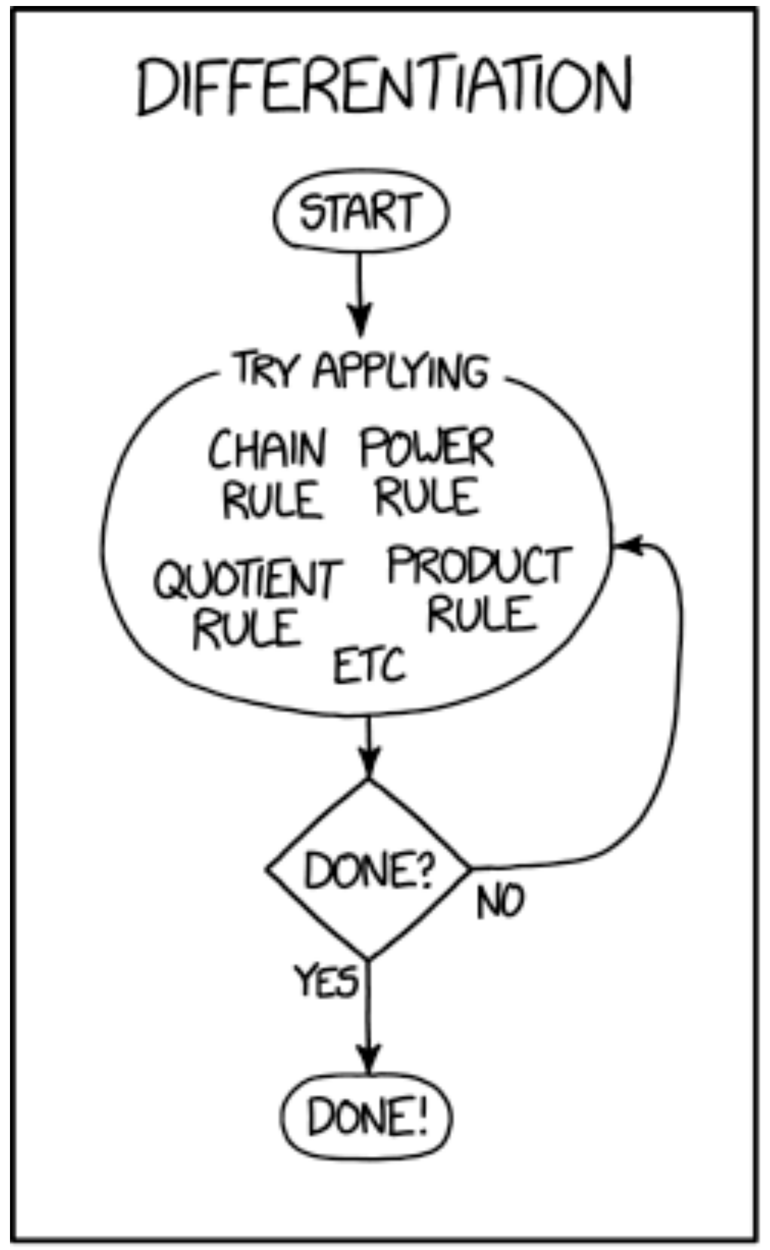

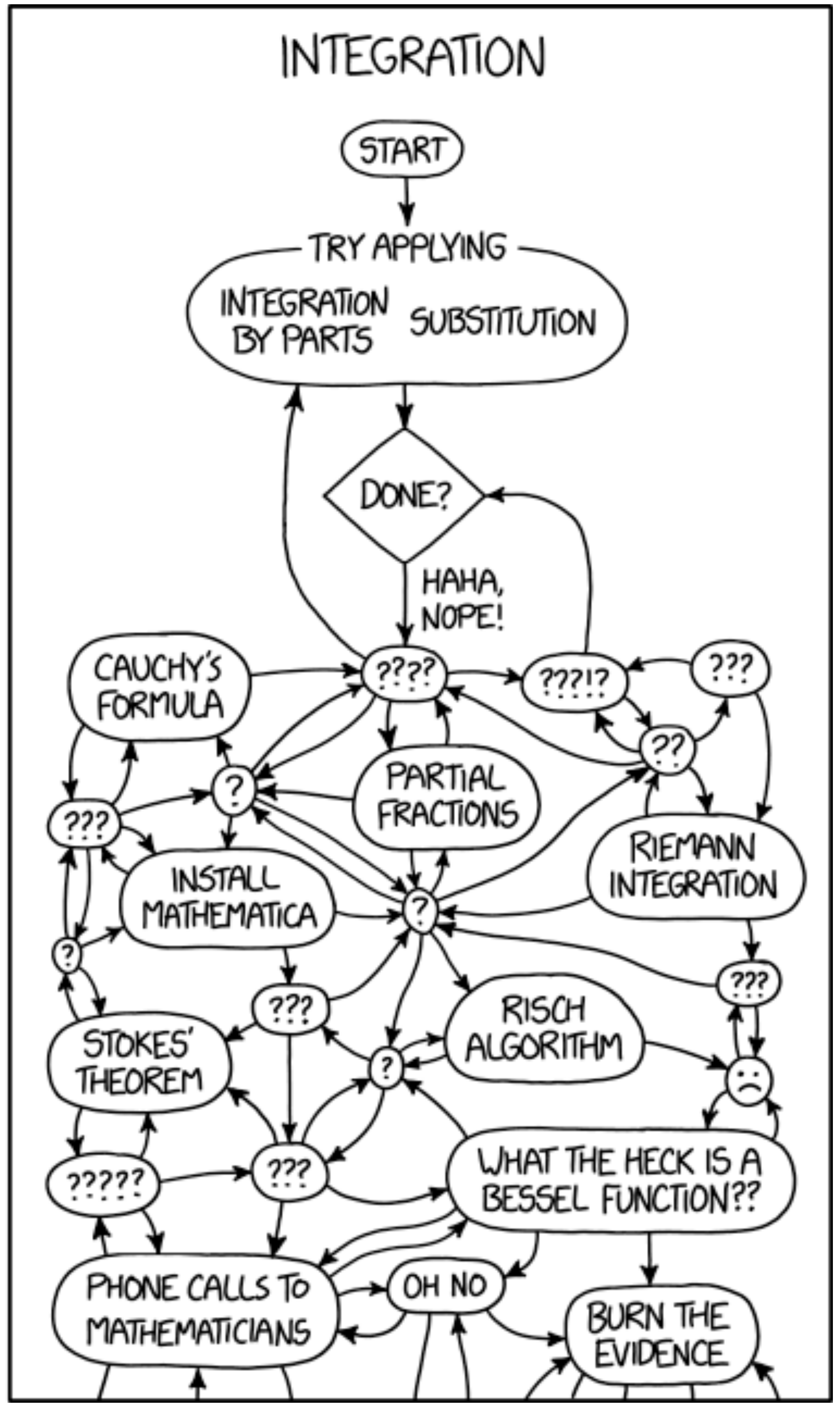

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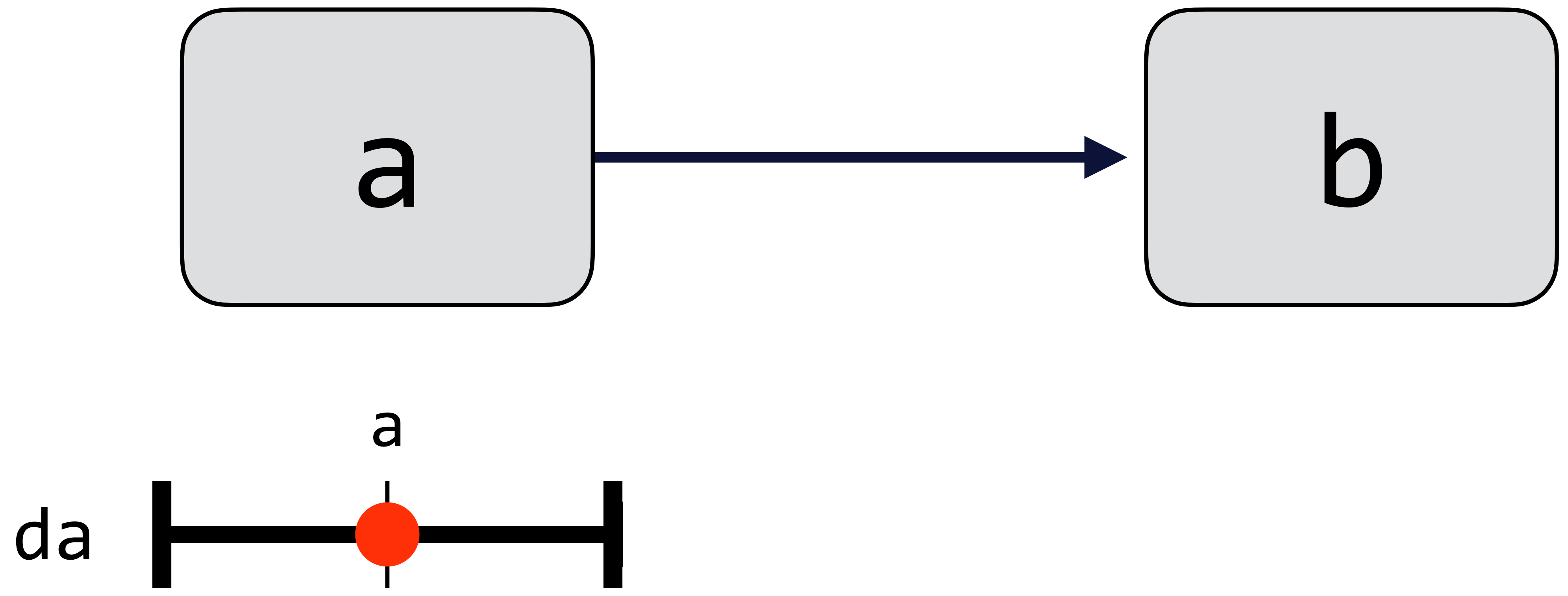

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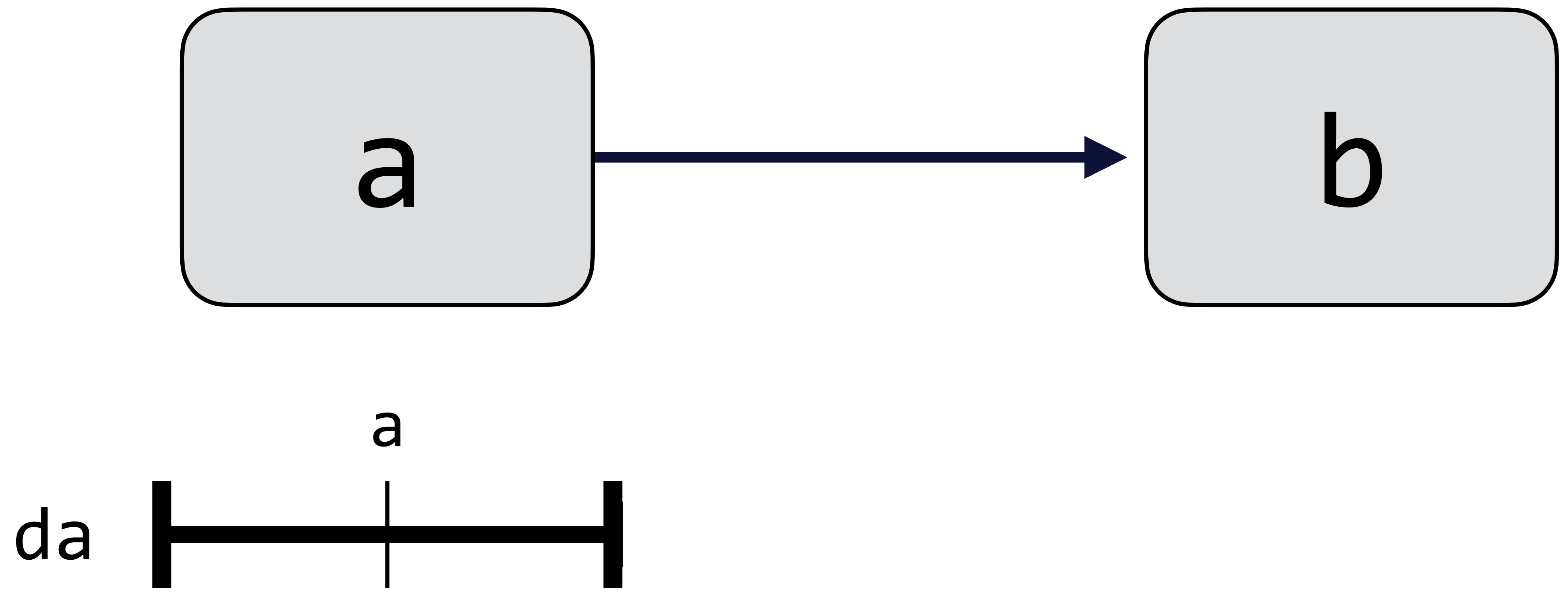

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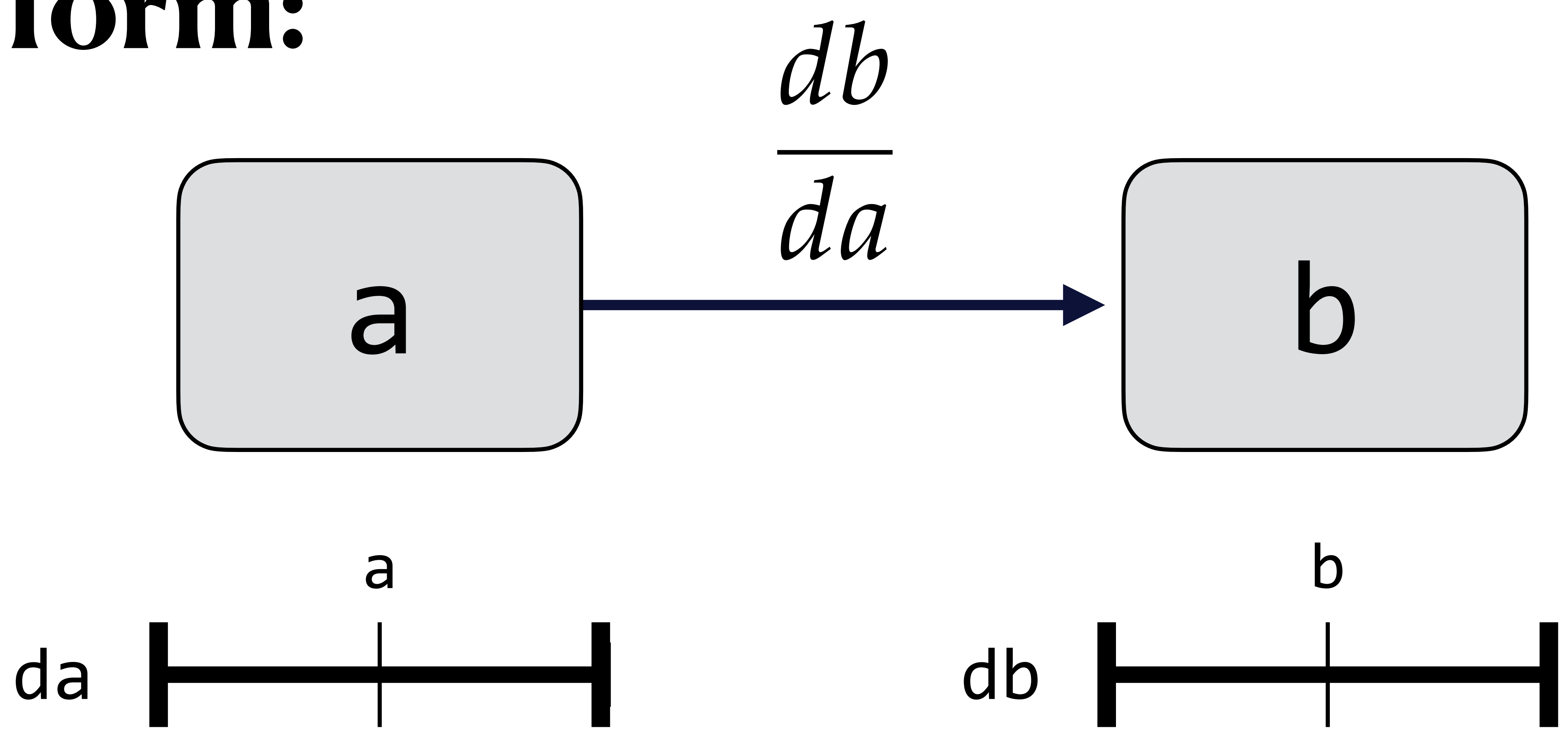

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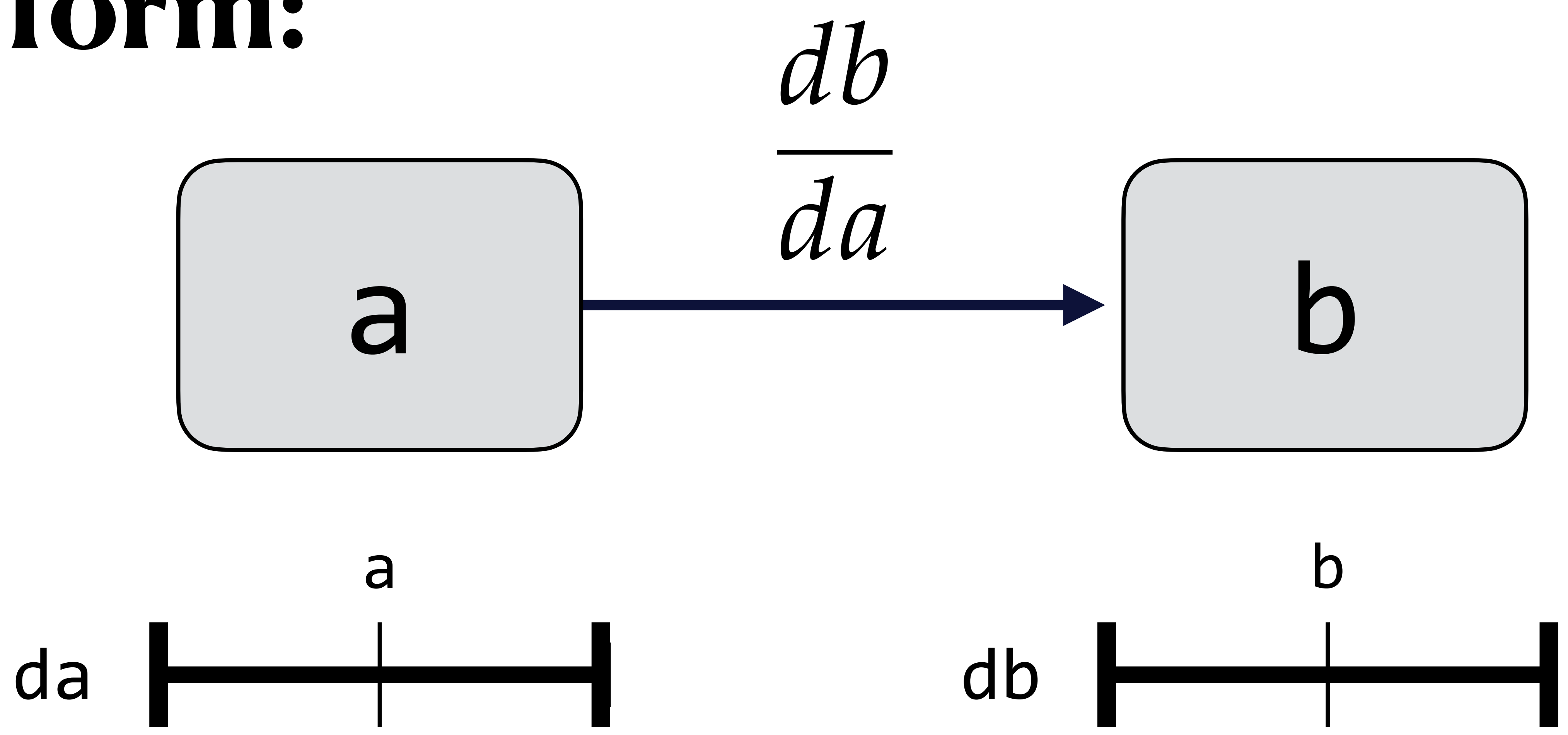

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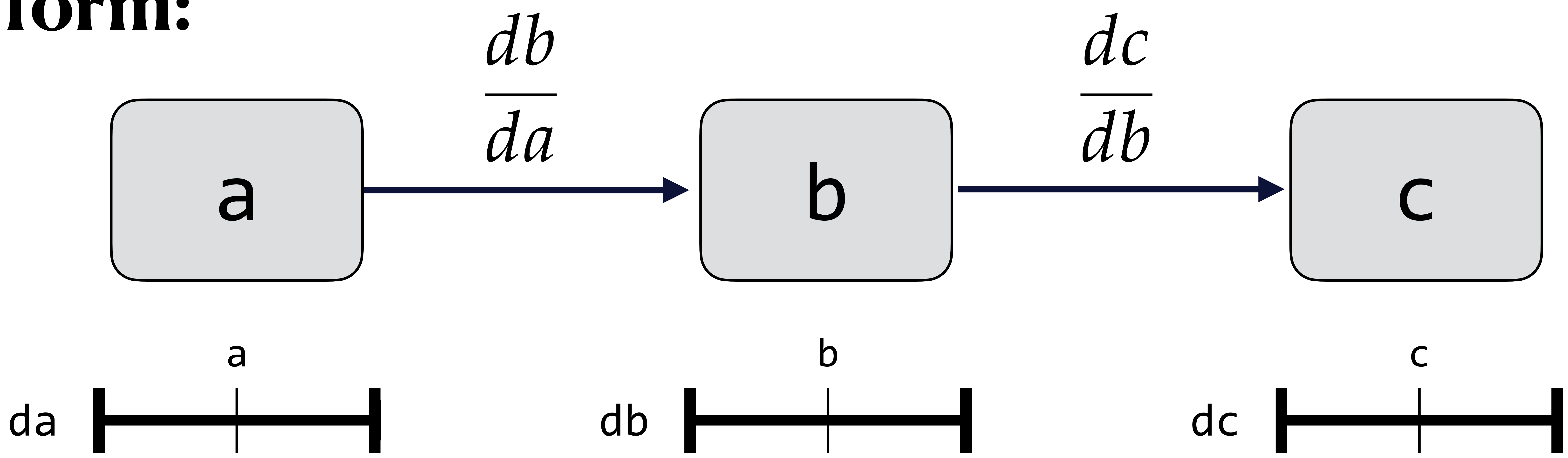

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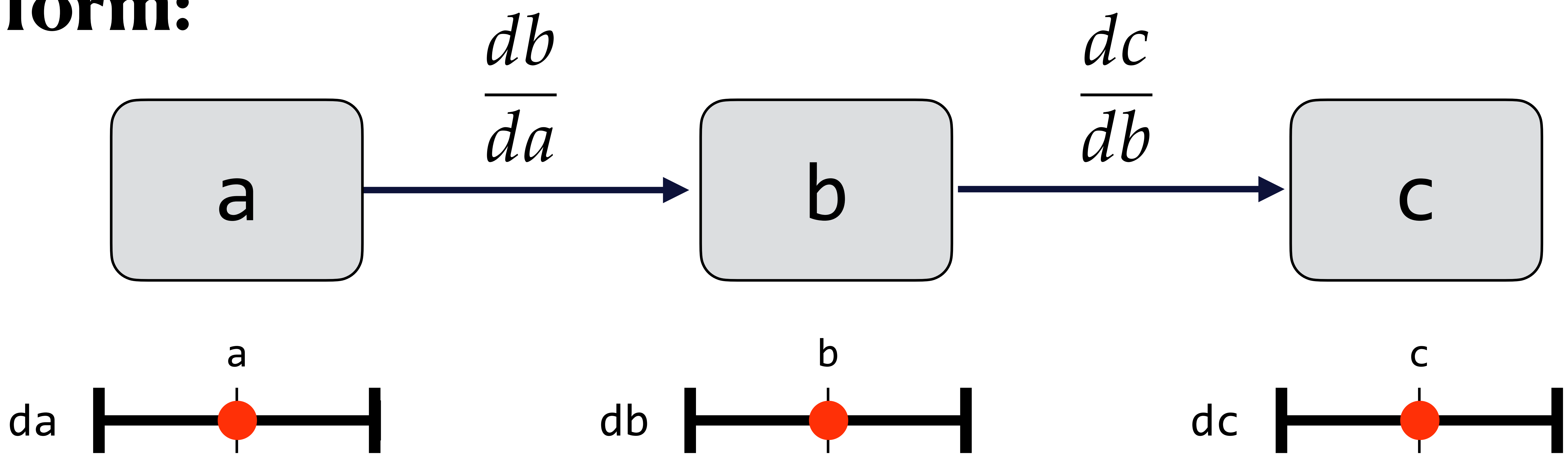

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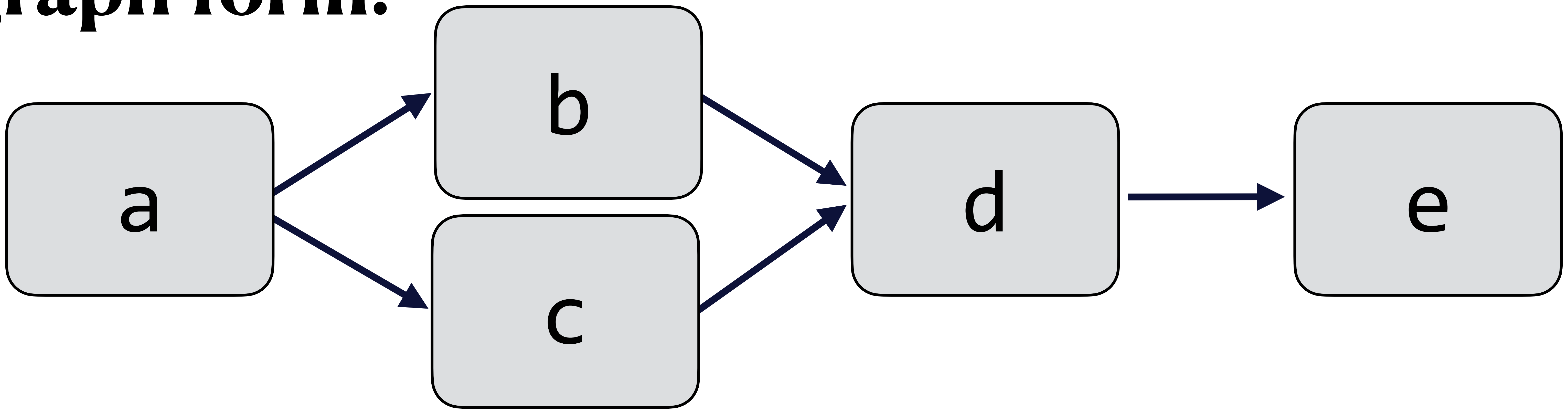

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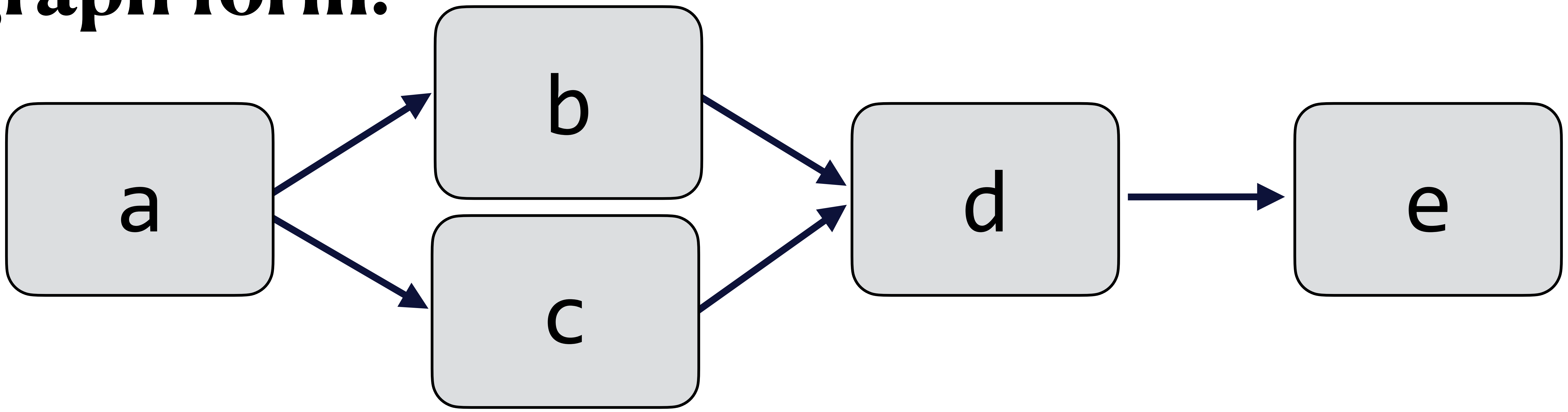

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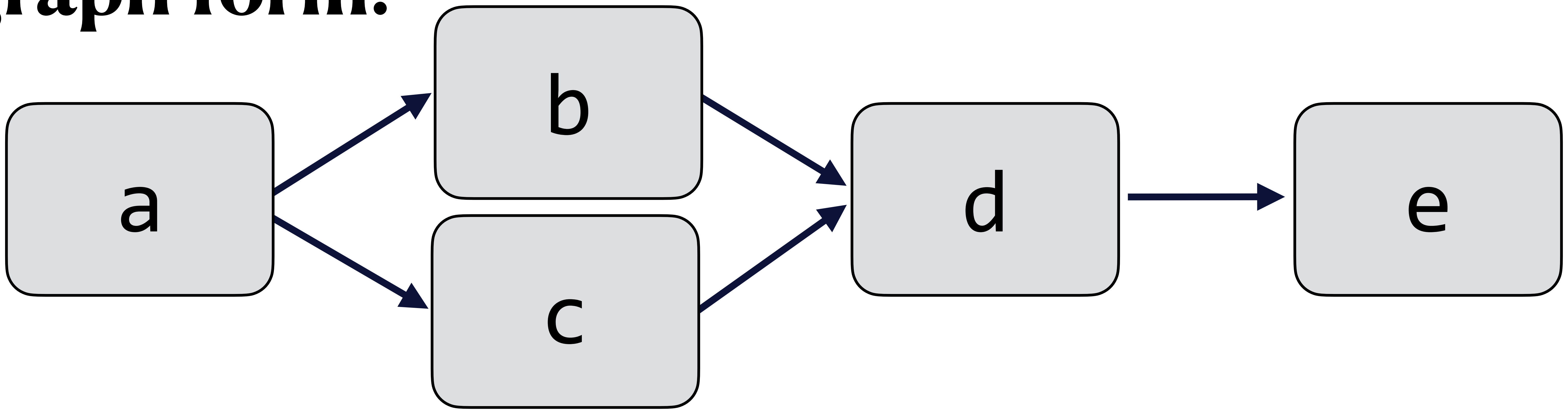

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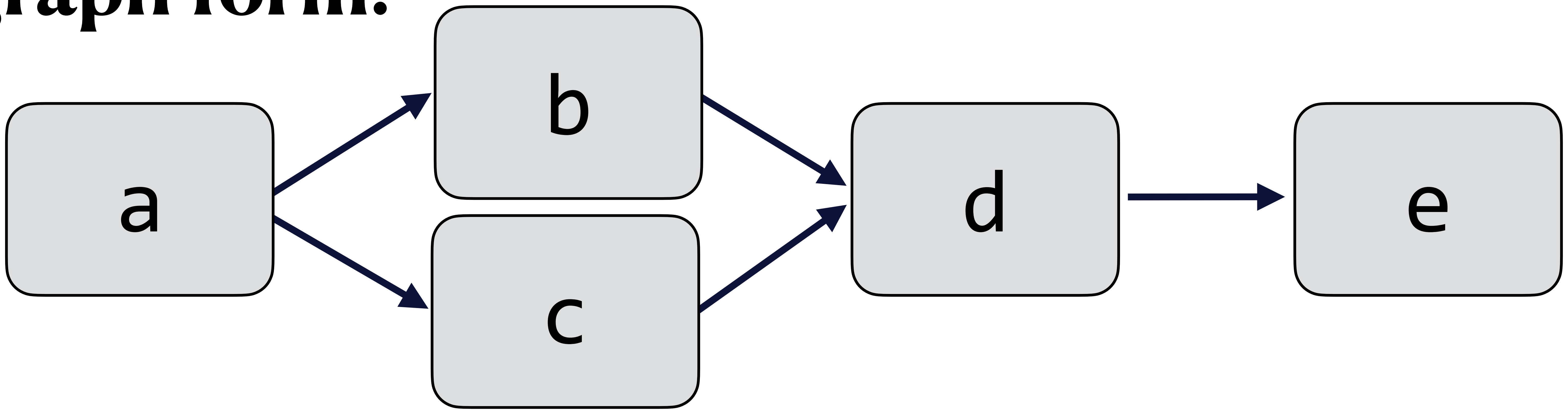

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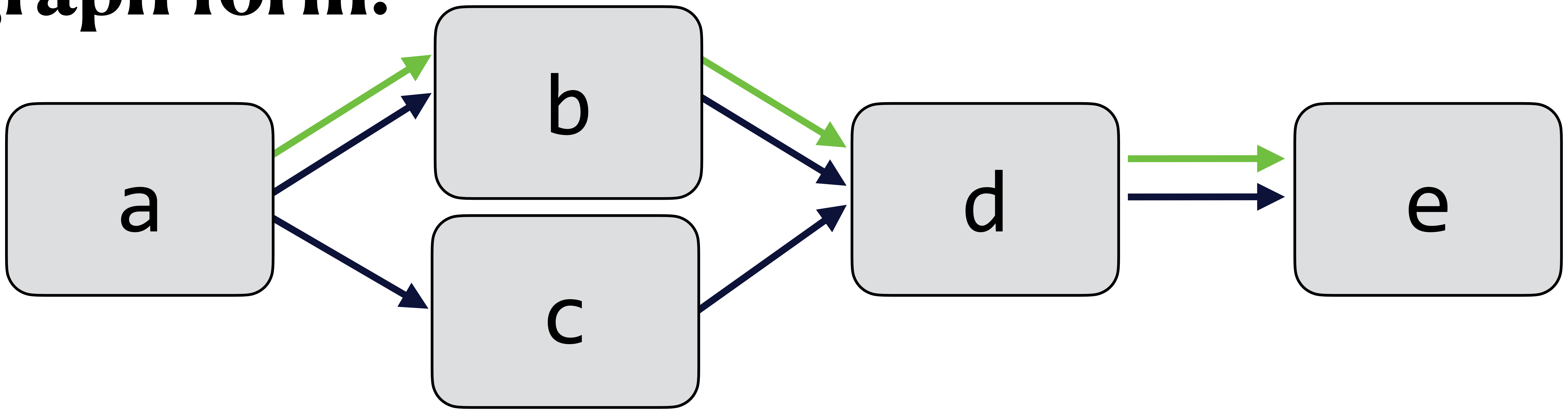

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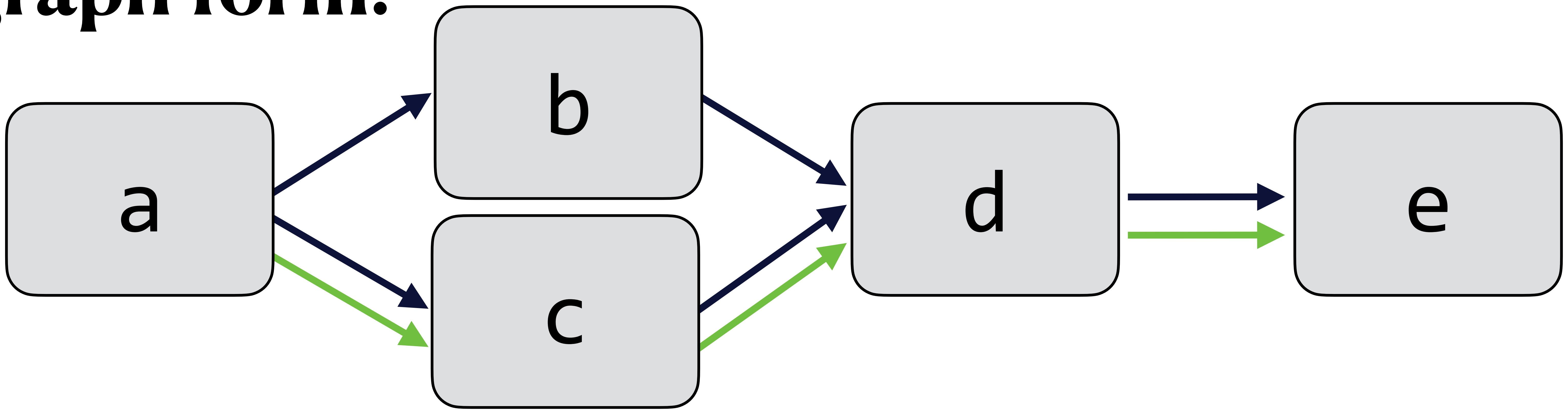

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Redundant computation

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

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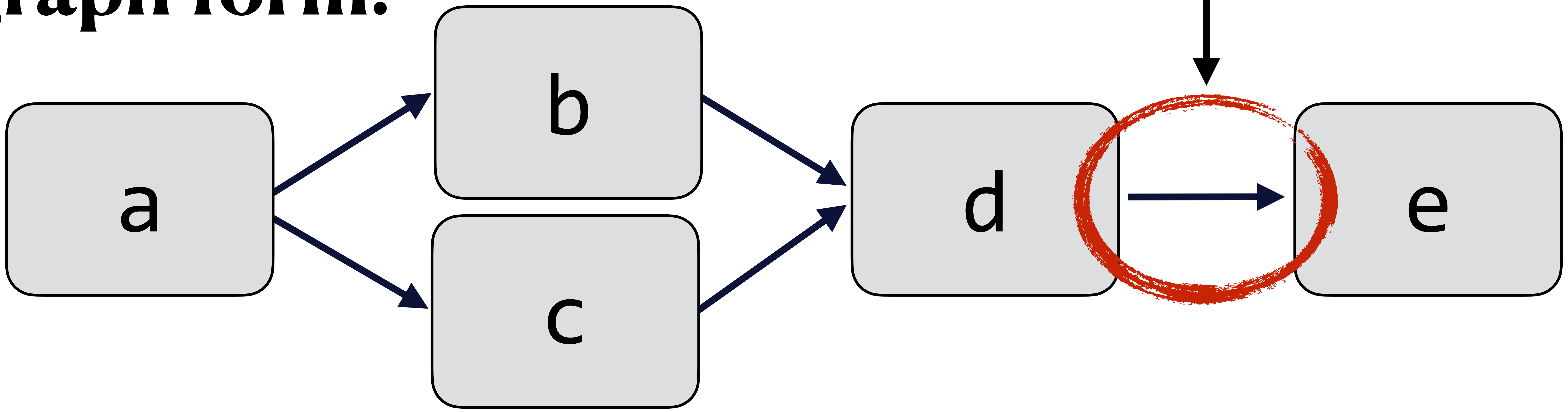

Cheap Gradient Principle

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.)

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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;
```

Original

Derivatives

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Original

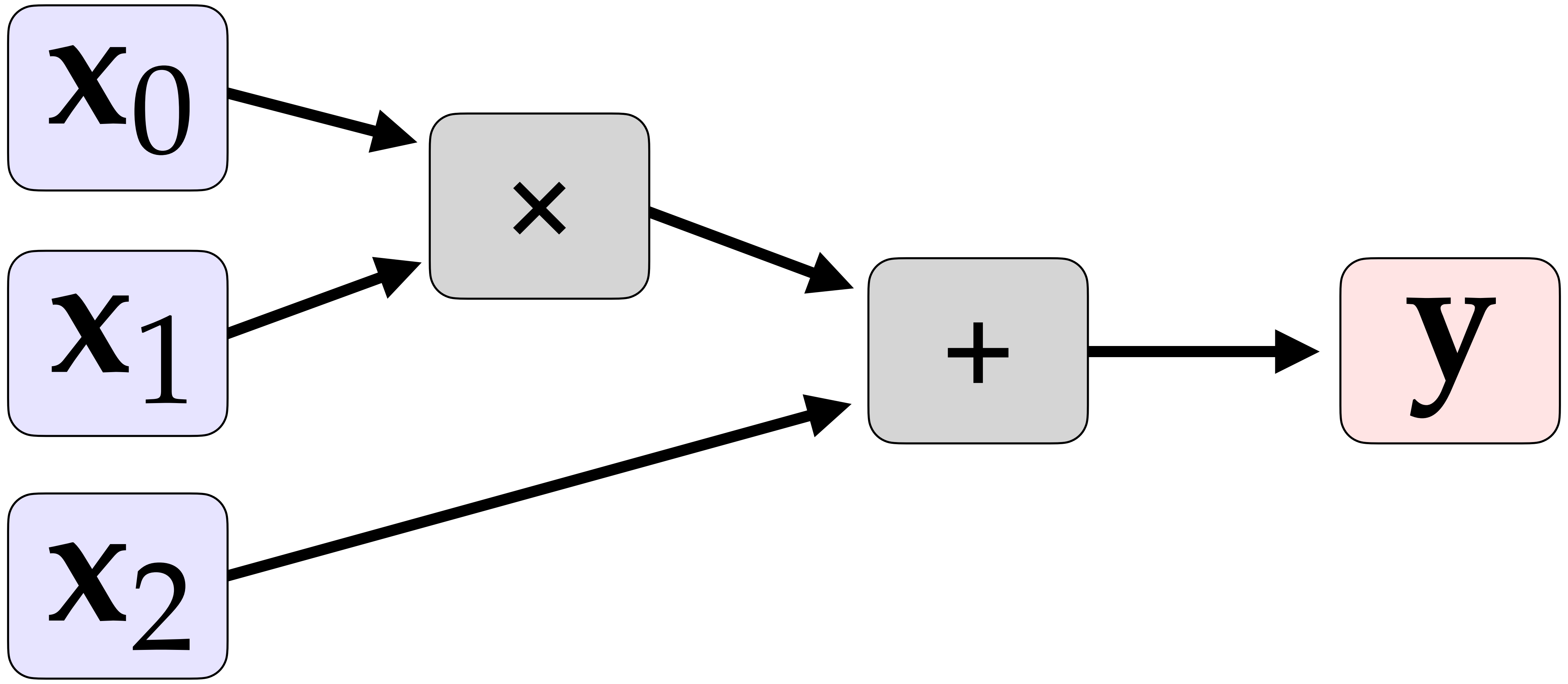
Derivatives

Differentiating a function with respect to an input

Differentiation depends on how variables are *connected*.

This is known as
Forward mode

$$\mathbf{y} = \mathbf{x}_0 \cdot \mathbf{x}_1 + \mathbf{x}_2$$



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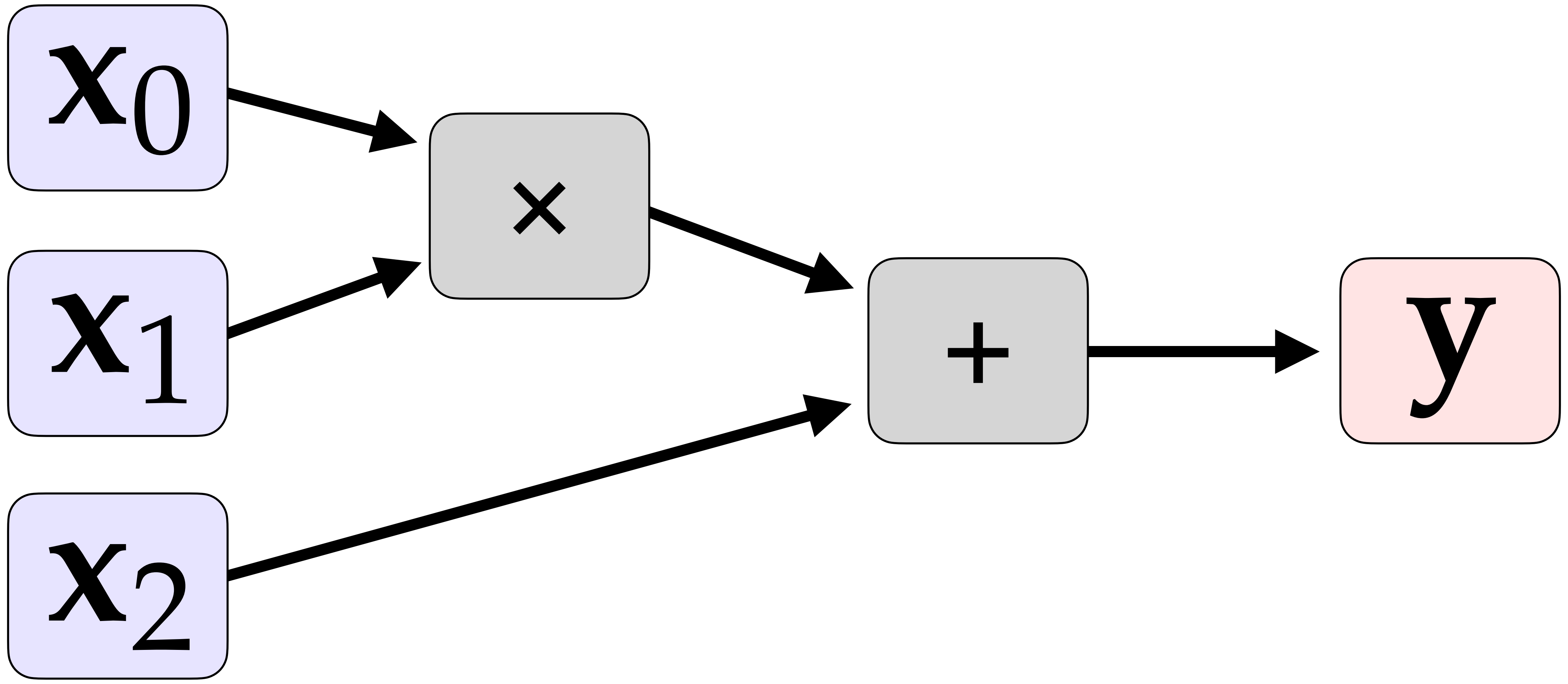

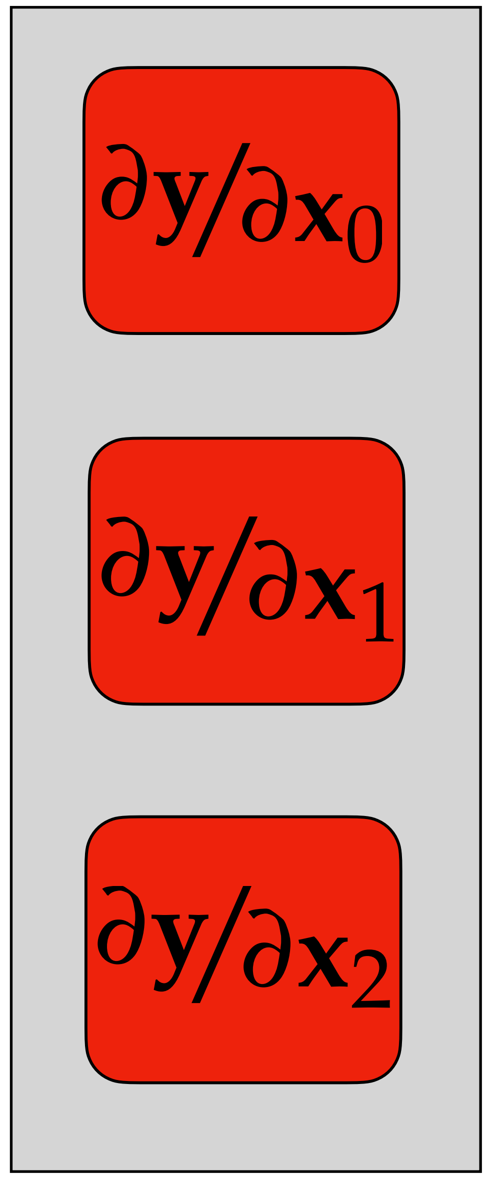

Gradient

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
```

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
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    def __add__(self, other: Number):
        return Number(
            value = self.value + other.value,
            grad  = self.grad + other.grad
        )
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Talk is cheap, show me the code!

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

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            value = self.value * other.value,
            grad  = self.grad*other.value + self.value*other.grad
        )
```

Talk is cheap, show me the code!

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

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class Number:
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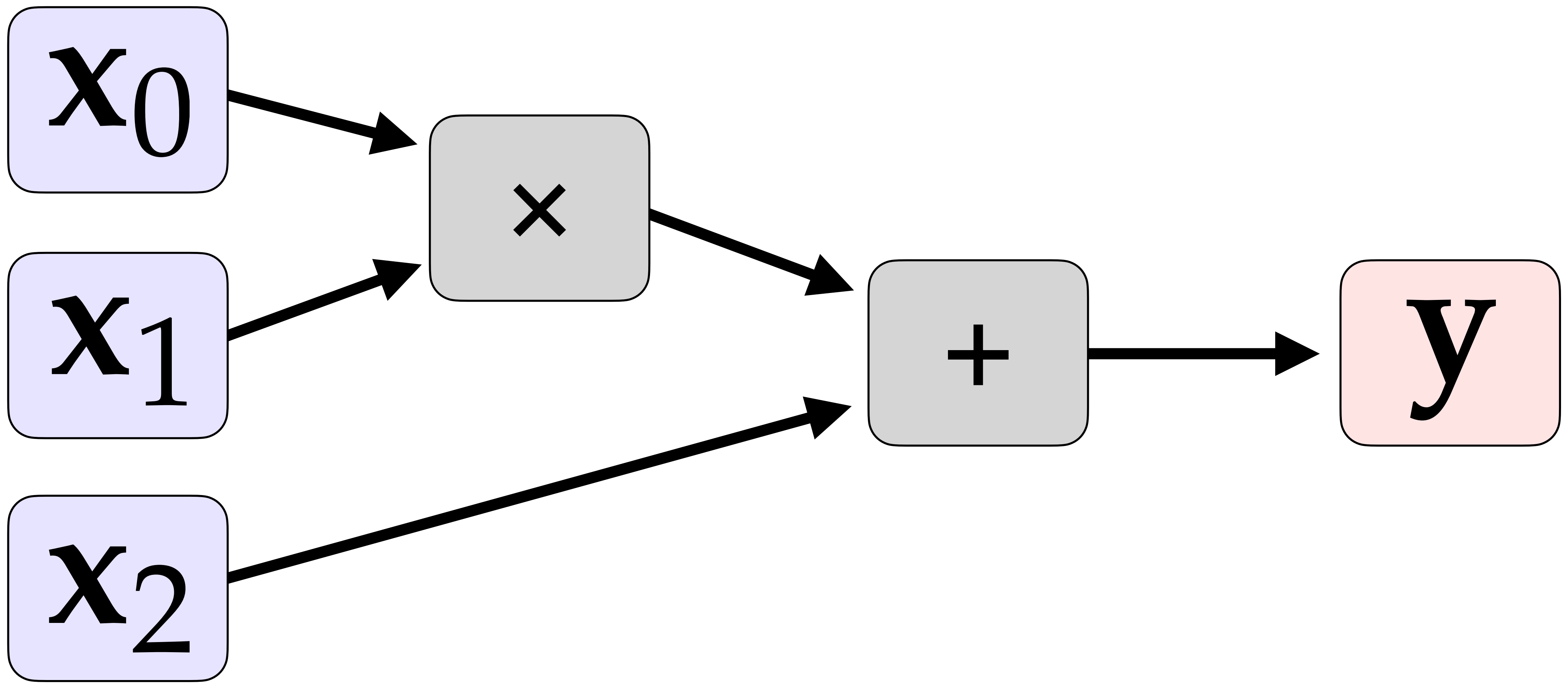
            grad  = self.grad*other.value + self.value*other.grad
        )
```

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

Demo time

Directionality of differentiation

$$\mathbf{y} = \mathbf{x}_0 \cdot \mathbf{x}_1 + \mathbf{x}_2$$



Directionality of differentiation

Reverse mode
aka. backward mode

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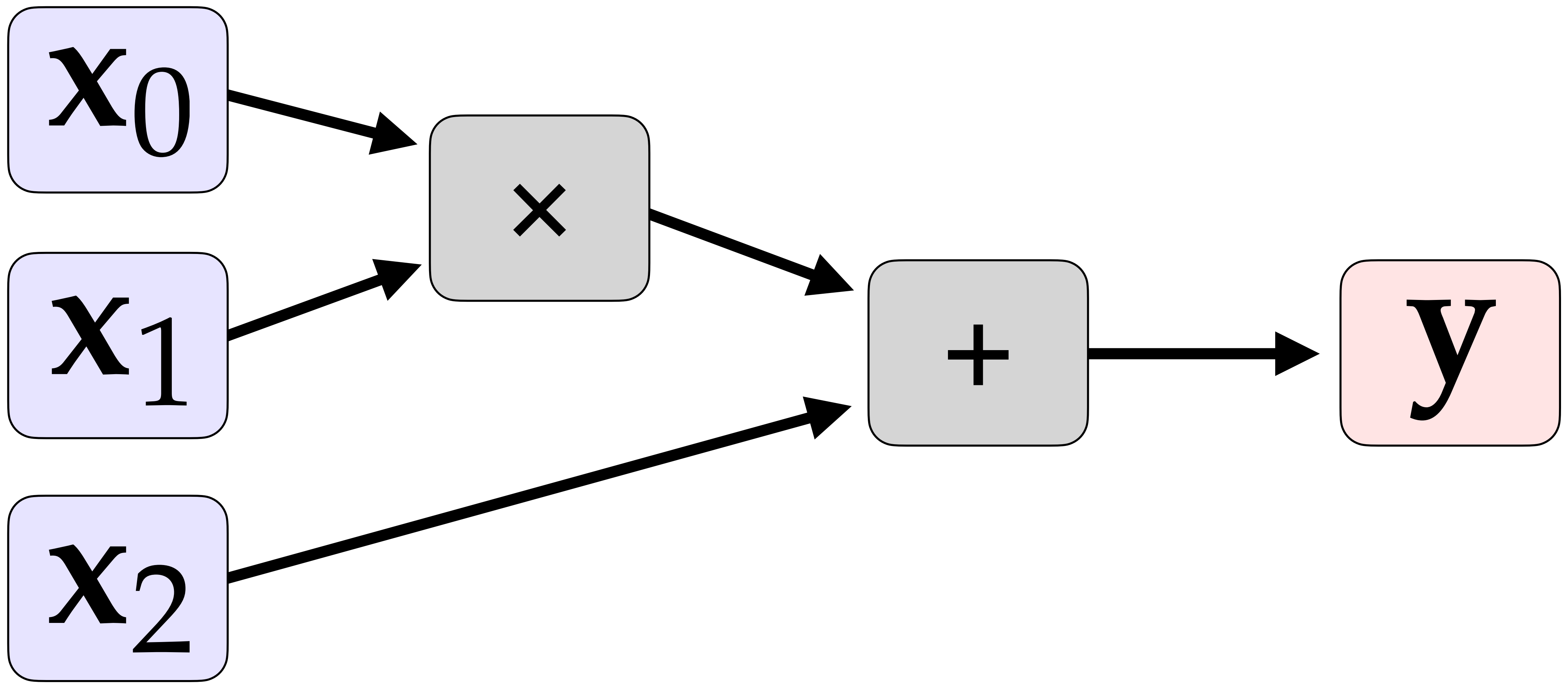

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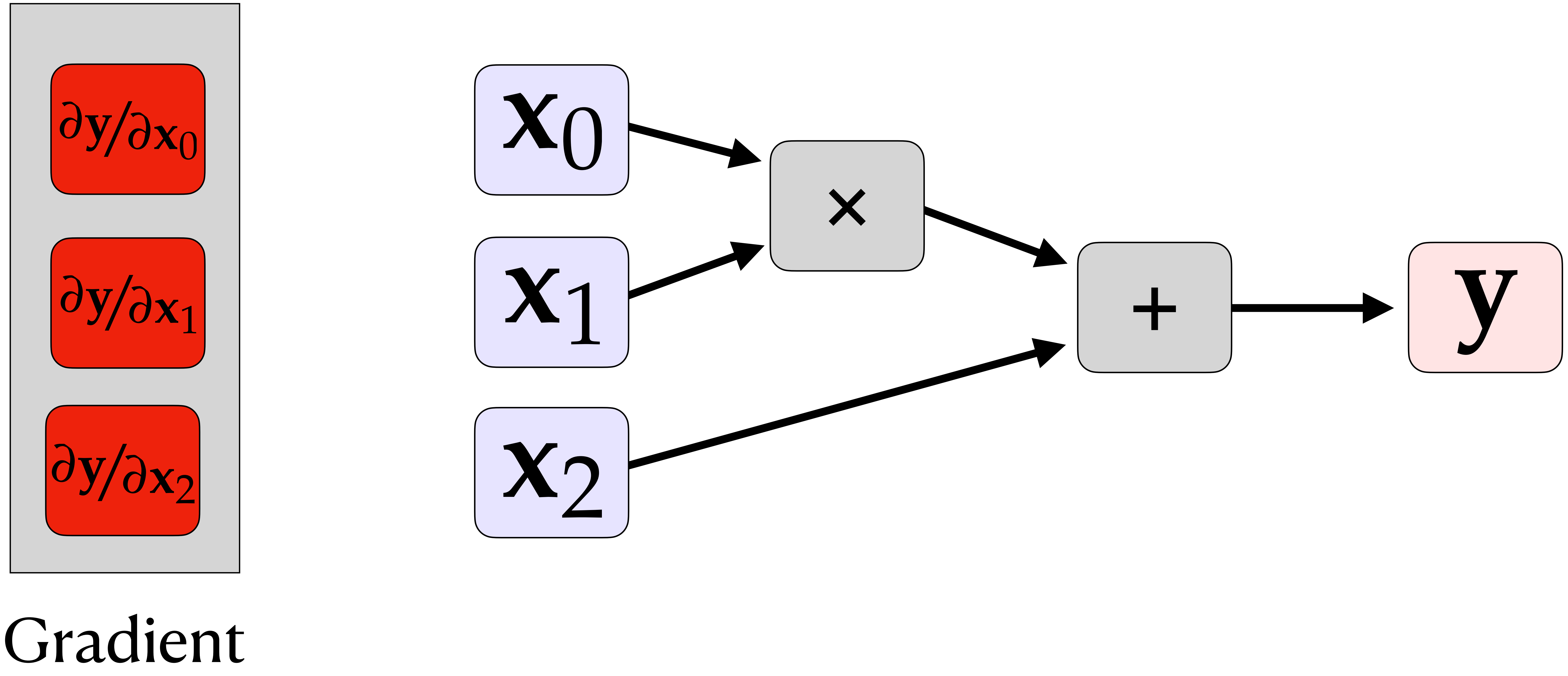

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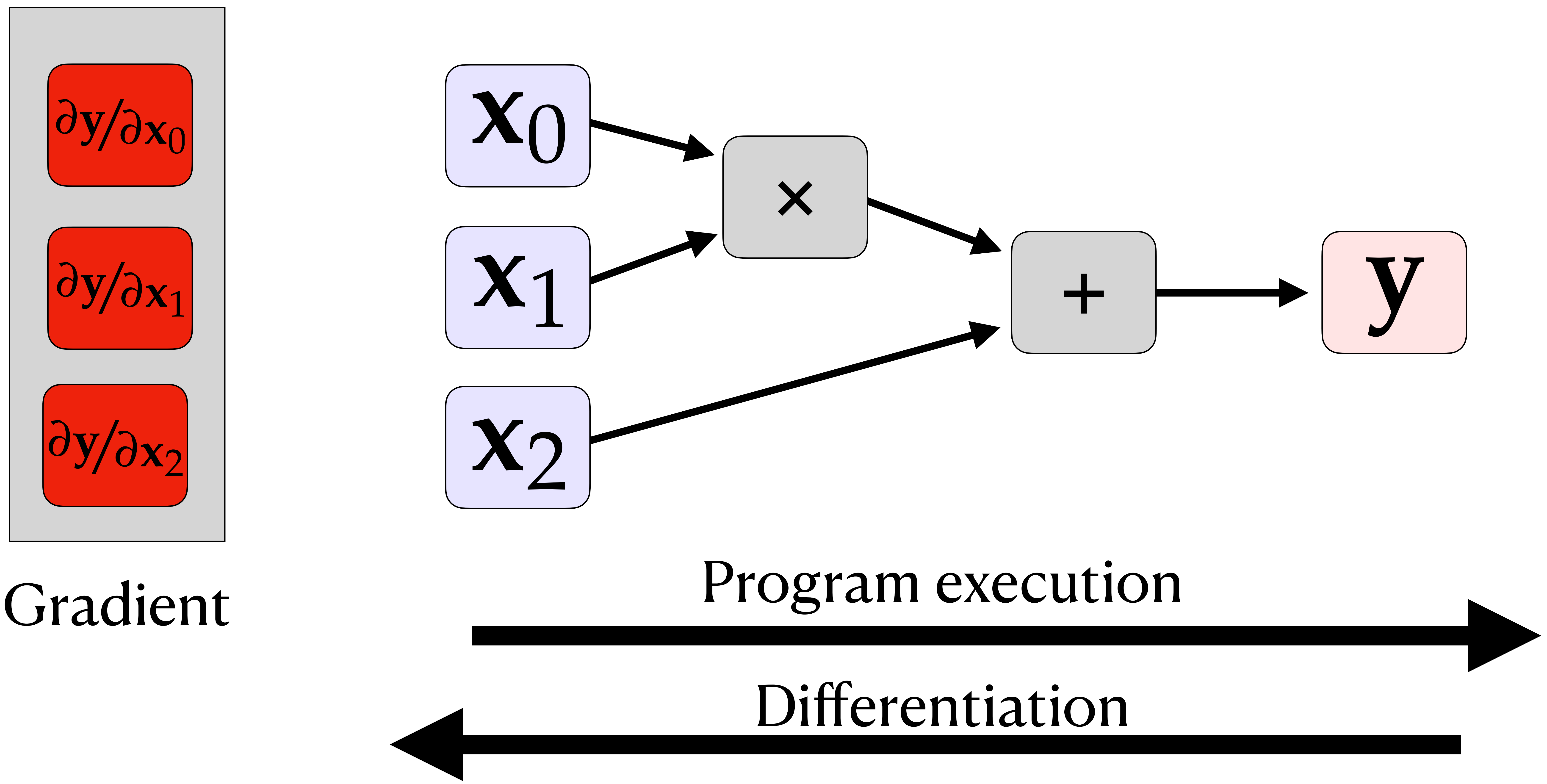

The Jacobian of multidimensional functions

Another way to think about forward/reverse mode AD

$$\mathbf{J}_f(\mathbf{x})$$

The Jacobian of multidimensional functions

Another way to think about forward/reverse mode AD

$$\mathbf{J}_f(\mathbf{x}) = \frac{f(\mathbf{x})}{\partial \mathbf{x}}$$

The Jacobian of multidimensional functions

Another way to think about forward/reverse mode AD

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

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

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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:

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Forward mode: computes $\mathbf{J}_f\,\mathbf{y}$

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

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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

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

Strategy 2: AD by recording onto a Tape

Differentiation task

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

Primal

```
a = α
b = -a
c = x · b
d = exp(c)
e = a · d
```

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Differentiation task

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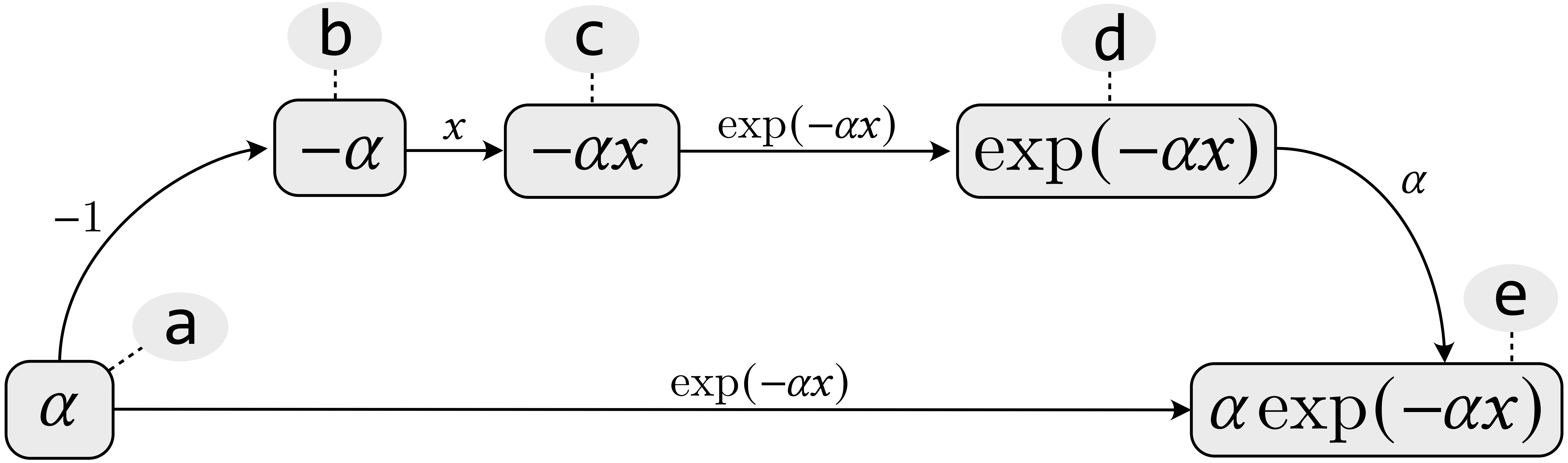
Tape / computation graph



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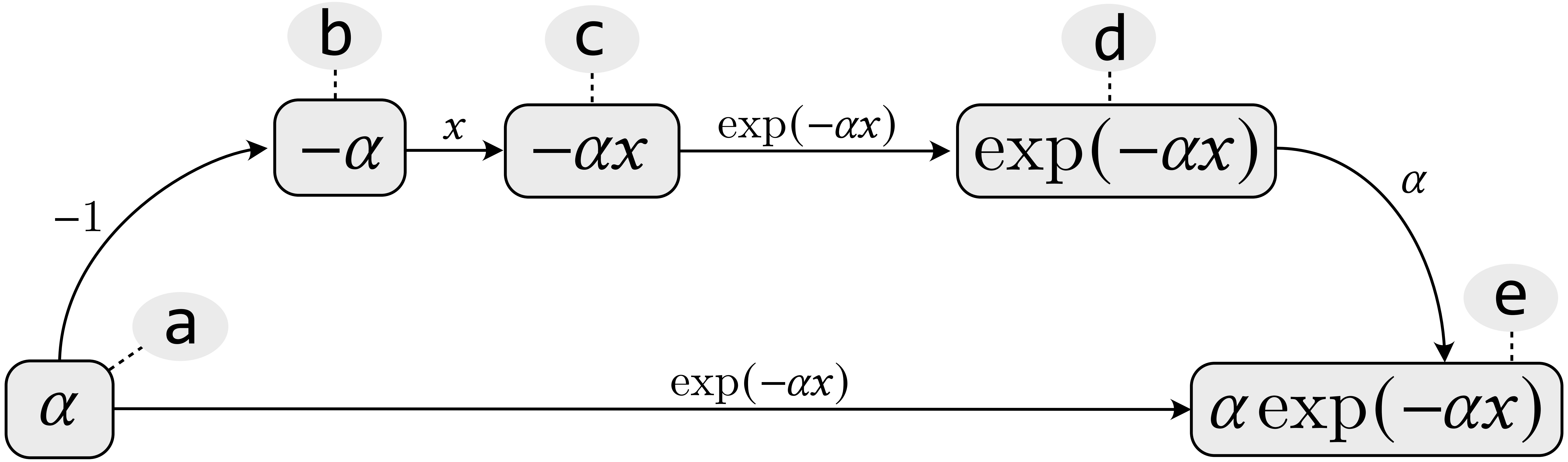

