Supervised Learning and Generalization

DSCC 251/451: Machine Learning with Limited Data

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Supervised Learning Review

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- Goal: learn the function that **best matches the dataset**

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  - Solution: learn the weights of a **parameterized function**

Parameterized Functions

Parameterized Functions

- A learning searches for a function f in a space of **possible functions**
- Parameters define a **family** of functions that share a common form
  - θ: general symbol for parameters/weights (usually represents **several**)
  - $\hat{y} = f(x; \theta)$: the function $f(x)$, **given parameters** θ
- Example: the **family of linear functions** $f(x) = mx + b$
  - $\theta = \{m, b\}$
  - This defines **all possible lines** (with different slopes and intercepts)
- Later: Neural Networks define their own family of functions

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- "Loss Function": a measure of how much the **predicted output** $\hat{y}$ **diverges** from the **true output** y
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- We always want to **minimize the loss/error**
  - This is a type of **optimization problem**, which is a huge subfield of math

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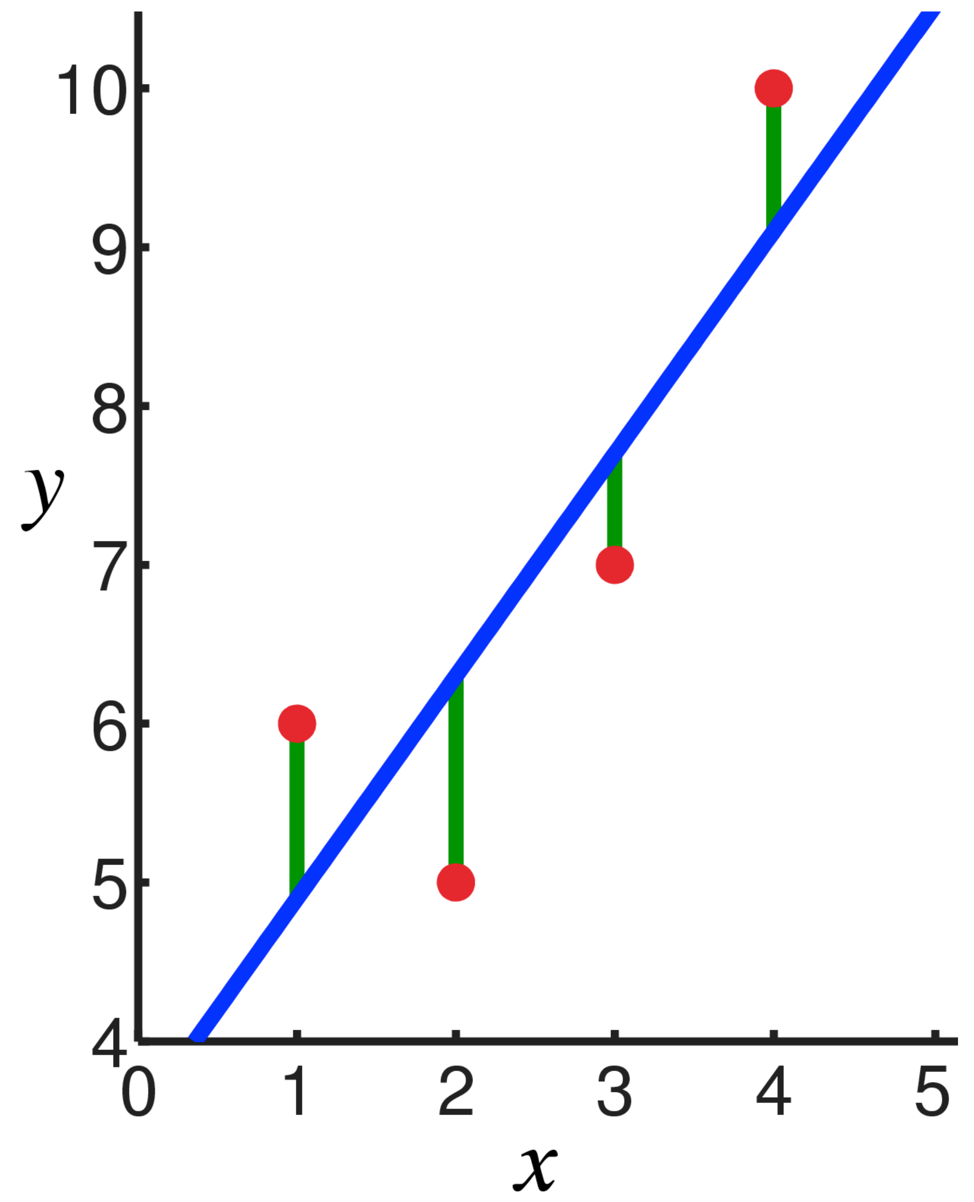
- Example: **Linear Regression** ("Least-Squares" method)

$$m^*, b^* = \arg\min_{m,b} \sum_i ((mx_i + b) - y_i)^2$$



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    - $\hat{y} = f(x) = x + \theta$

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- Lastly **learn the optimal value of θ** (i.e. the value that **minimizes the loss**)

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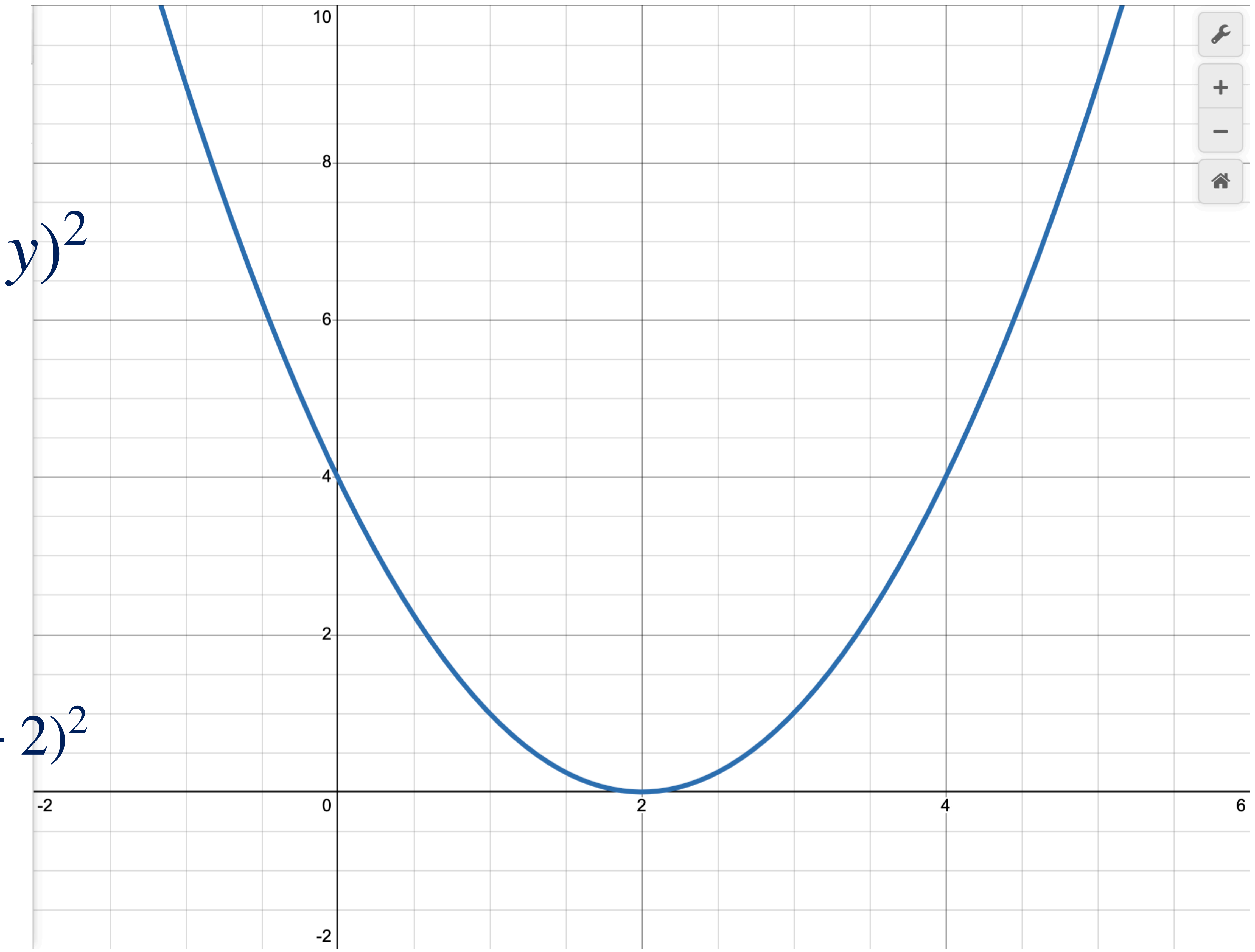

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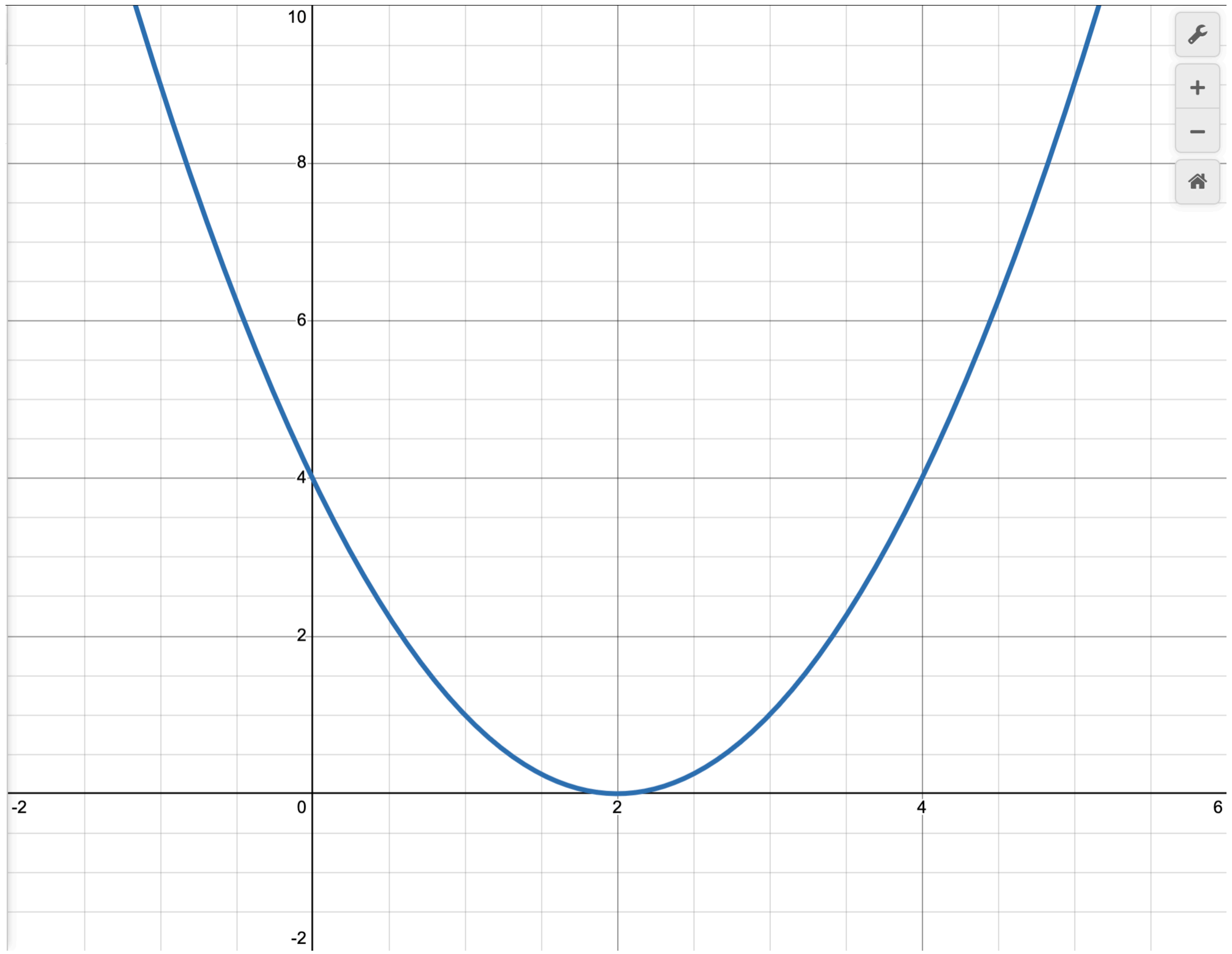

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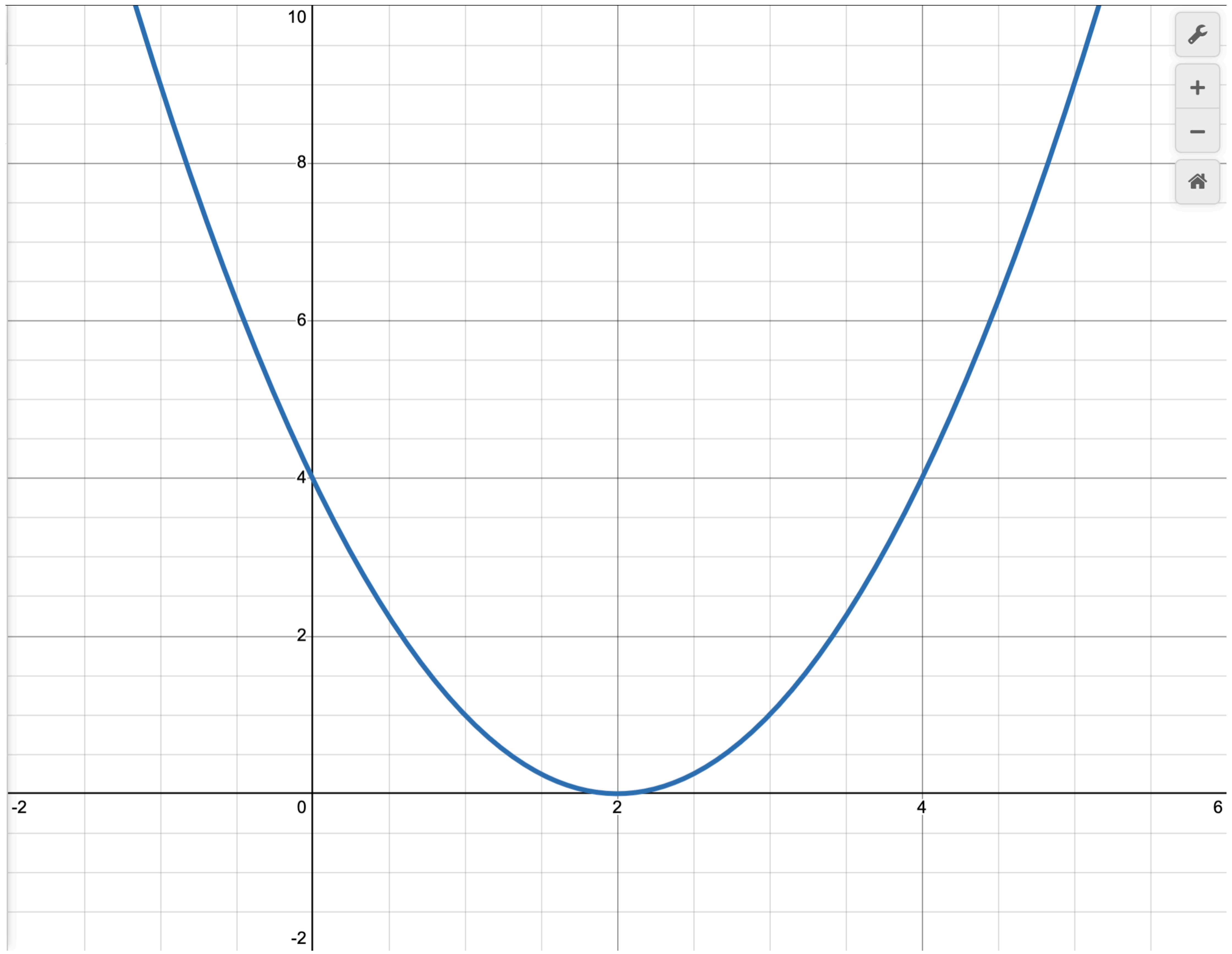

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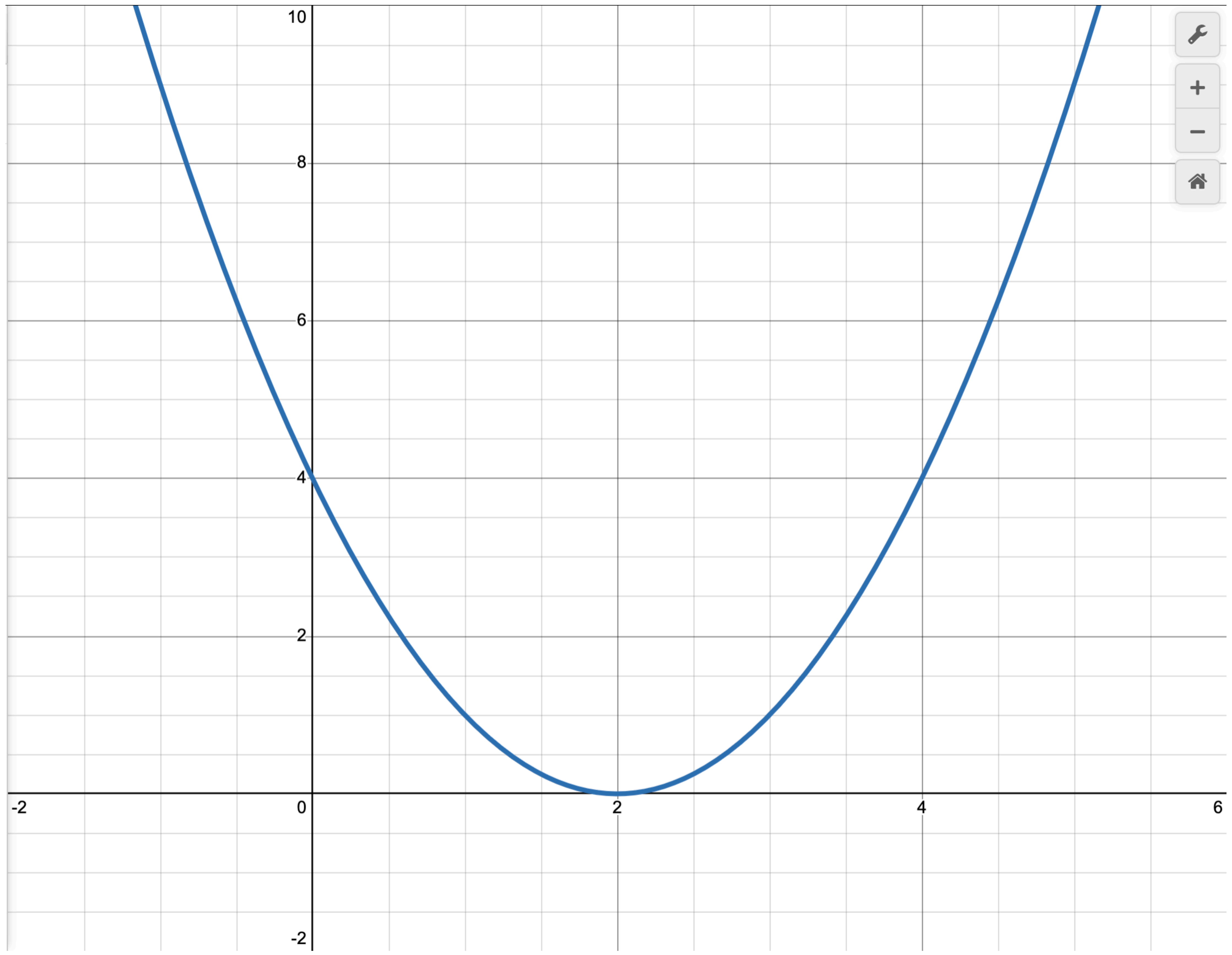

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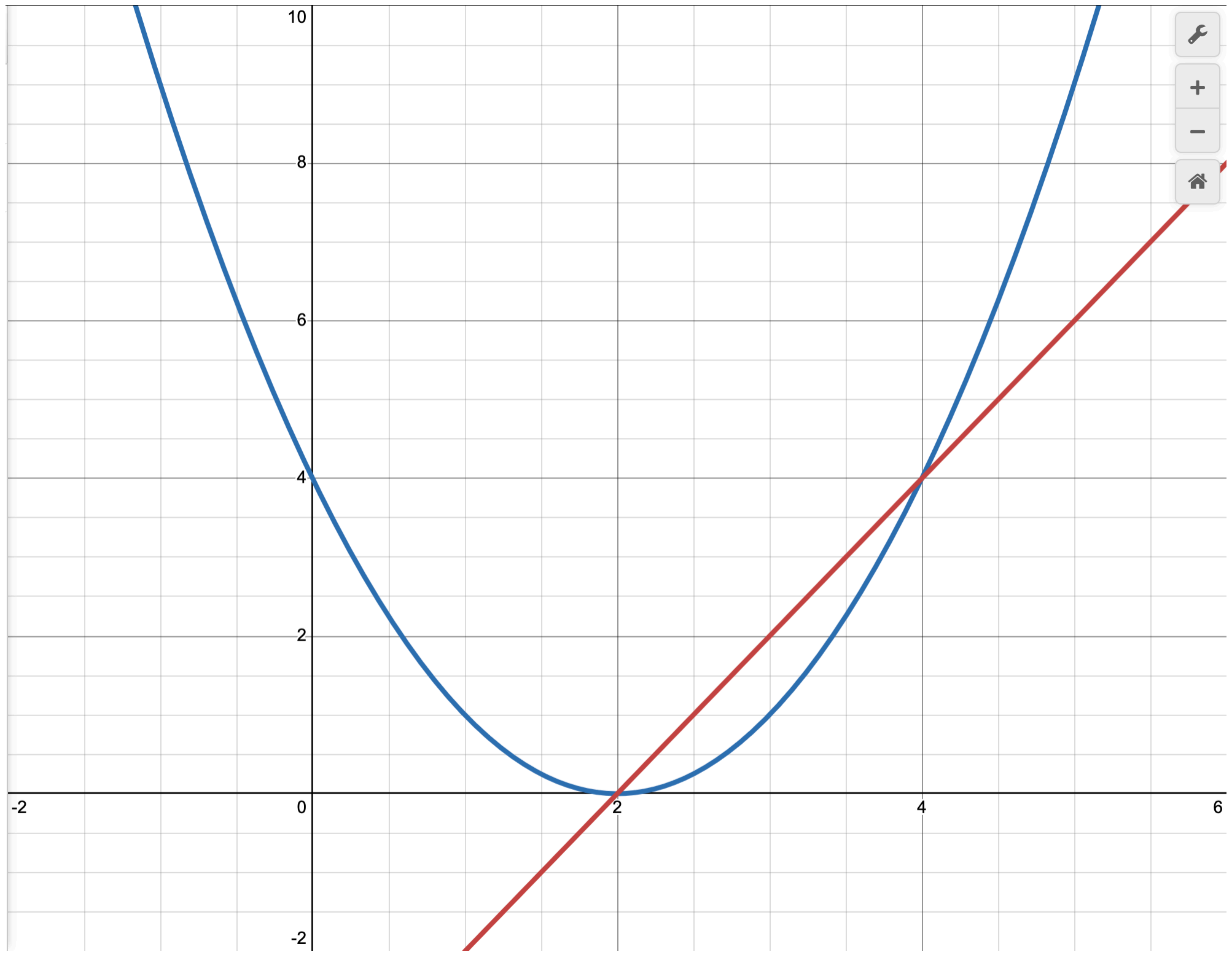

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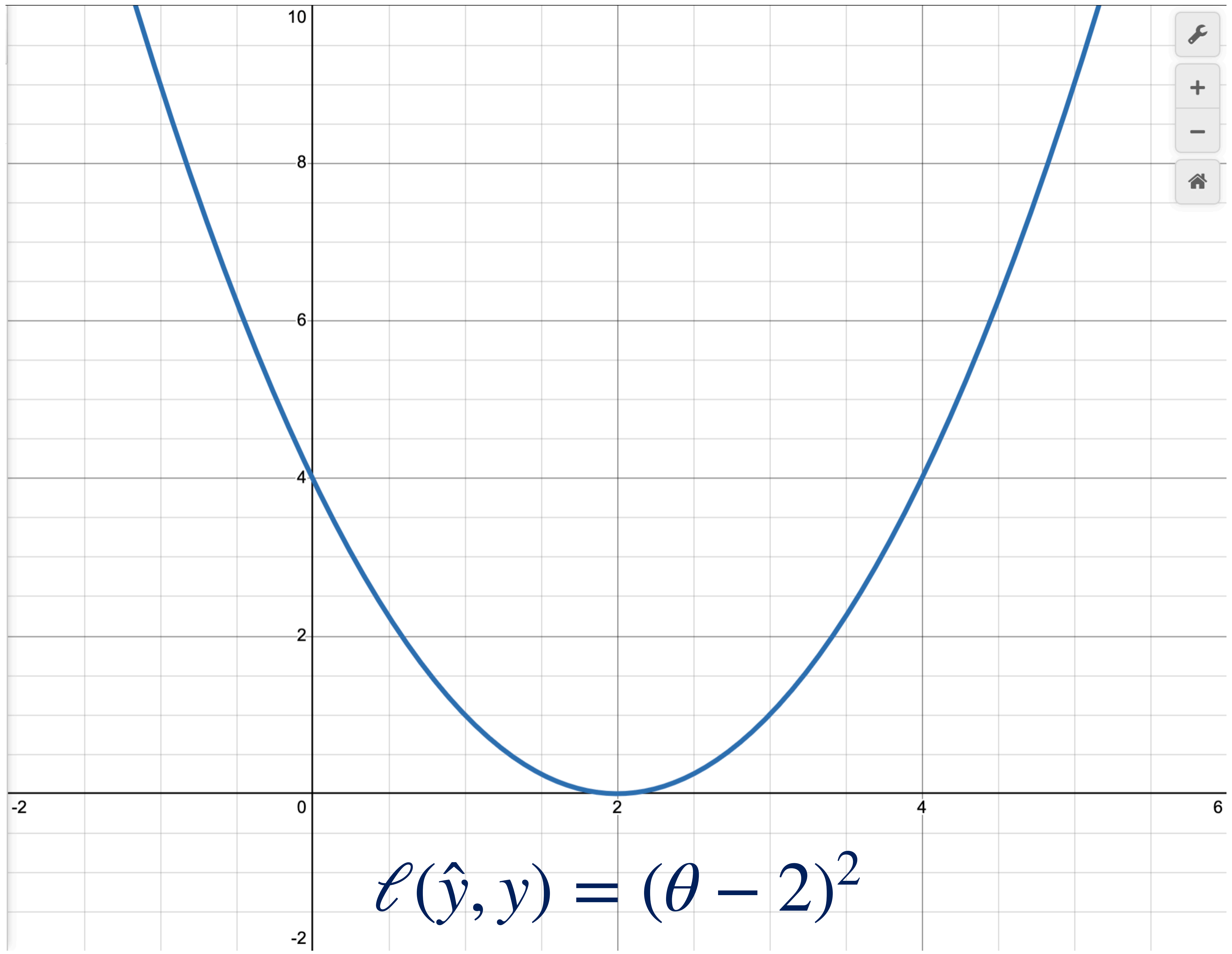

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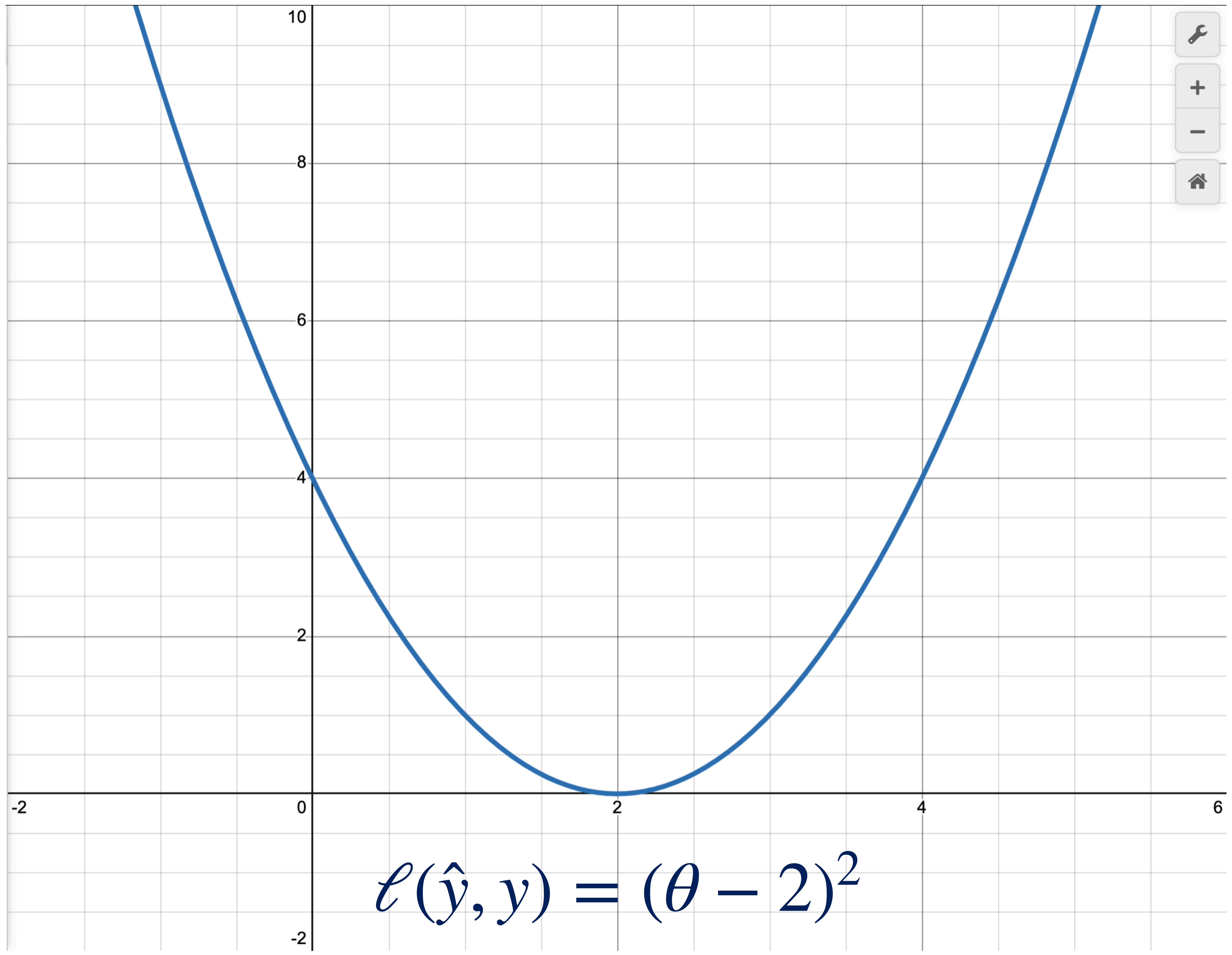

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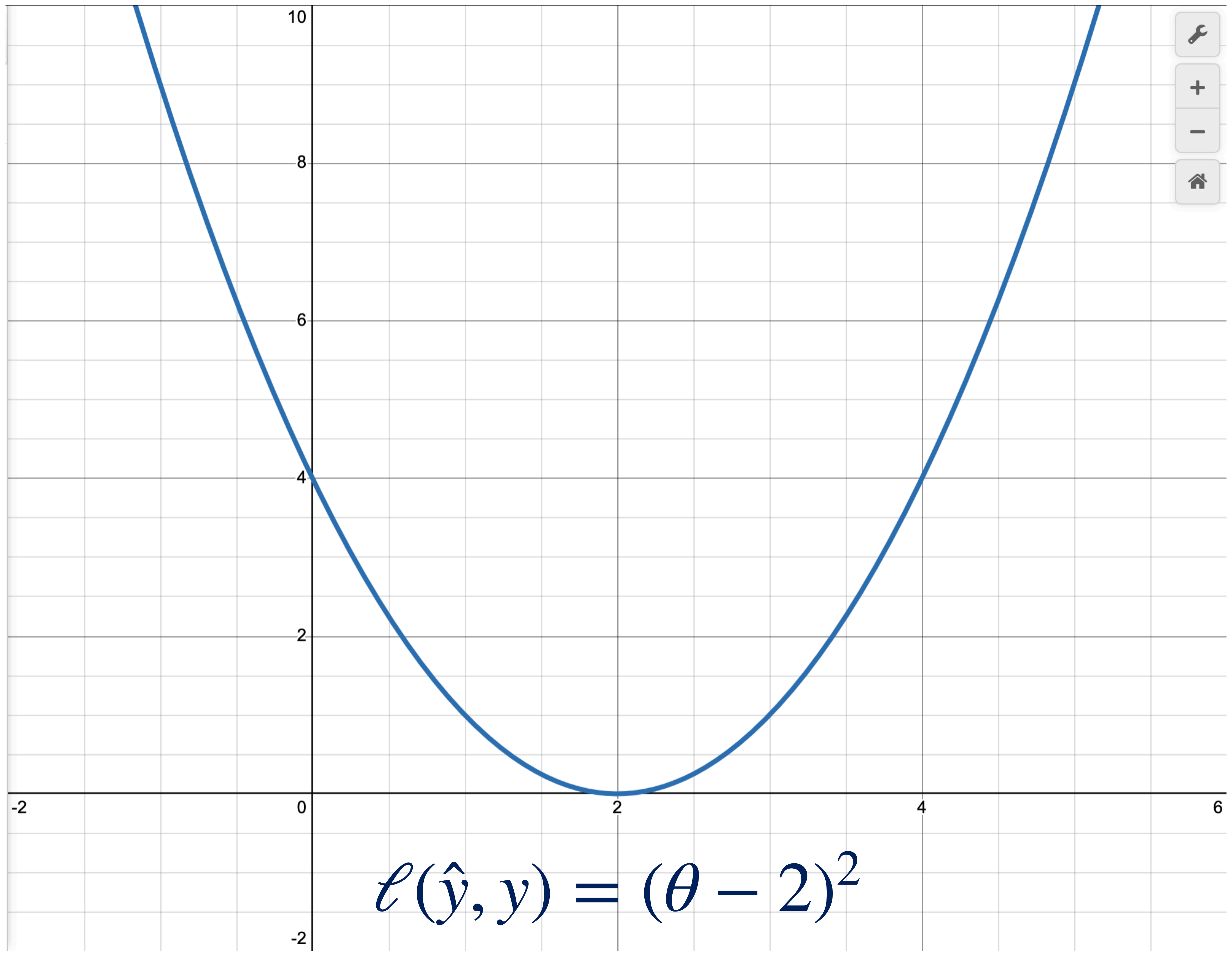

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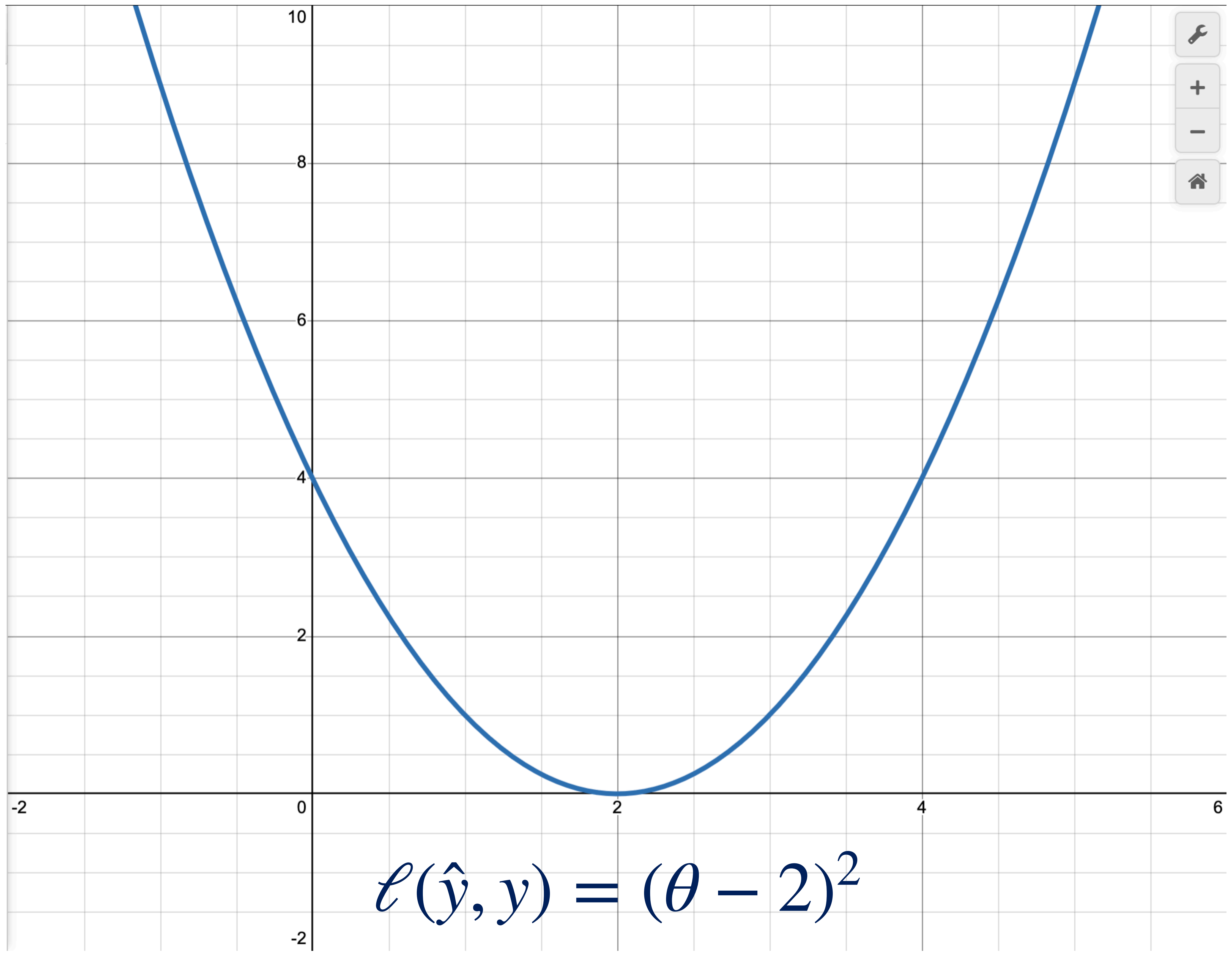
- For this example **ONLY**, solving for one datapoint solves the whole problem



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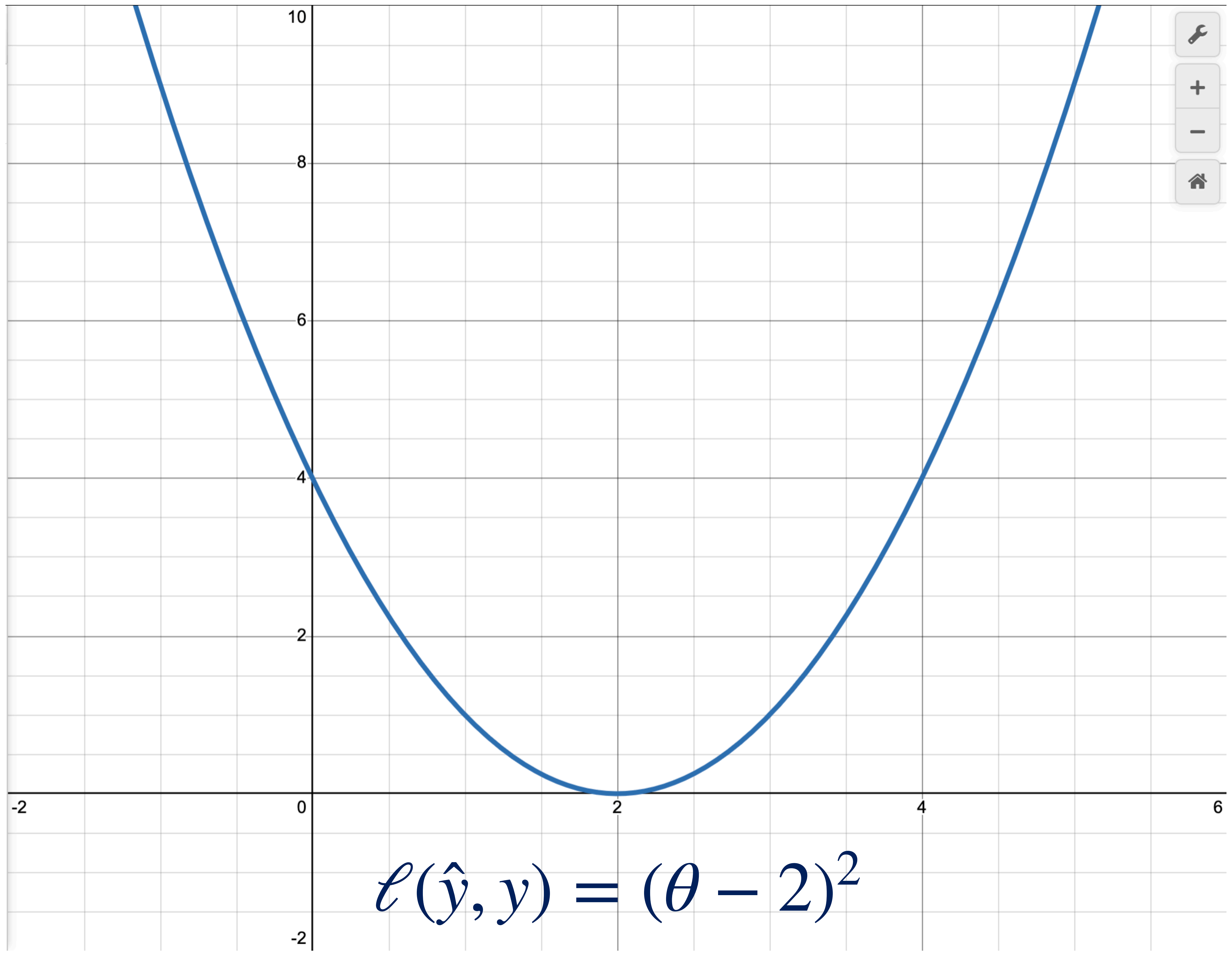

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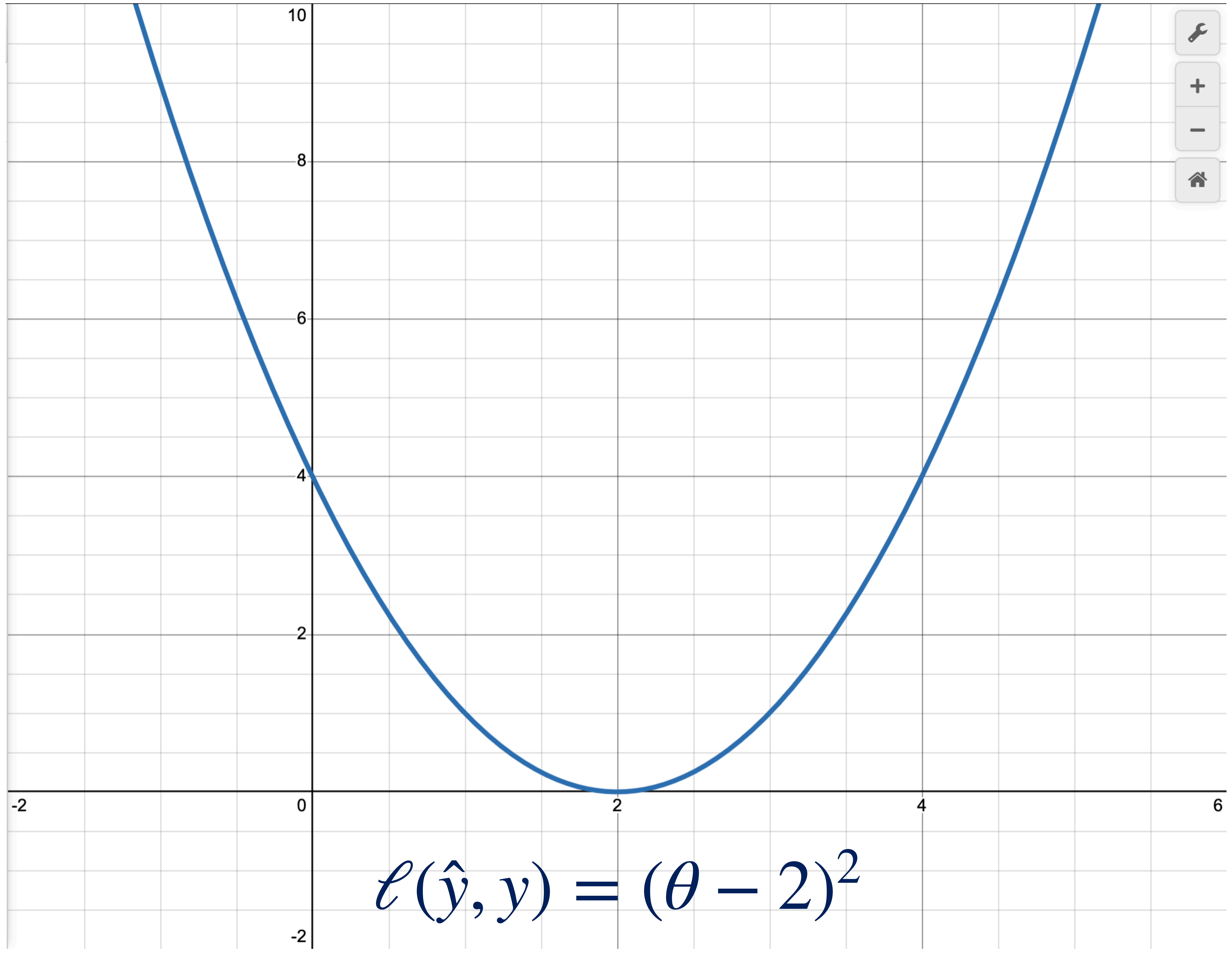

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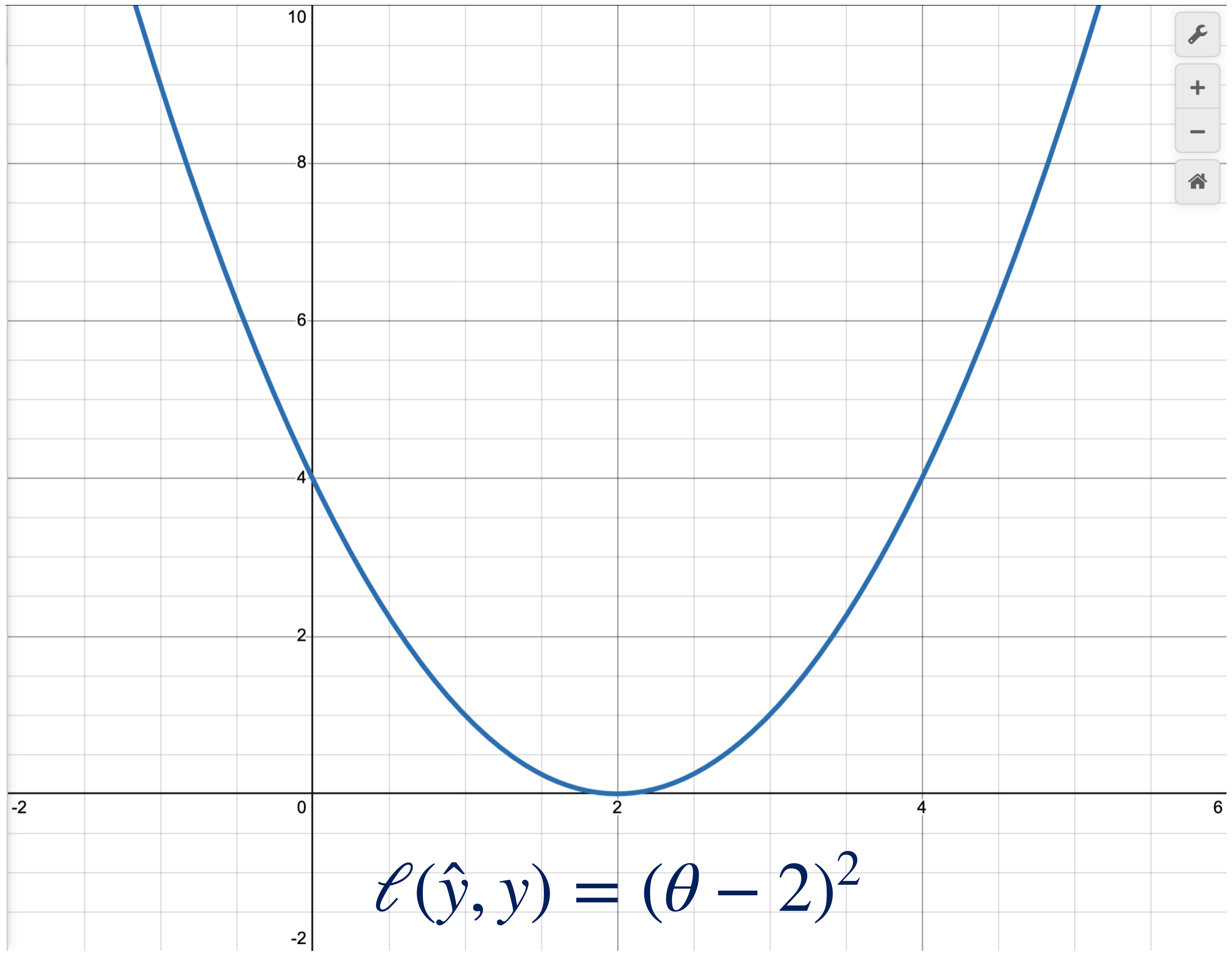

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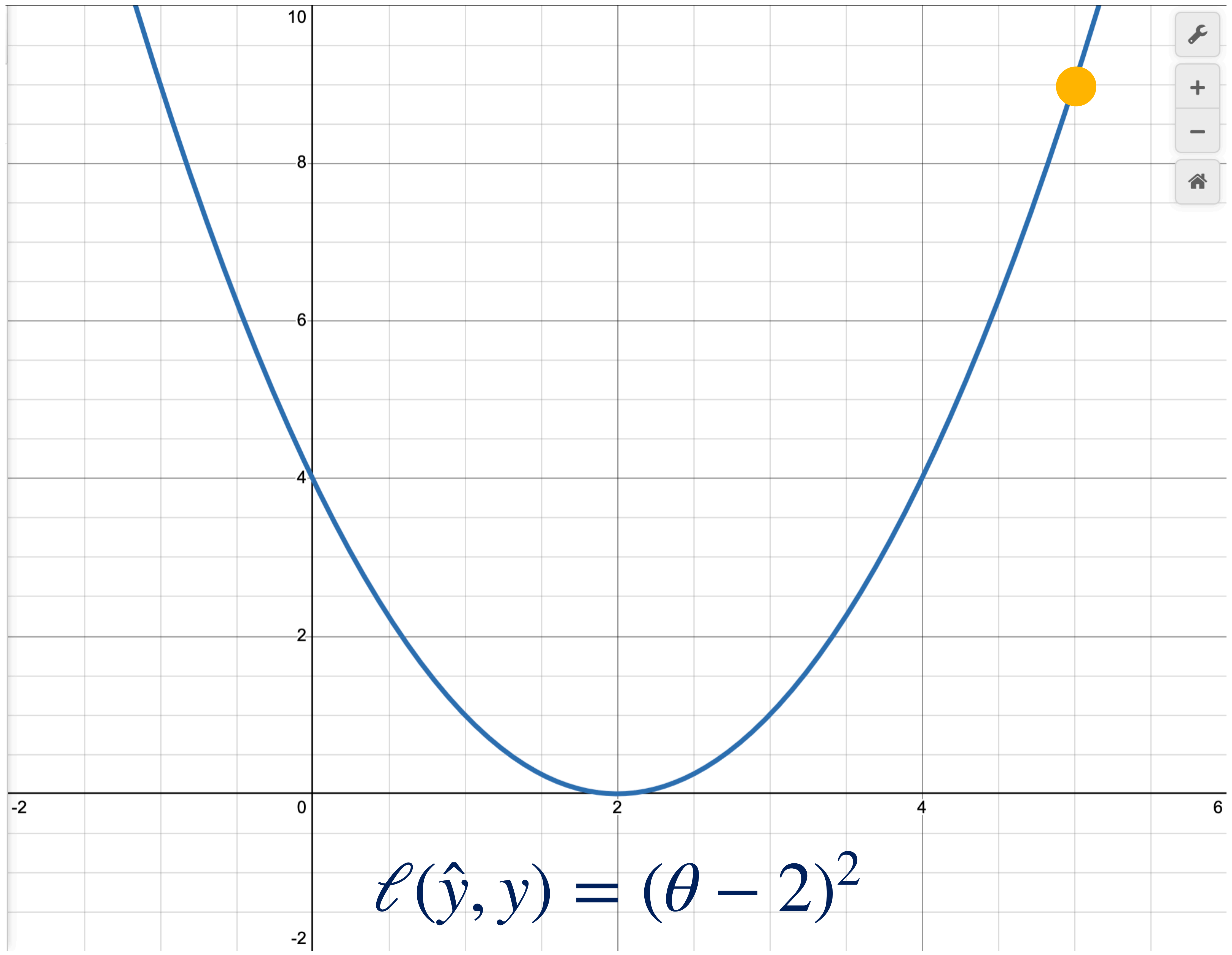

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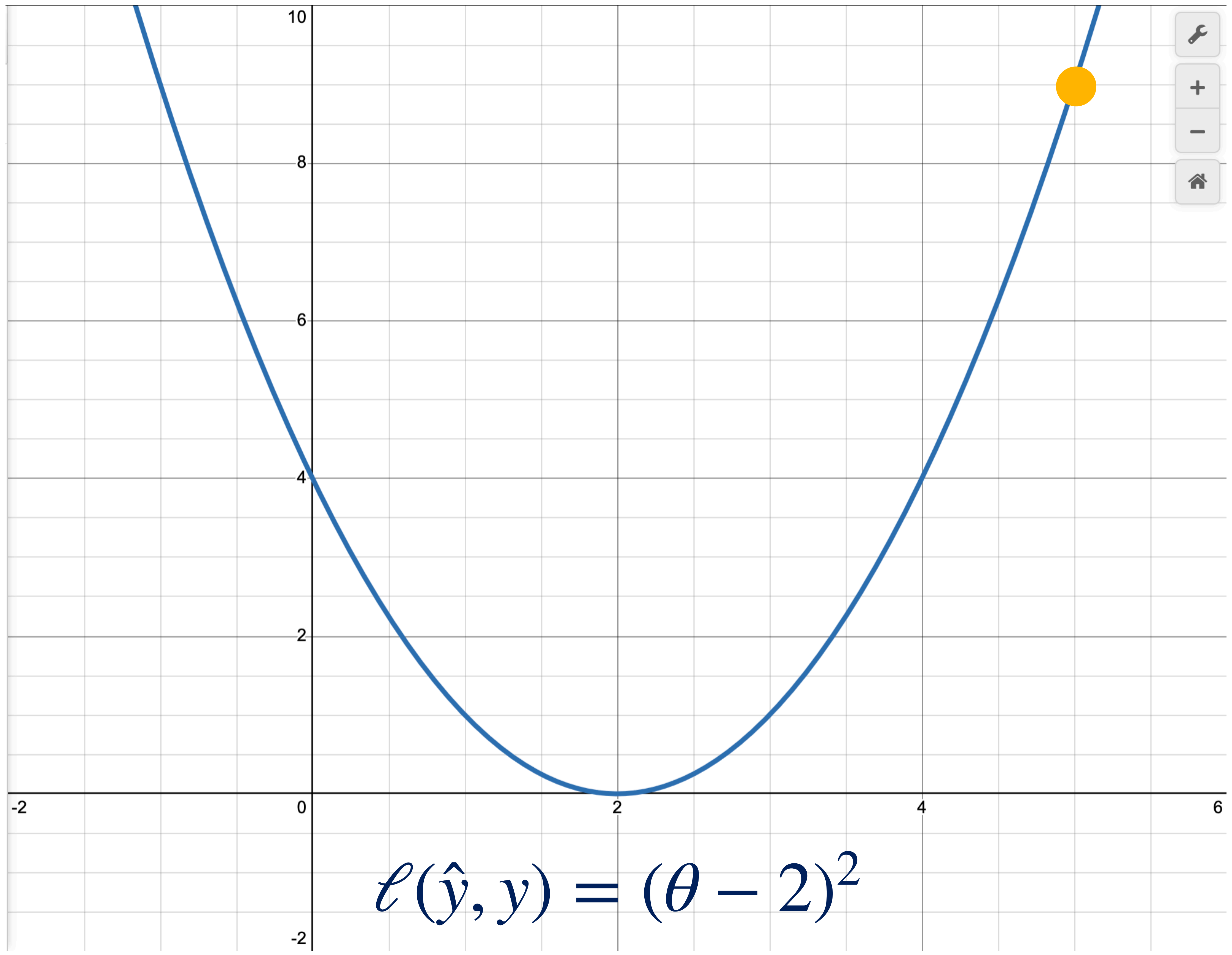

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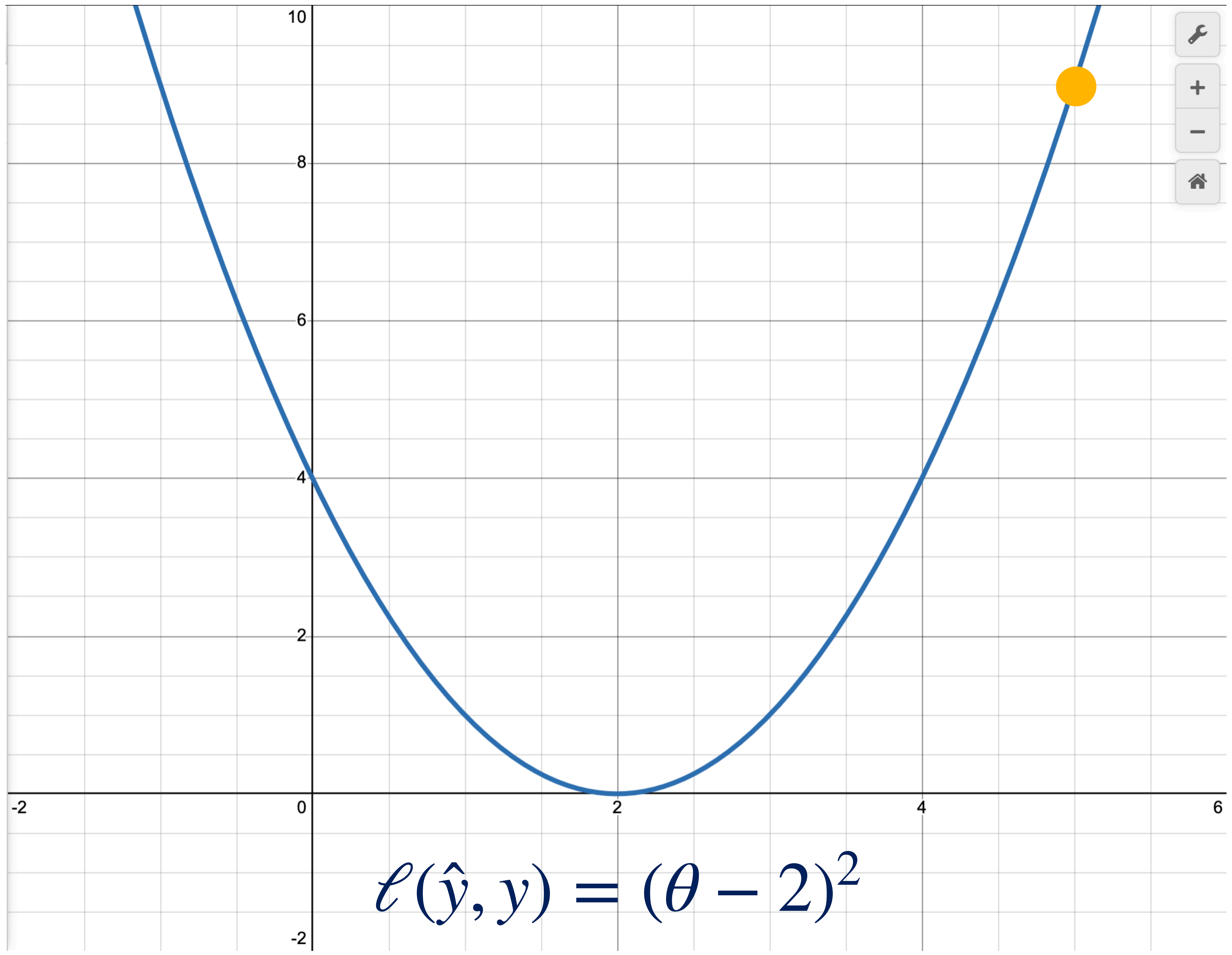

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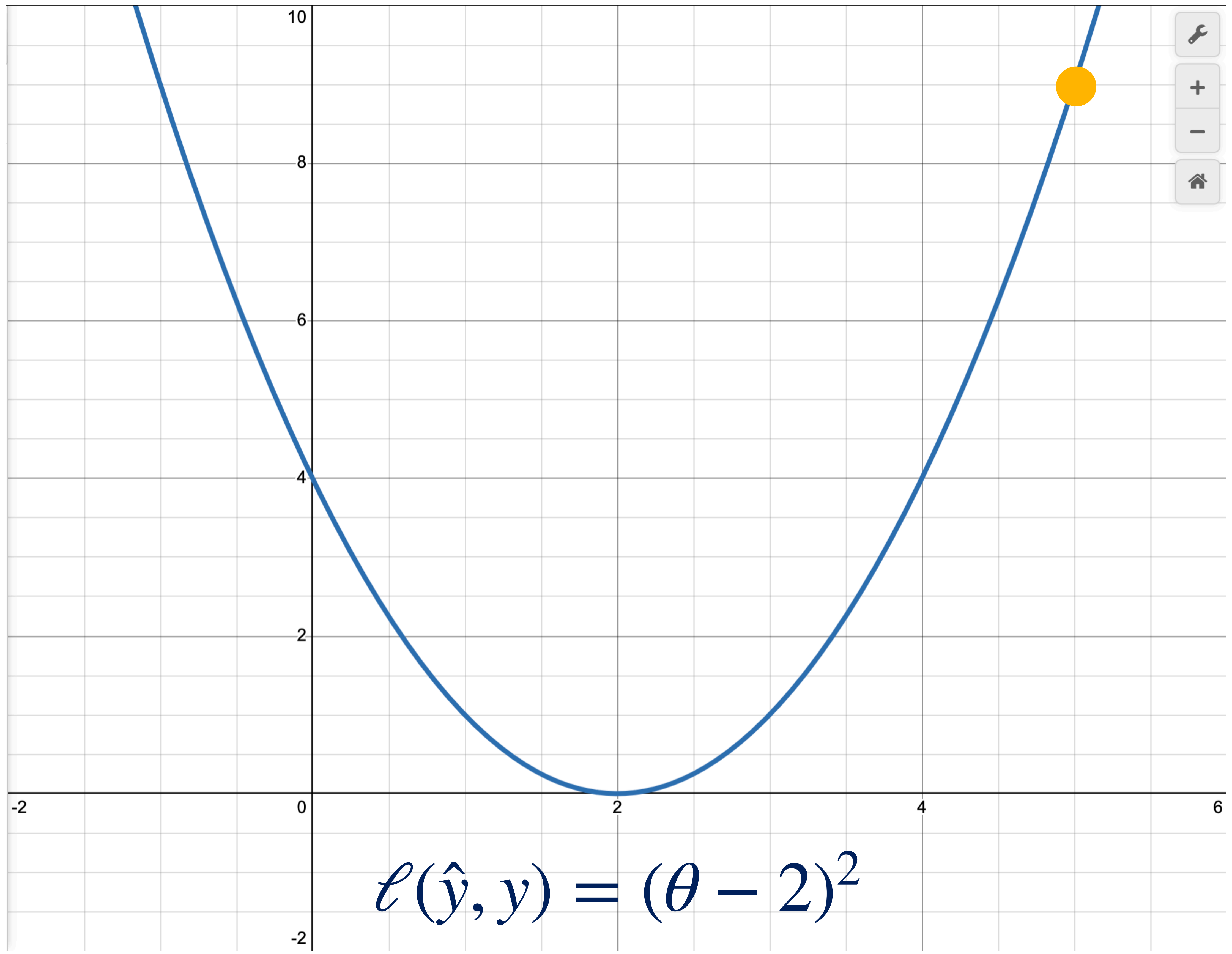

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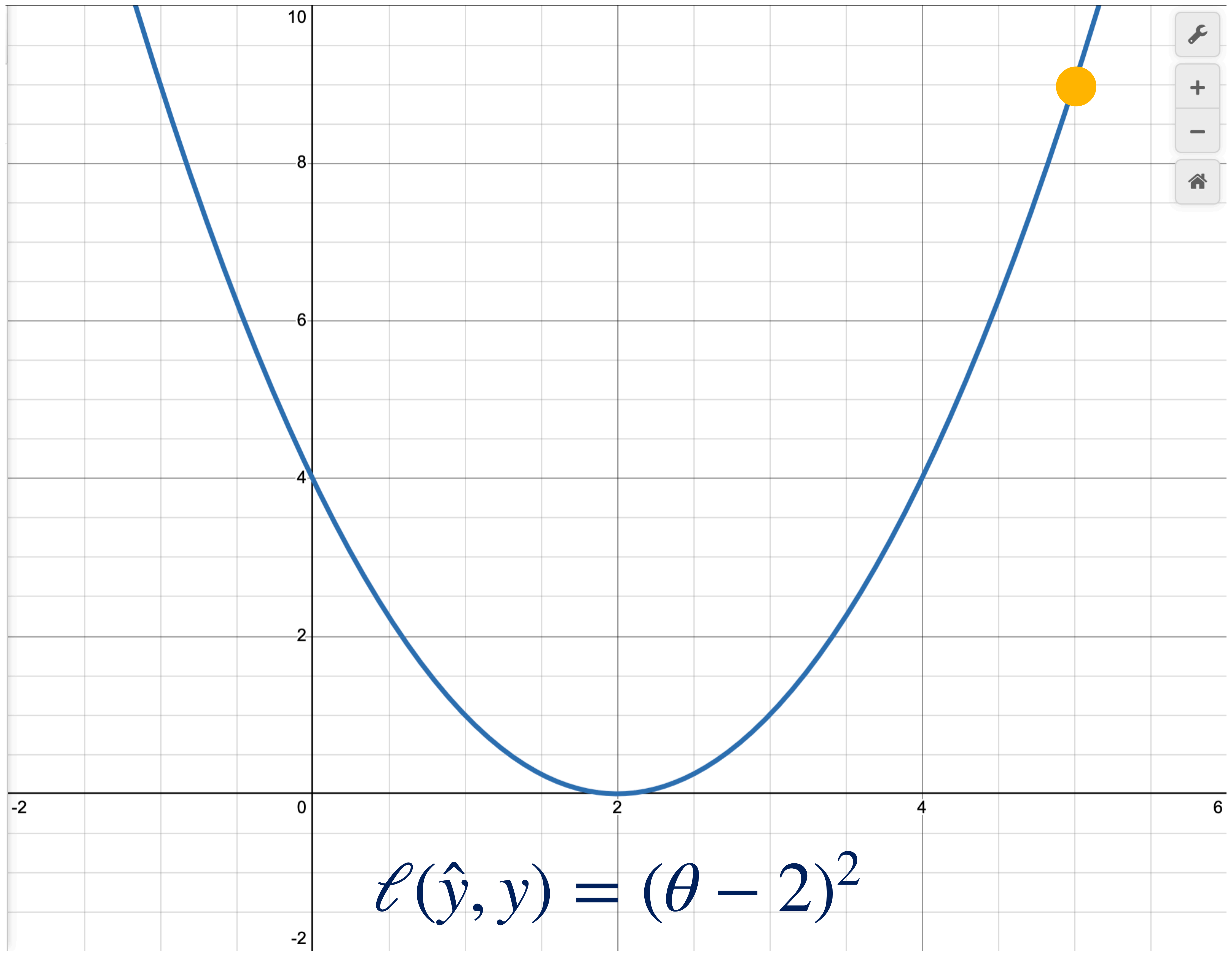

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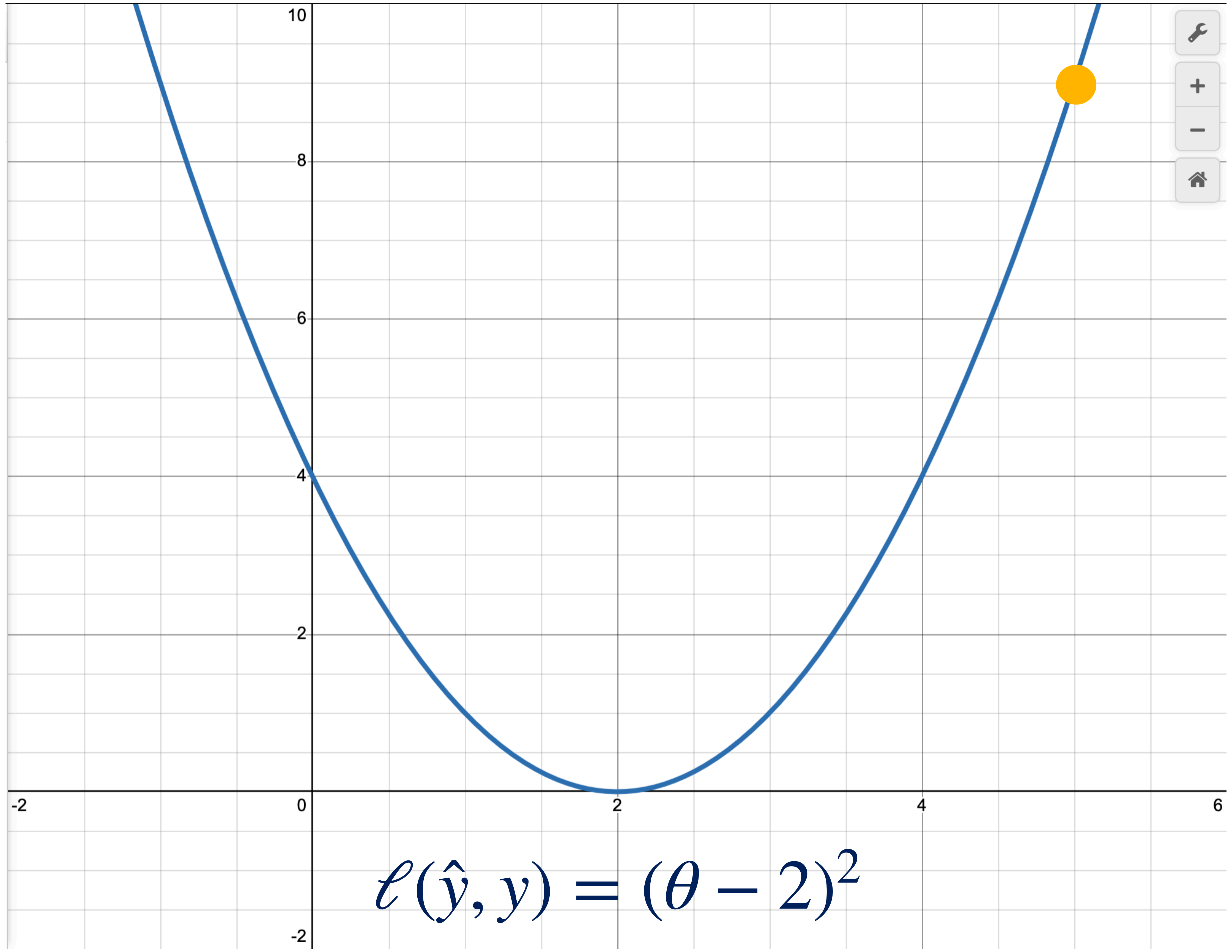
  - Adjust θ by the **negative of the slope** (because we want to **minimize** the function)
- First step:



$$\ell(\hat{y}, y) = (\theta - 2)^2$$

$$\ell'(\hat{y}, y) = 2\theta - 4$$

Gradient Descent (first try)

- At each step of the algorithm:
  - Calculate the **slope at the current point**
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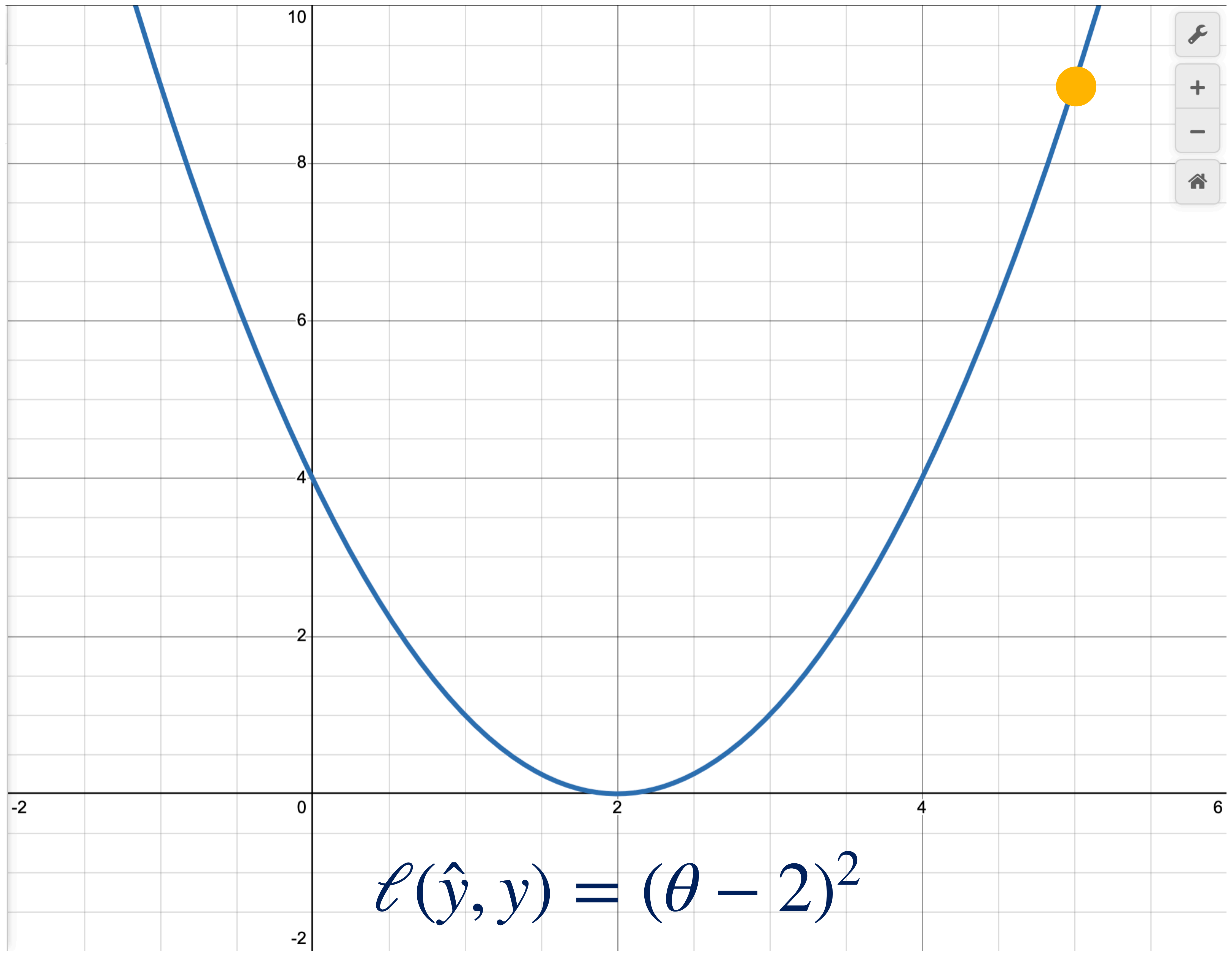
- First step:
  - Plug in θ to derivative:



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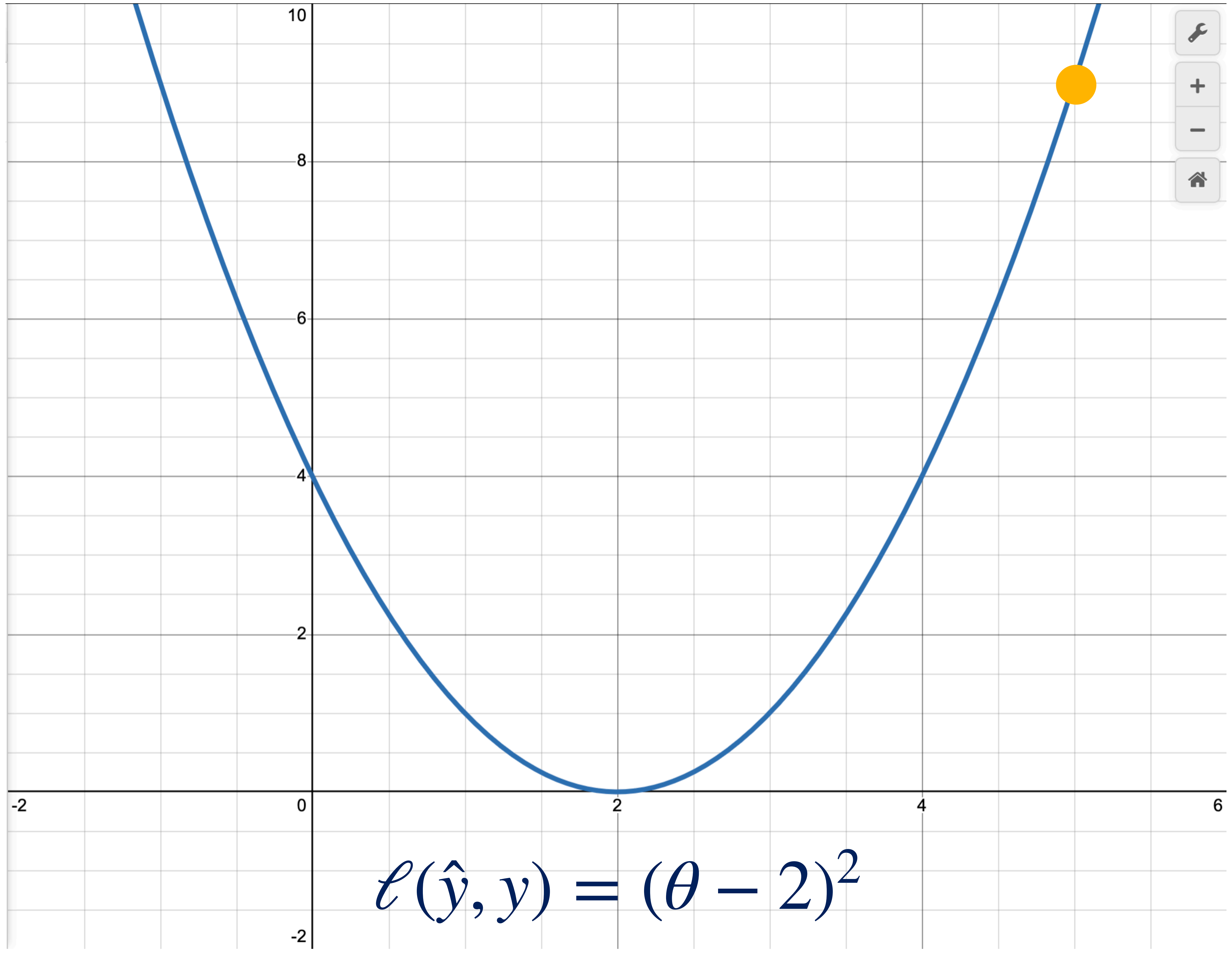