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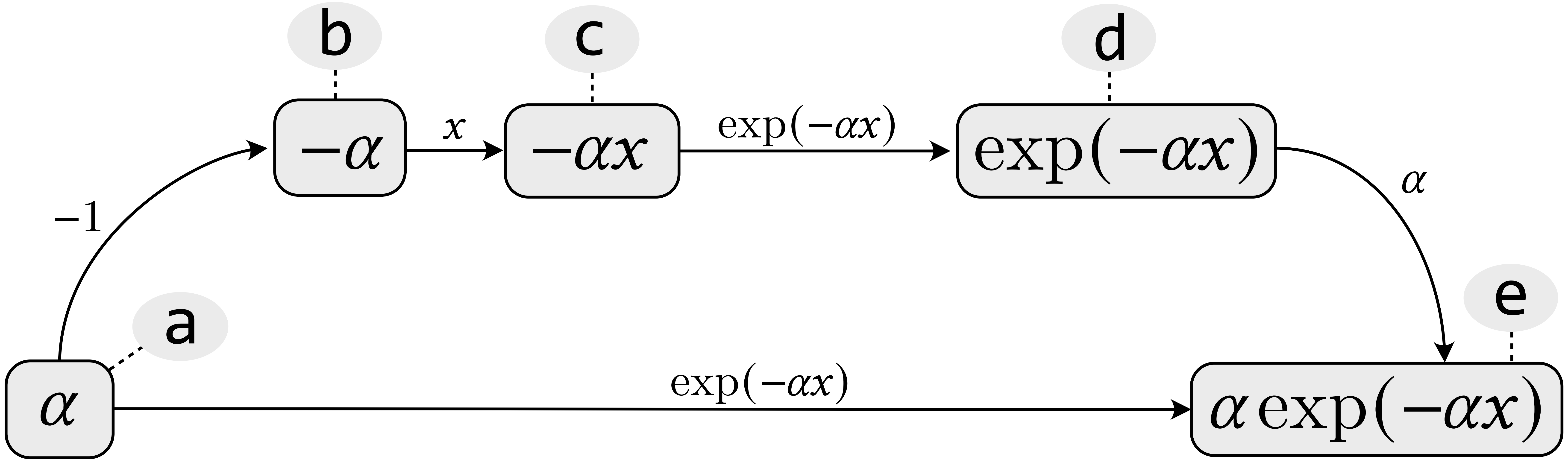

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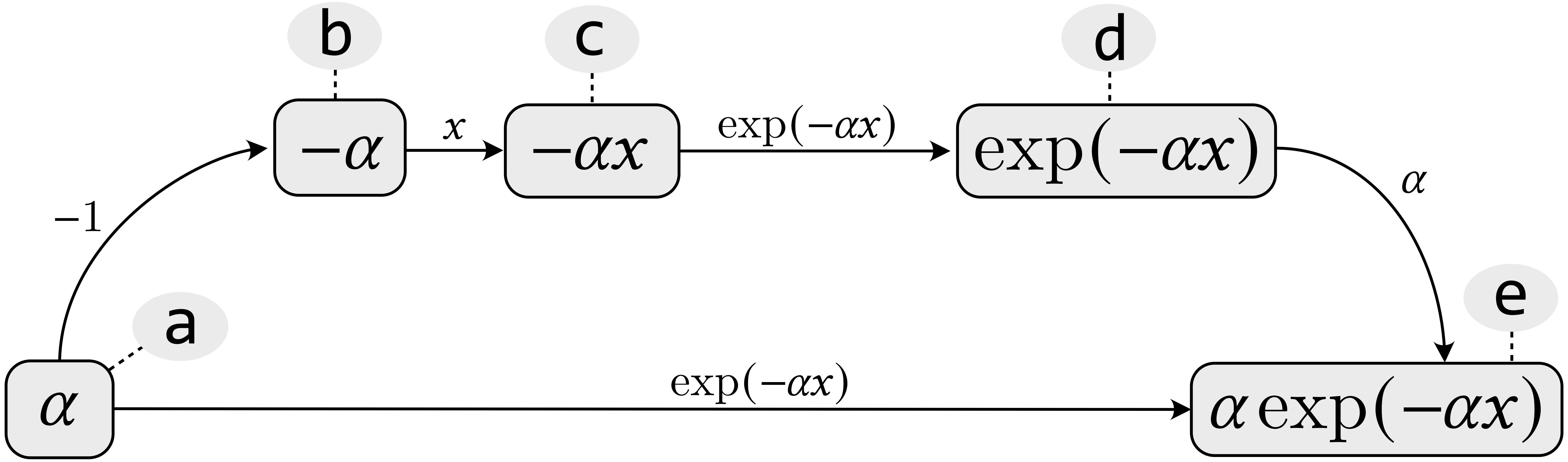

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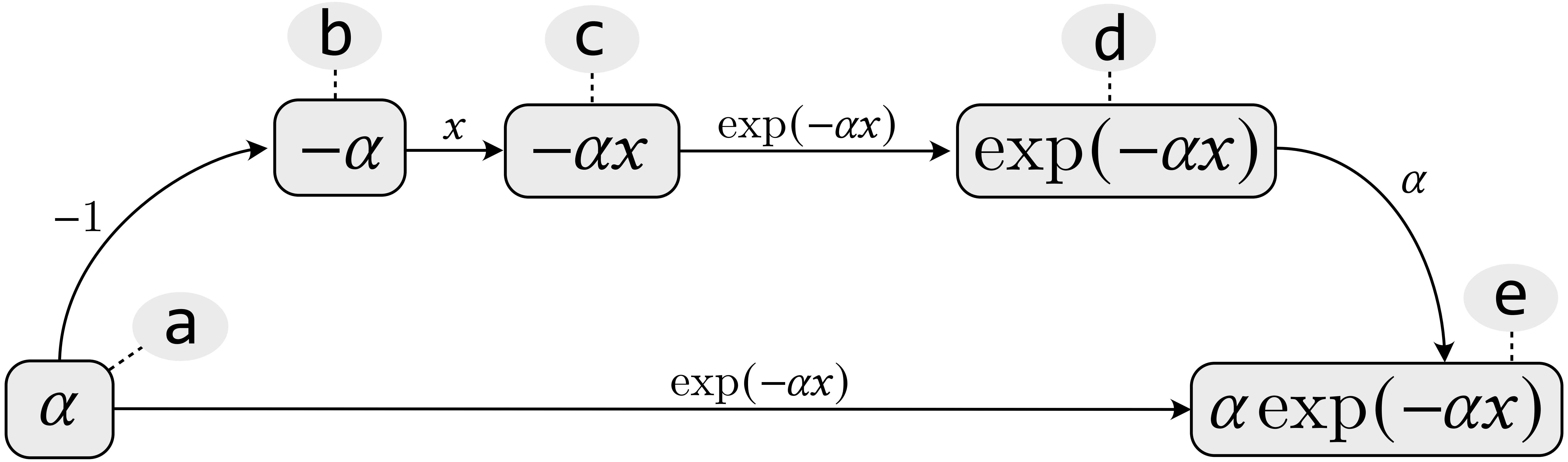

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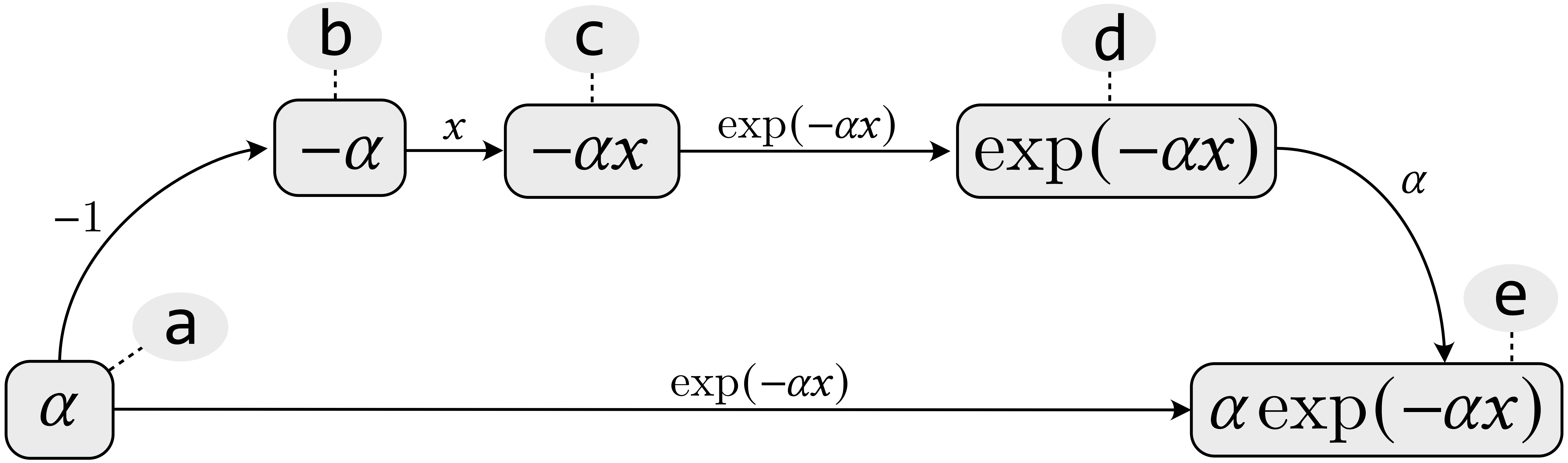

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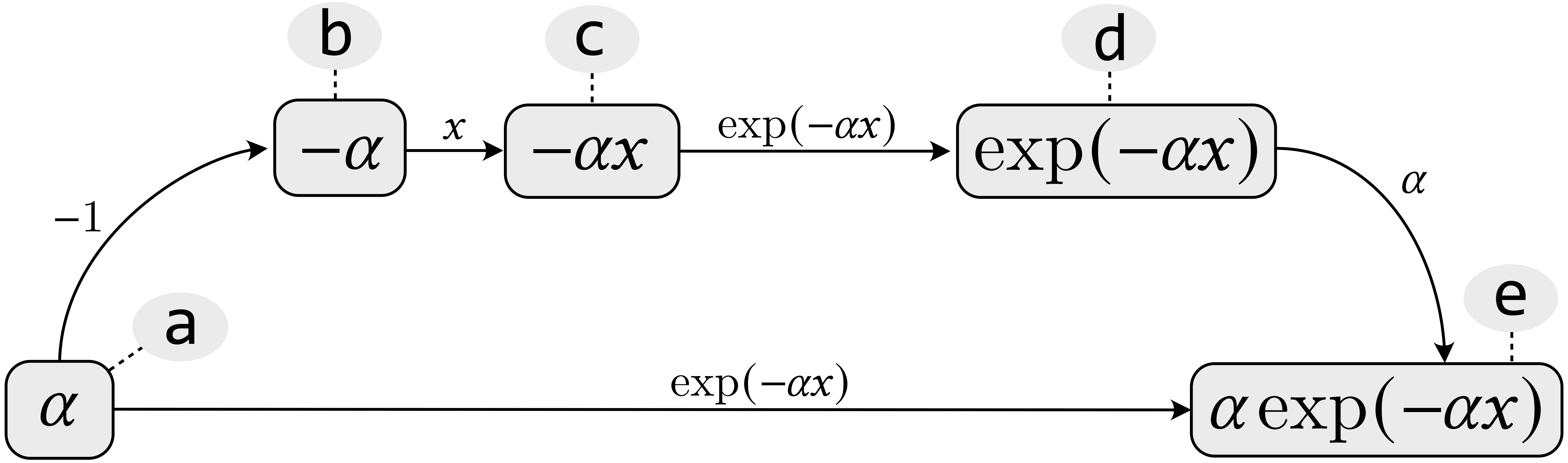

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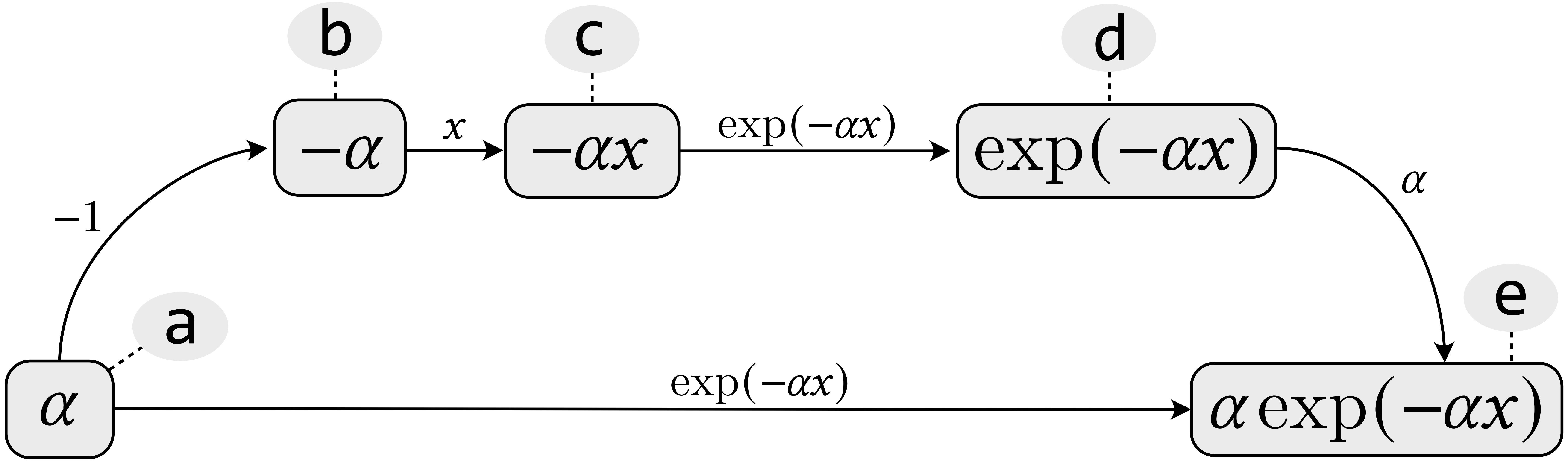

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Reverse mode

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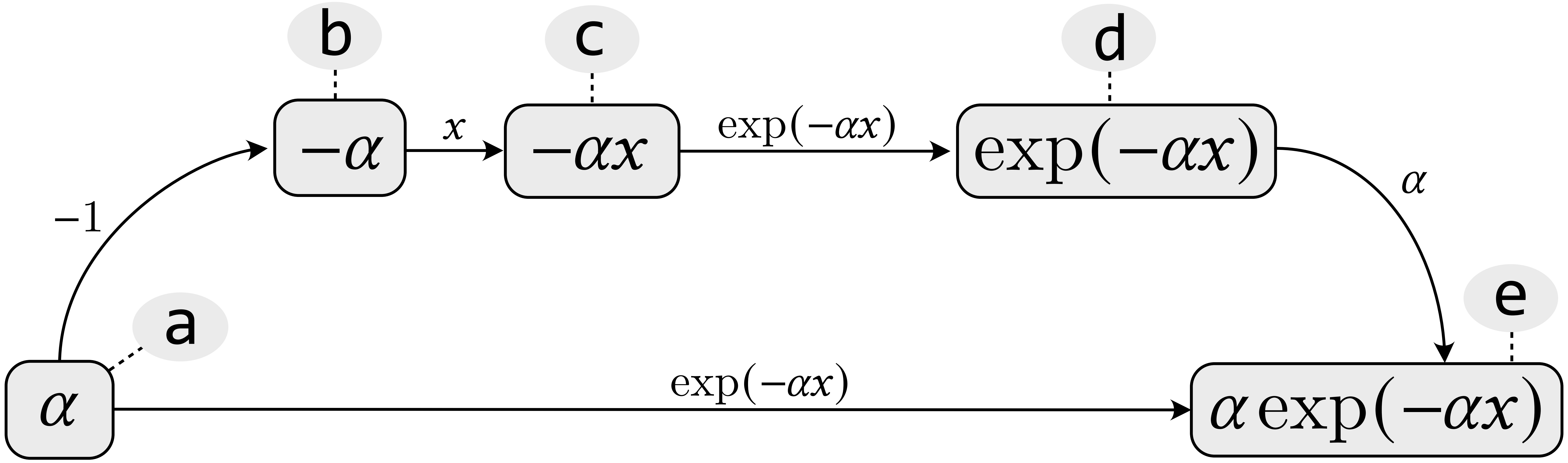

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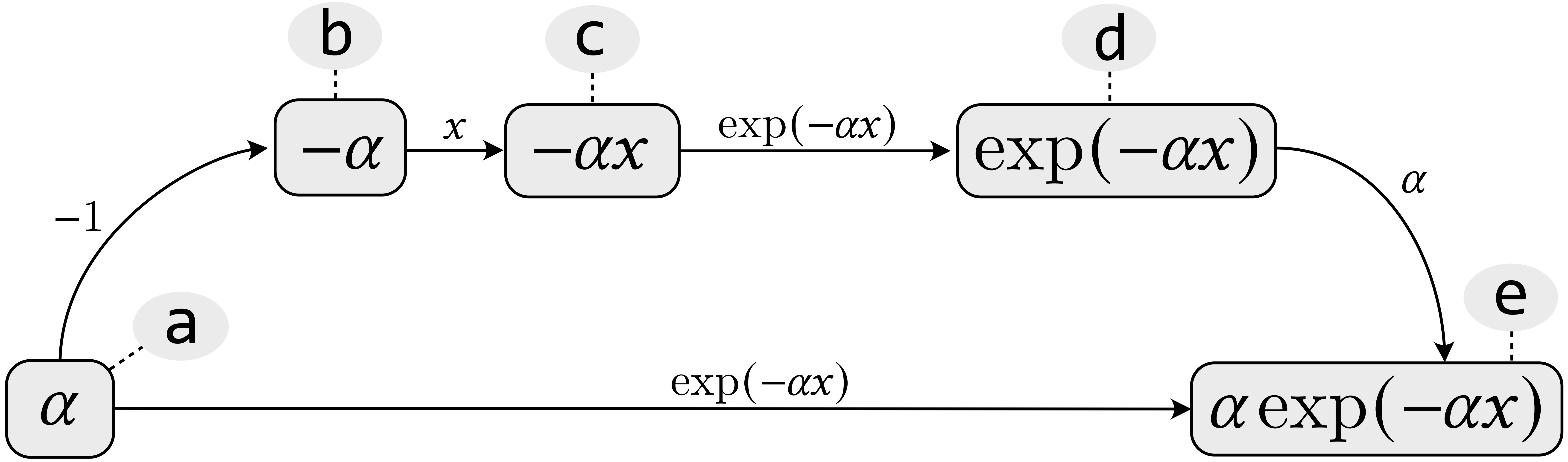

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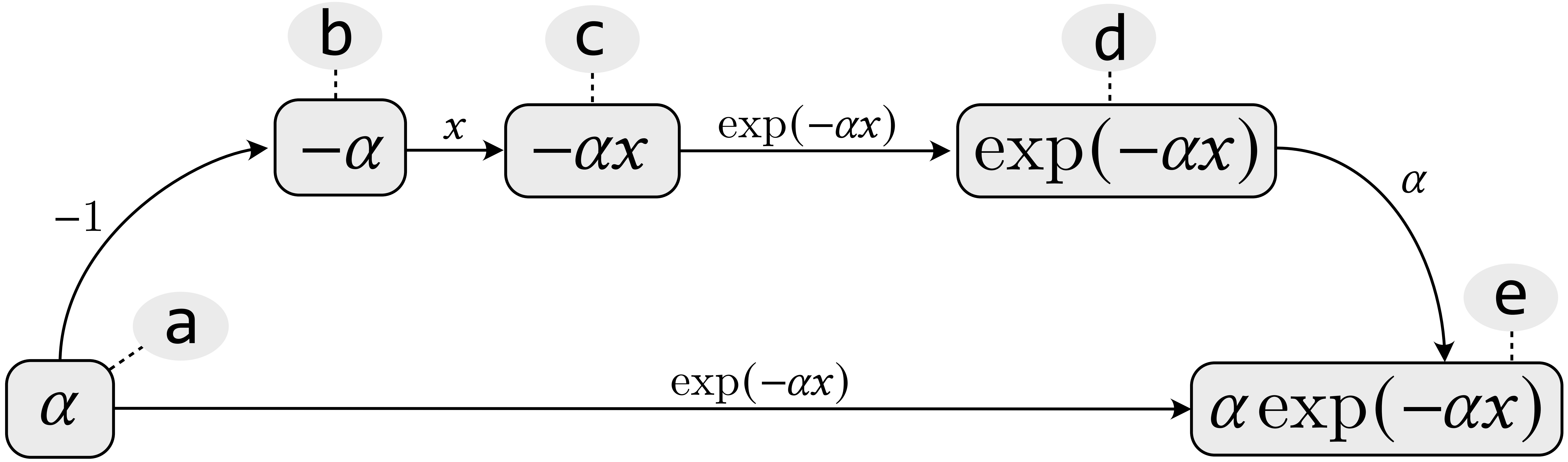

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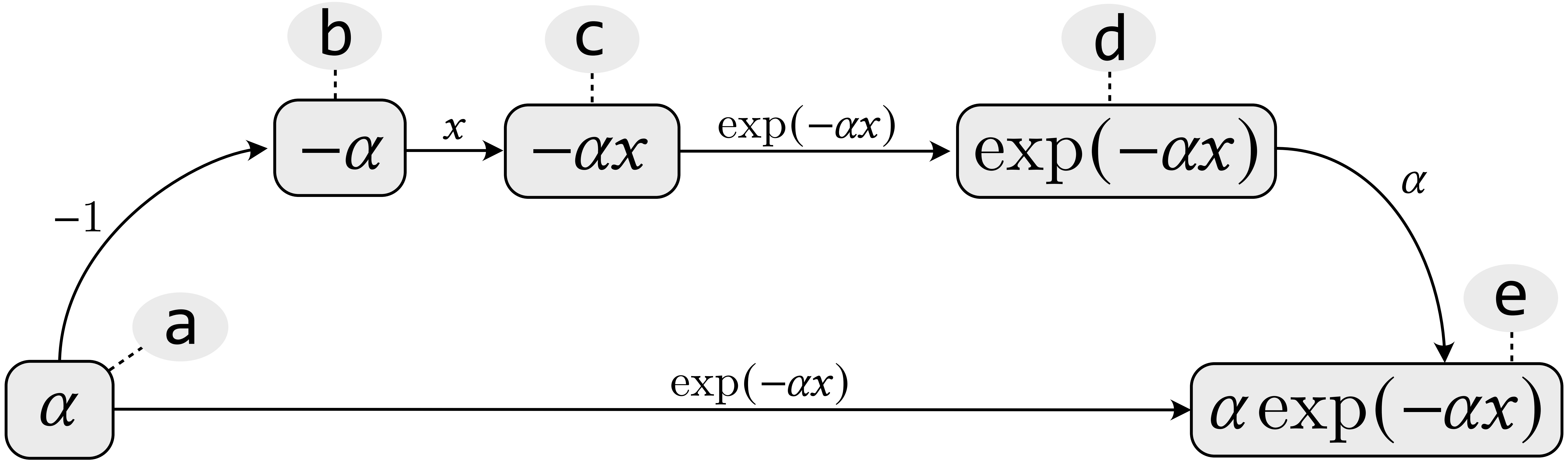

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Reverse mode

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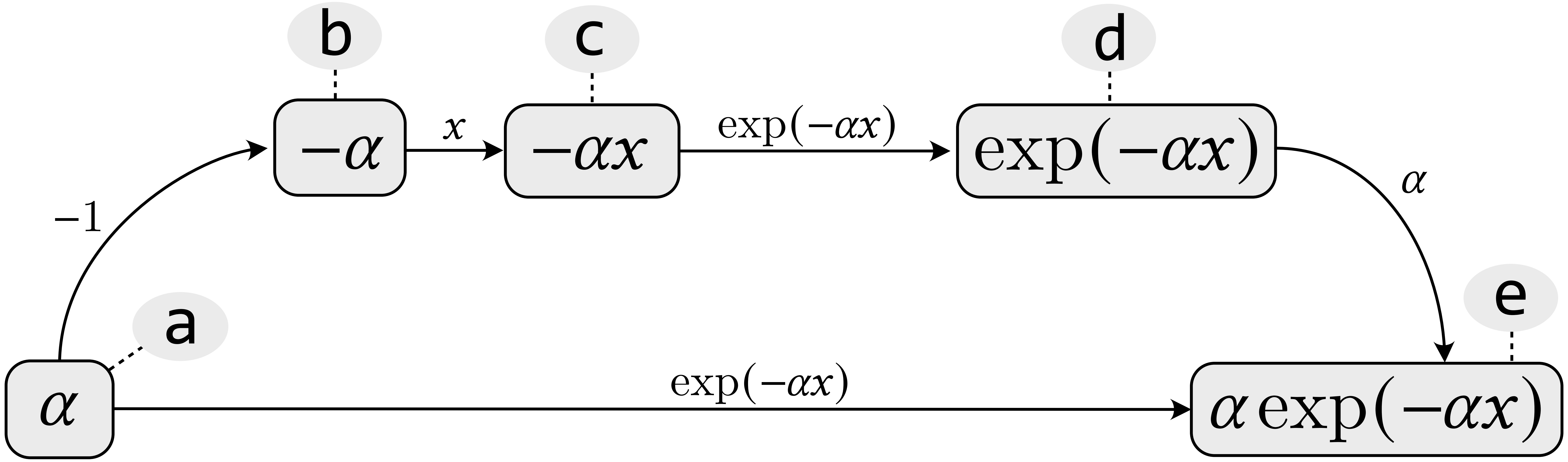