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- First step:
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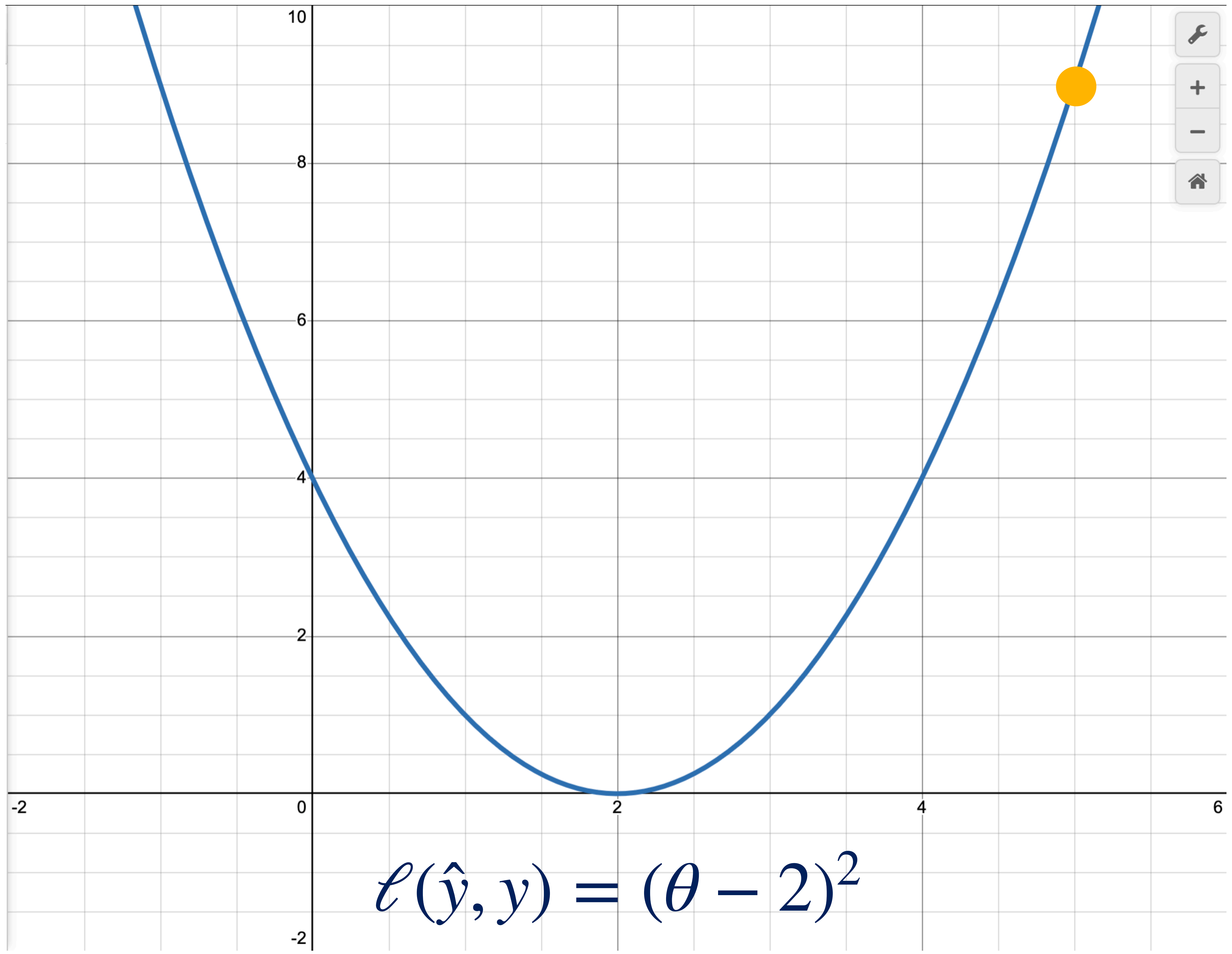
  - Update θ:



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- At each step of the algorithm:
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- First step:
  - Plug in θ to derivative:
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  - Update θ:
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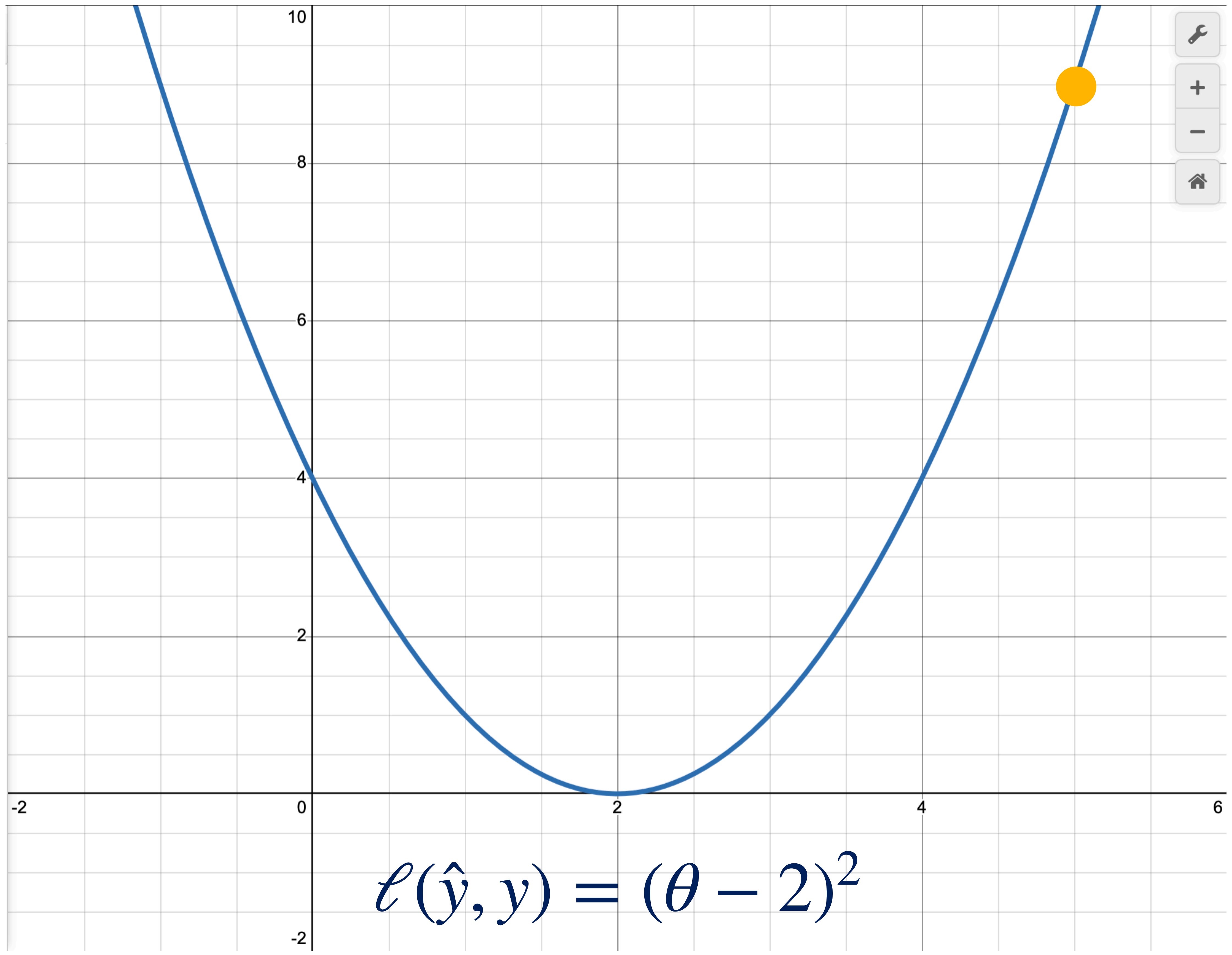

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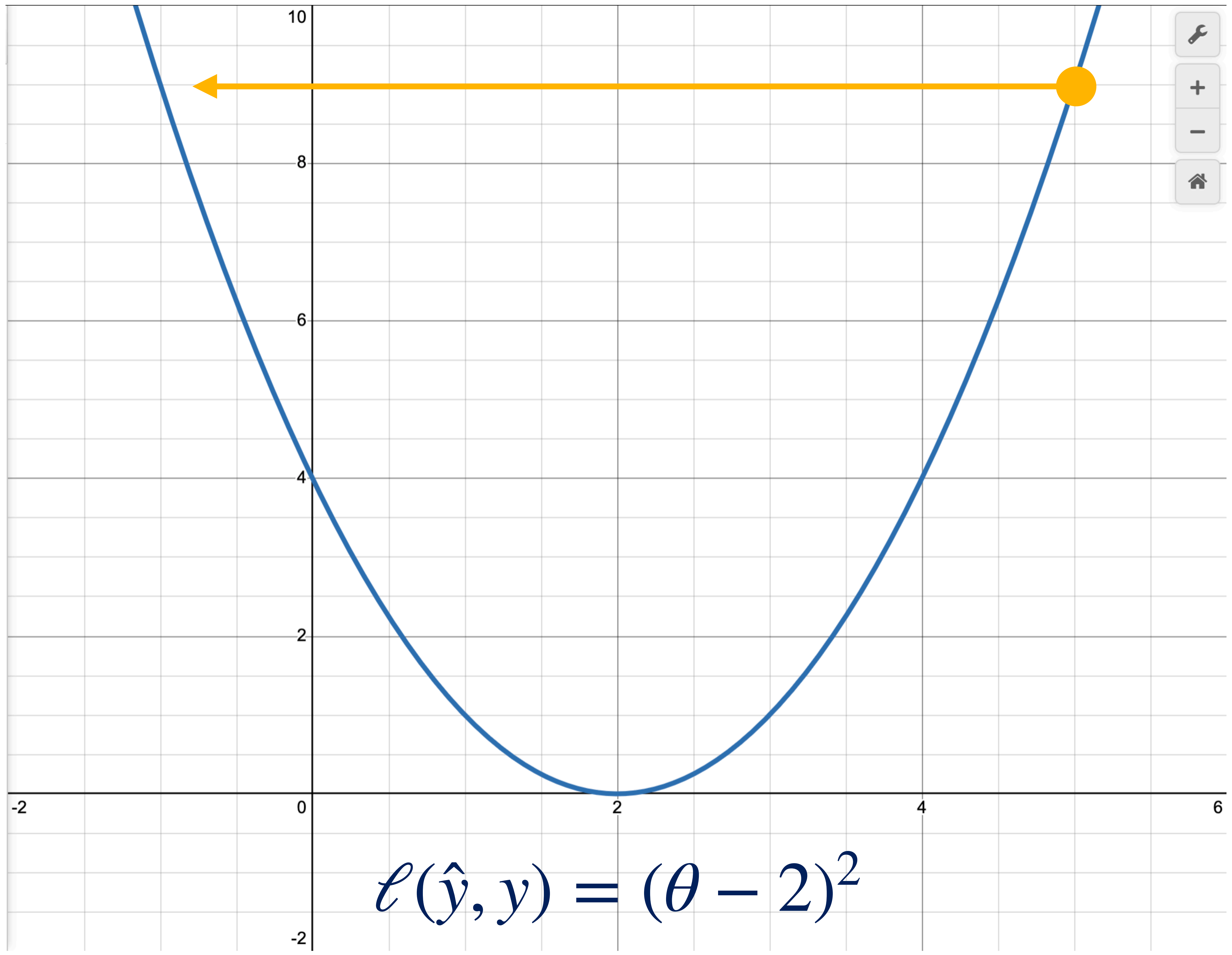

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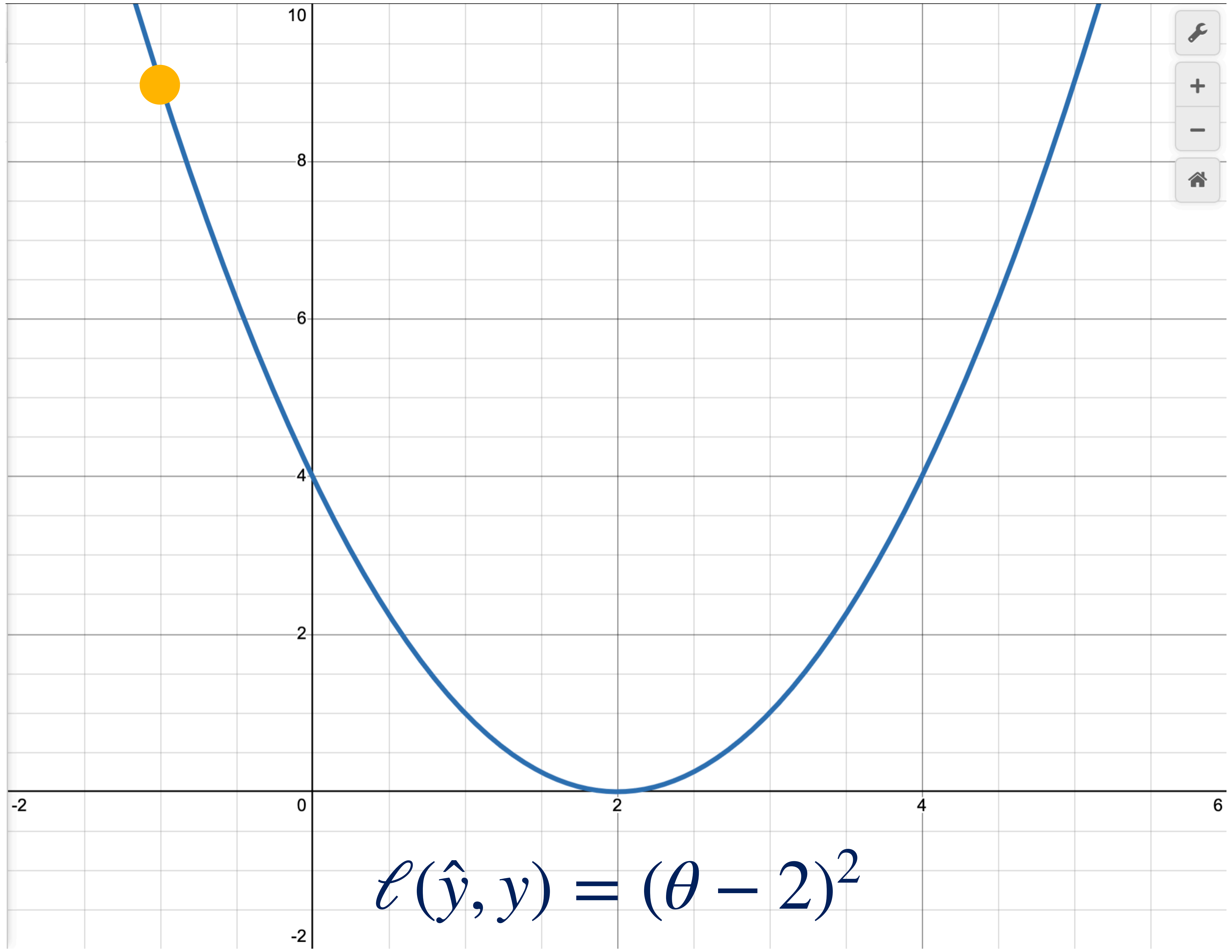

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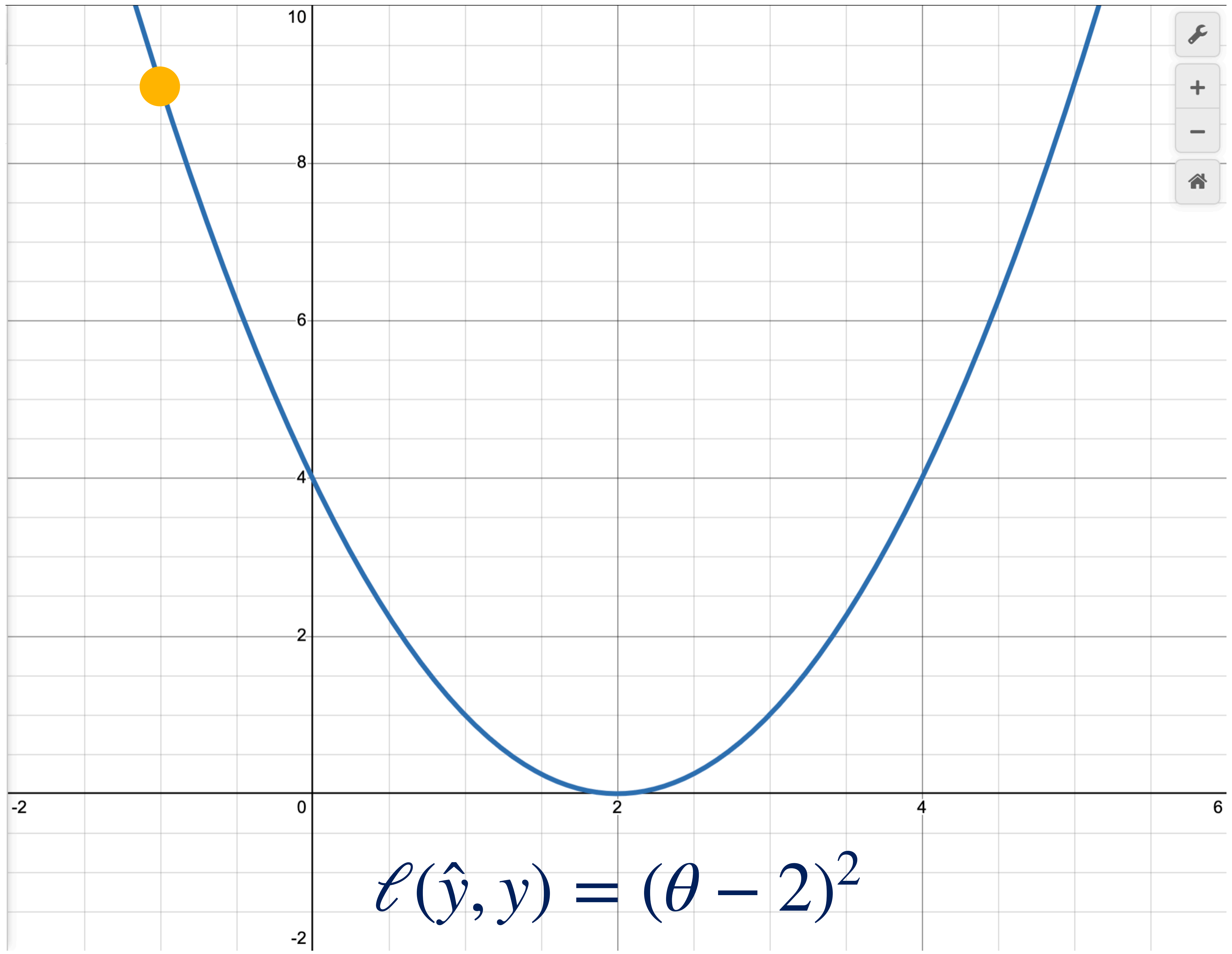
Gradient Descent (first try)

- Second step:



$$\ell(\hat{y}, y) = (\theta - 2)^2$$

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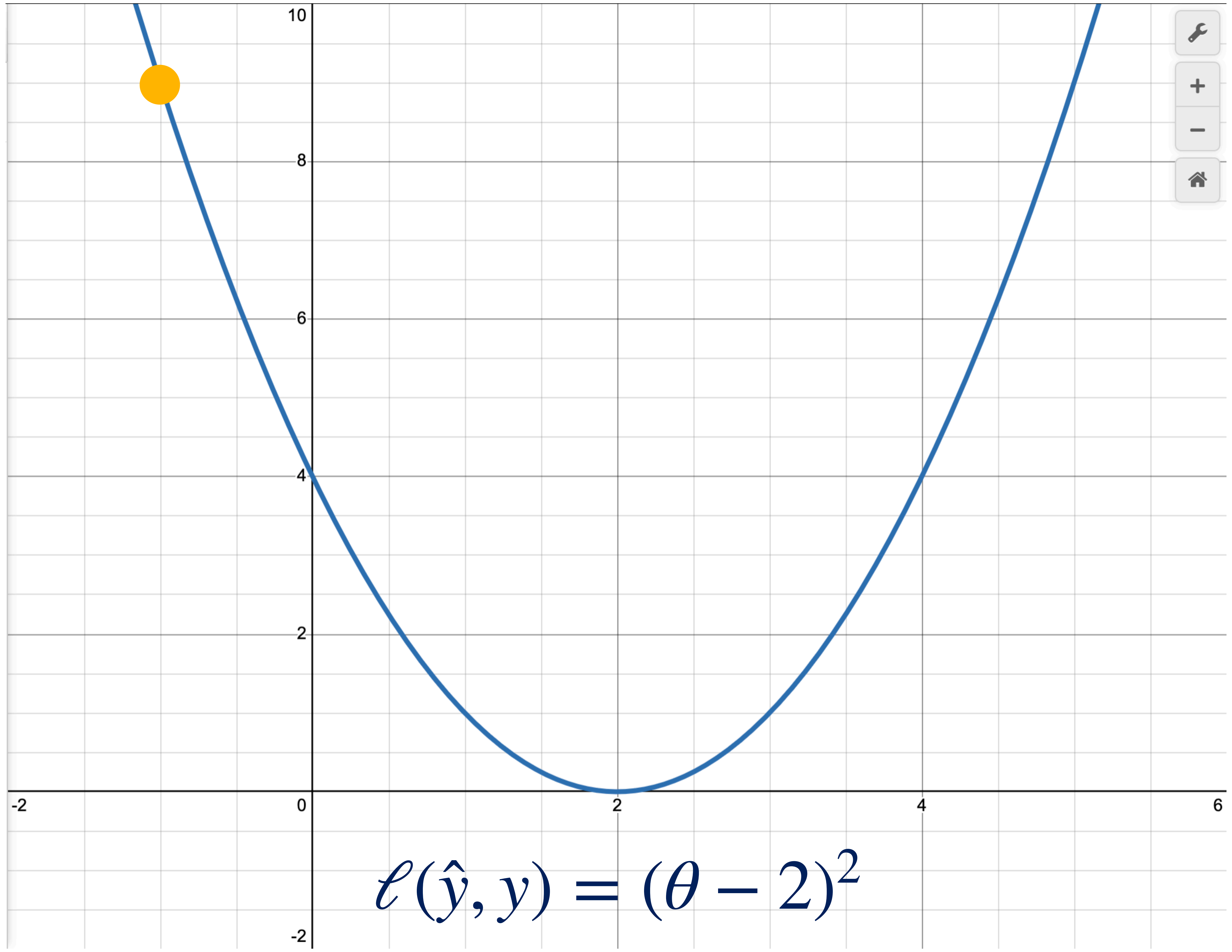
Gradient Descent (first try)

- Second step:
  - Plug in new θ_1:



$$\ell(\hat{y}, y) = (\theta - 2)^2$$

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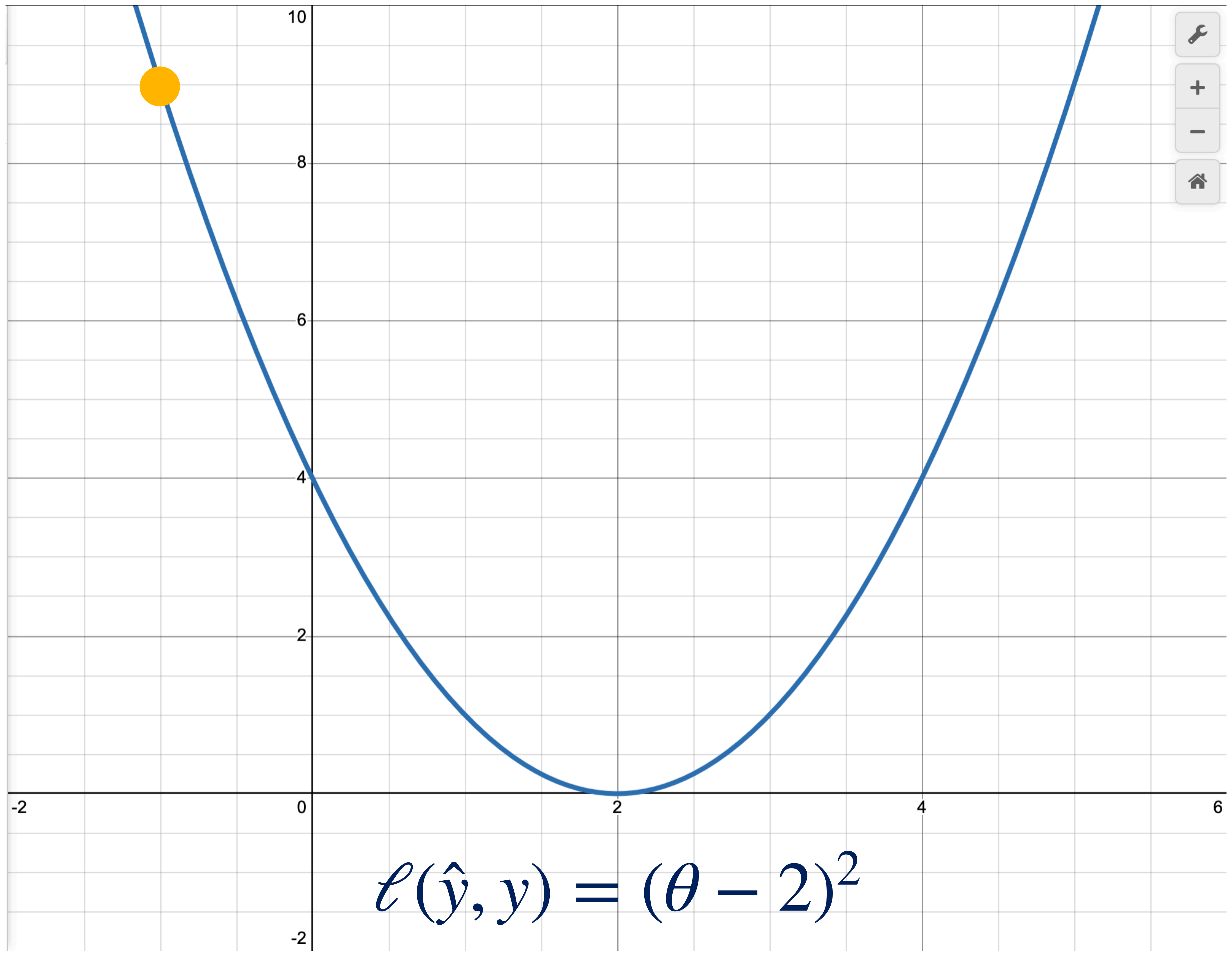
Gradient Descent (first try)

- Second step:
  - Plug in new θ_1:
    - $2 \cdot (-1) - 4 = -6$



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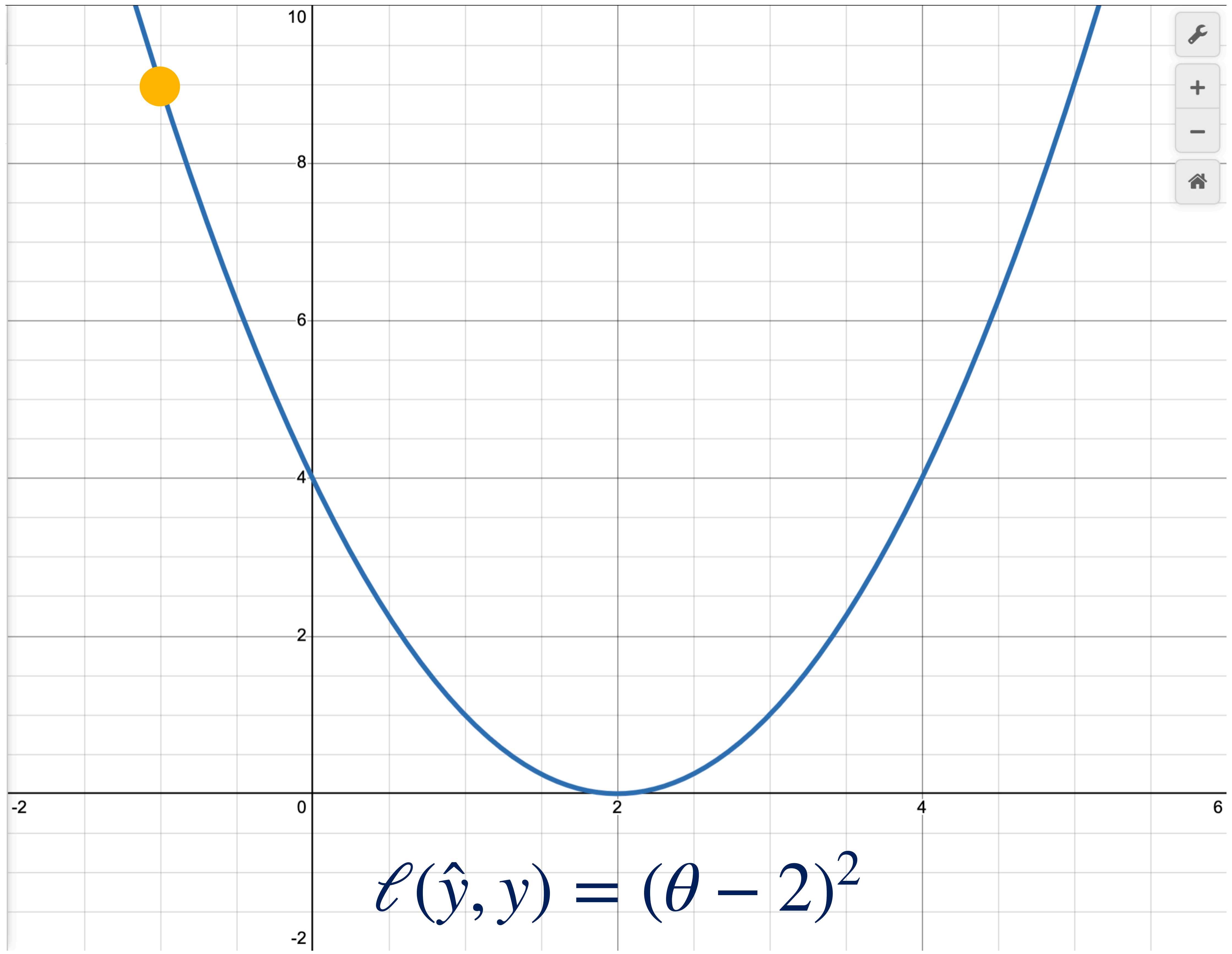

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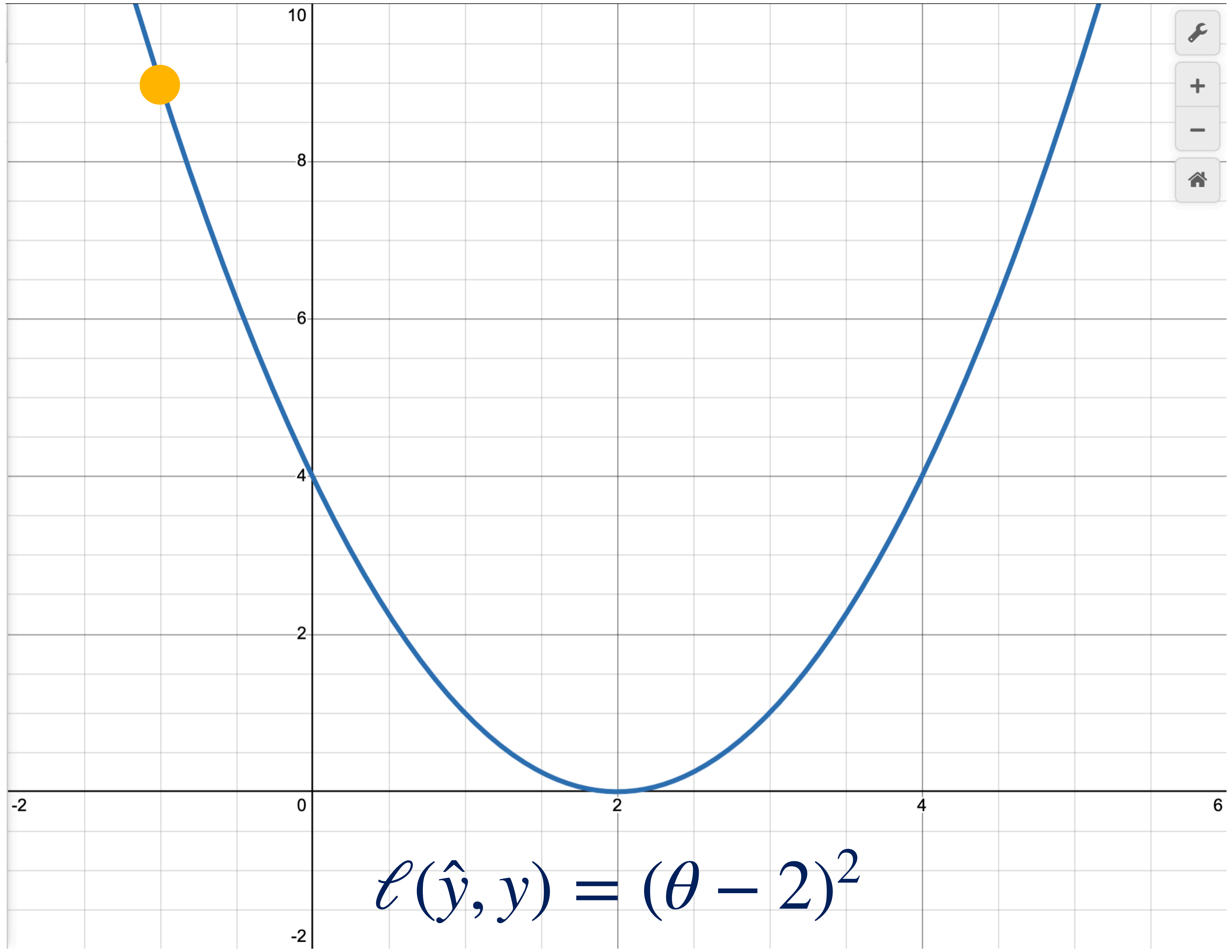
Gradient Descent (first try)

- Second step:
  - Plug in new θ_1:
    - $2 \cdot (-1) - 4 = -6$
  - Update θ:
    - $\theta_2 = \theta_1 - (-6) = 5$



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- Second step:
  - Plug in new θ_1:
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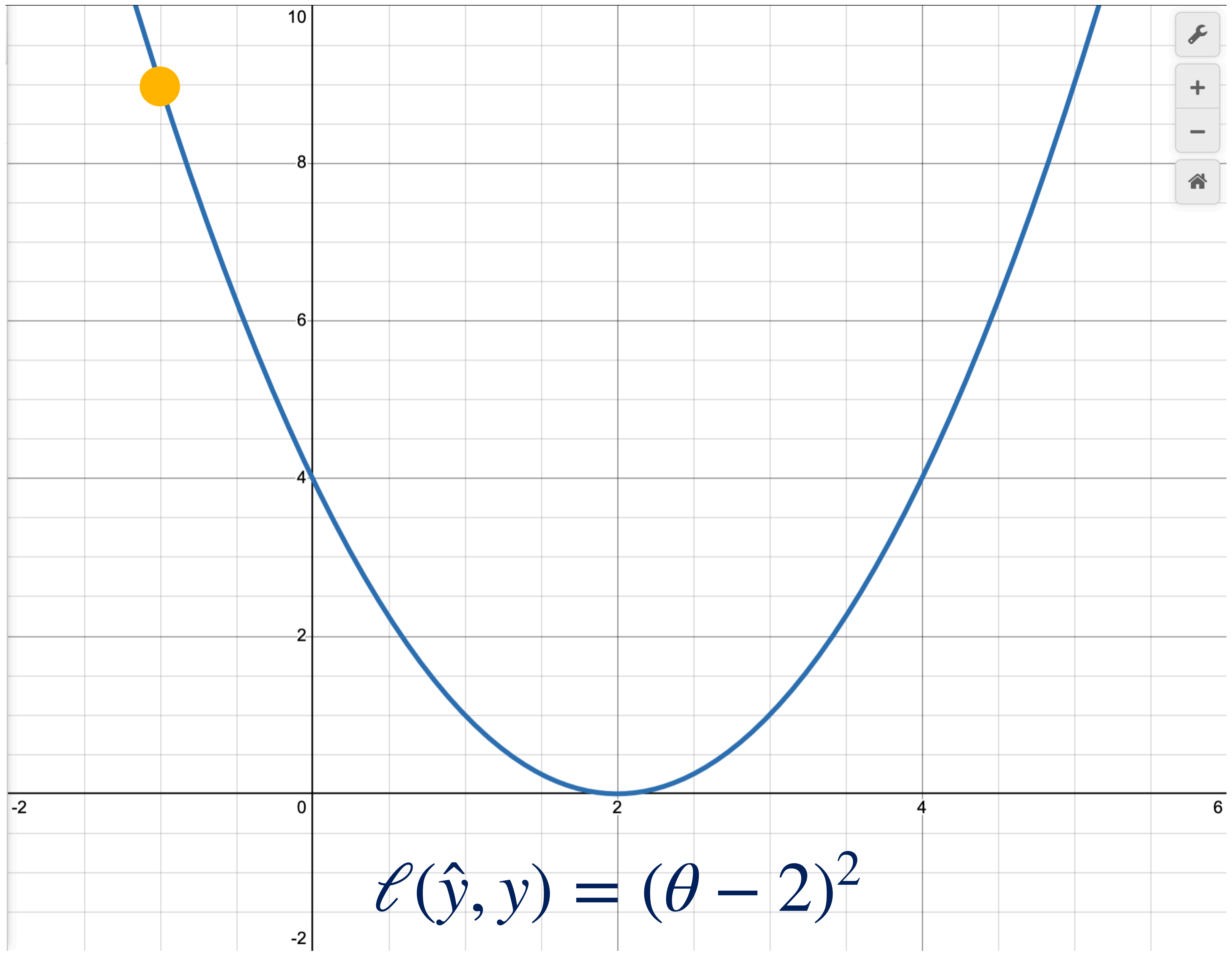
- Whoops! We're **back where we started!**



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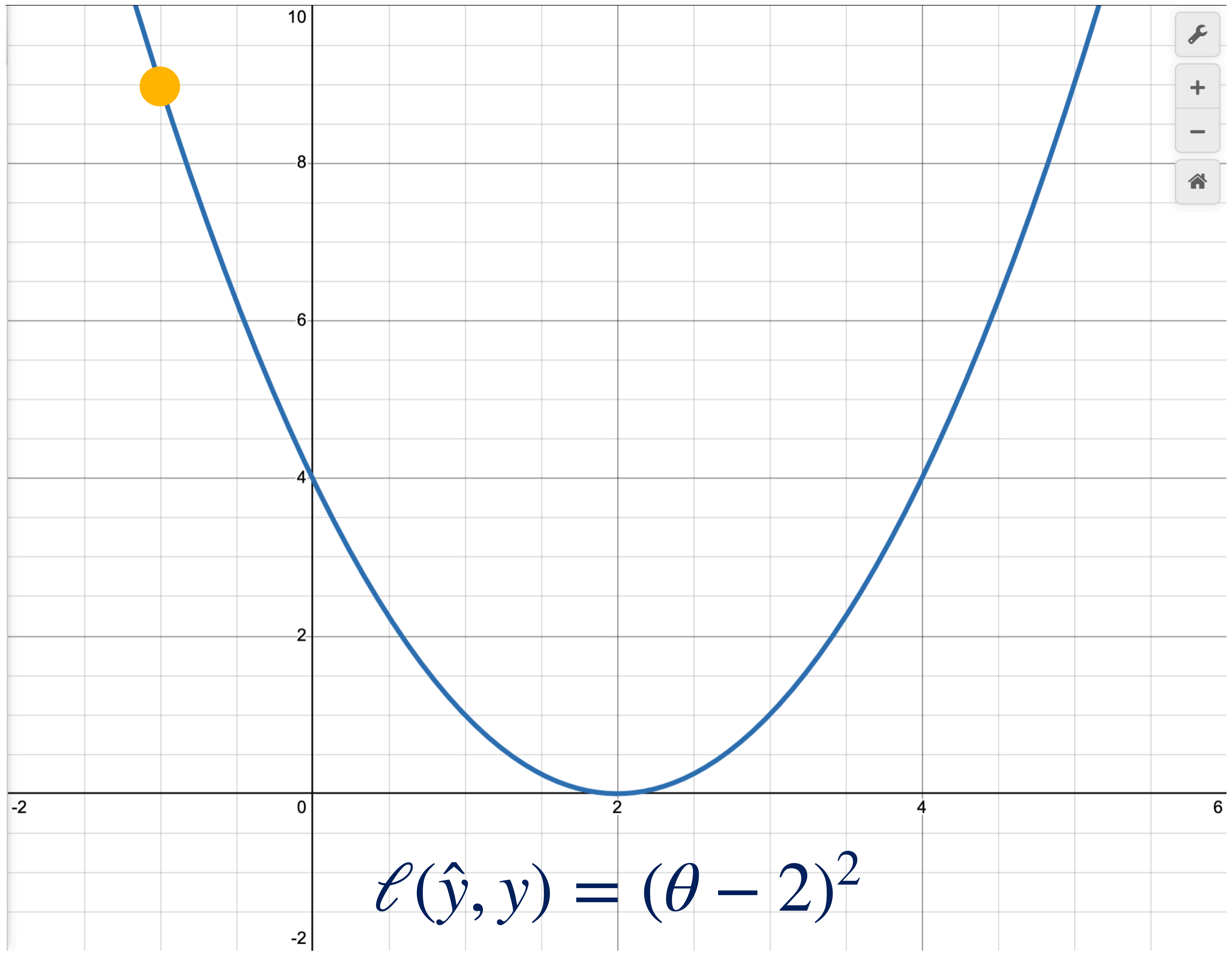
  - This process would **"bounce back and forth"** forever!



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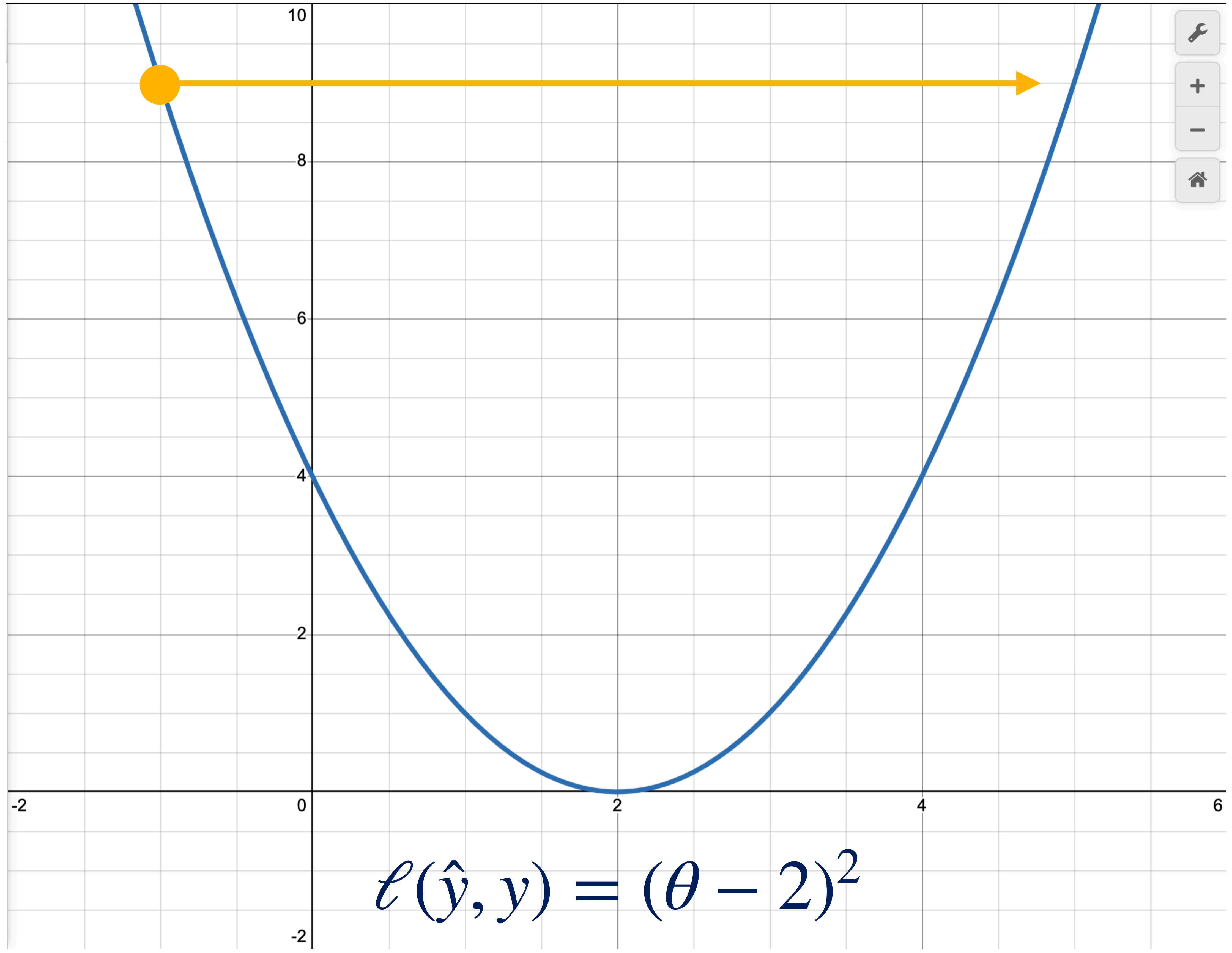

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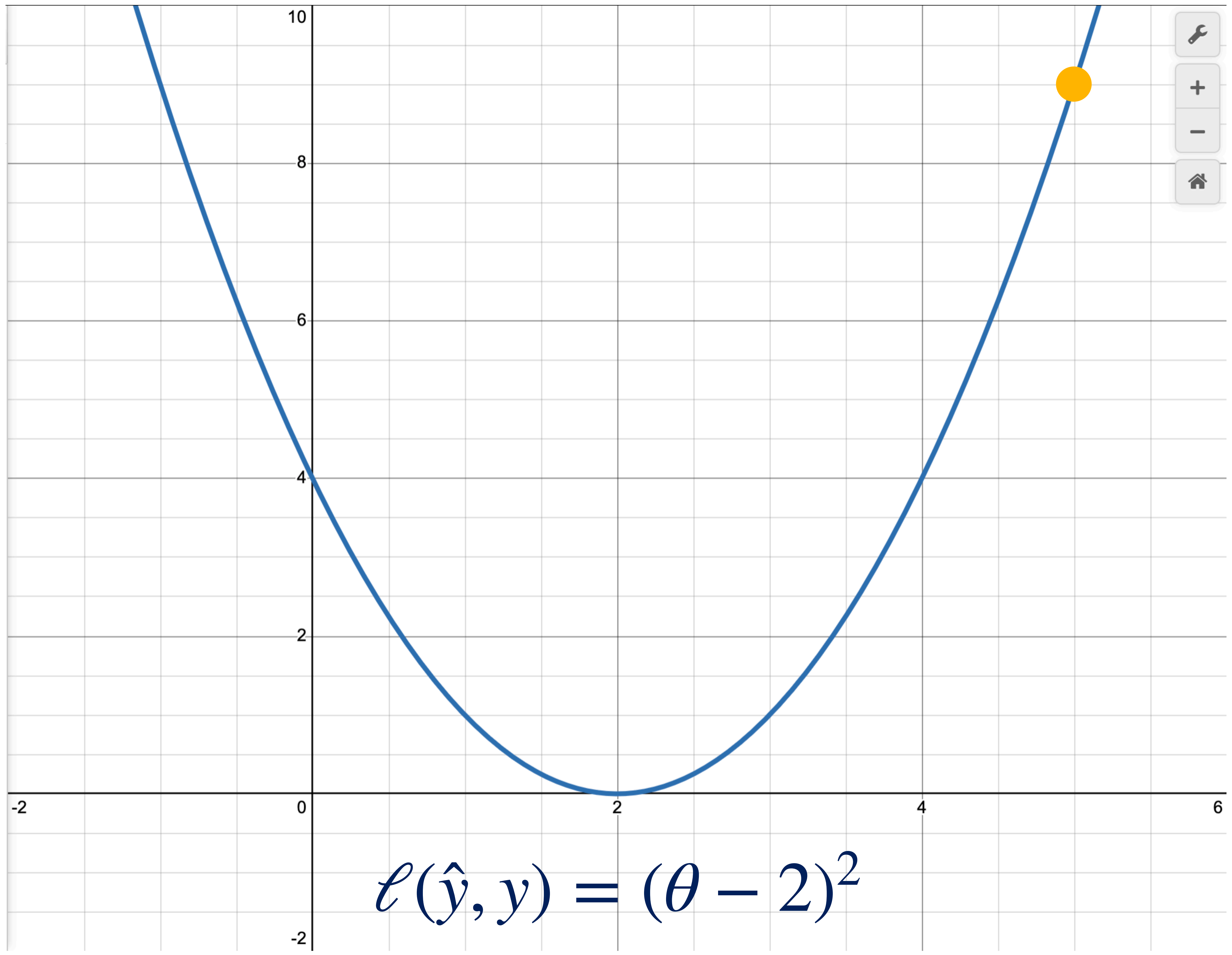
Gradient Descent (second try)



$$\ell(\hat{y}, y) = (\theta - 2)^2$$

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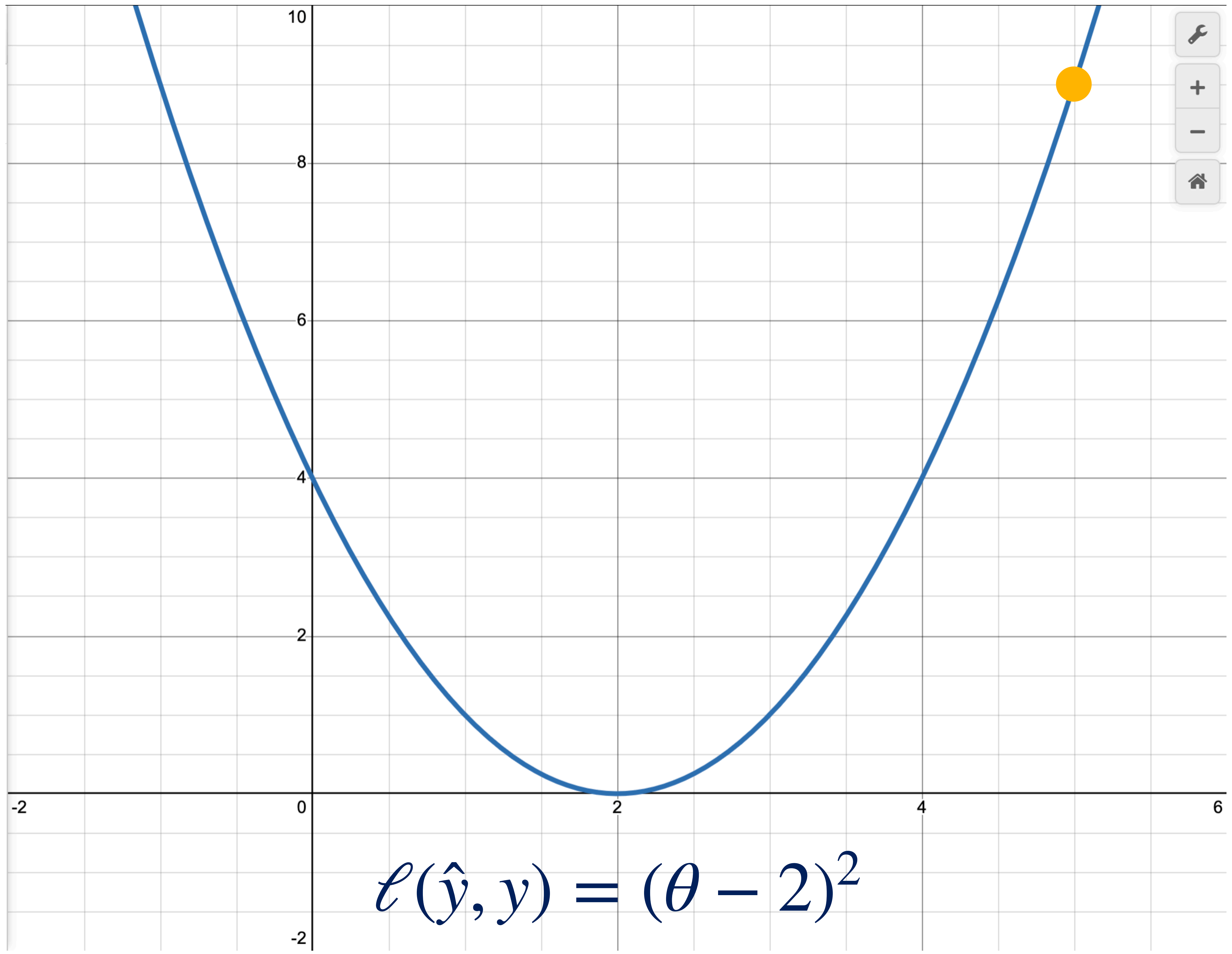
Gradient Descent (second try)

- What if we adjusted θ by a **fraction** of the slope? (Say, 0.75)



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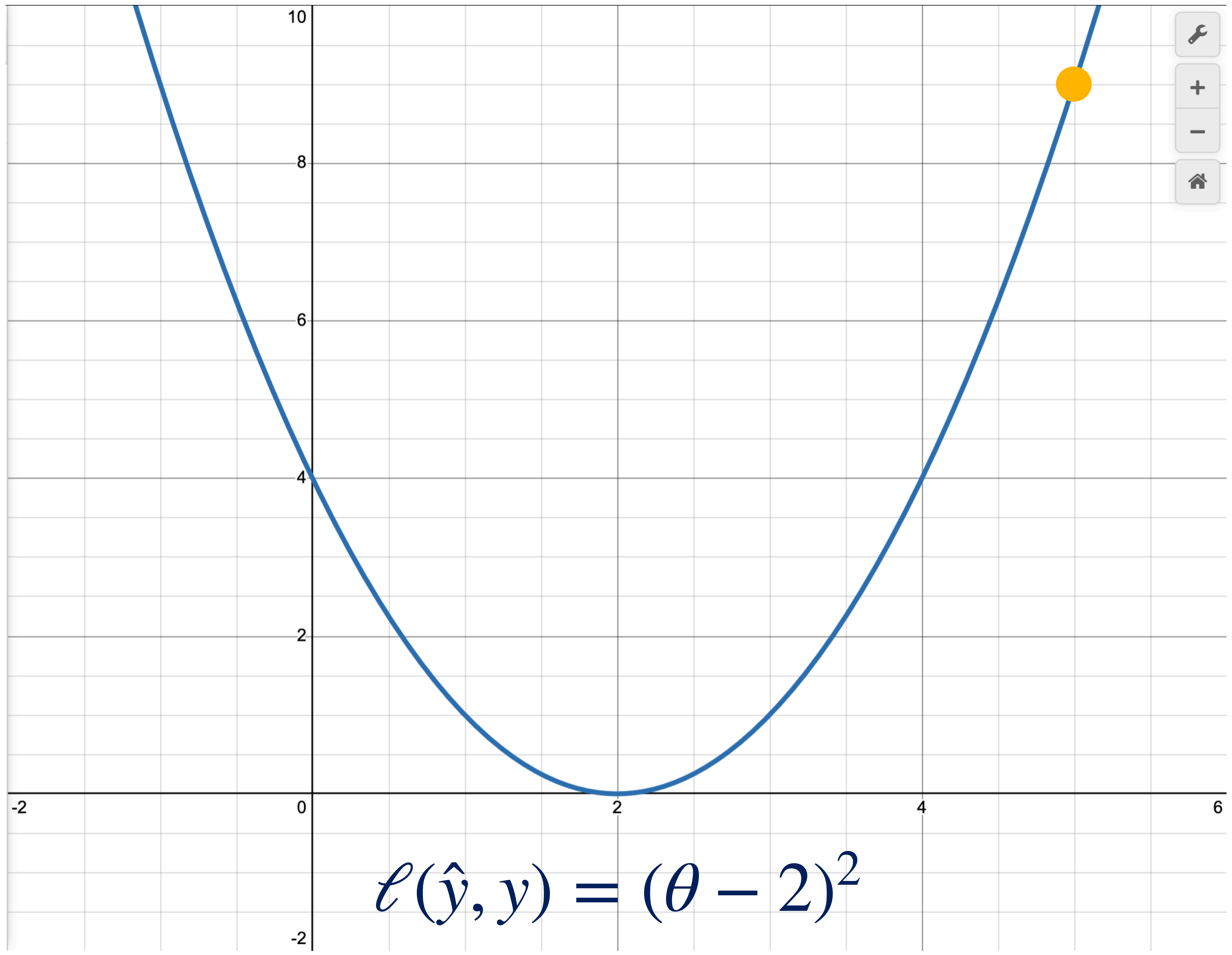
Gradient Descent (second try)

- What if we adjusted θ by a **fraction** of the slope? (Say, 0.75)
- Let's start again:



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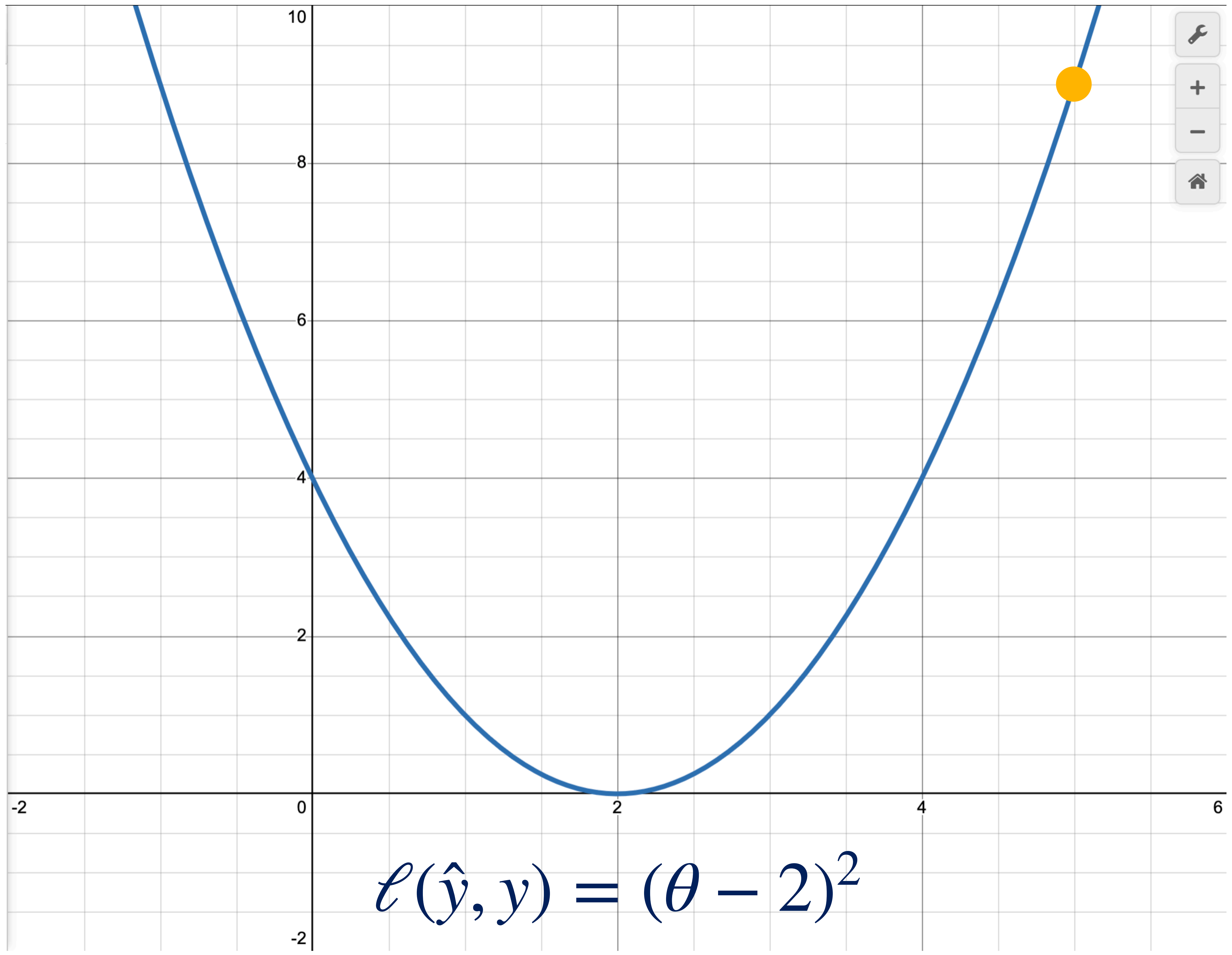
Gradient Descent (second try)

- What if we adjusted θ by a **fraction** of the slope? (Say, 0.75)
- Let's start again:
    - Plug in θ_0 to derivative:



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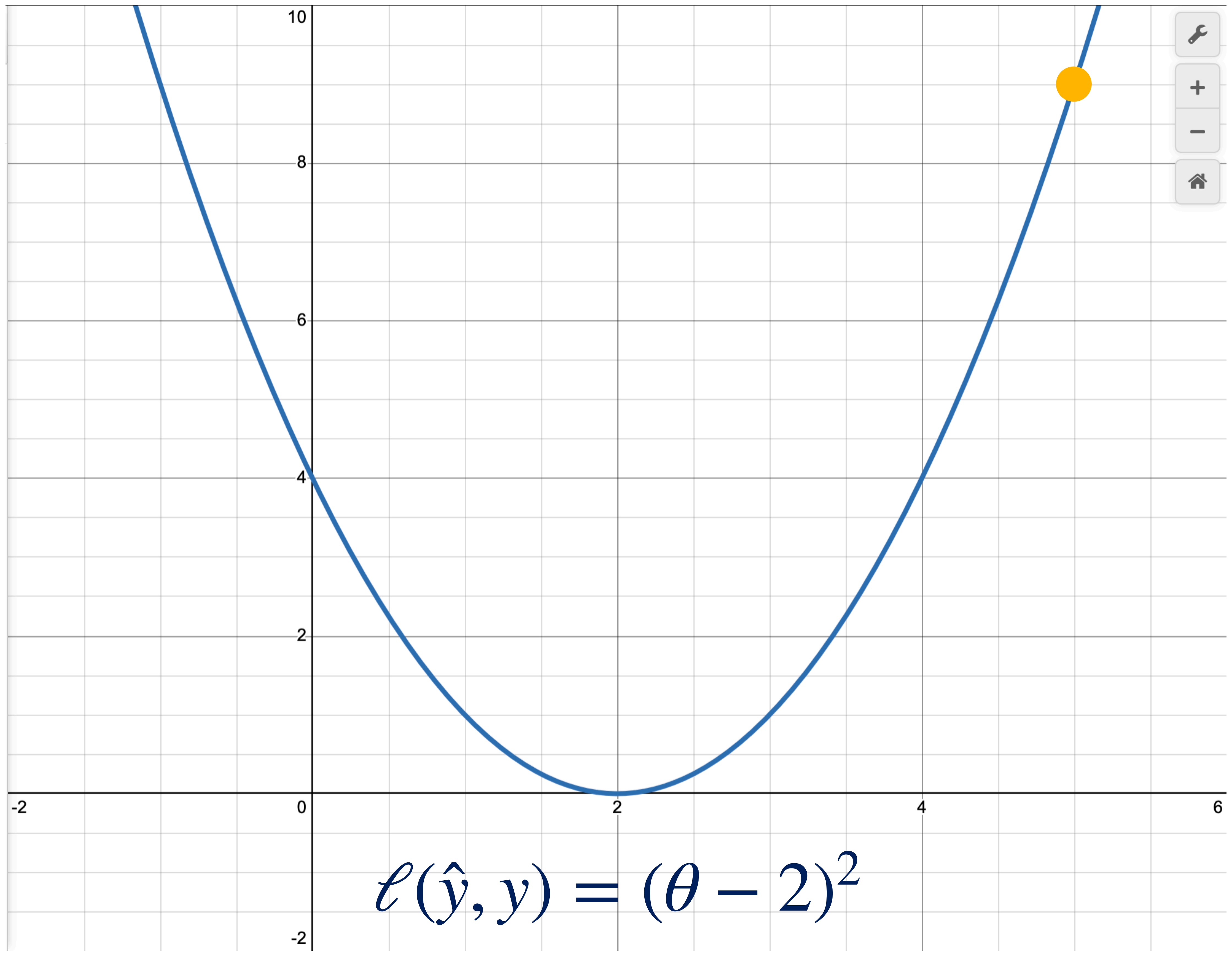

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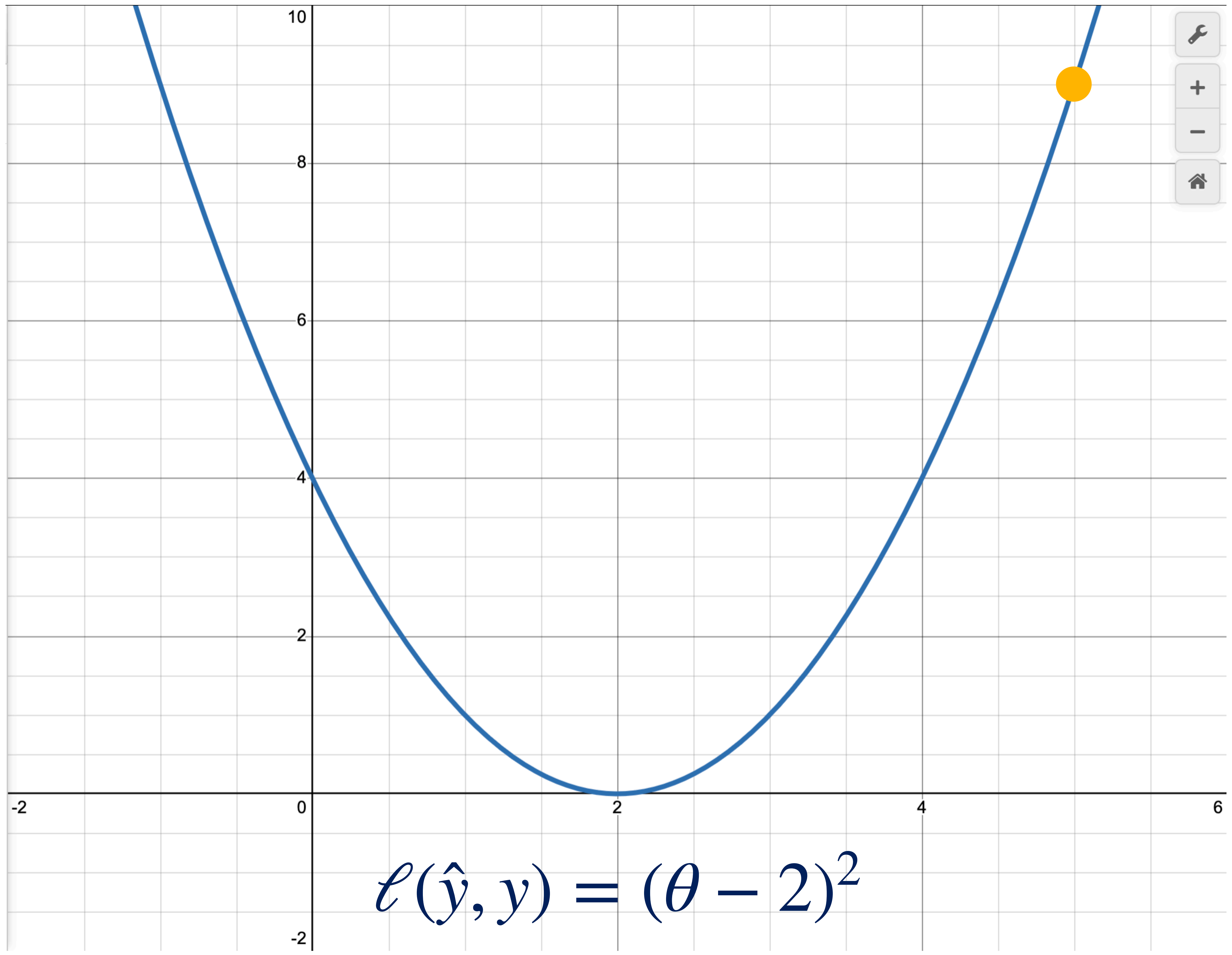

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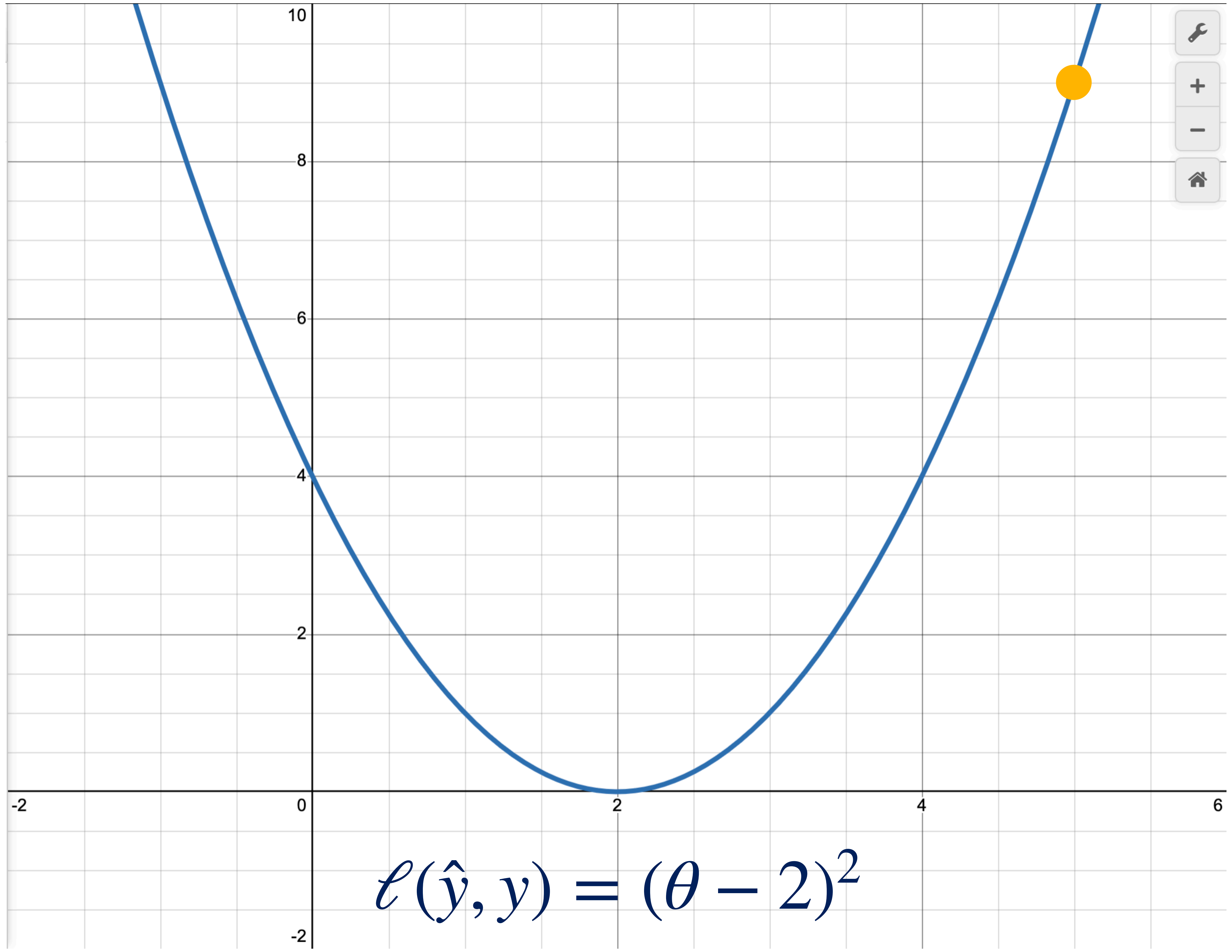
  - Update θ:
    - $\theta_1 = \theta_0 - 0.75 \cdot 6 = 0.5$



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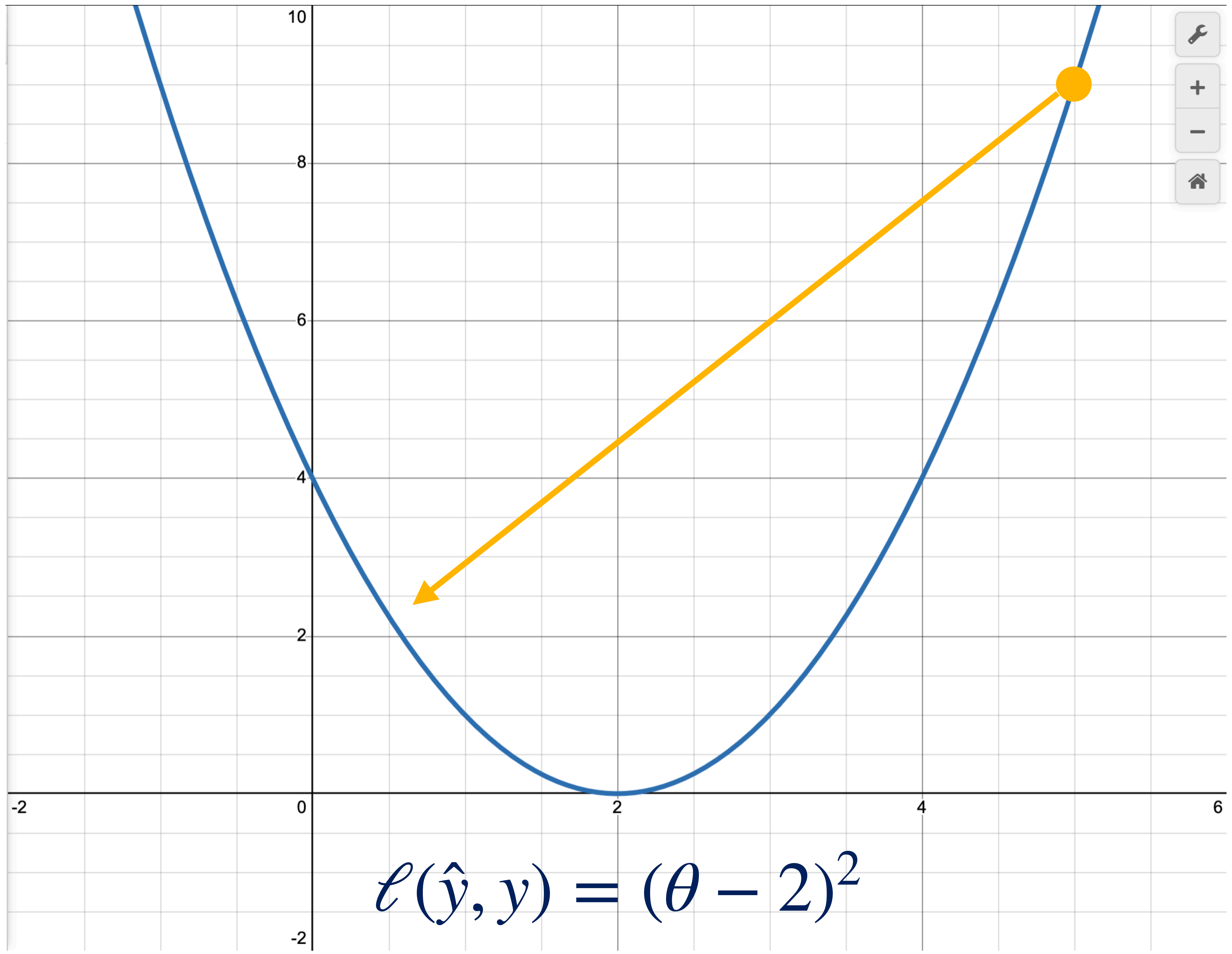

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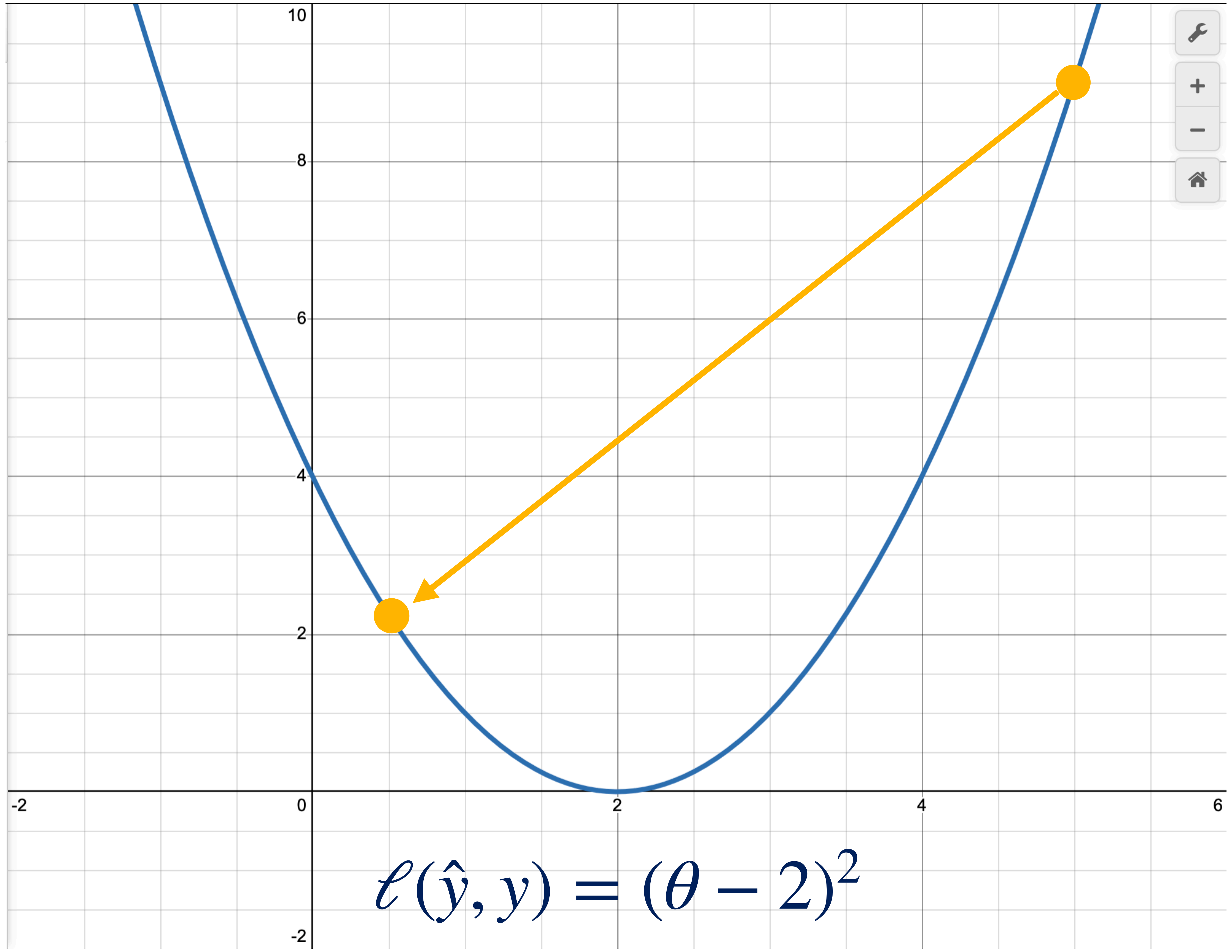