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```

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
```

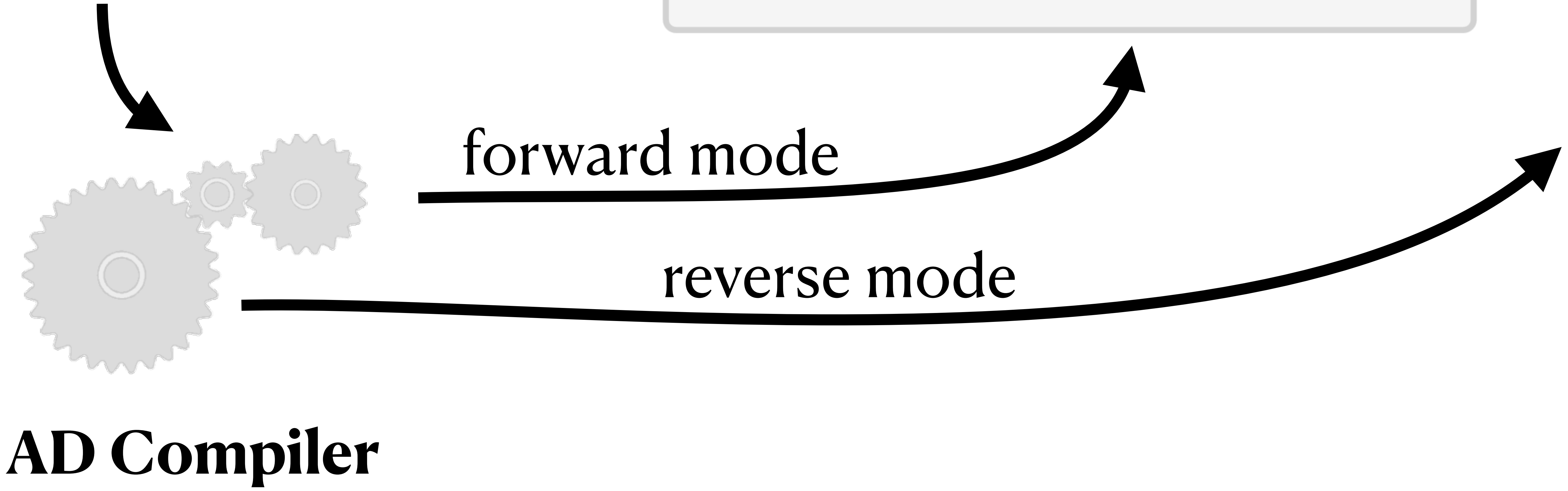
Strategy 3: AD by code transformation

(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
```

```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

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.

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.

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

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AD Implementation strategies

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

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AD Implementation strategies

Dual numbers

Simple and efficient.

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).

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.

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

Forward mode

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.

Reverse mode

Dual numbers

Does not make sense for reverse mode.

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

Forward mode

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.

Reverse mode

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Does not make sense for reverse mode.

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What everyone uses in practice.

Technique tree

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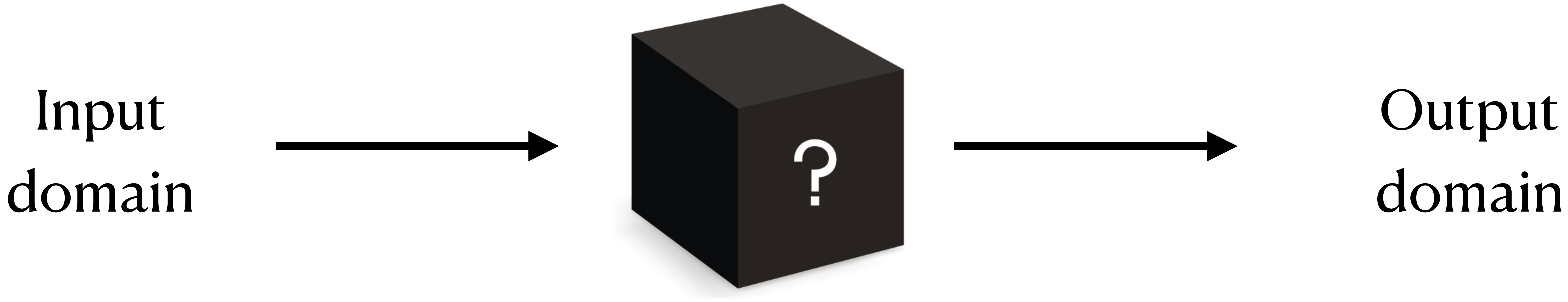
We have gradients.

Now, what?

"Inverse problems"

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

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



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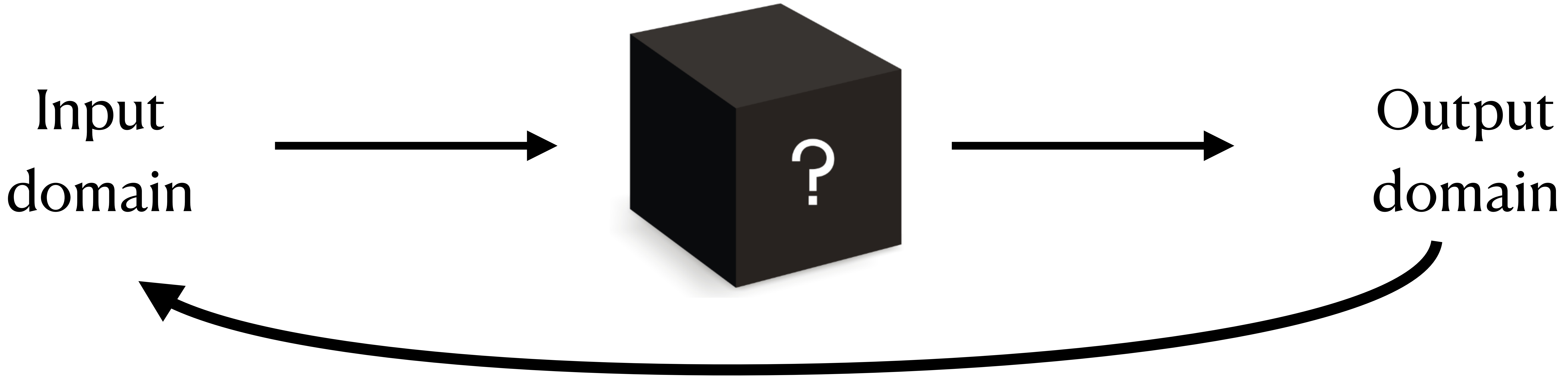
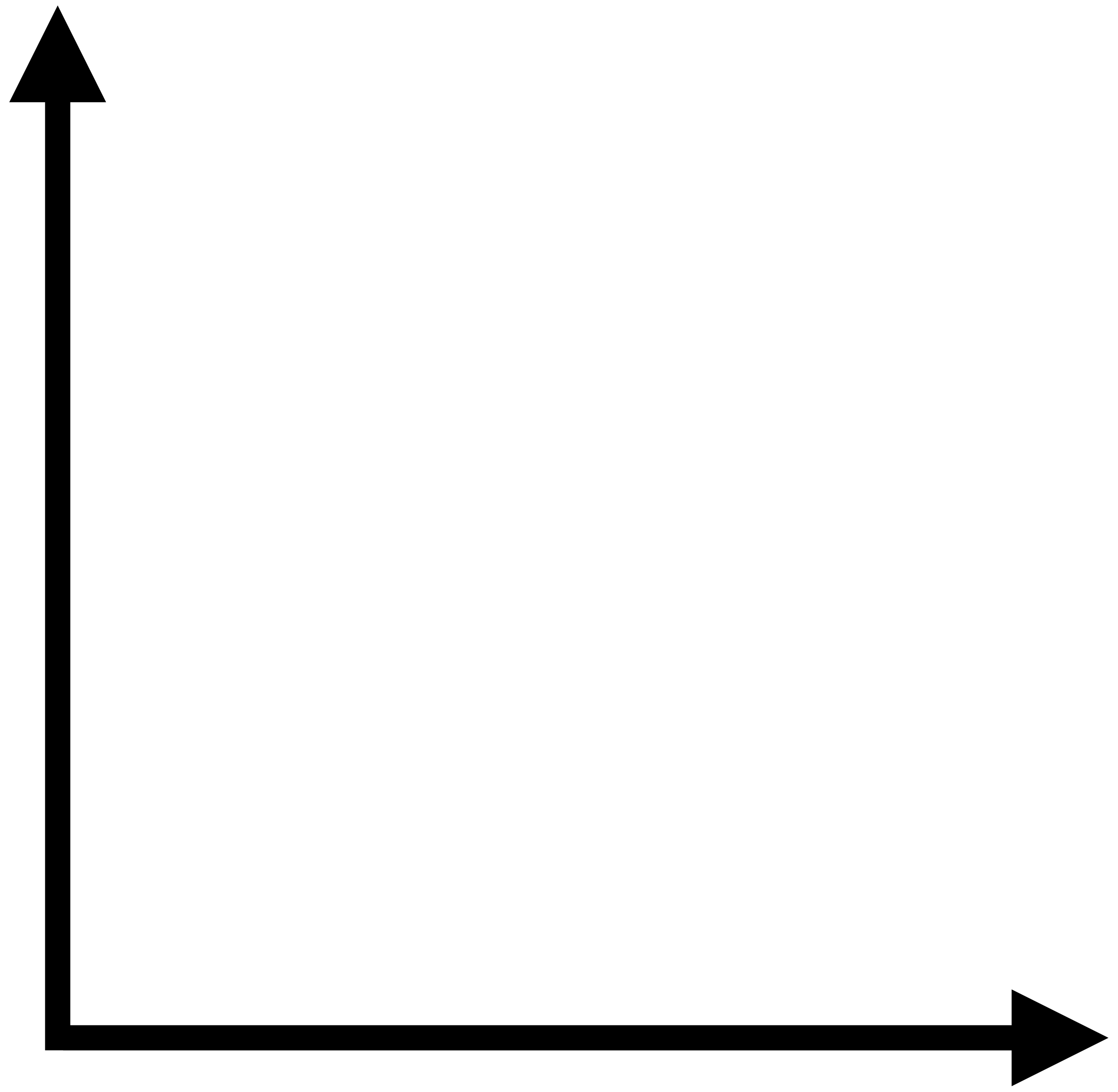


$$f^{-1}(\mathbf{x}) \ ?$$

Two important kinds of inverse problems



Root finding

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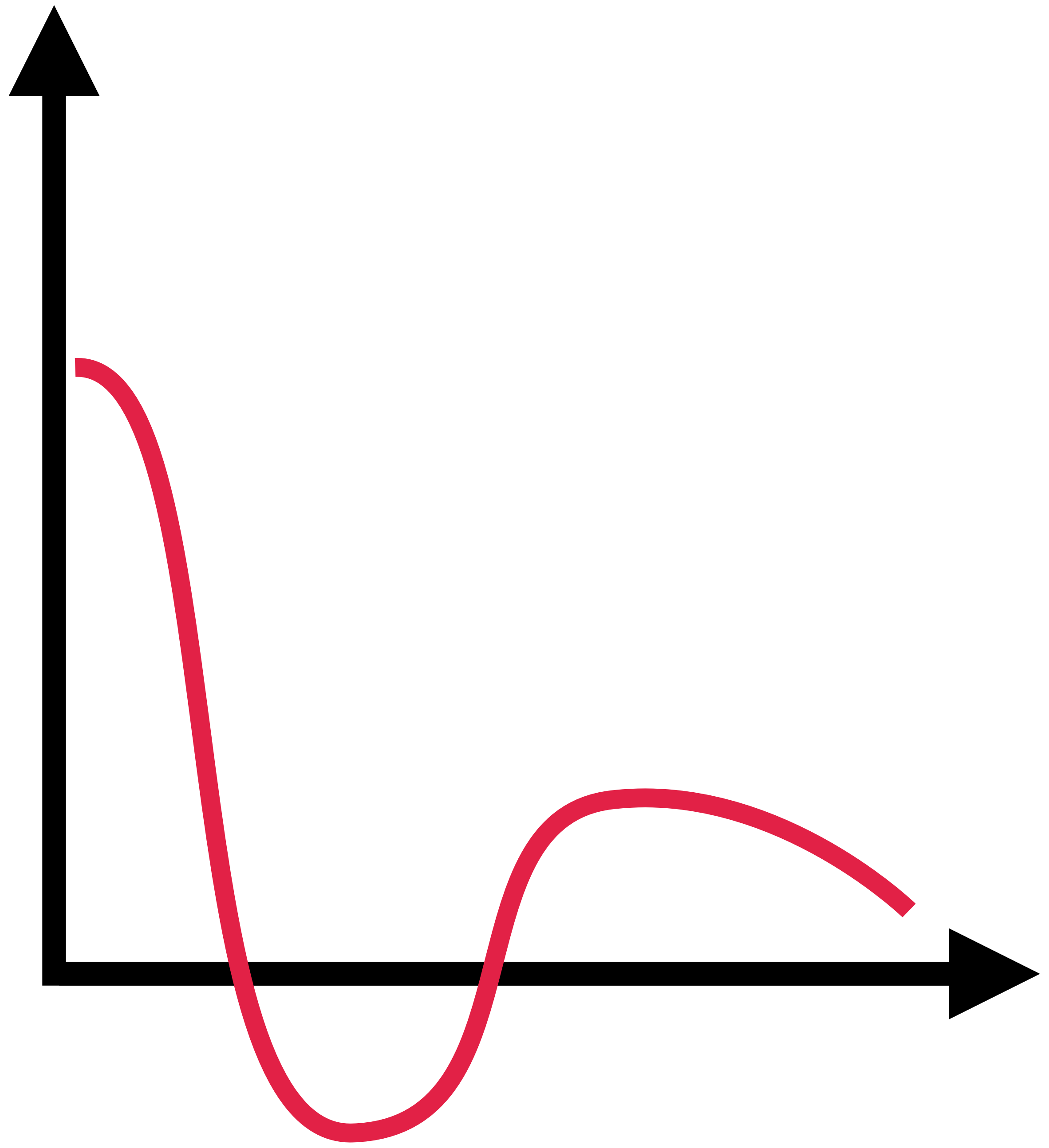

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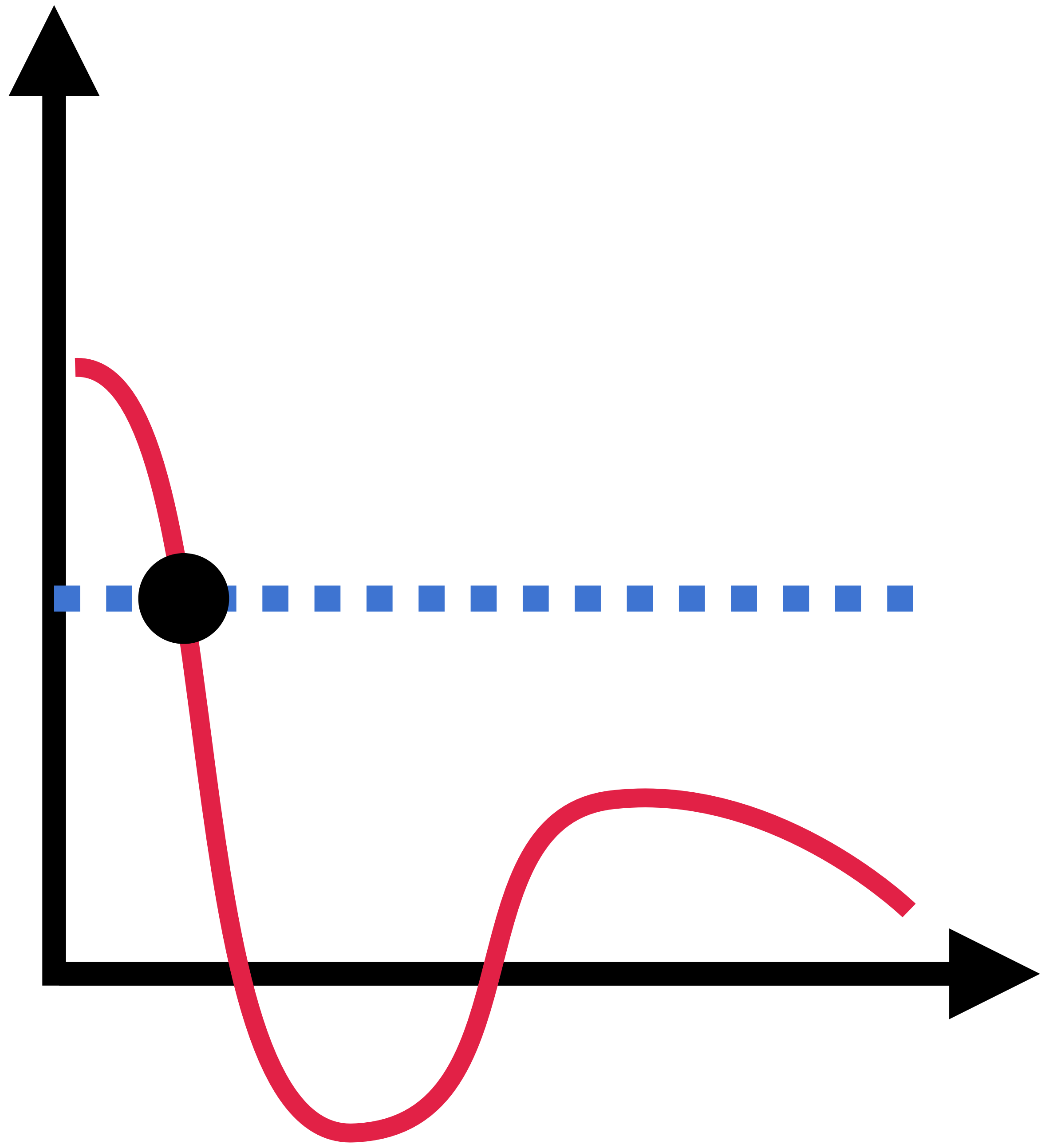

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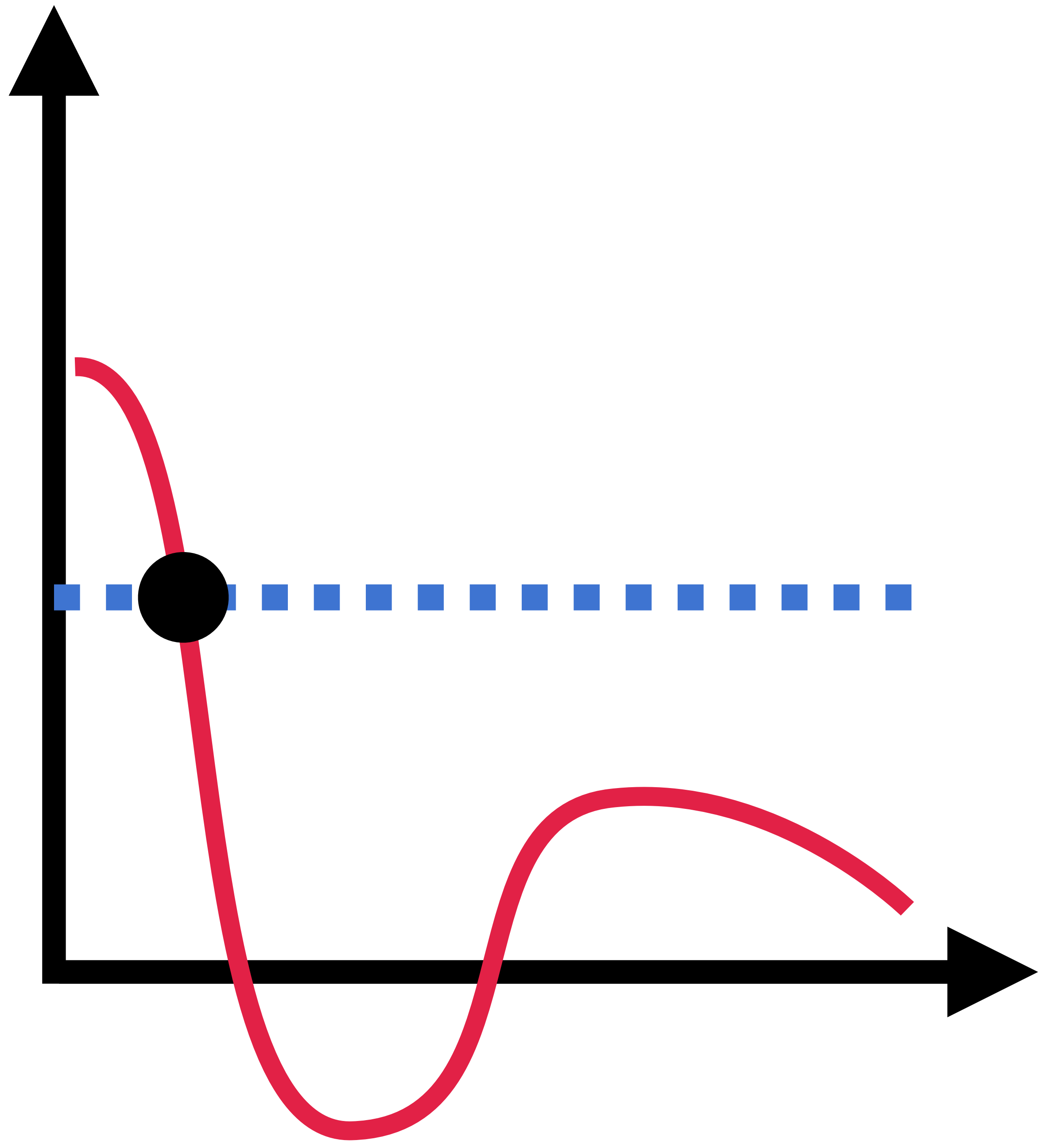

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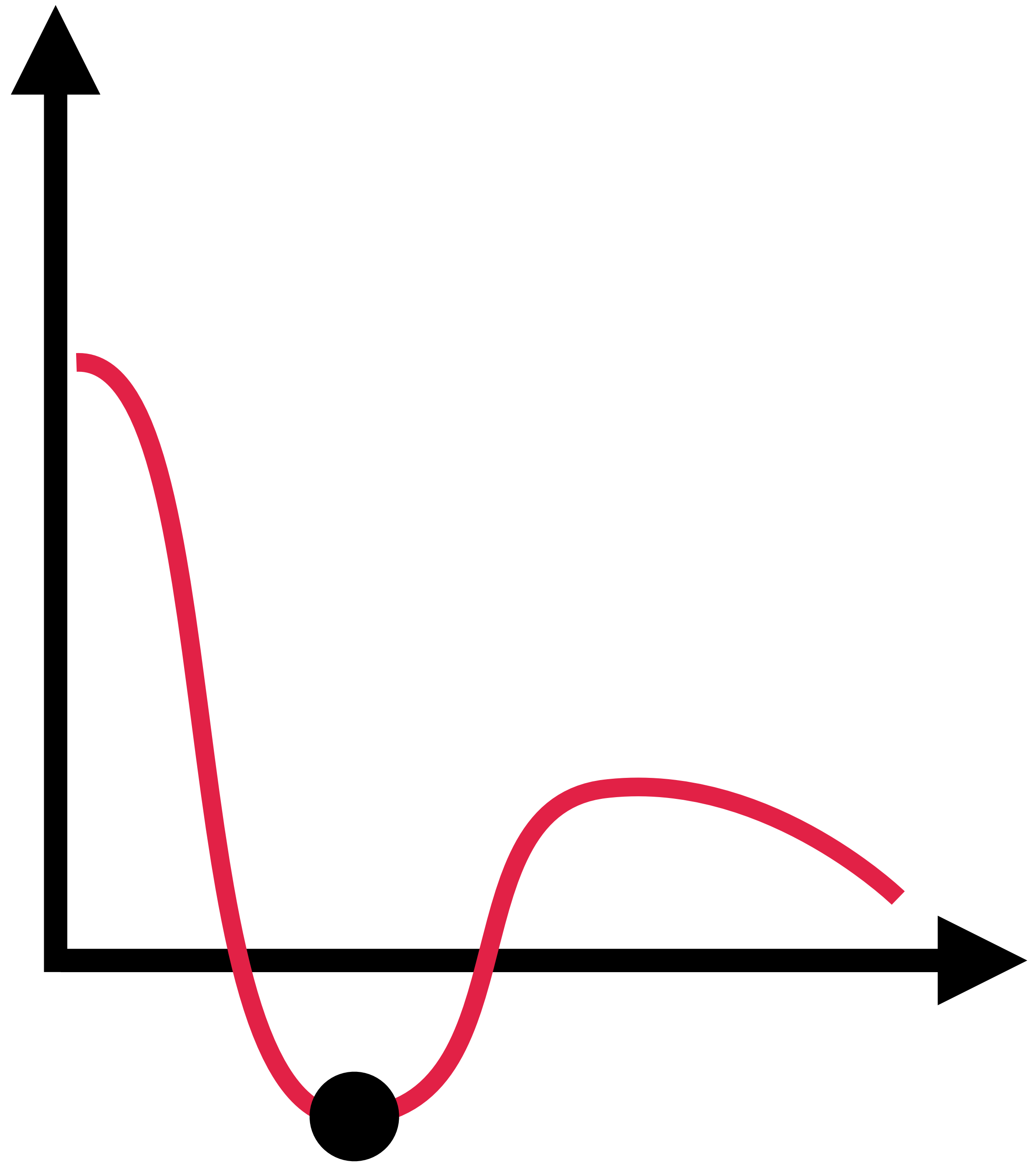

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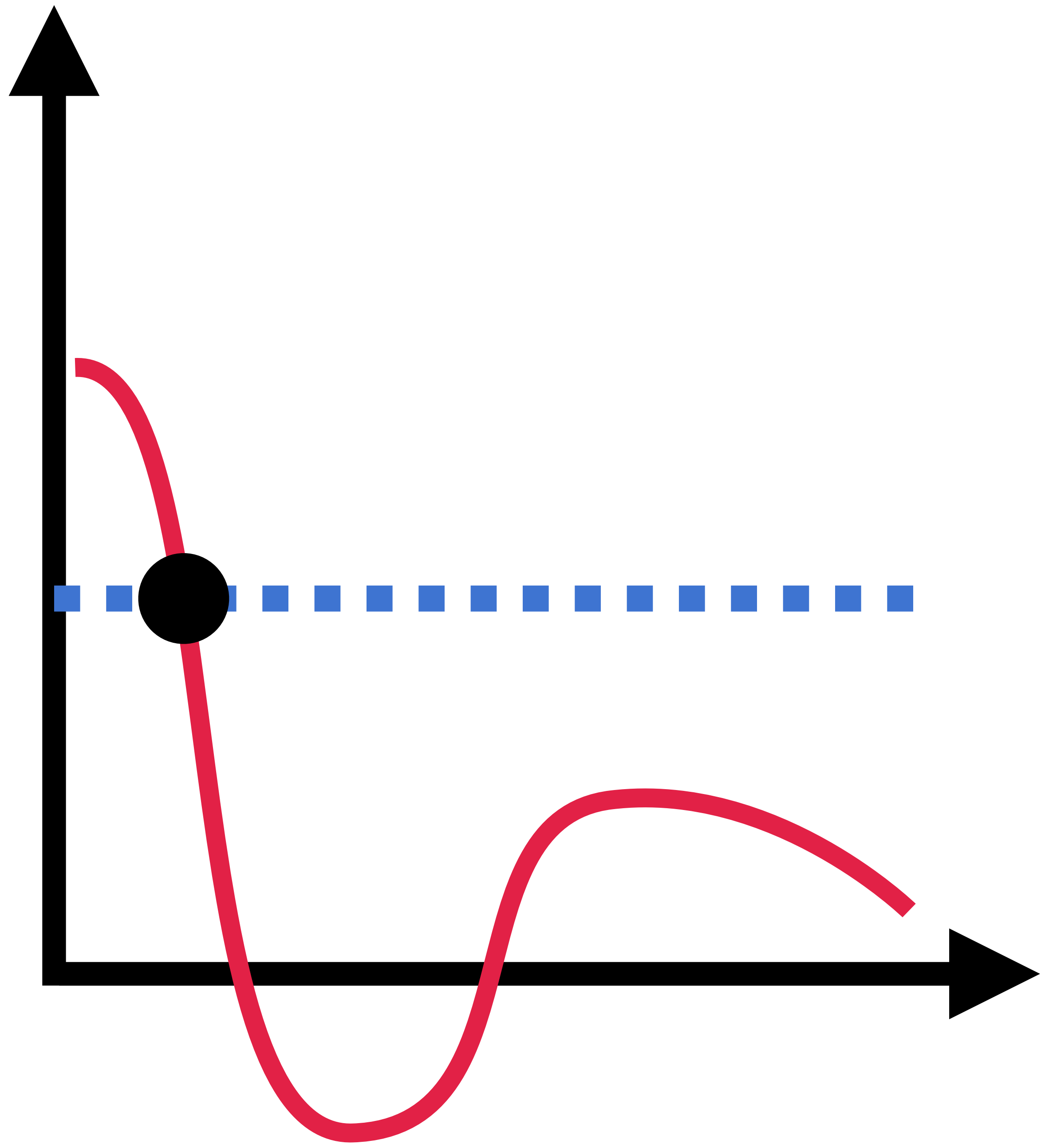

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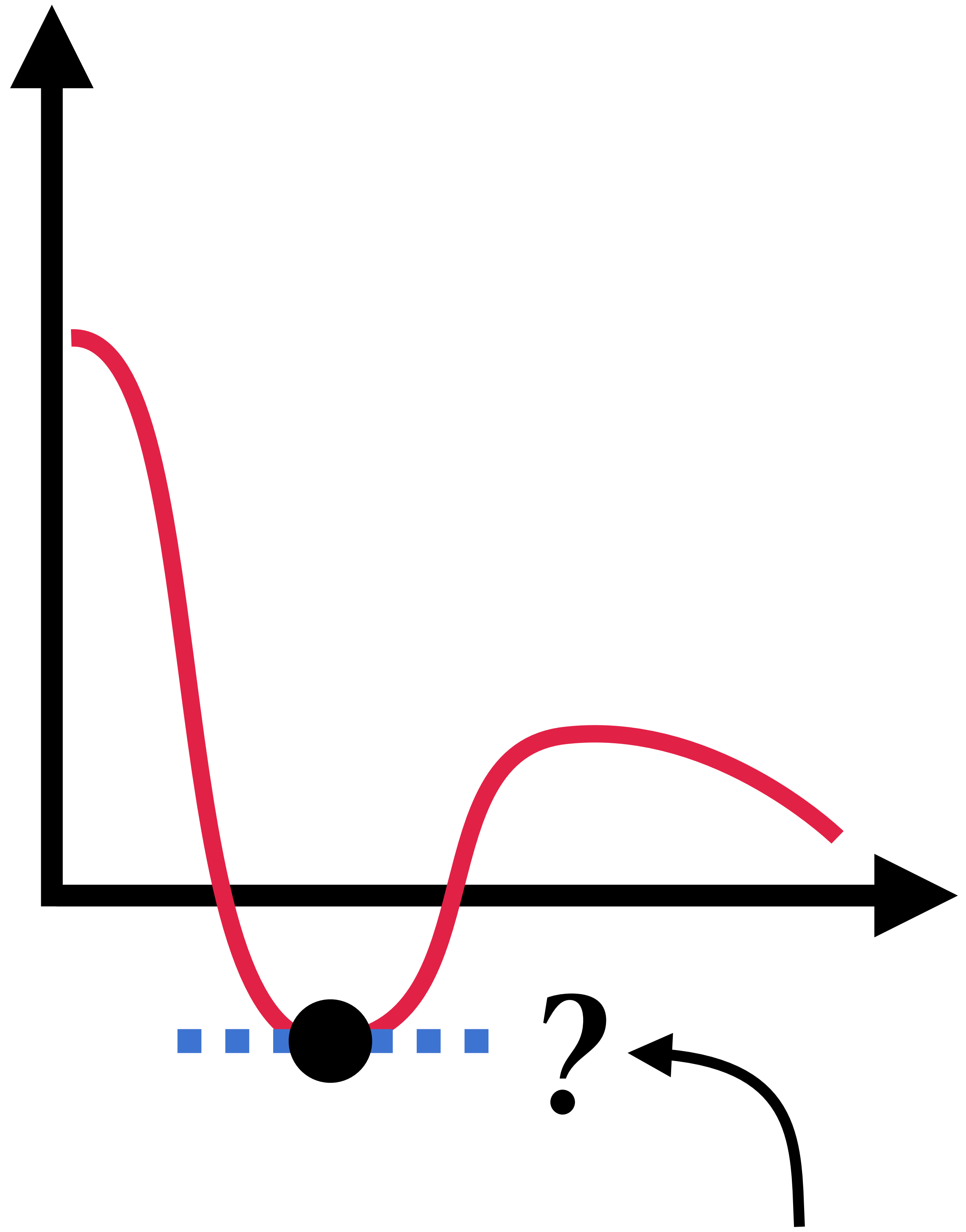

minimum Y value unknown, so this isn't exactly the same as root finding

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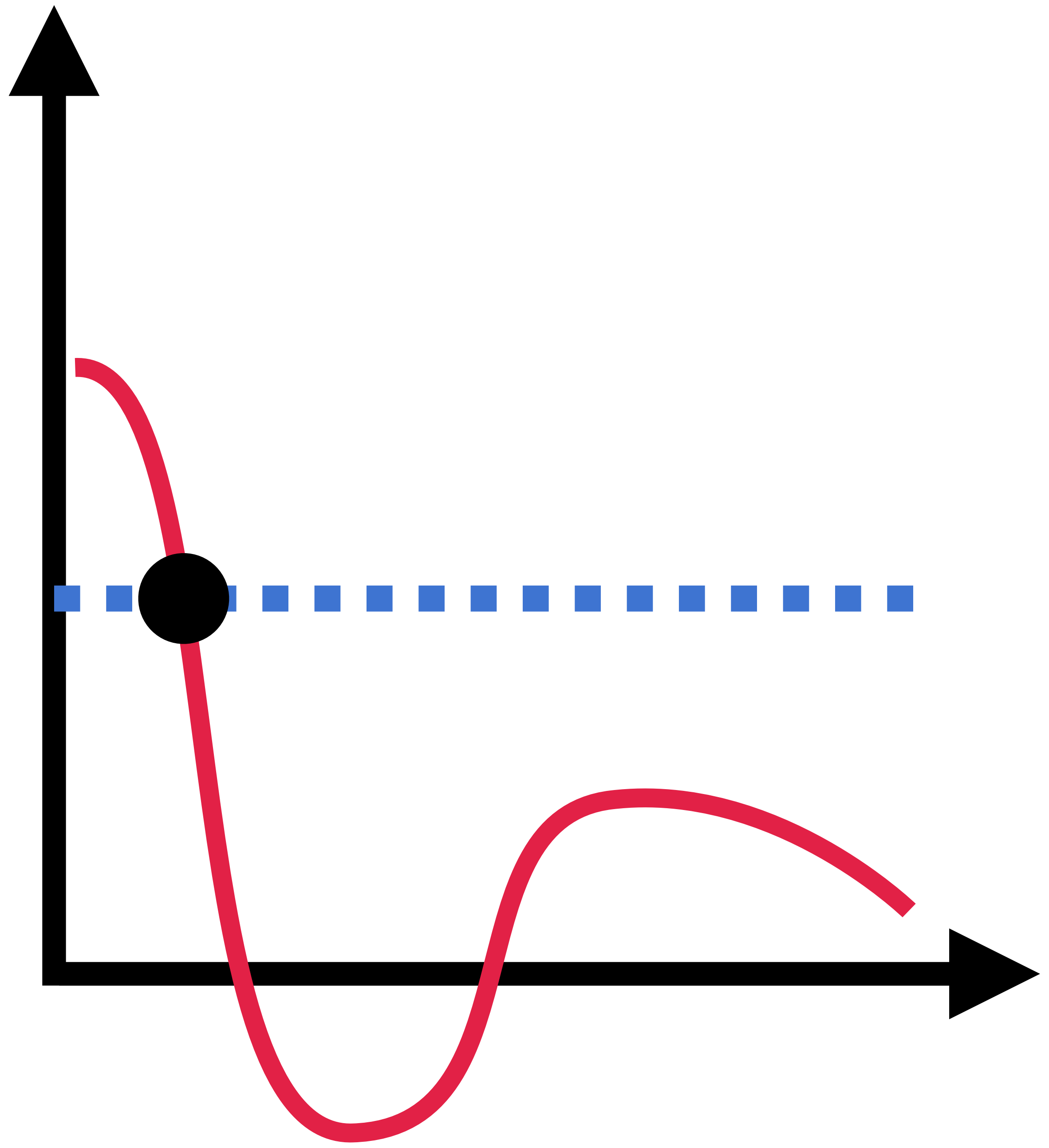

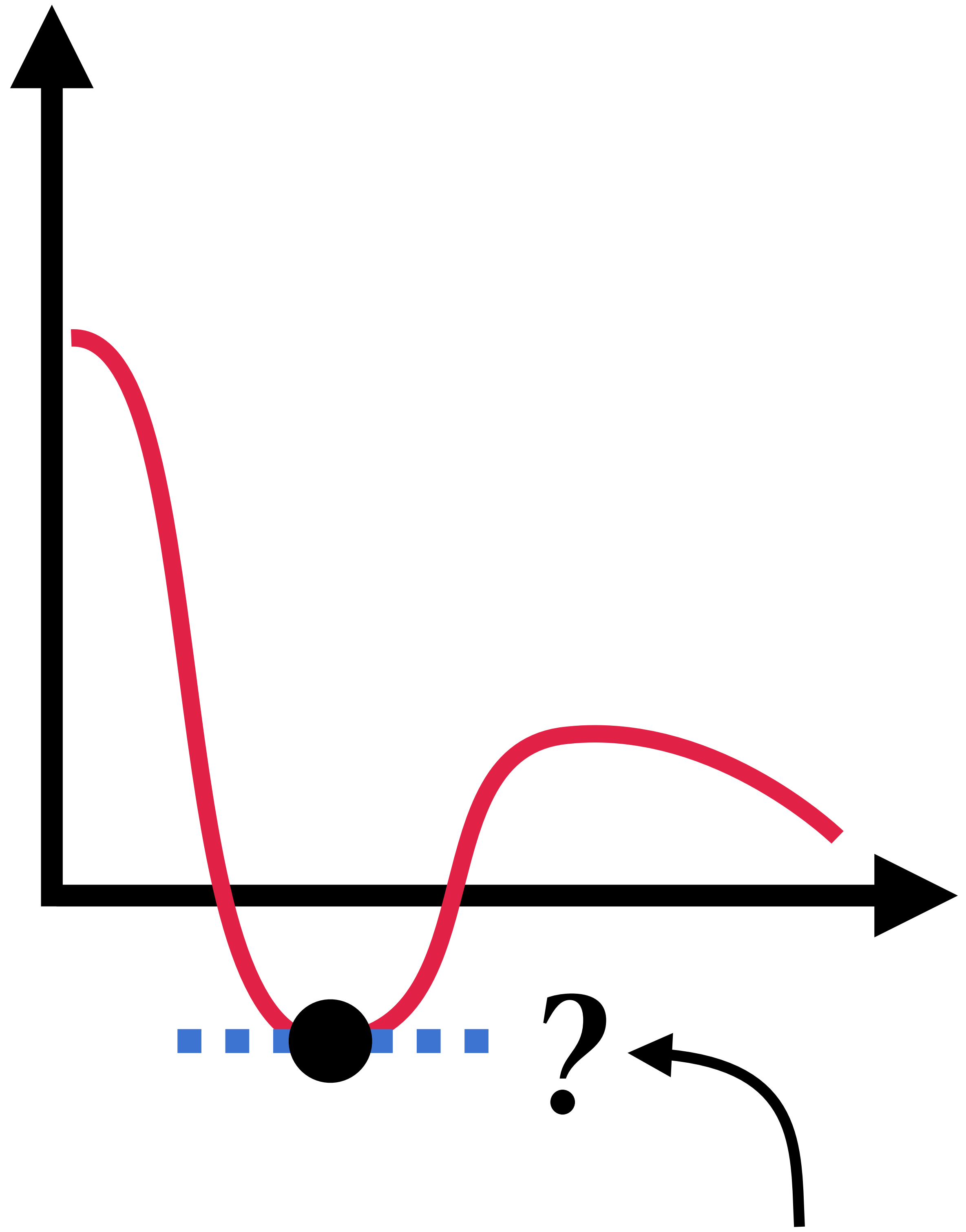

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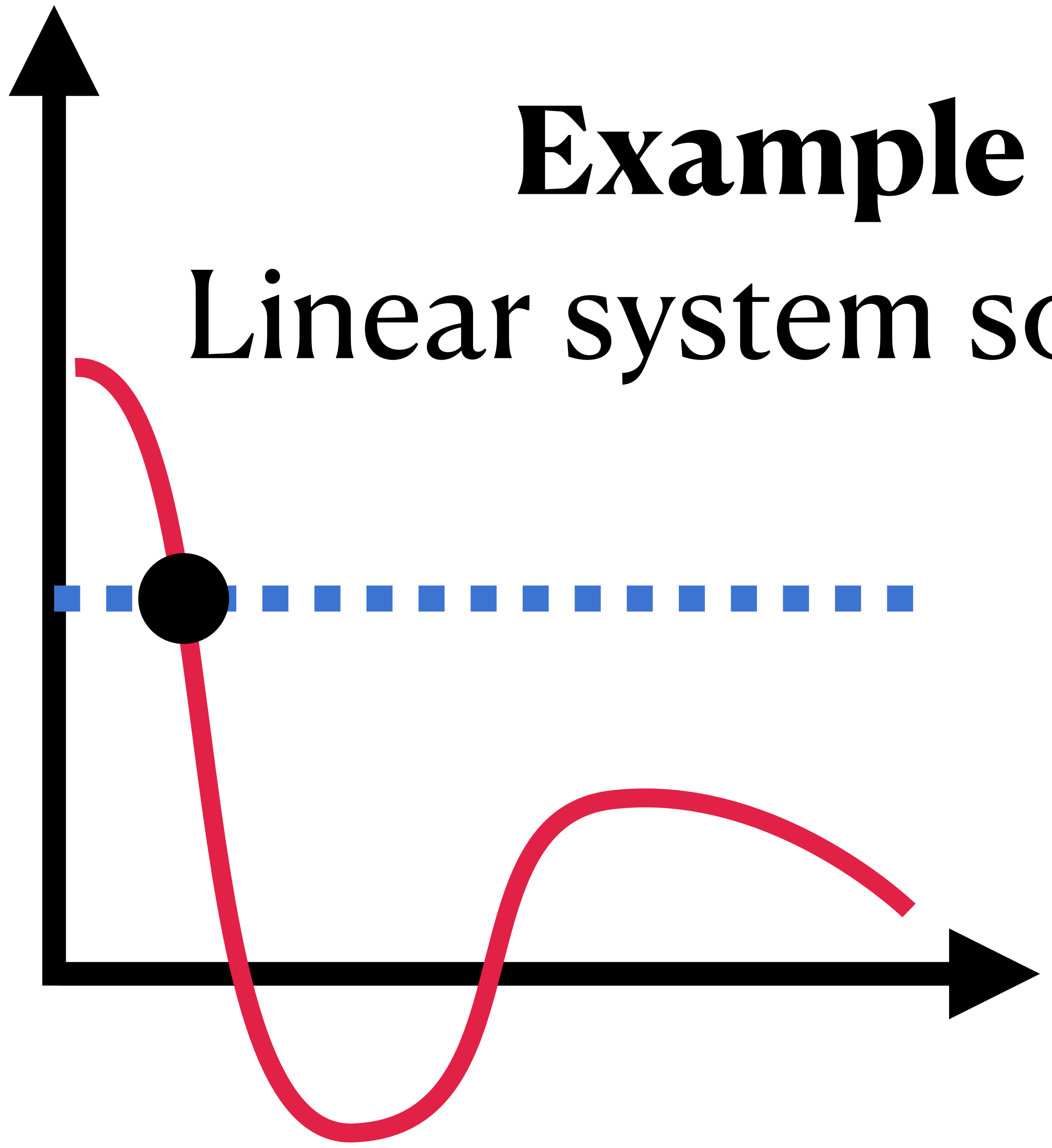

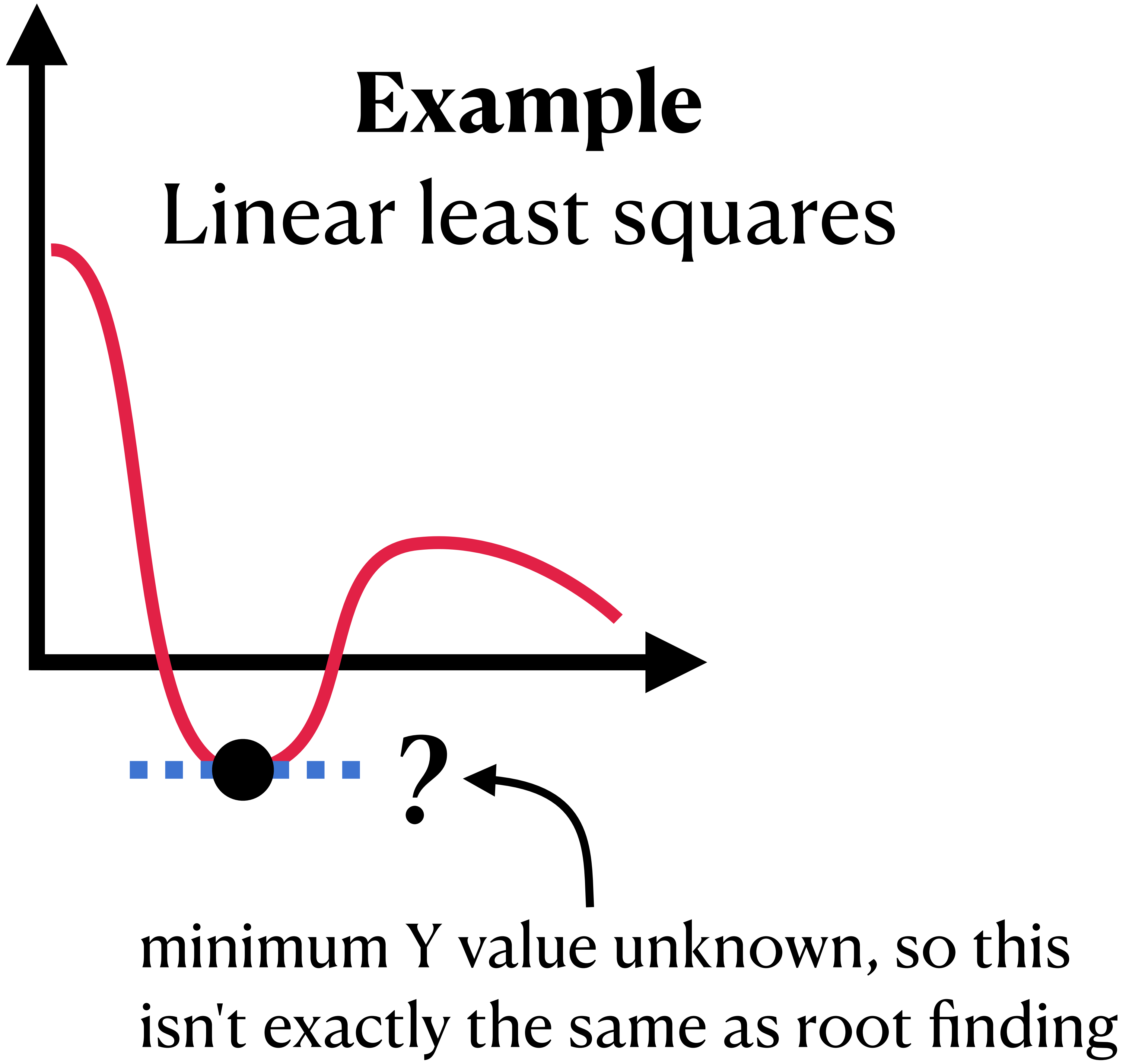

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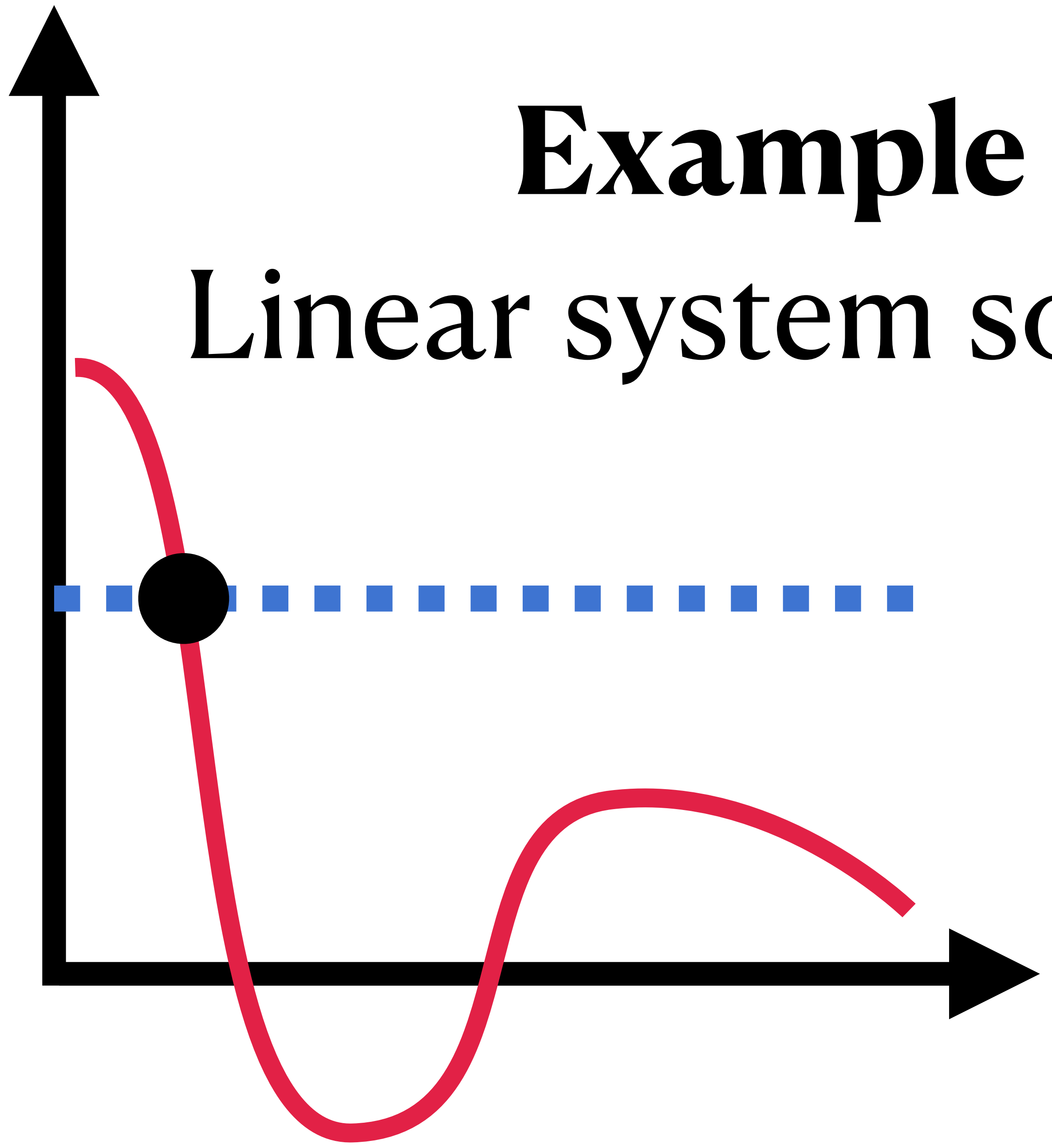
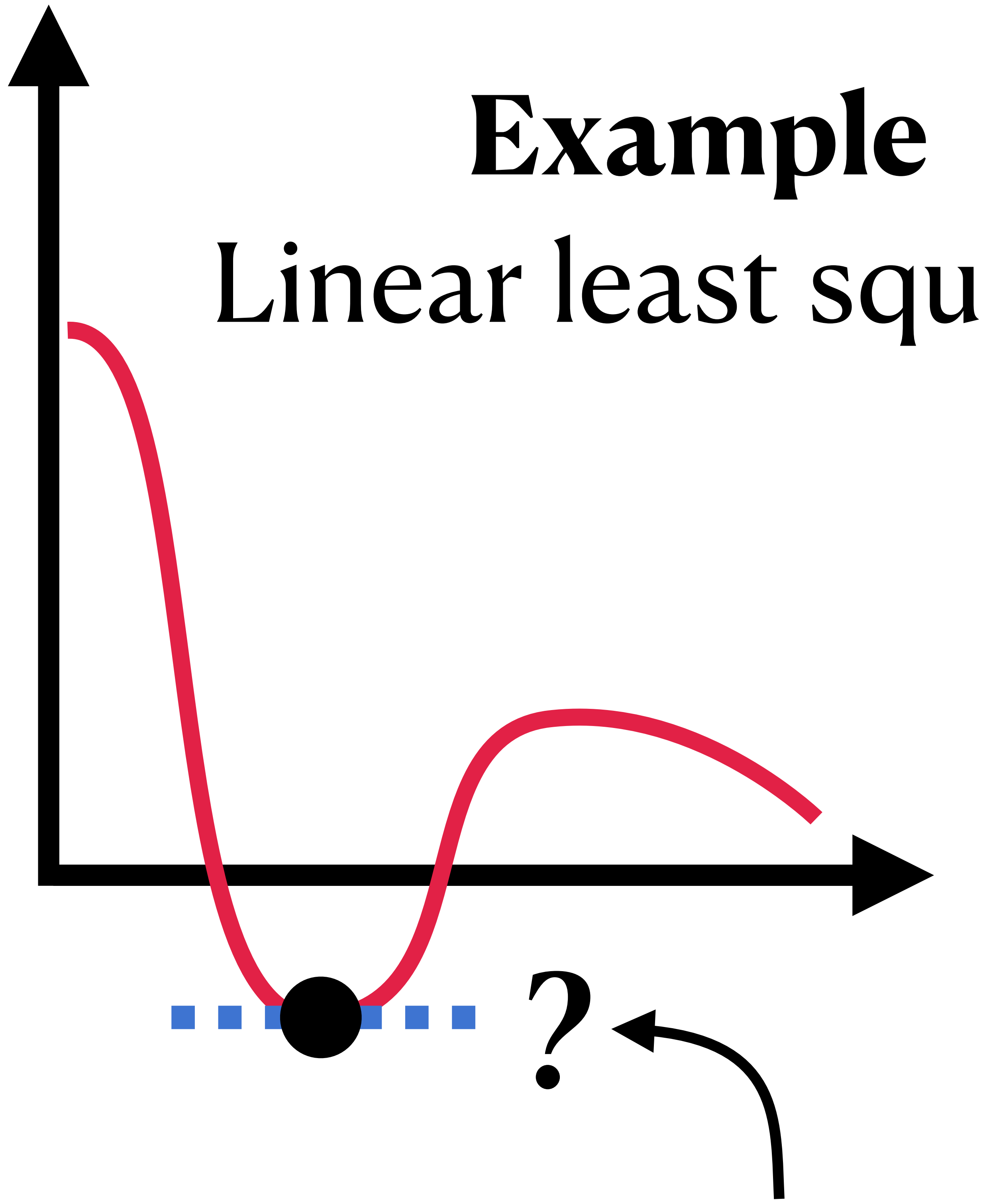


Example
Linear system solving



Example
Linear least squares

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

Conversion:
normal equations

Root finding ⟷ Optimization

problems can often be converted

Root finding

Let's start with a simple 1D problem

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

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

How many solutions?

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

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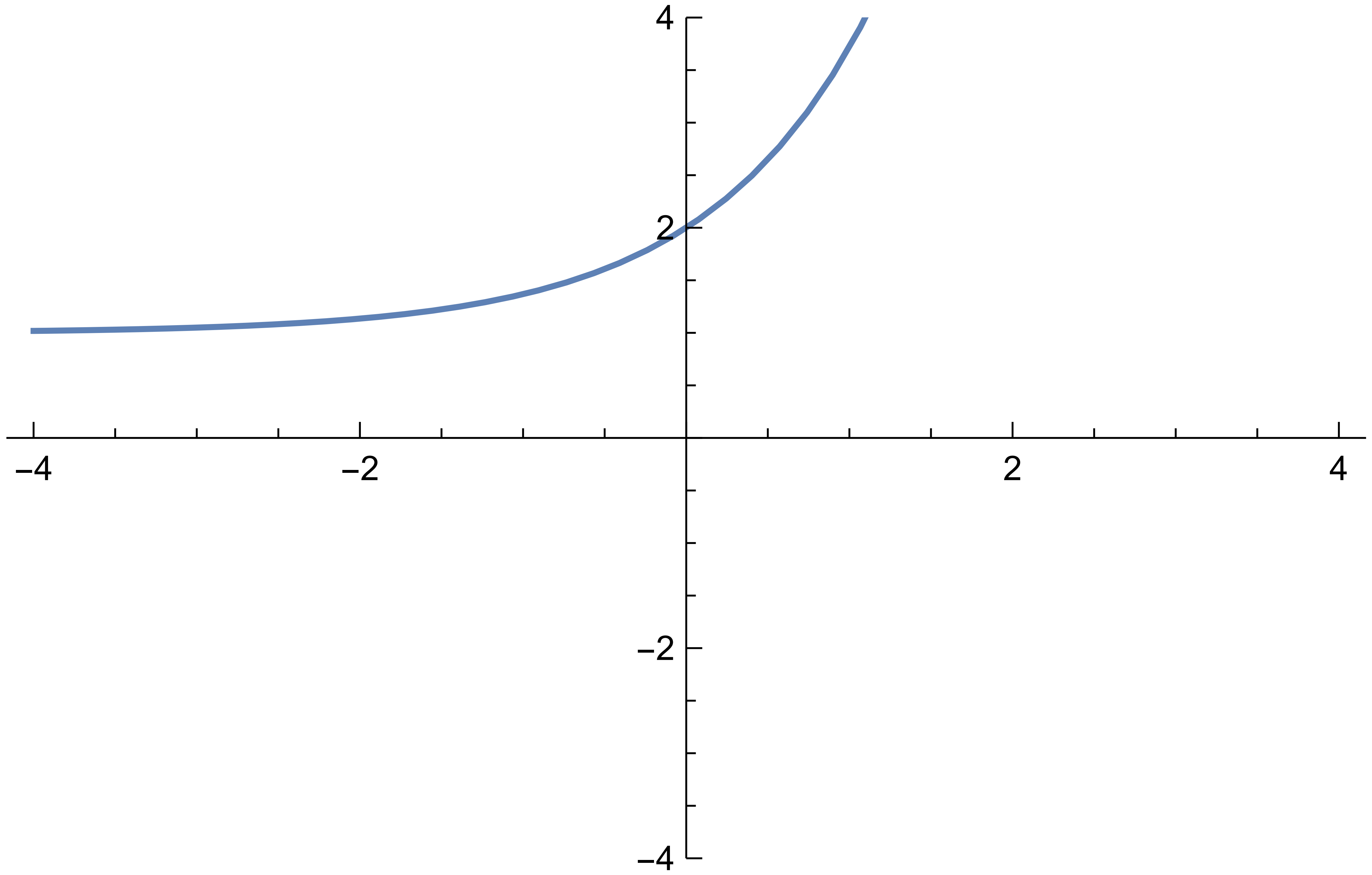

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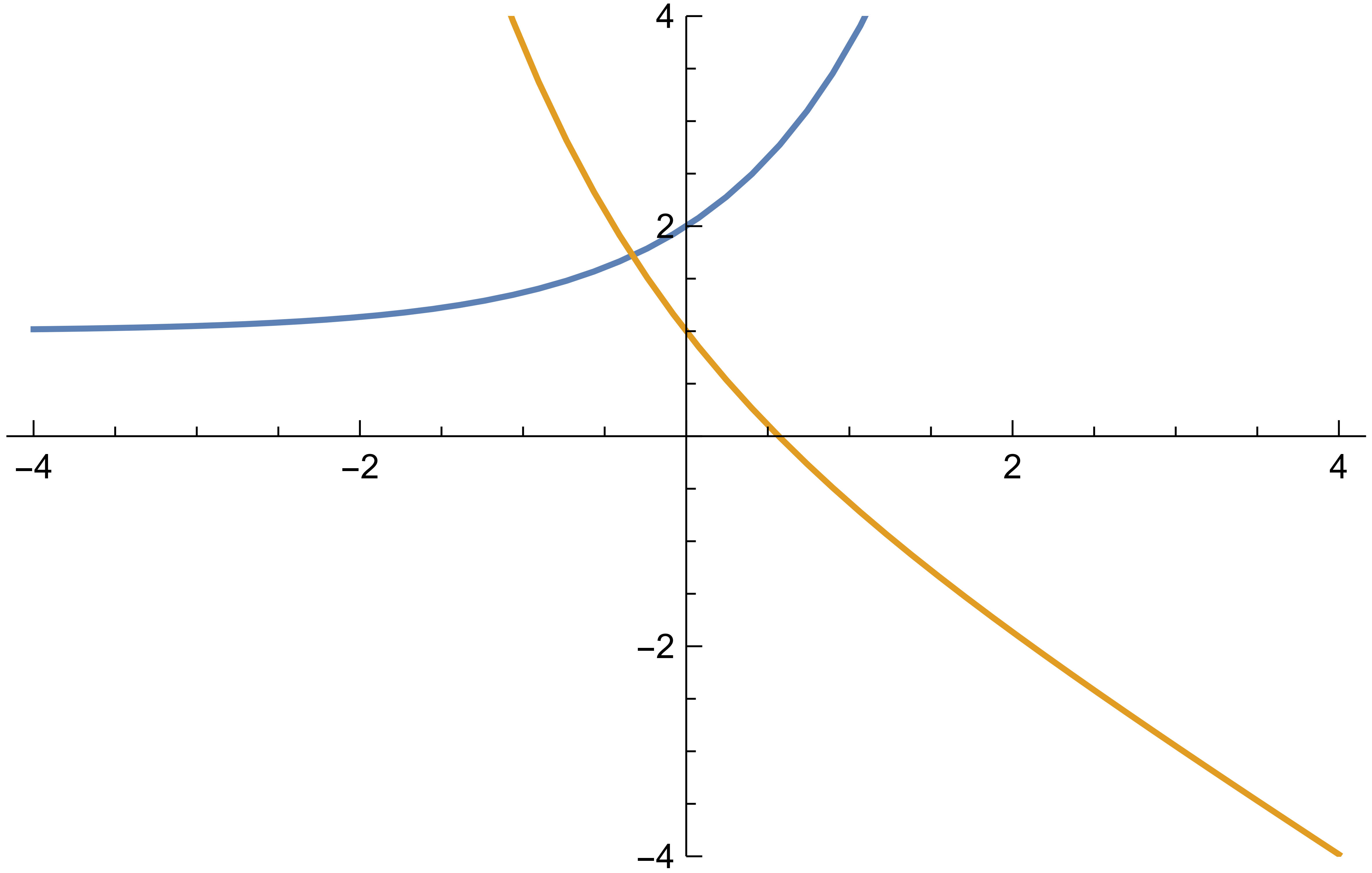

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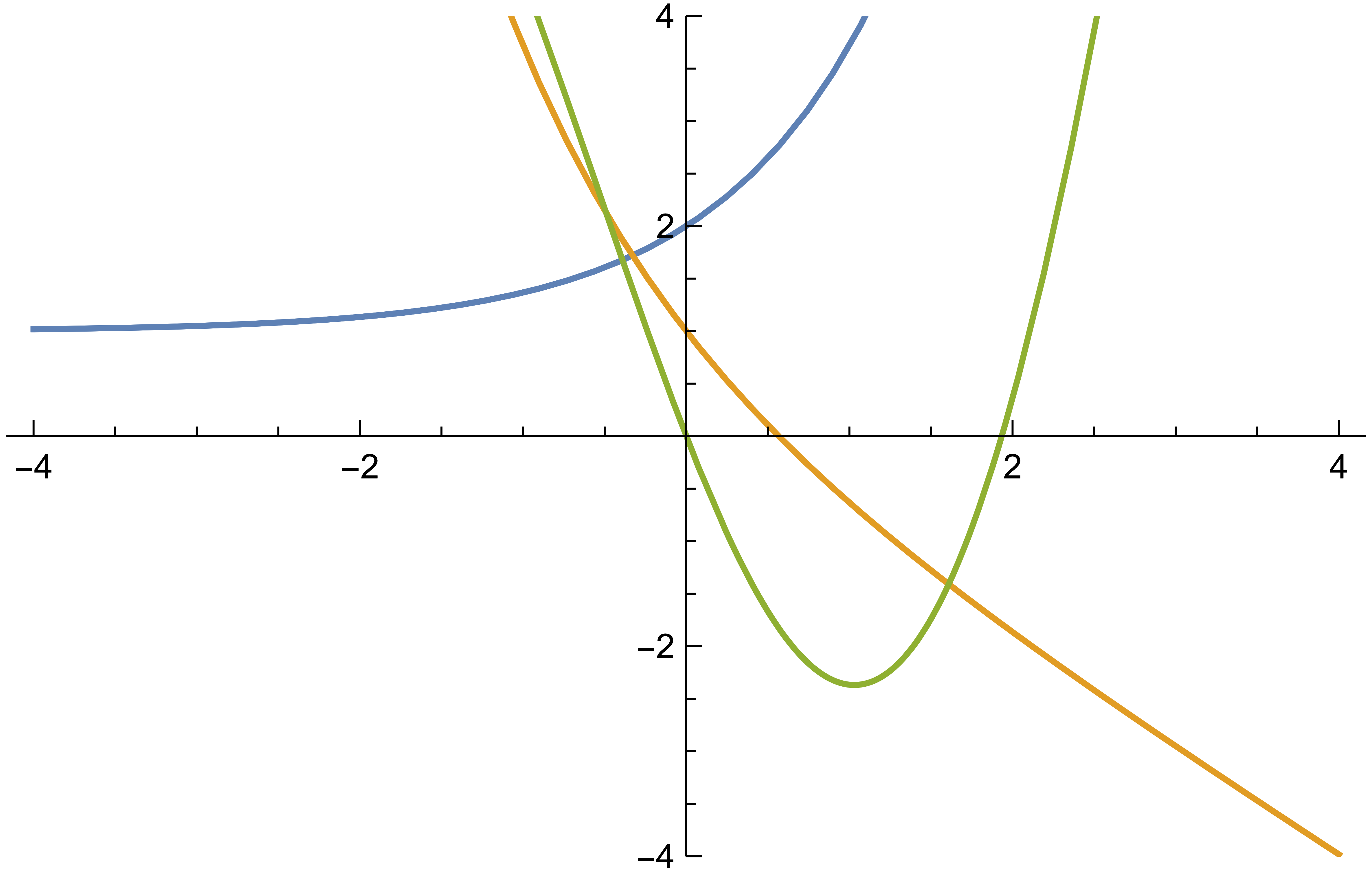

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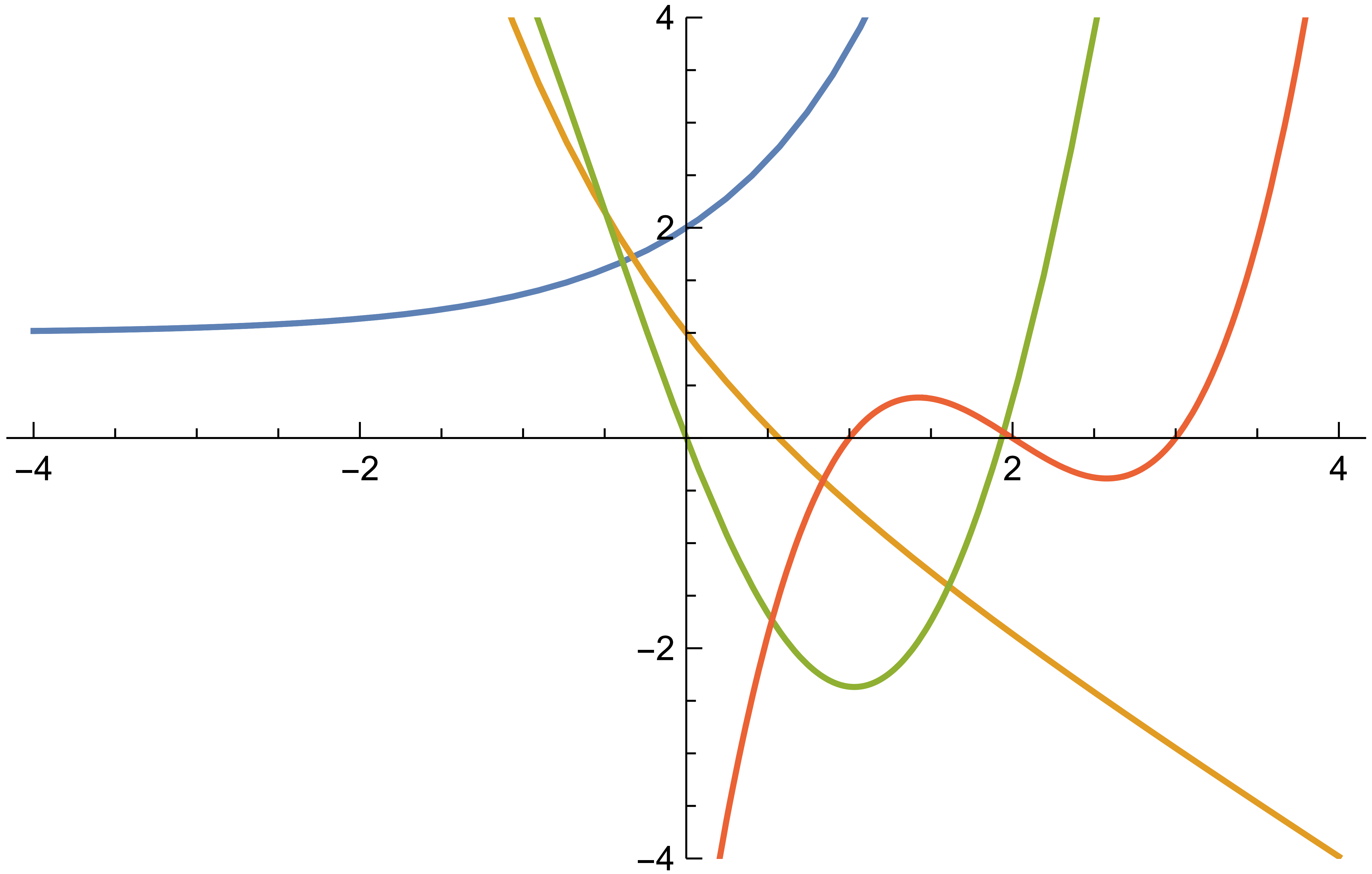

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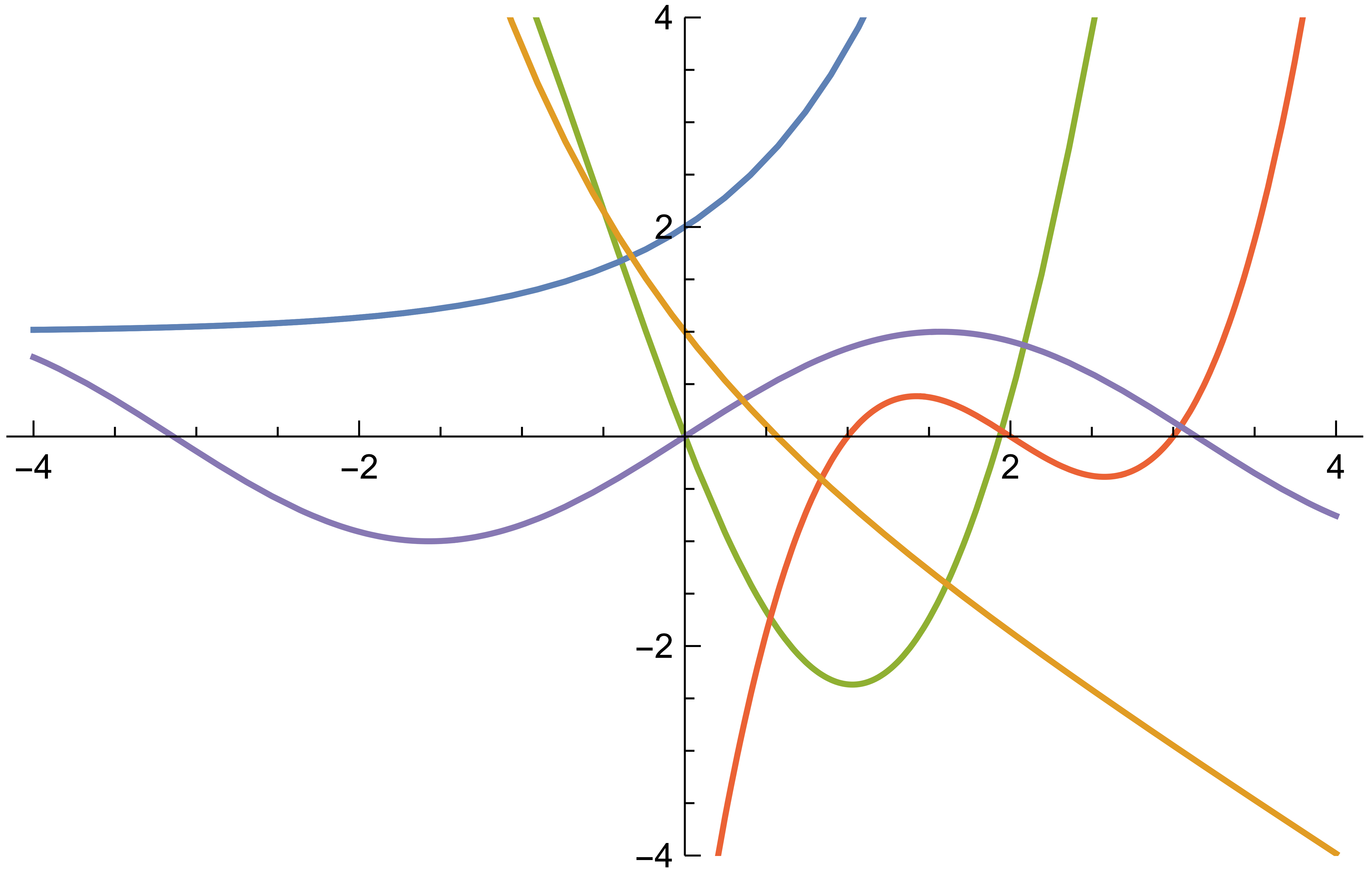