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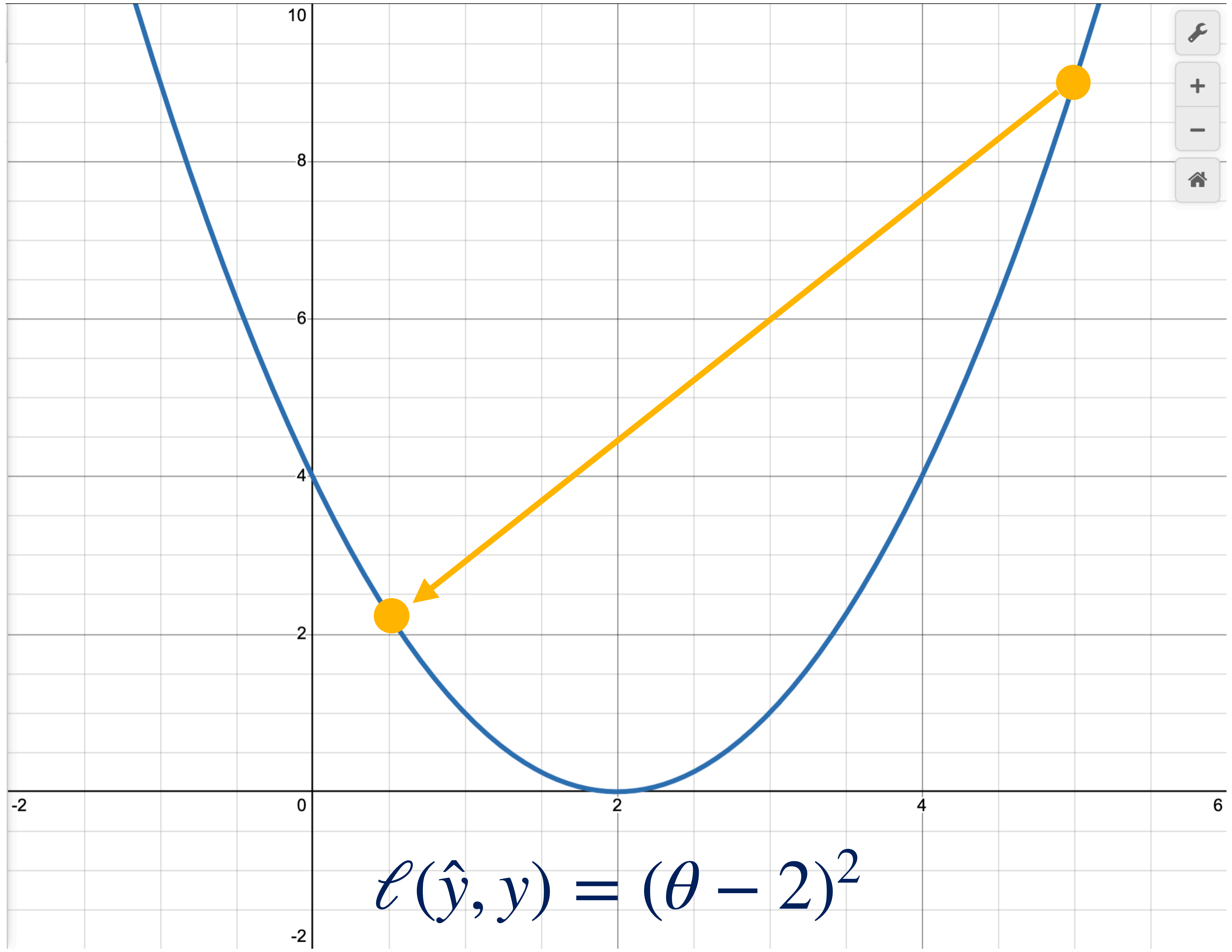
Gradient Descent (second try)

- Second step:



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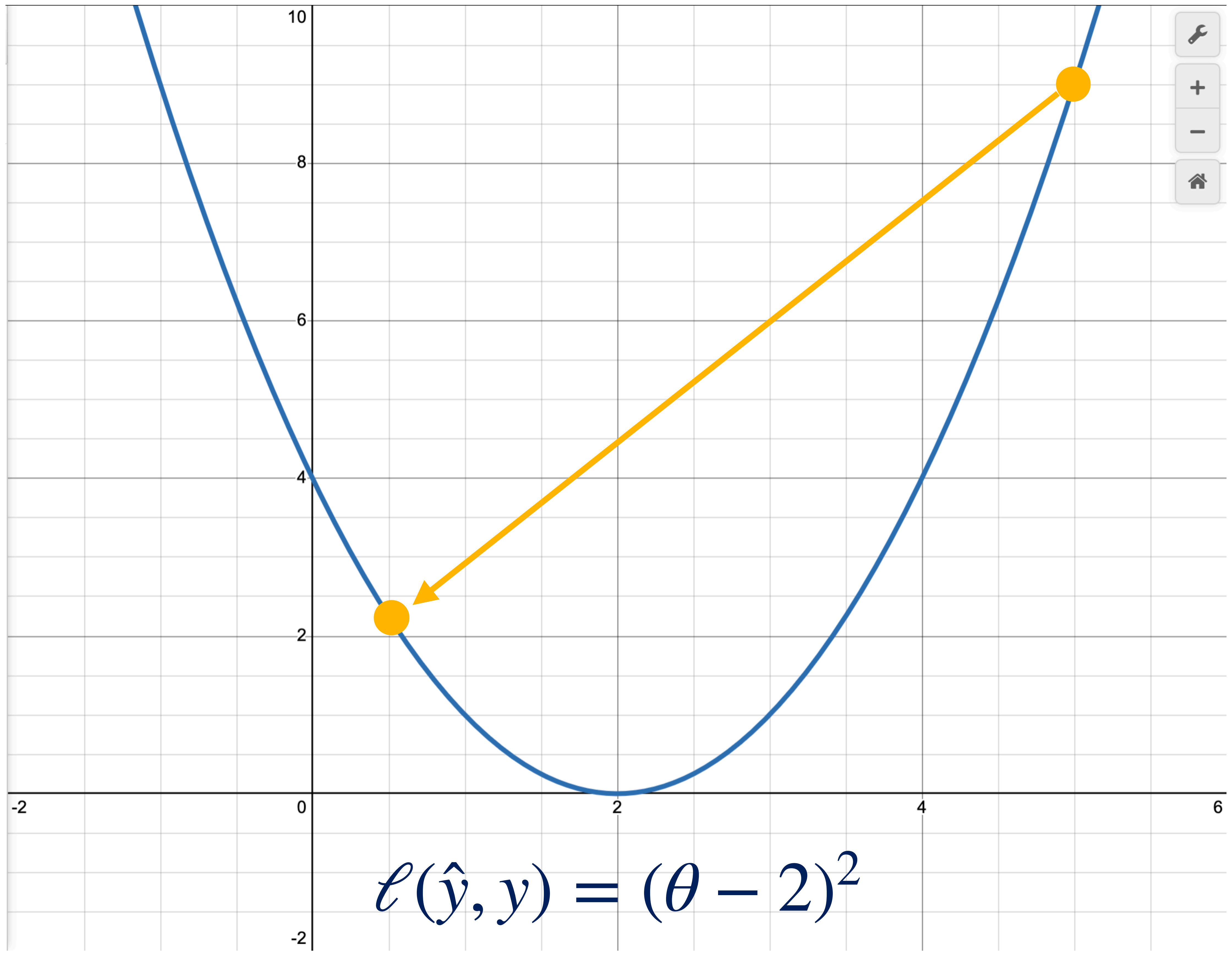

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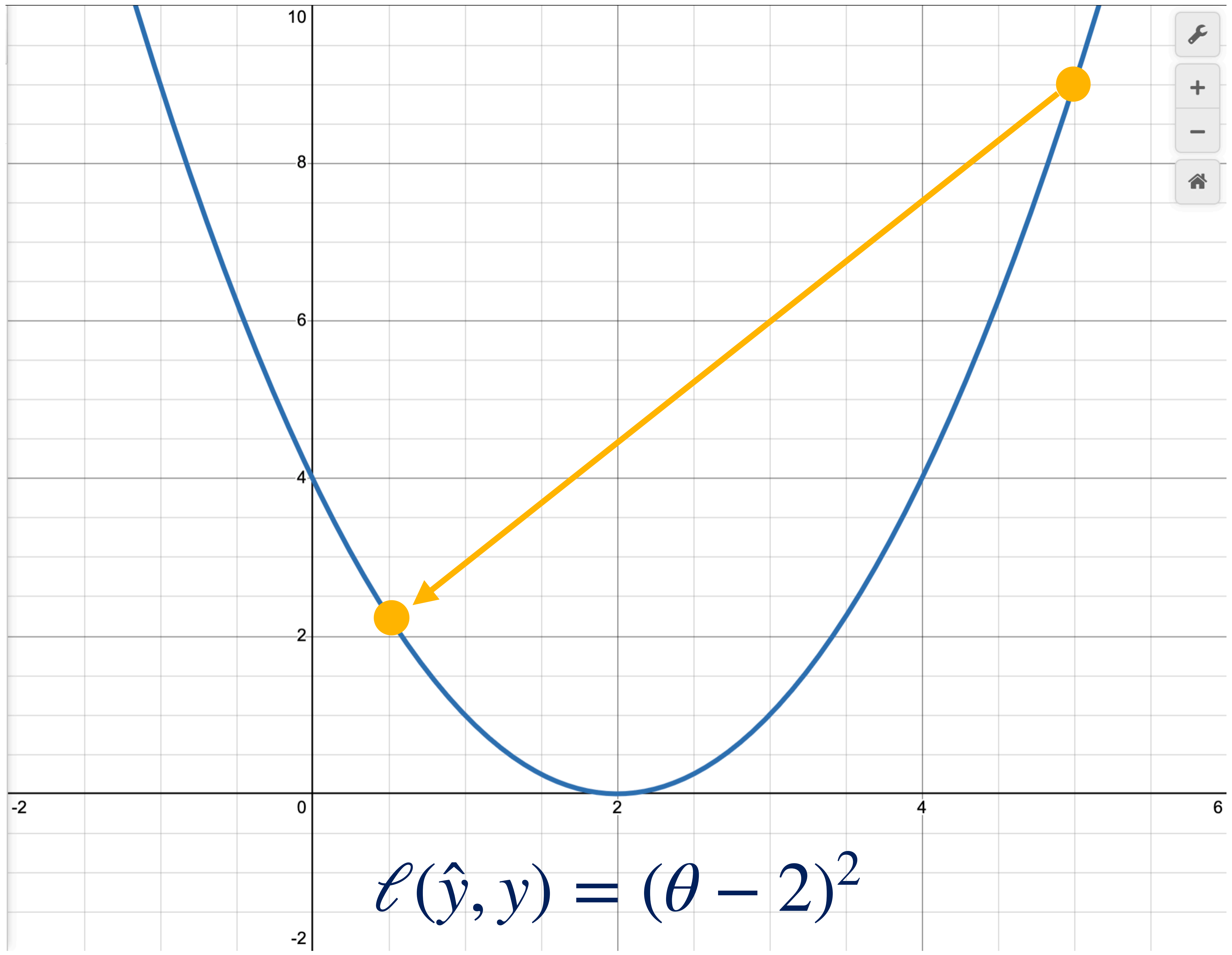
Gradient Descent (second try)

- Second step:
  - Plug in θ_1 to derivative:
    - $2 \cdot 0.5 - 4 = -3$



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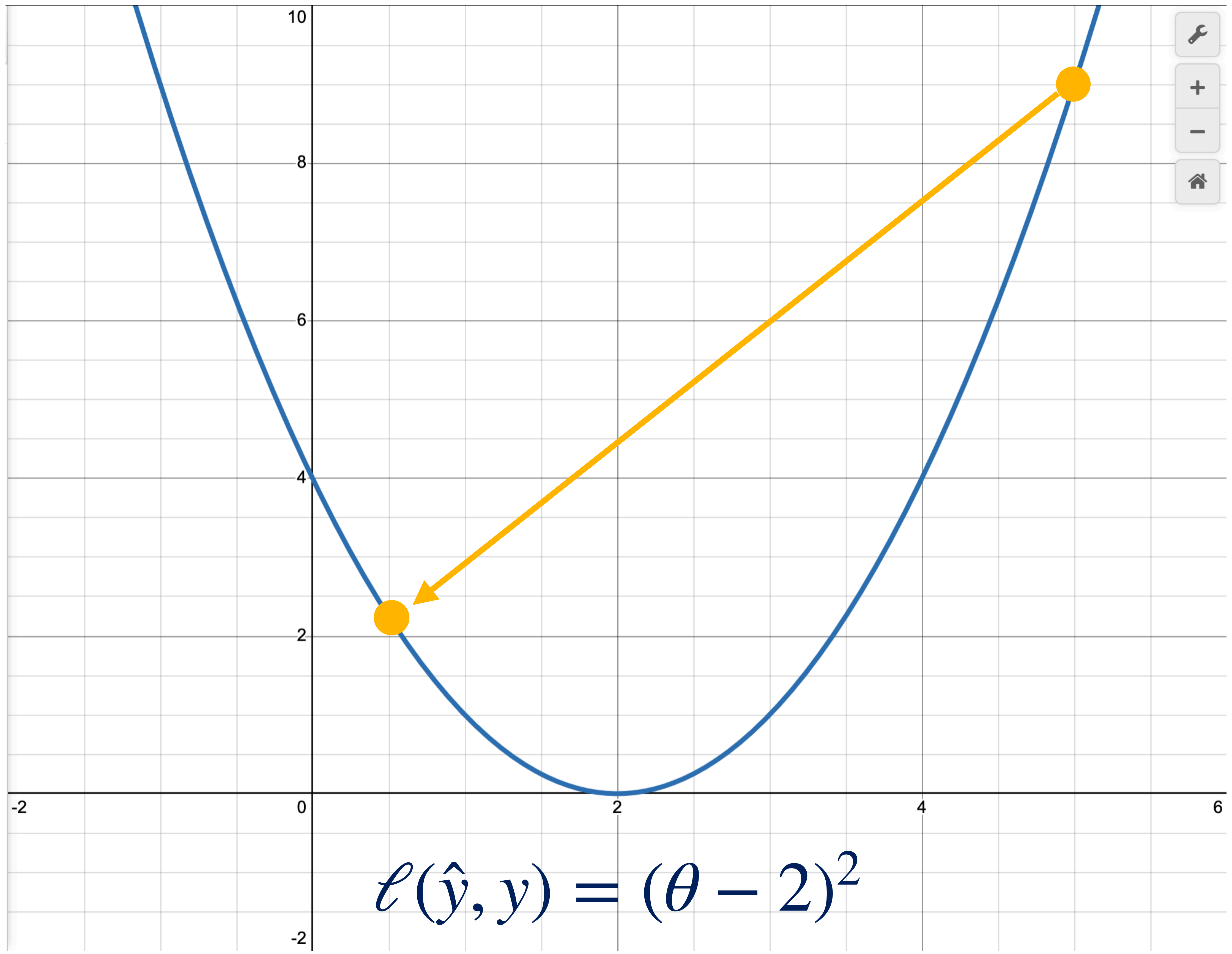

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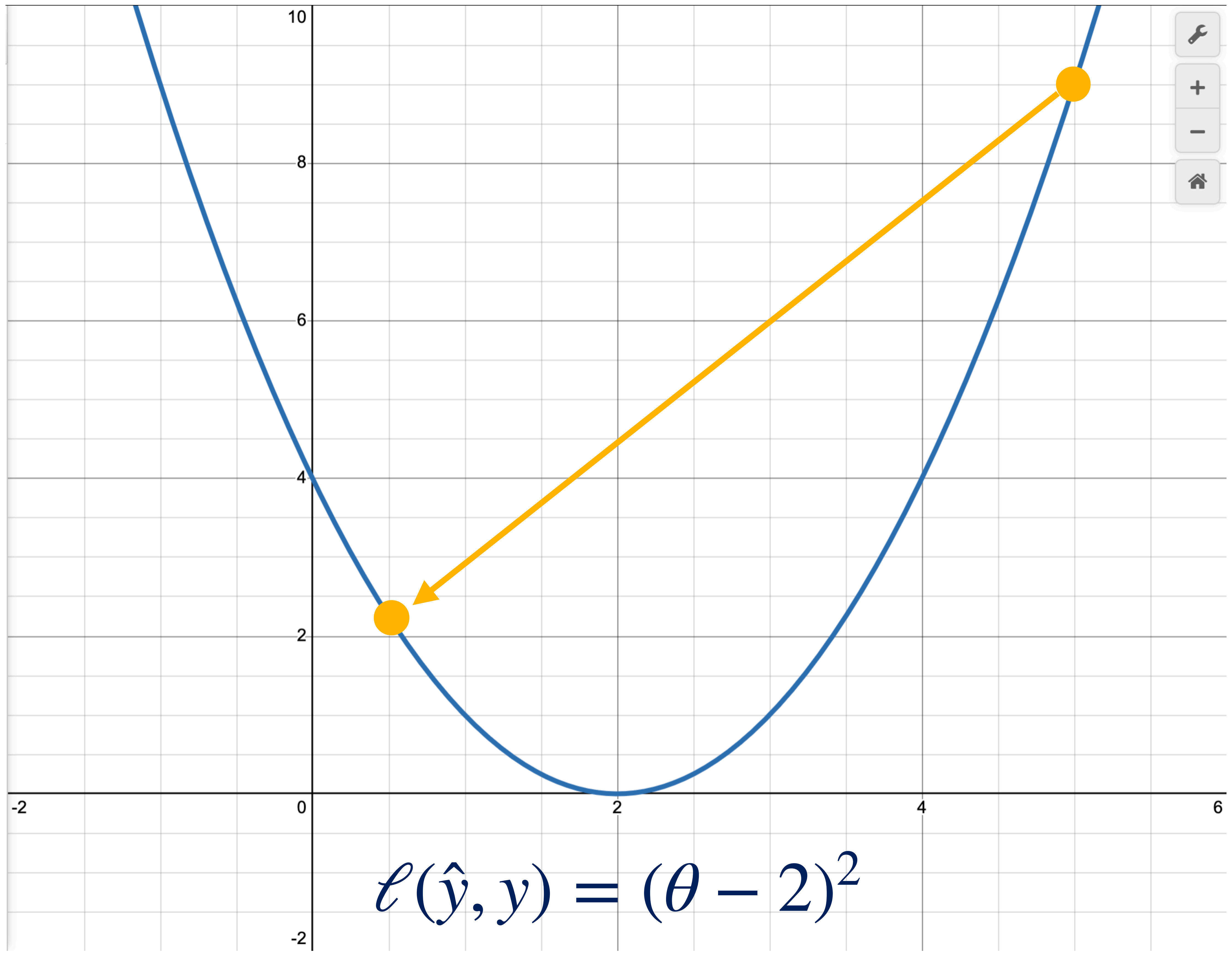
Gradient Descent (second try)

- Second step:
  - Plug in θ_1 to derivative:
    - $2 \cdot 0.5 - 4 = -3$
  - Update θ:
    - $\theta_2 = \theta_1 - 0.75 \cdot (-3) = 2.25$



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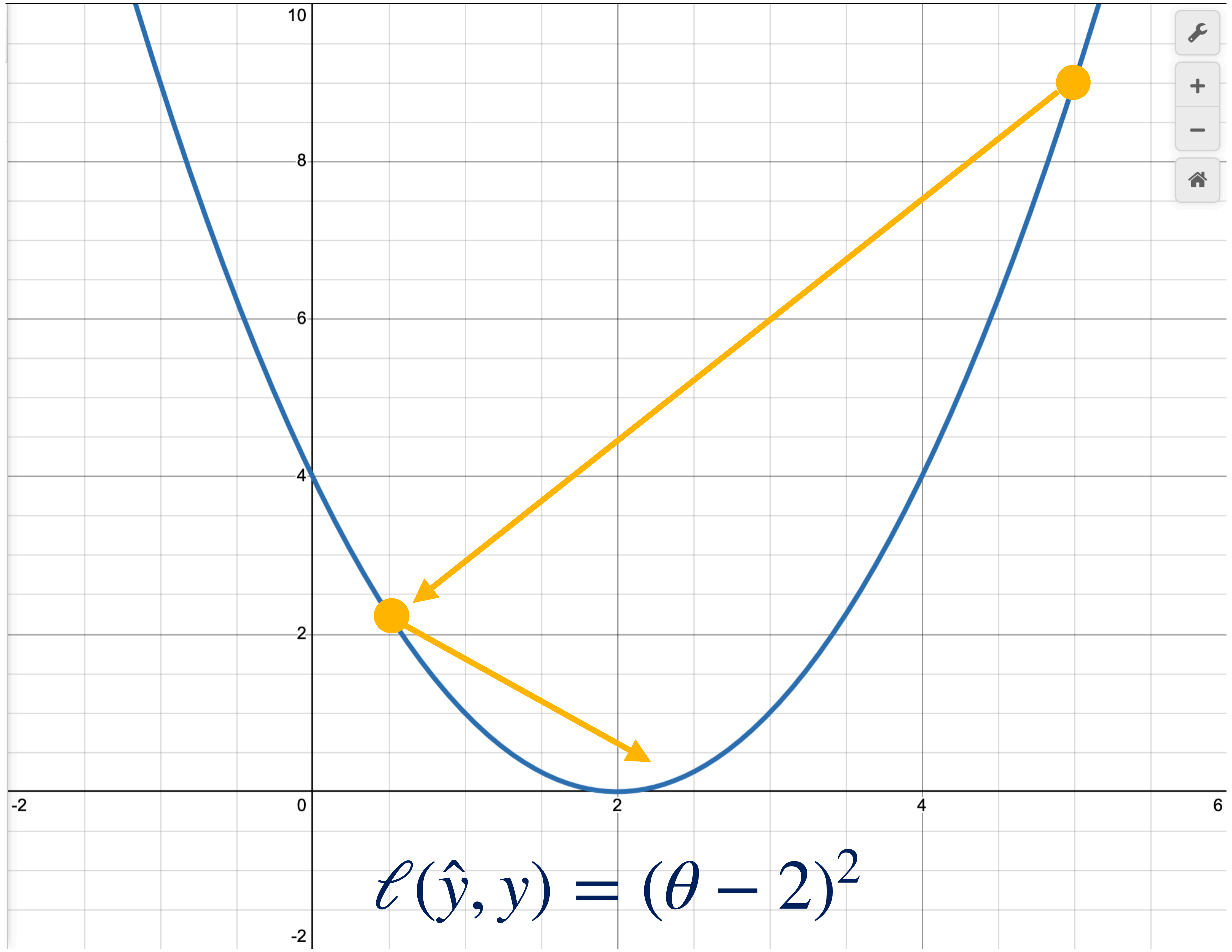

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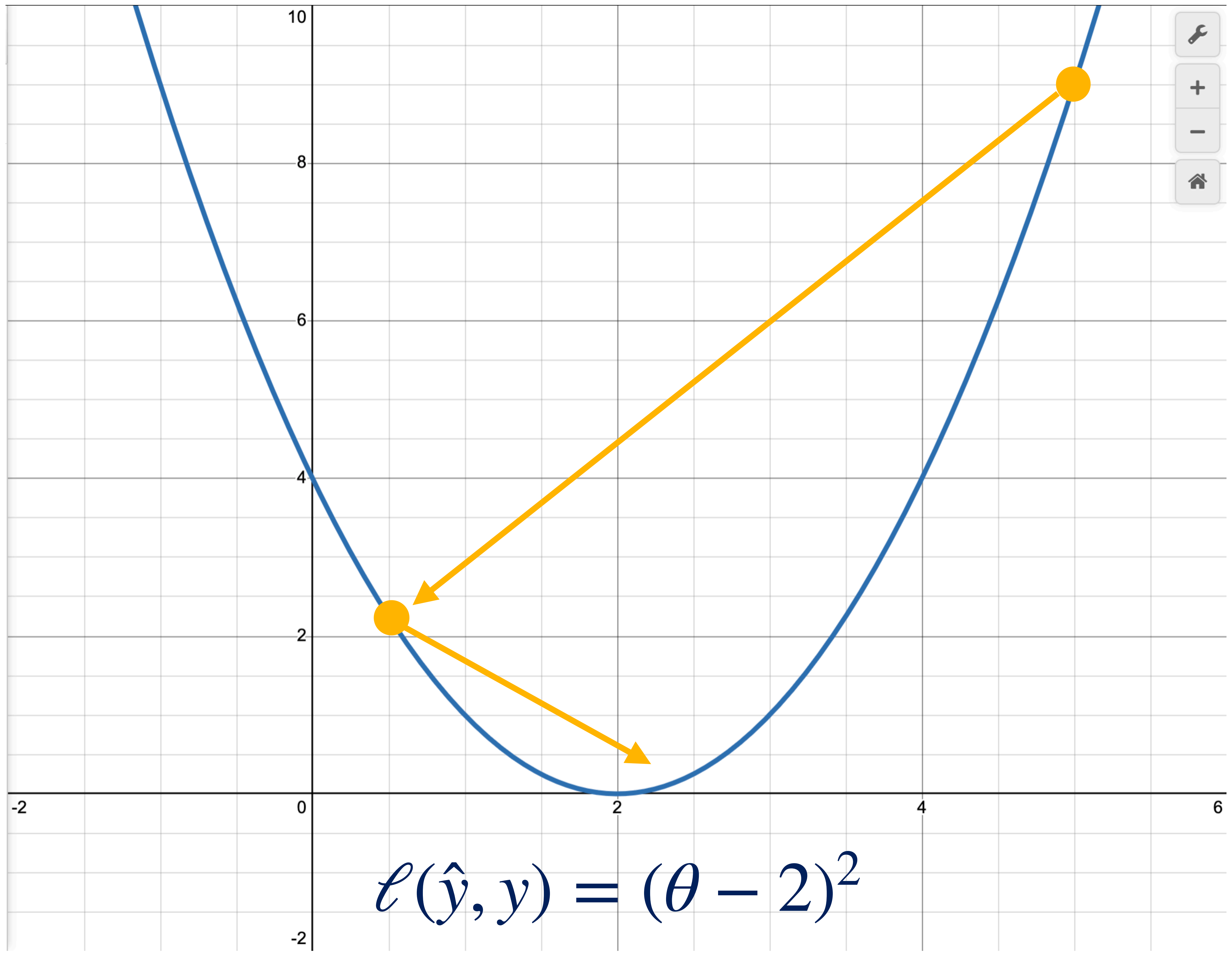
- (This is looking better)



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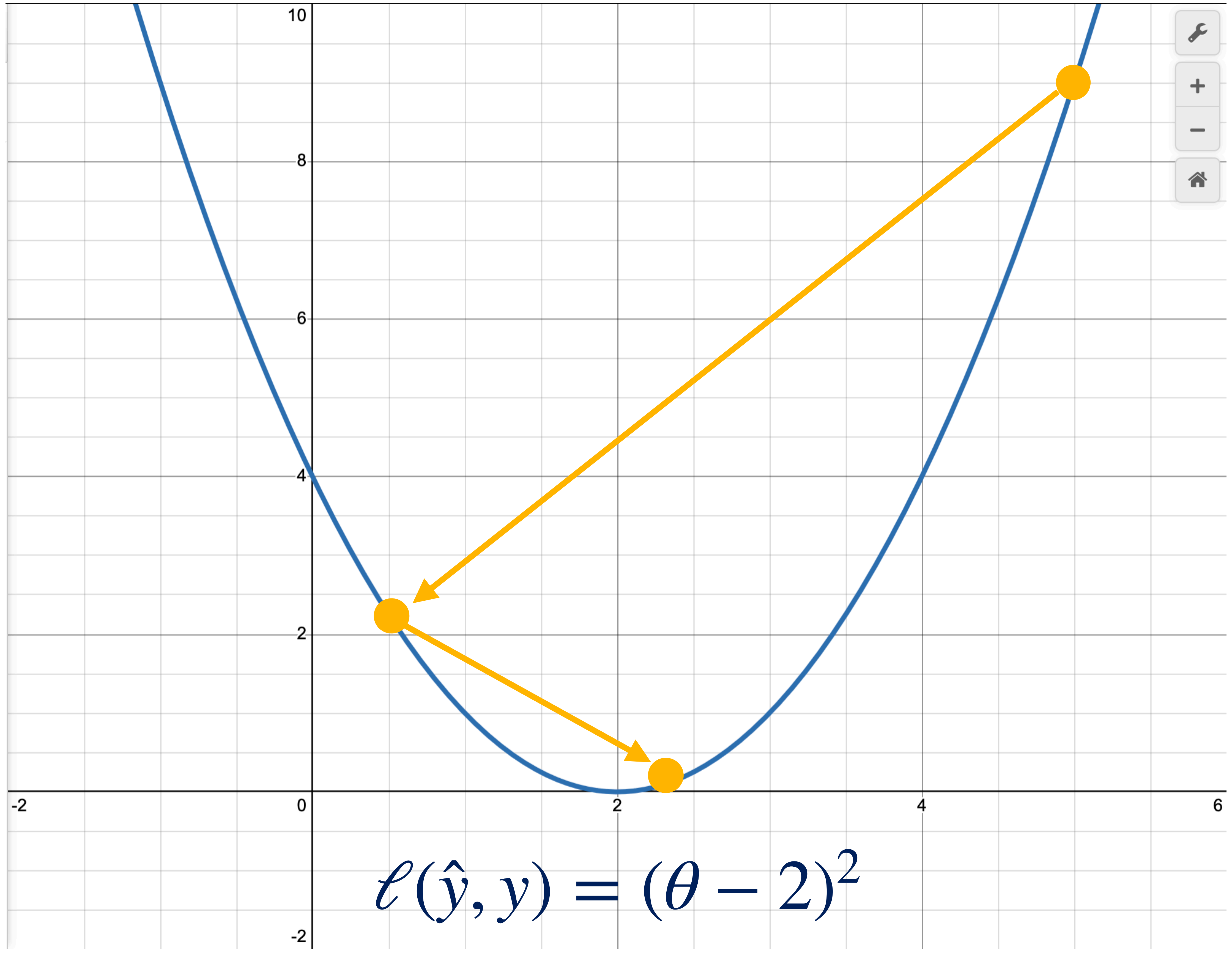
Gradient Descent (second try)



$$\ell(\hat{y}, y) = (\theta - 2)^2$$

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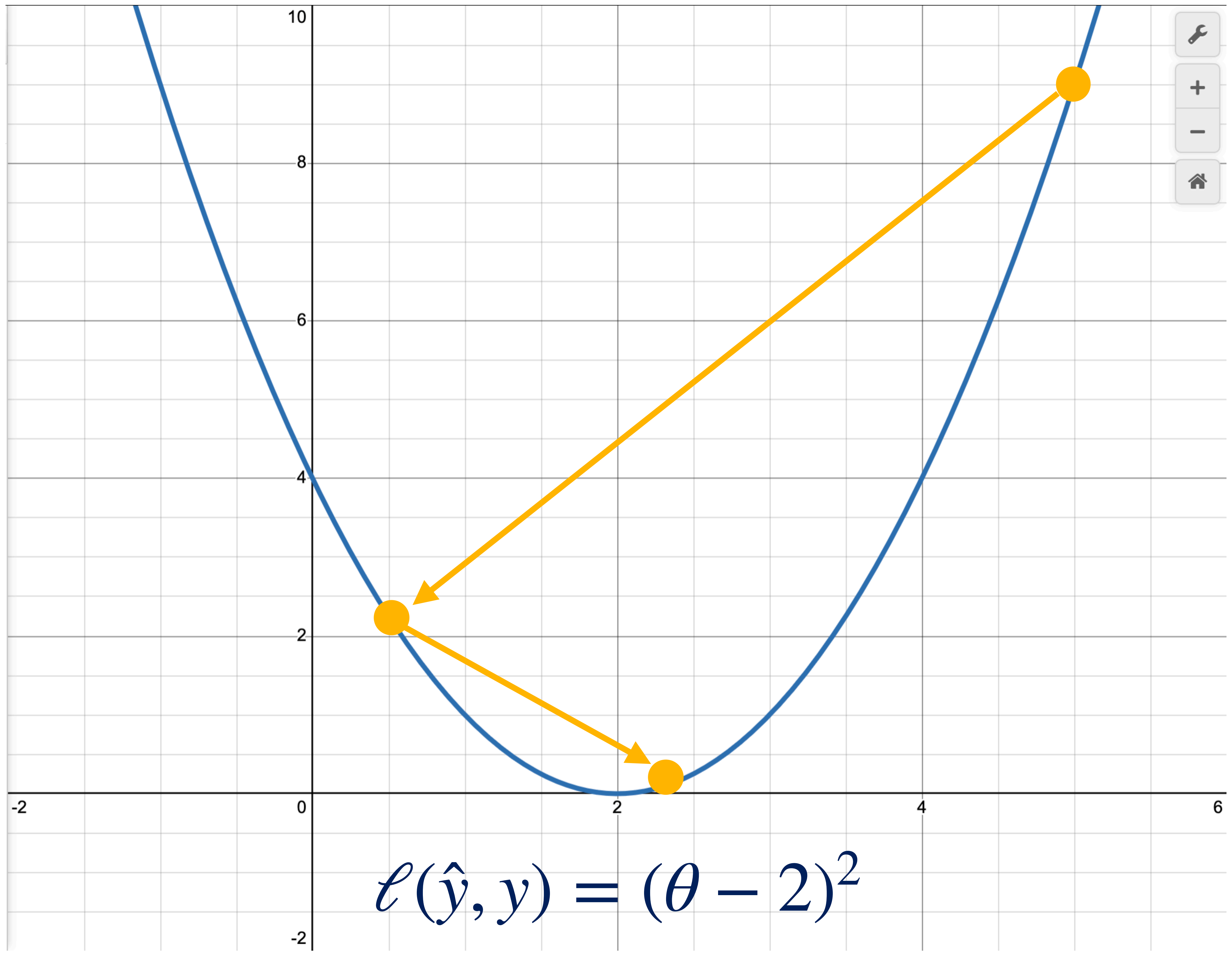
Gradient Descent (second try)

- Third step:
  - Plug in θ_2 to derivative:
    - $2 \cdot 2.25 - 4 = 0.5$
  - Update θ:
    - $\theta_3 = \theta_2 - 0.75 \cdot 0.5 = 1.875$



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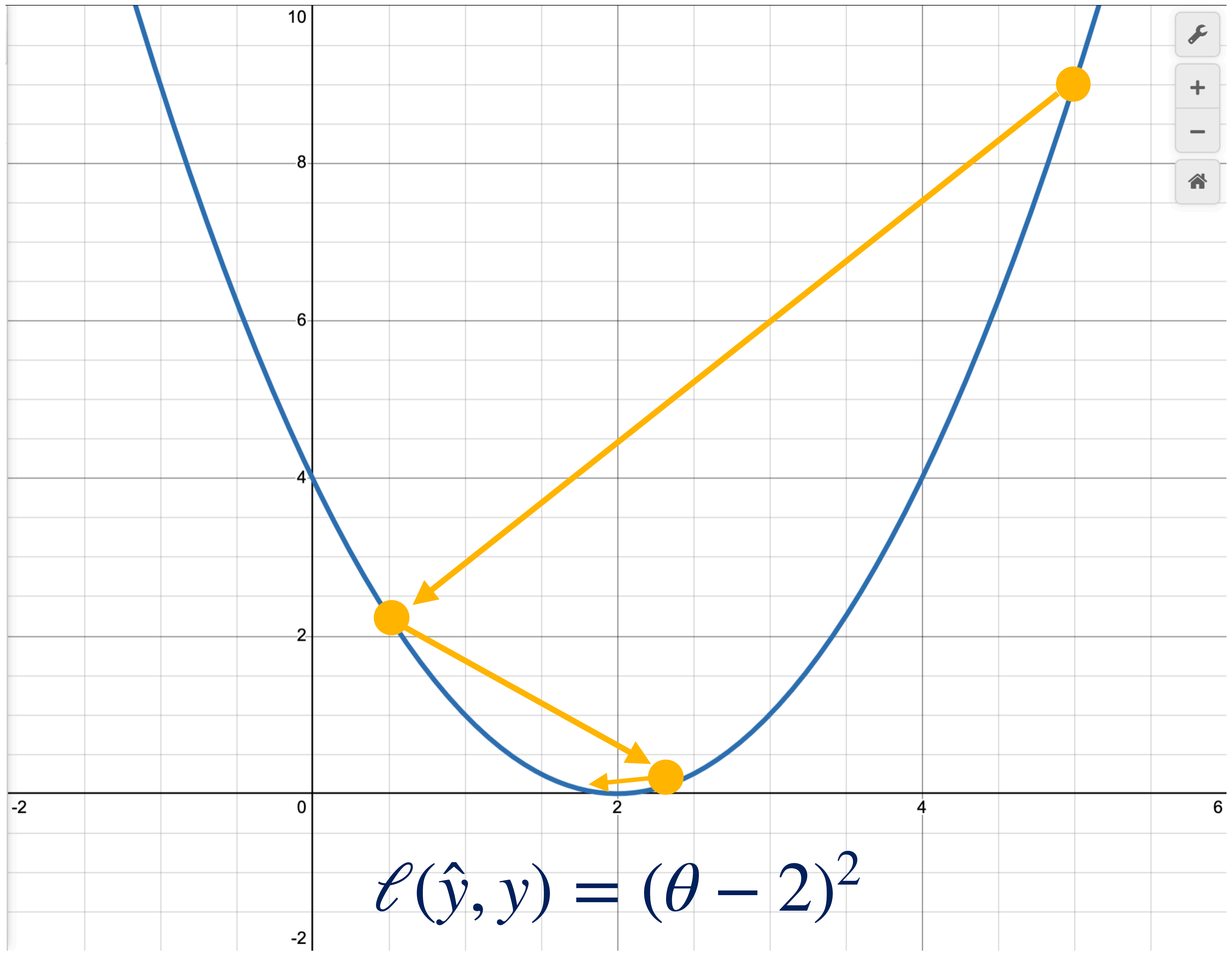

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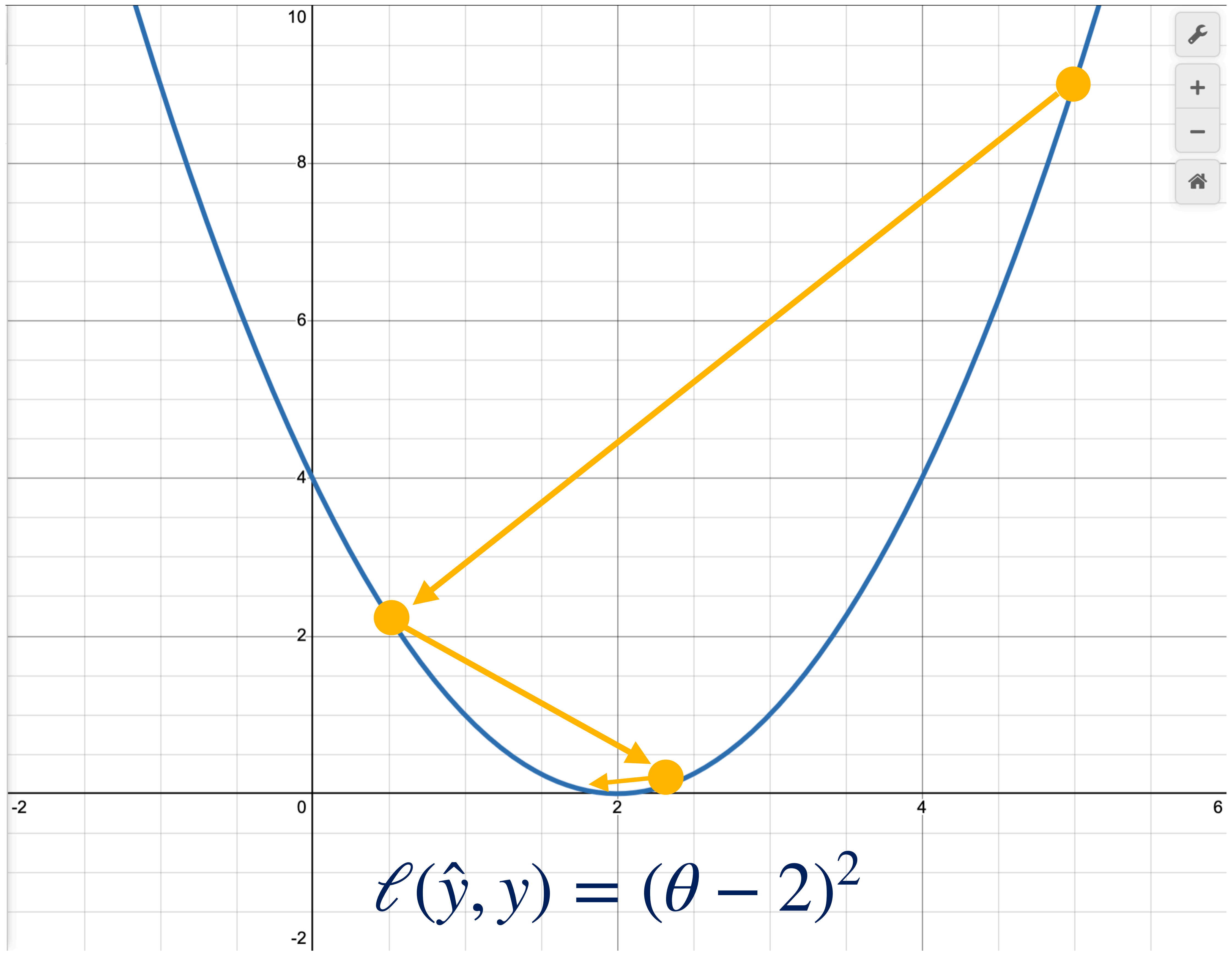
- **Loss gets lower with every step!**