  - $\sin(x) = 0$



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Common assumptions

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

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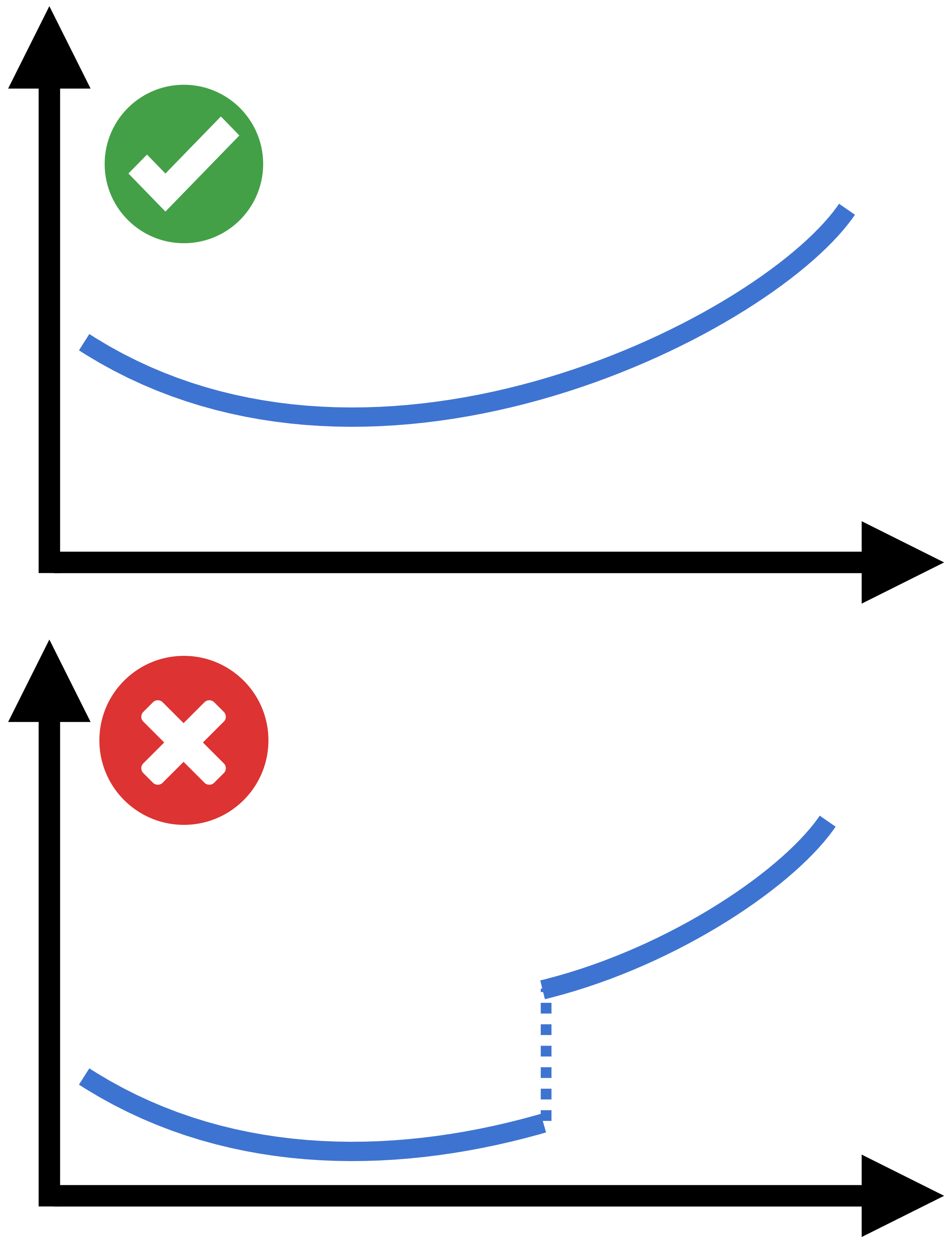

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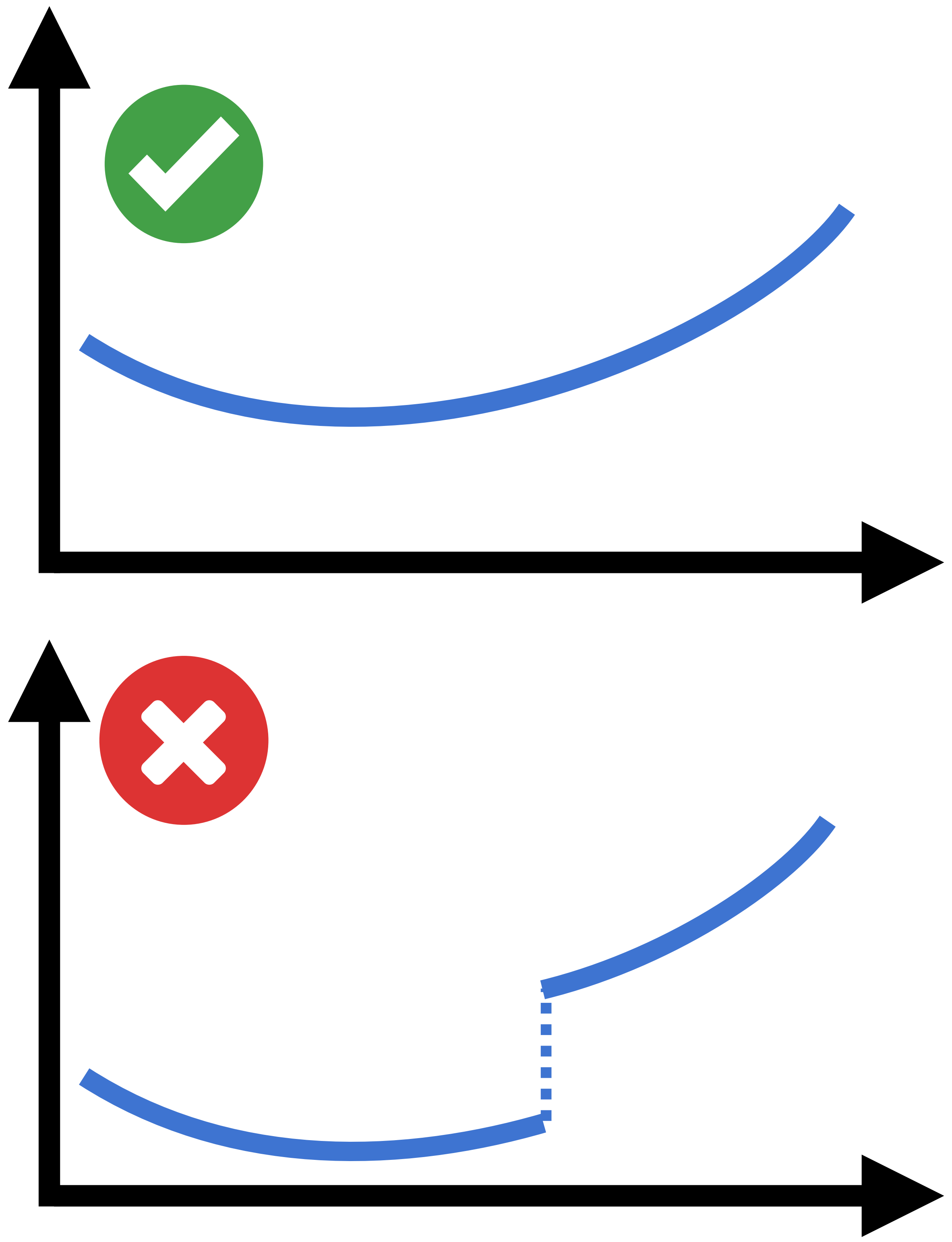

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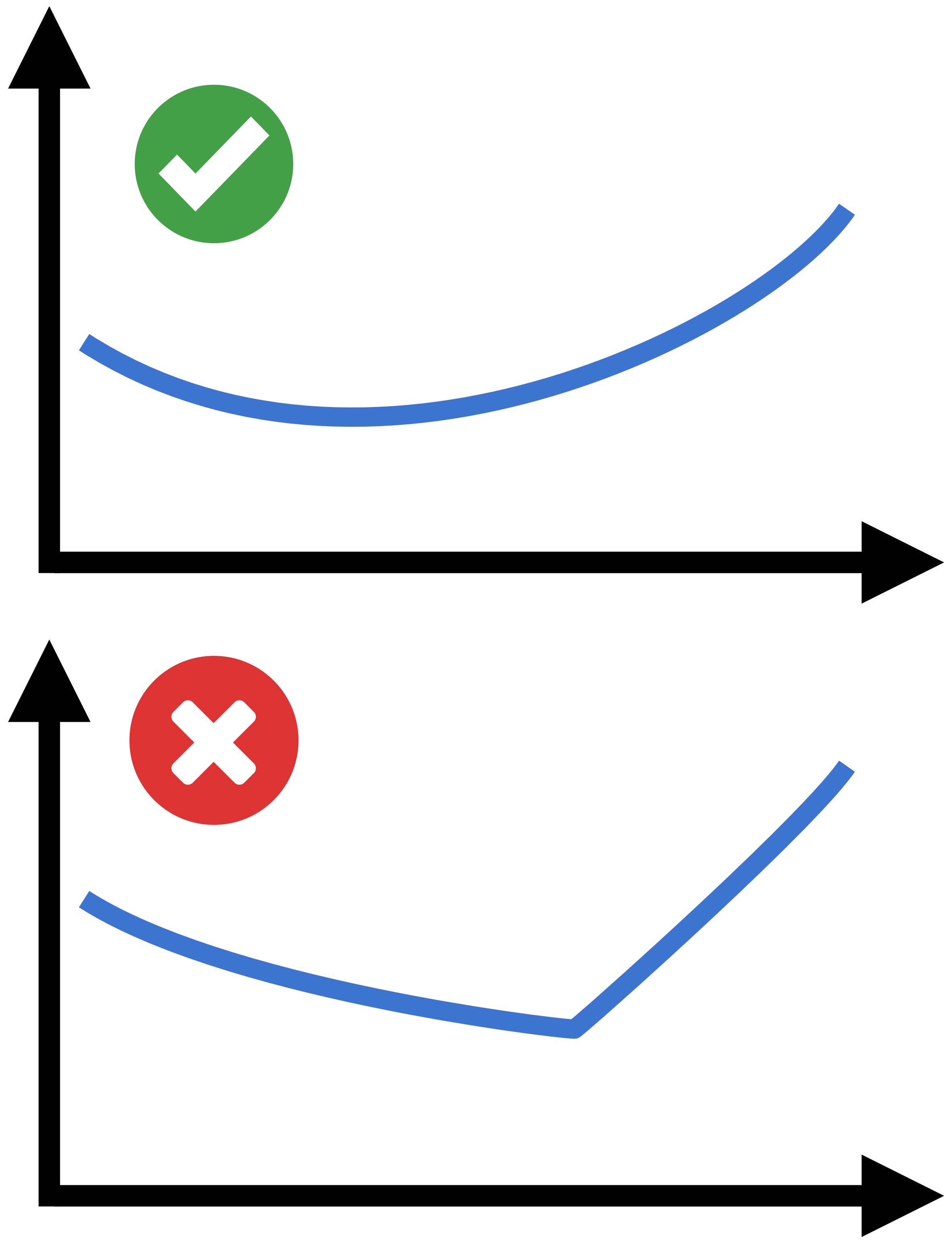

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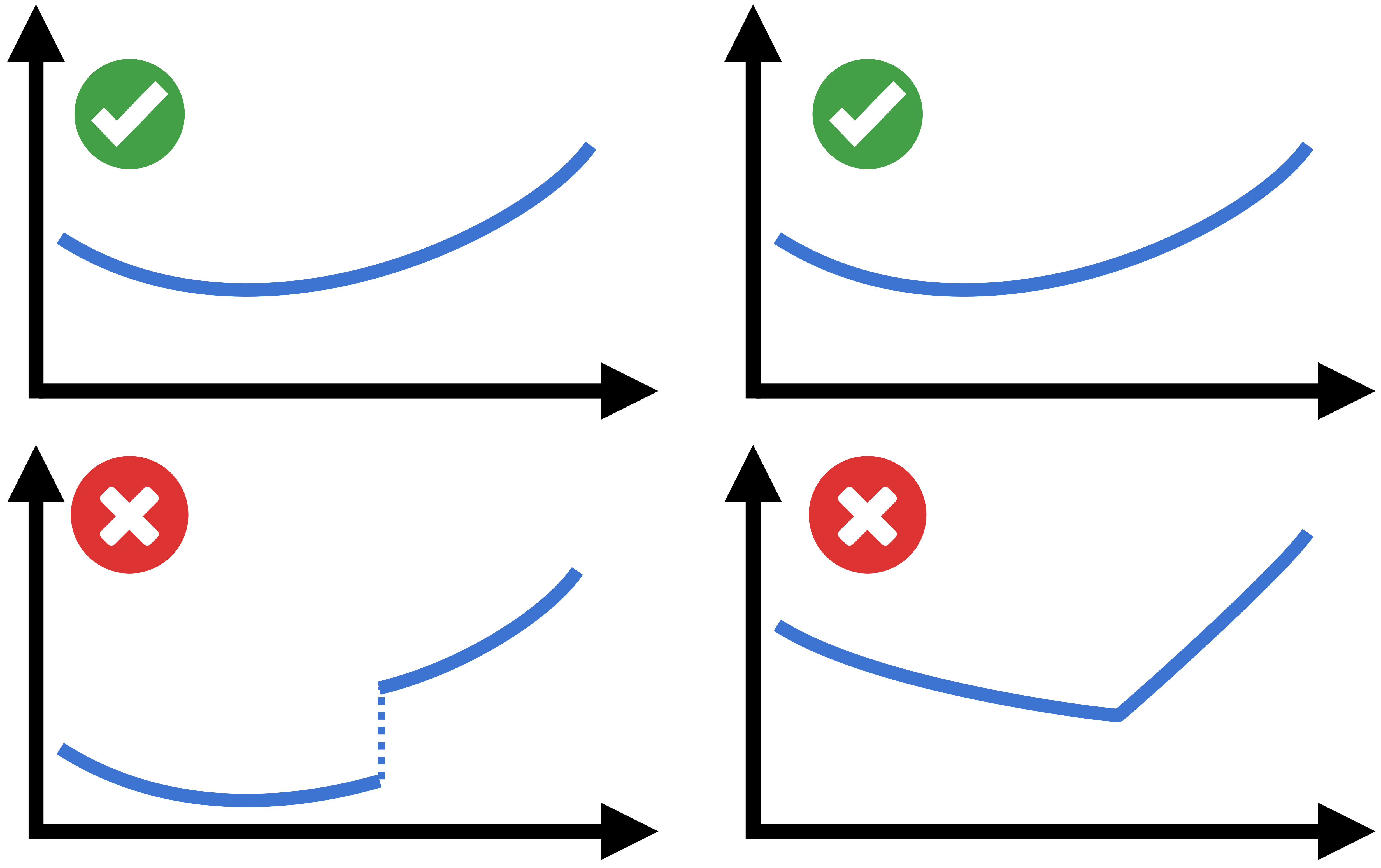

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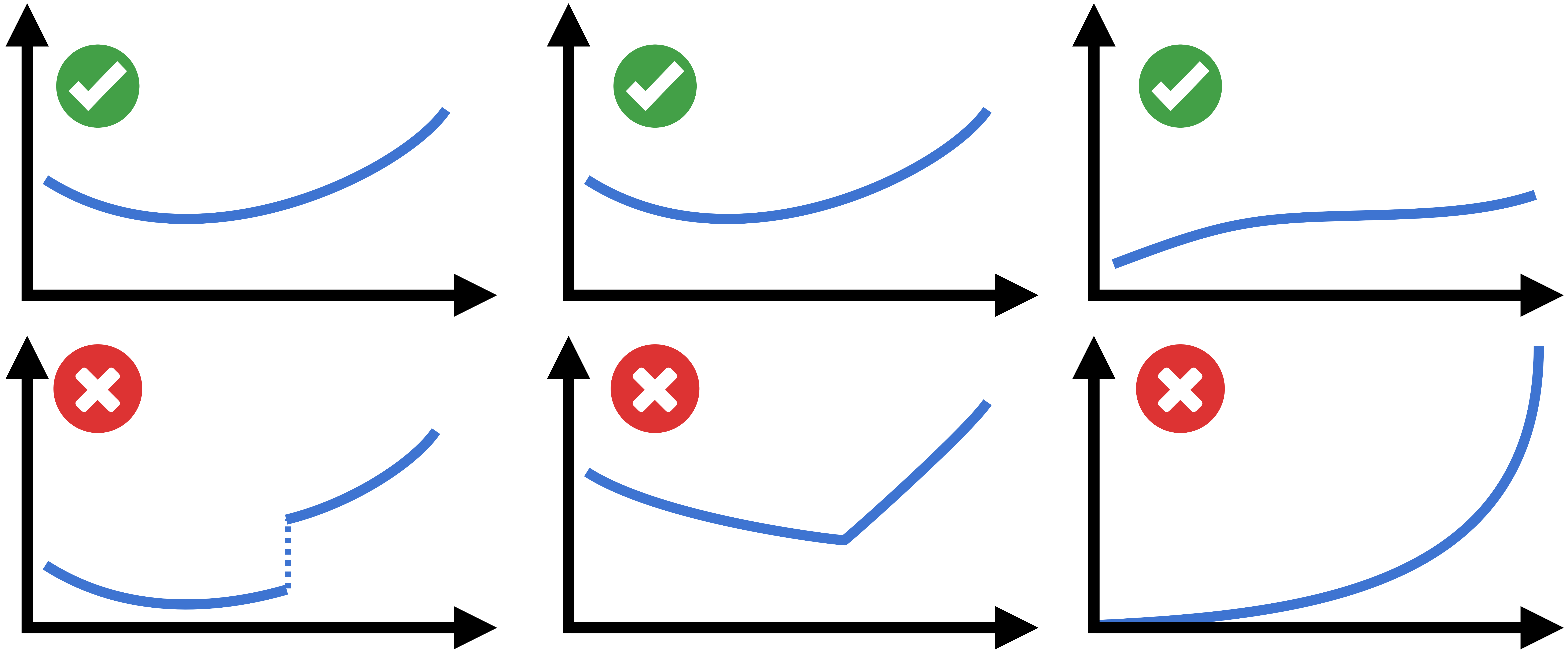

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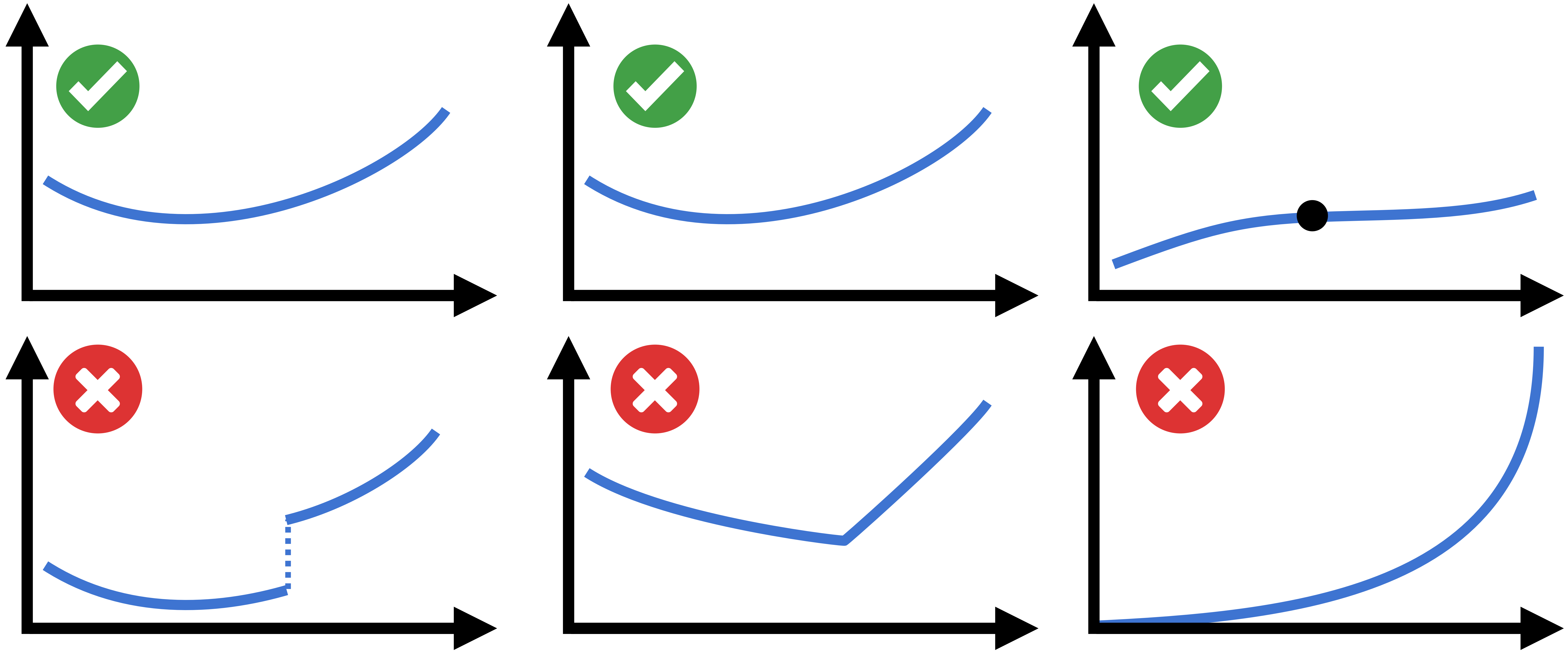

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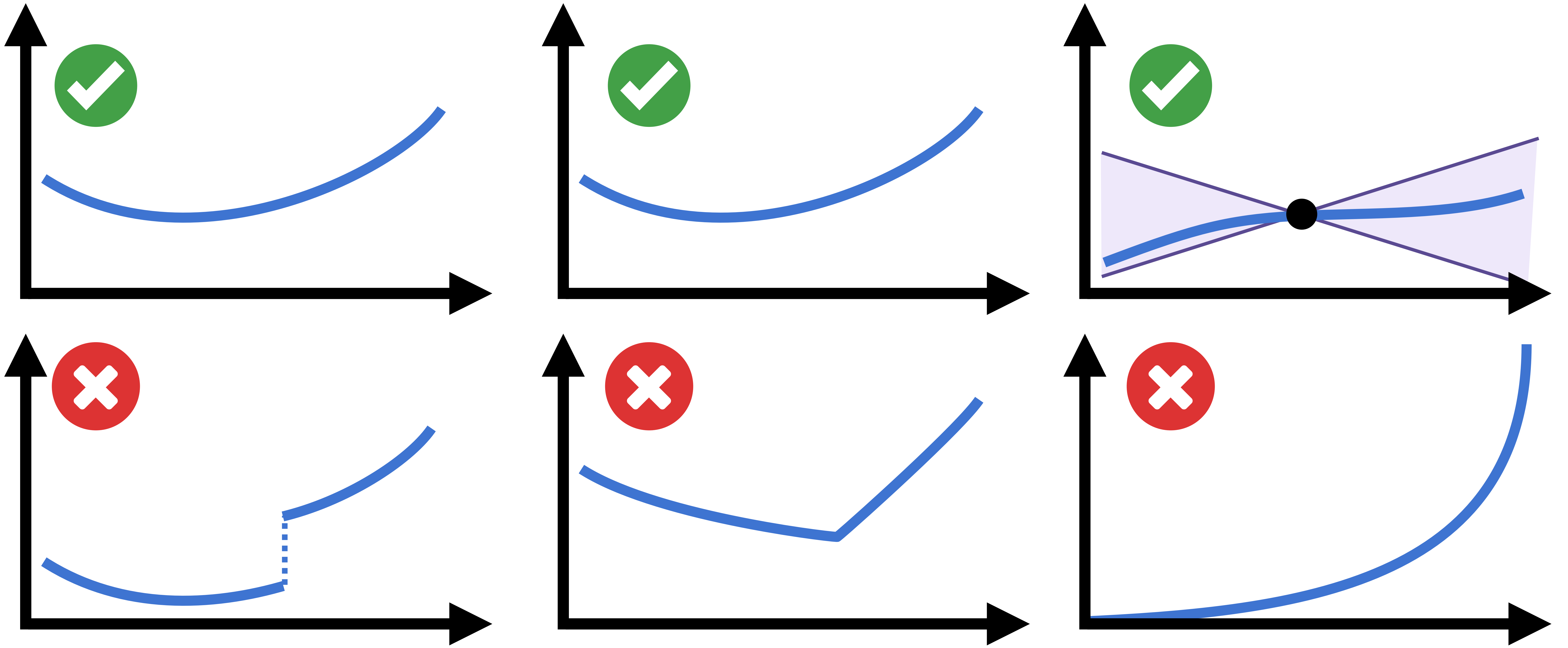

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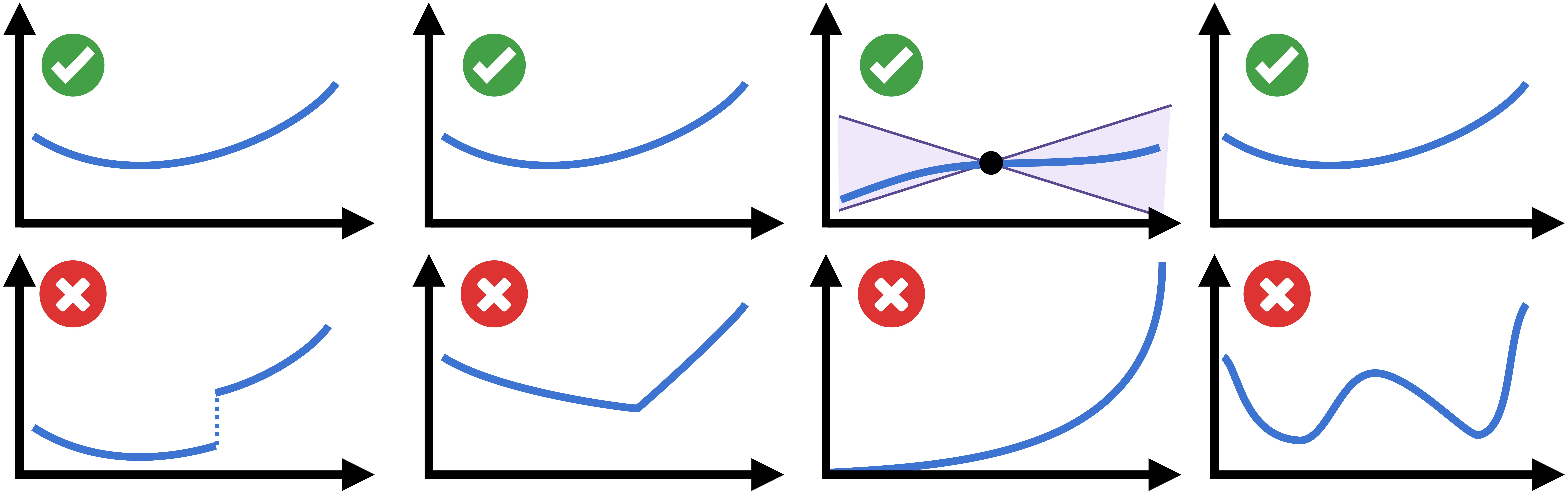

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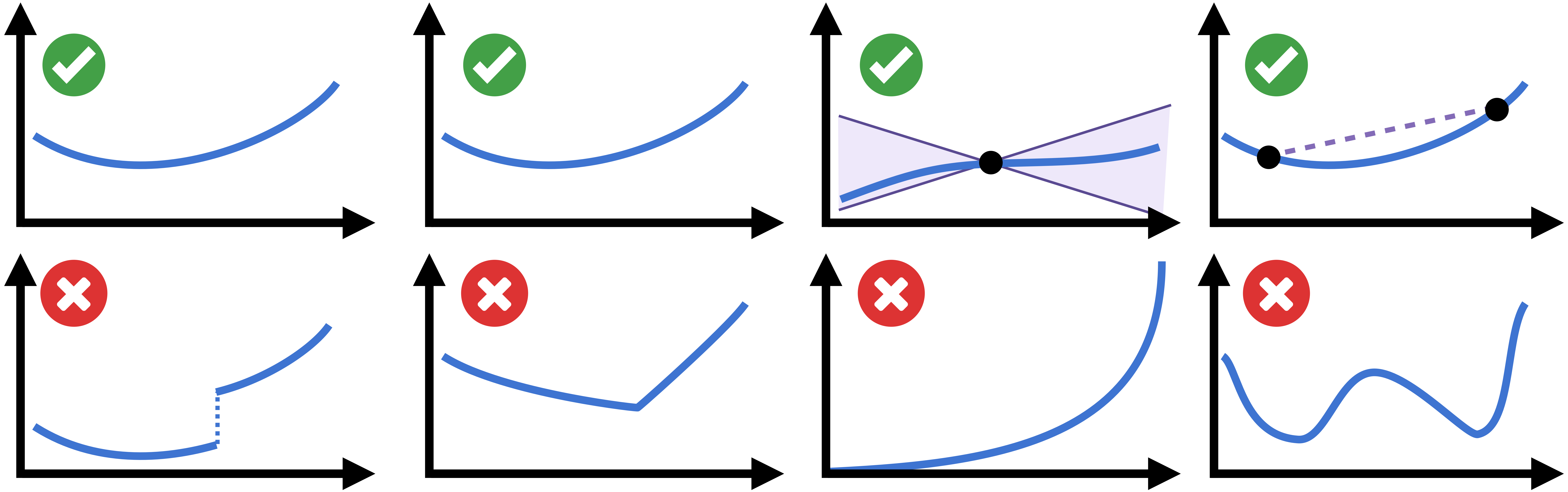

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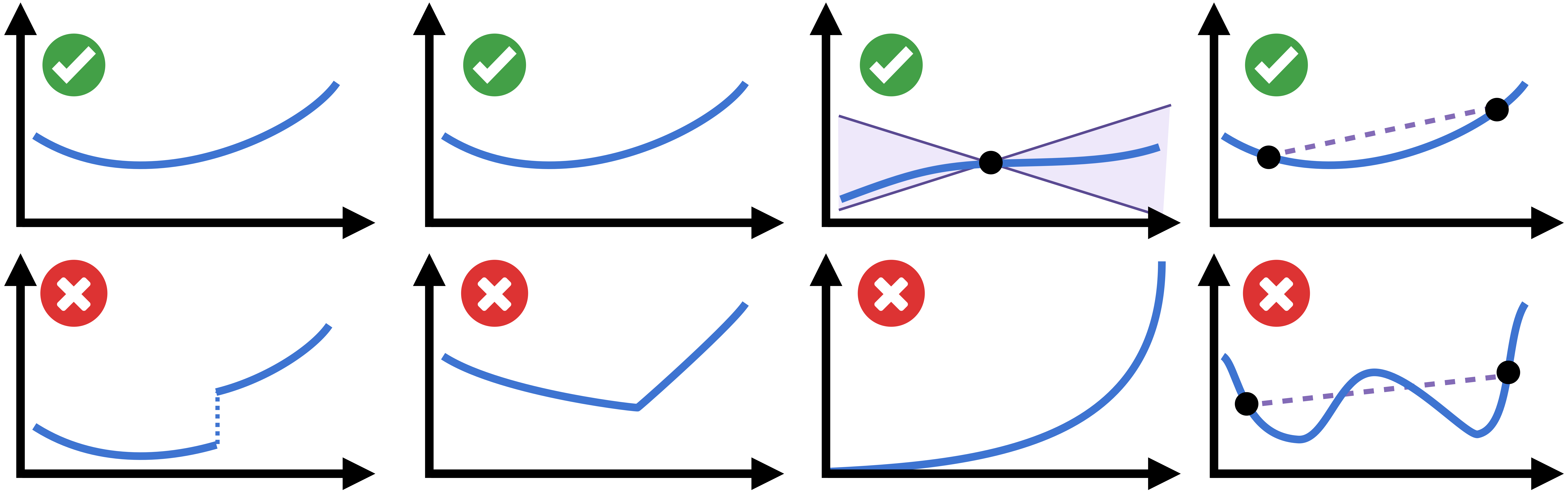

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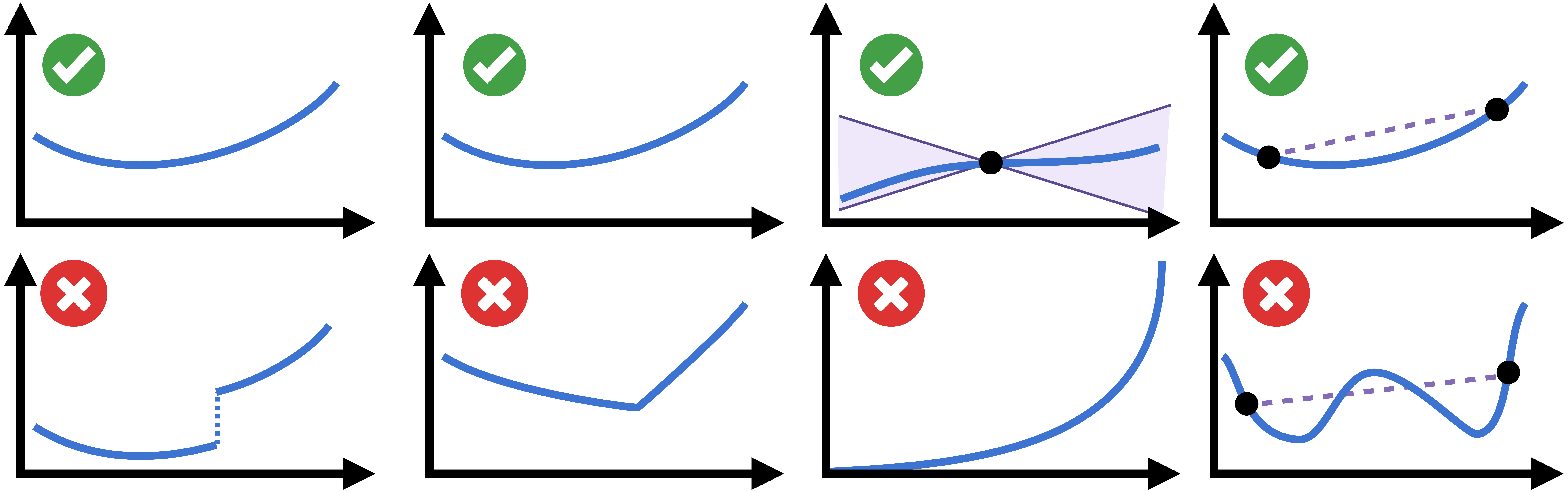

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Mostly used for optimization.

A model problem

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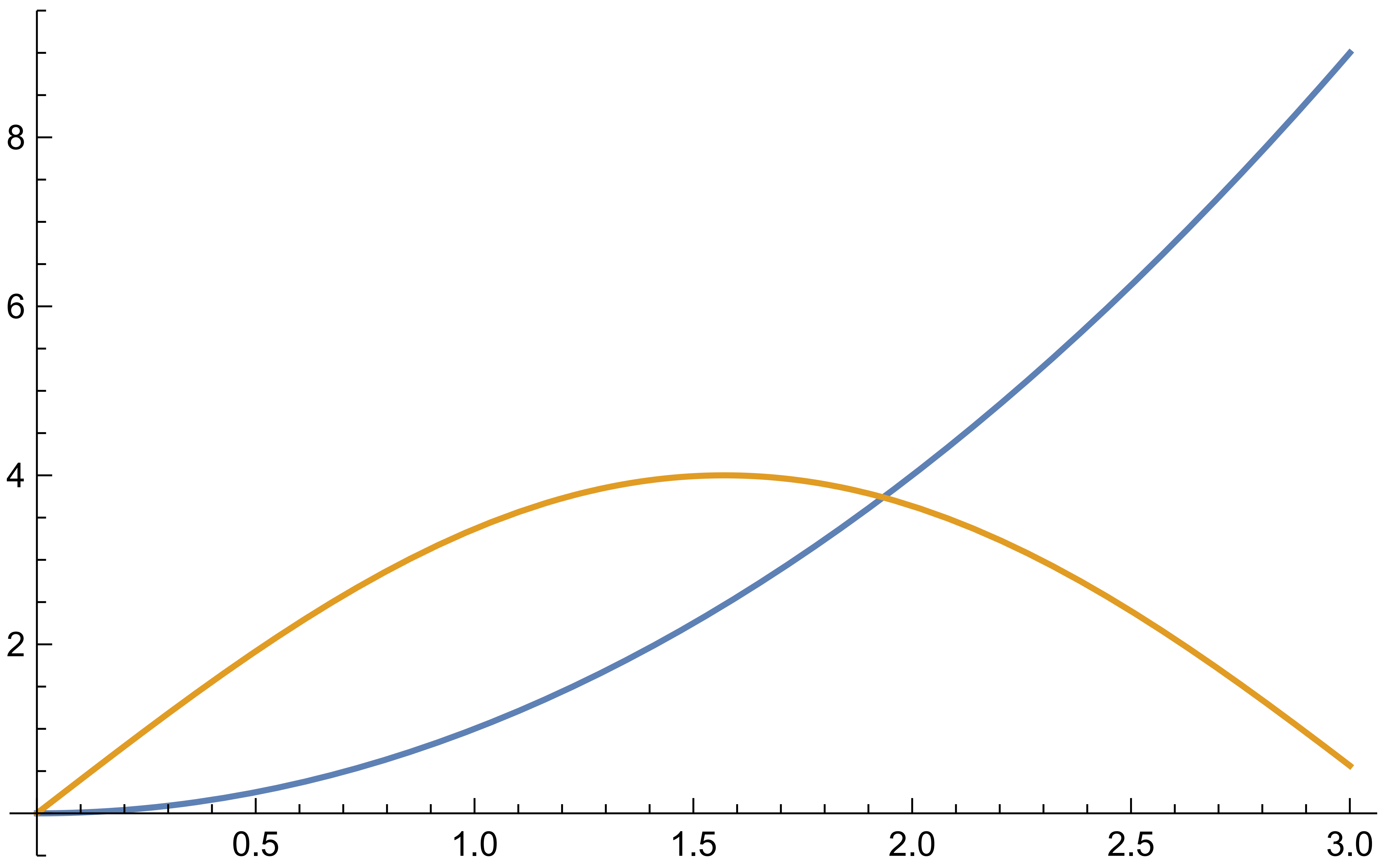

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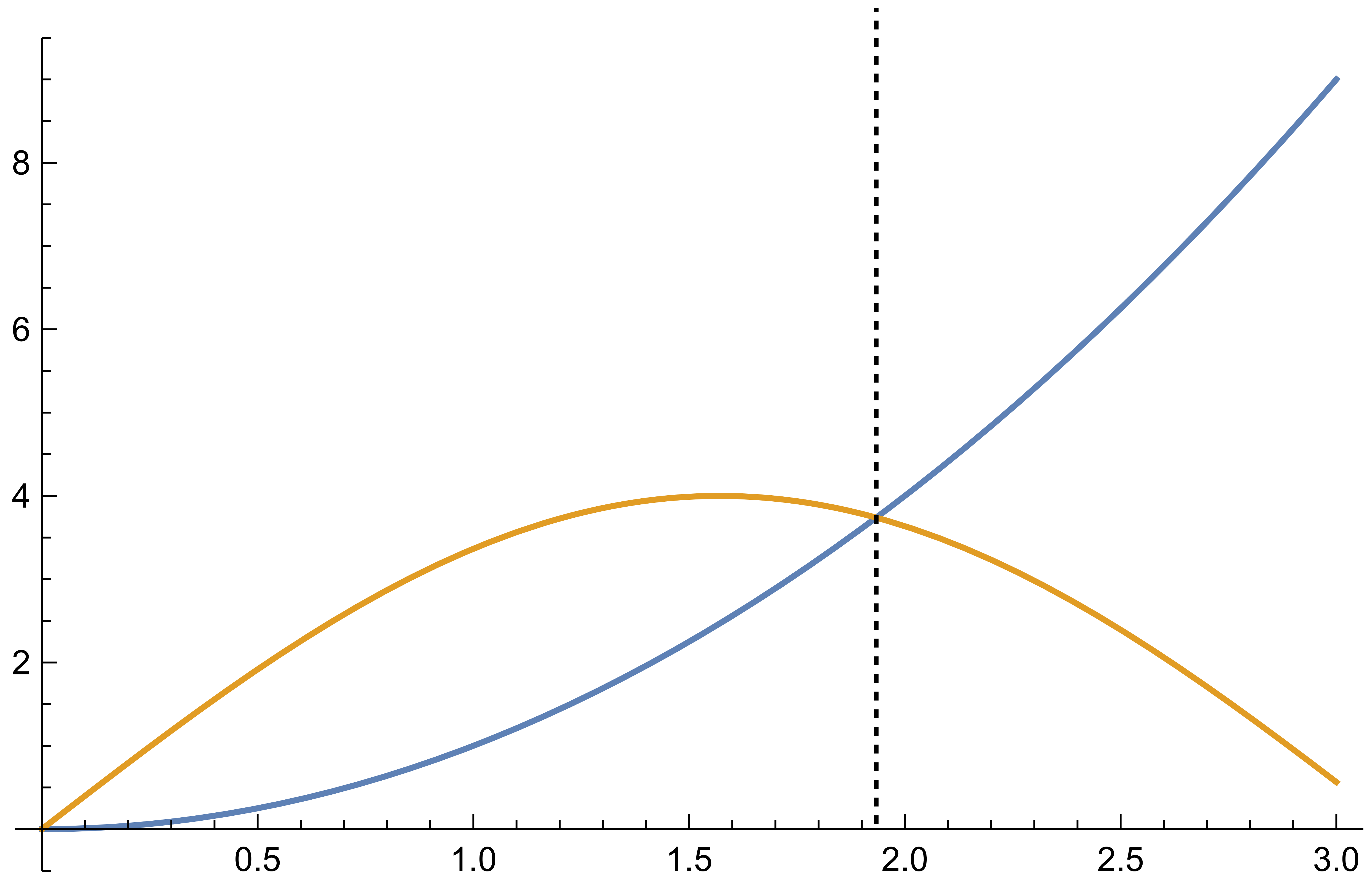

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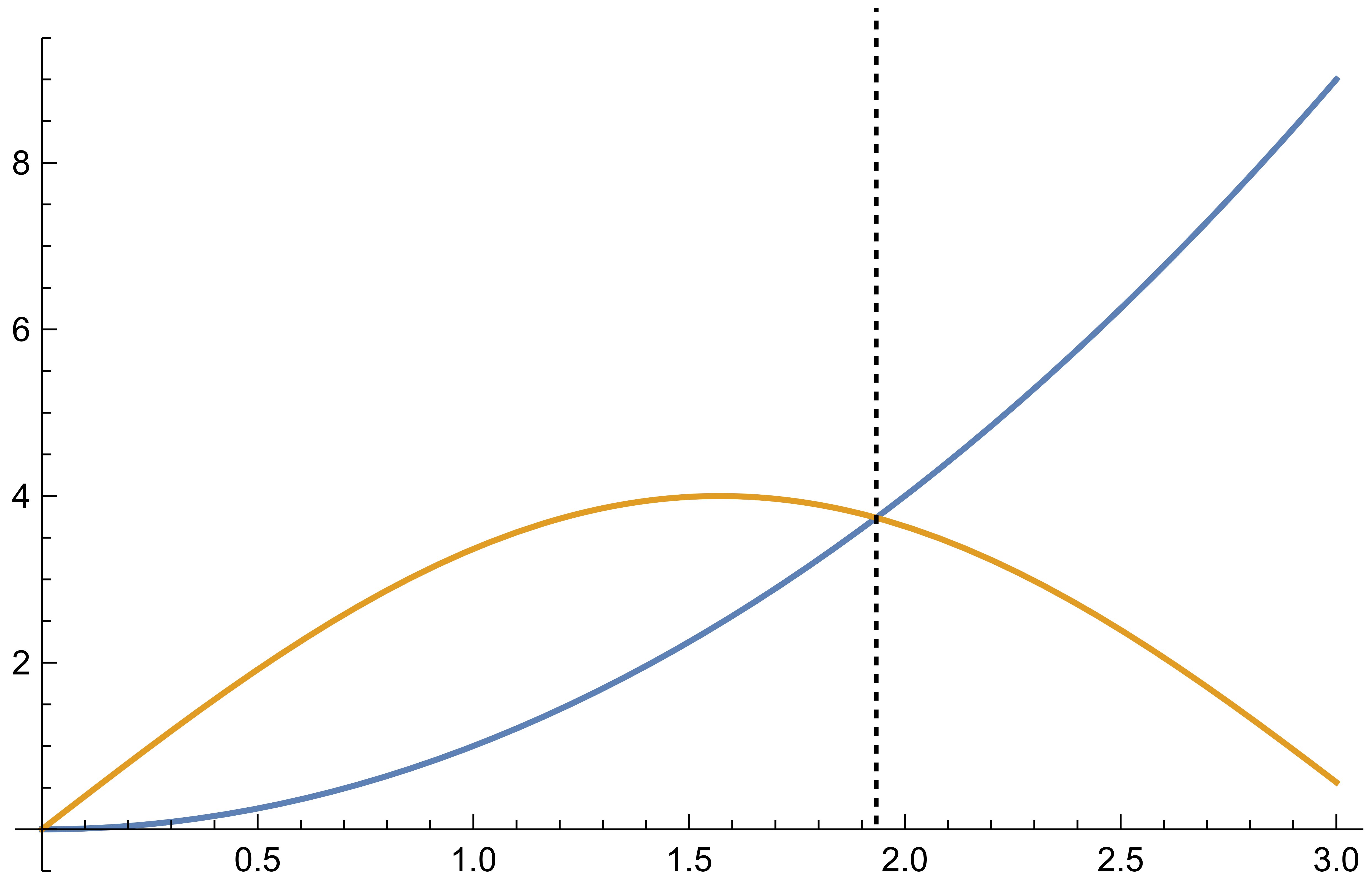

A model problem

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

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

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

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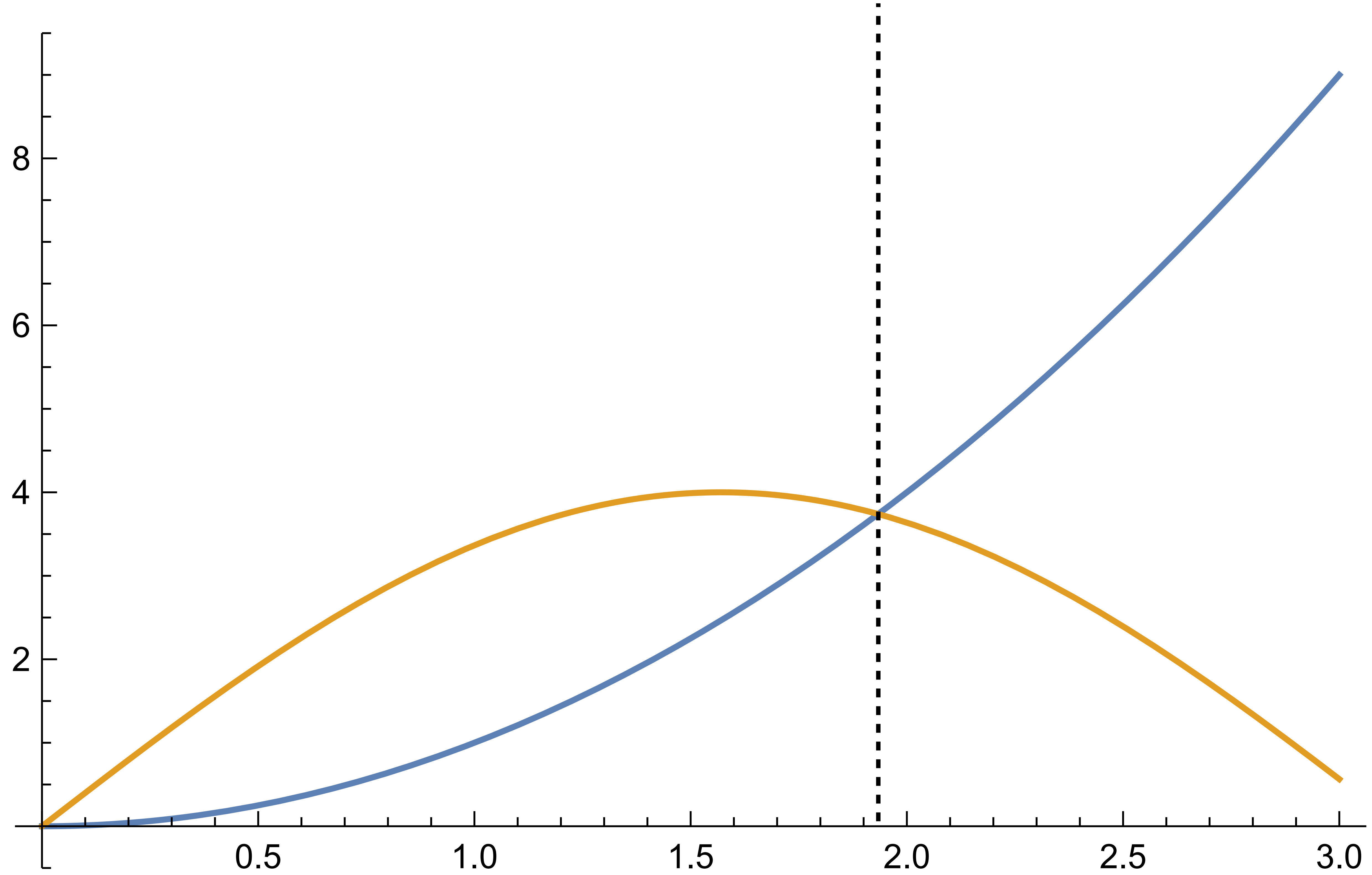

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Can more or less read off solution from graph, *how difficult can it be?*

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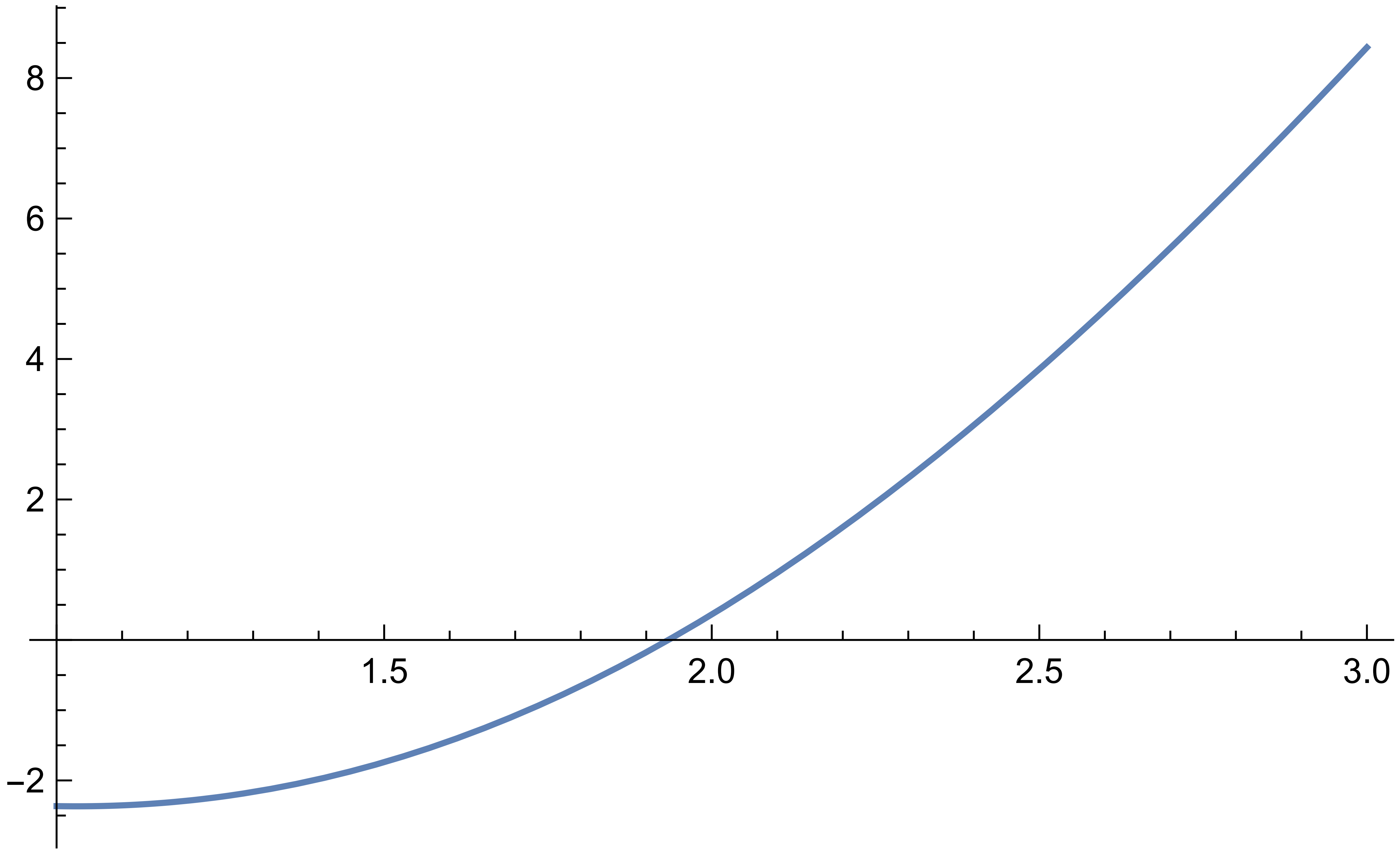

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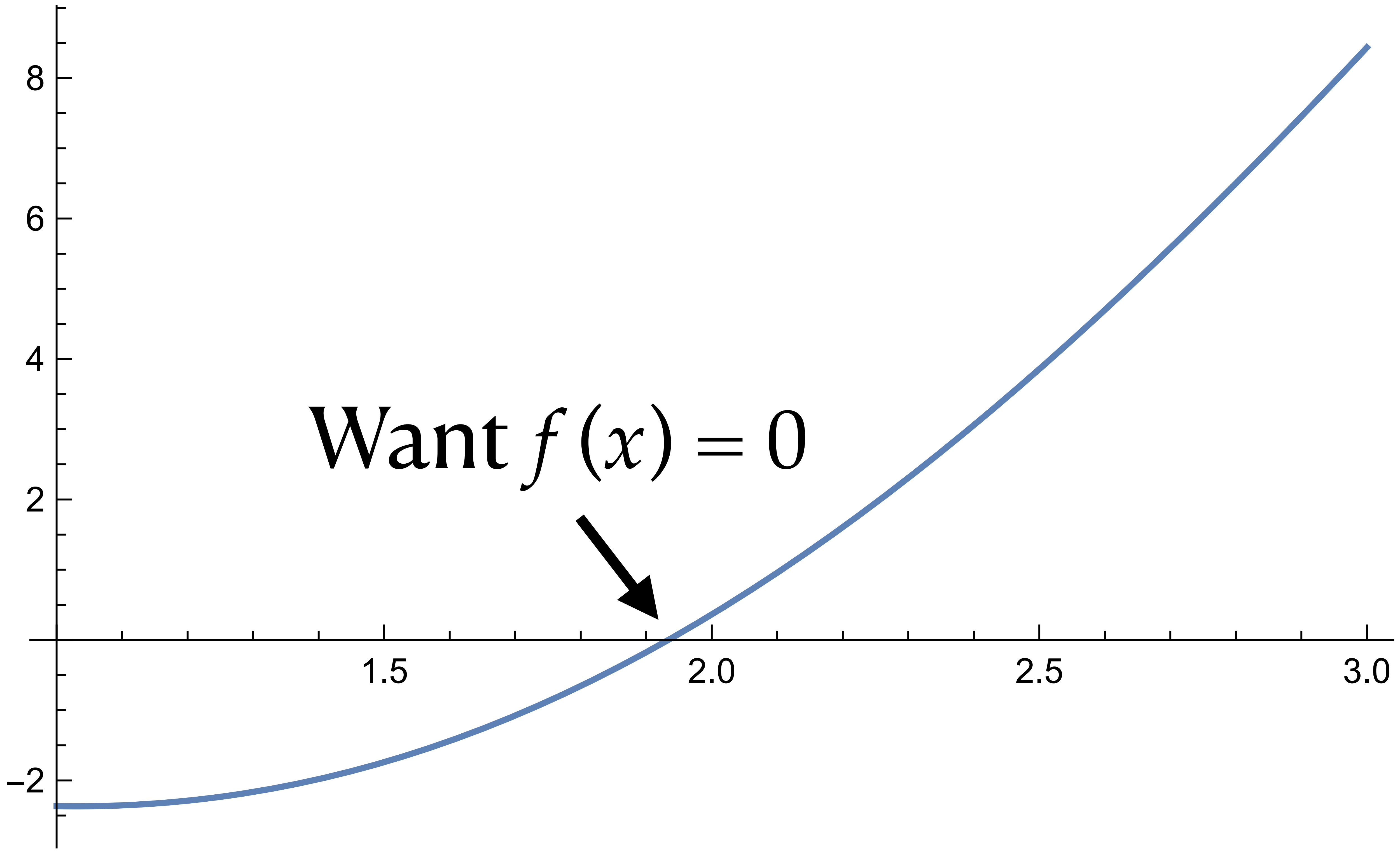

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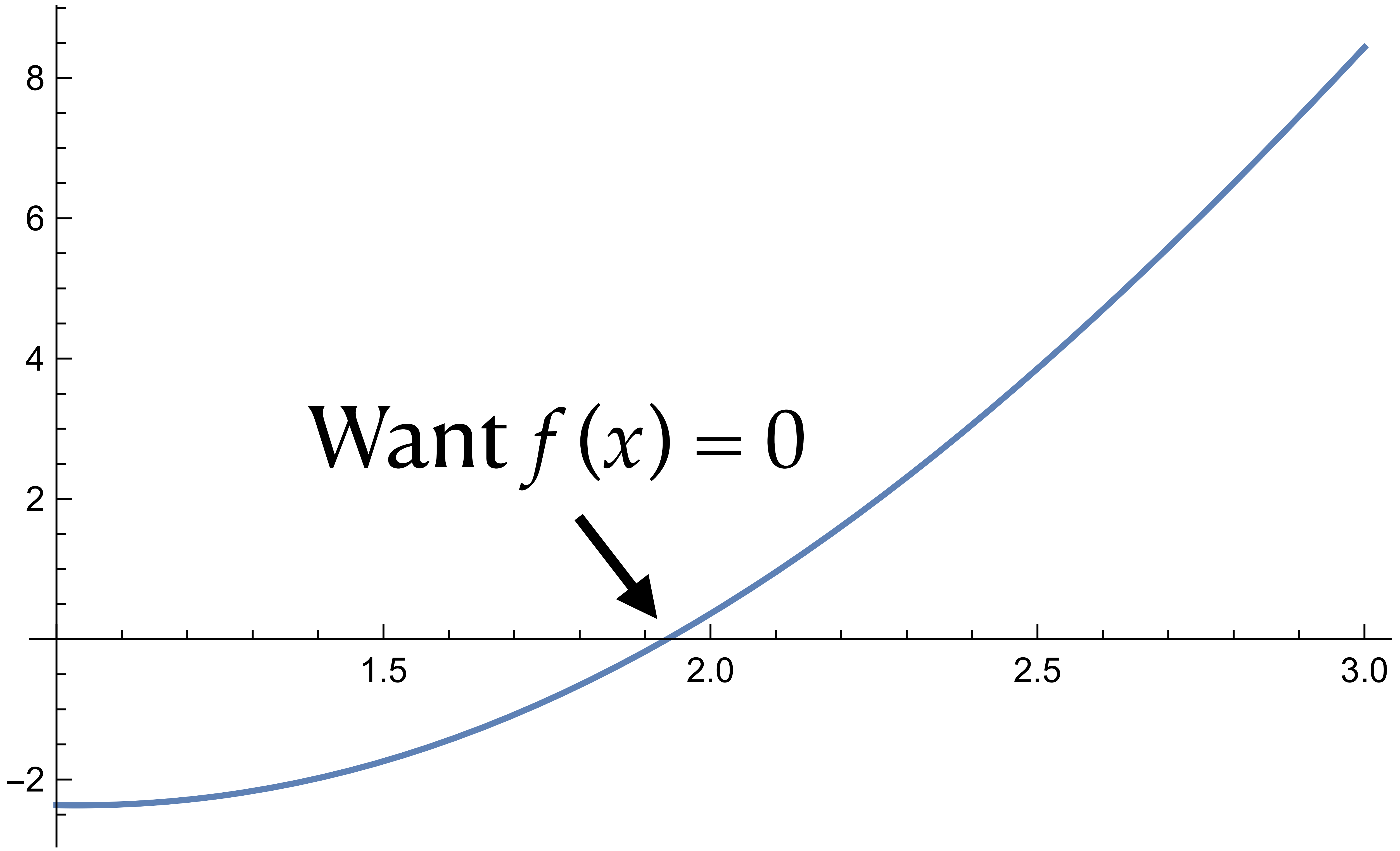
*Plot required thousands of function evaluations, each one is potentially **very expensive** (evaluating f(x) once: test a new drug compound on patients, build a rocket and collect a sample on Mars.)*



Intermediate Value Theorem

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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 every value between y_0 and y_1.

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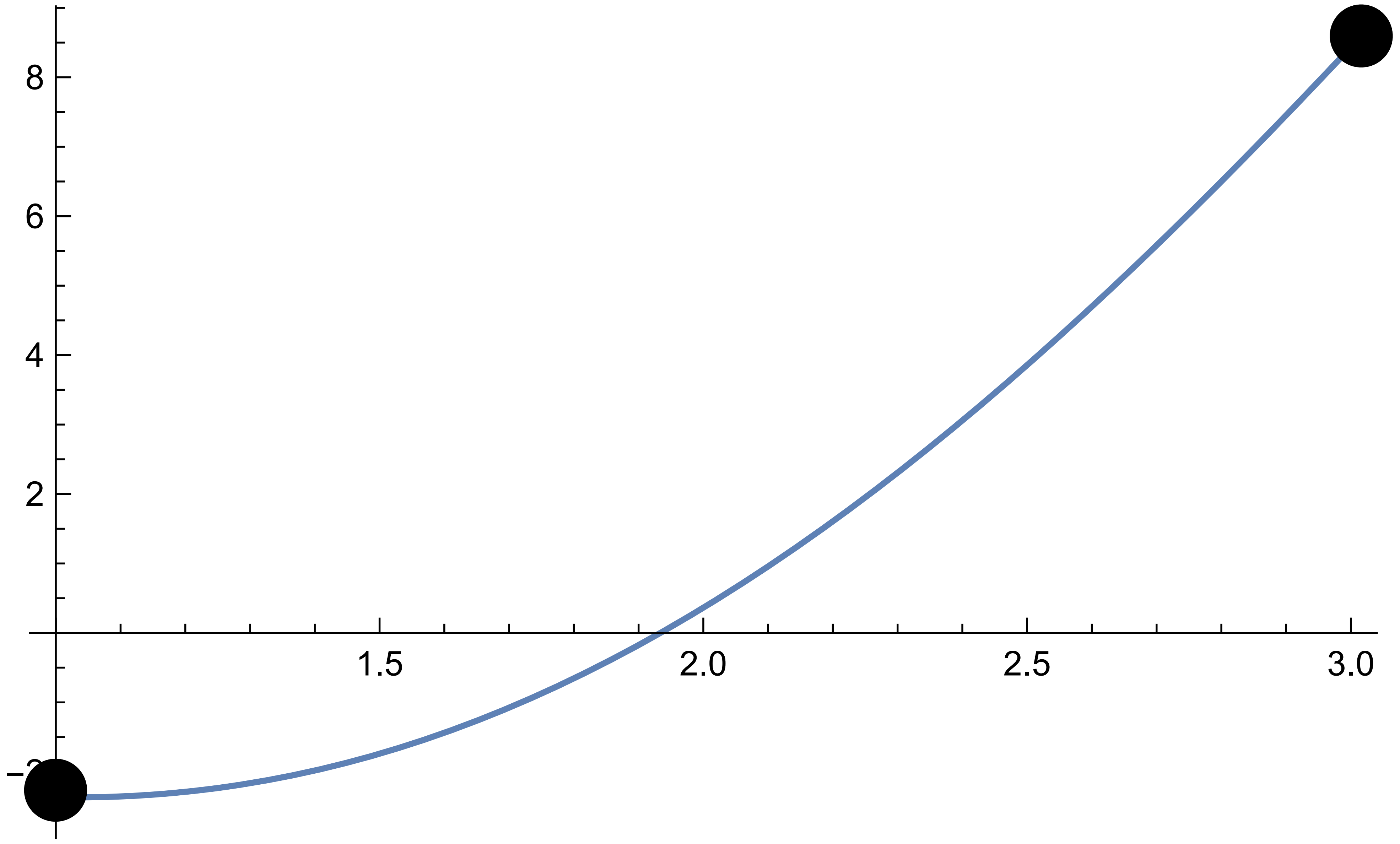
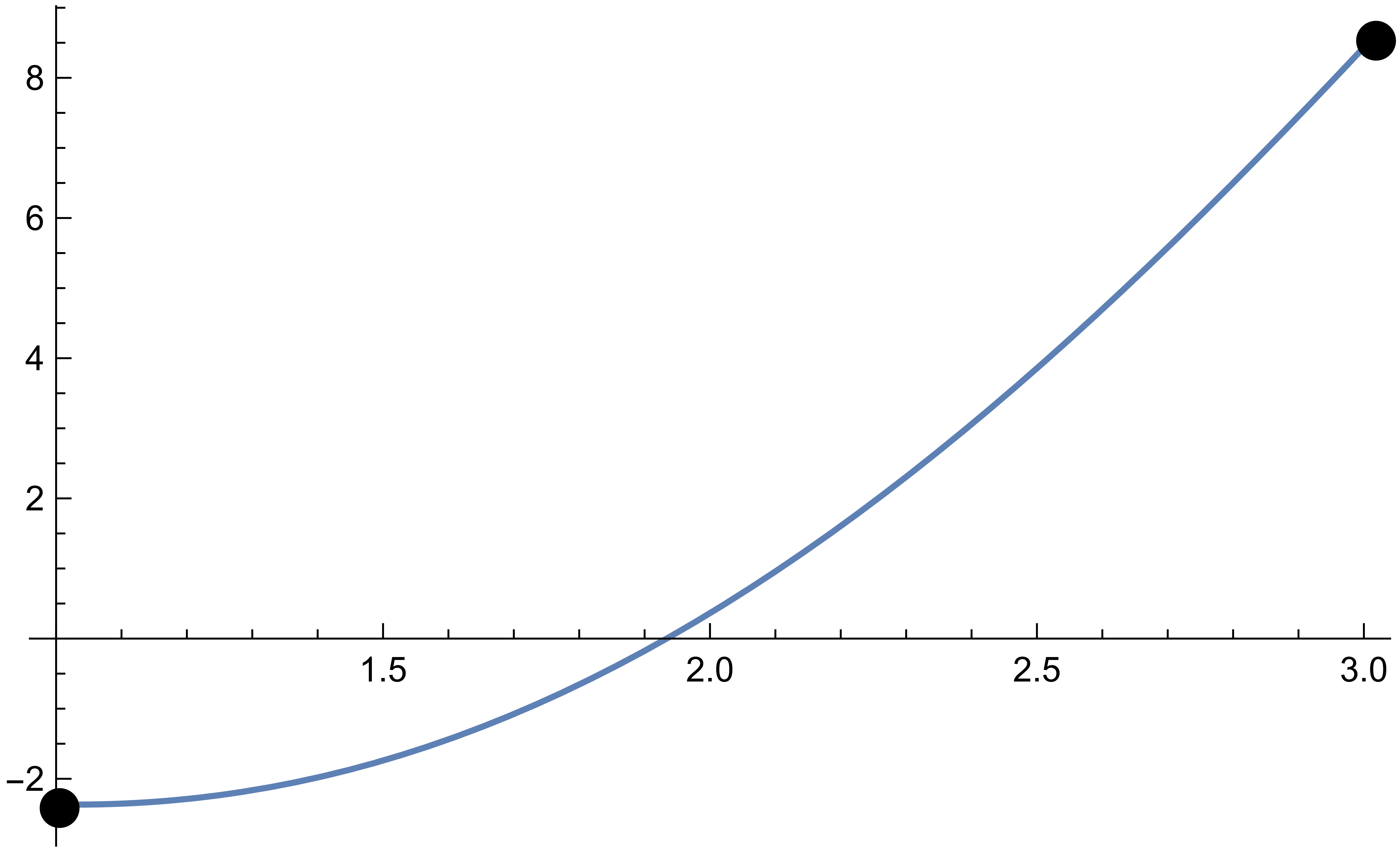


Use of continuity in our model problem



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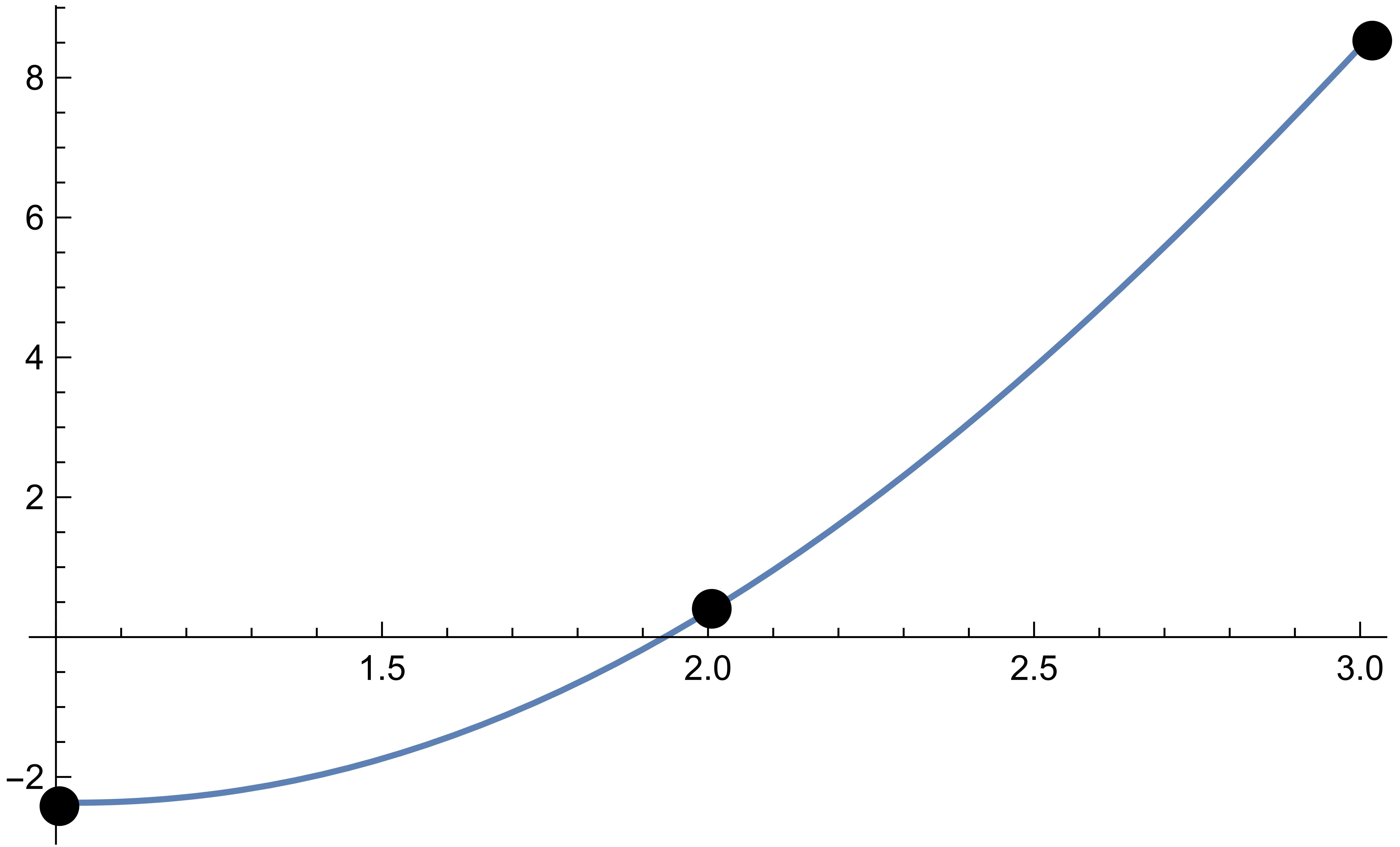

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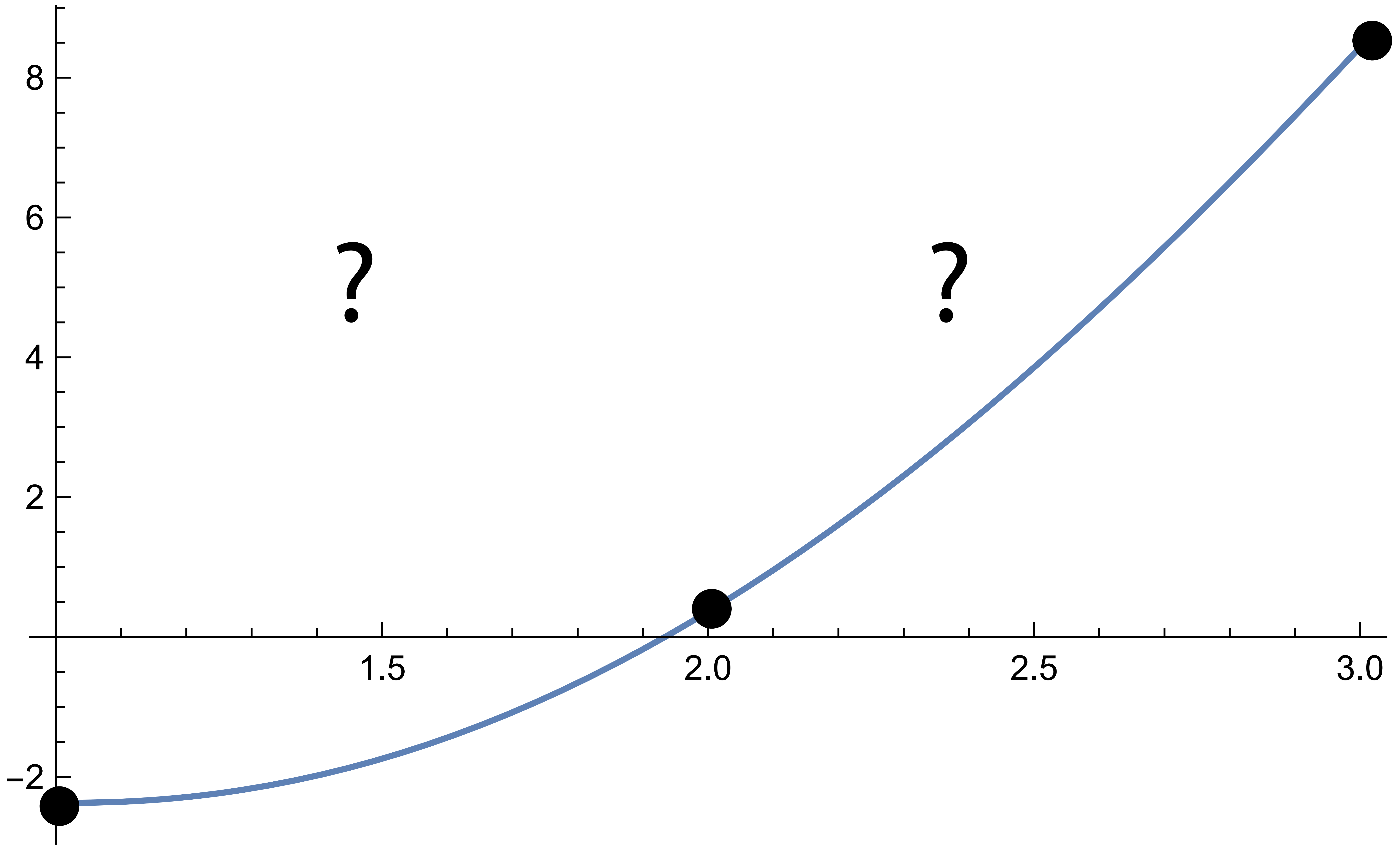

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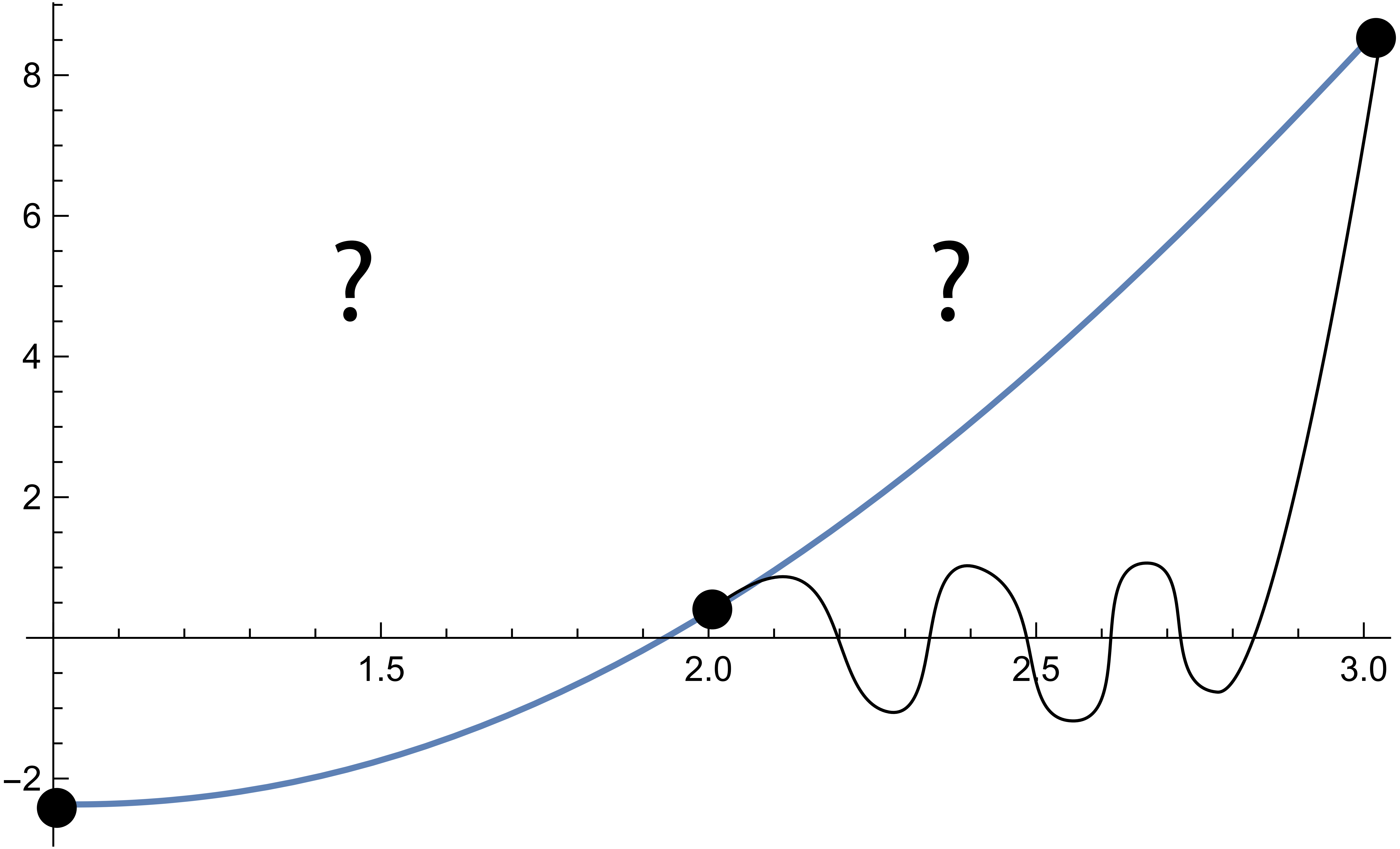

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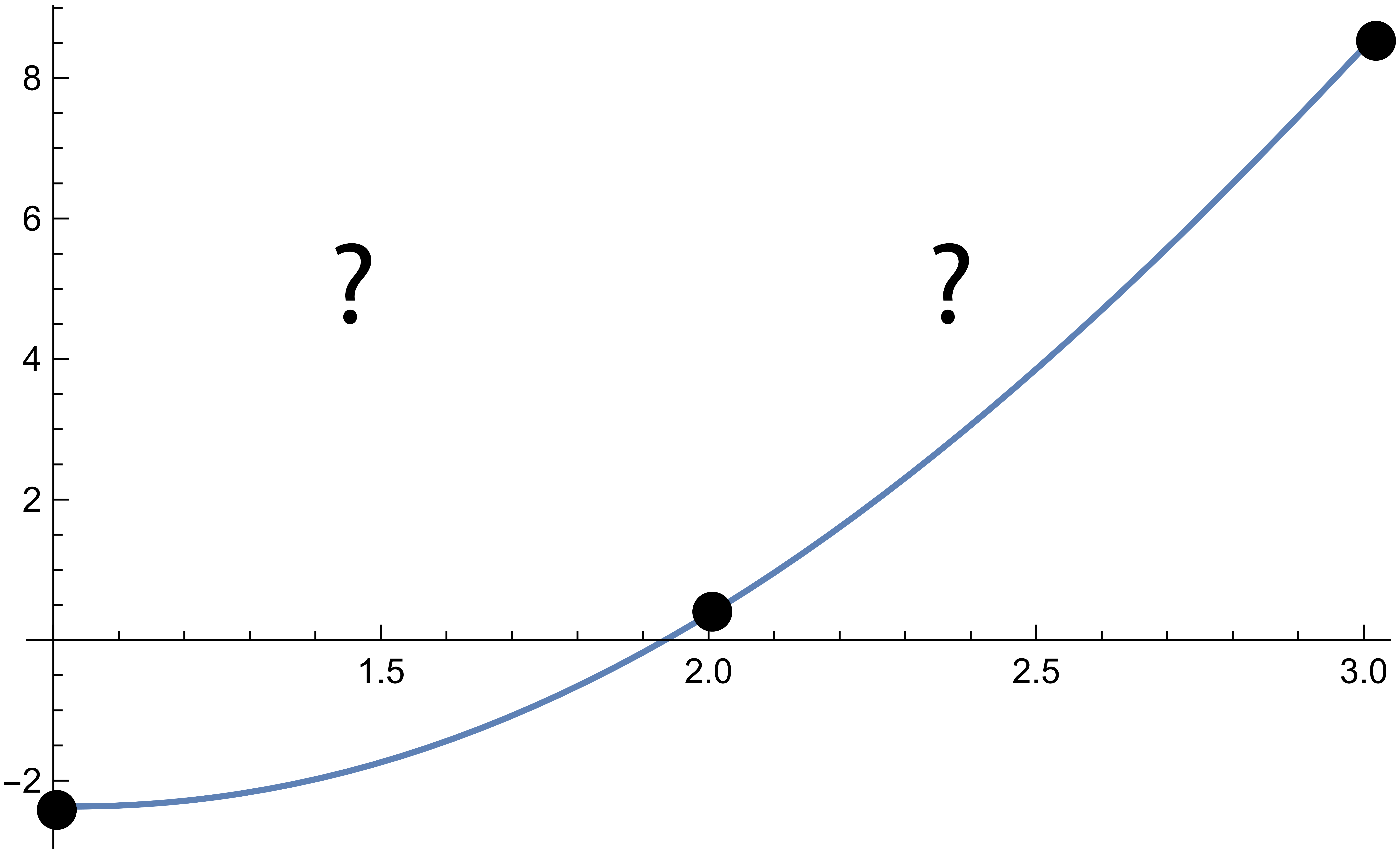

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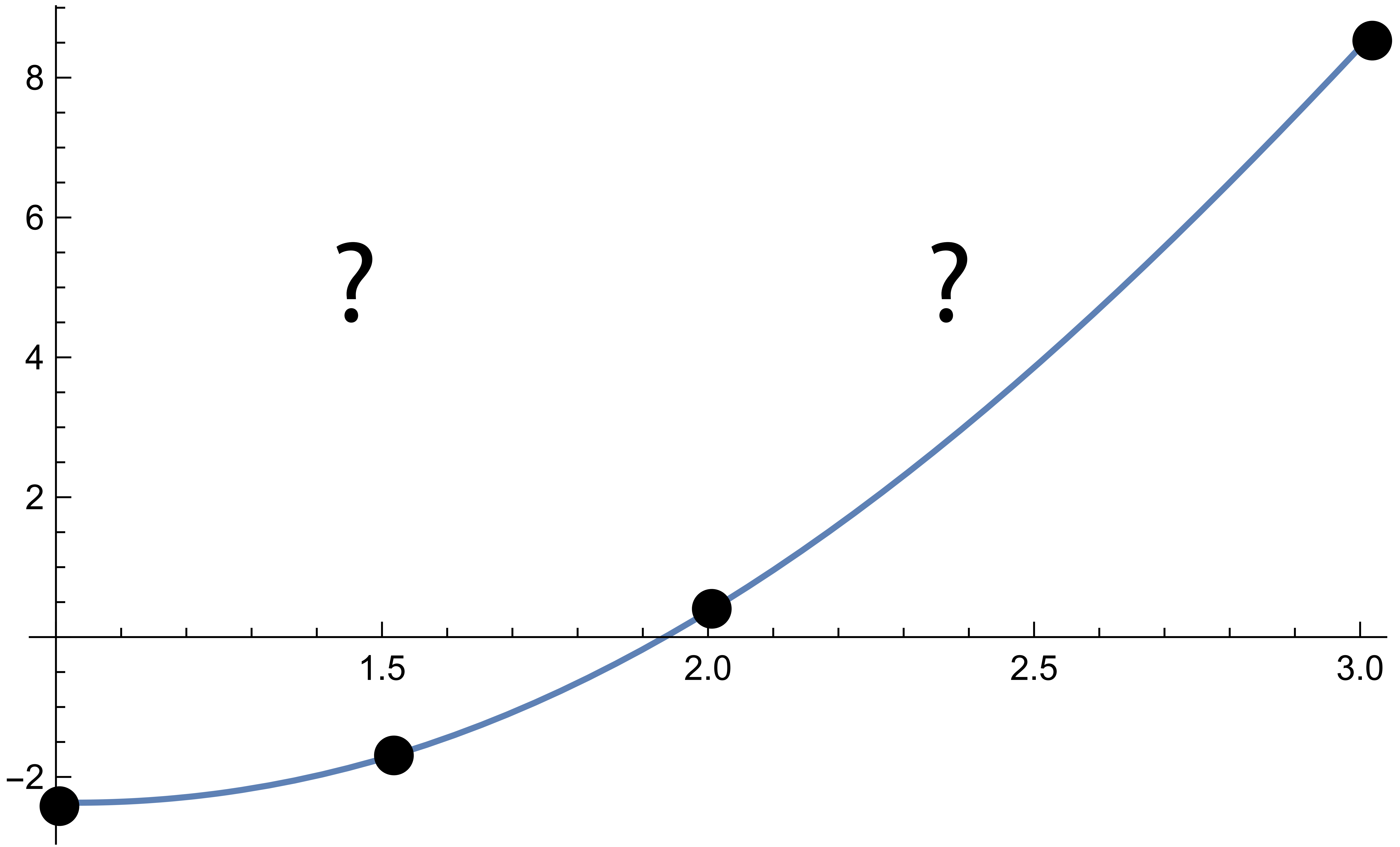

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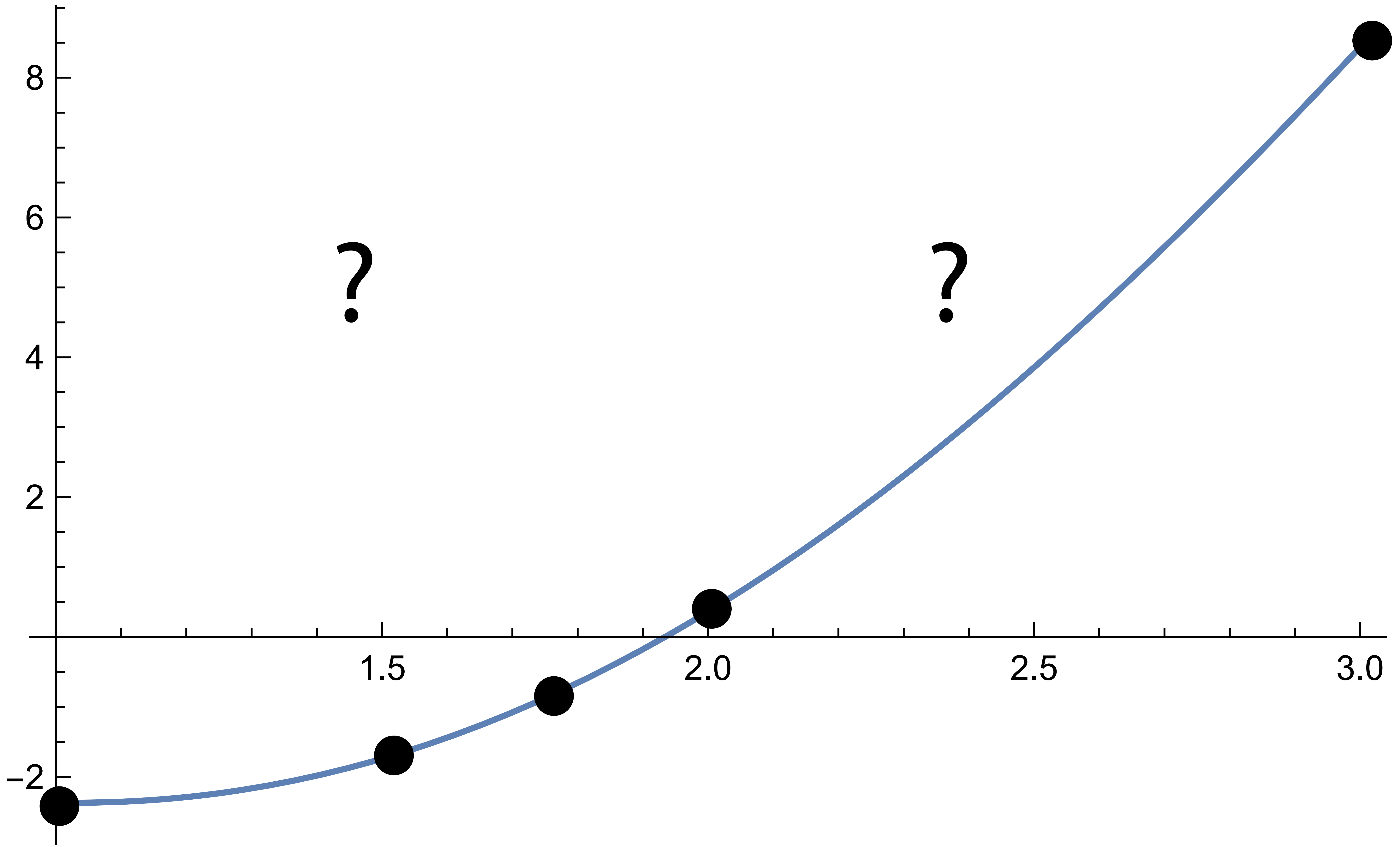

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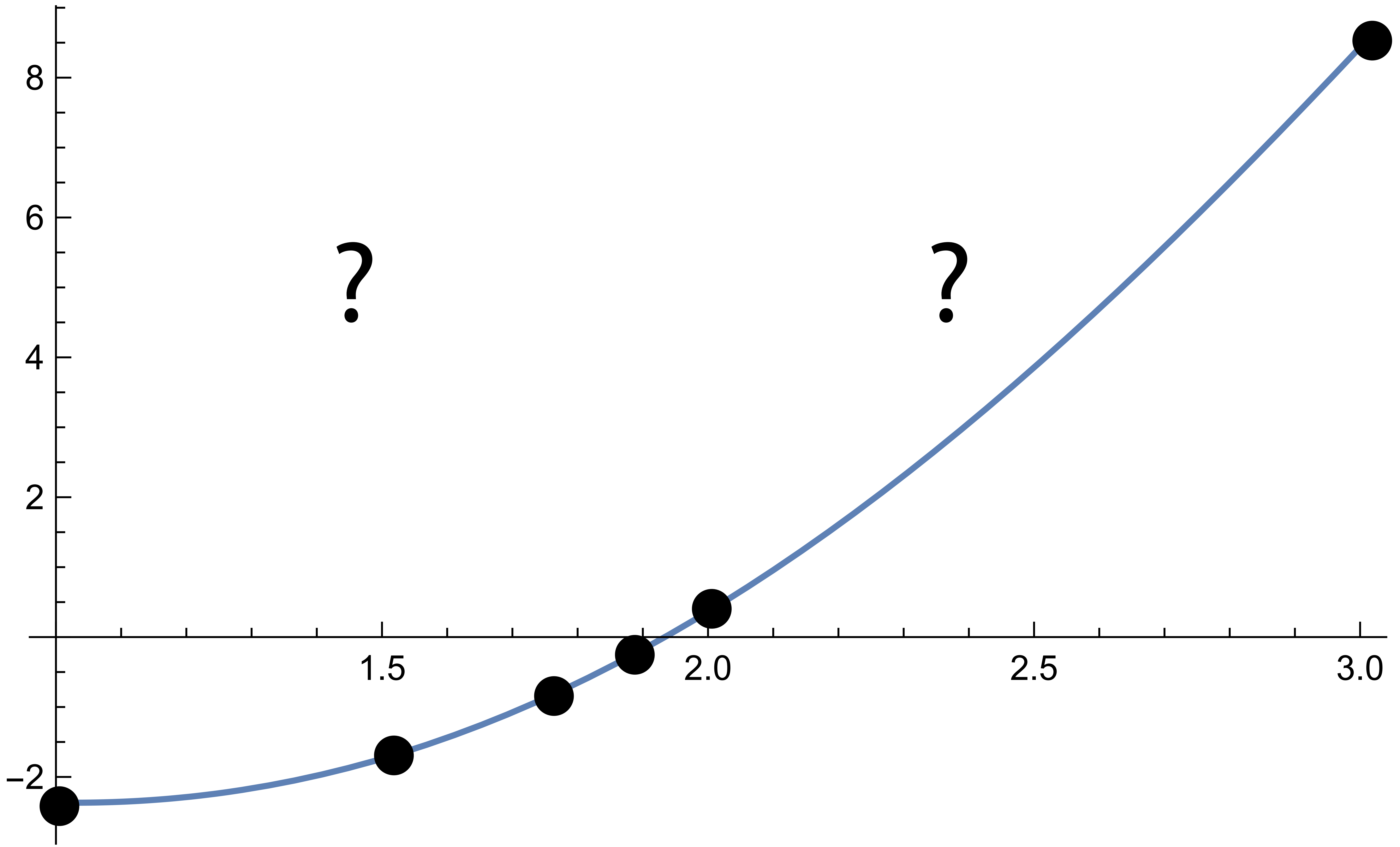
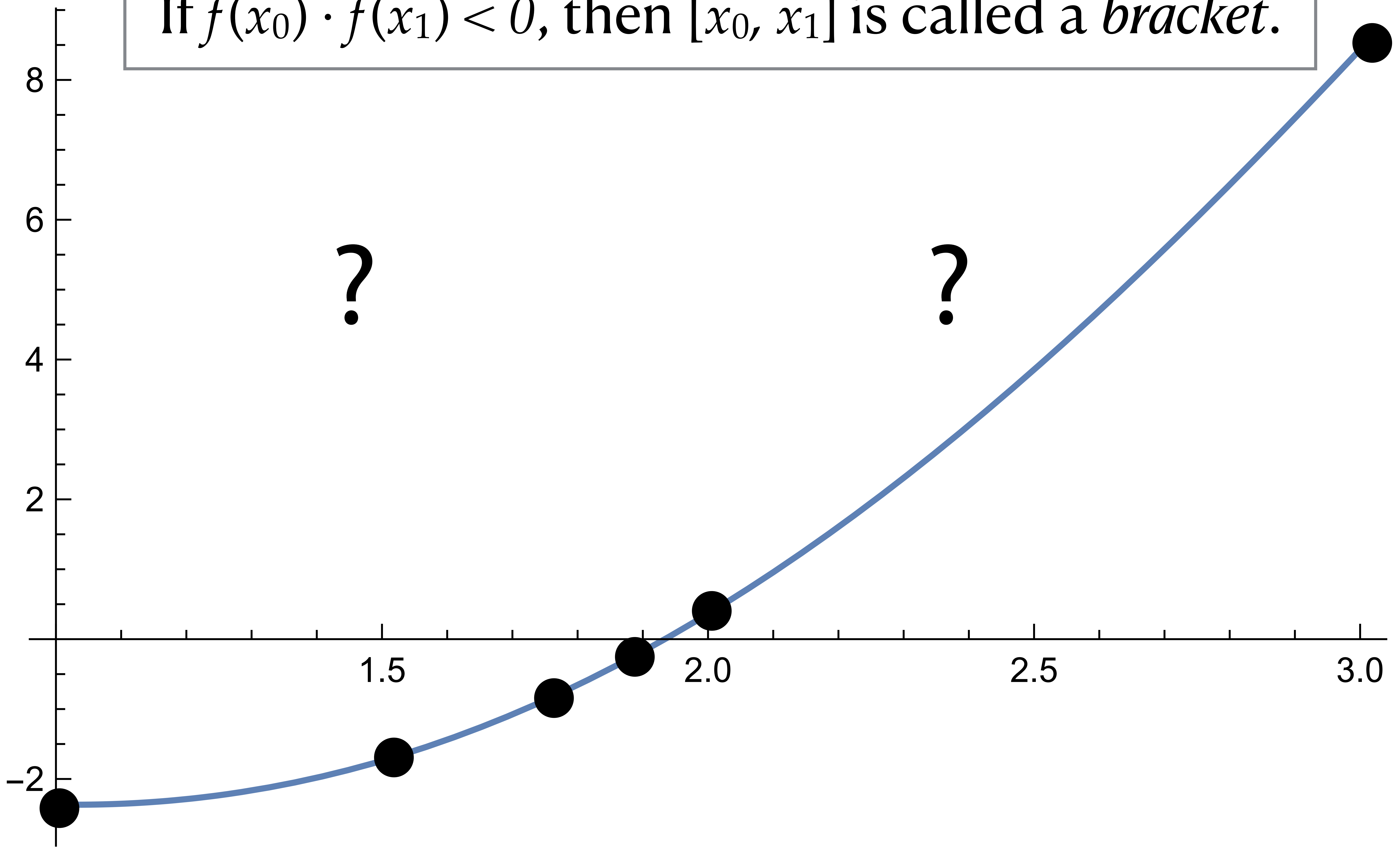


Use of continuity in our model problem

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

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Is this code optimal?

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    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
```