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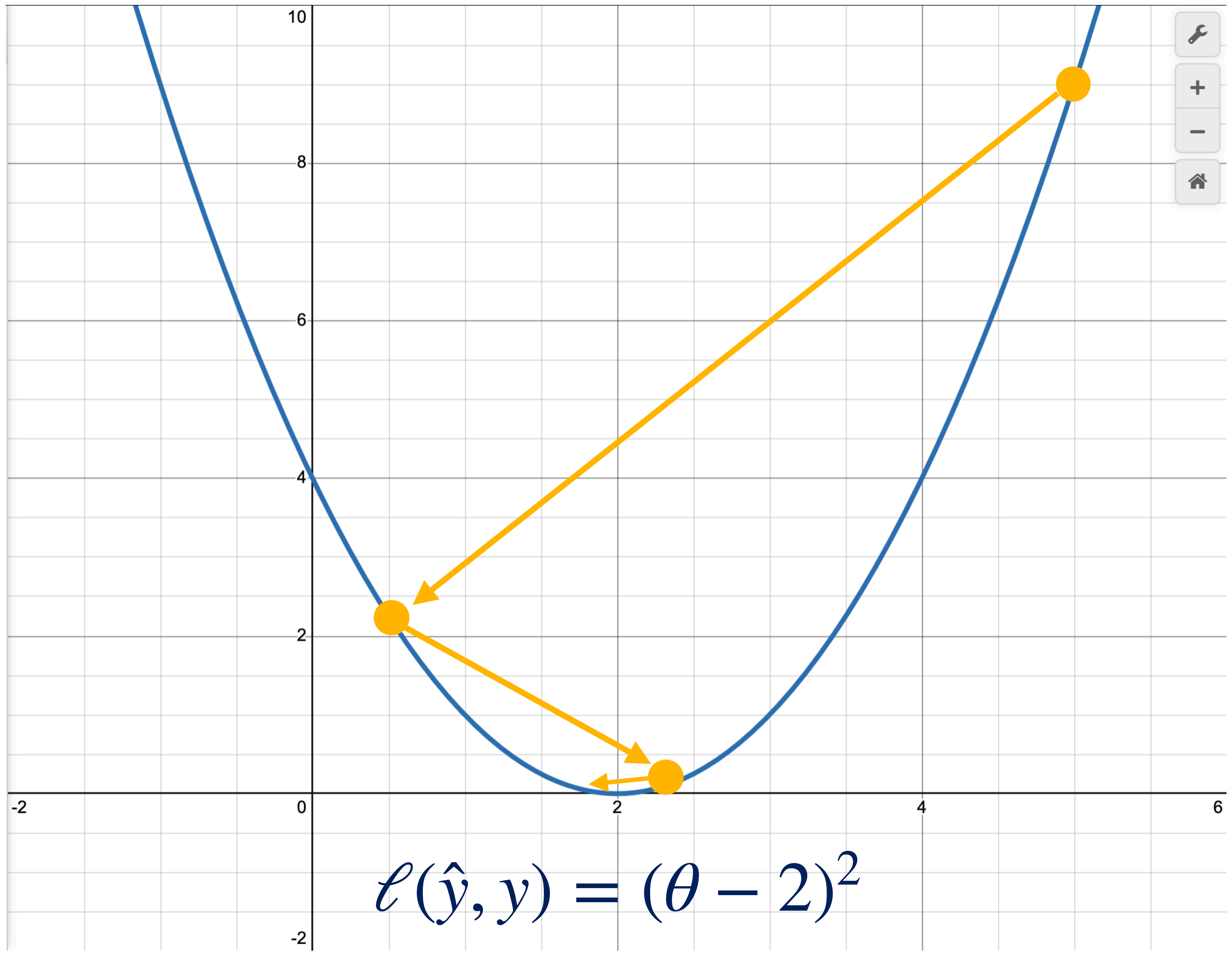
- **Loss gets lower with every step!**
- θ gets **arbitrarily close to the optimal value** with more steps



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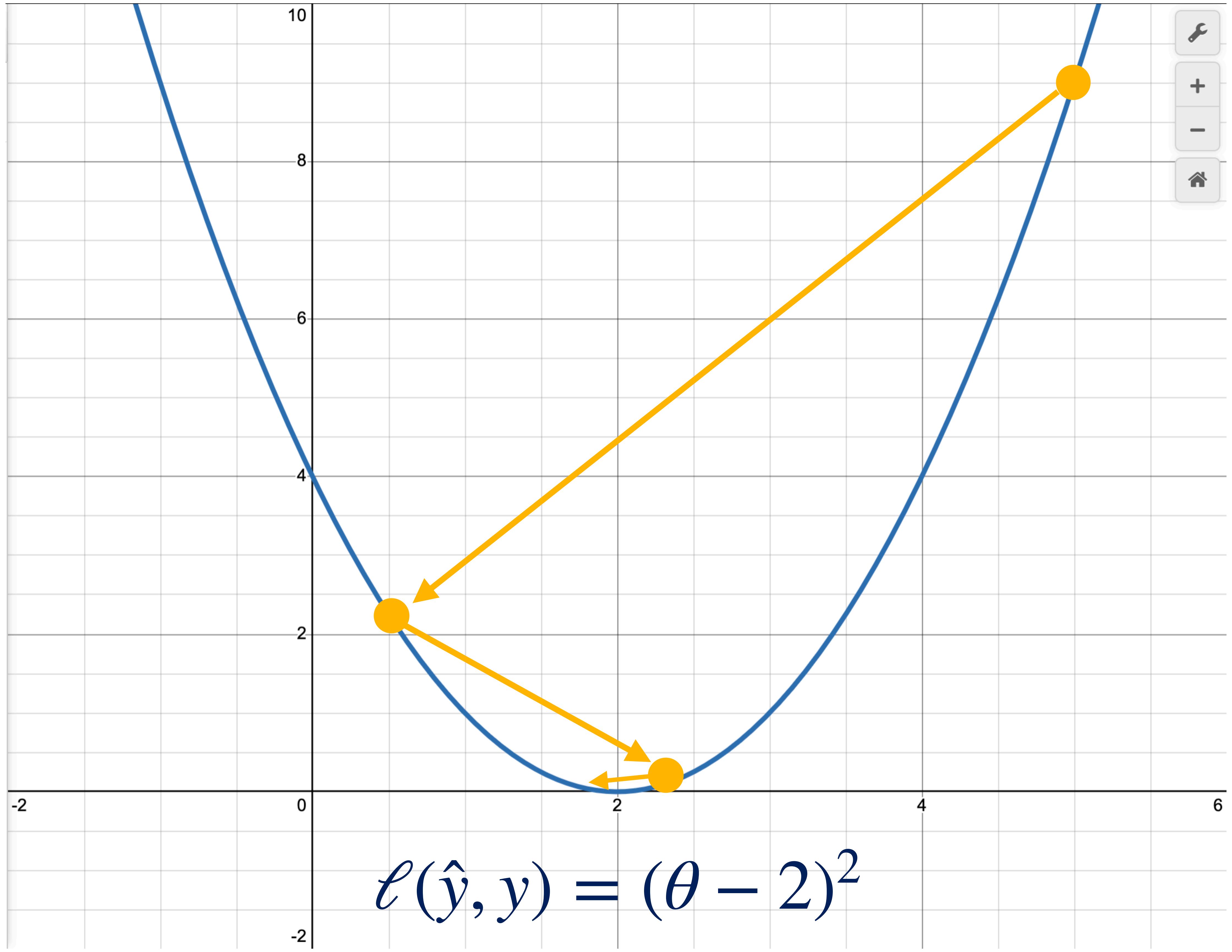
Learning Rate



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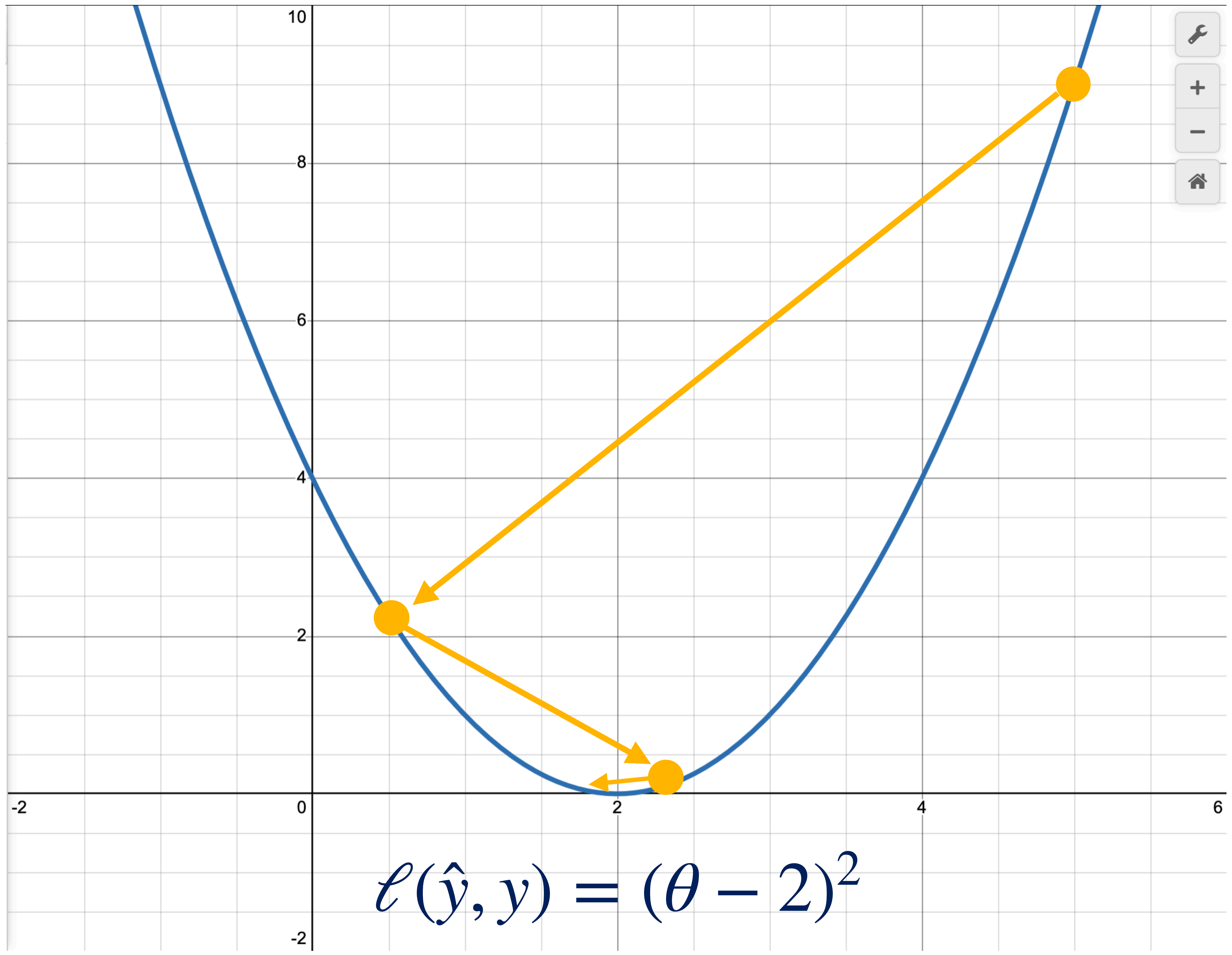
Learning Rate

- The fraction by which we multiplied our adjustment is called the **Learning Rate**



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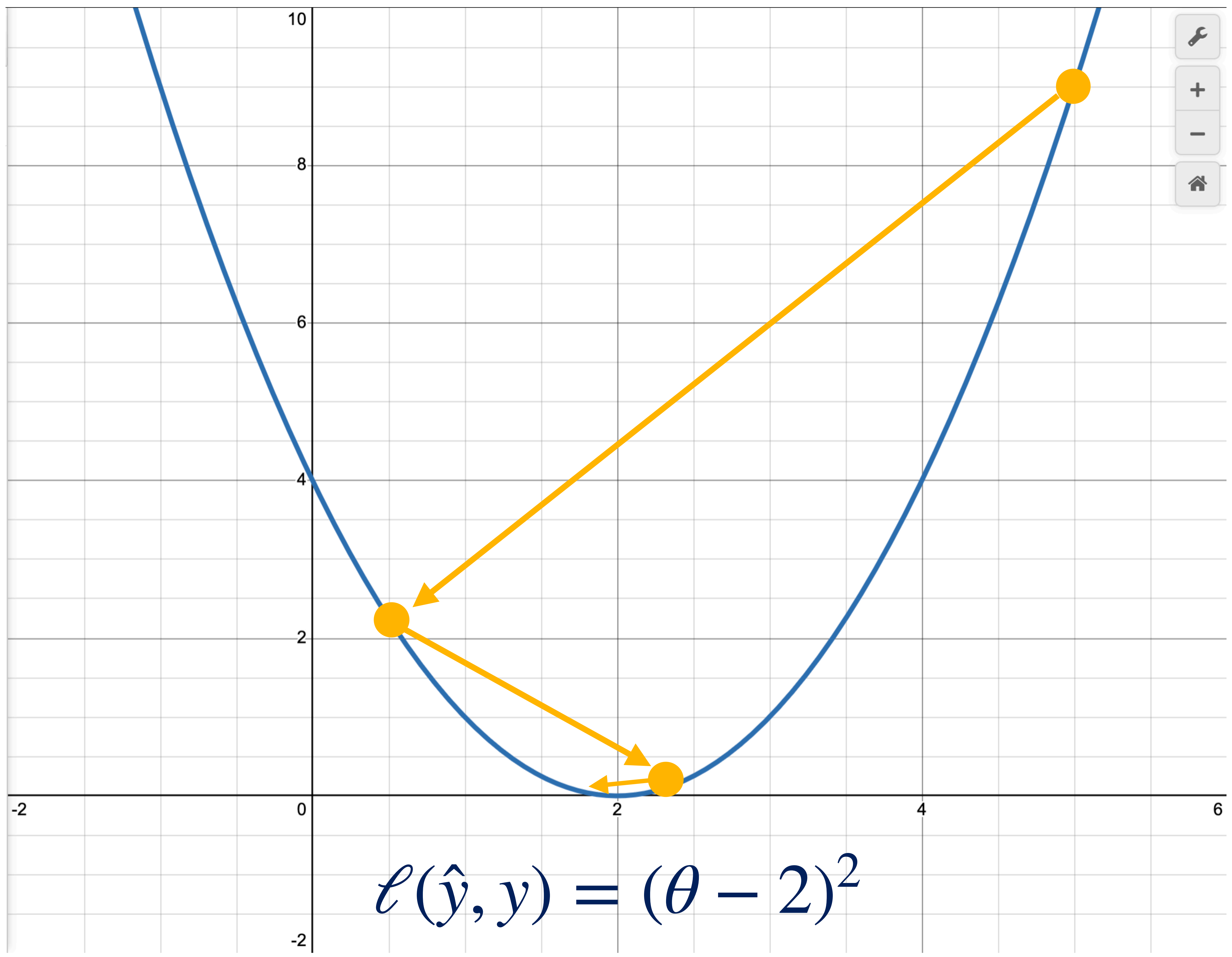
Learning Rate

- The fraction by which we multiplied our adjustment is called the **Learning Rate**
- In practice, LR is chosen by **trial and error** (called "tuning")



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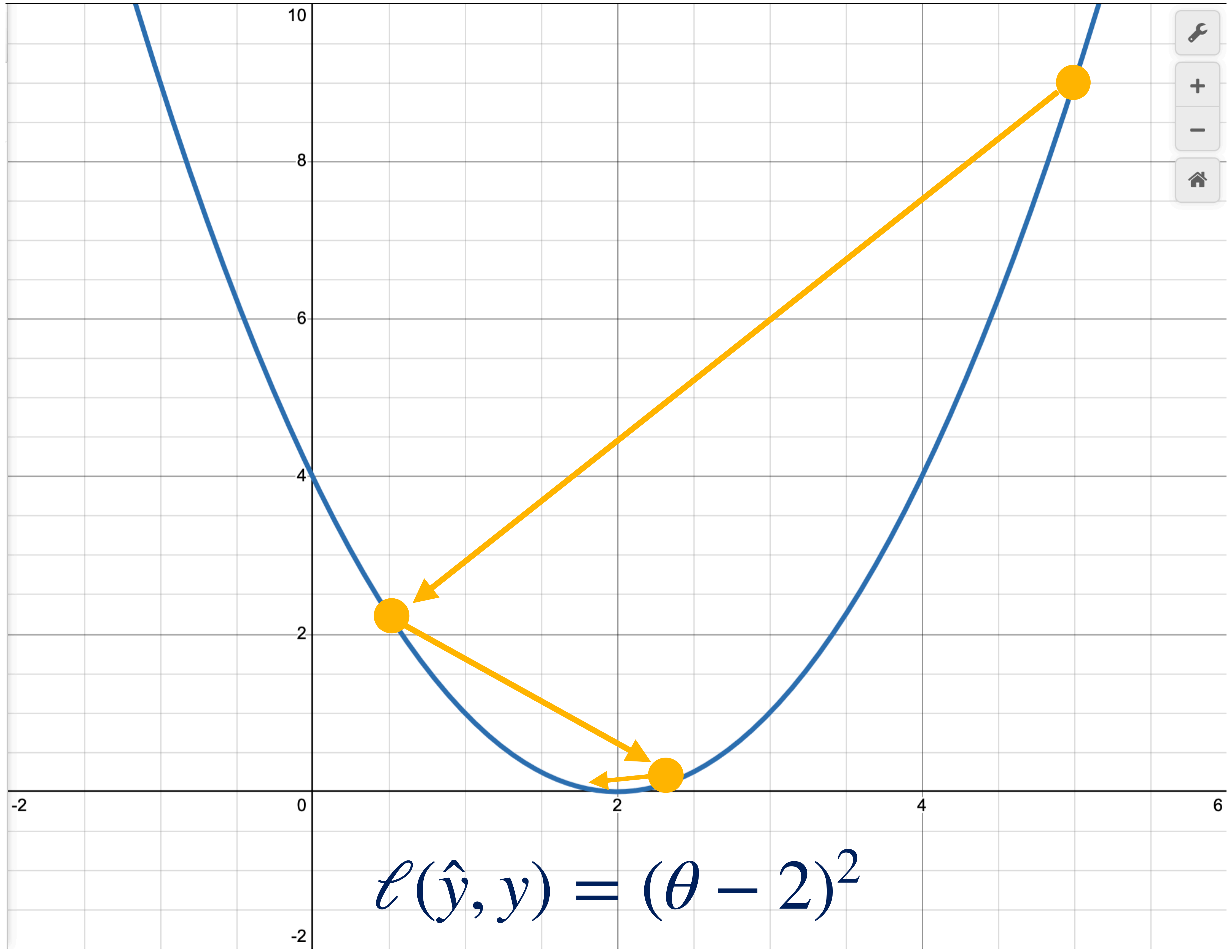
Learning Rate

- The fraction by which we multiplied our adjustment is called the **Learning Rate**
- In practice, LR is chosen by **trial and error** (called "tuning")
- Risks of different values
  - Too high → **"bouncing around"** and missing an optimum
  - Too low → taking **many steps** to reach the optimum



$$\ell(\hat{y}, y) = (\theta - 2)^2$$

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Supervised Paradigms

Supervised Paradigms

- **Classification**: model outputs **discrete categories**
  - E.g. **binary** classification: spam/not-spam, human/bot, true/false
  - **Multi-class:** dog/cat/other, choosing word from finite vocabulary
  - Almost always outputs a **probability distribution**
    - Often achieved with the **sigmoid** or **softmax function**

Supervised Paradigms

- **Classification**: model outputs **discrete categories**
  - E.g. **binary** classification: spam/not-spam, human/bot, true/false
  - **Multi-class:** dog/cat/other, choosing word from finite vocabulary
  - Almost always outputs a **probability distribution**
    - Often achieved with the **sigmoid** or **softmax function**
- **Regression**: model outputs a **continuous number**
  - E.g. predicting the price of a house, sales numbers

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- **Neural Networks**: hierarchical **non-linear transformations** of input features
  - Examples: Feedforward, CNNs, RNNs, Transformers, etc.
  - **Quickly overfit** to limited data (without regularization + other tricks)

Model Generalization

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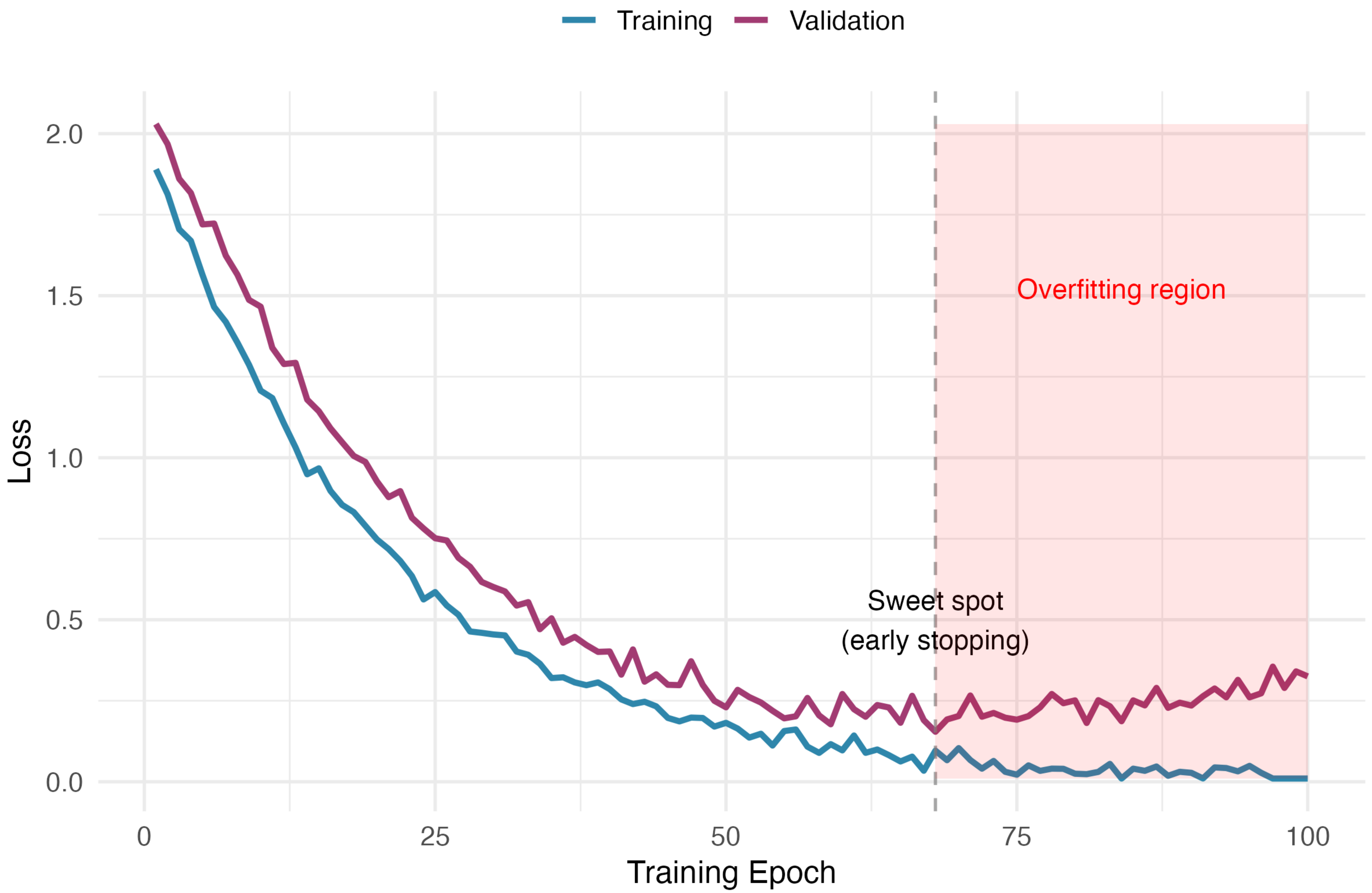
- What is overfitting?

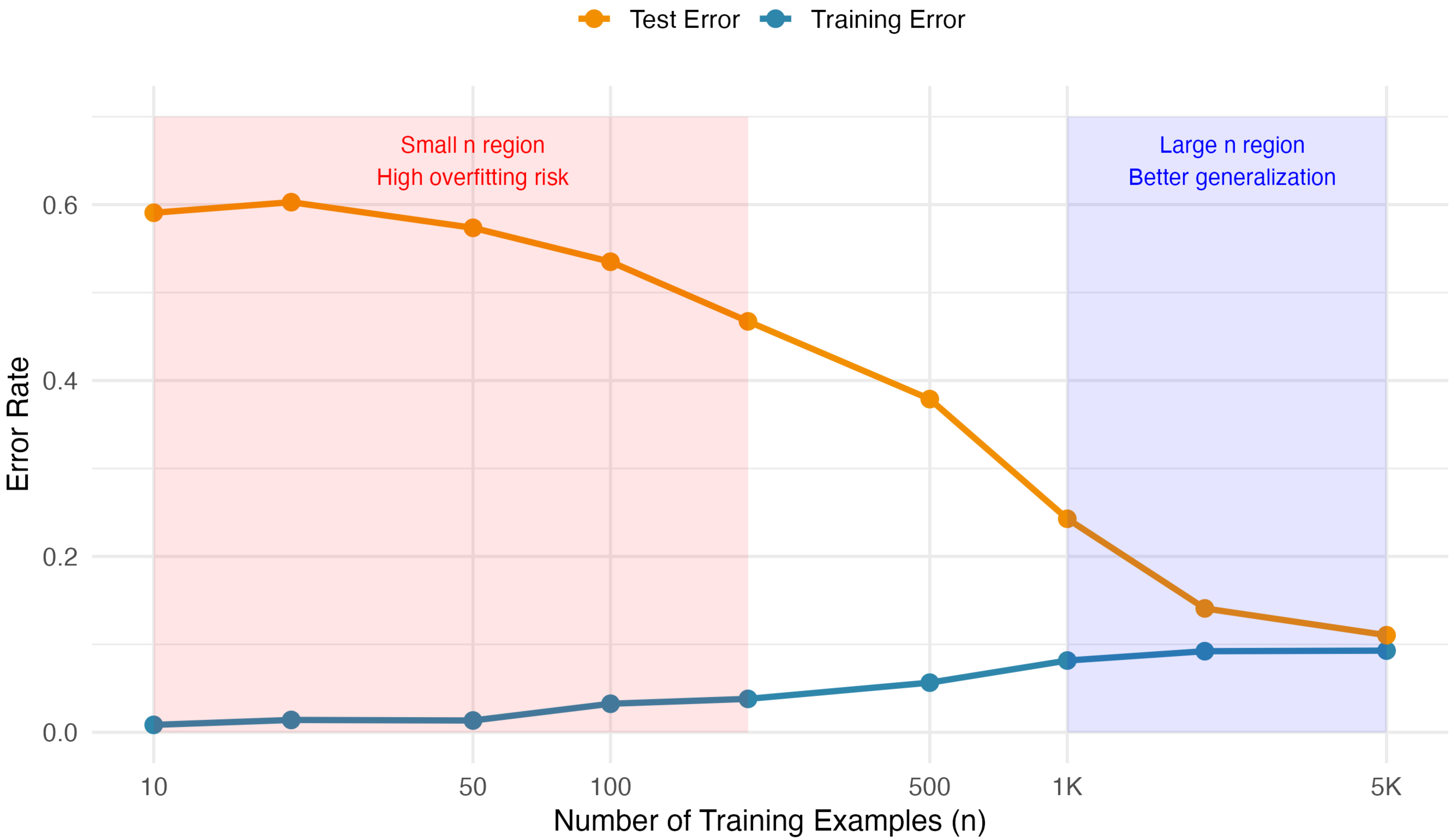
What Overfitting Looks Like

Training loss keeps improving, but validation loss increases

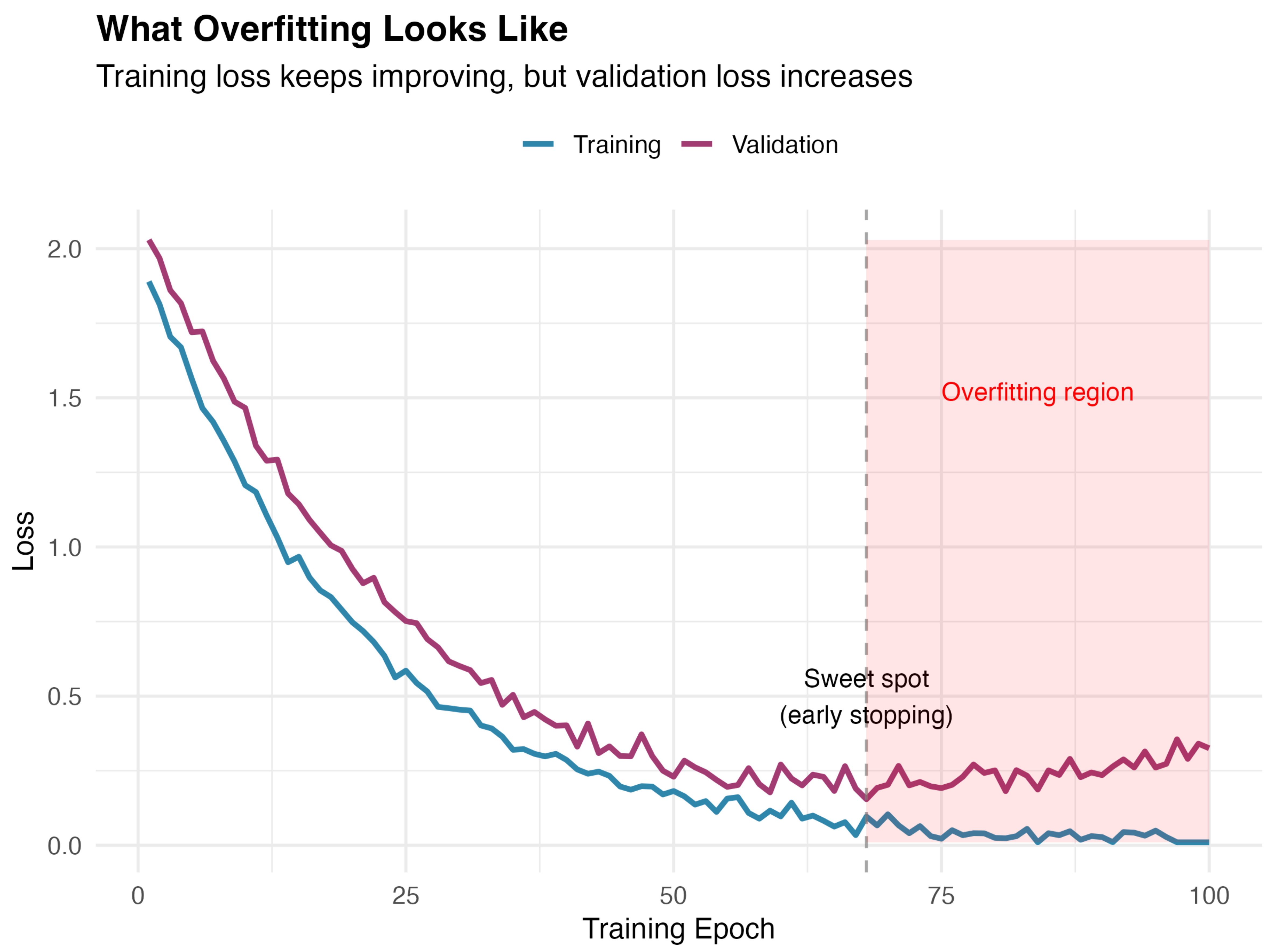


The Generalization Gap Depends on Data Size

This is the fundamental picture of the course



Why does overfitting happen?



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- Model overfitting depends on **two key factors**:
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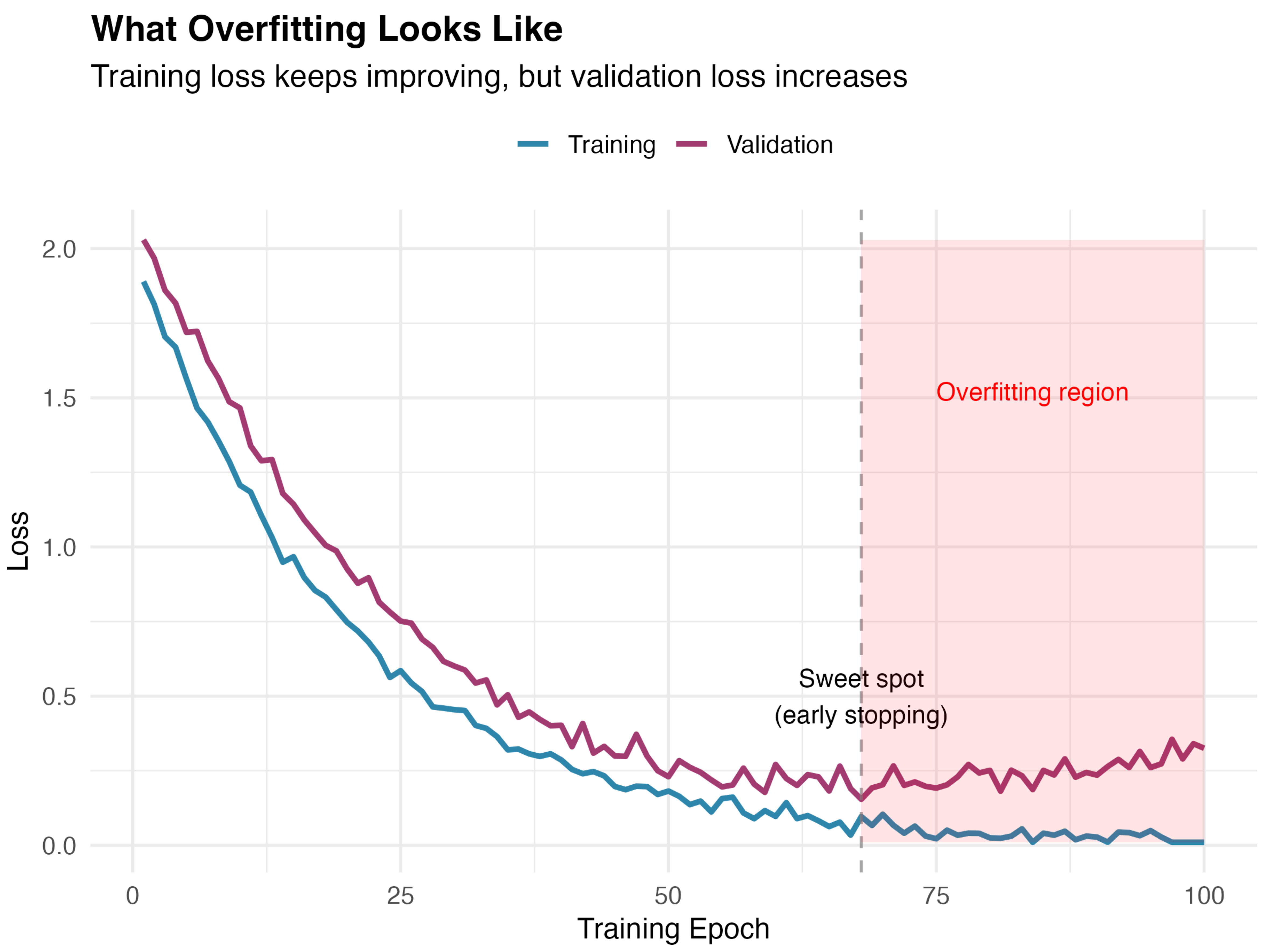
  - **Model complexity**: what capacity does the model have to **fit complex patterns?**