Is this code optimal?

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

Bisection search

function → f, *"bracket"* → l, r, *stopping criterion thresholds* → eps1, eps2

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Does not use function values!
(only their sign is relevant)

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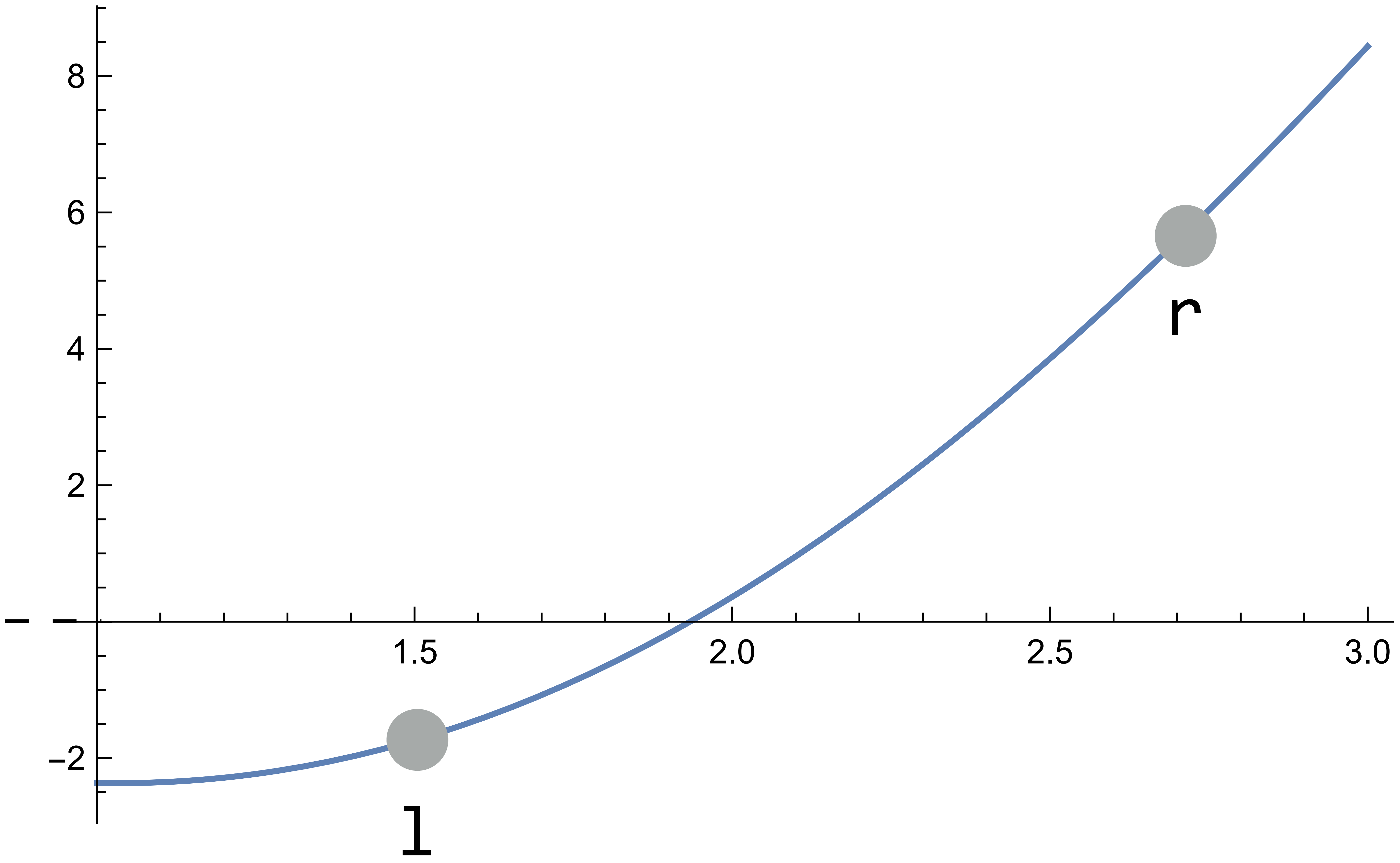

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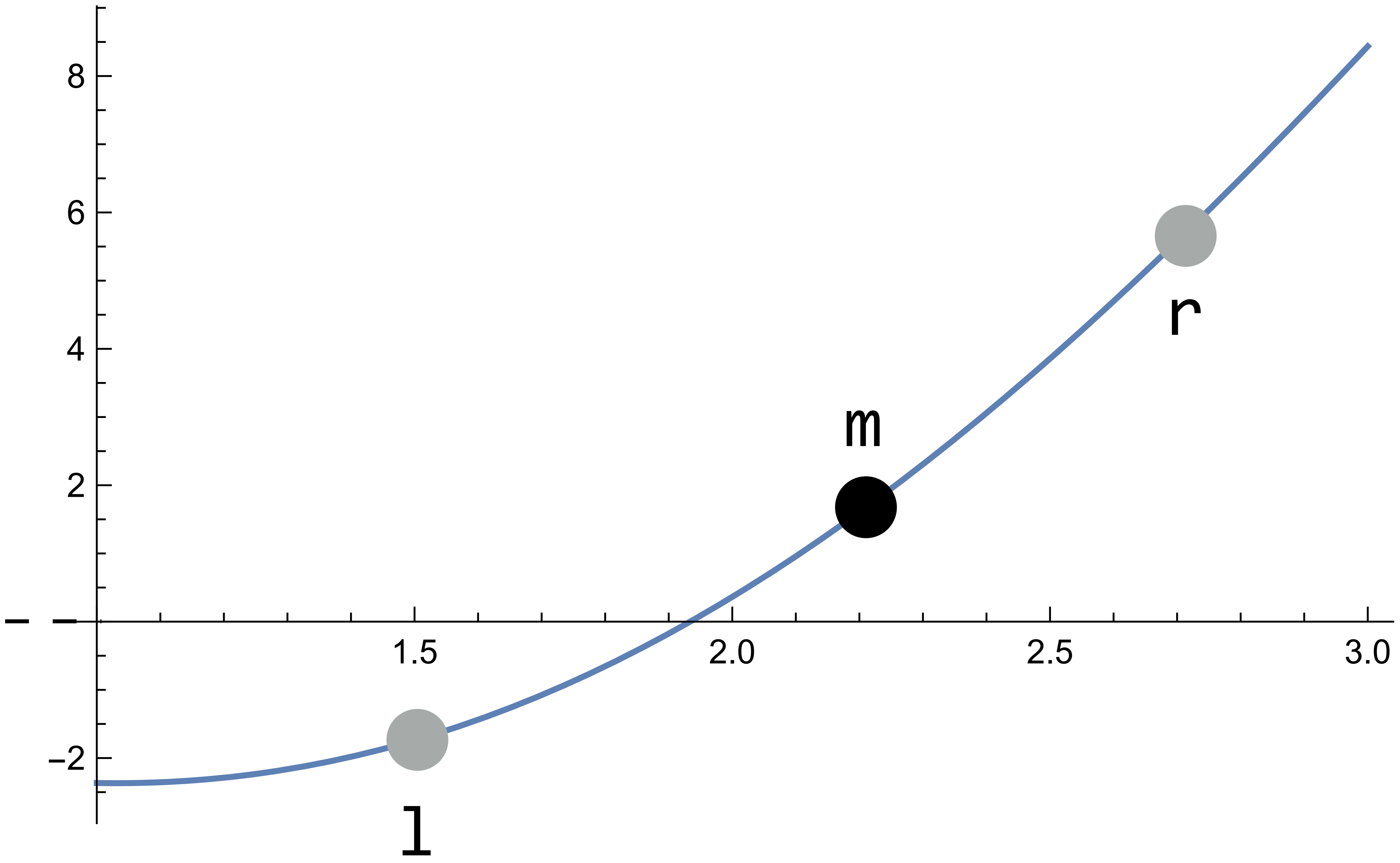

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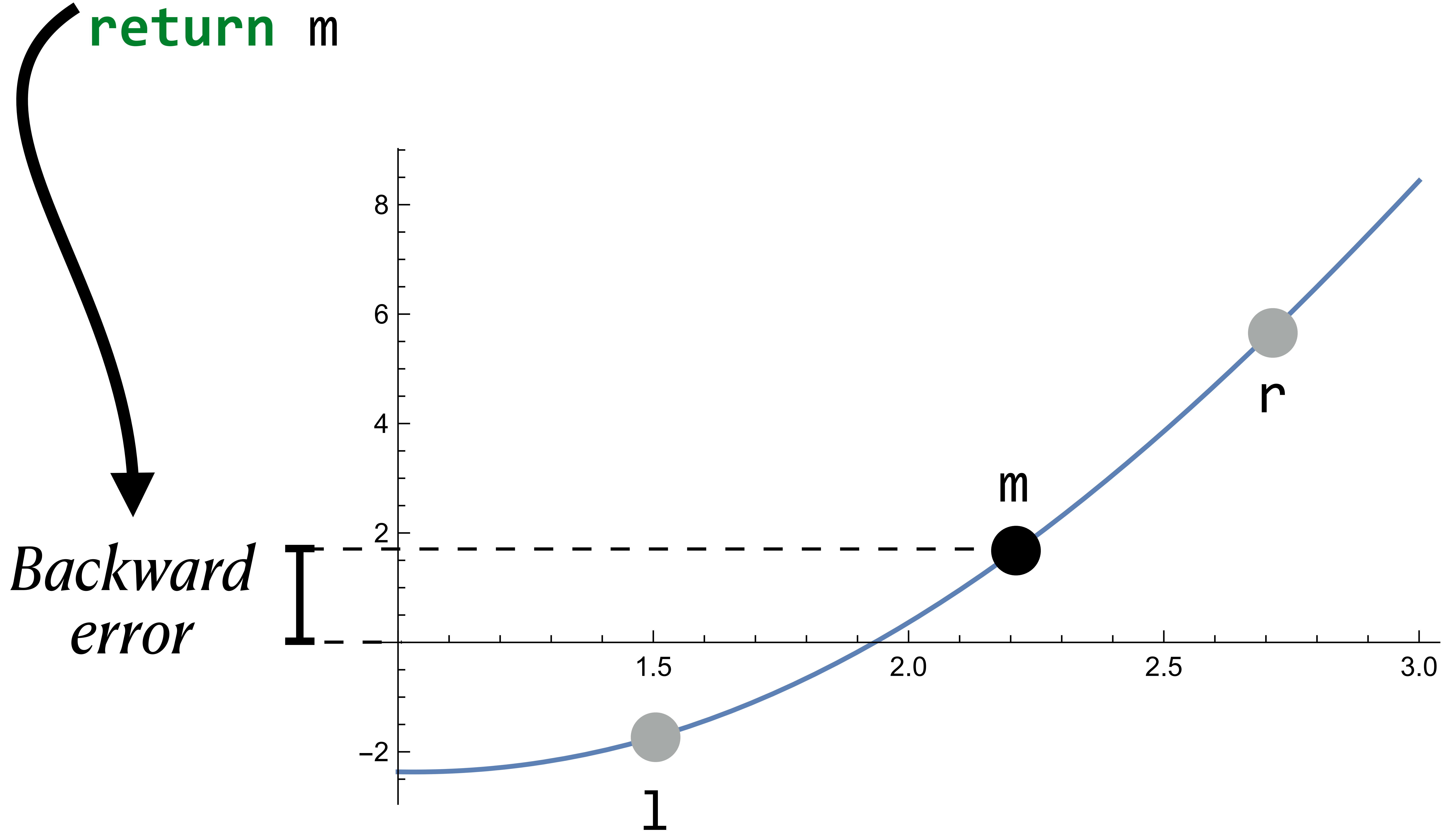

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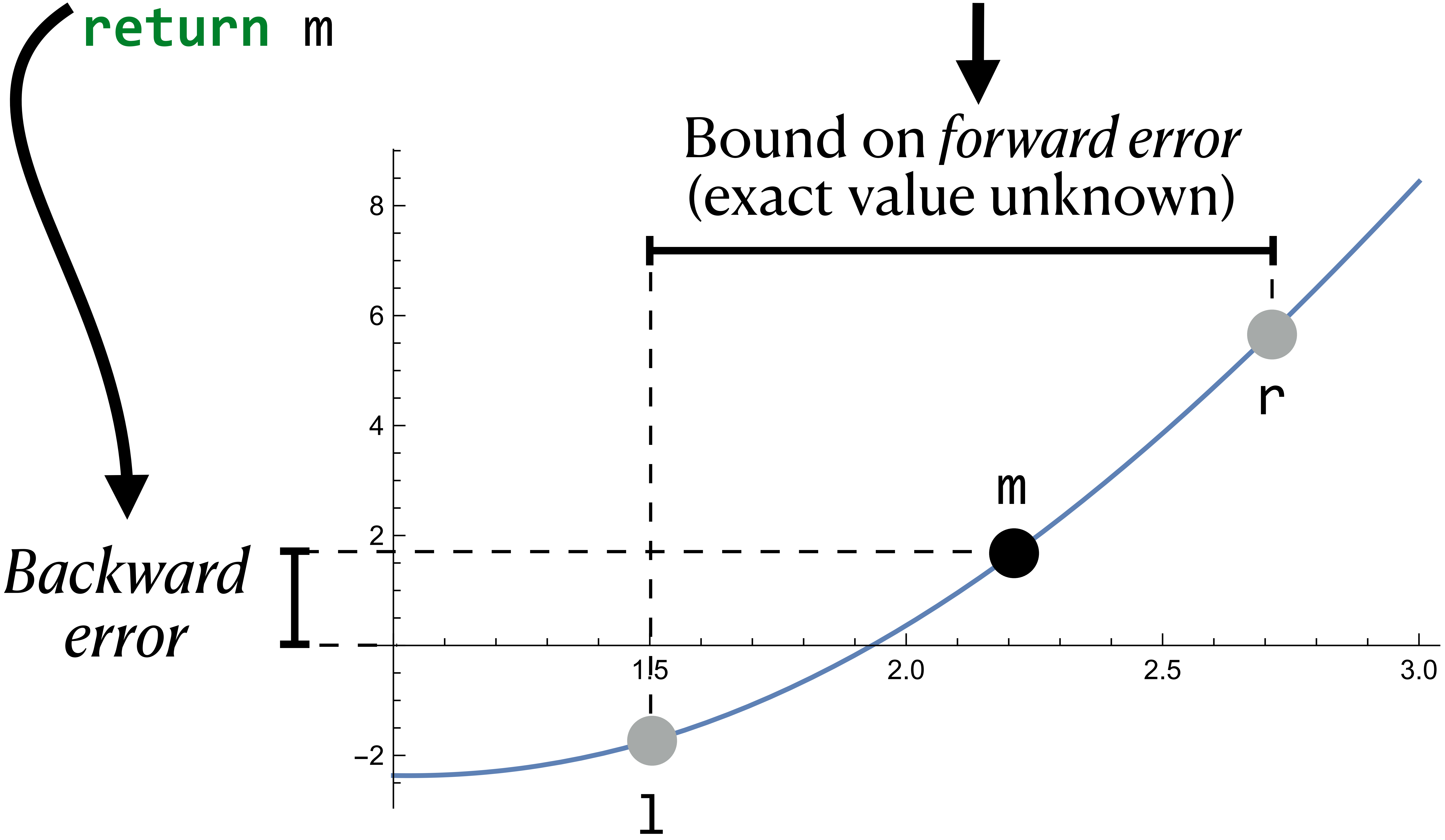

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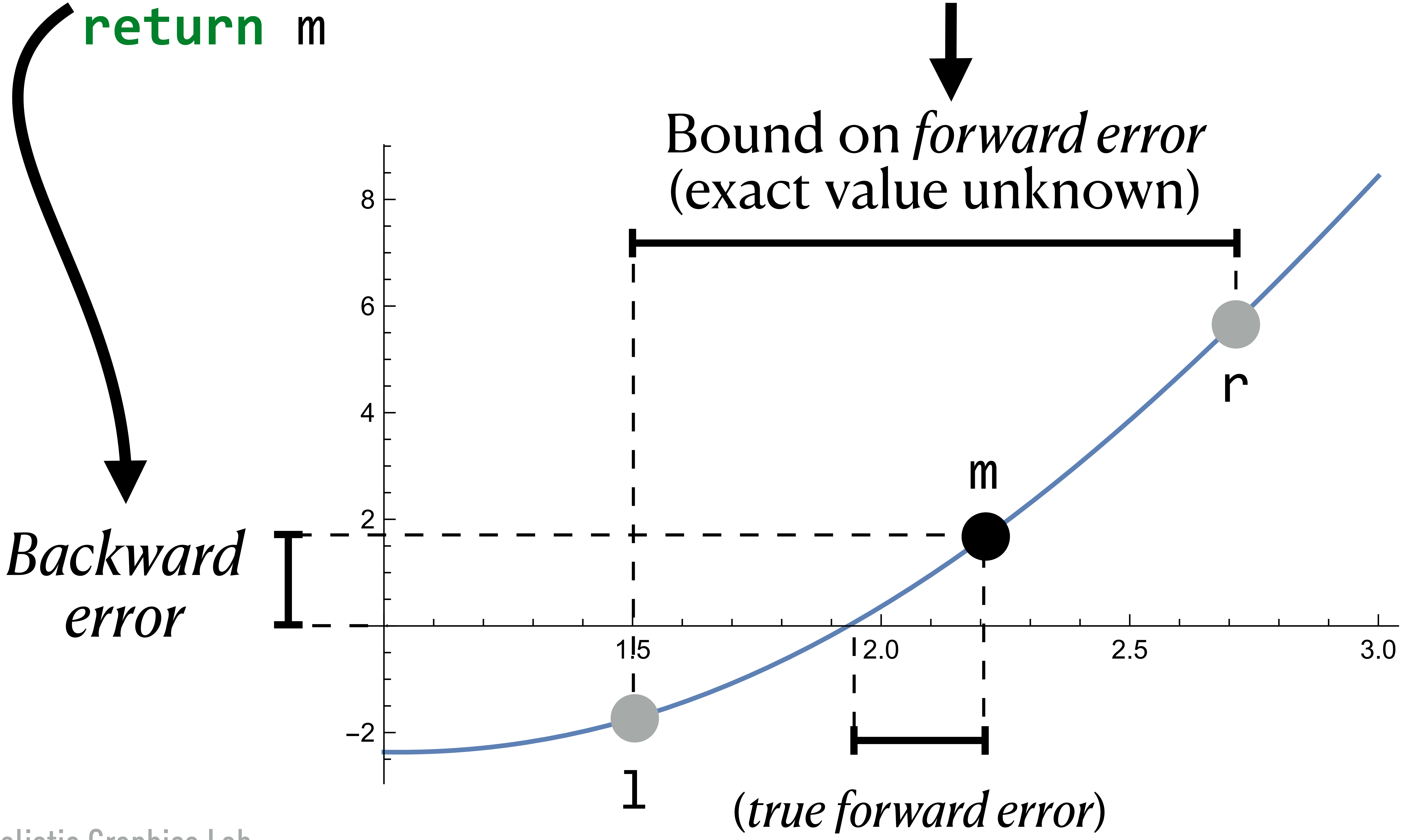

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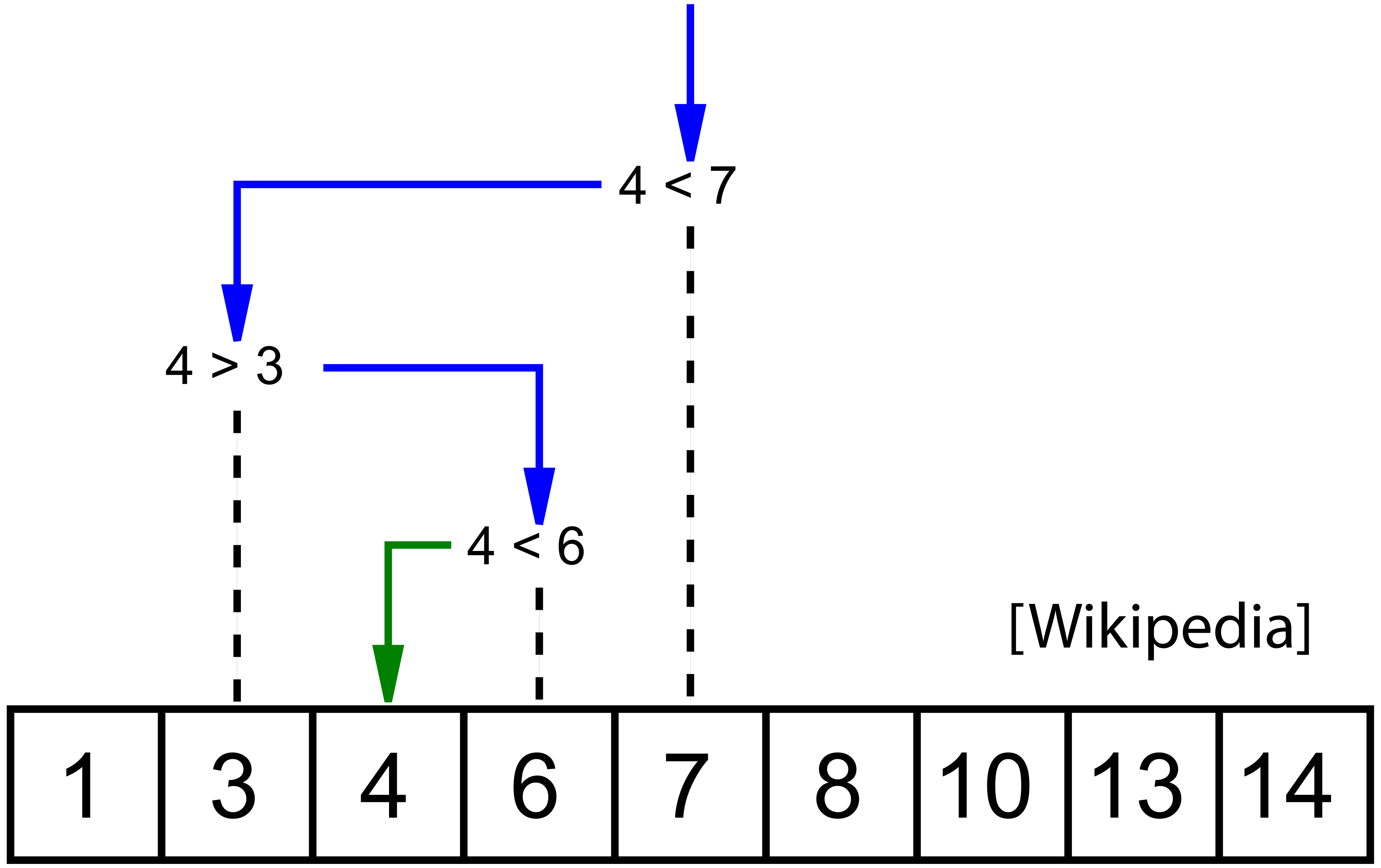

[Wikipedia]

Binary search for 4 in sorted list.

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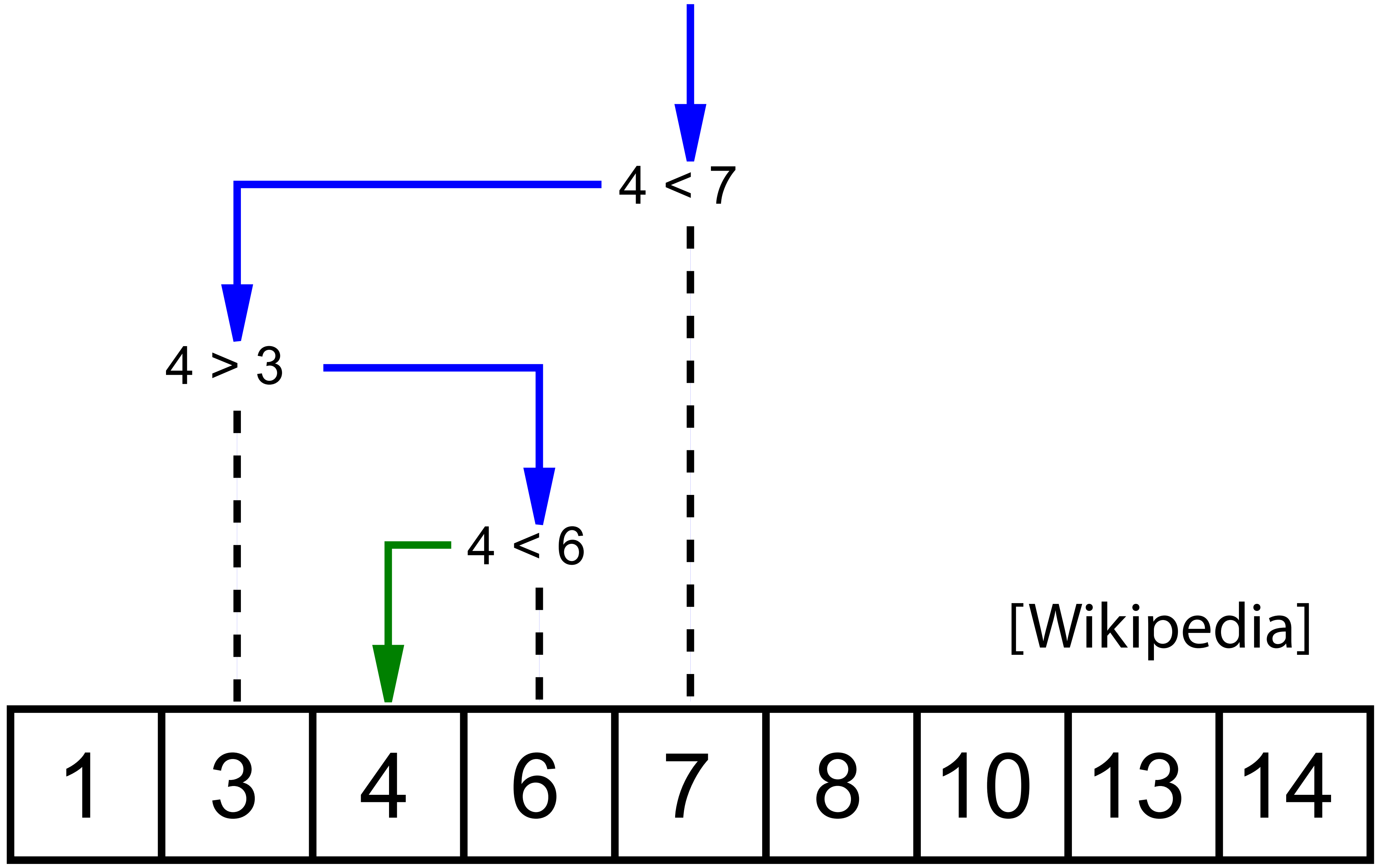

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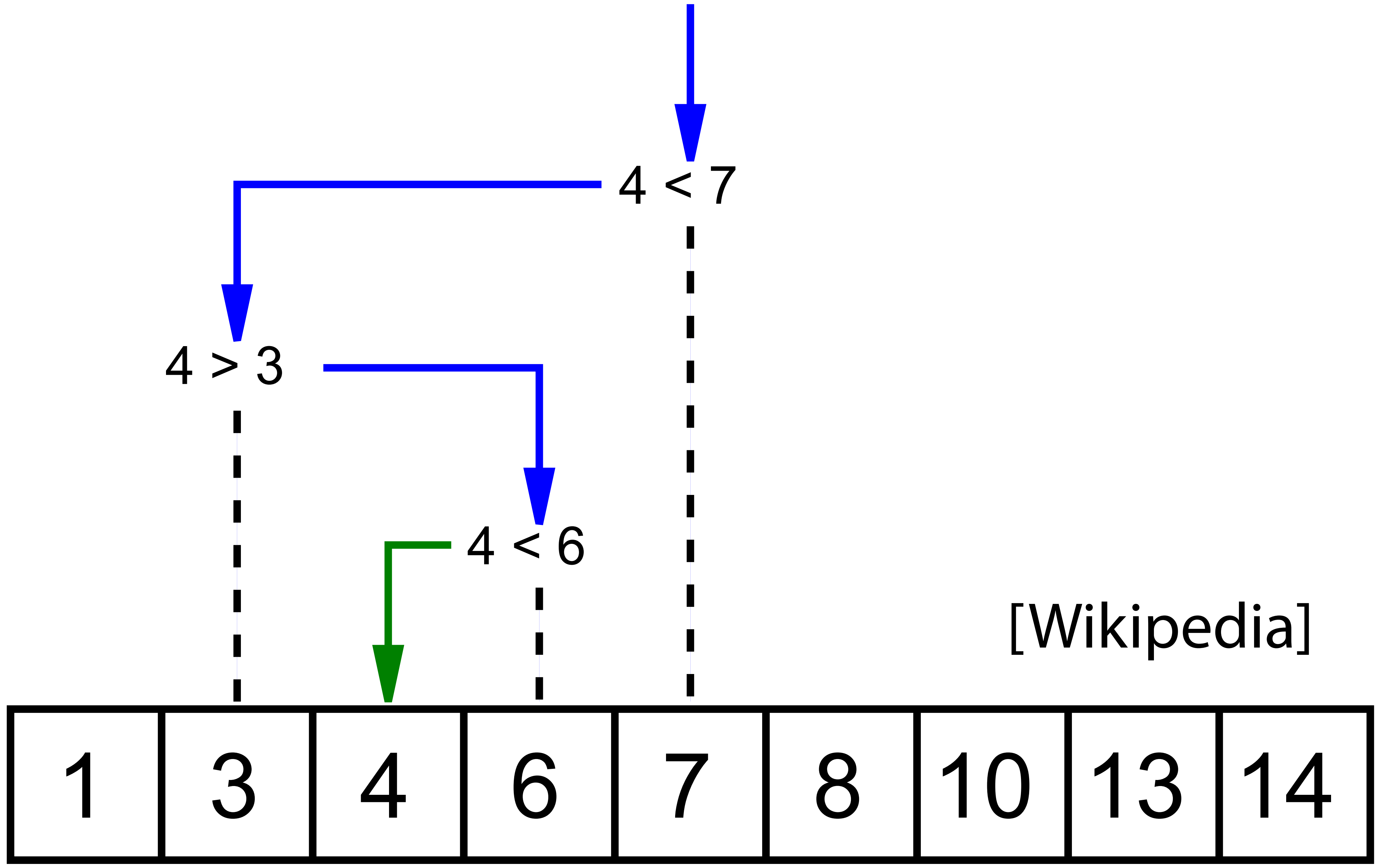

Binary search for 4 in sorted list.

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

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

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- 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) : $r - l$

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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
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1.500000	−1.739980	2.000000	0.362810
1.750000	−0.873444	2.000000	0.362810
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[Heath]

Midpoint = **1.933**838

True solution = 1.93375376282..

(13 iterations for ~4 digits)

Newton's method

- Based on first-order Taylor expansion:

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

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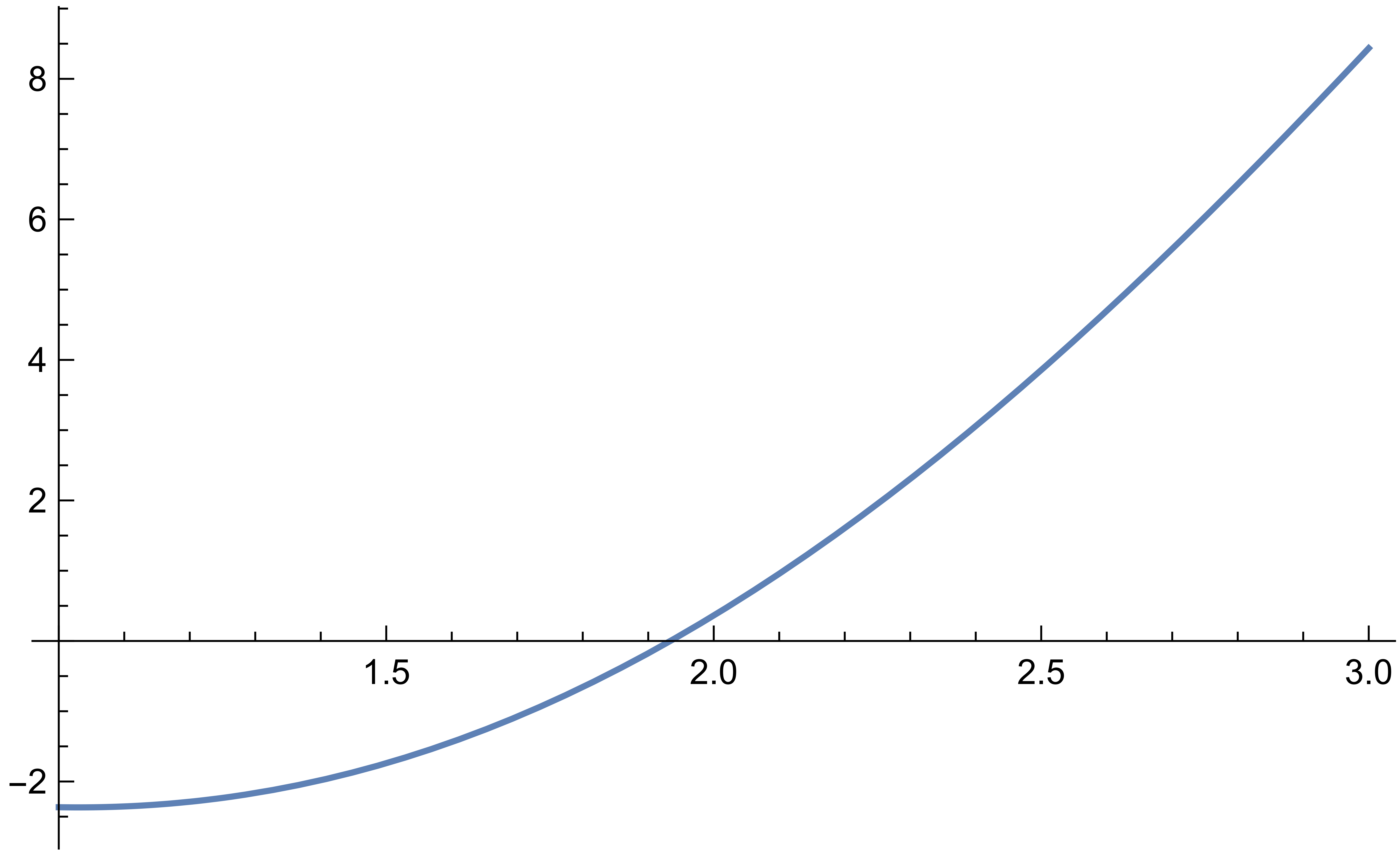
- Move to that position, and repeat..

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

Visualization of Newton's method



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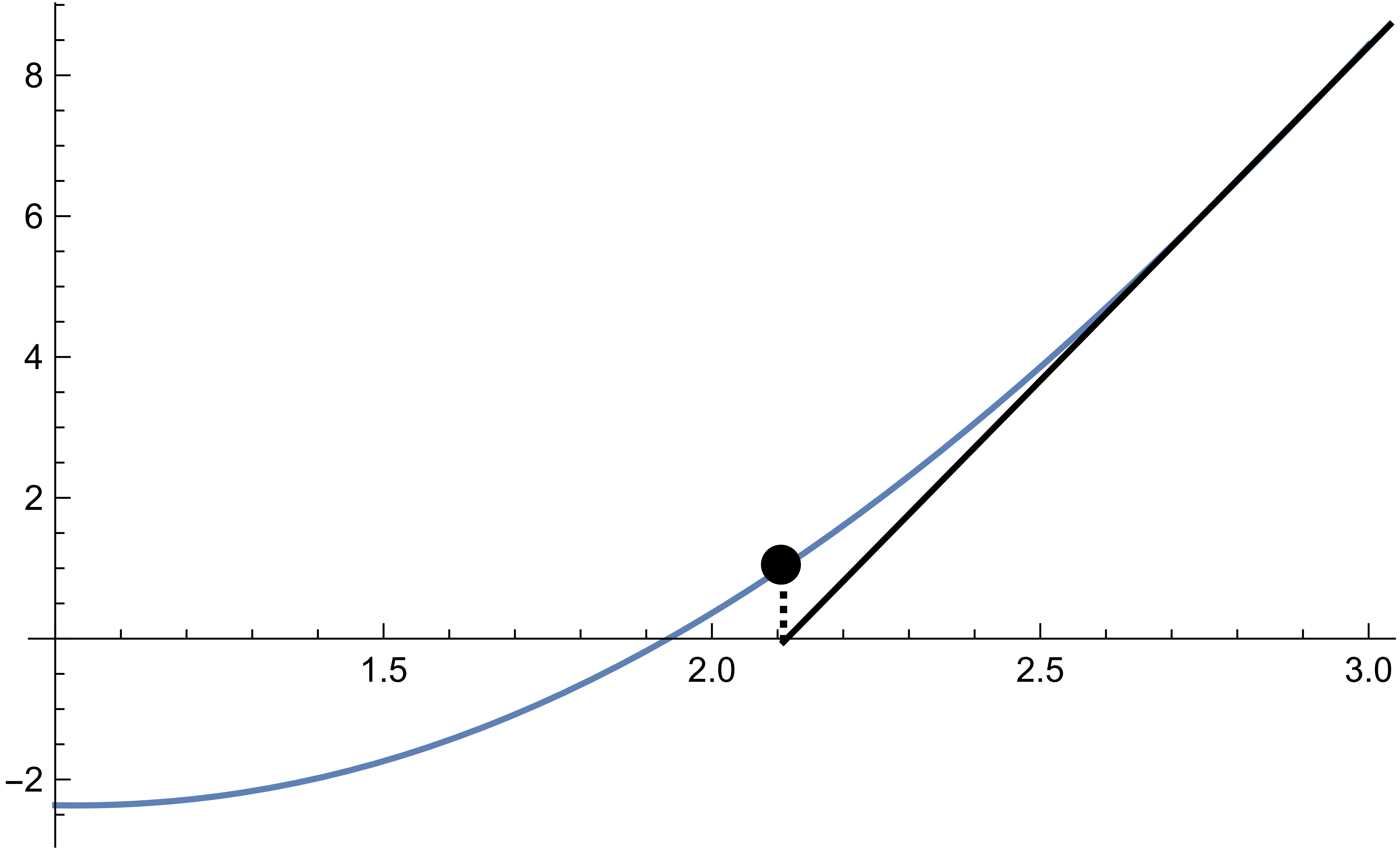

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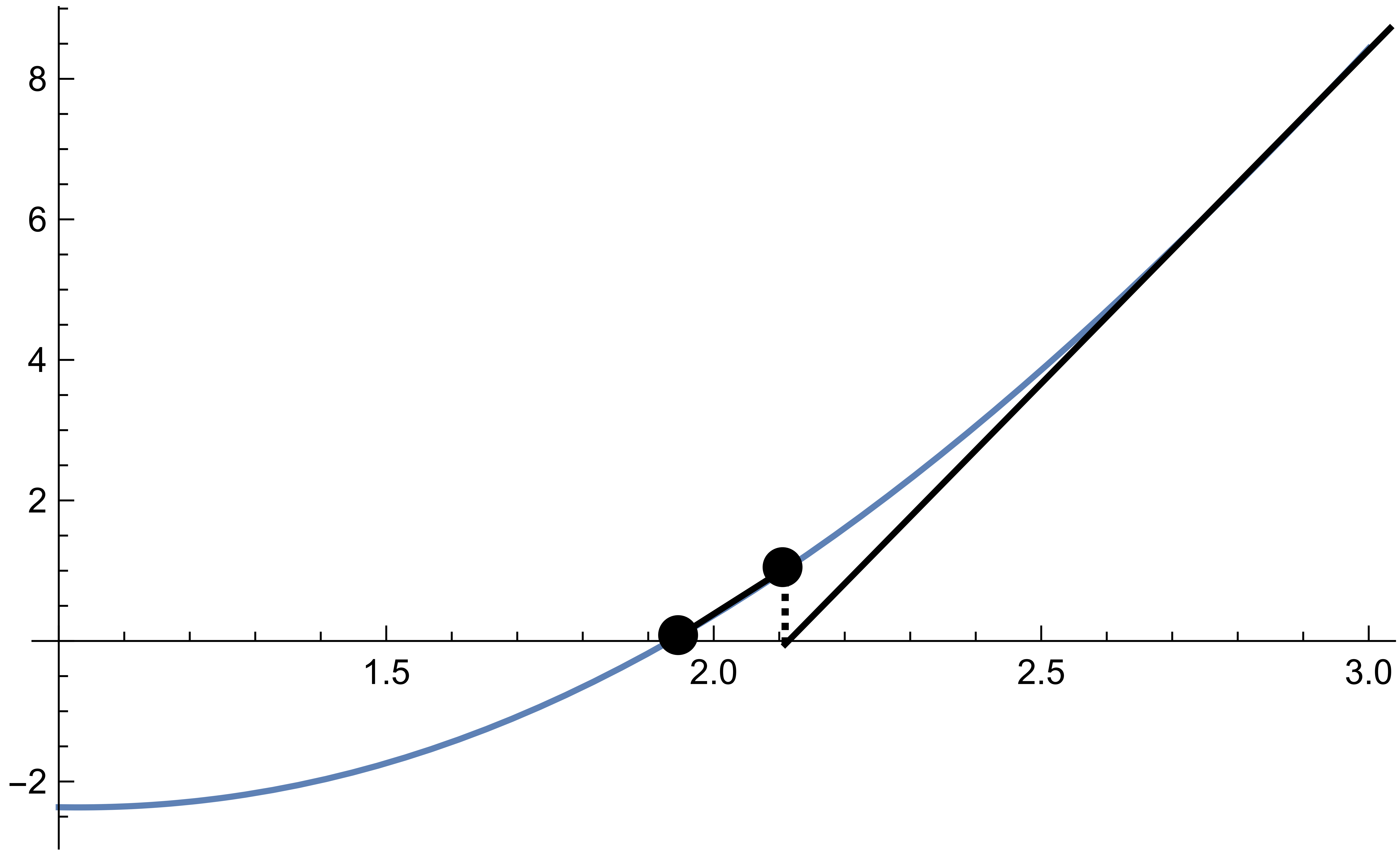

Convergence of Newton's method

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Newton's method requires the derivative of f. Here,

$$f'(x) = 2x - 4\cos x$$

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x	$f(x)$	$f'(x)$	h
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2.153058	1.294772	6.505771	−0.199019
<u>1.9</u>54039	0.108438	5.403795	−0.020067
<u>1.933</u>972	0.001152	5.288919	−0.000218
<u>1.933754</u>	0.000000	5.287670	0.000000

(5 iterations for ~7 digits)

[Heath]

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[Heath]

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

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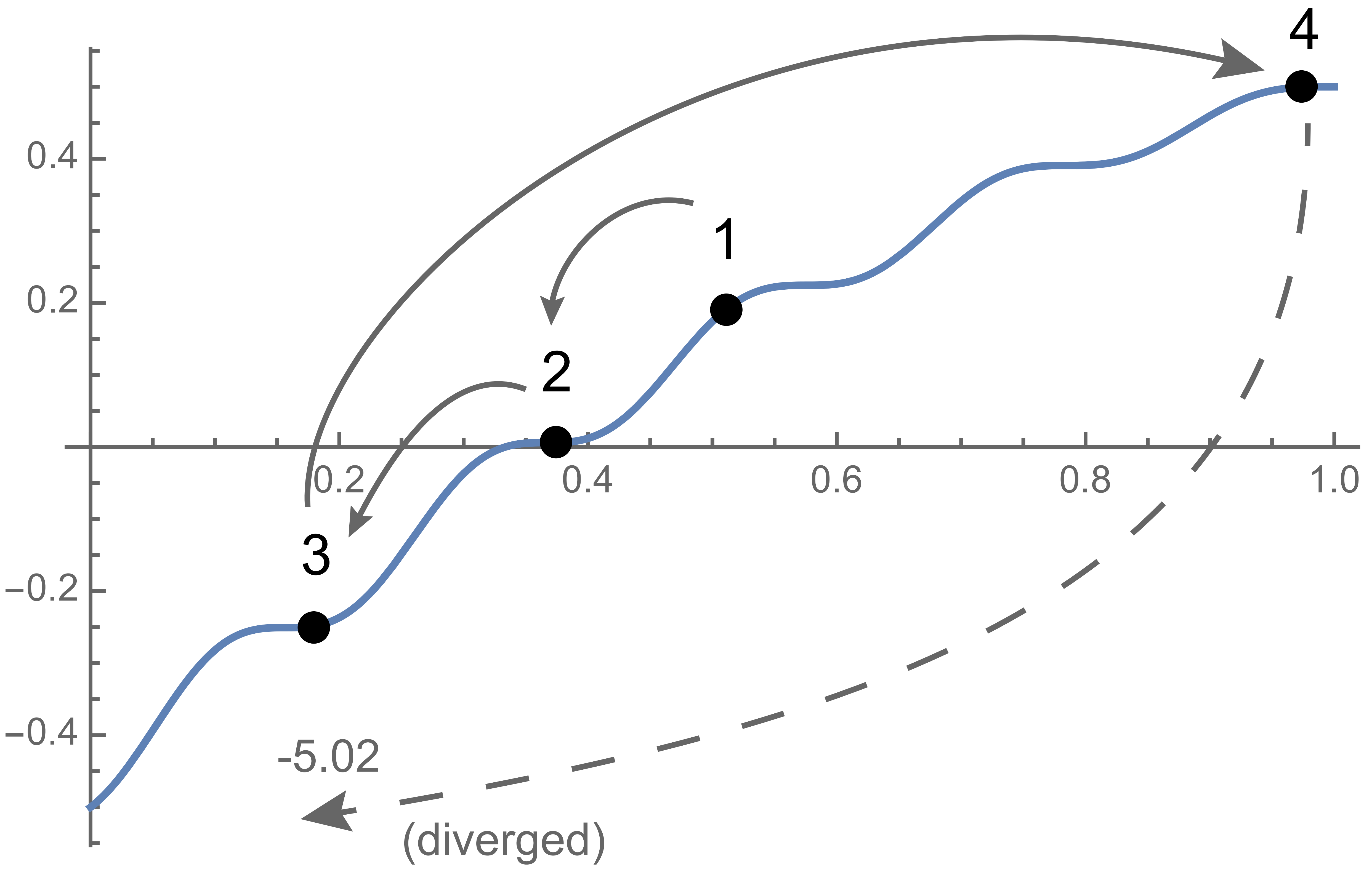
Failure cases of Newton's Method



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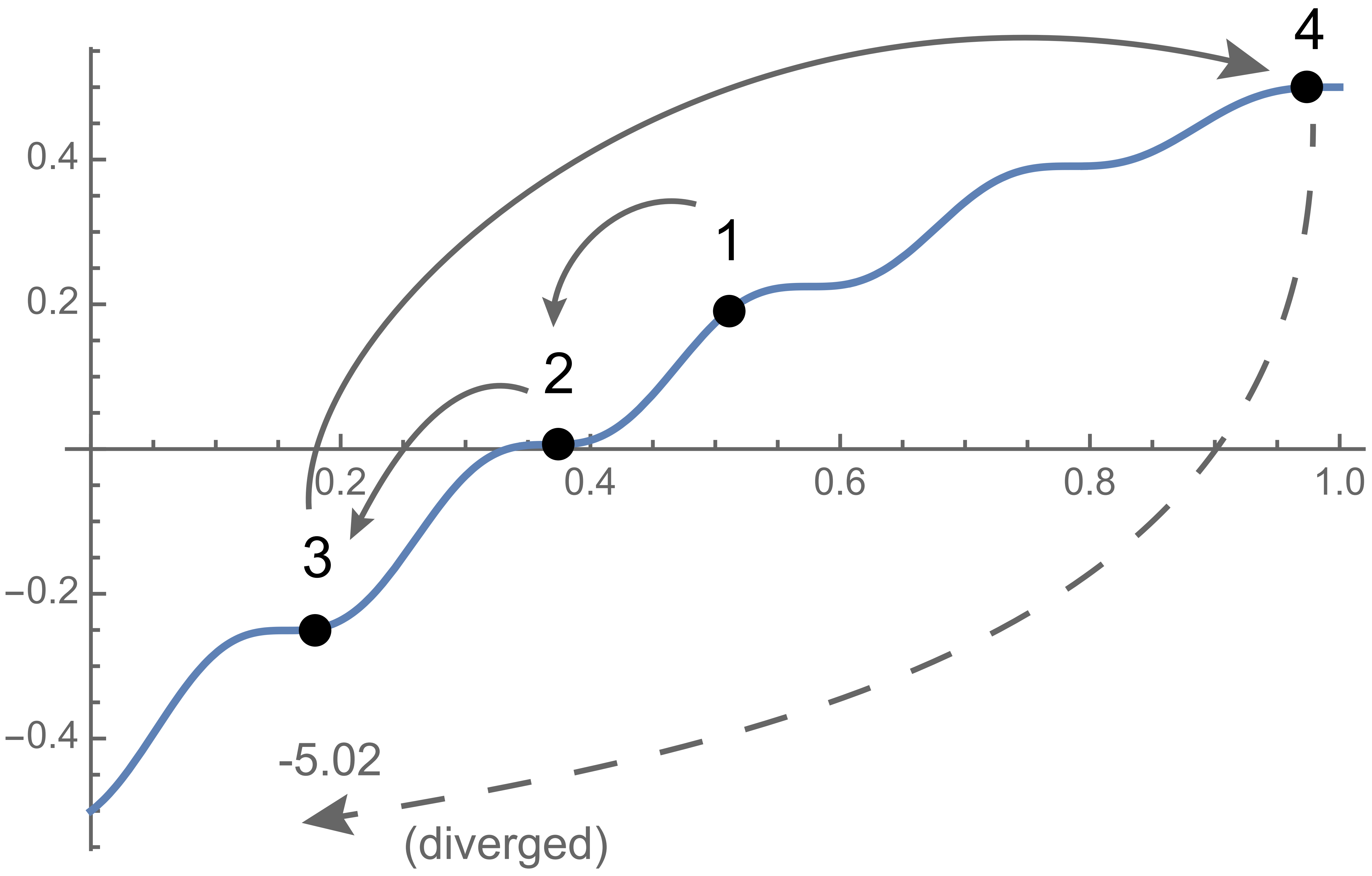

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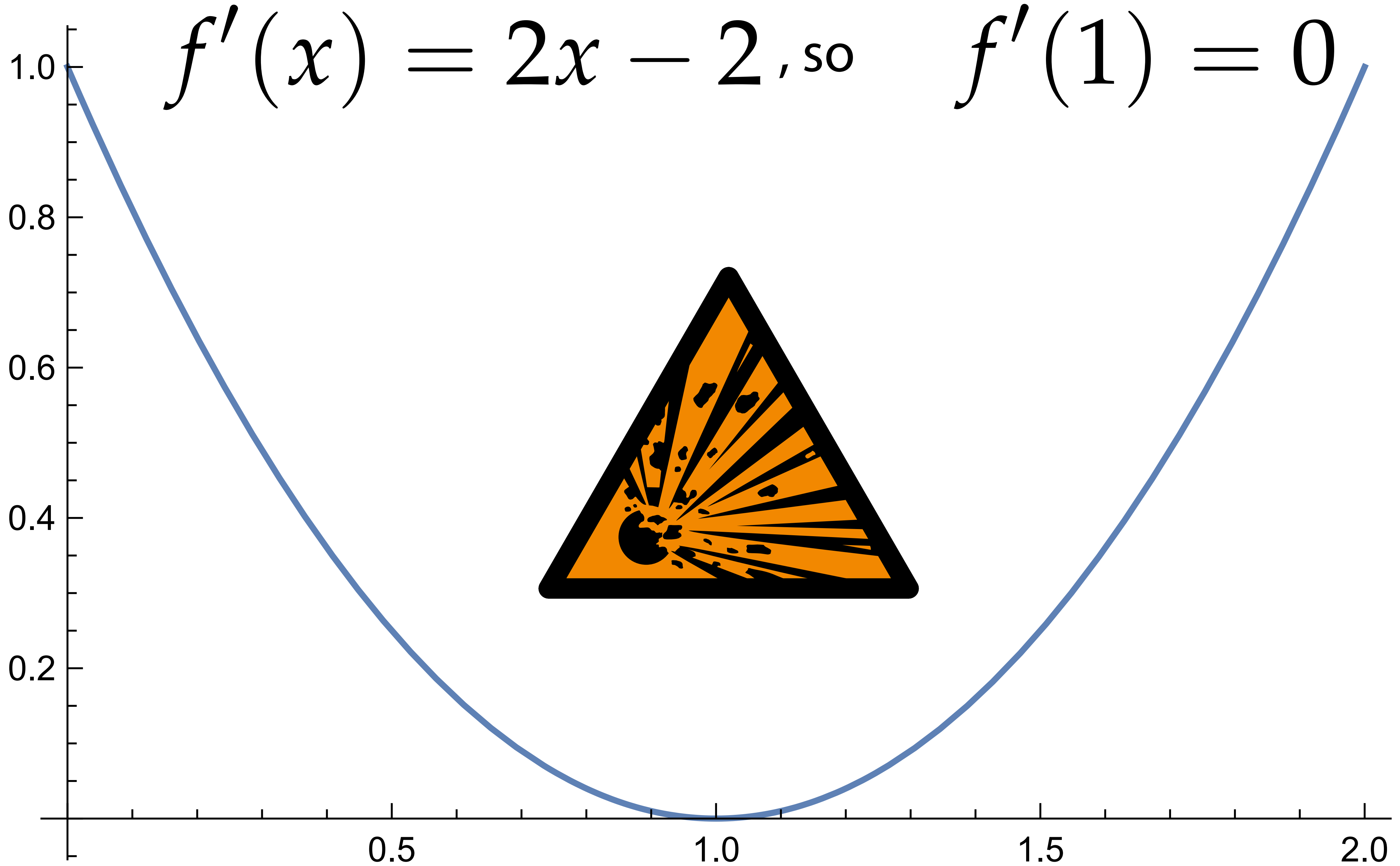

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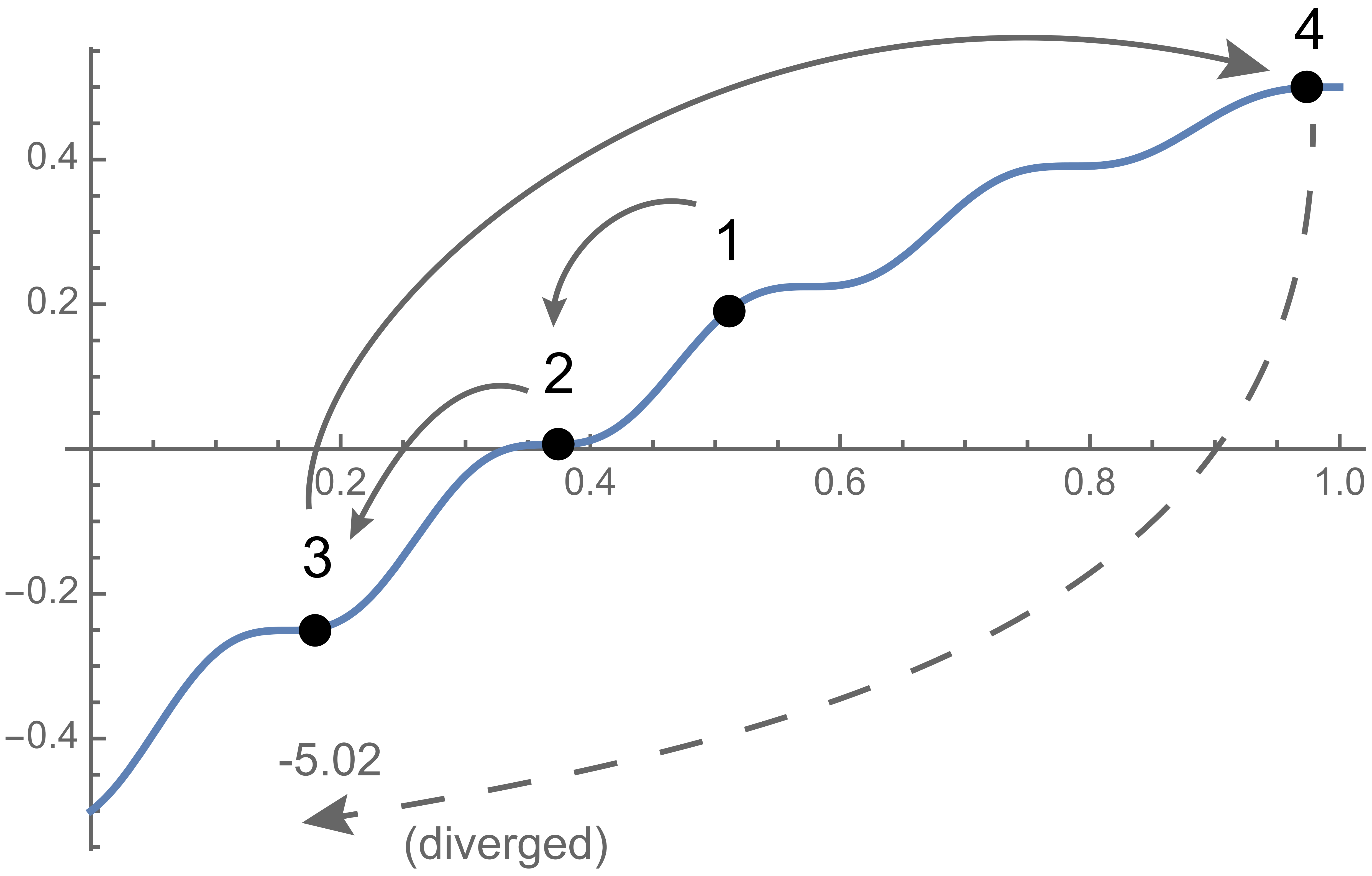

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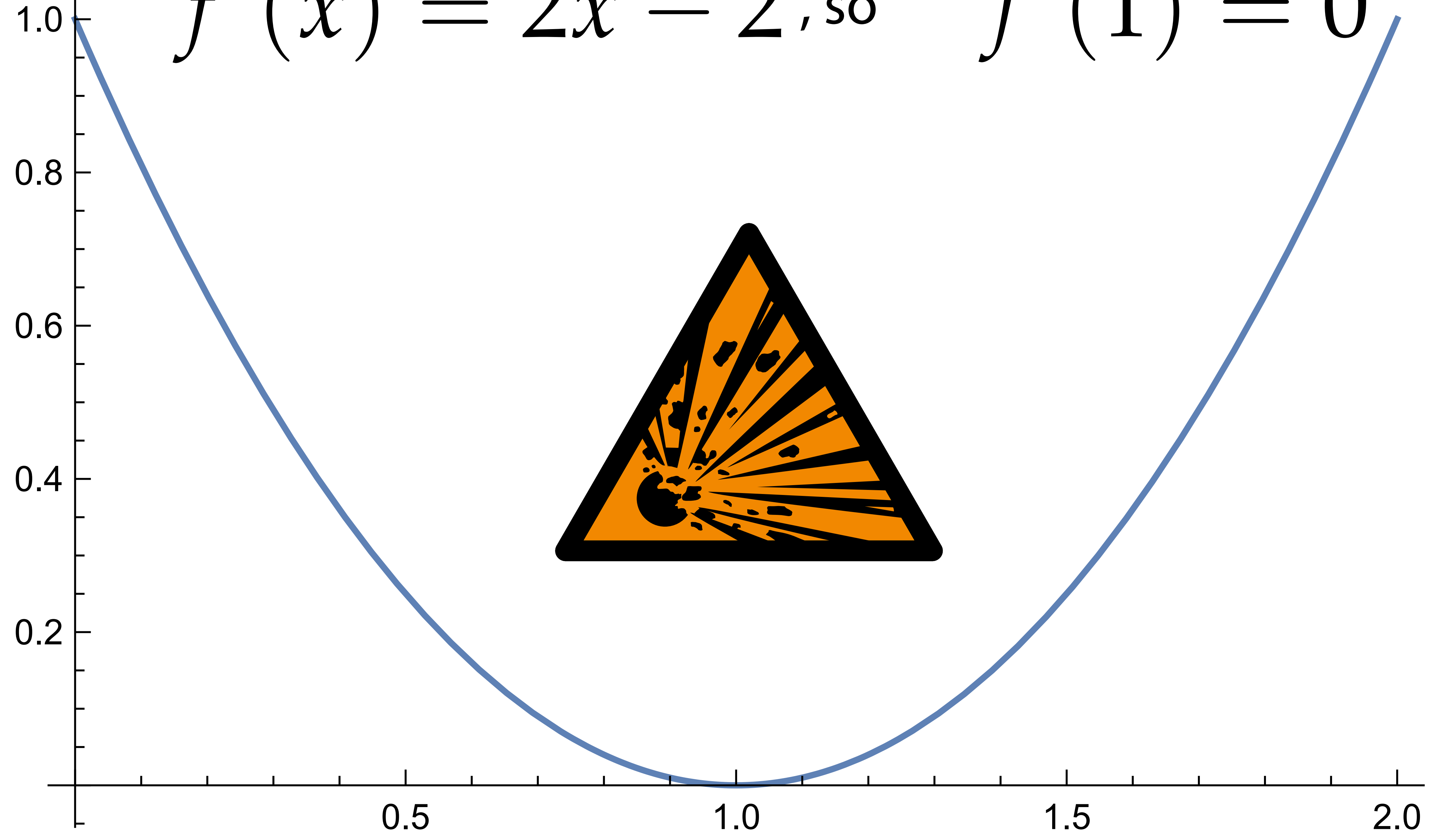

In theory: division by zero at $x = 1$.

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

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  - Assumes input and output spaces have matching dimension.

Relation to Character Animation

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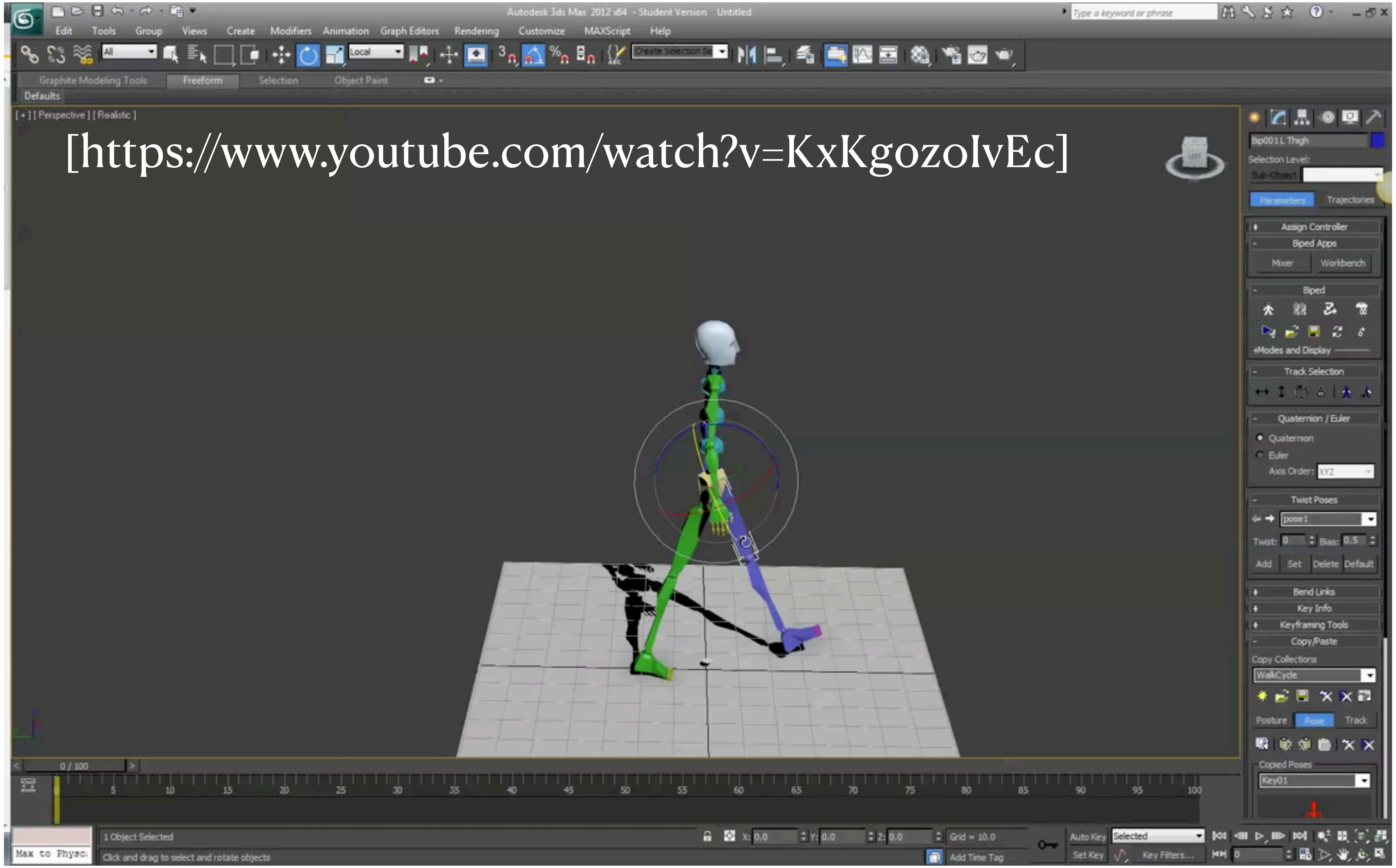
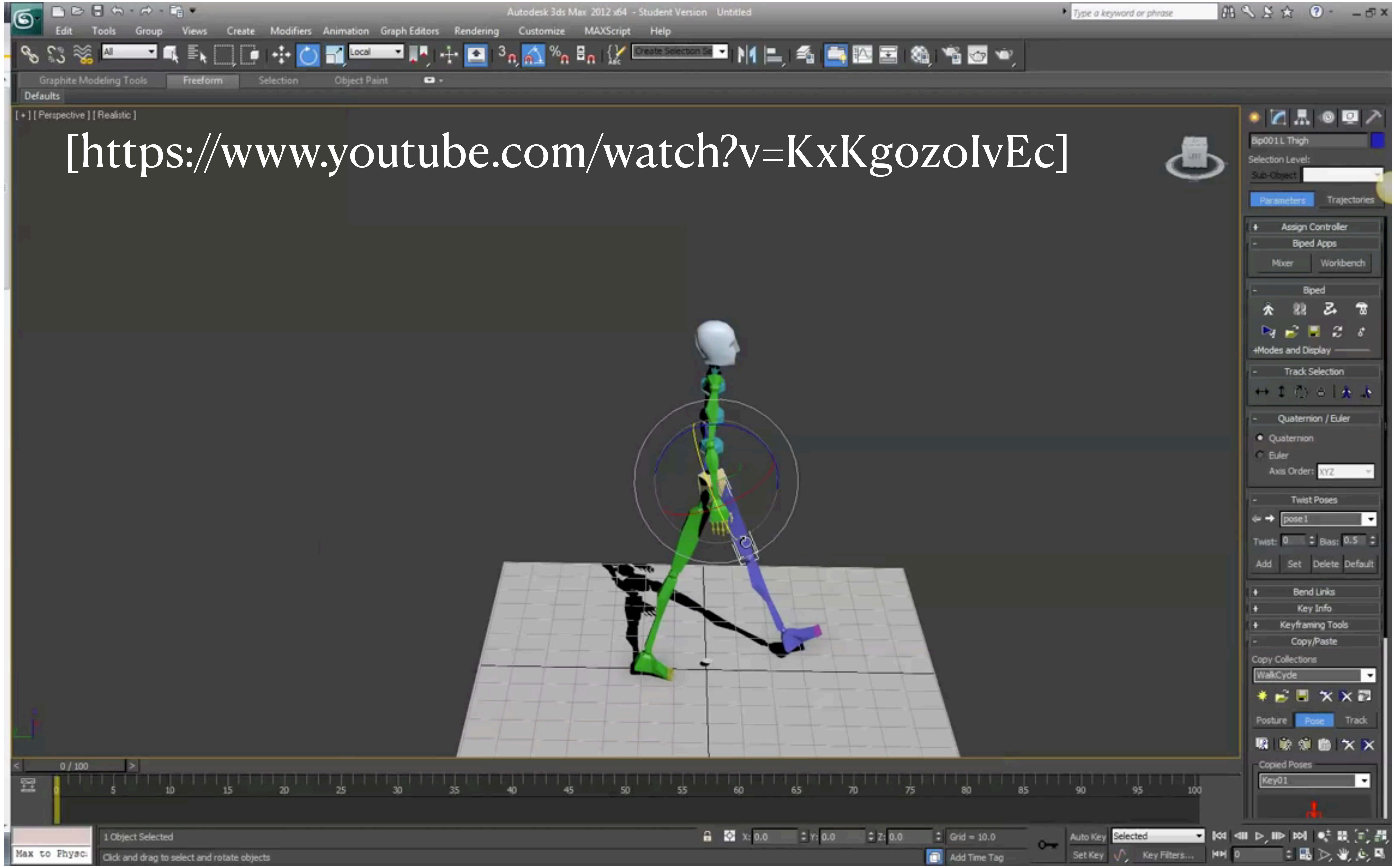
Connection to Character Animation



[https://www.youtube.com/watch?v=KxKgozoIvEc]

Connection to Character Animation



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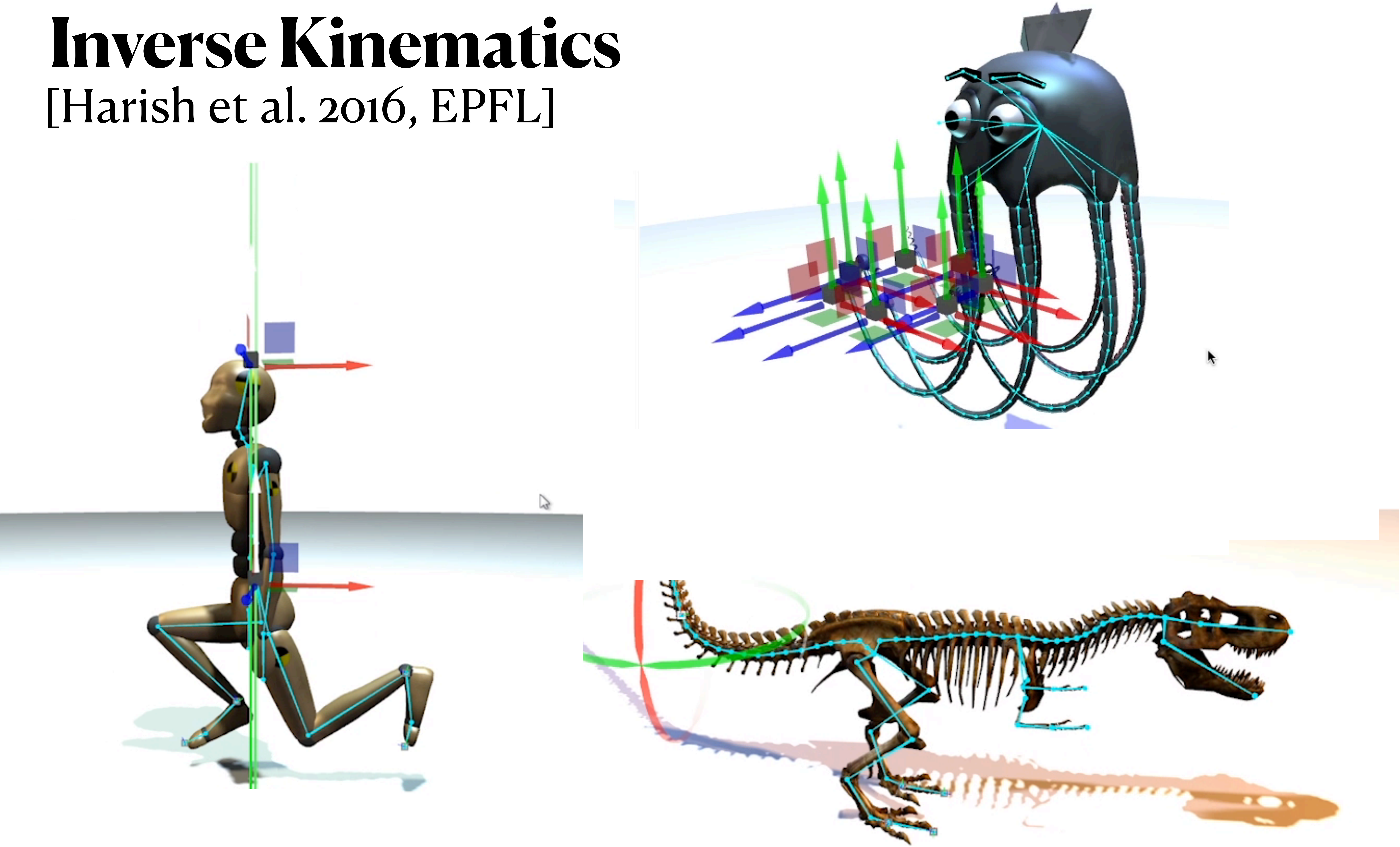
Inverse Kinematics
[Harish et al. 2016, EPFL]



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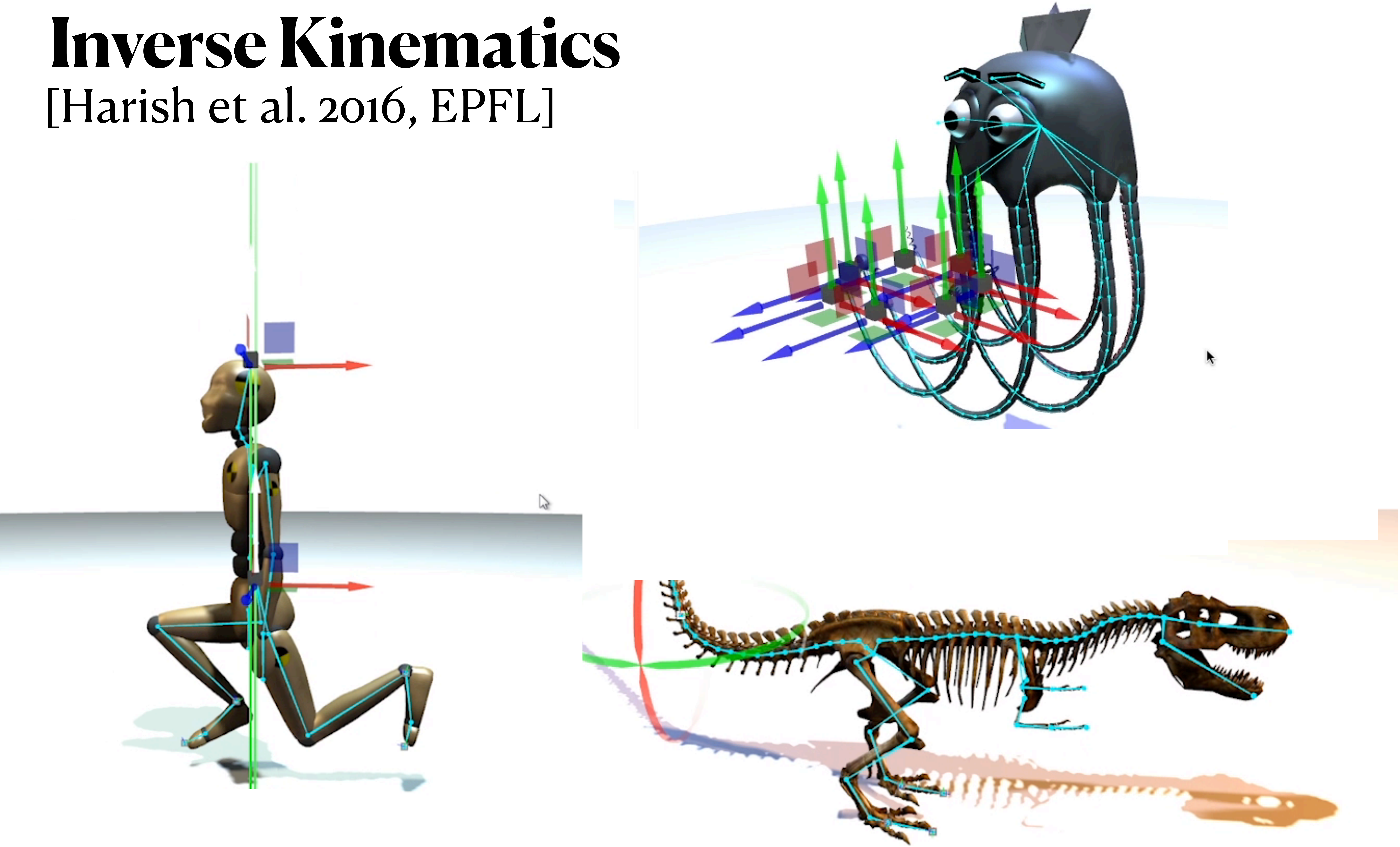
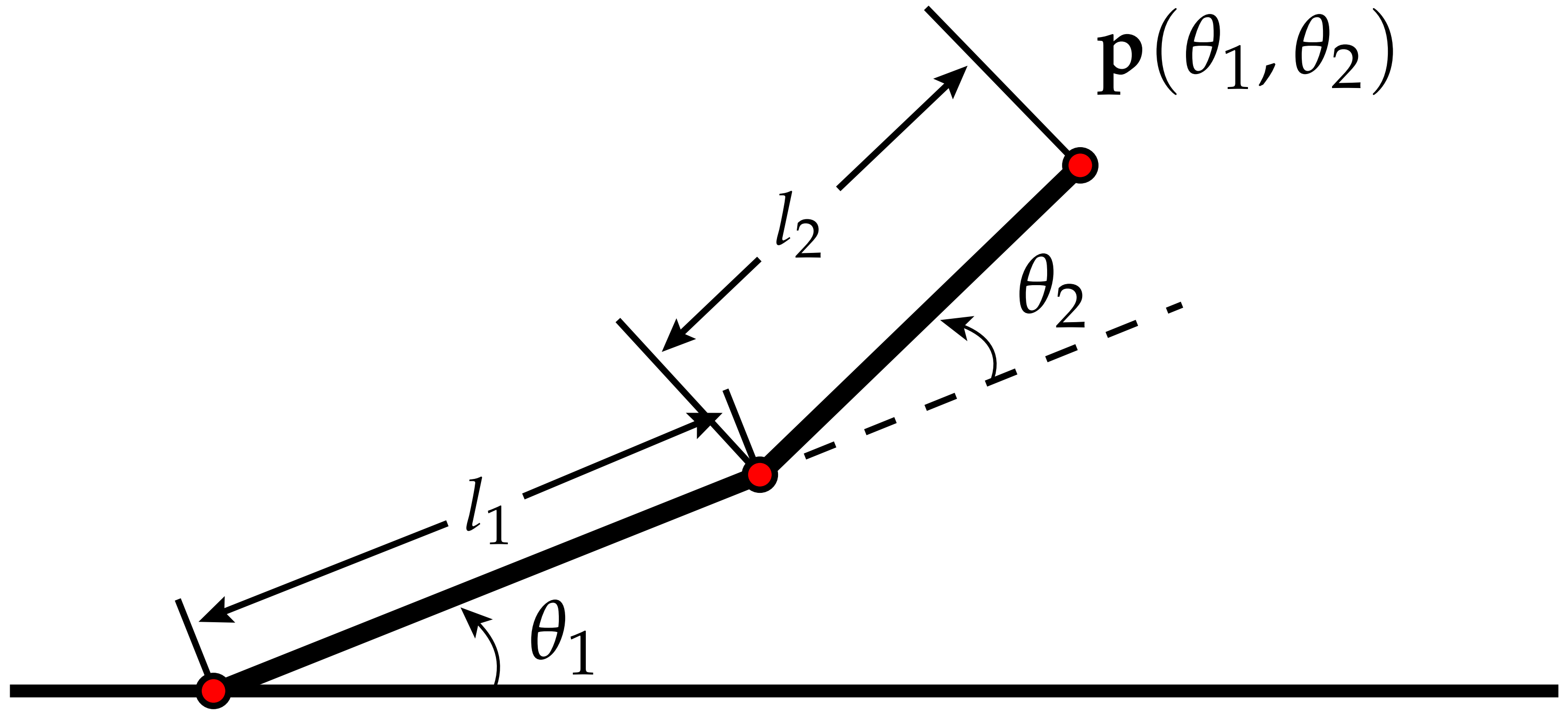