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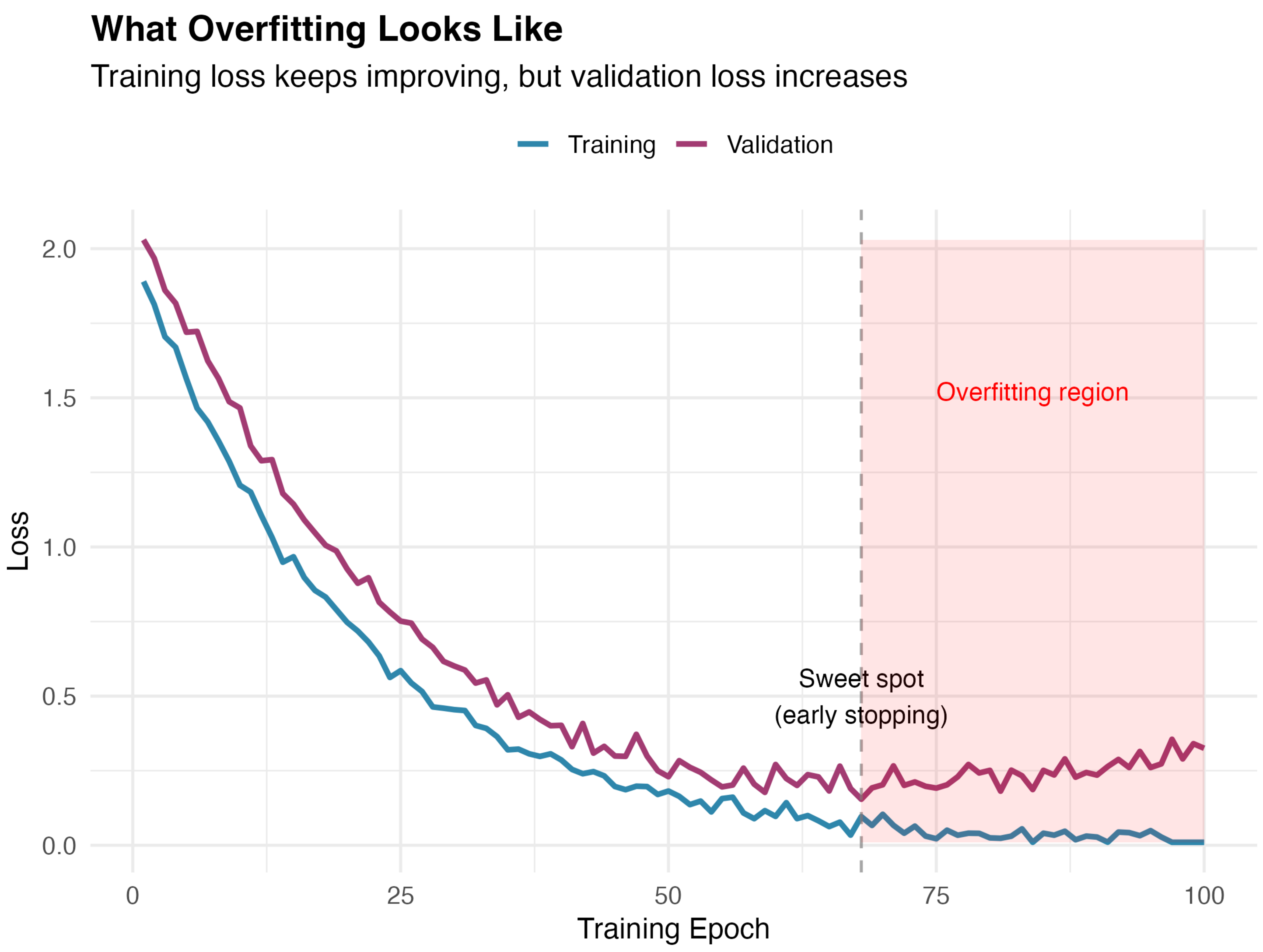
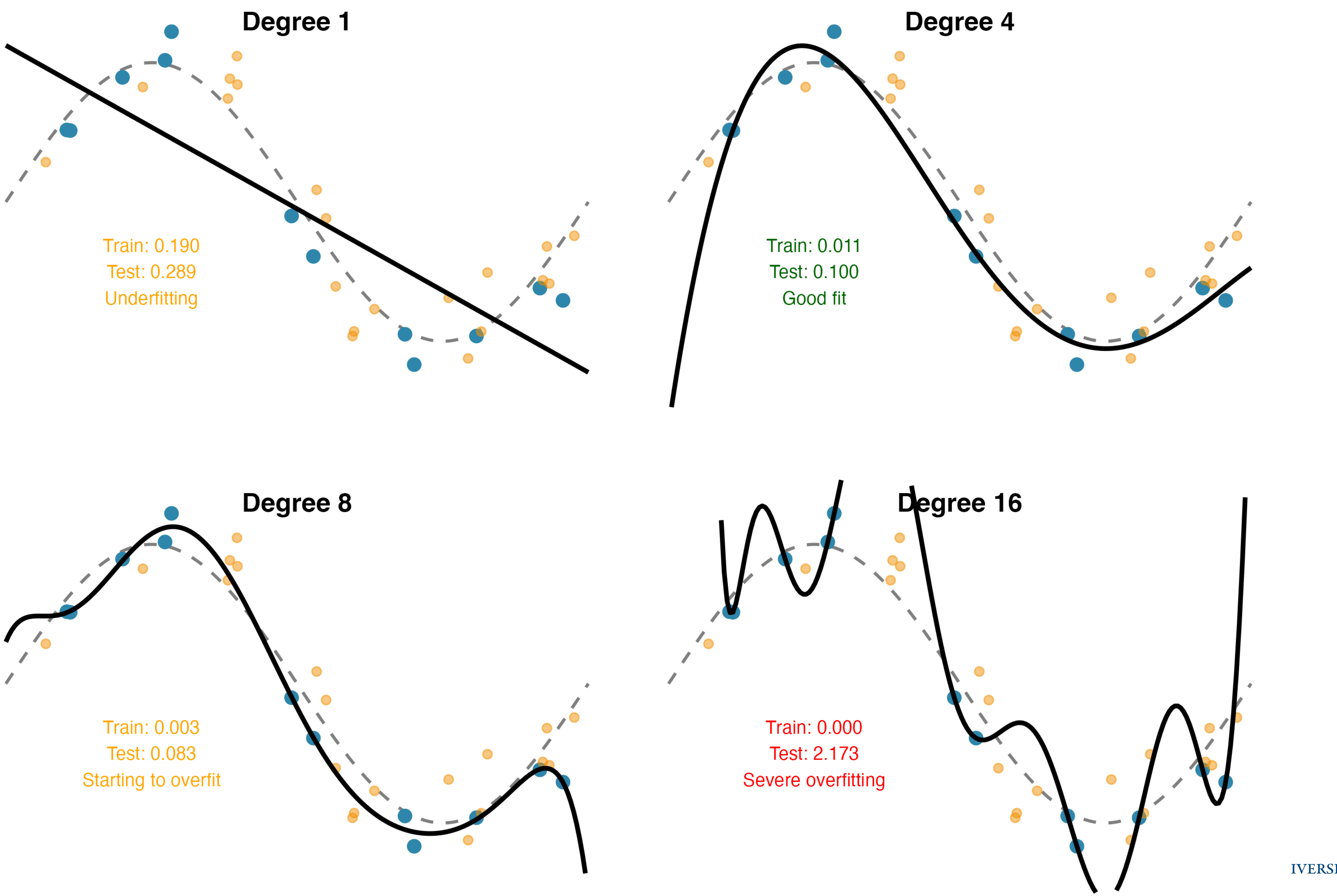
- The latter is classically demonstrated with **polynomial regression** (next slide)



Model Complexity vs. Overfitting
Blue = training data, Orange = test data, Dashed = true function



Bias and Variance

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  - Example: fitting a **linear regression** to **non-linear data**
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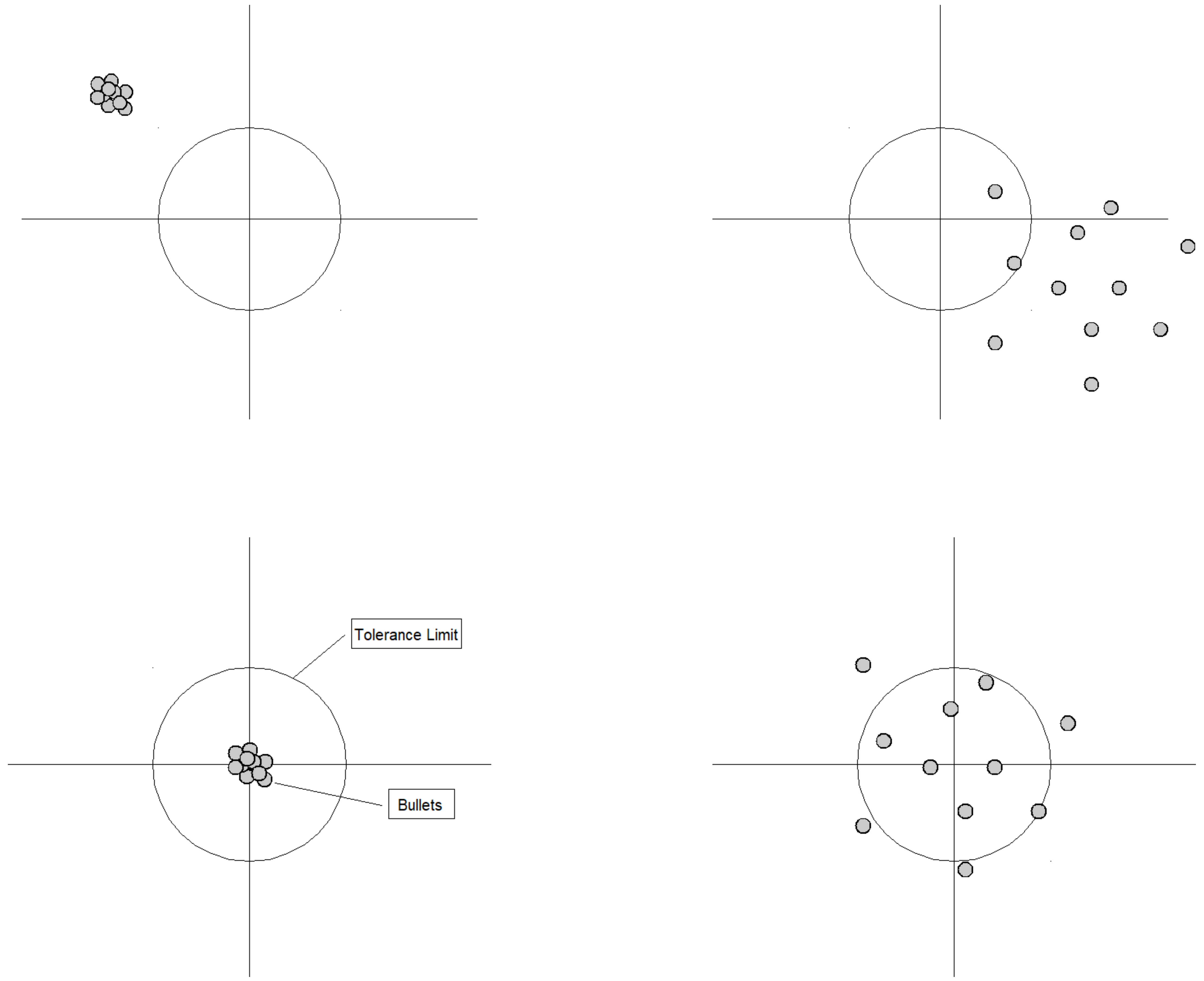
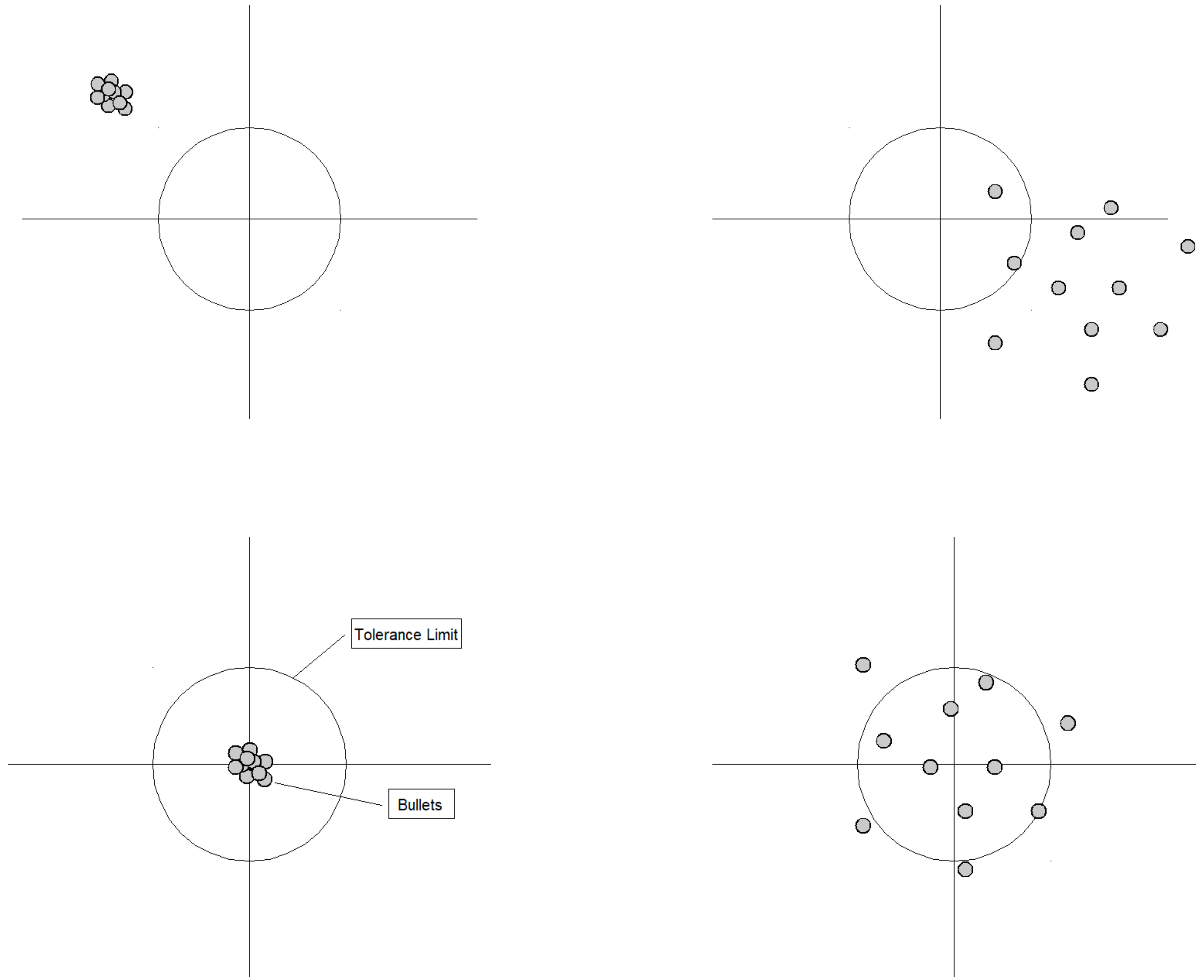
- Bias and Variance inherently form a **tradeoff** - we can't minimize both at once

Bias and Variance



Bias and Variance

high bias
low variance



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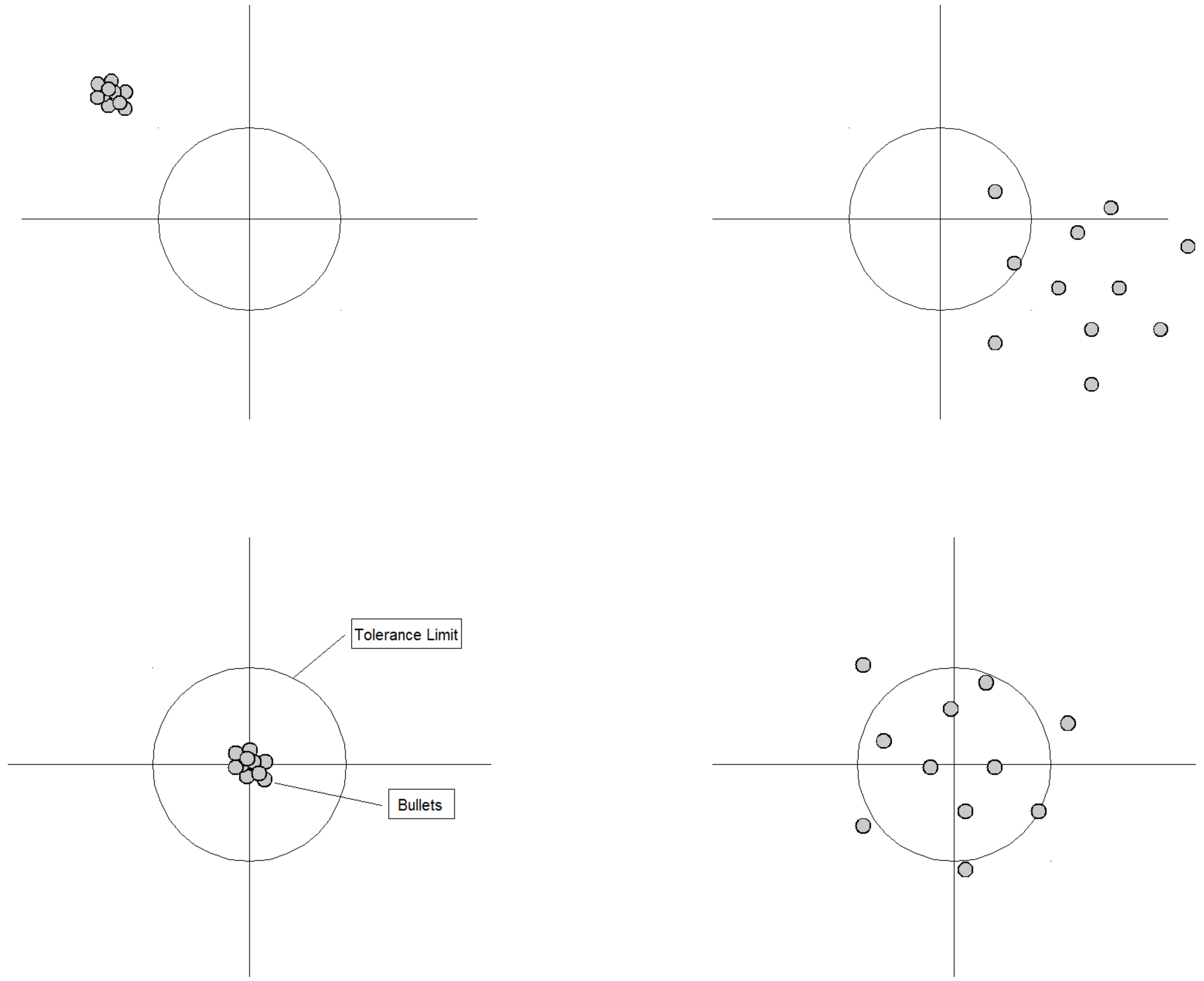

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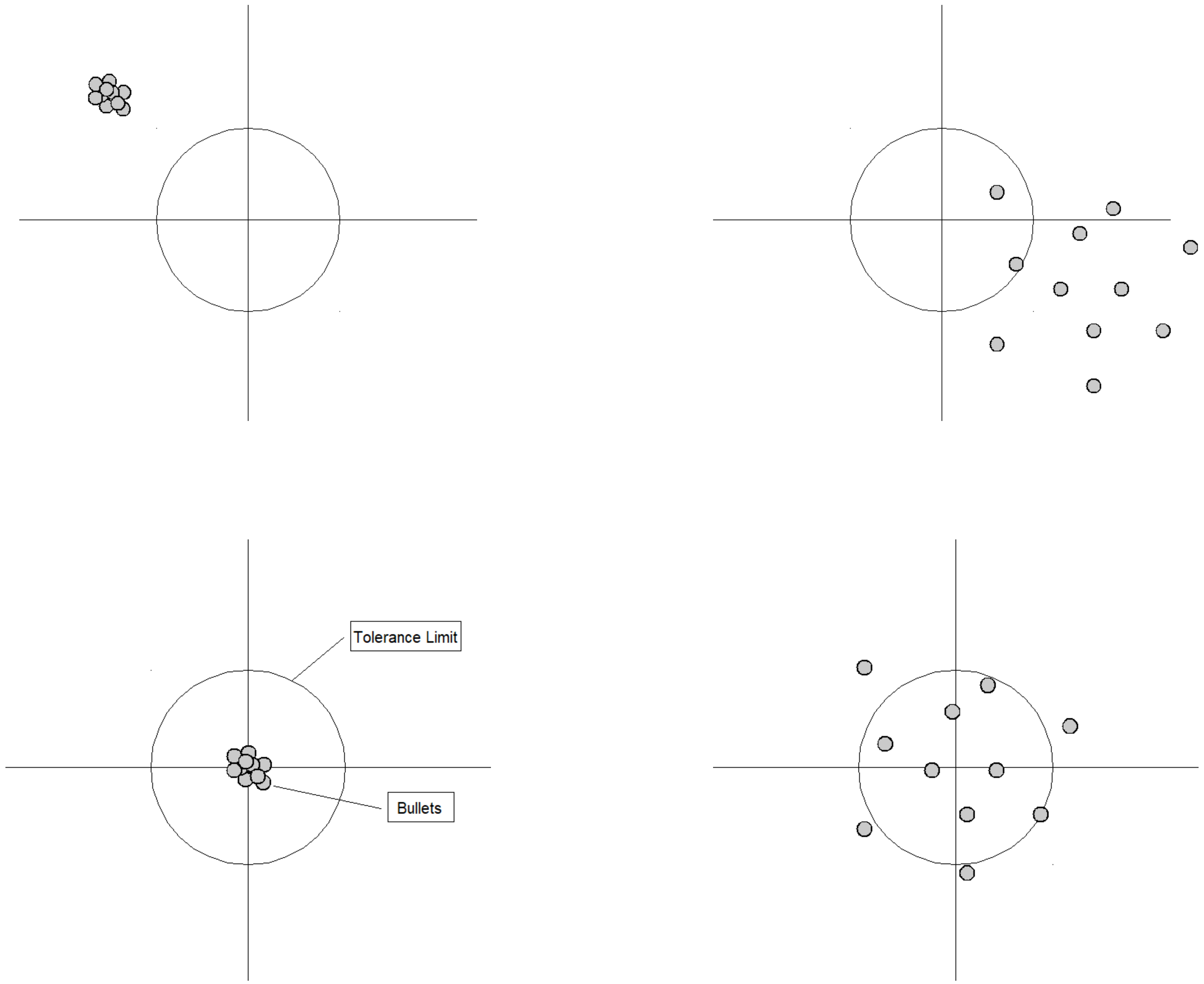

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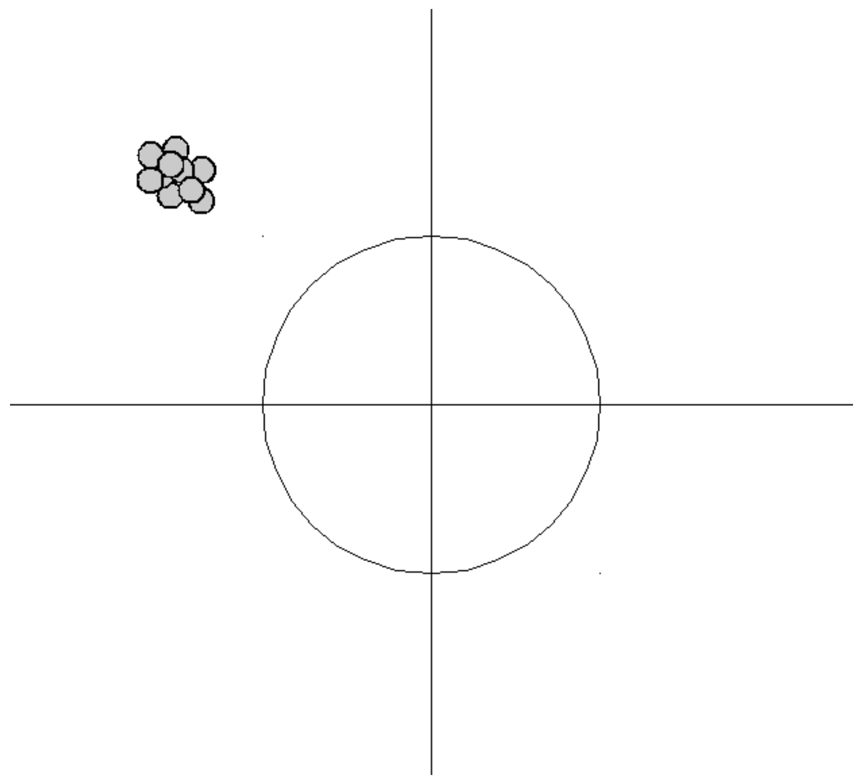

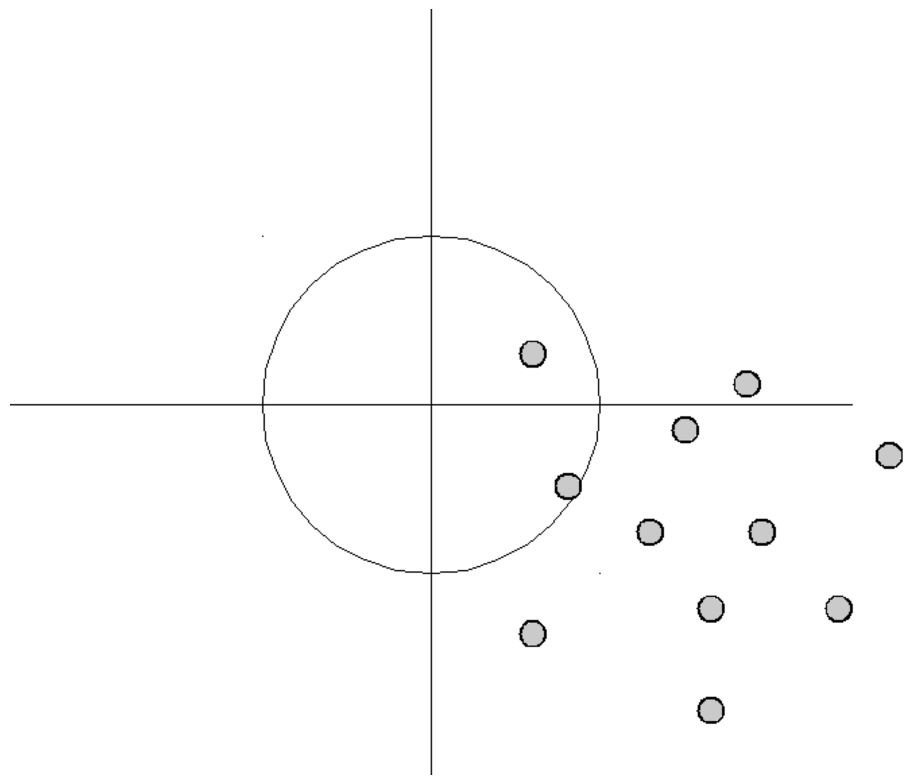

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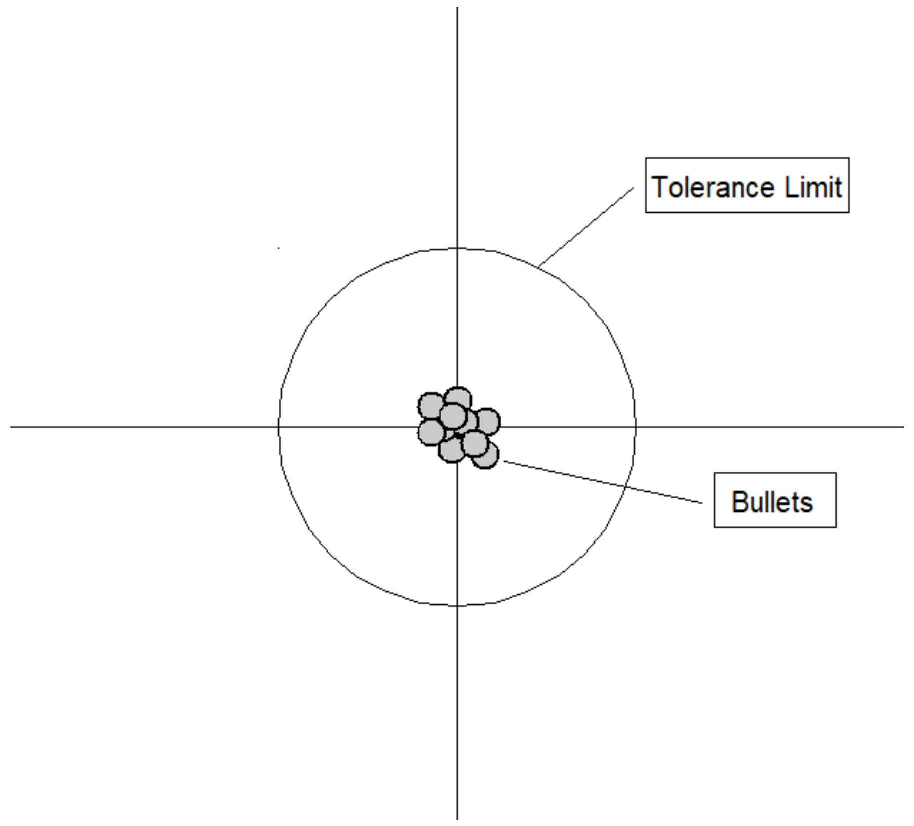

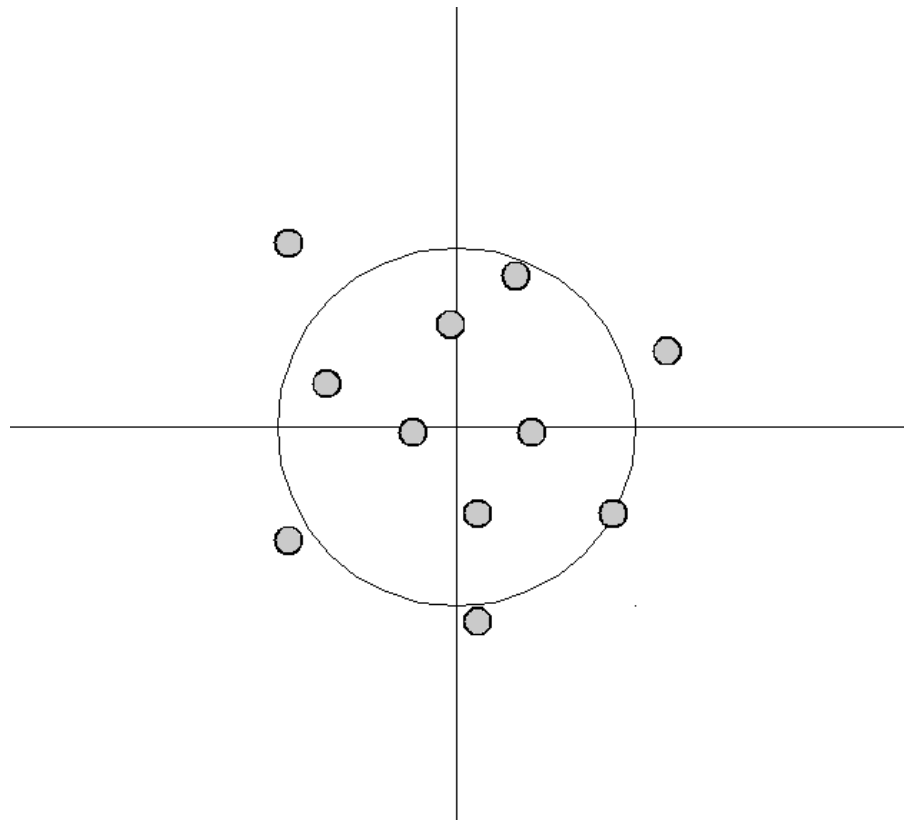

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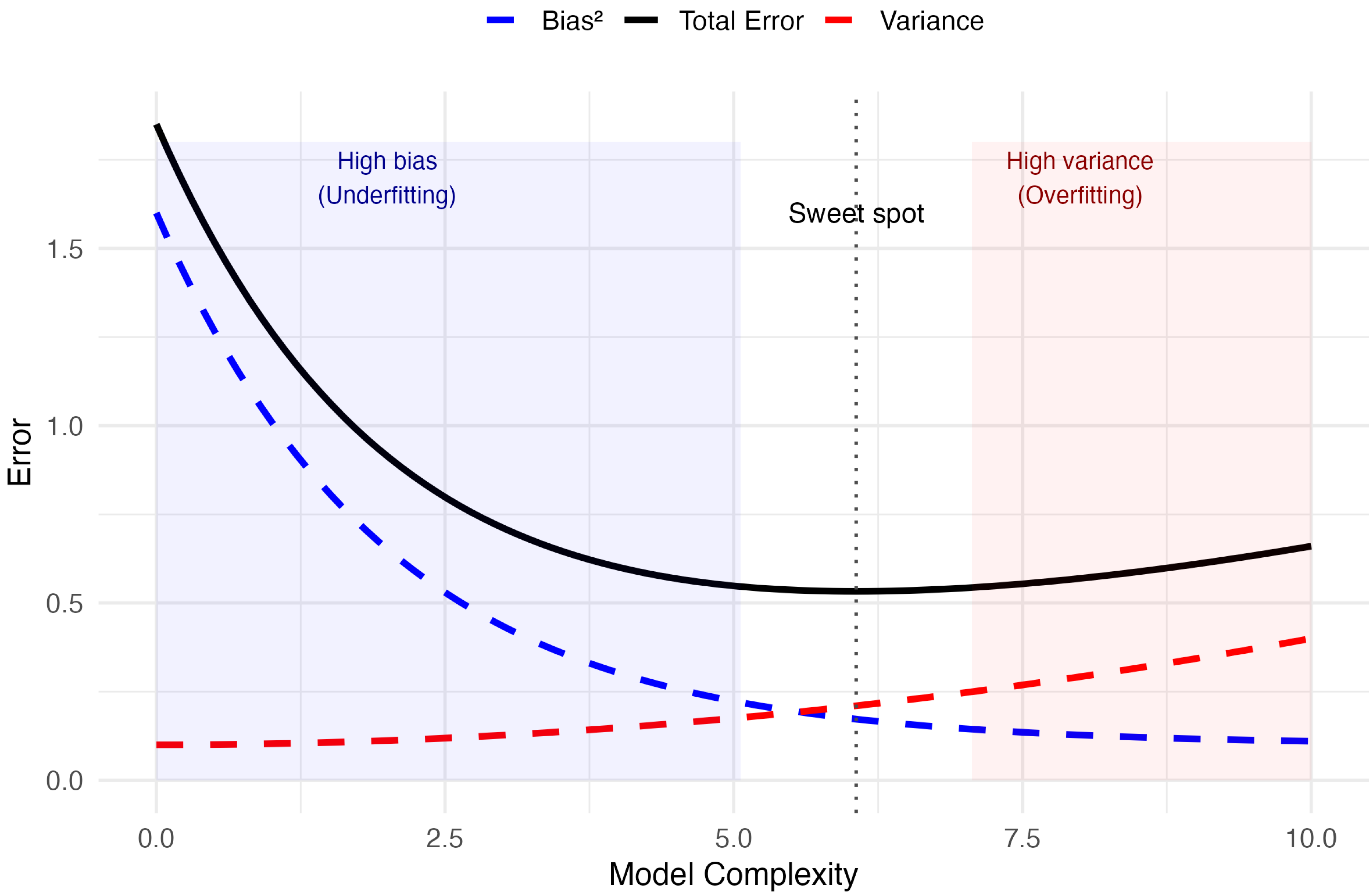
The Bias-Variance Tradeoff

Total error is minimized at intermediate complexity



Mitigating Overfitting

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  - Based on the "L2 Norm" (**Euclidian Distance**) of the weight vector
  - Strength controlled by **hyperparameter** λ**:** loss += $\lambda\Sigma\theta_i^2$
- **L1 Regularization**: penalizes large weights (in a different way)
  - Based on "L1 Norm" aka **"Manhattan Distance"** of the weight vector
  - Tends to **drive some weights to zero** (creating a sparse model)
  - loss += $\lambda\Sigma|\theta_i|$

L1 and L2 Visualized

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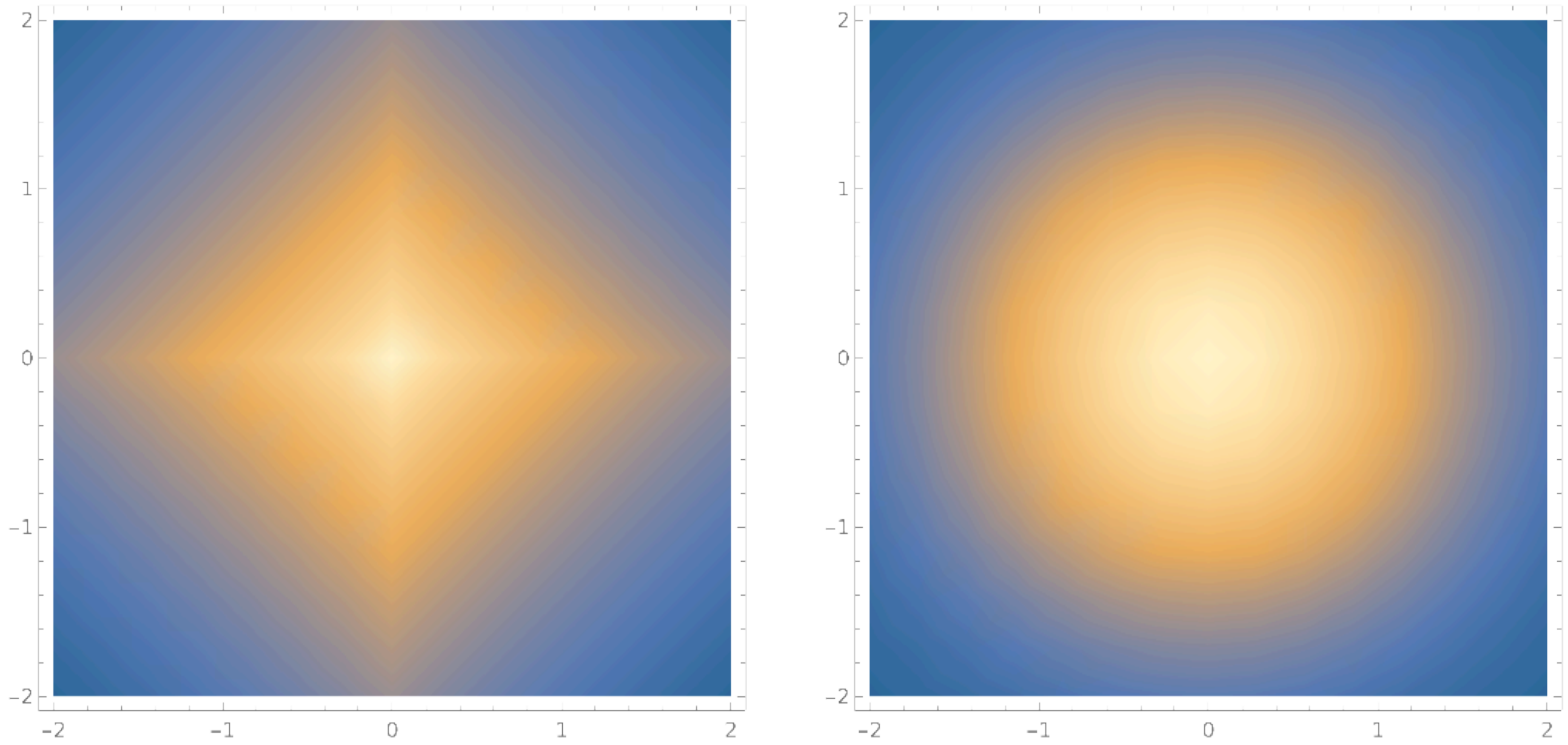