Inverse Kinematics via Newton's method

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



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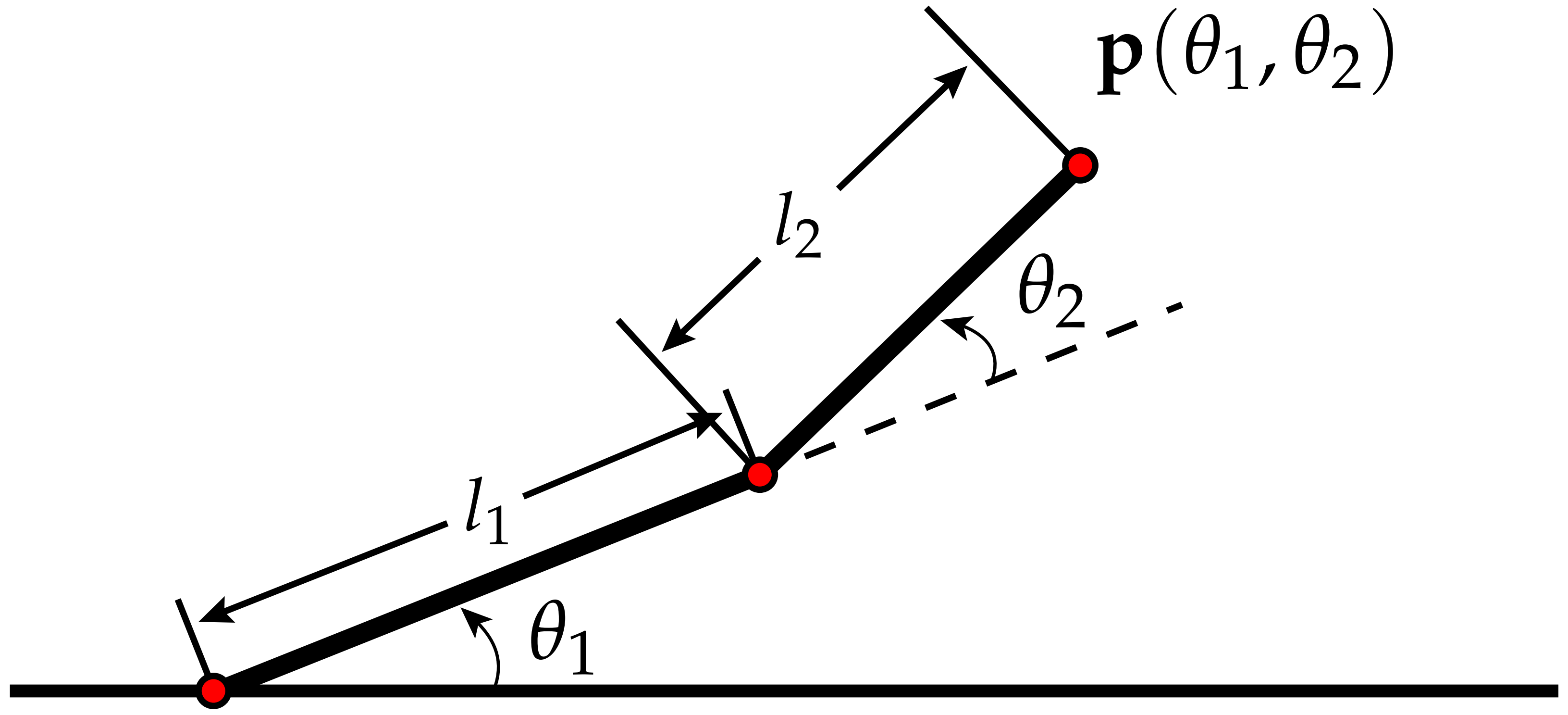

Idea: solve with Newton's method

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

Inverse Kinematics via Newton's method

n unknowns

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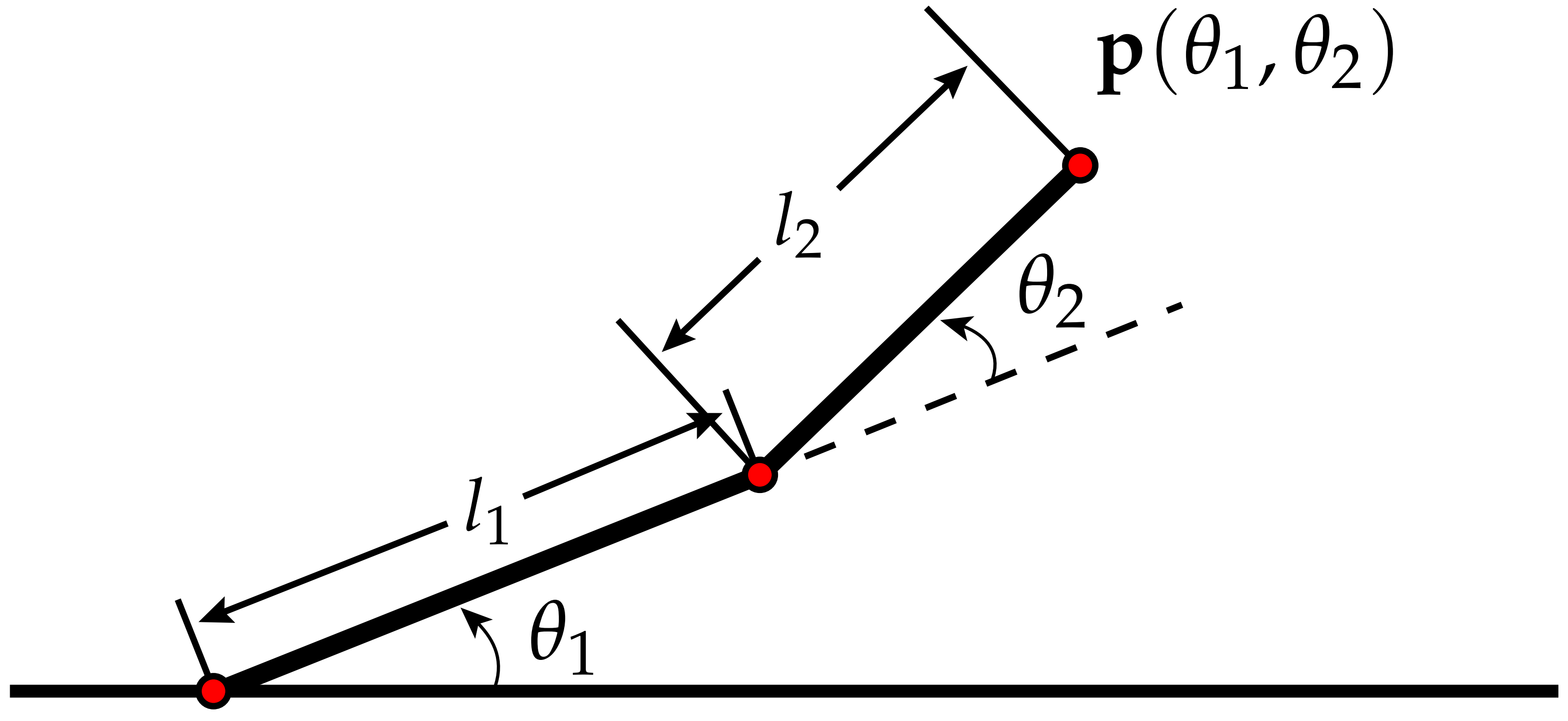
2 equations



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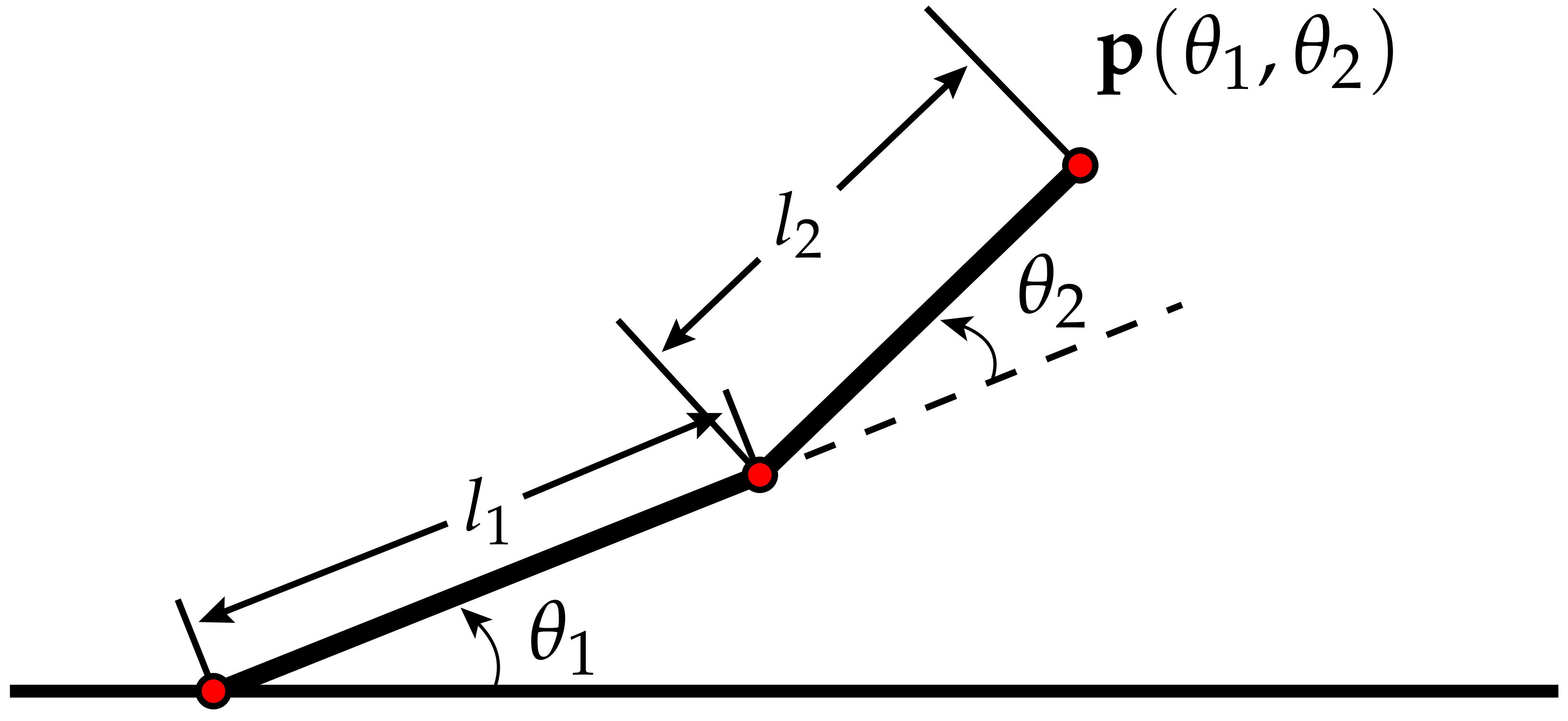

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Idea 2: solve with Newton's method + pseudoinverse

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

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

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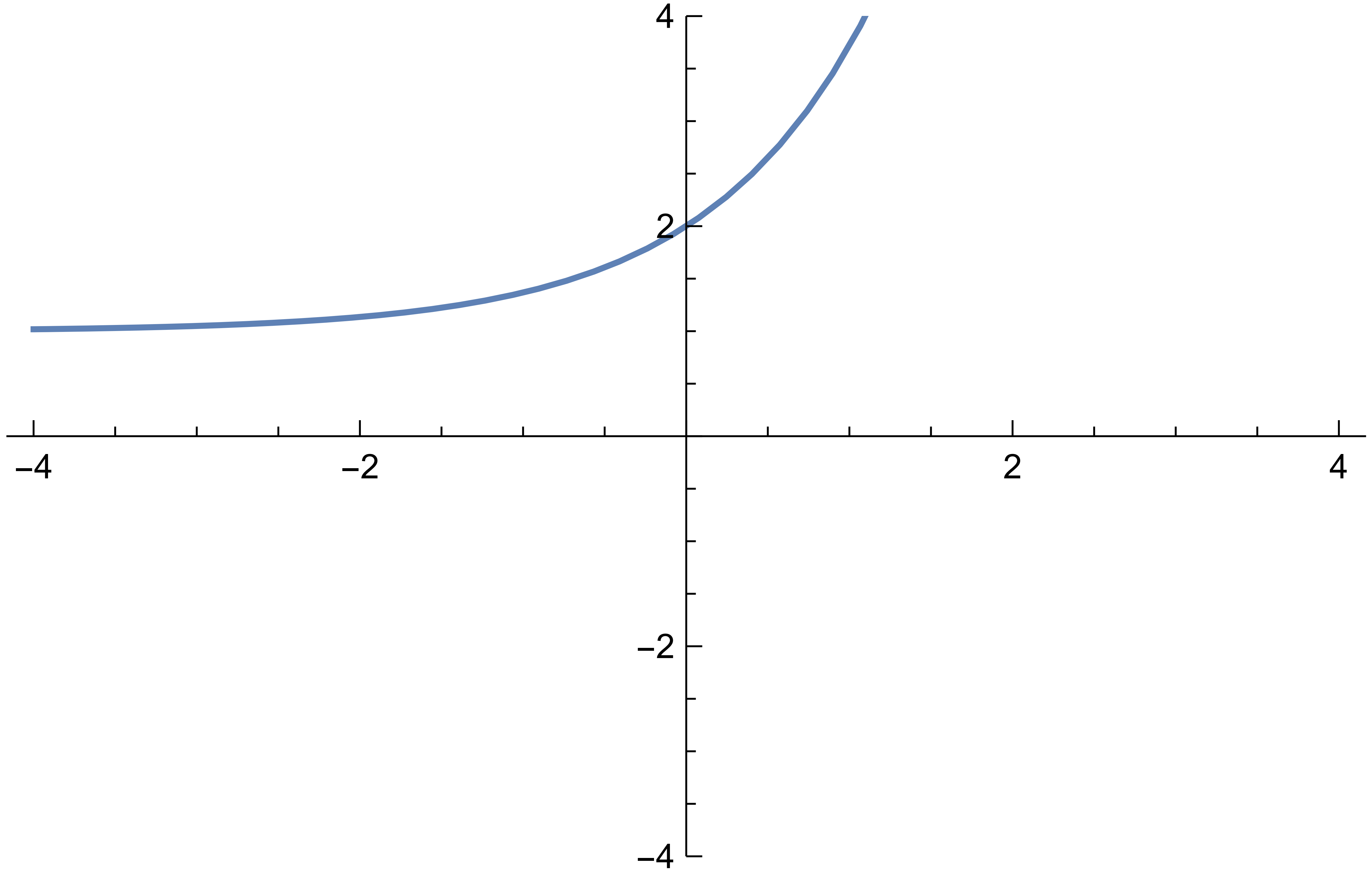

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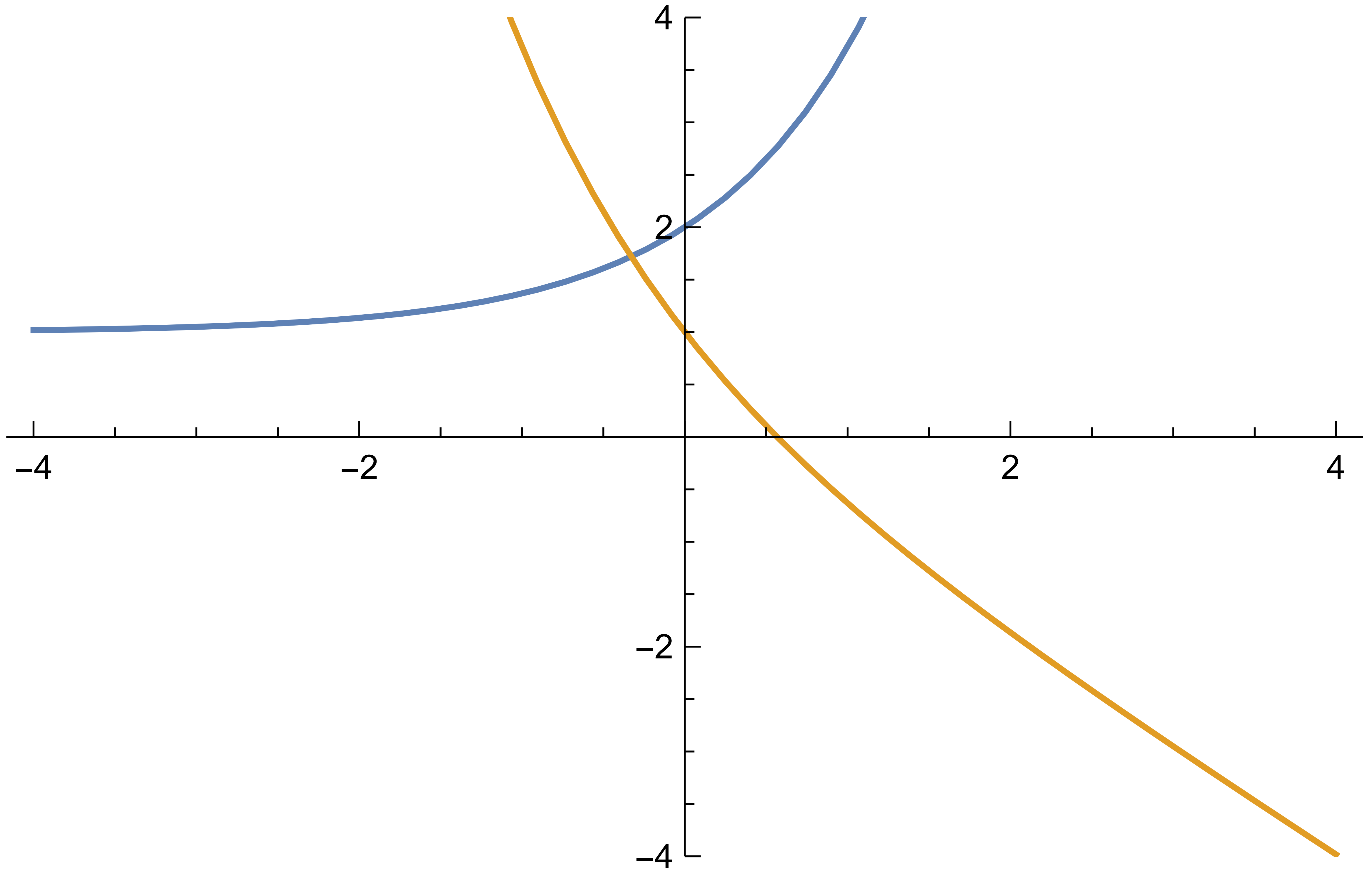

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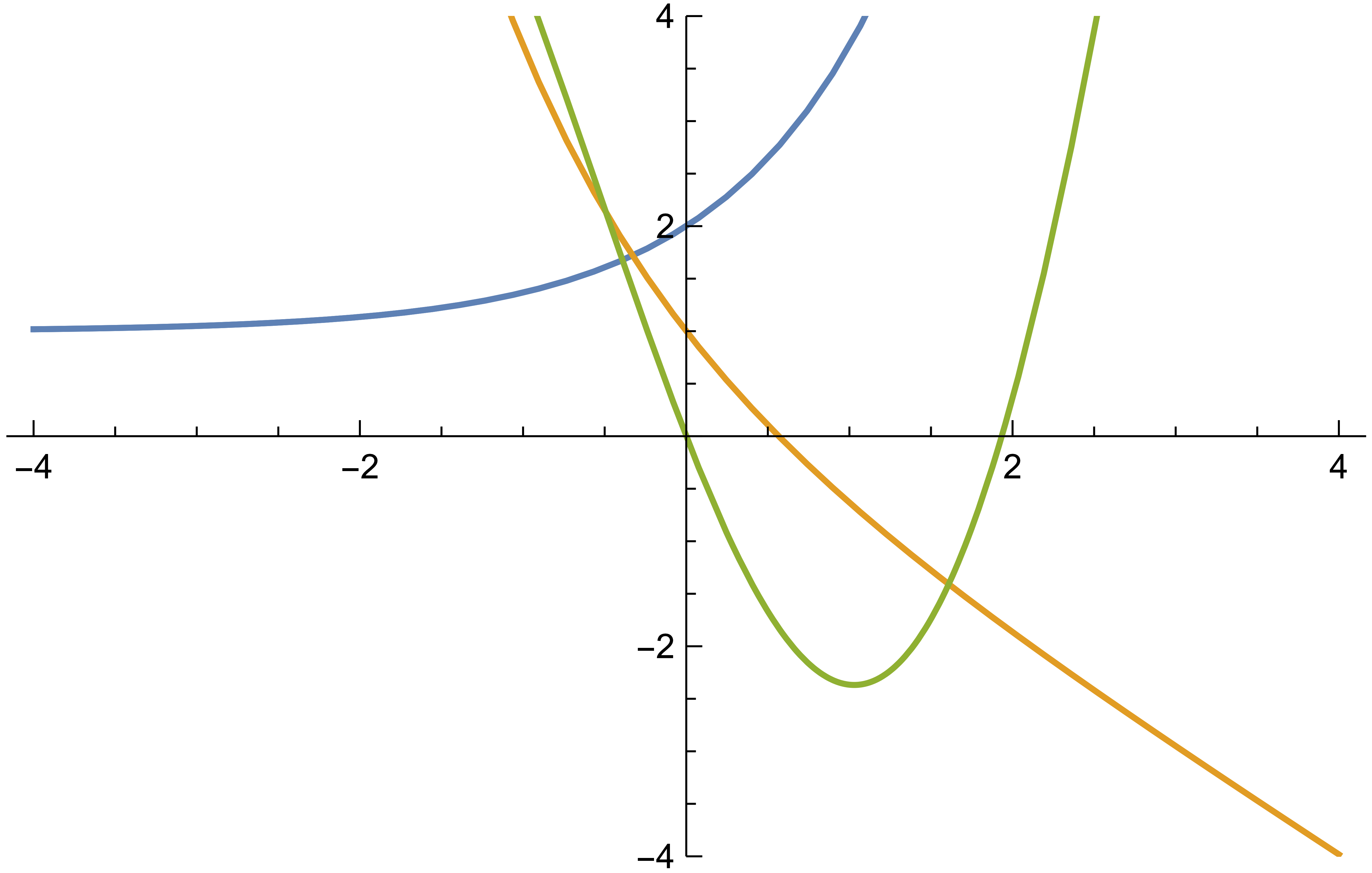

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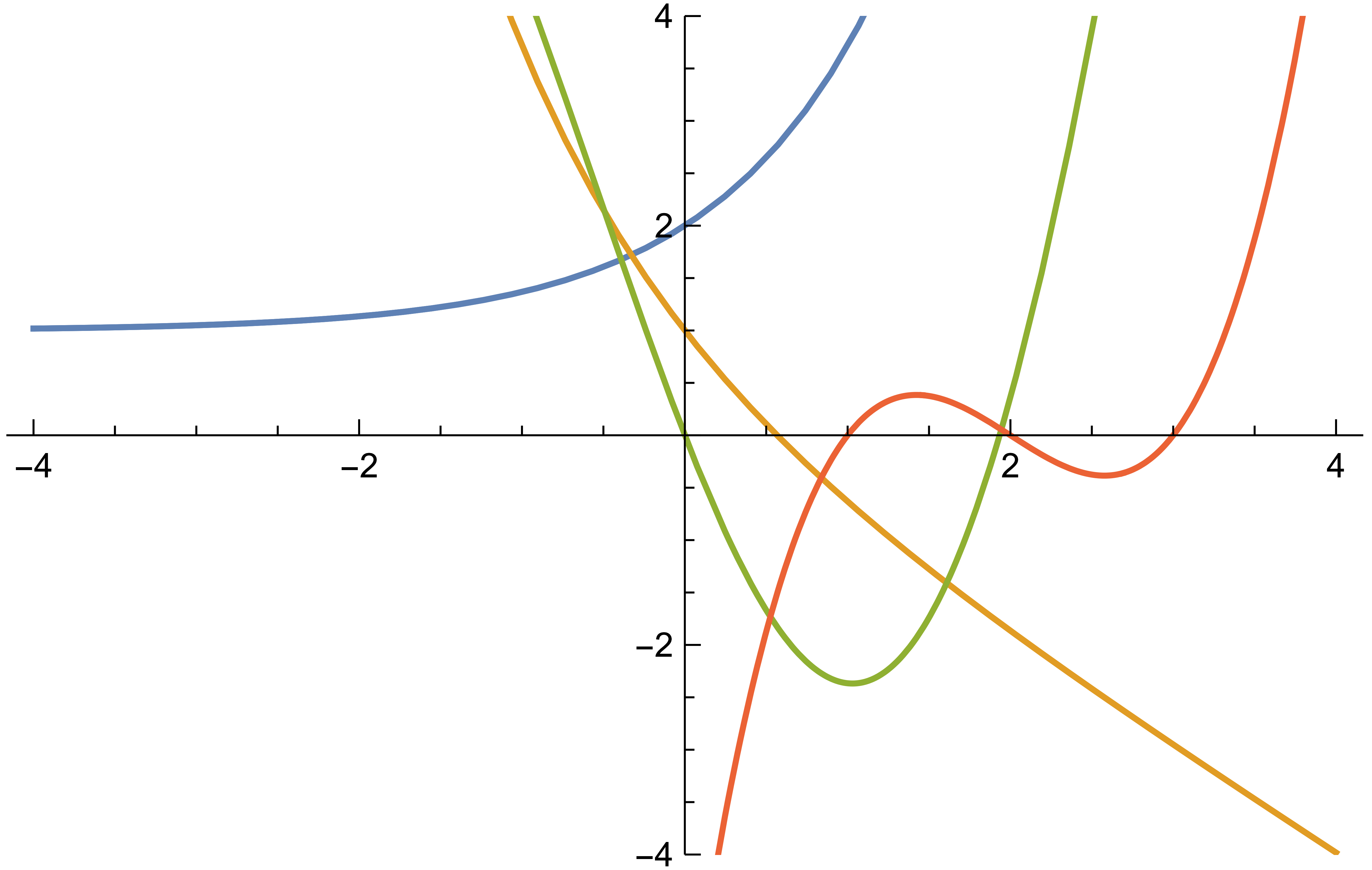

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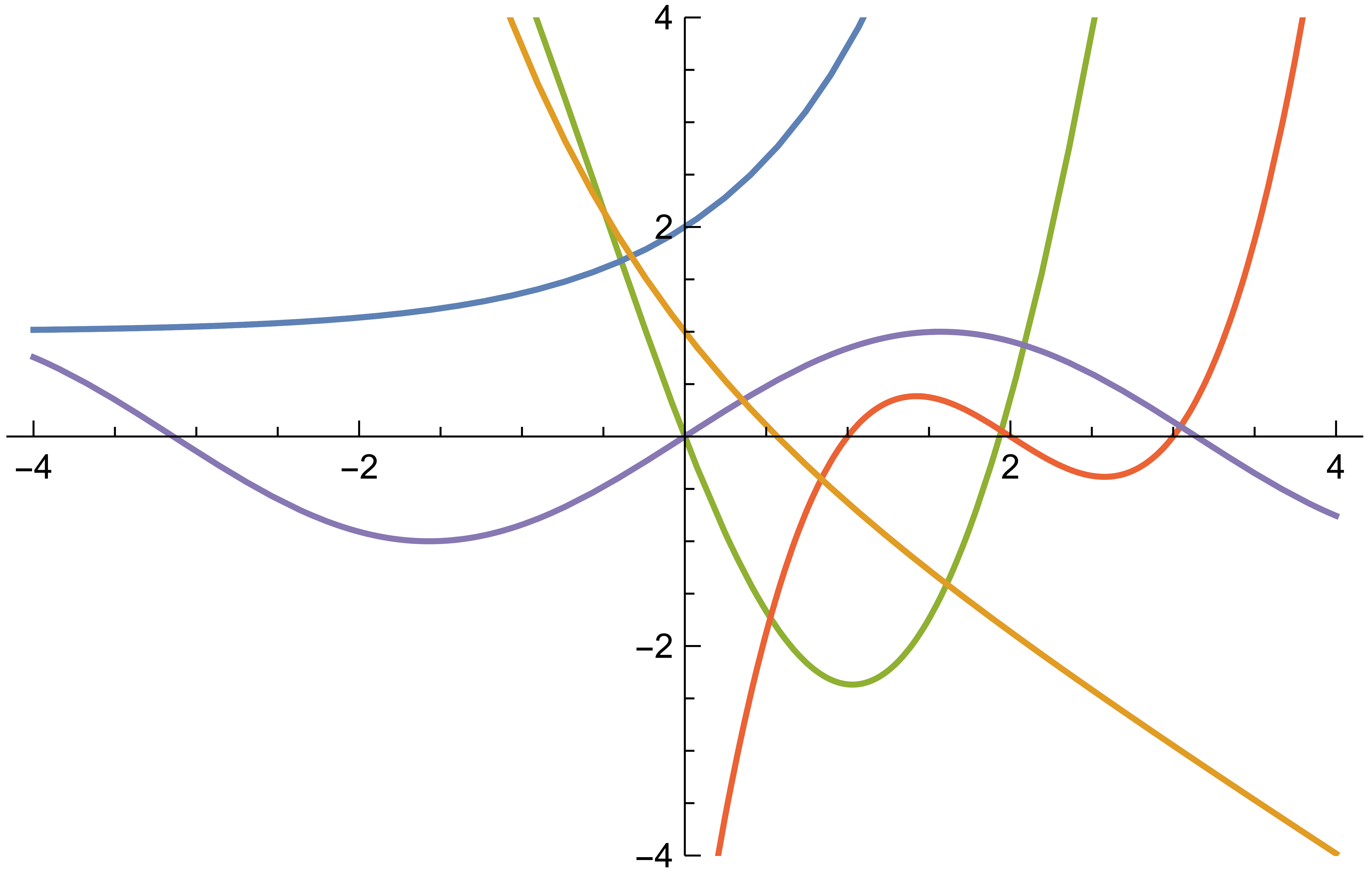
  - $\sin(x) = 0$



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

Common assumptions

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

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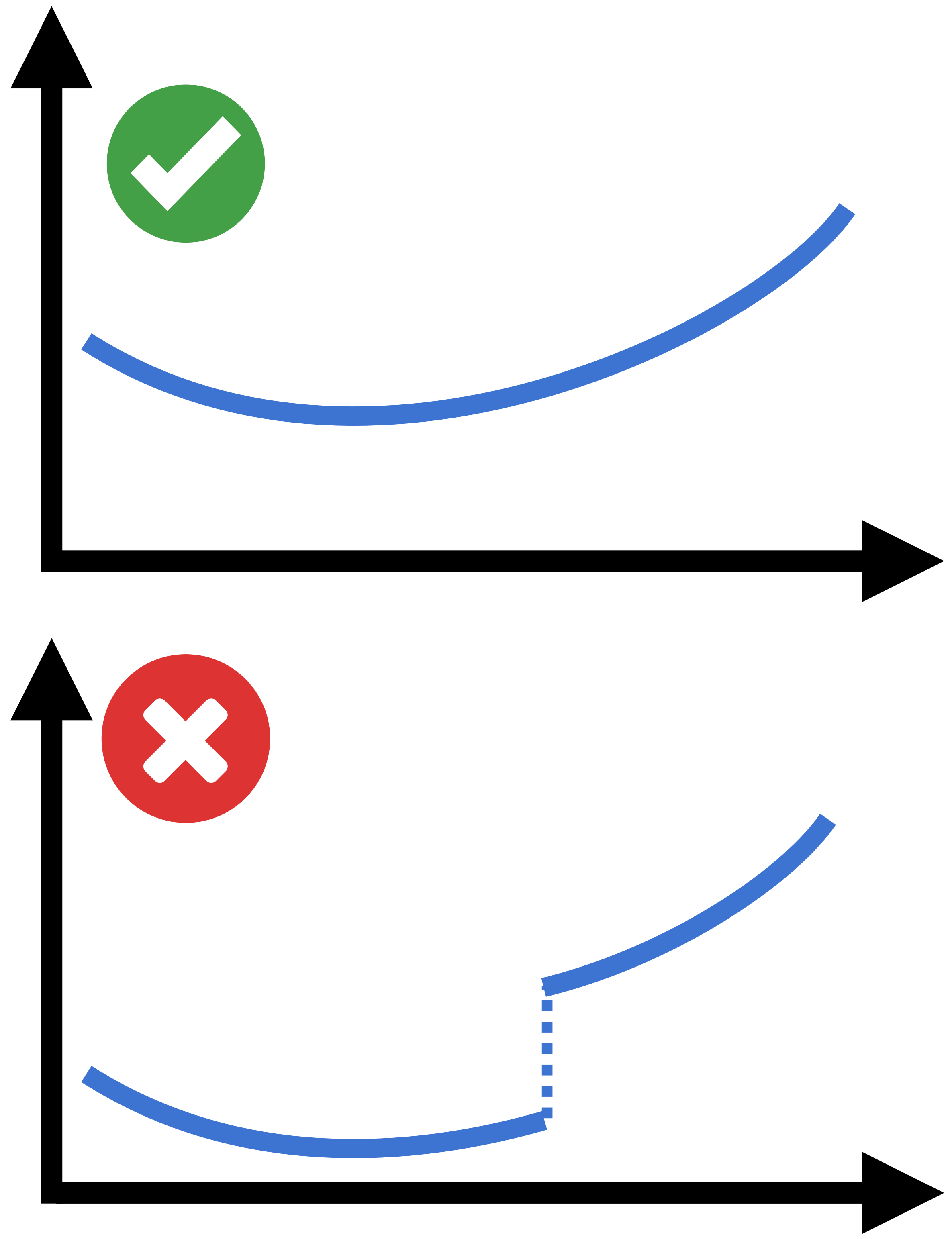

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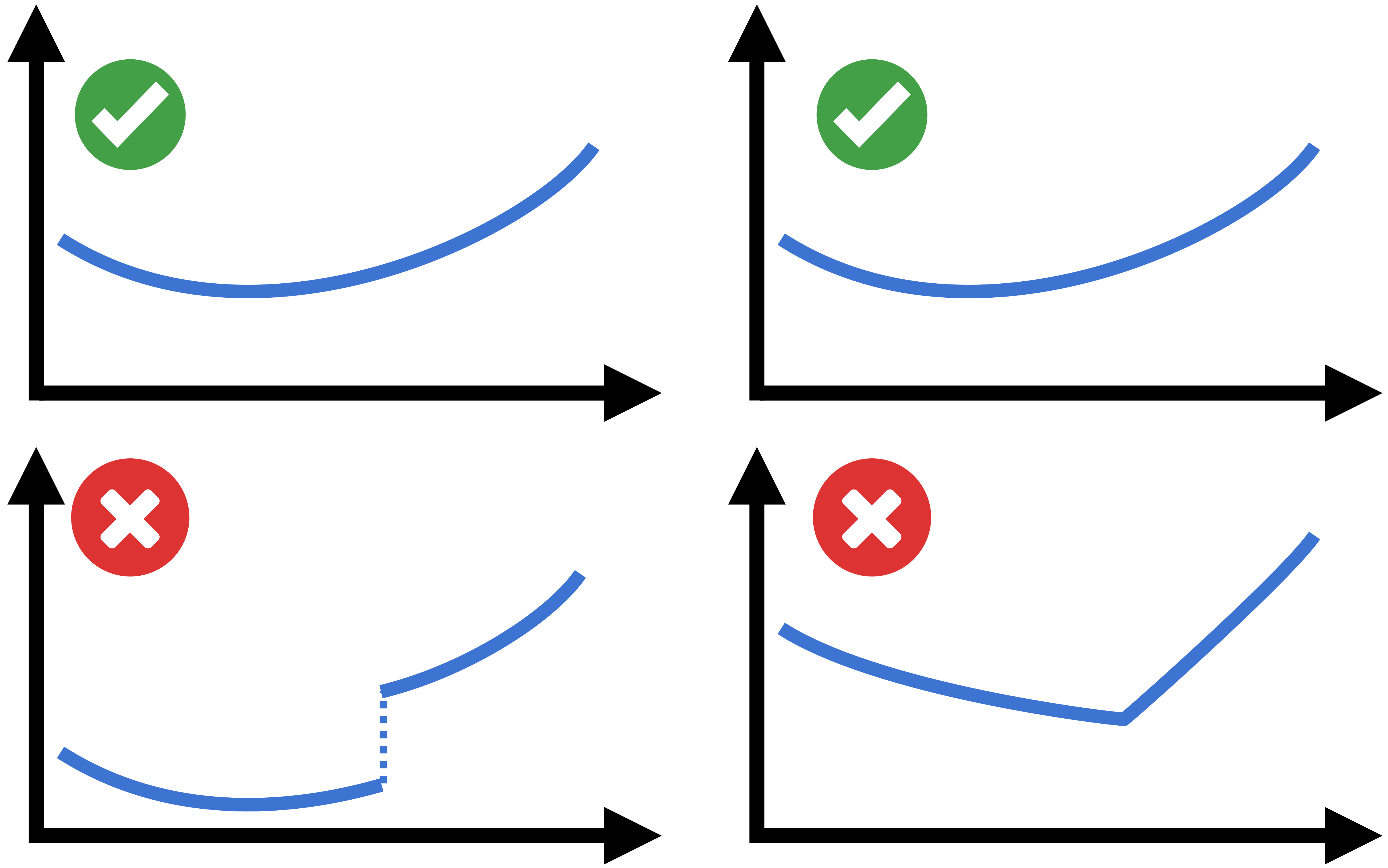

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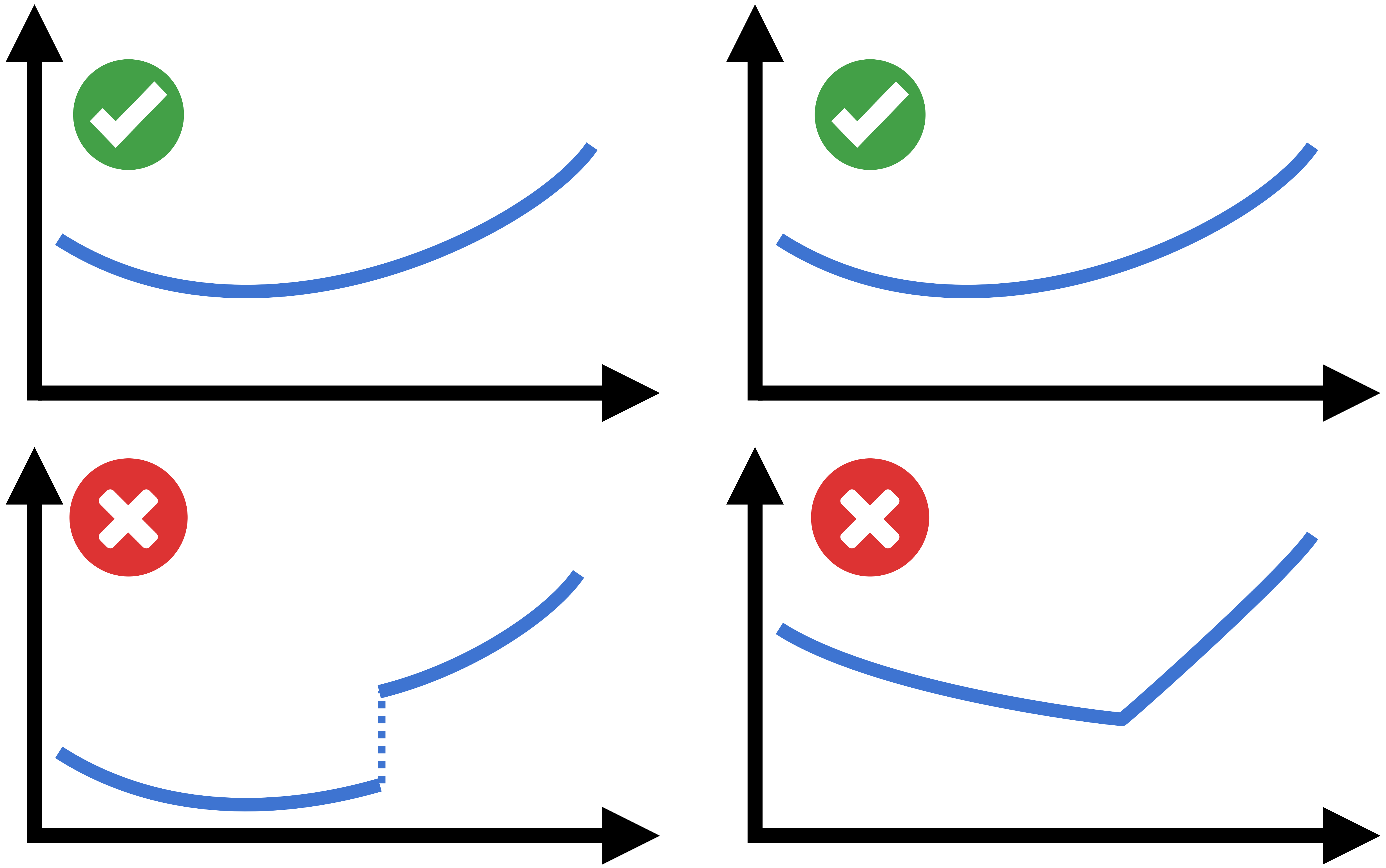

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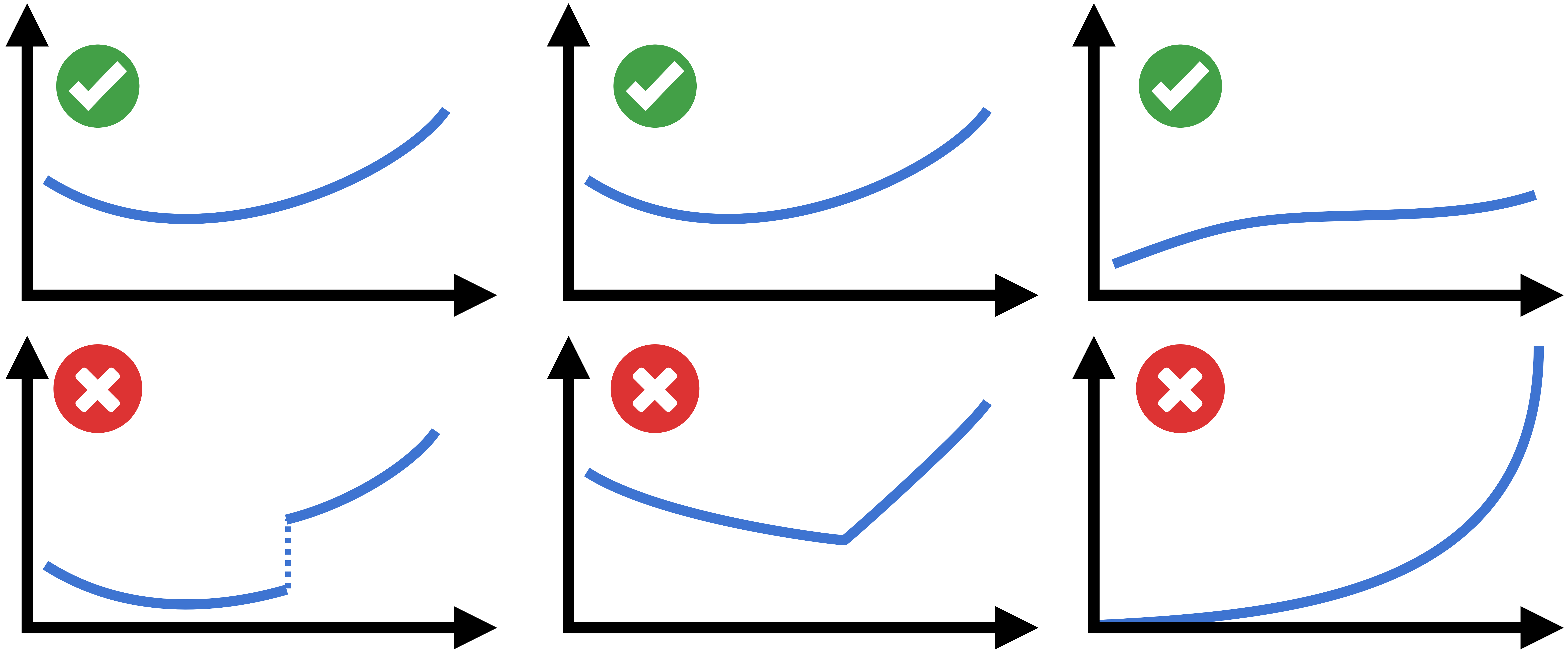

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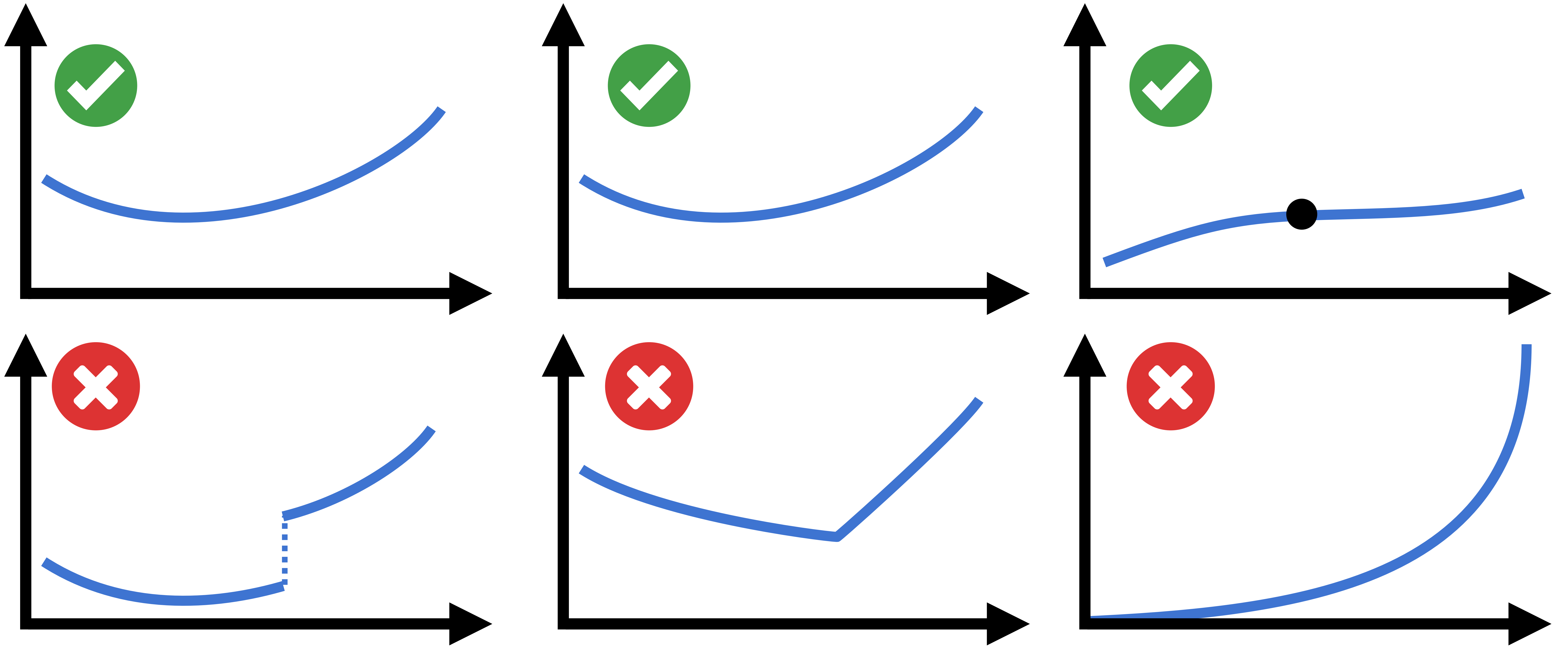

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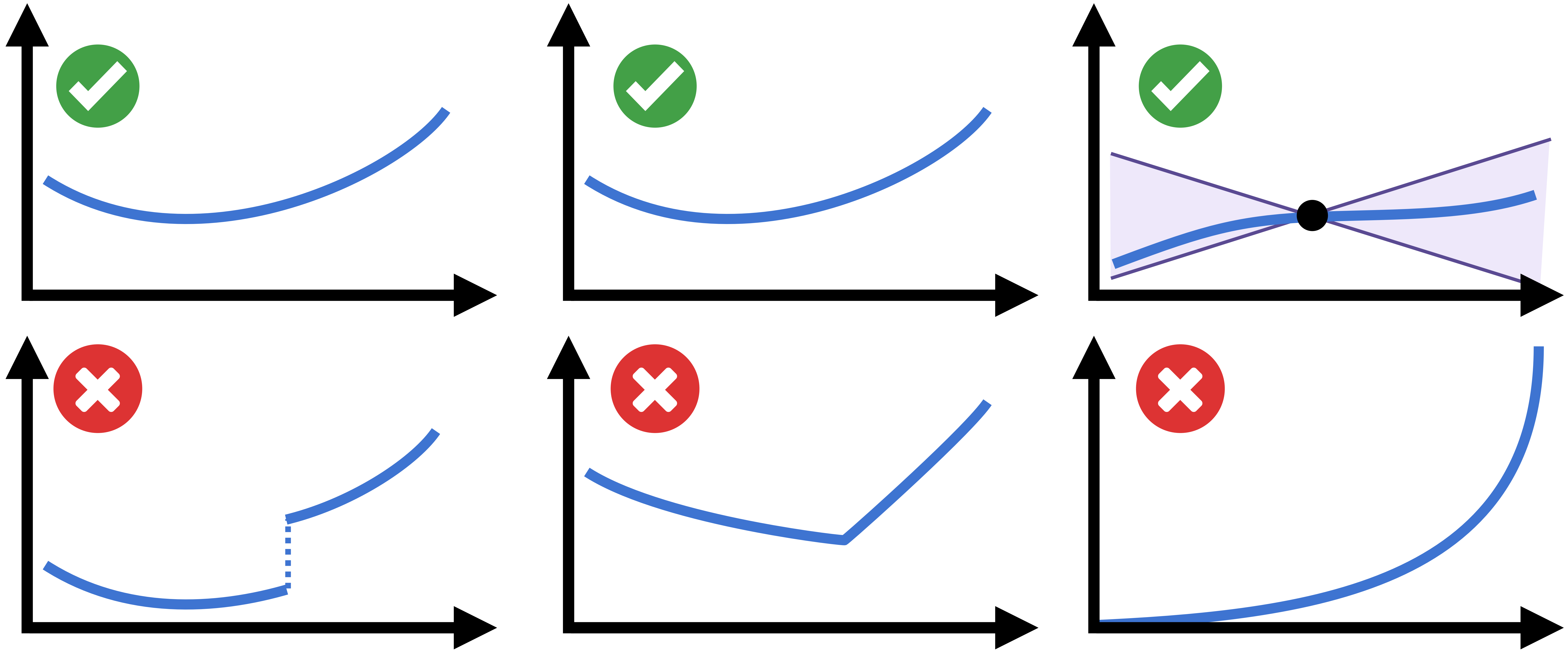

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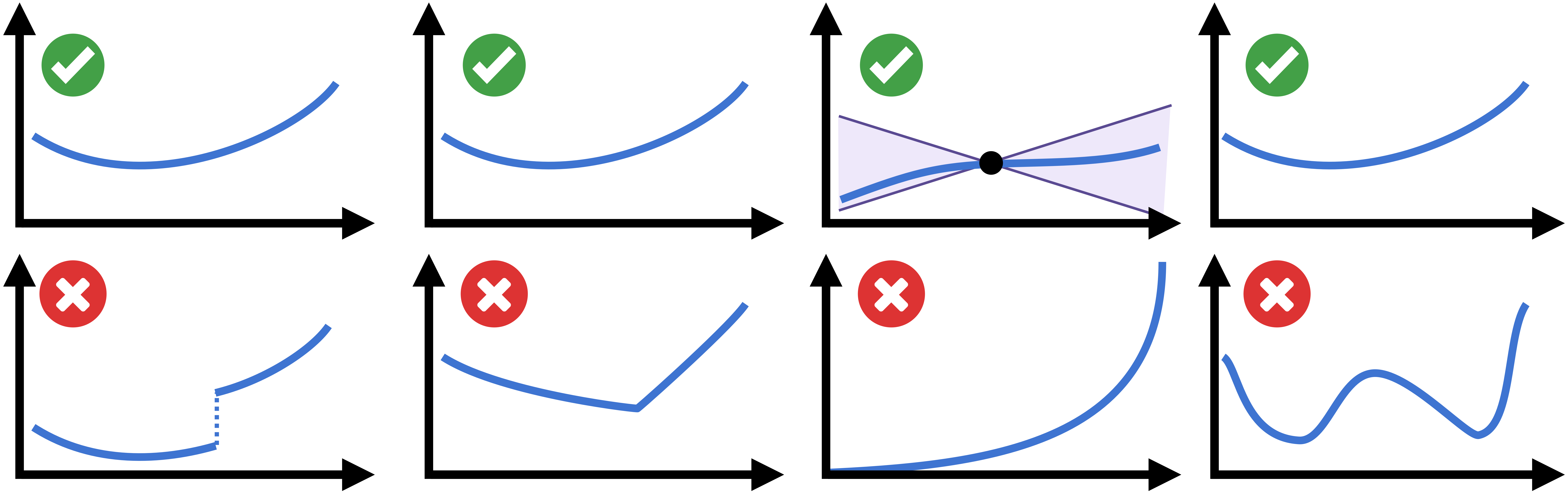

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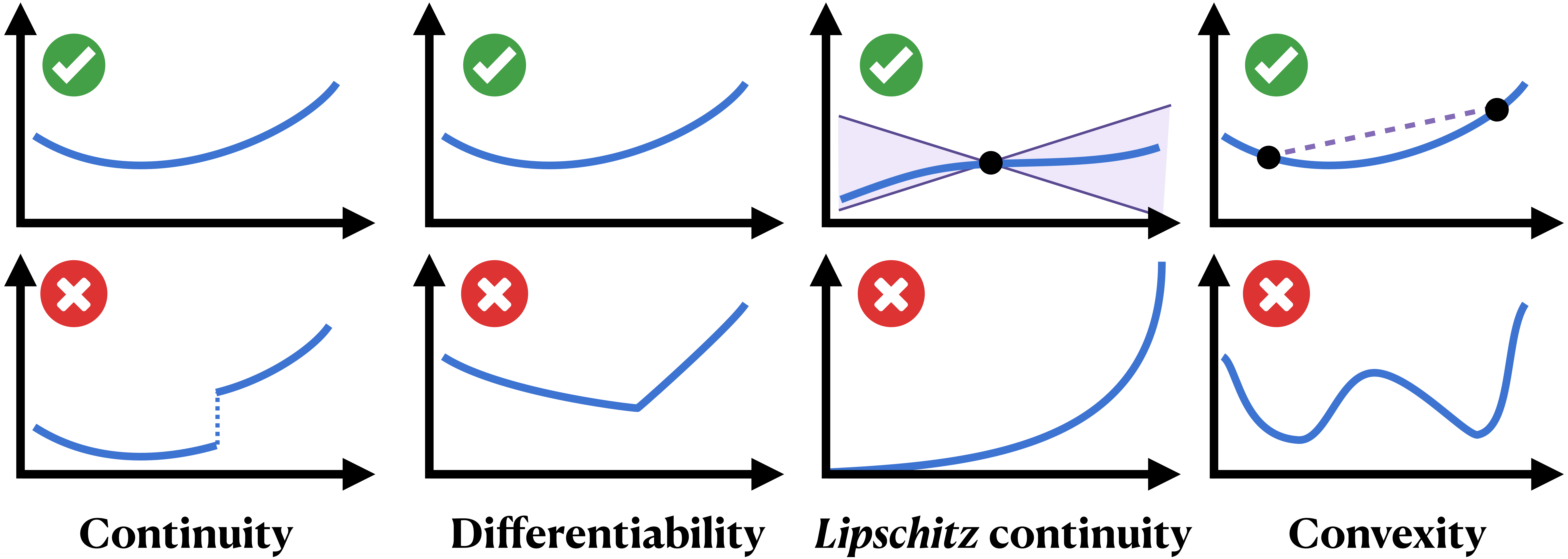

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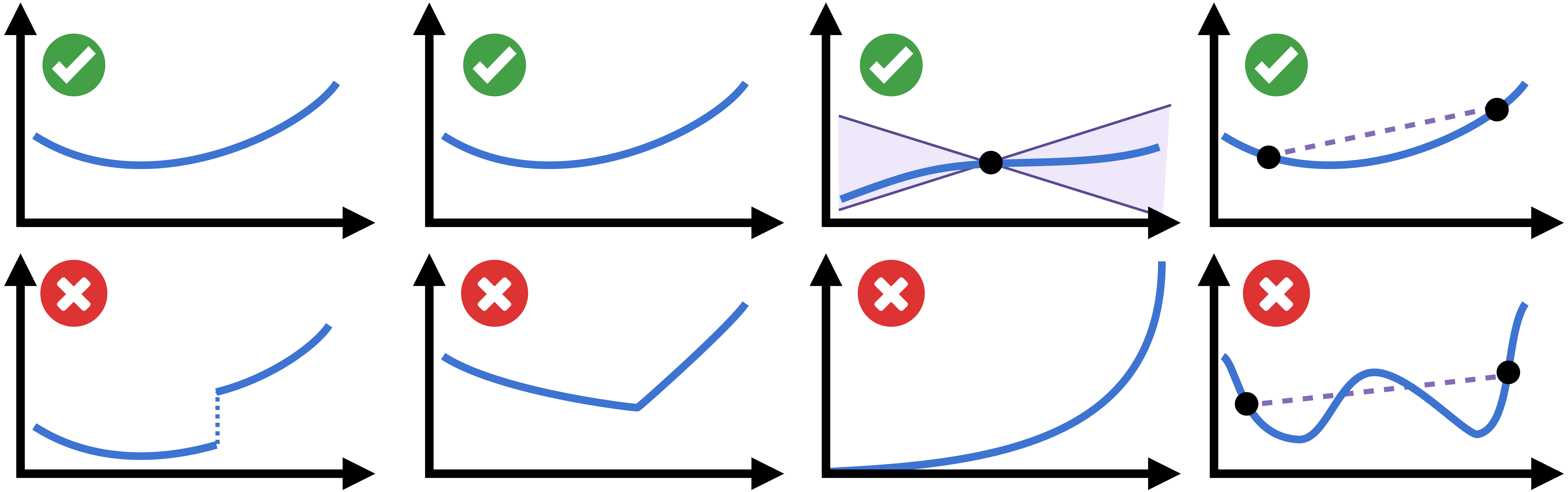

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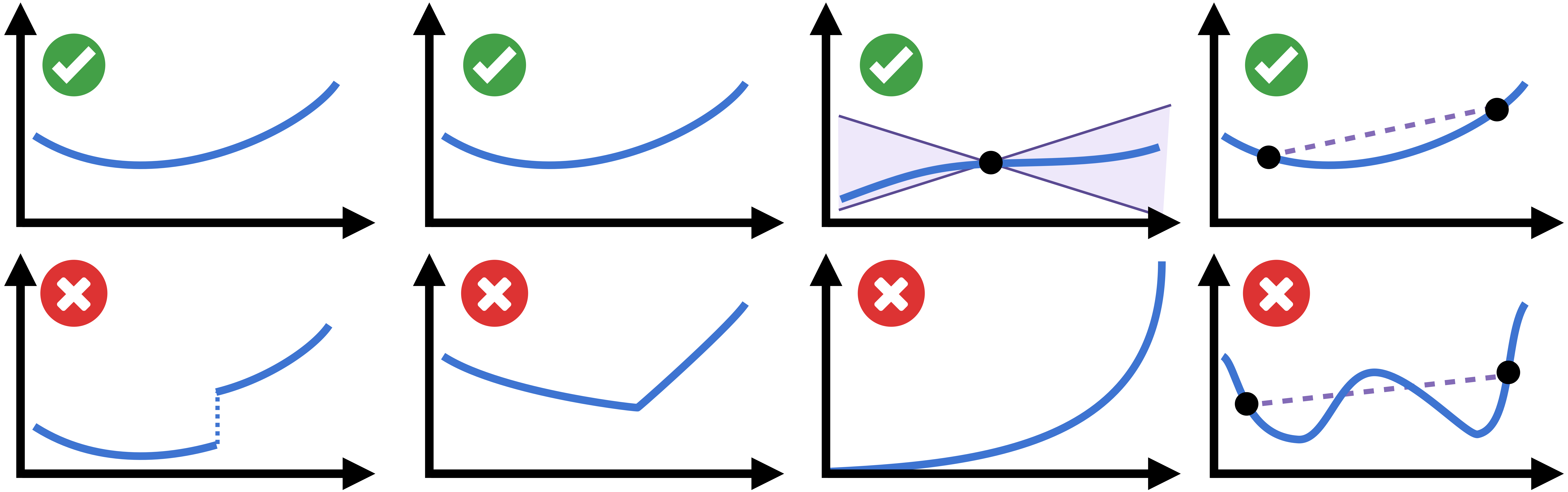

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Mostly used for optimization.

A model problem

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

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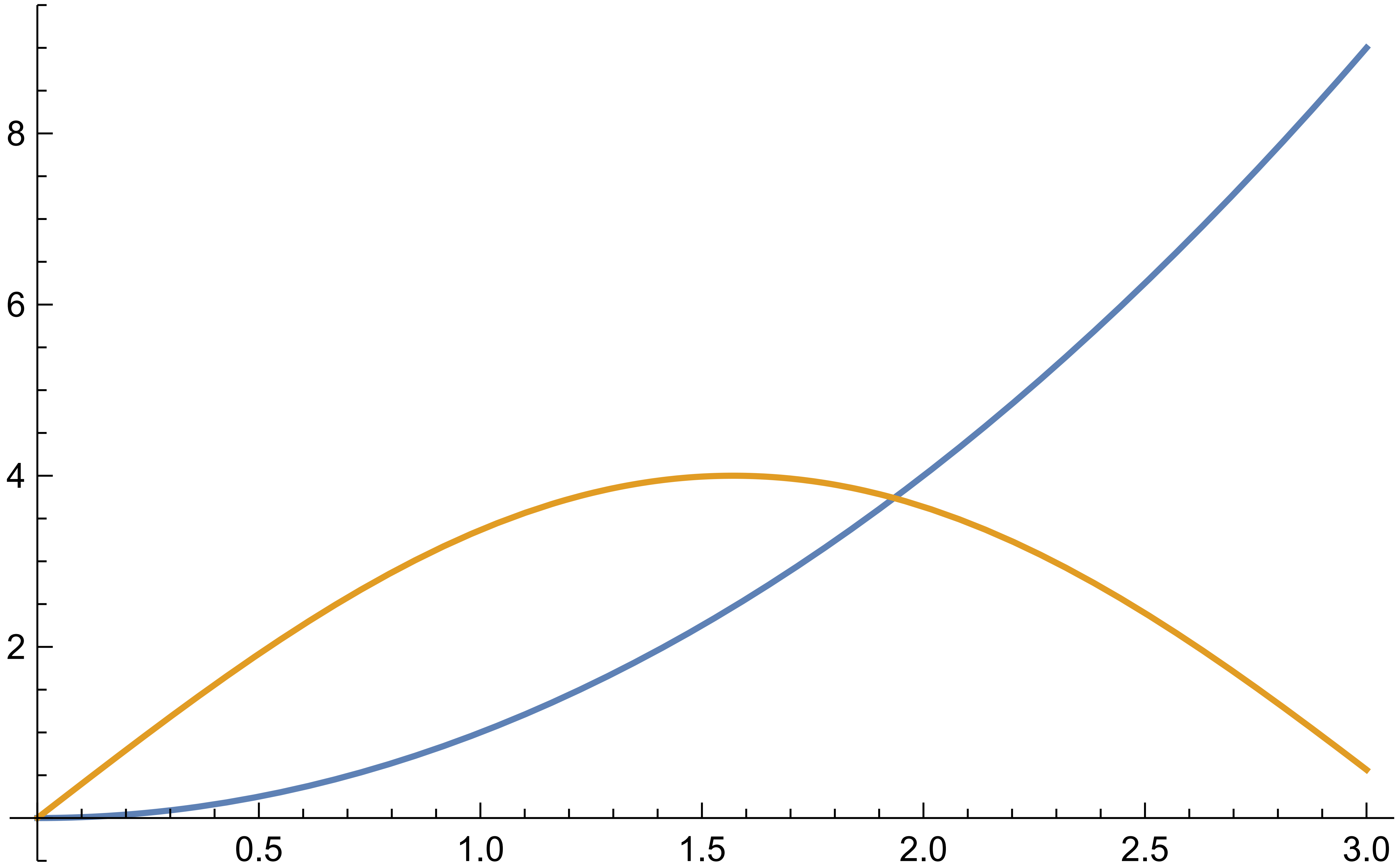

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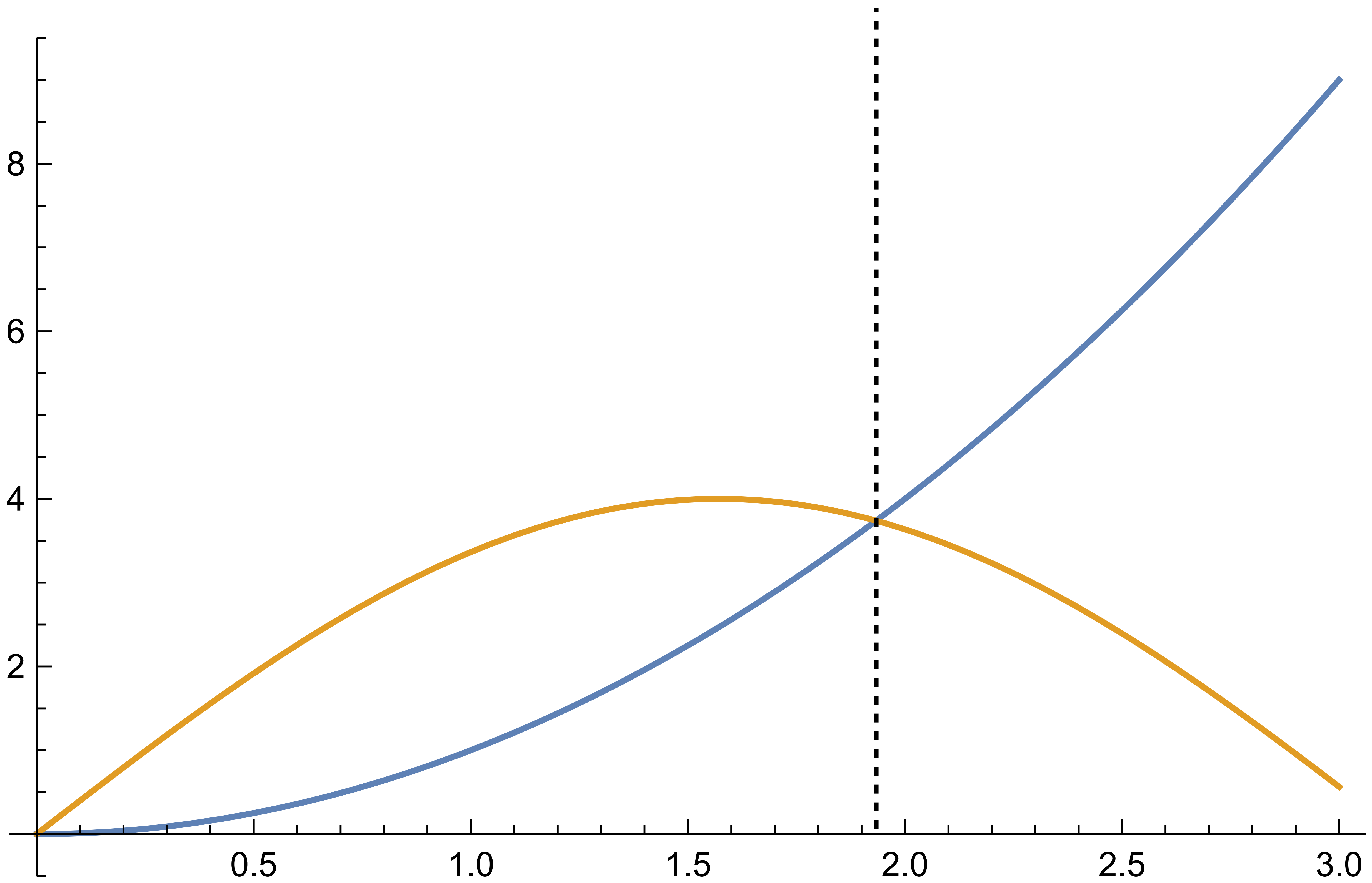
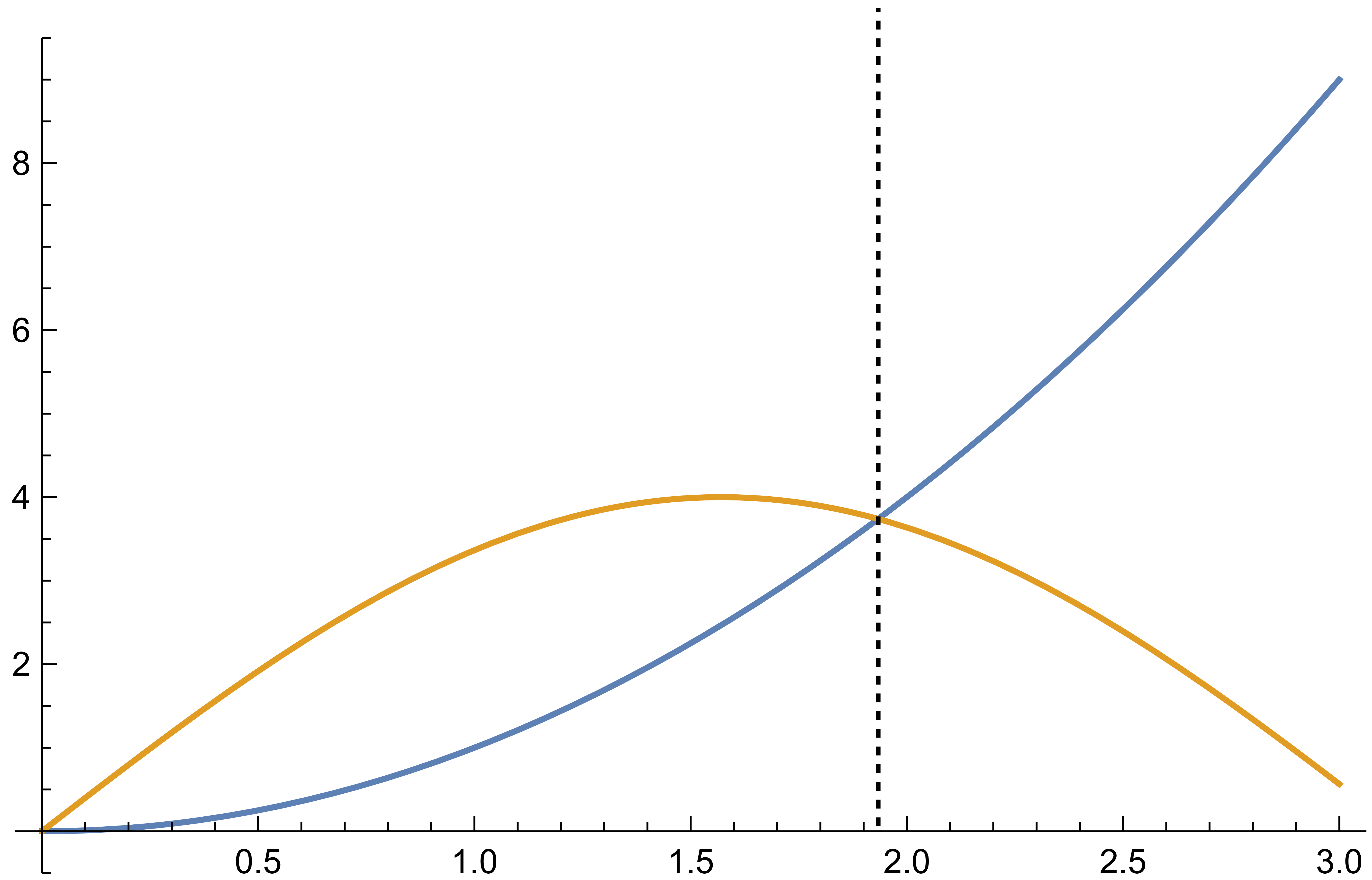


A model problem

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

Solution is not analytic!



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.

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

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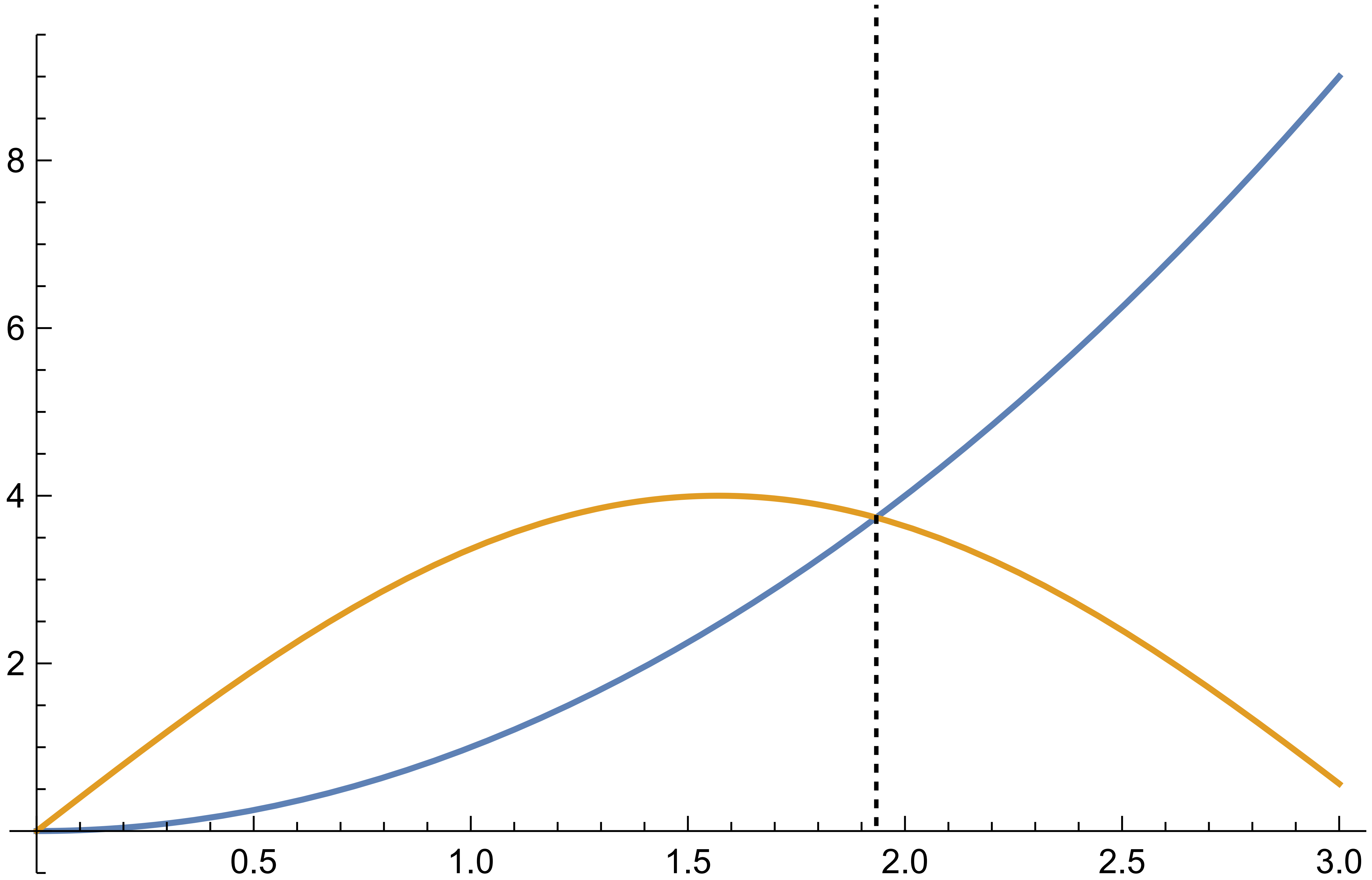
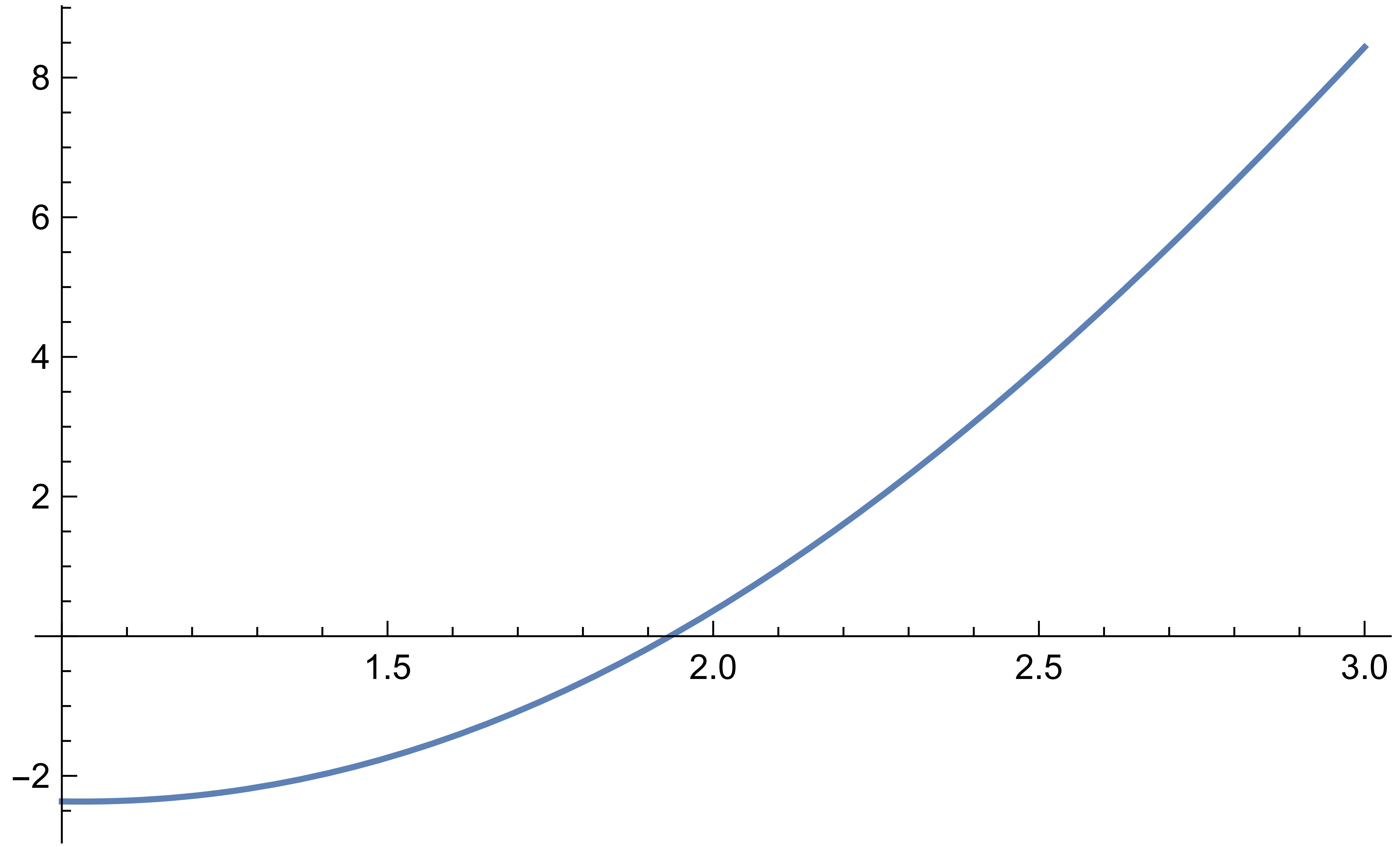


A model problem

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

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



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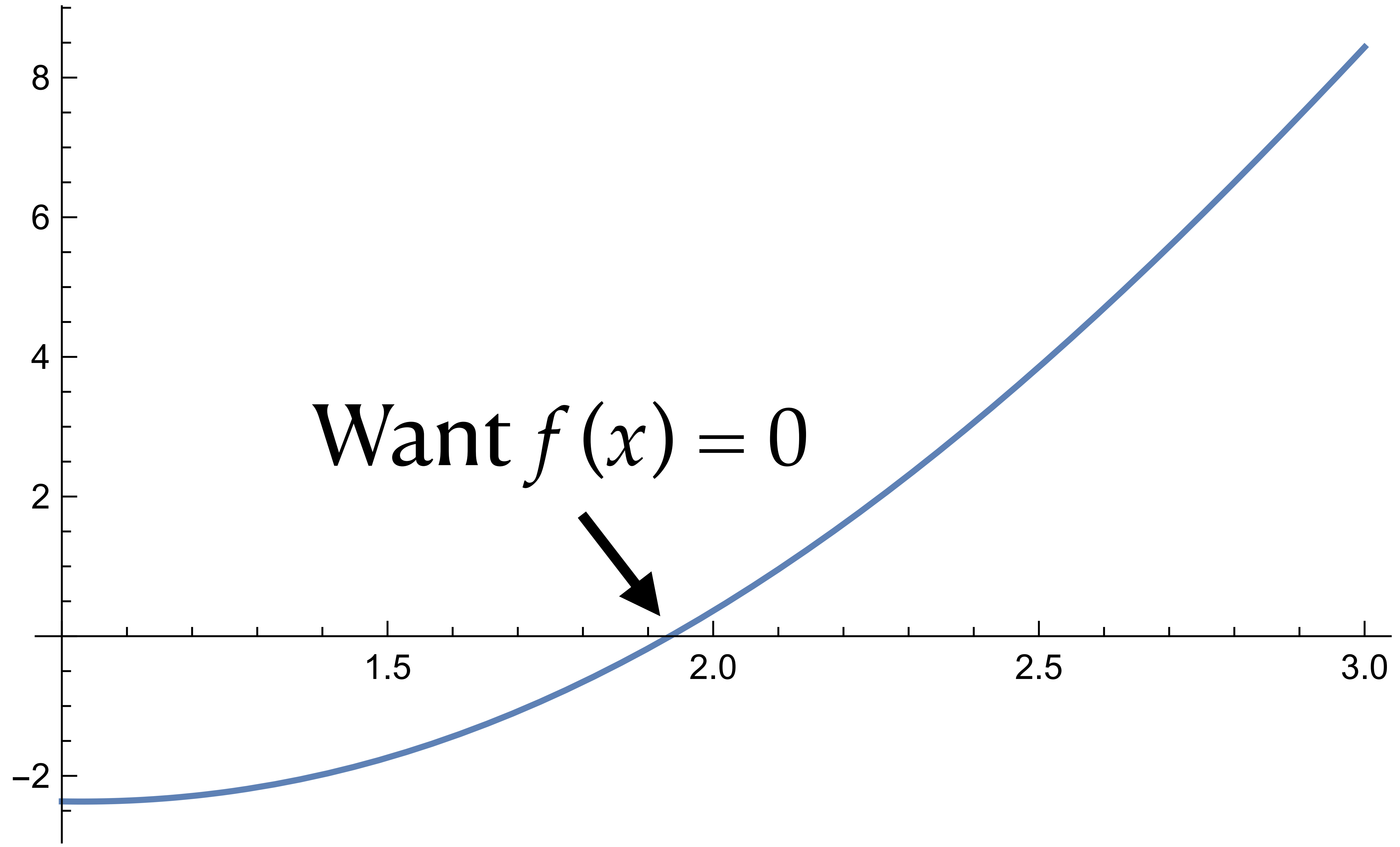

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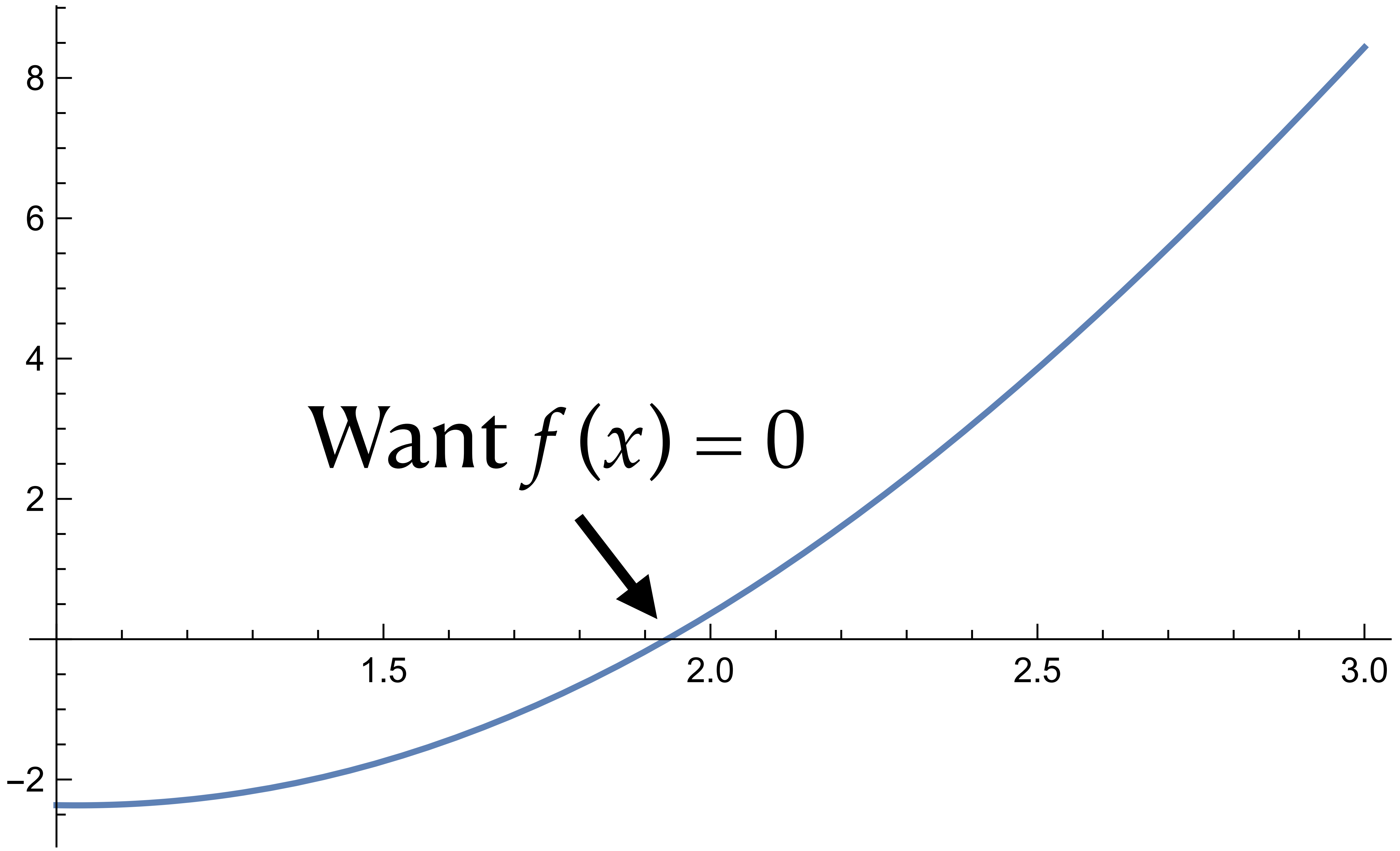
*Plot required thousands of function evaluations, each one is potentially **very expensive** (evaluating $f(x)$ once: test a new drug compound on patients, build a rocket and collect a sample on Mars.)*



Intermediate Value Theorem

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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
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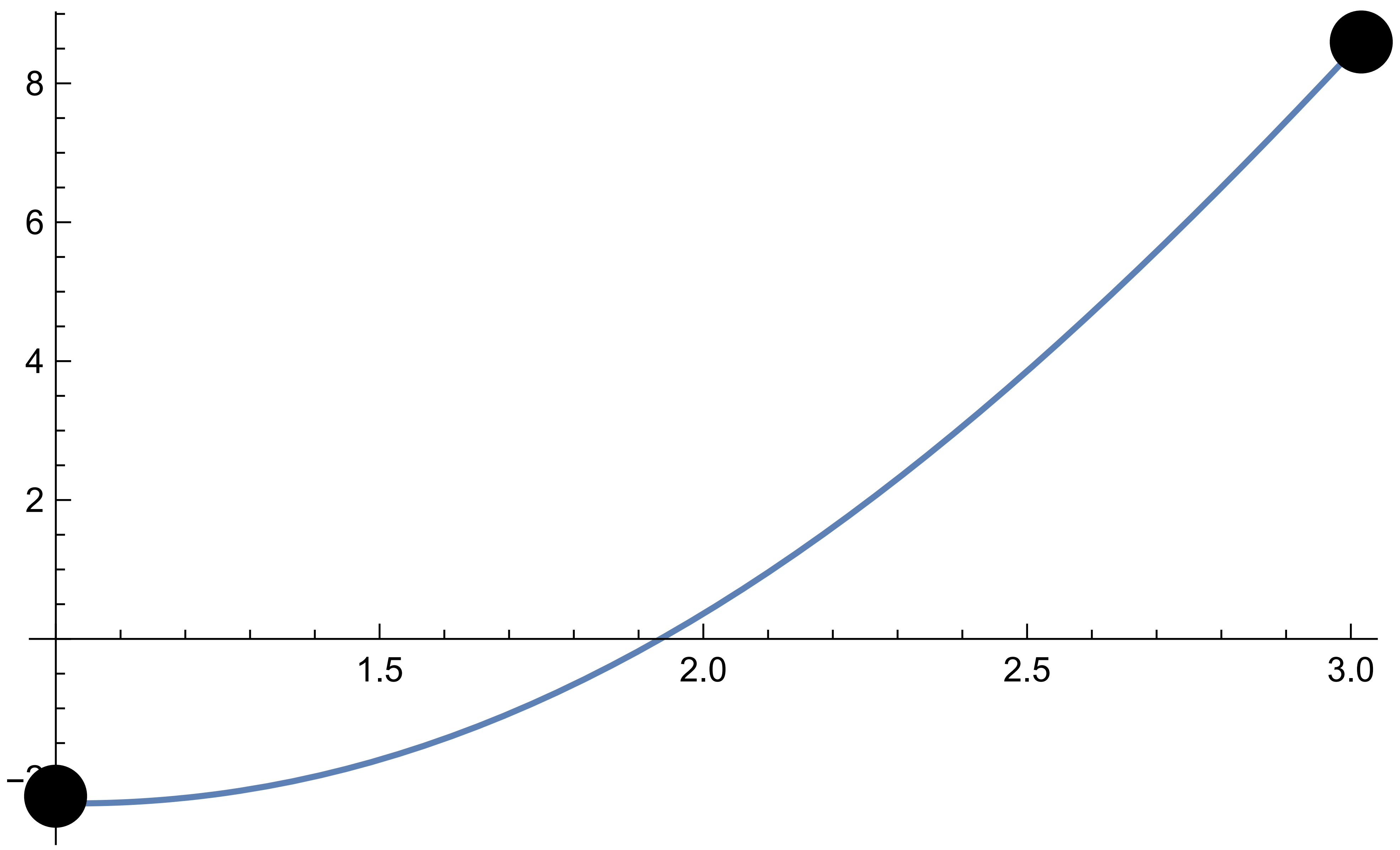
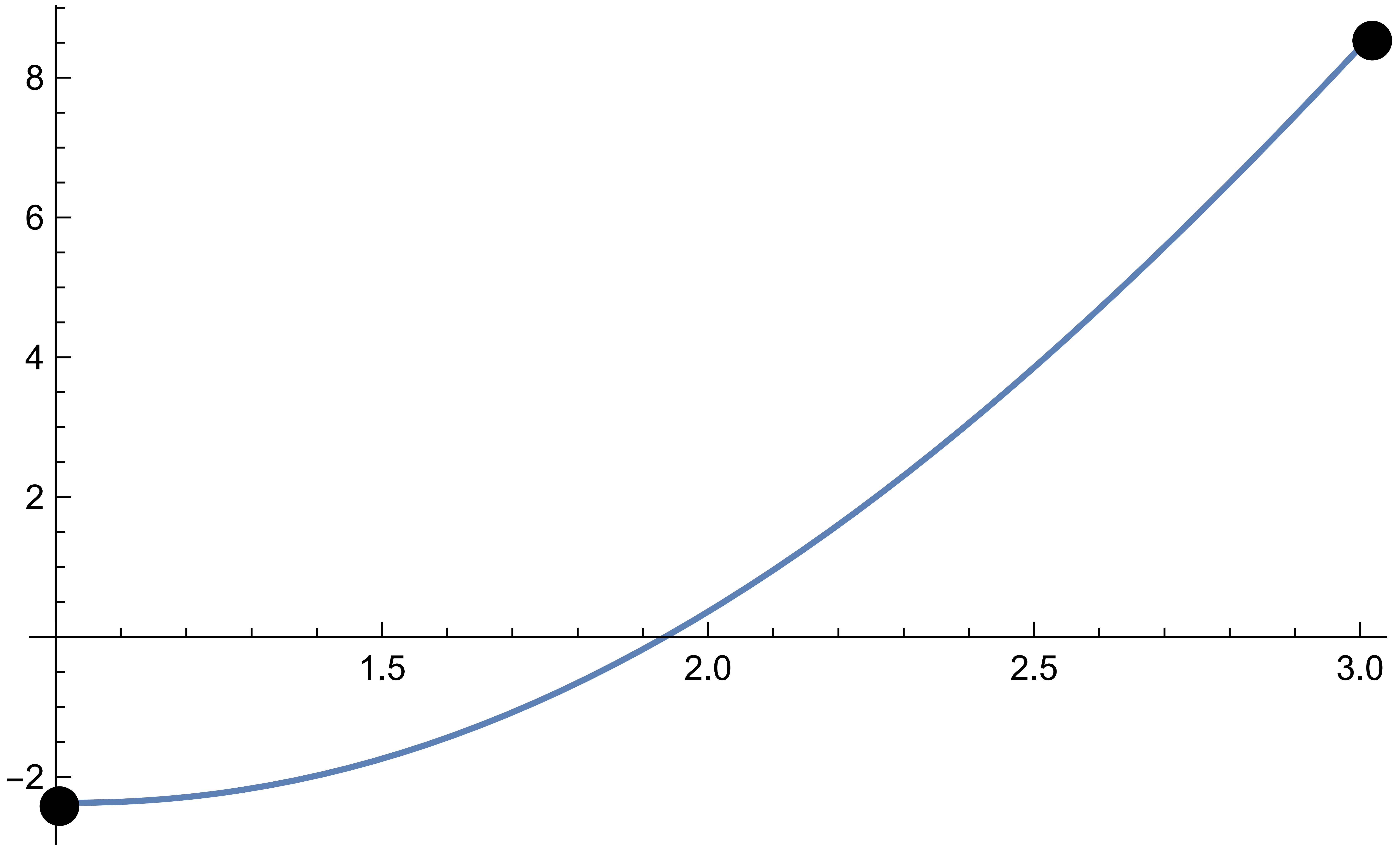


Use of continuity in our model problem



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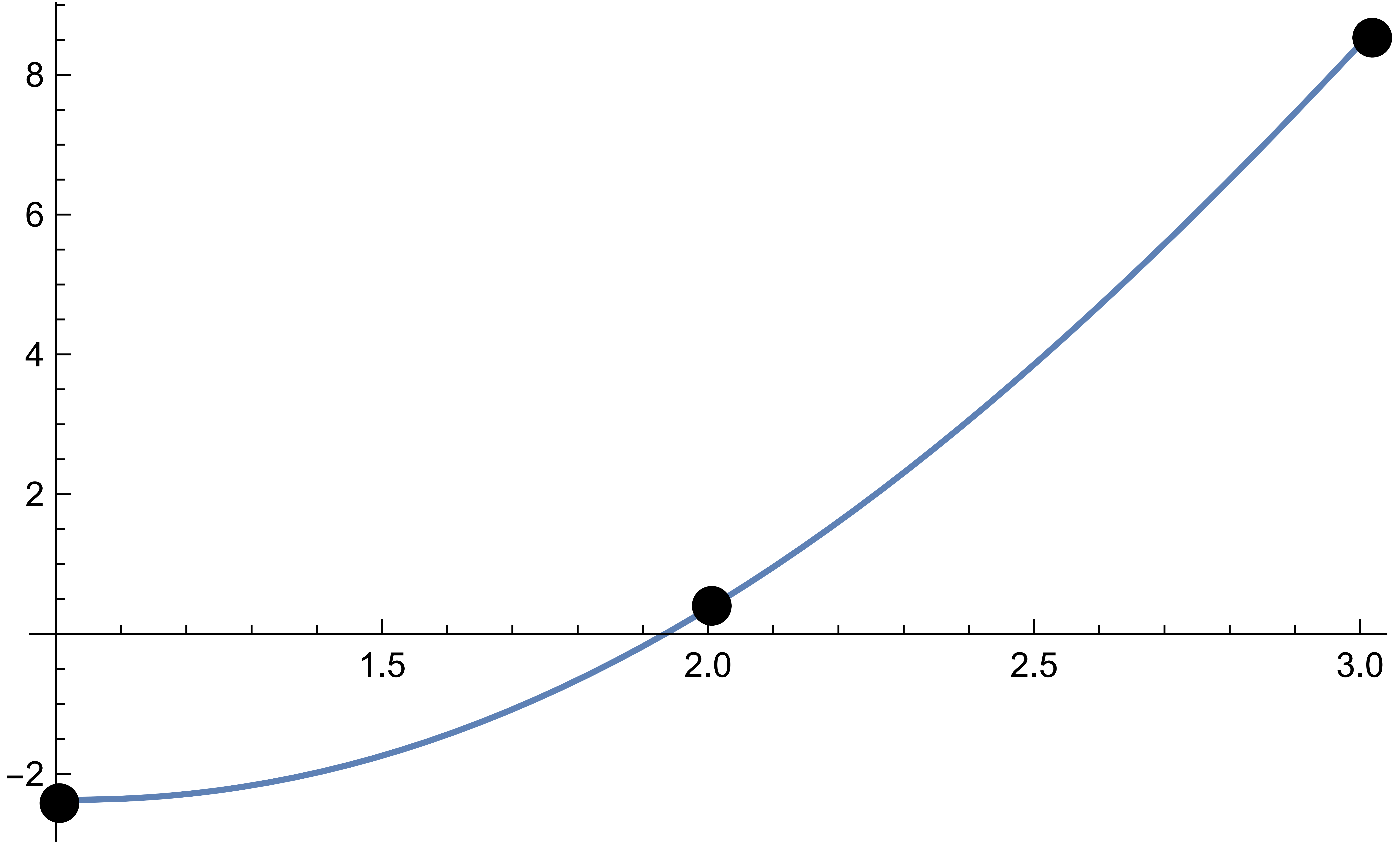

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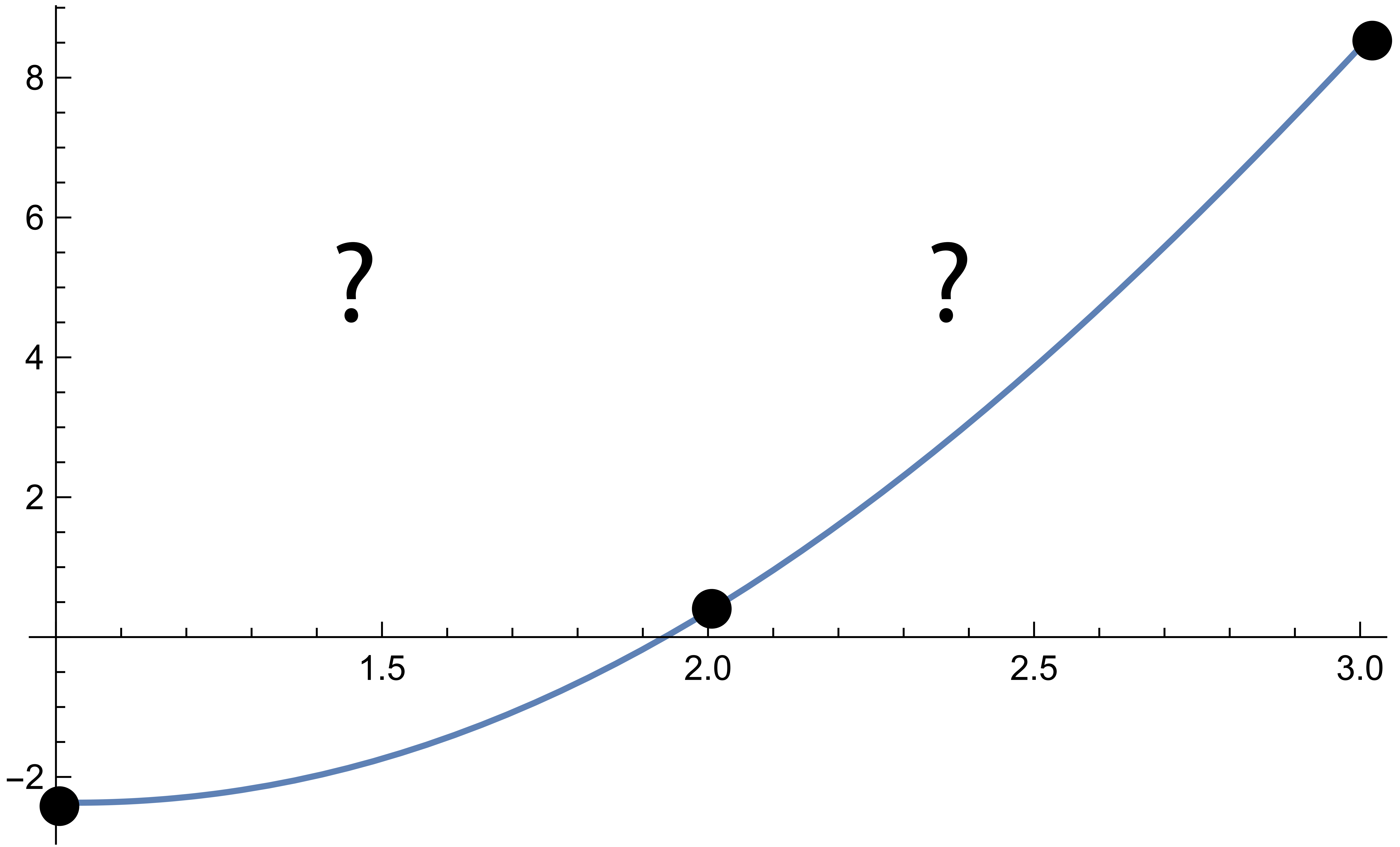

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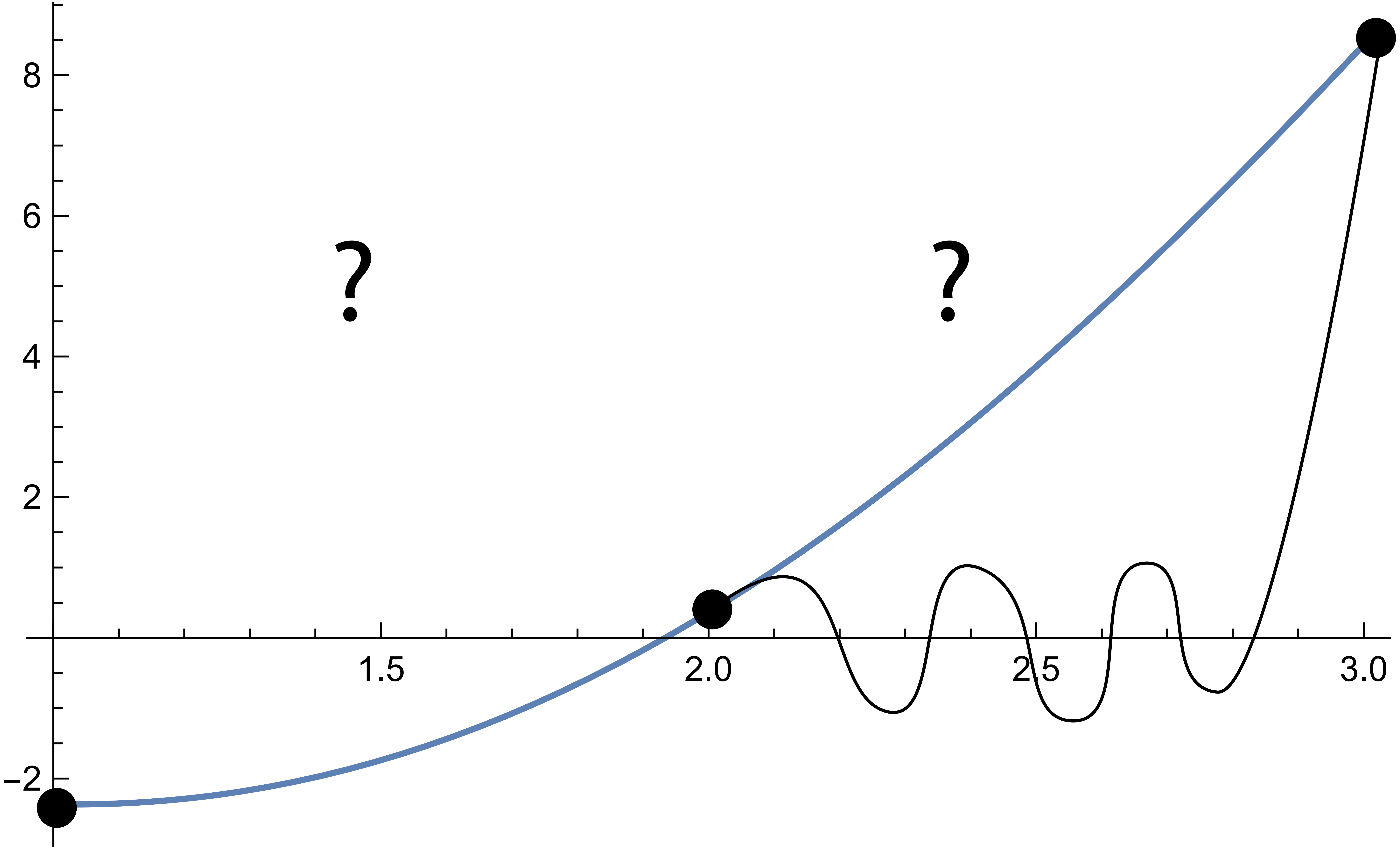

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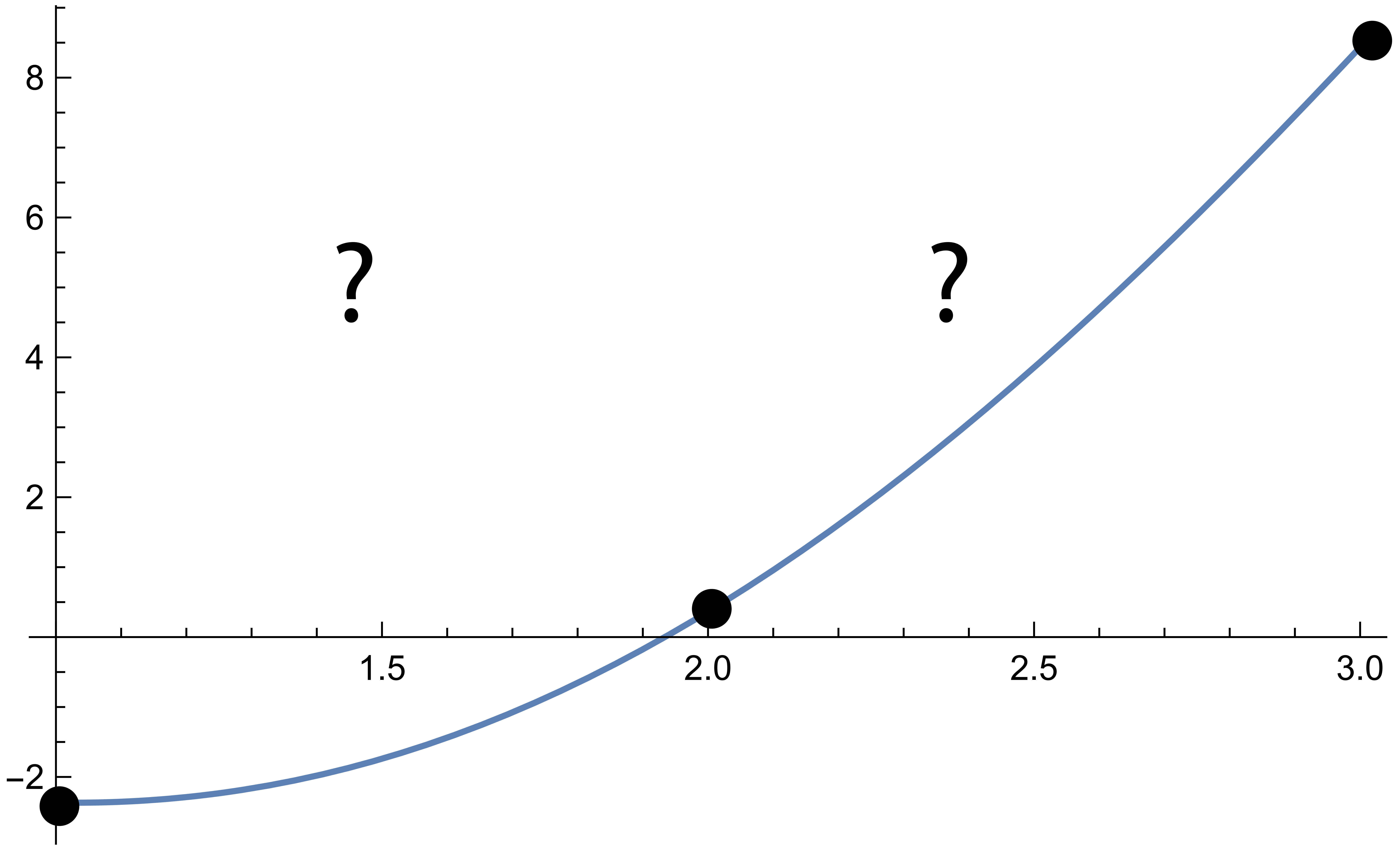

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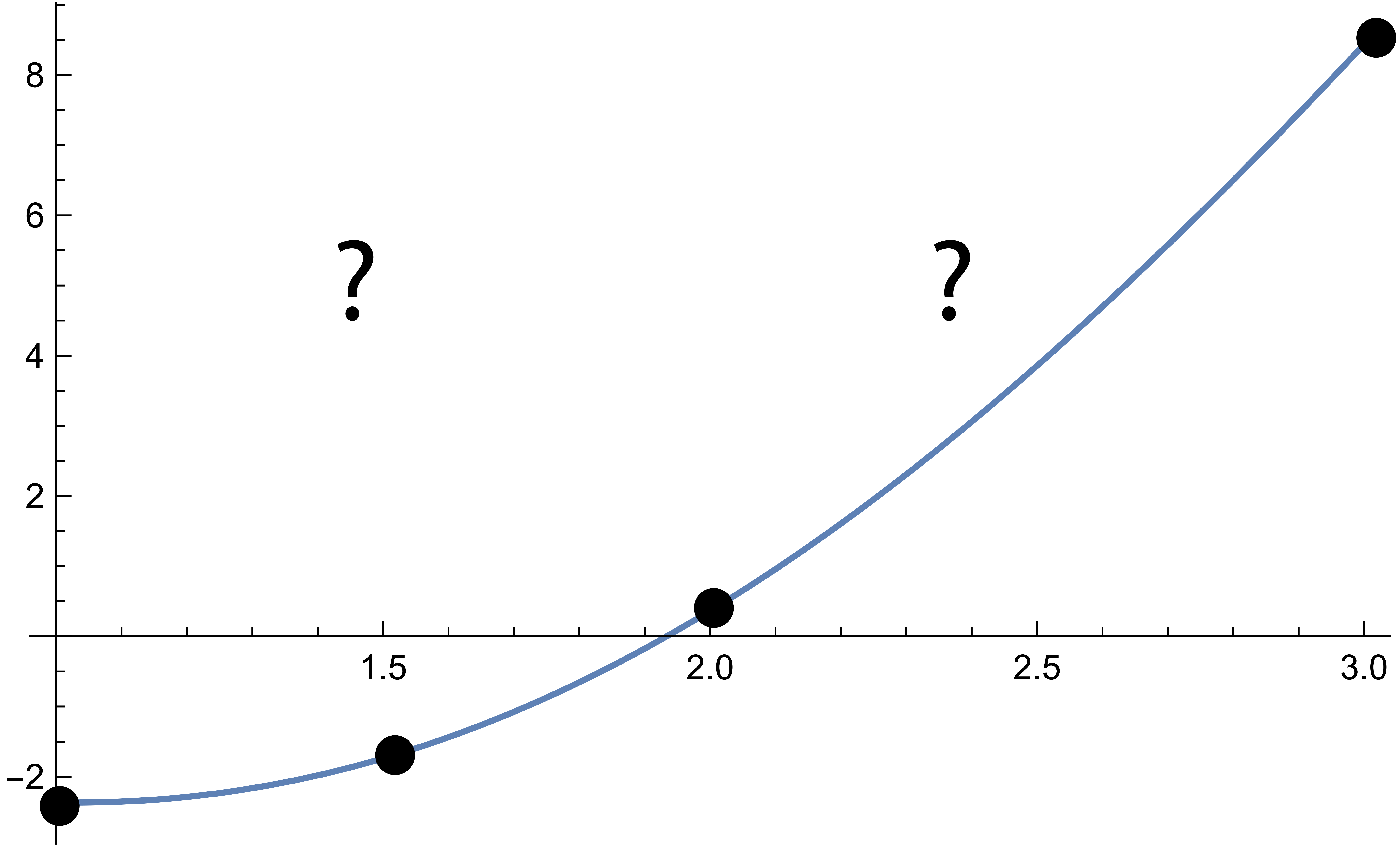

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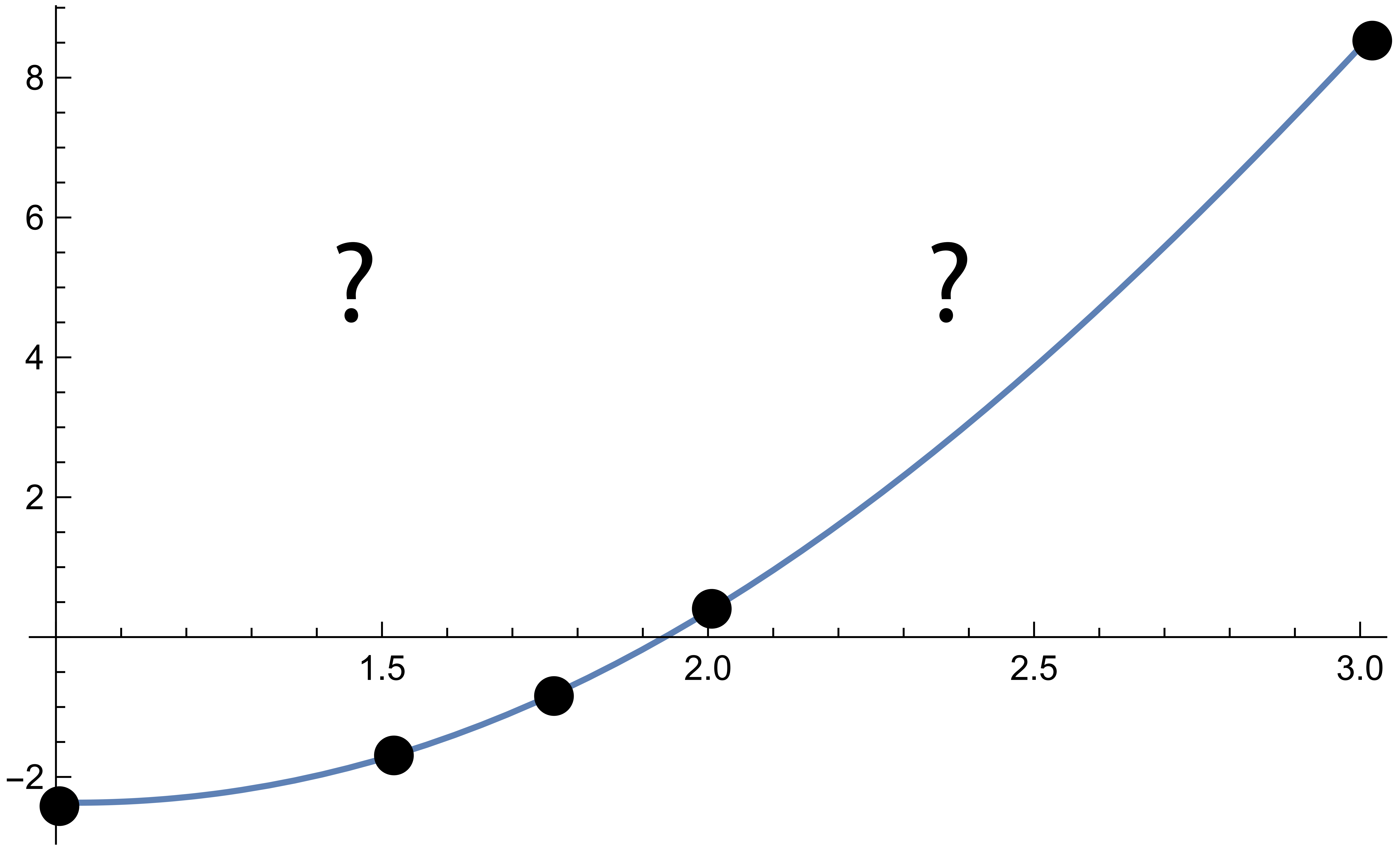

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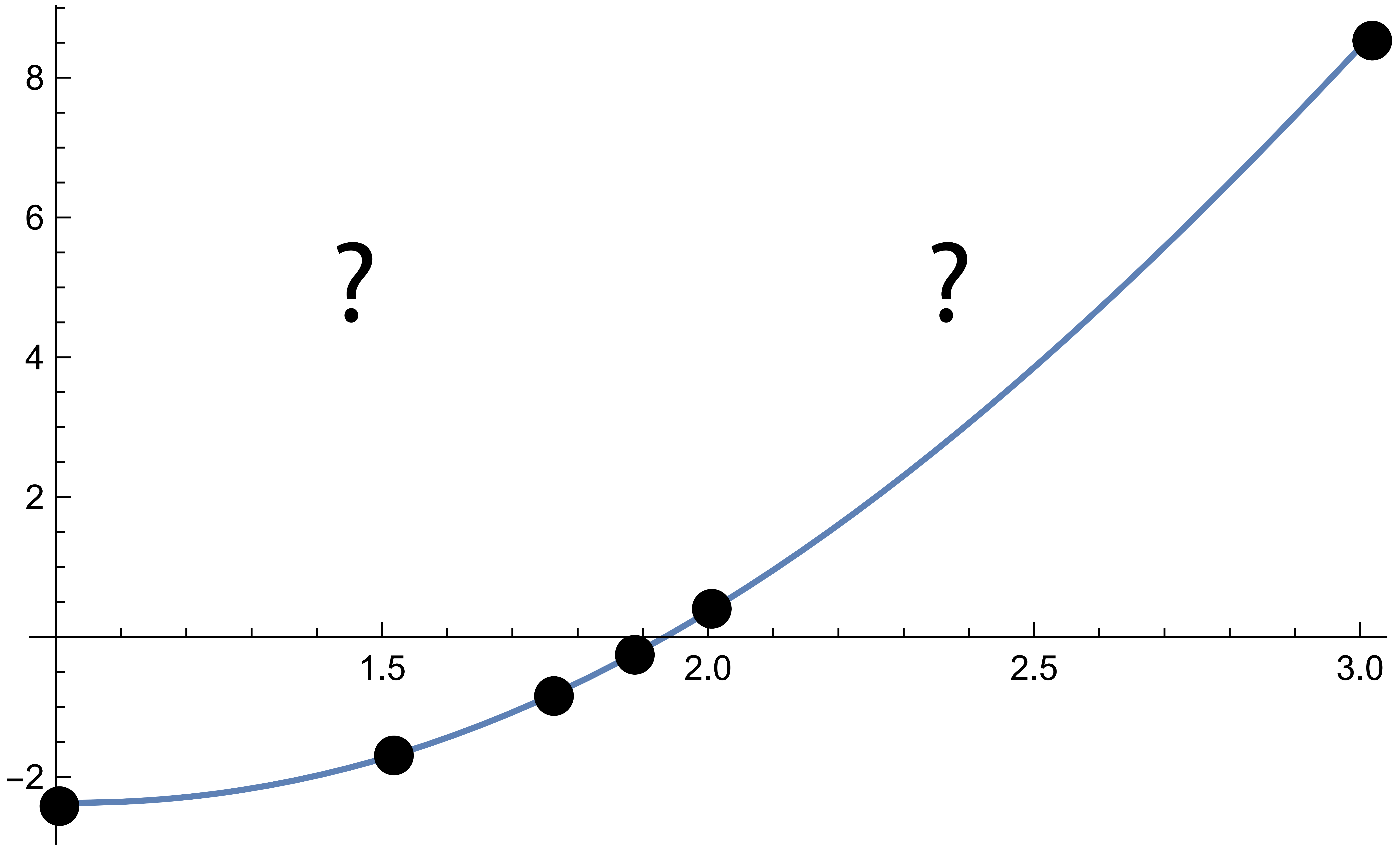
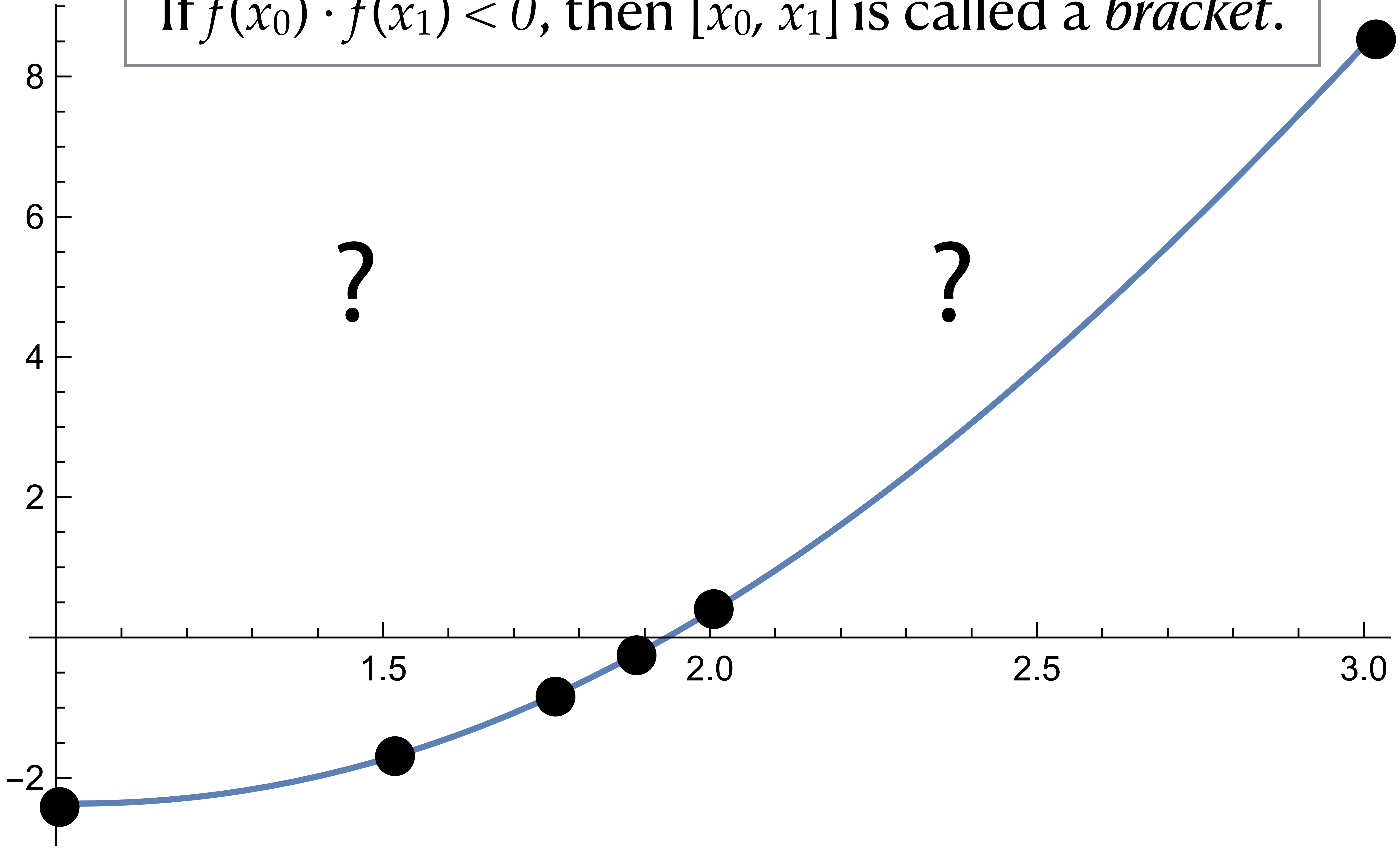


Use of continuity in our model problem

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:
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Does not use function values!
(only their sign is relevant)

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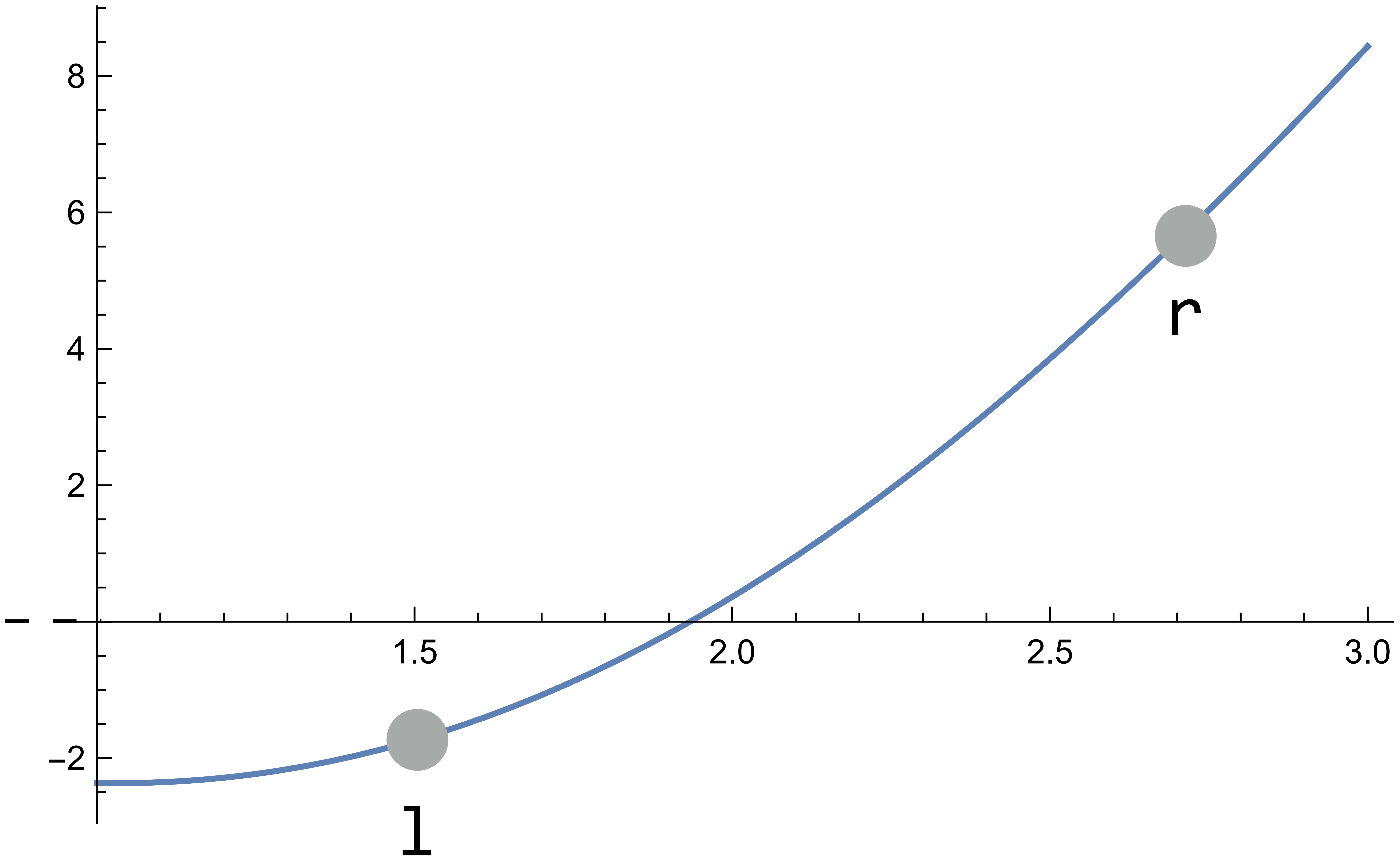

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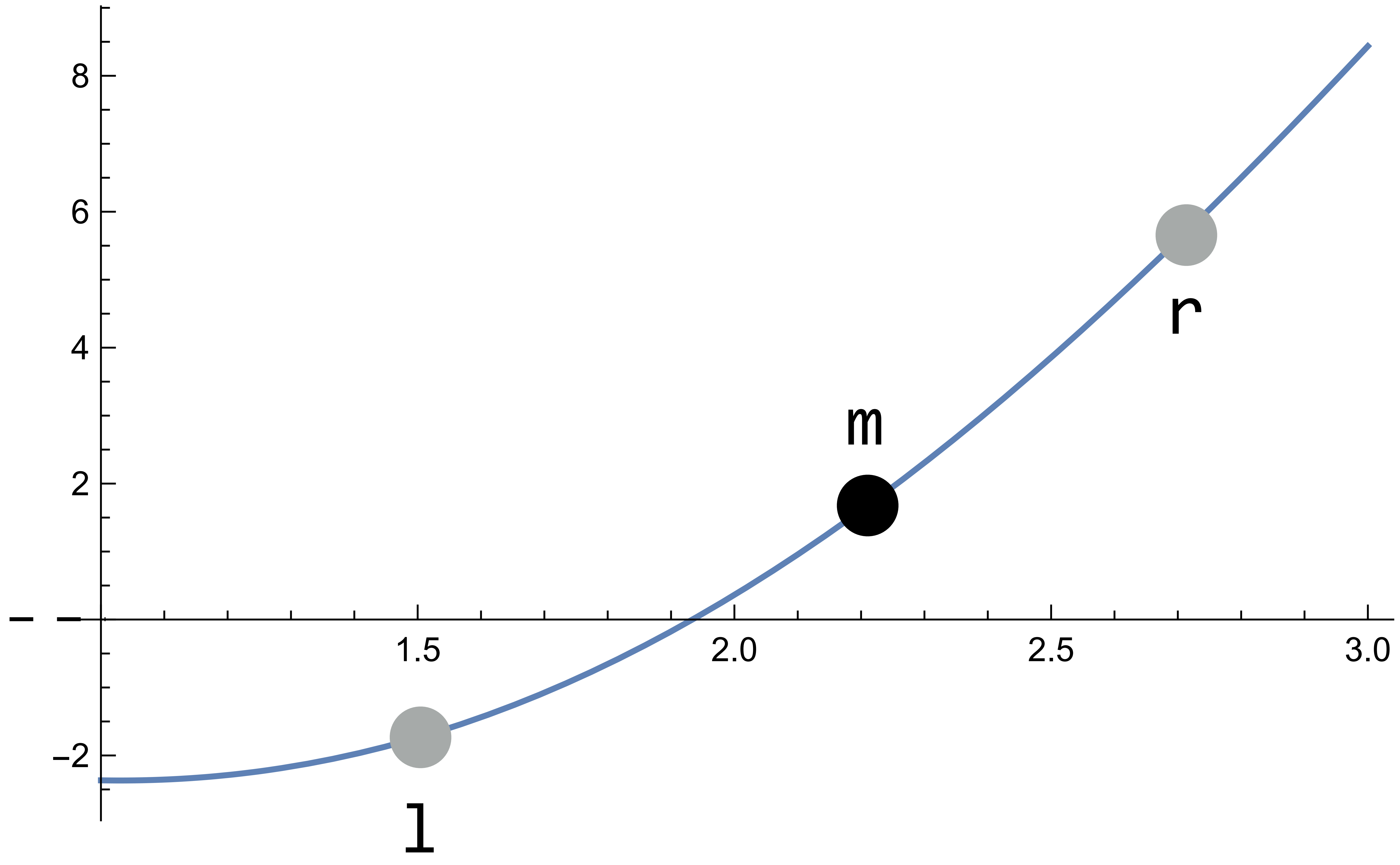

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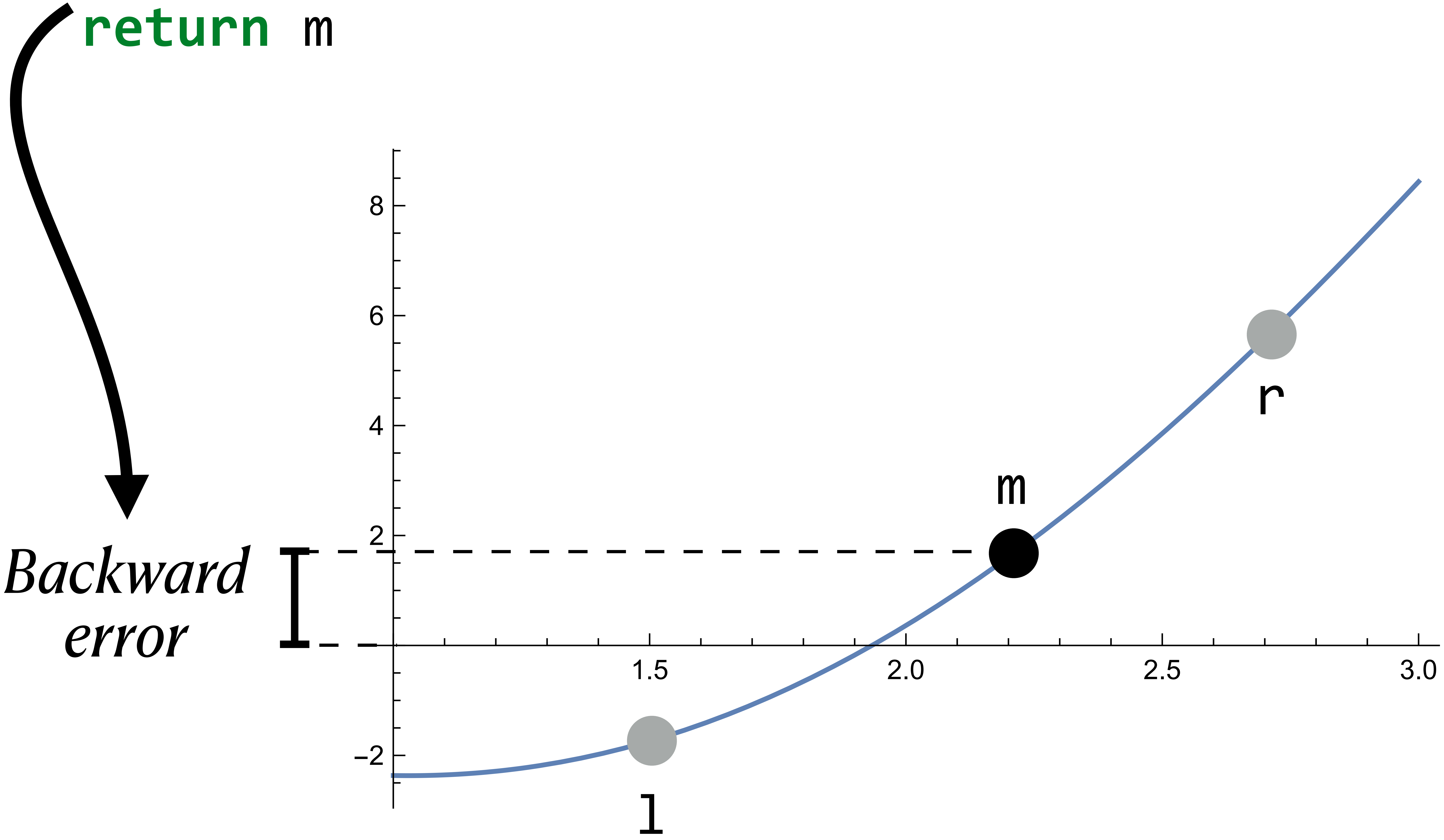