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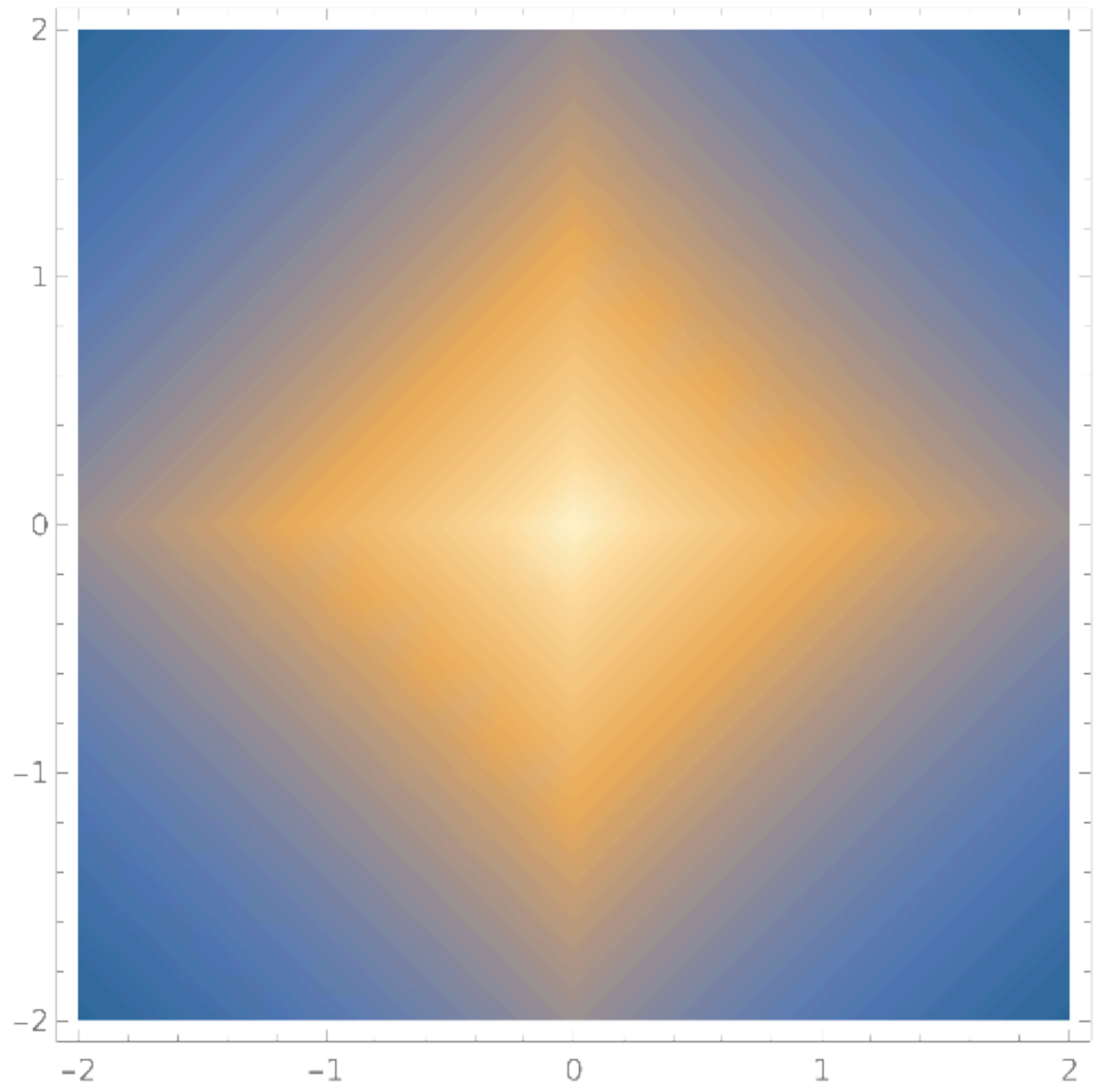
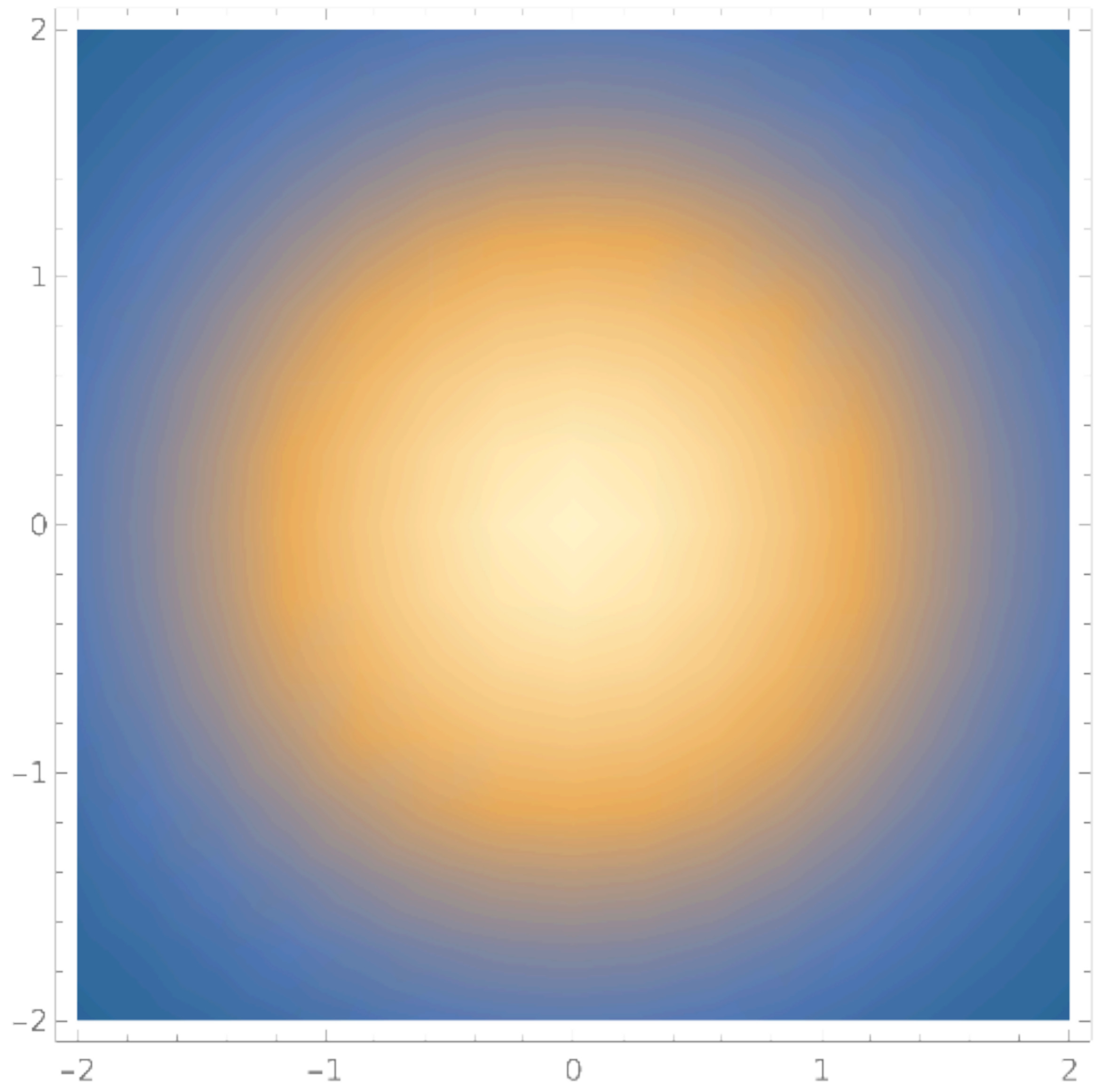
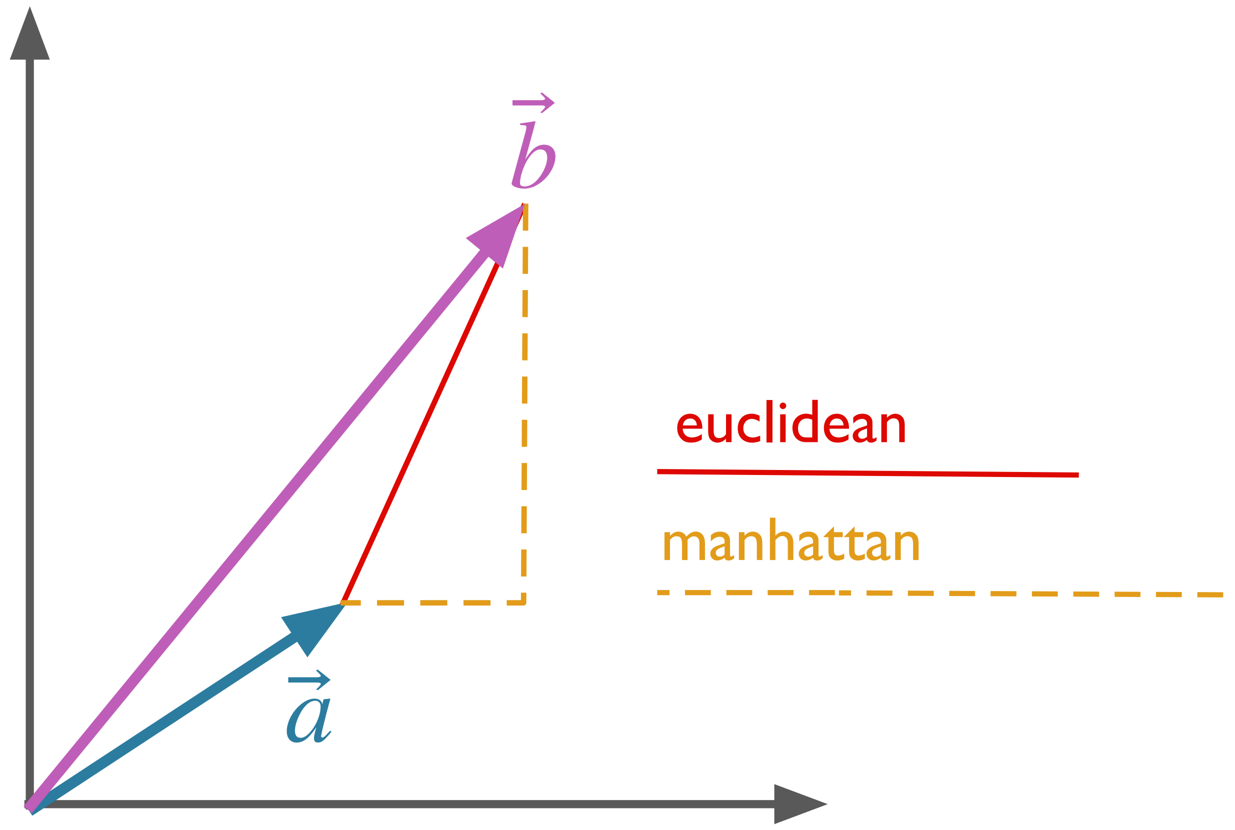


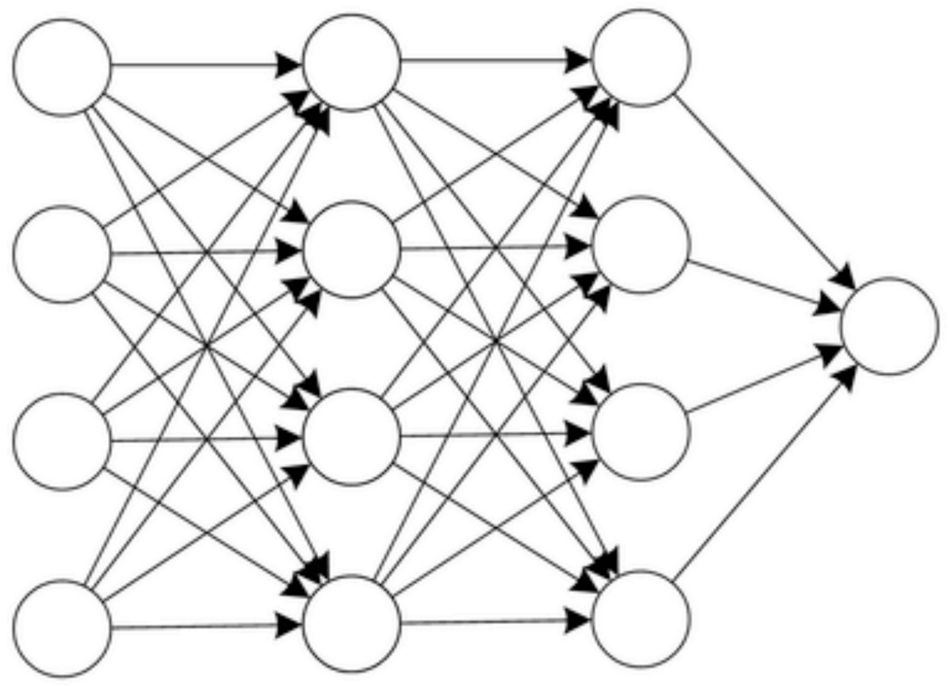
L1



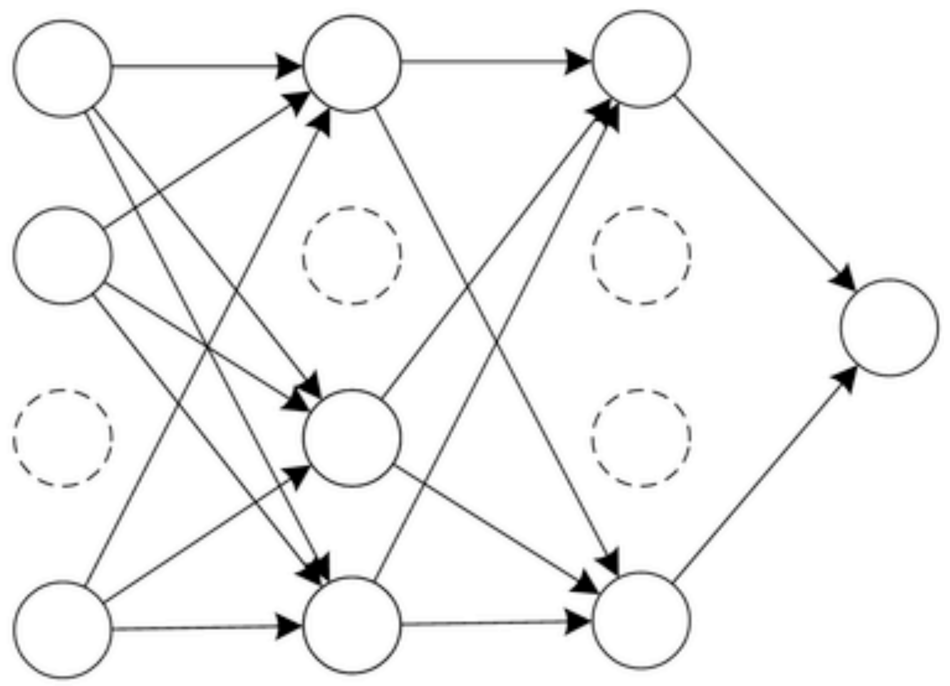
L2



Dropout



(a) Standard Neural Network



(b) Network after Dropout

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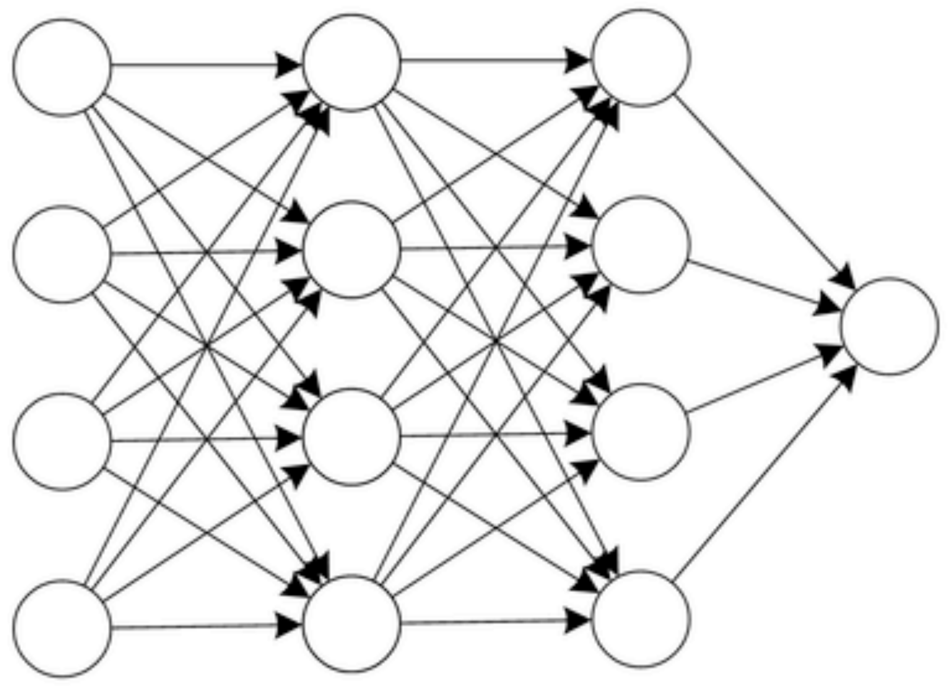
- Mostly used in **neural networks** (or other models with many parameters)



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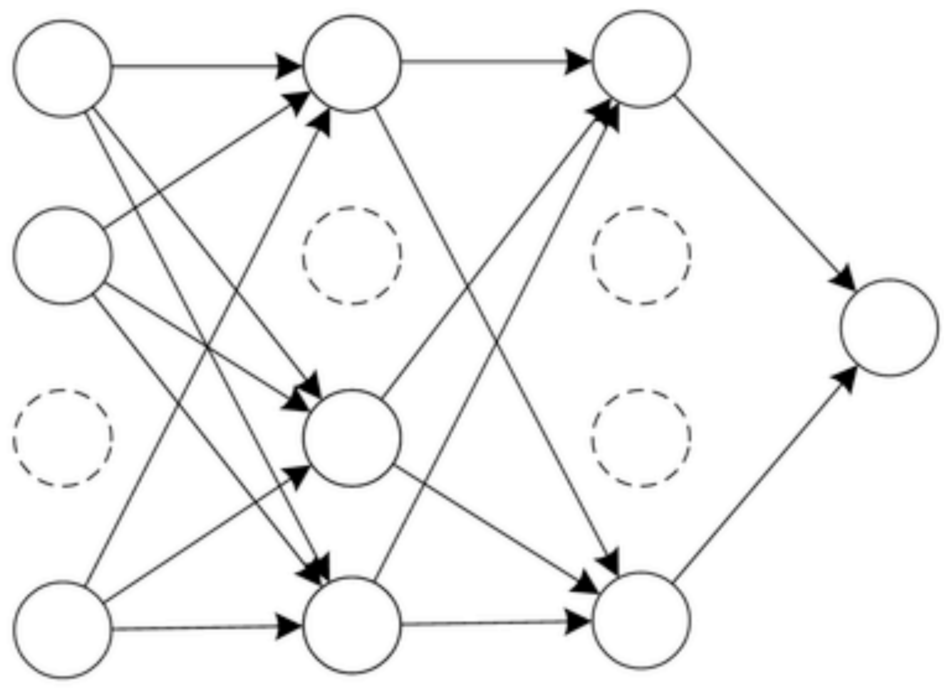

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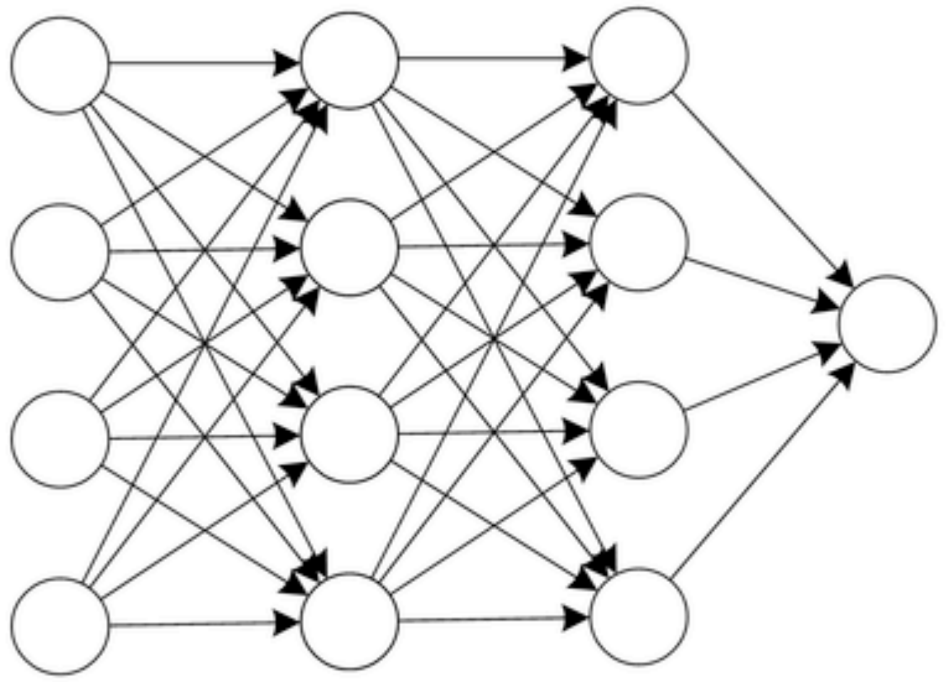

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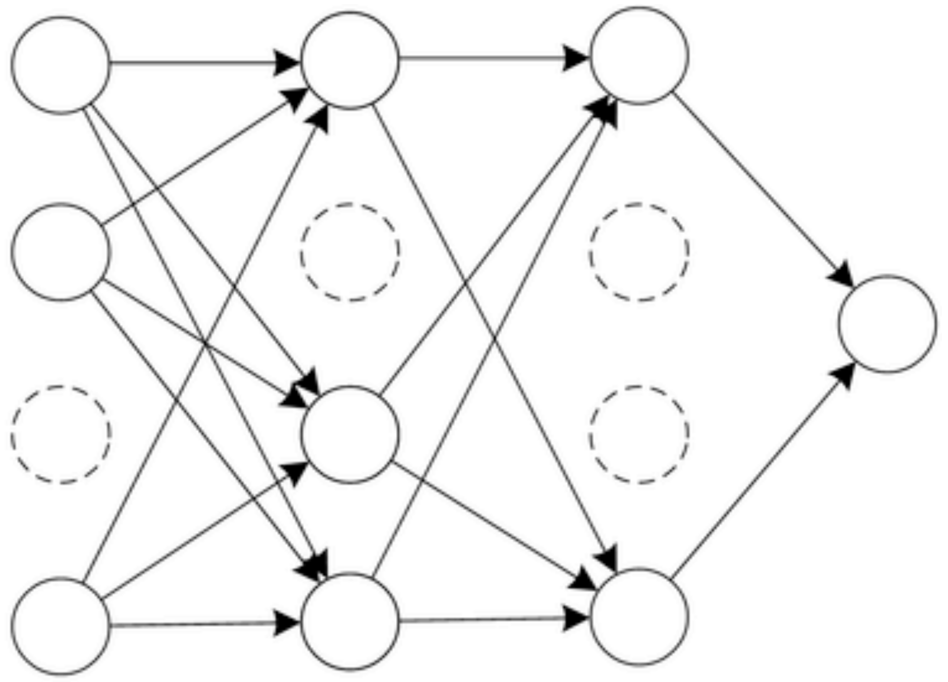

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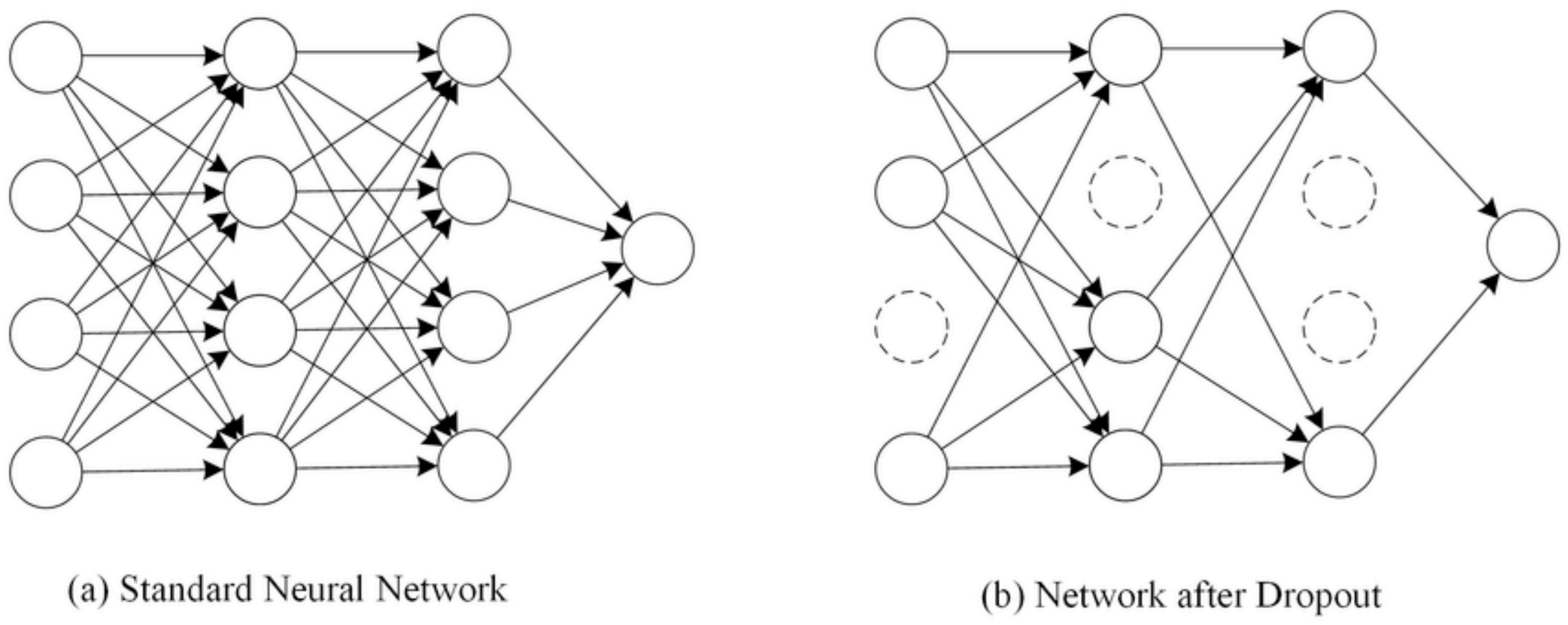
- Forces the network to use **redundant representations**
  - Put another way, avoids **memorizing examples** with **single parameters**



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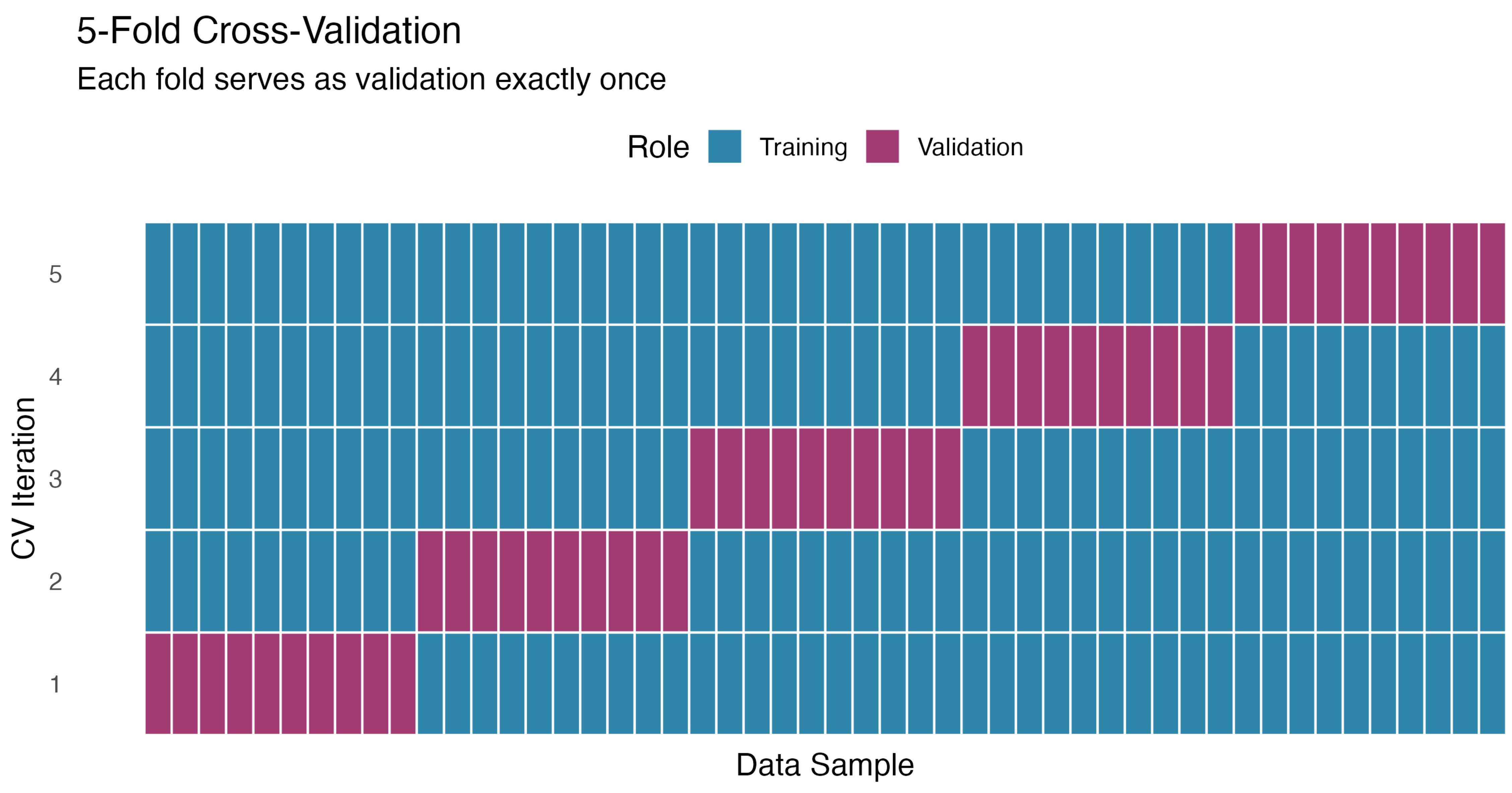
- **Data Augmentation**: more later; idea is to **artificially expand** the training set

Final point: Cross-Validation



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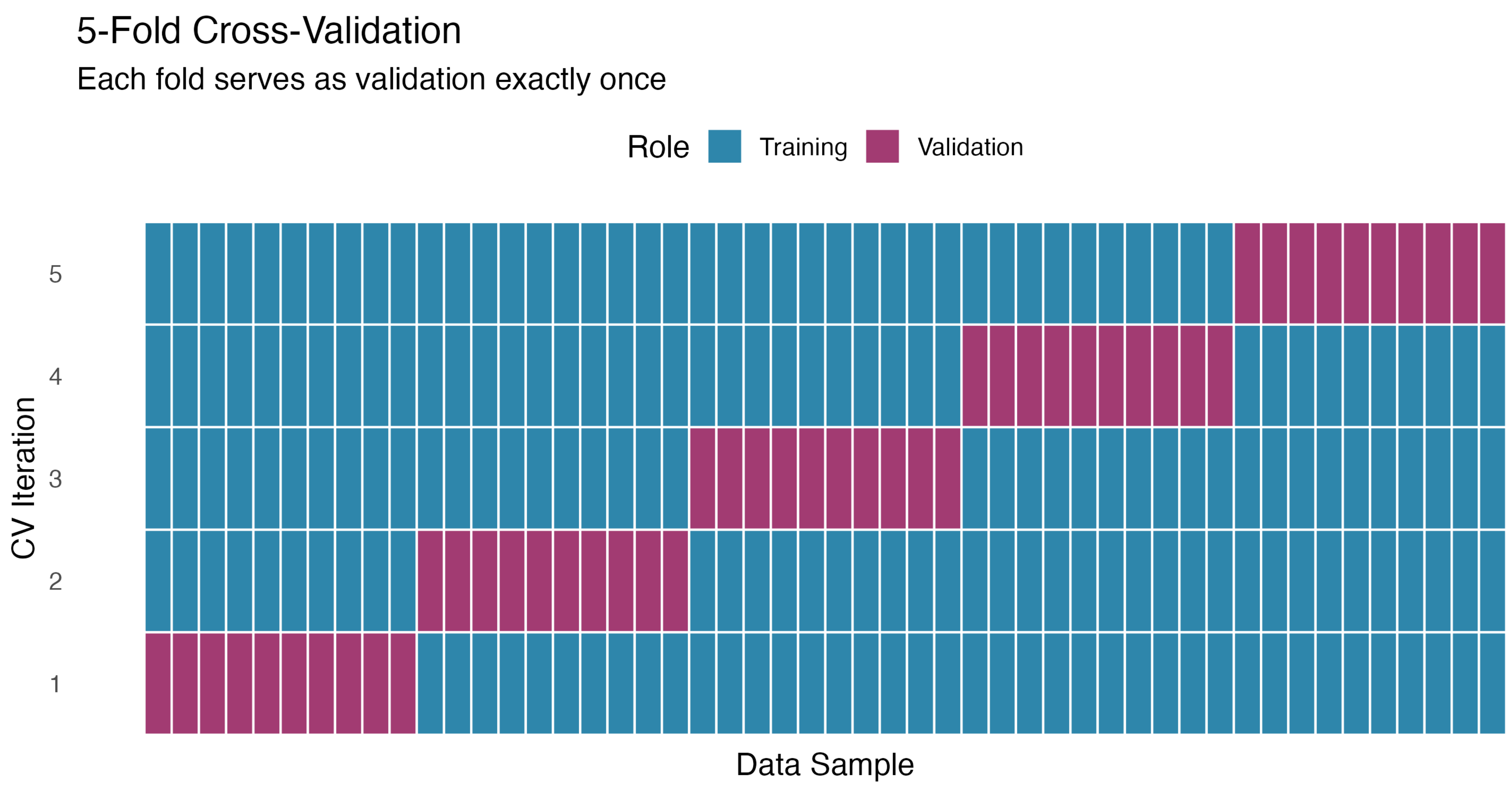

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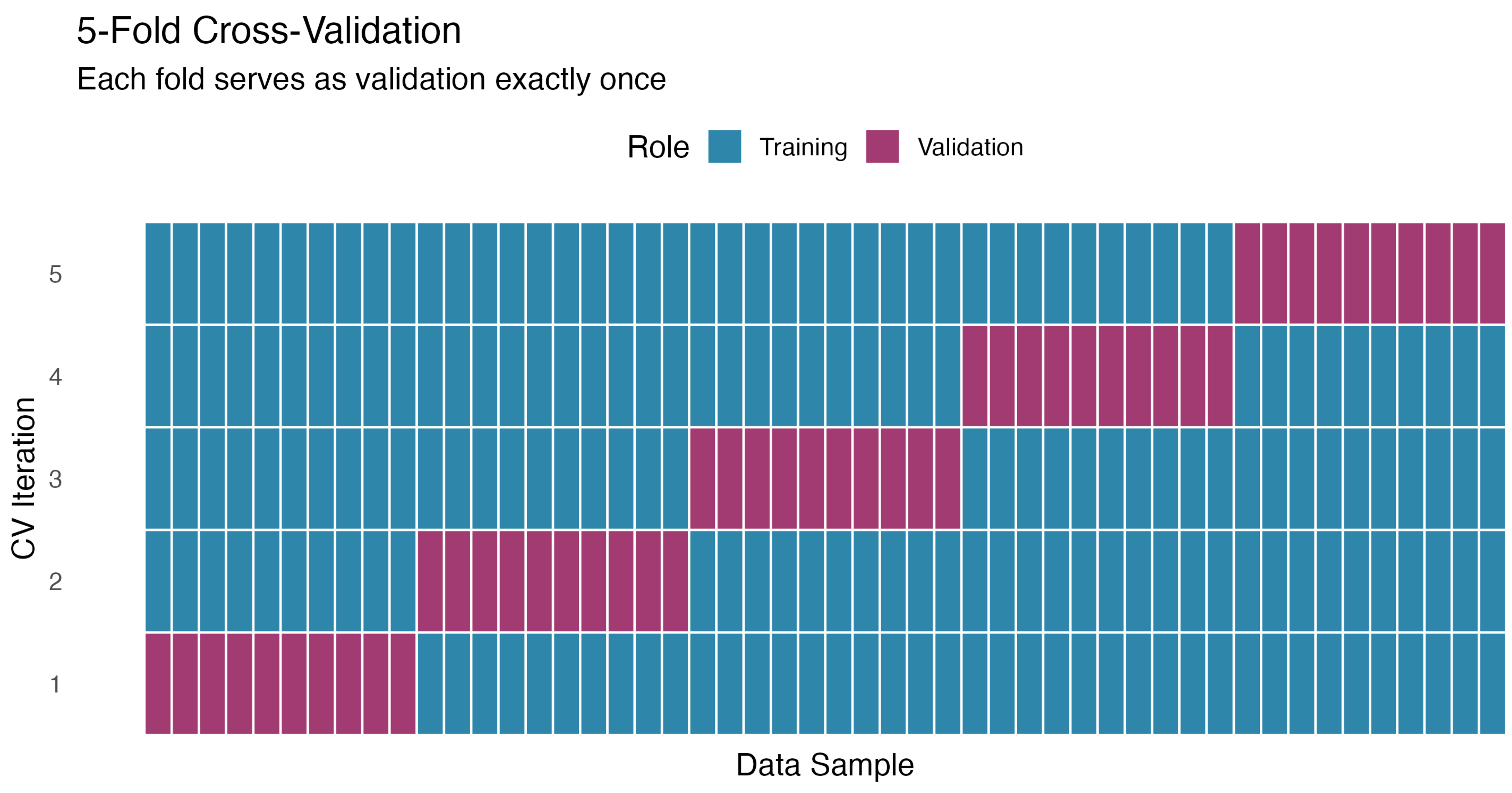
  - Do this **K times**, then **average the result**



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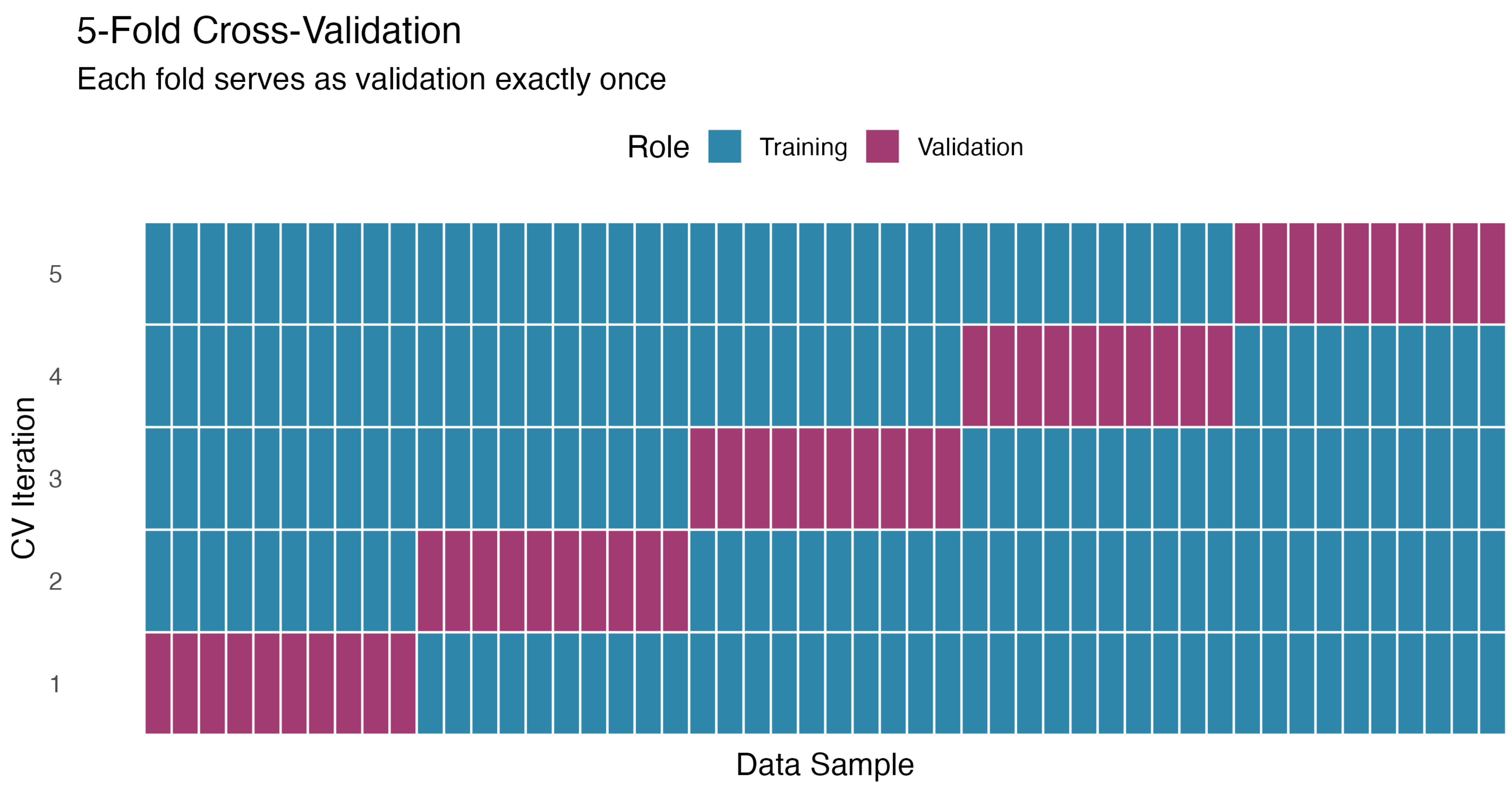
- Gives a **more reliable estimate** of generalization



5-Fold Cross-Validation

Each fold serves as validation exactly once