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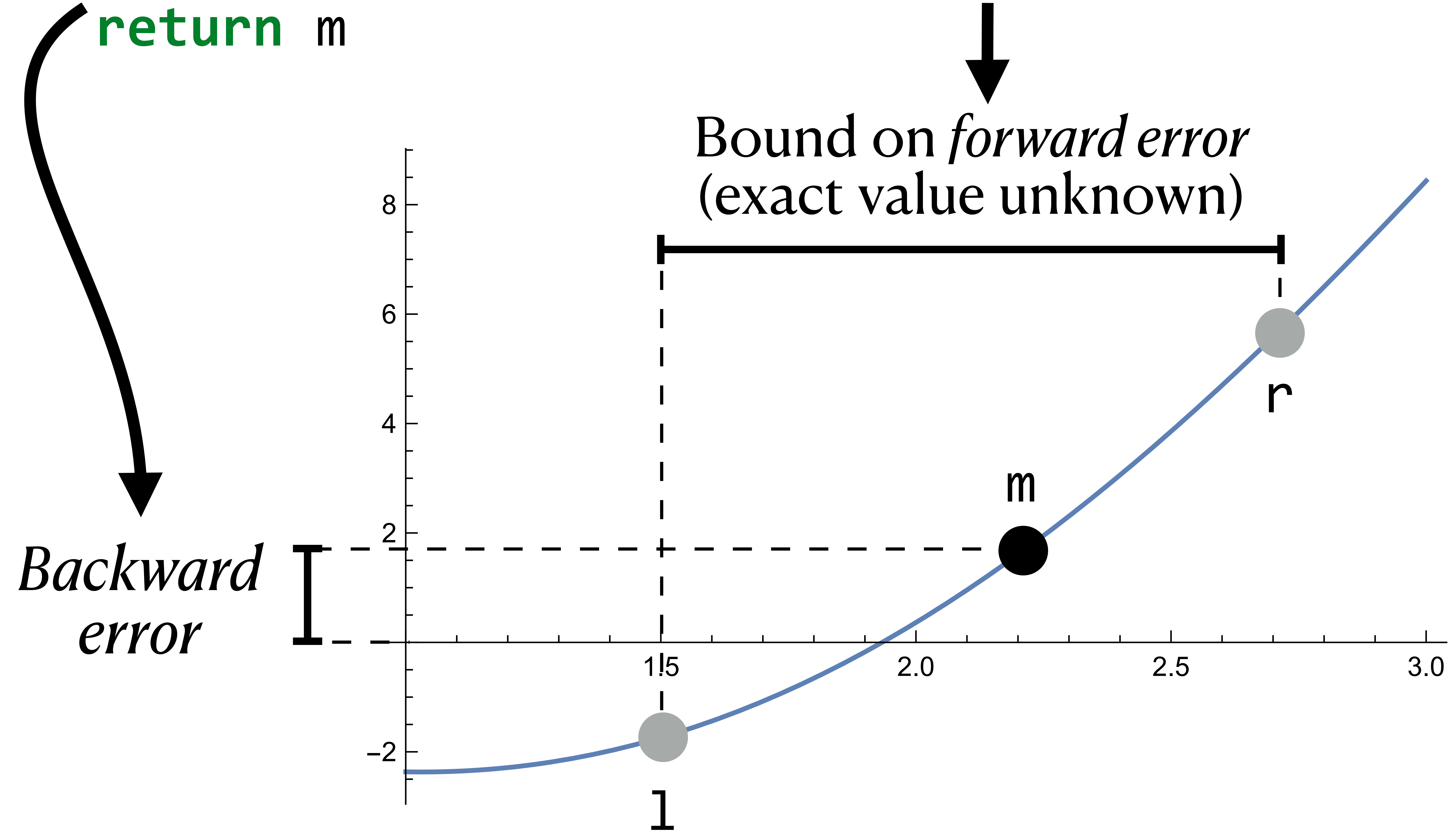

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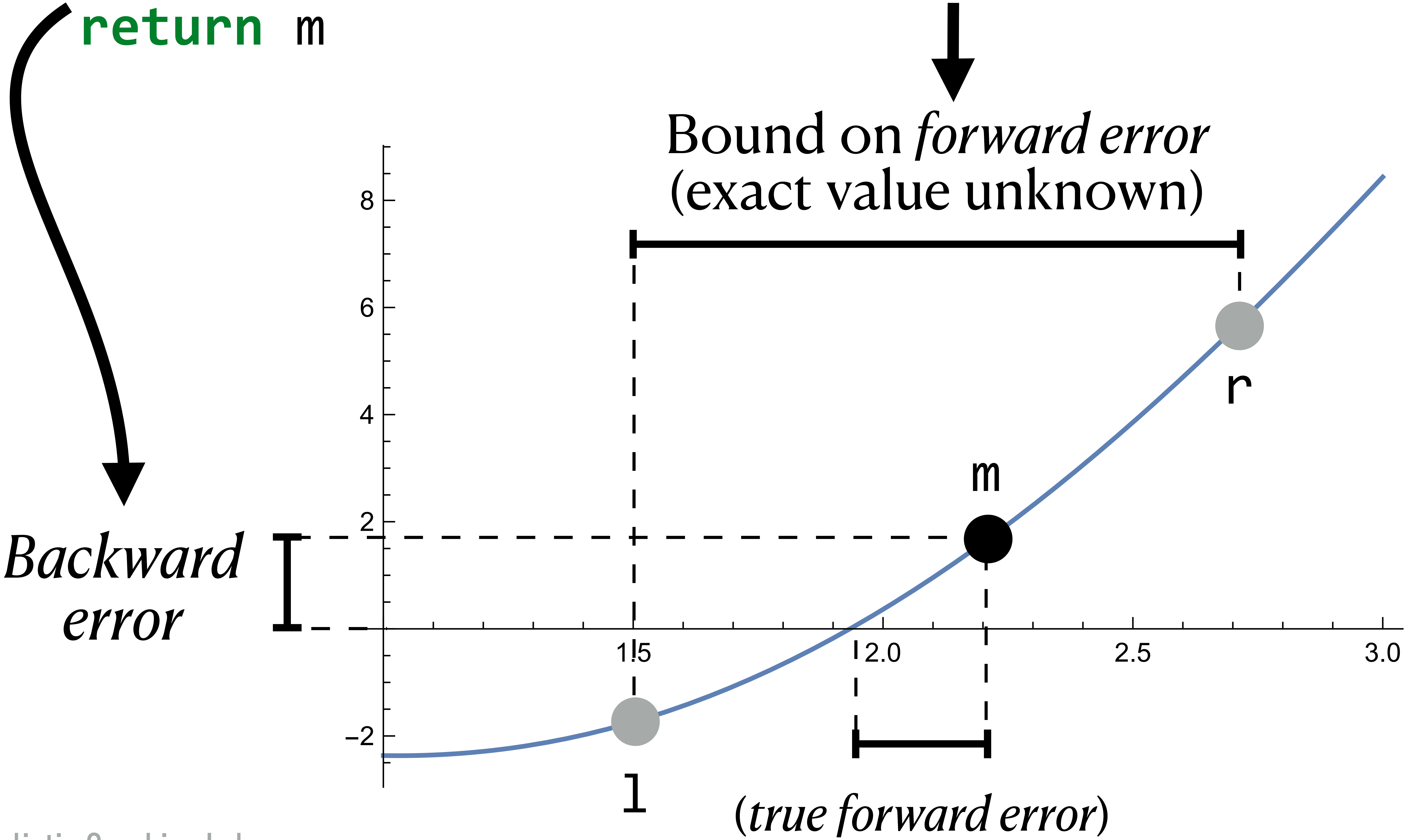
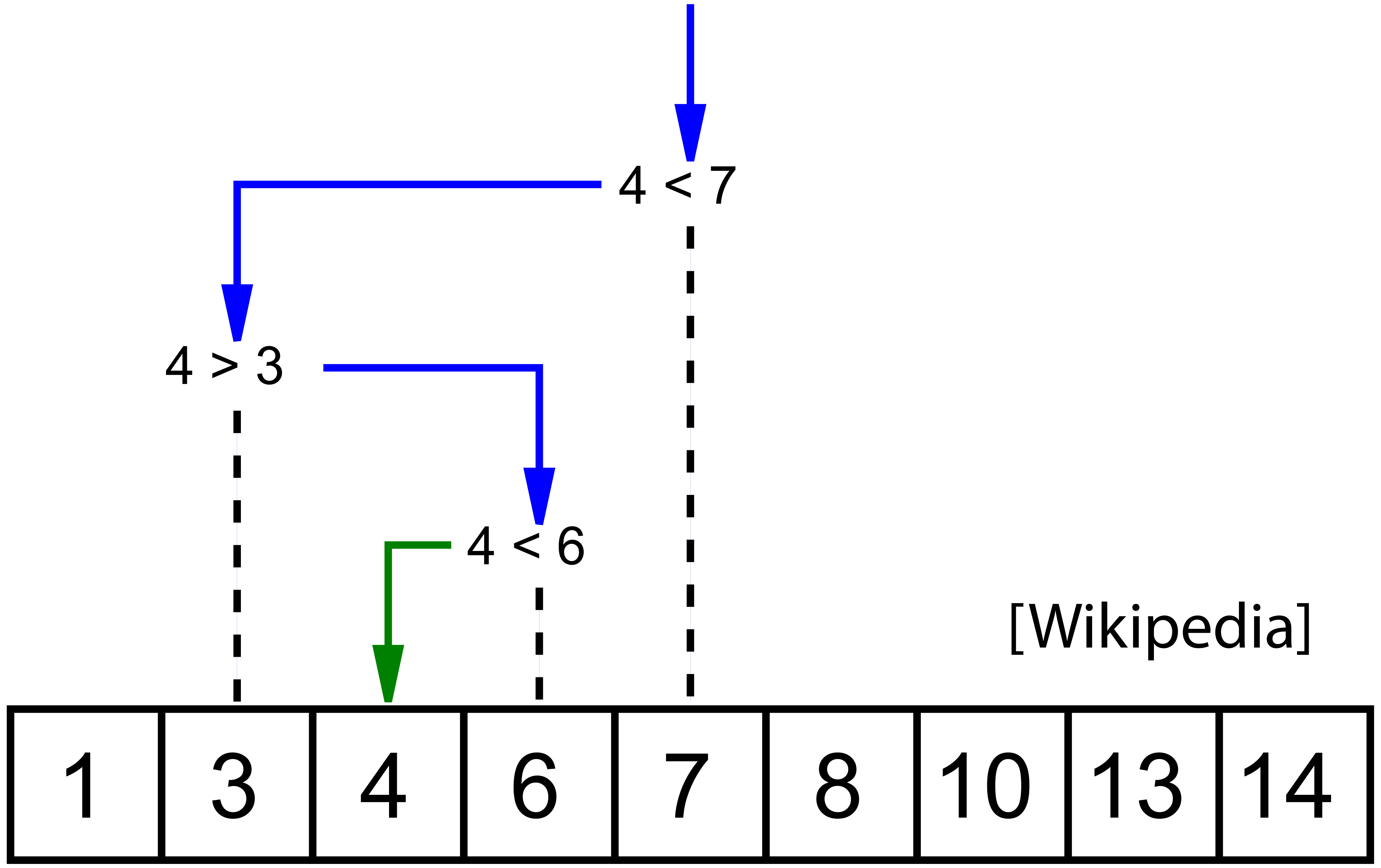


Does this seem at all familiar?



Binary search for 4 in sorted list.

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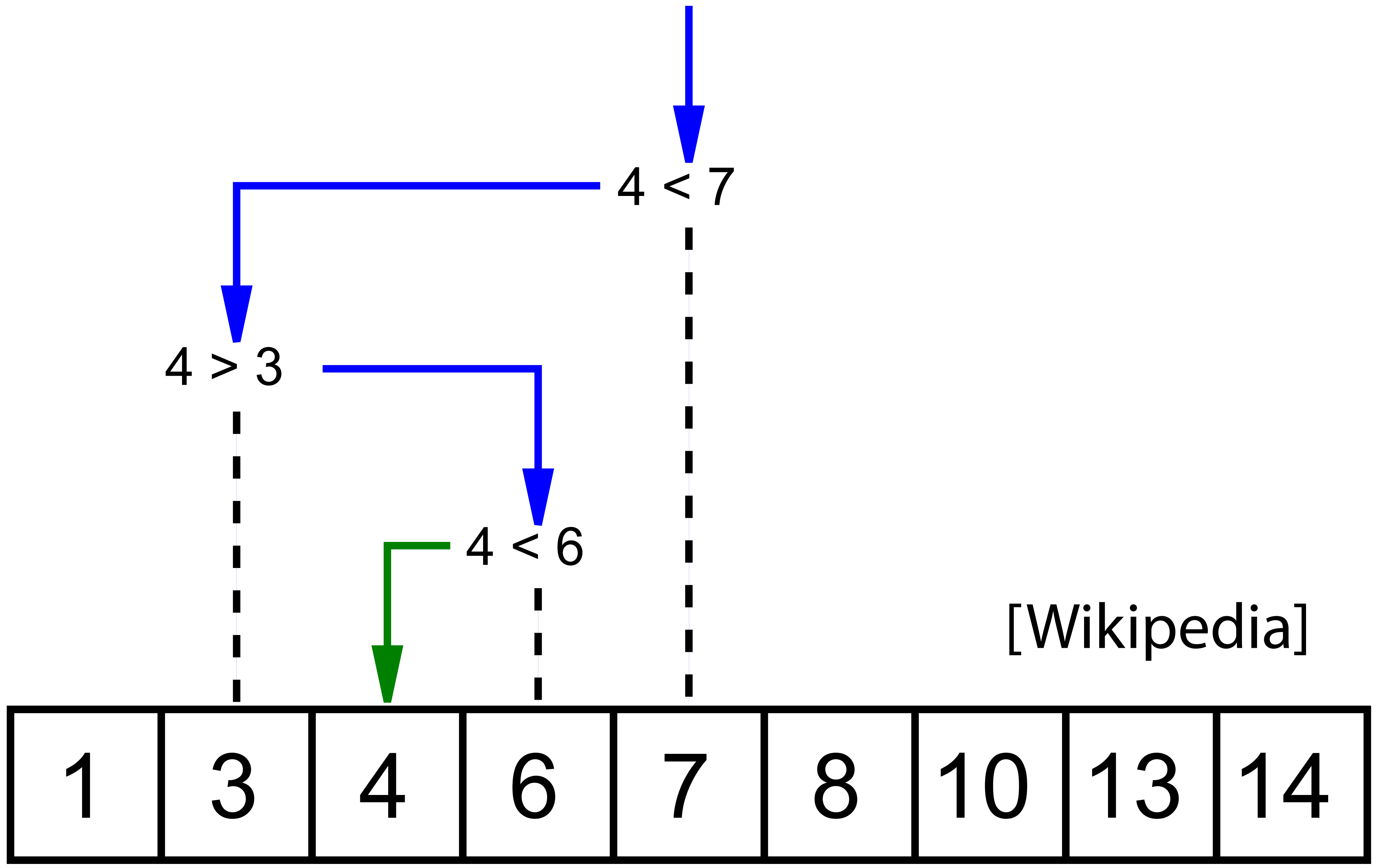

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Complexity of (discrete) algorithm: $O(\log n)$

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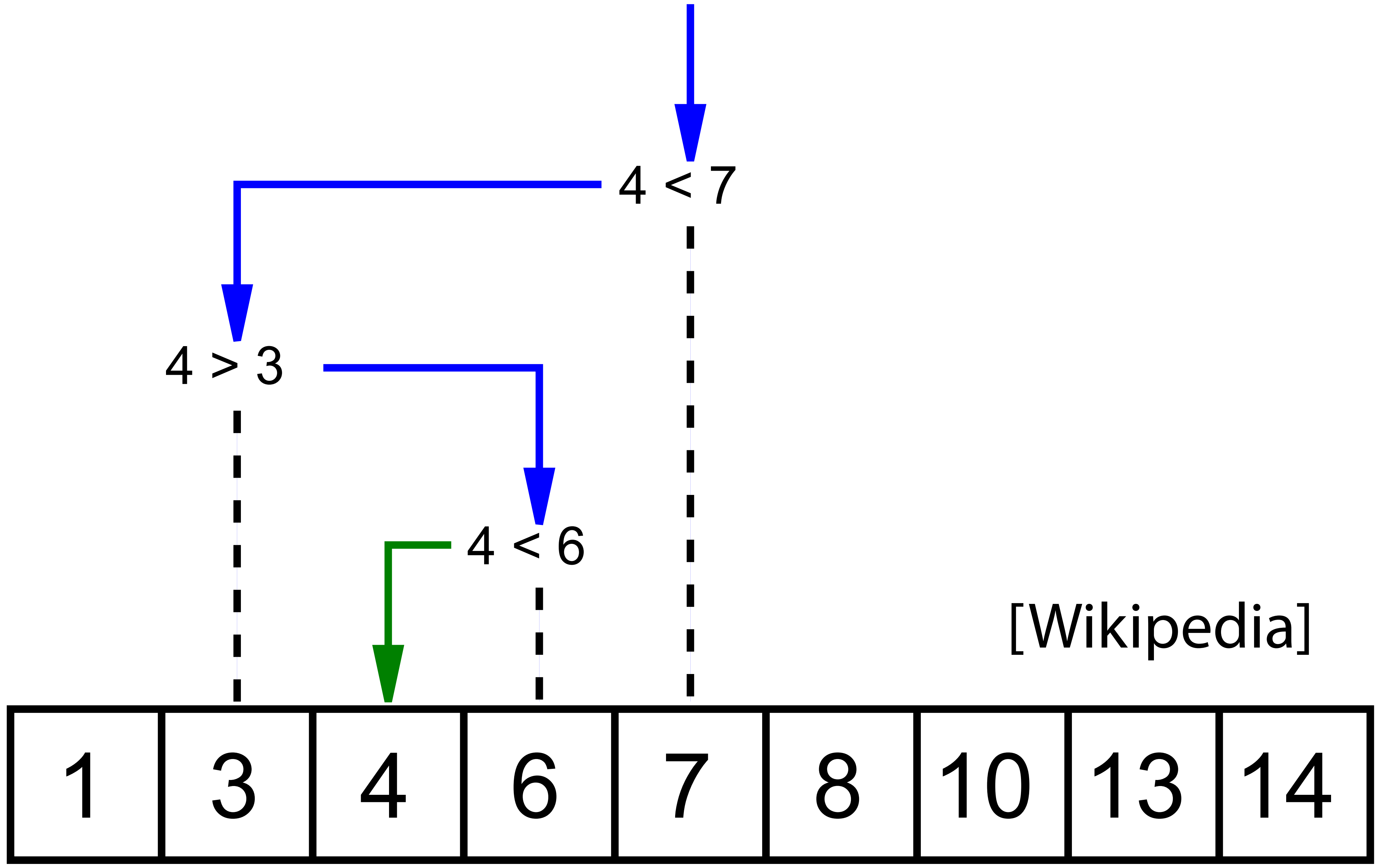

Binary search for 4 in sorted list.

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:

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- 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) : $r - l$

Convergence order and rate of bisection

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In other words: **order** of convergence = 1 (*linear*)
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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
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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
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l	$f(l)$	r	$f(r)$
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[Heath]

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[Heath]

Midpoint = **1.933**838

True solution = 1.93375376282..

(13 iterations for ~4 digits)

Newton's method

- Based on first-order Taylor expansion:

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

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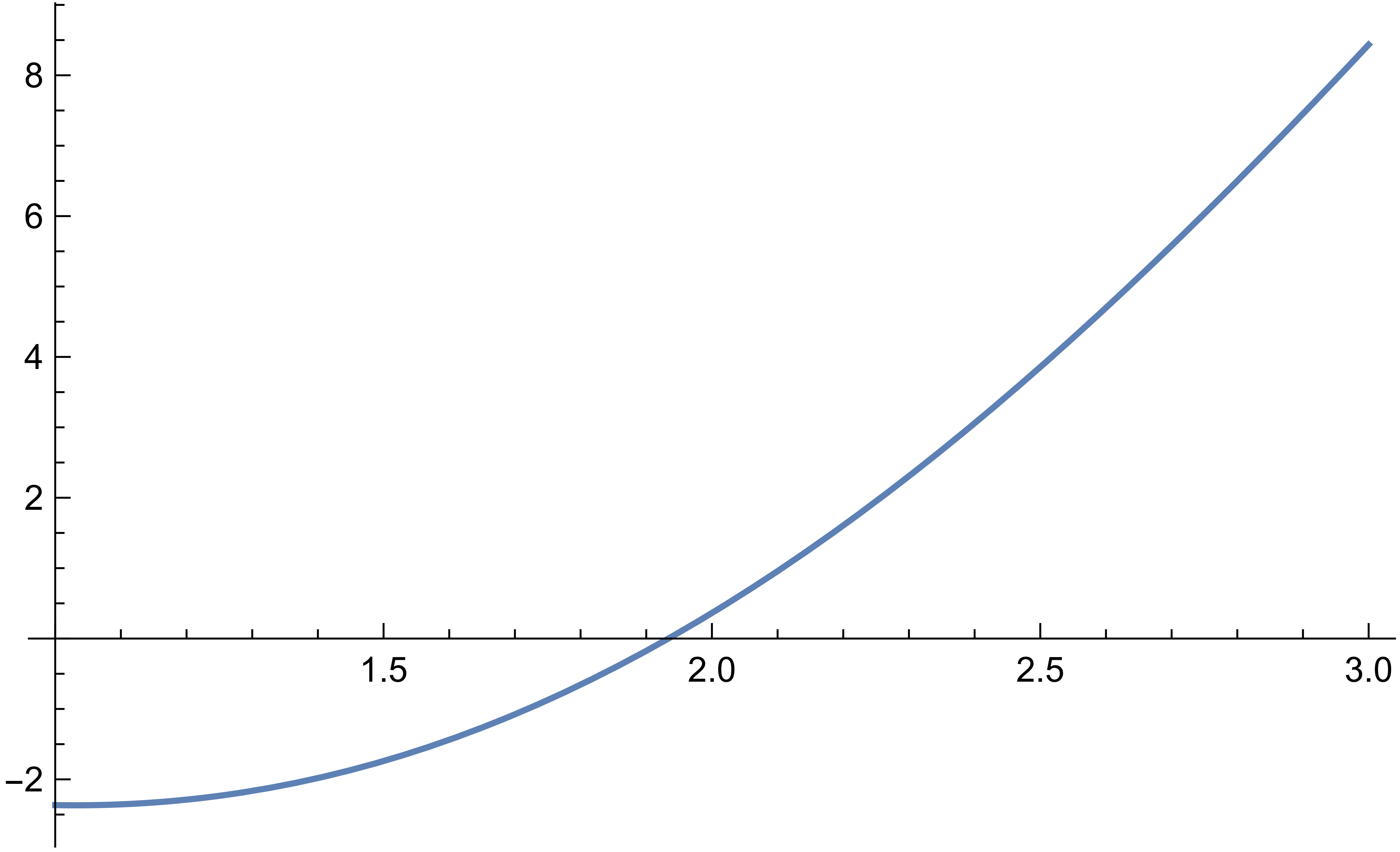
- Move to that position, and repeat..

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

Visualization of Newton's method



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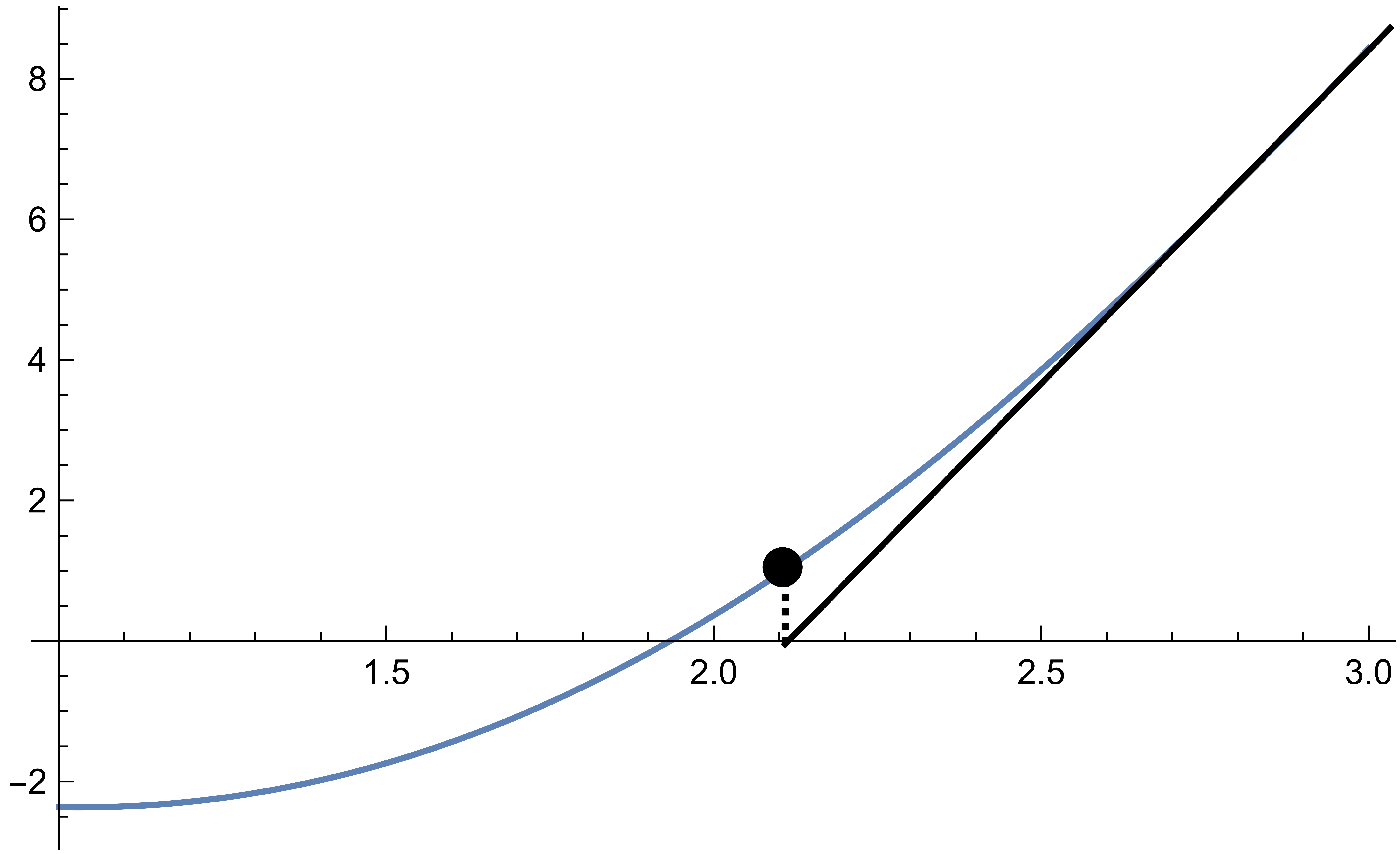

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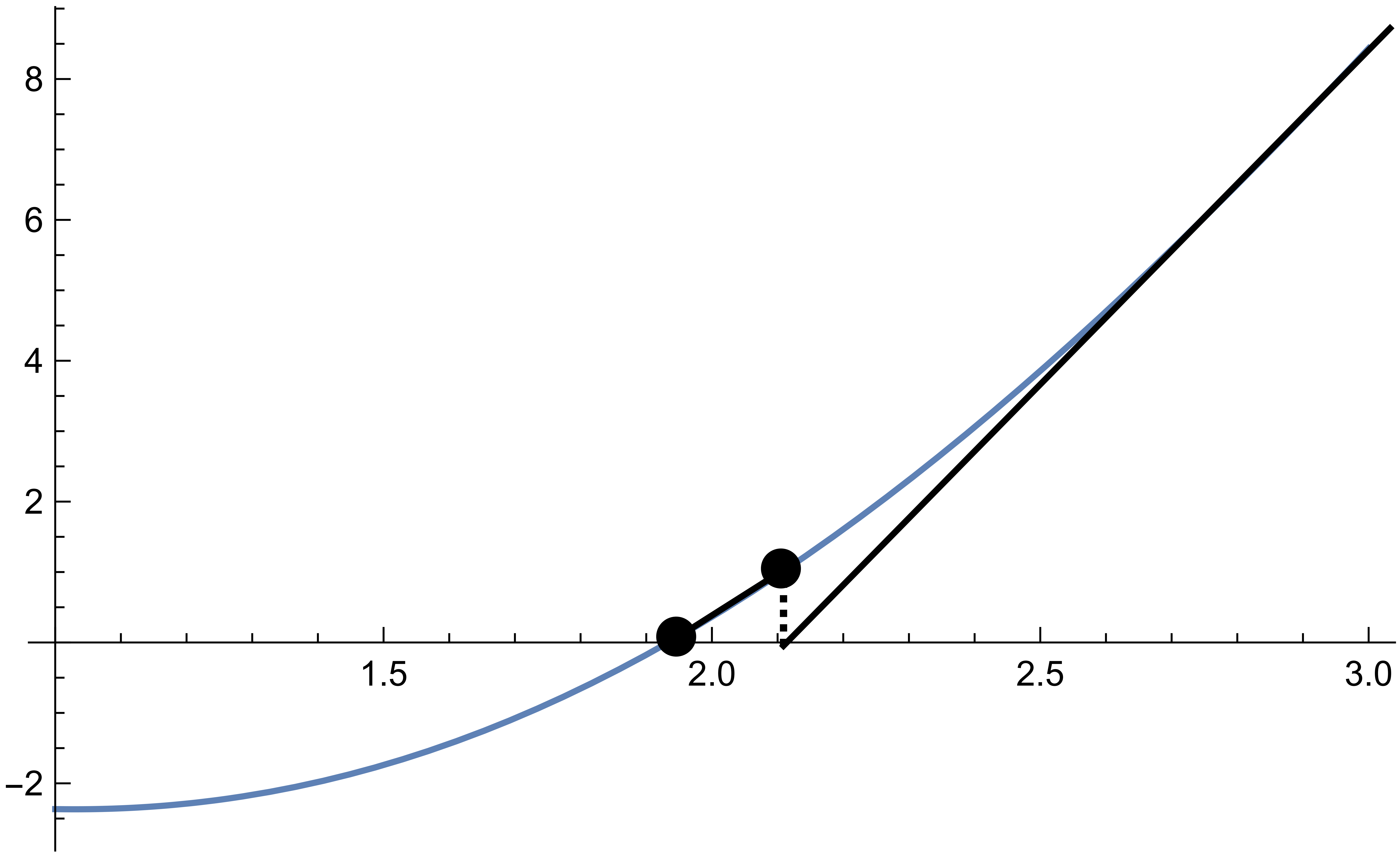

Convergence of Newton's method

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

Newton's method requires the derivative of f. Here,

$$f'(x) = 2x - 4\cos x$$

Convergence of Newton's method

x	$f(x)$	$f'(x)$	h
3.000000	8.435520	9.959970	−0.846942
2.153058	1.294772	6.505771	−0.199019
1.954039	0.108438	5.403795	−0.020067
1.933972	0.001152	5.288919	−0.000218
1.933754	0.000000	5.287670	0.000000

(5 iterations for ~7 digits)

[Heath]

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[Heath]

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

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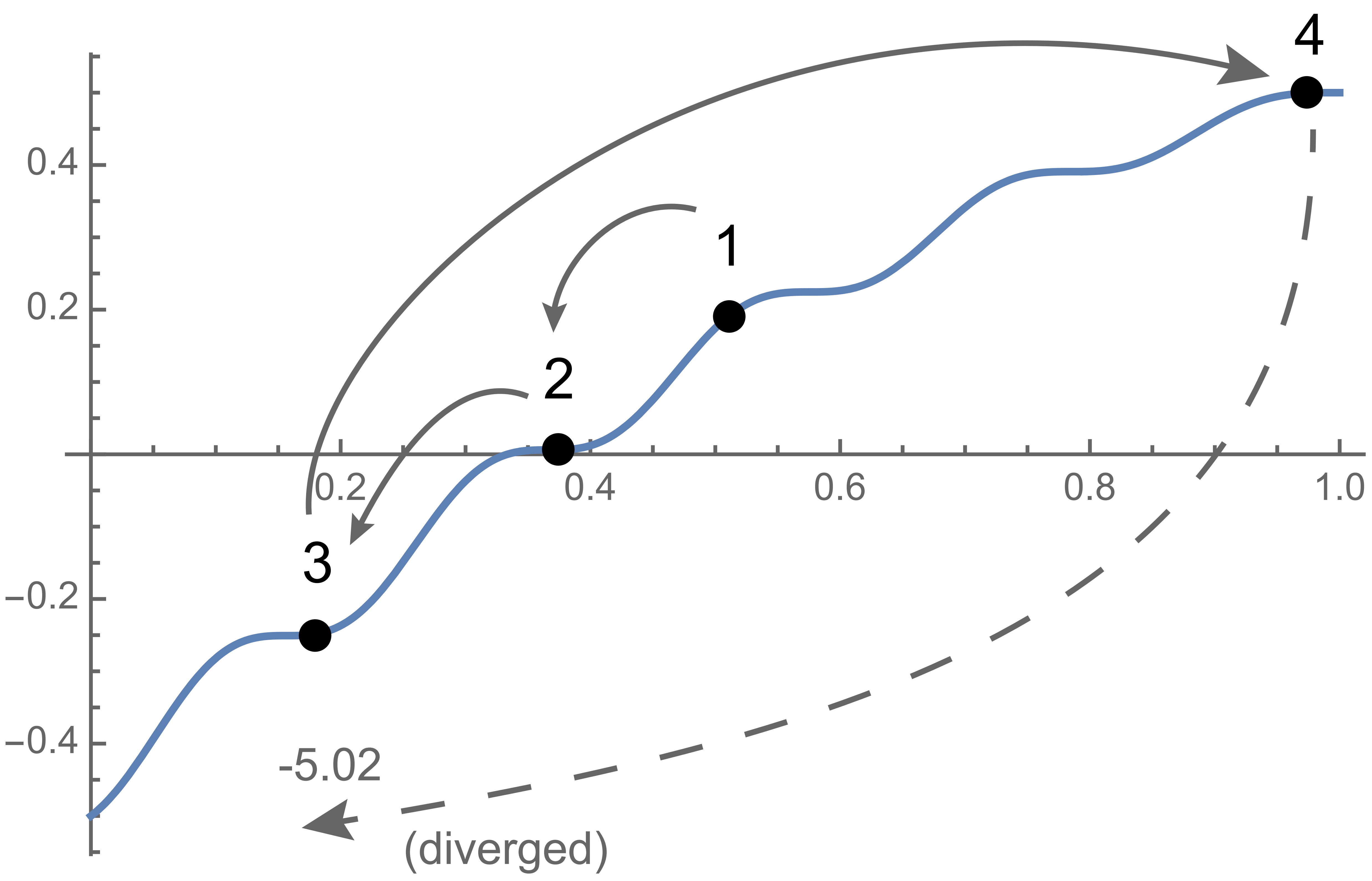
Failure cases of Newton's Method



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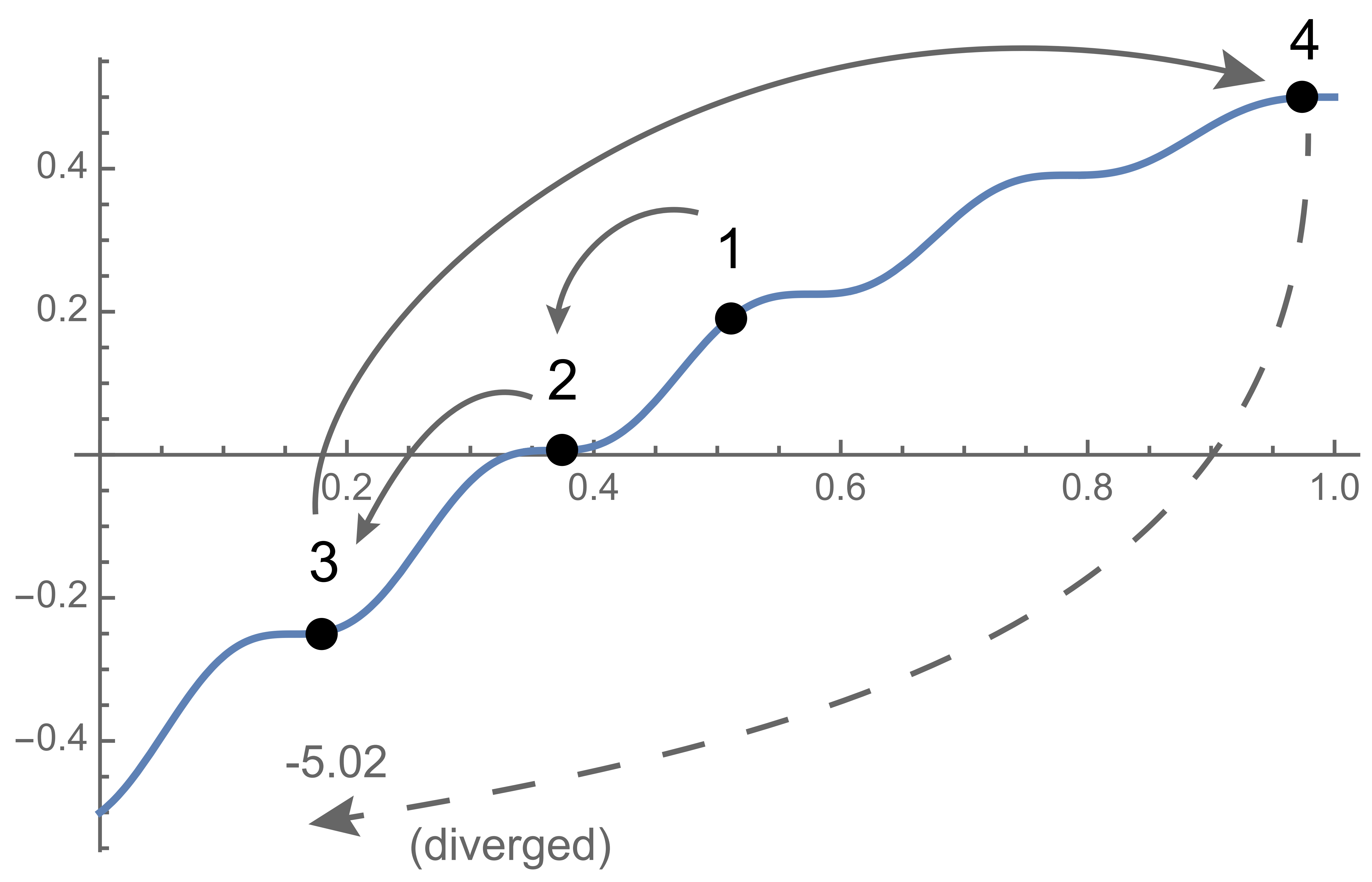
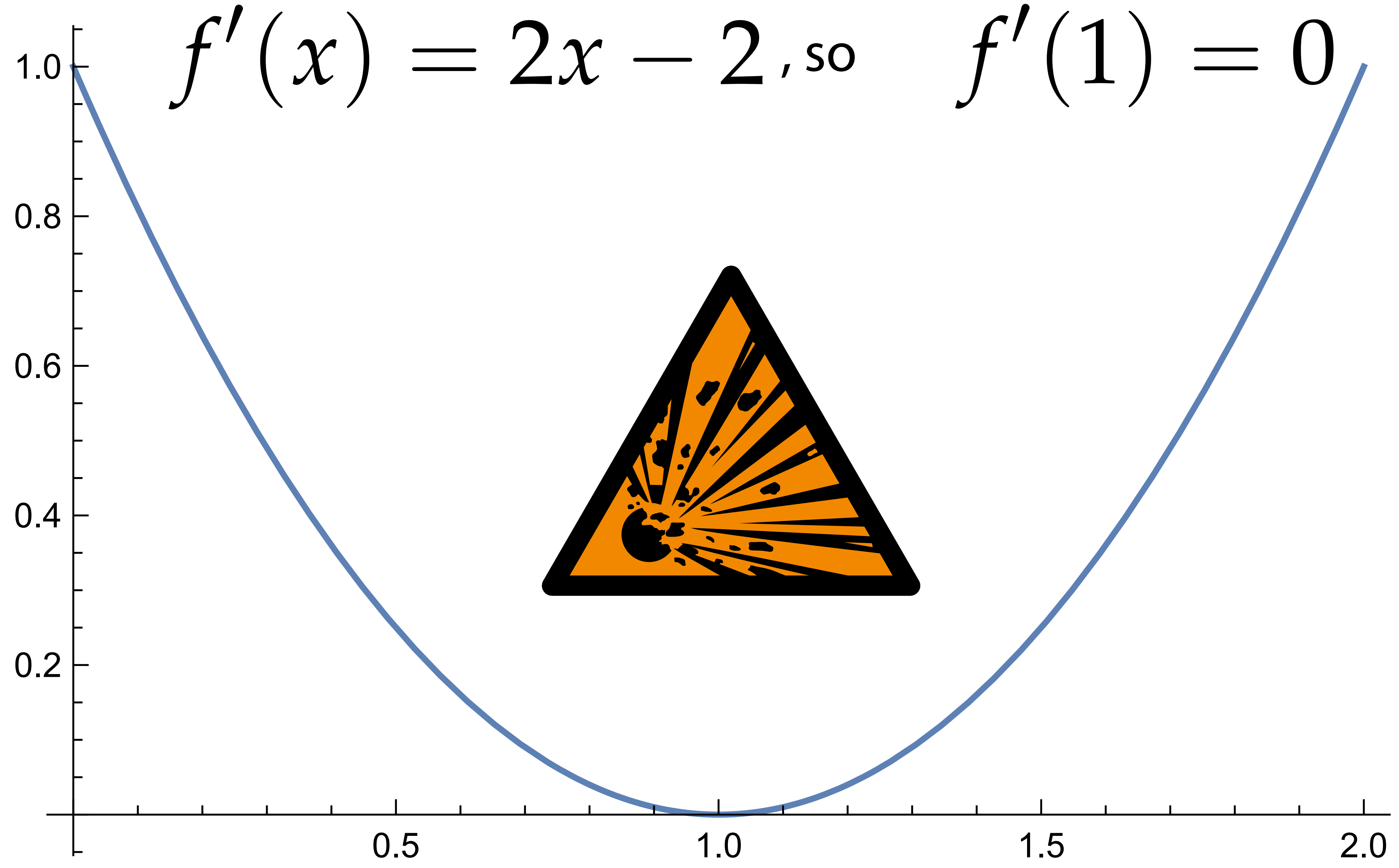


$$f(x) = (x-1)^2$$

$$f'(x) = 2x - 2$$, so $$f'(1) = 0$$



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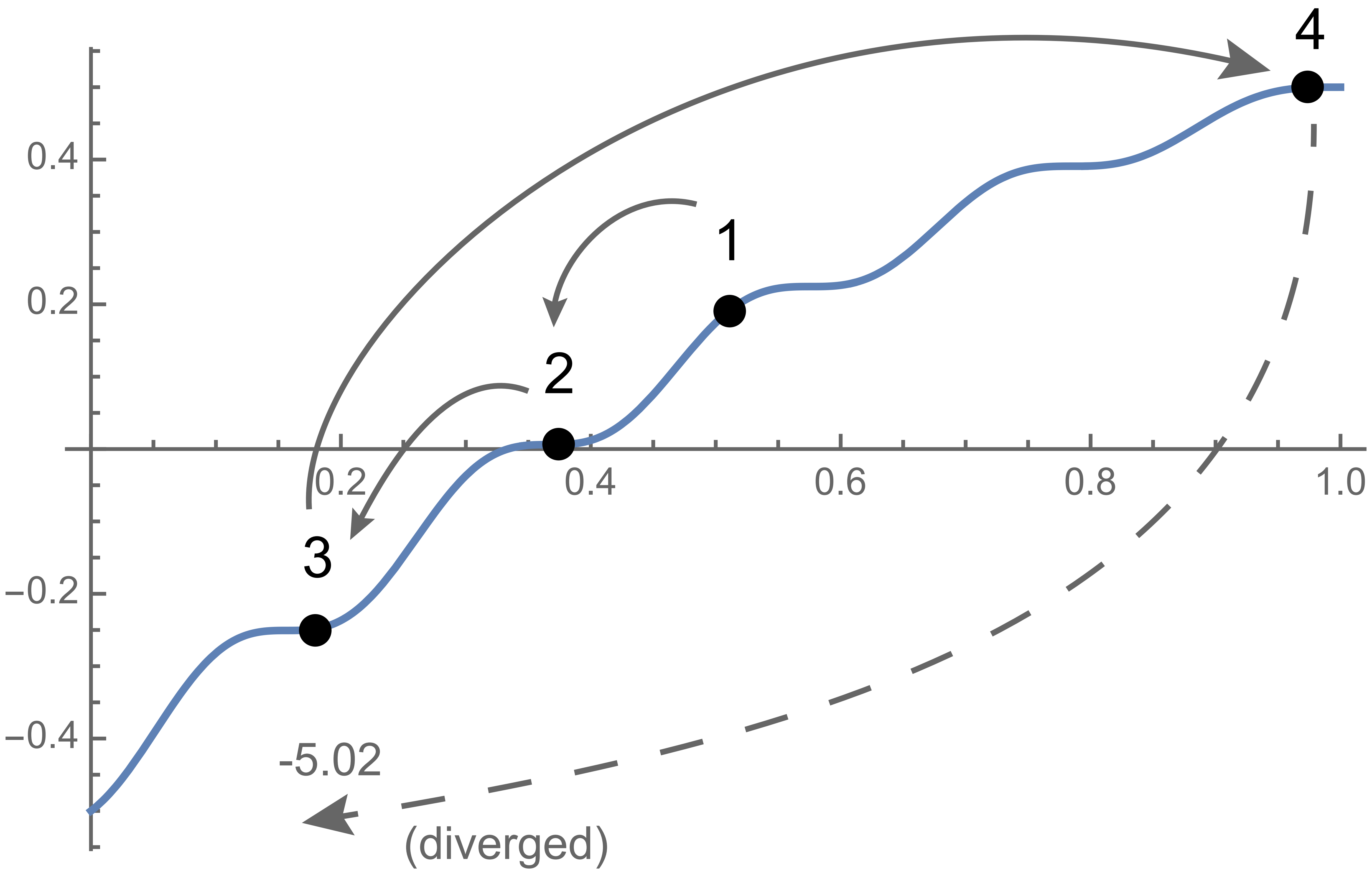

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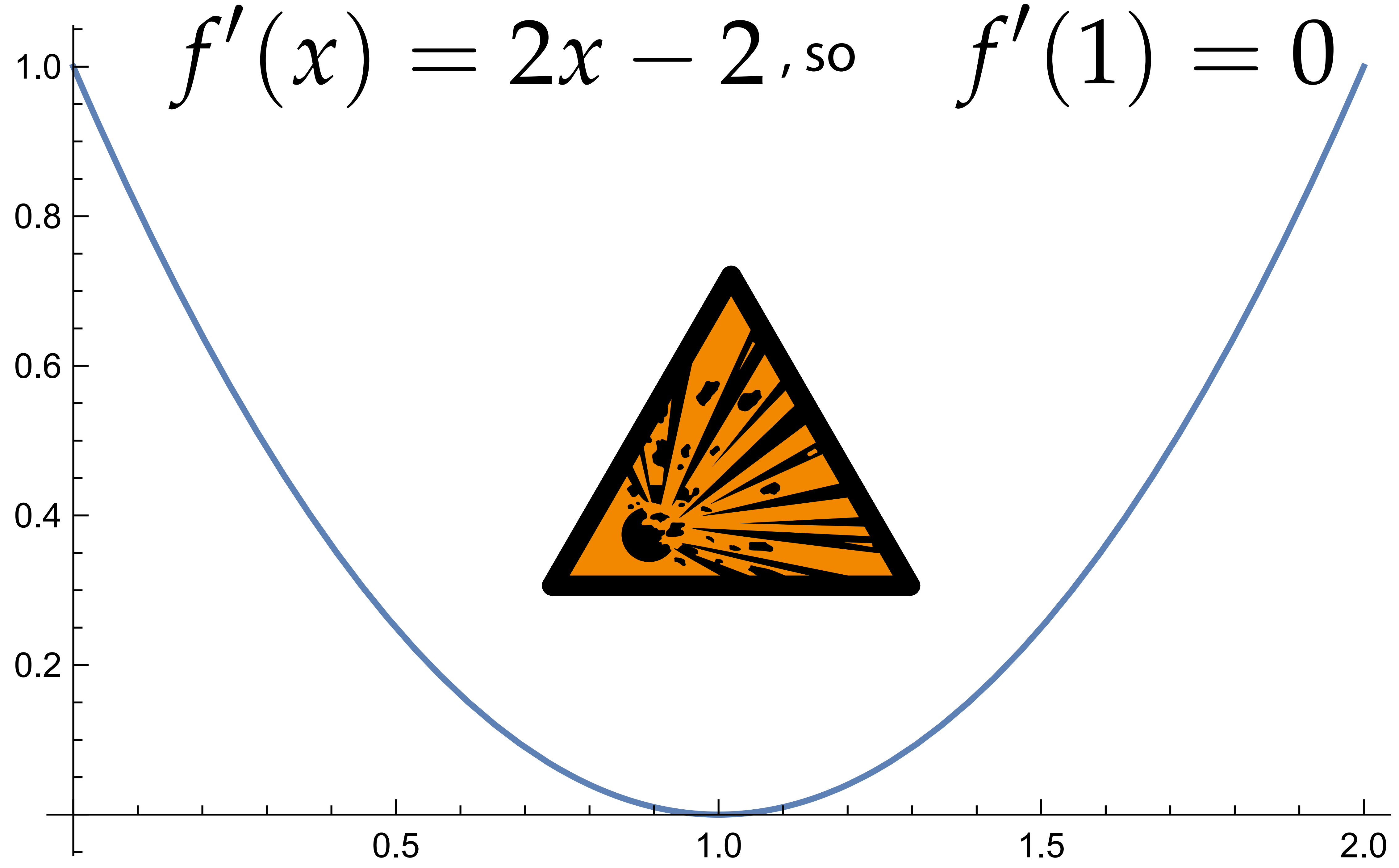

In theory: division by zero at $x = 1$.

In practice: slow convergence.

N dimensions

Multivariate root finding

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

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

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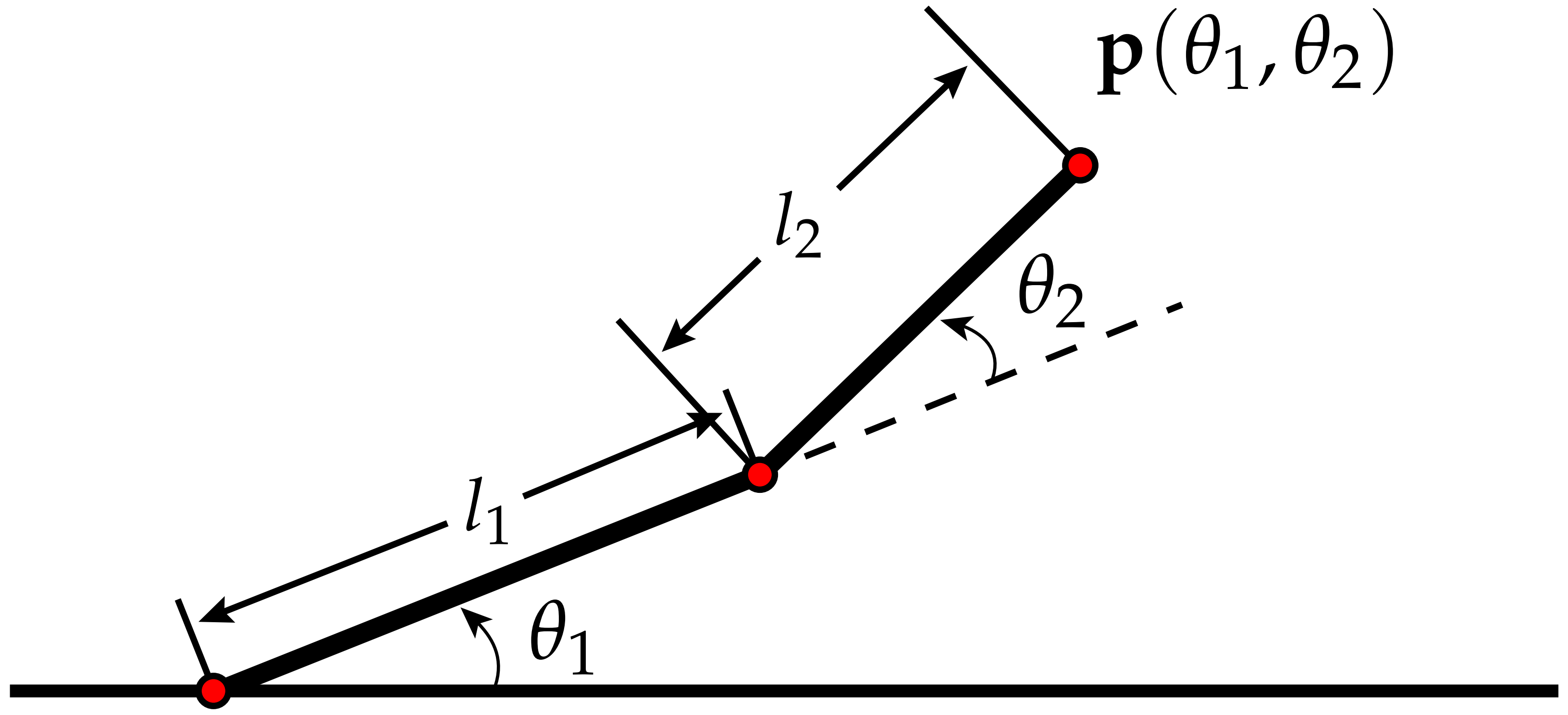
  - Assumes input and output spaces have matching dimension.

HW3: Inverse Kinematics via Newton's method

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



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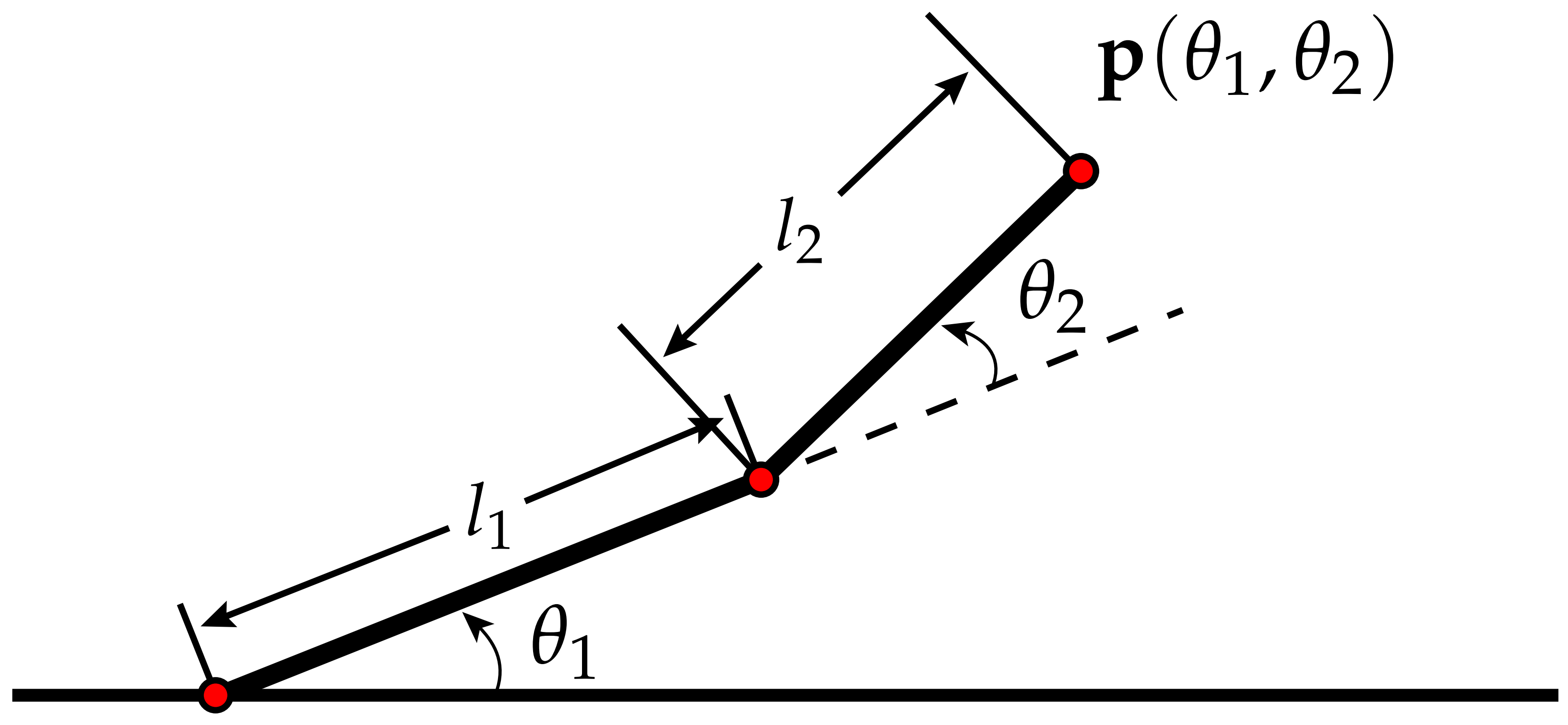

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n unknowns

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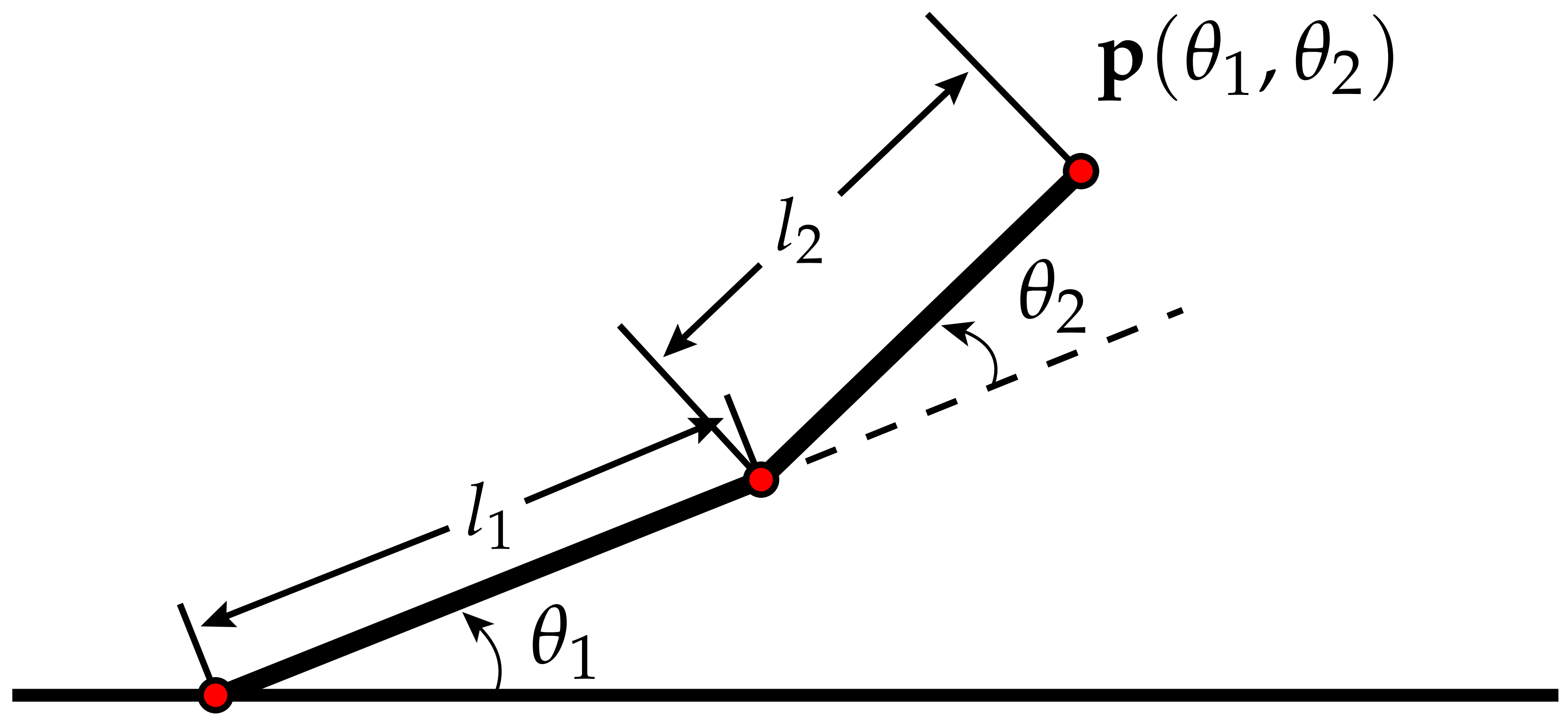

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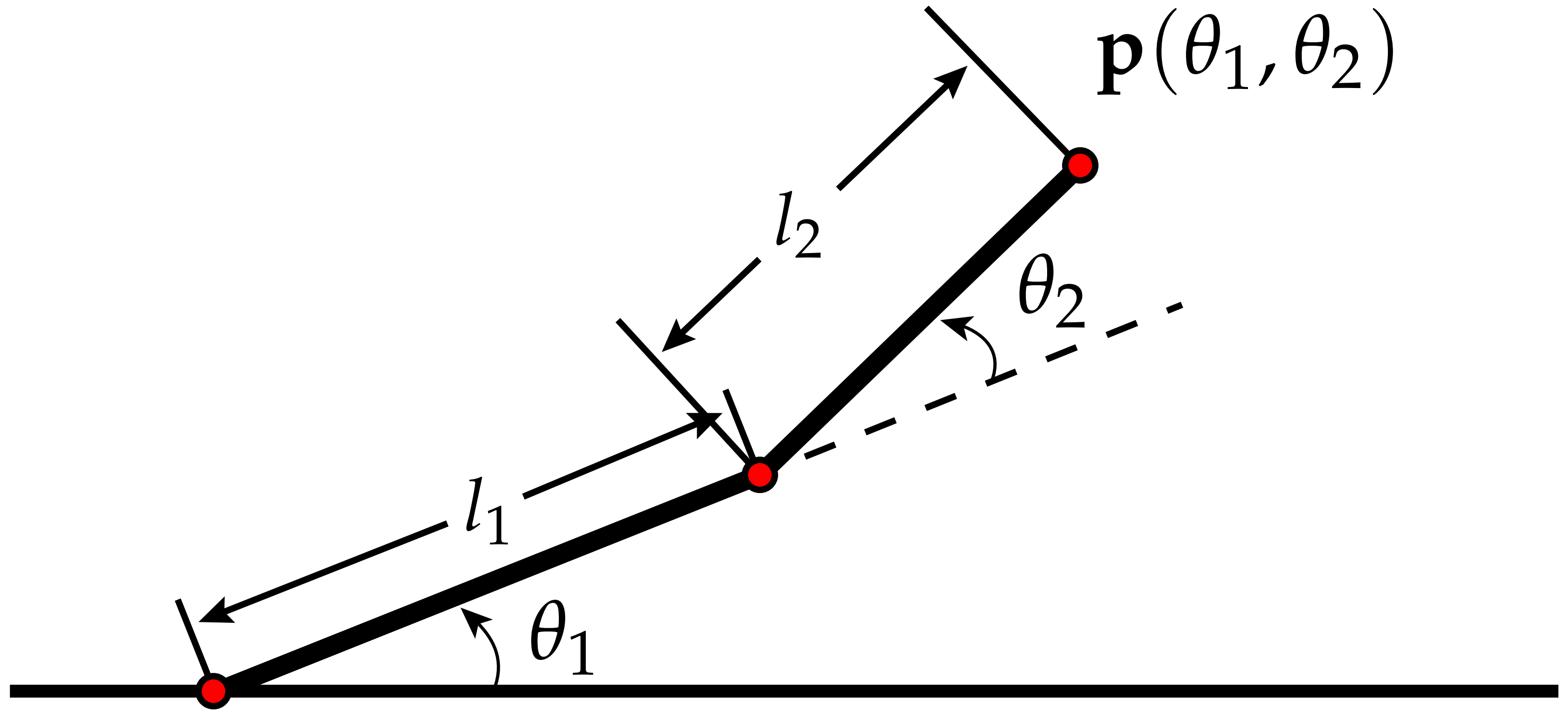

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Idea 2: solve with Newton's method + pseudoinverse

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

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"

A benchmark problem

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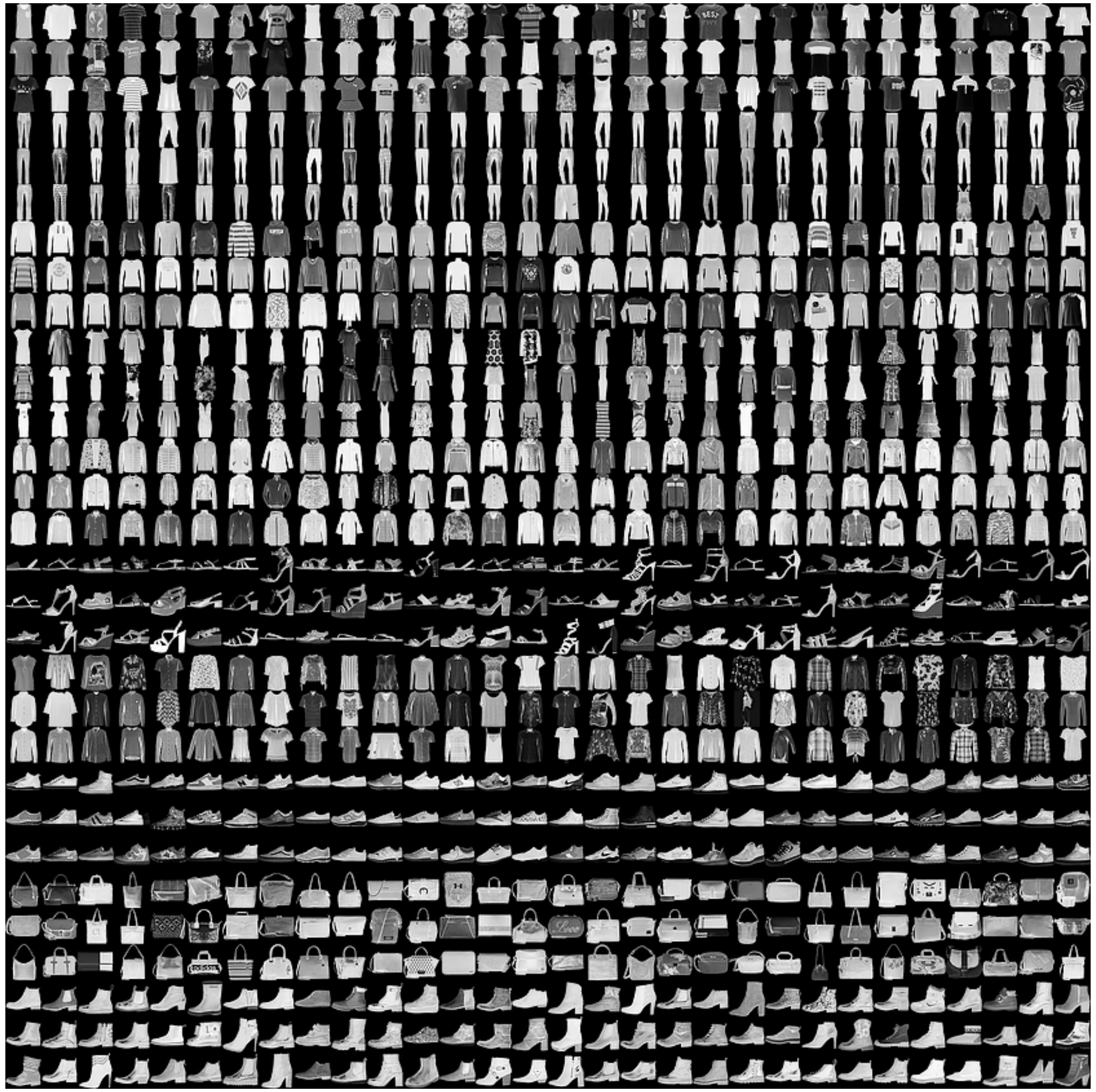

zalando


60'000 training images
10'000 testing images