EE2211 Introduction to Machine Learning

Lecture 8

Vincent Tan
vtan@nus.edu.sg

Electrical and Computer Engineering Department
National University of Singapore

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Thomas, Helen, Xinchao, Kar-Ann, Chen Khong, Robby, and Haizhou

Course Contents

- Introduction and Preliminaries (Xinchao)
  - Introduction
  - Data Engineering
  - Introduction to Probability and Statistics
- Fundamental Machine Learning Algorithms I (Vincent)
  - Systems of linear equations
  - Least squares, Linear regression
  - Ridge regression, Polynomial regression
- Fundamental Machine Learning Algorithms II (Vincent)
  - Over-fitting, bias/variance trade-off
  - Optimization, Gradient descent
  - Decision Trees, Random Forest
- Performance and More Algorithms (Xinchao)
  - Performance Issues
  - K-means Clustering
  - Neural Networks

Fundamental ML Algorithms: Optimization, Gradient Descent

Module III Contents

- Overfitting, underfitting and model complexity
- Regularization
- Bias-variance trade-off
- Loss function
- Optimization
- Gradient descent
- Decision trees
- Random forest

Review

- Supervised learning: given feature(s) x, we want to predict target y $y \in \mathbb{R}$ (regression) $y \in \{-1, +1\}$ bin. classif.

Review

- Supervised learning: given feature(s) x, we want to predict target y
- Most supervised learning algorithms can be formulated as the following optimization problem

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, \mathbf{Data\text{-}Loss}(\mathbf{w}) + \lambda \mathbf{Regularization}(\mathbf{w})$$

- **Data-Loss(w)** quantifies fitting error to training set given parameters **w:** smaller error => better fit to training data
- **Regularization(w)** penalizes more complex models

Review

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- **Data-Loss(w)** quantifies fitting error to training set given parameters **w**: smaller error => better fit to training data
- **Regularization(w)** penalizes more complex models
- For example, in the case of polynomial regression (previous lectures):

$$\underset{\mathbf{w}}{\operatorname{argmin}} \underbrace{(\mathbf{Pw}-\mathbf{y})^T(\mathbf{Pw}-\mathbf{y})}_{\textbf{Data-Loss(w)}} + \underbrace{\lambda \mathbf{w}^T\mathbf{w}}_{\textbf{Reg(w)}}$$

Review

- For polynomial regression (previous lectures)

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, C(\mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}}\, (\mathbf{P}\mathbf{w} - \mathbf{y})^T(\mathbf{P}\mathbf{w} - \mathbf{y}) + \lambda \mathbf{w}^T\mathbf{w}$$

Review

- For polynomial regression (previous lectures)

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$$= \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{m} (\mathbf{p}_i^T\mathbf{w} - y_i)^2 + \lambda \mathbf{w}^T\mathbf{w}$$

$\mathbf{p}_i^T\mathbf{w}$ is prediction of i-th training sample

y_i is target of i-th training sample

Review

- For polynomial regression (previous lectures)

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- Linear regression with 2 features, $\mathbf{p}_i = \begin{bmatrix} 1 \\ x_{1,i} \\ x_{2,i} \end{bmatrix}$
  - — Bias/Offset
  - — Feature 1 of i-th sample
  - — Feature 2 of i-th sample

Review

$P^T P + \lambda I$ is invertible.

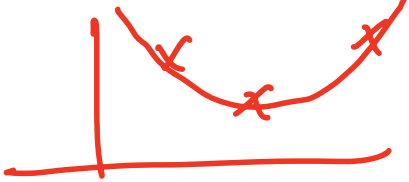
- For polynomial regression (previous lectures)

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, C(\mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}}\, \underbrace{(\mathbf{P}\mathbf{w}-\mathbf{y})^T(\mathbf{P}\mathbf{w}-\mathbf{y})}_{\text{data-loss}} + \underbrace{\lambda \mathbf{w}^T\mathbf{w}}_{\text{regularization.}}$$

L_2 loss

$$= \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{m} (\mathbf{p}_i^T\mathbf{w} - y_i)^2 + \lambda \mathbf{w}^T\mathbf{w}$$

- Linear regression with 2 features, $\mathbf{p}_i = \begin{bmatrix} 1 \\ x_{1,i} \\ x_{2,i} \end{bmatrix}$
  - 1 — Bias/Offset
  - $x_{1,i}$ — Feature 1 of i-th sample (height)
  - $x_{2,i}$ — Feature 2 of i-th sample (weight)
- Quadratic regression with 1 feature, $\mathbf{p}_i = \begin{bmatrix} 1 \\ x_i \\ x_i^2 \end{bmatrix}$
  - 1 — Bias/Offset
  - x_i — x is feature of i-th sample
  - x_i^2 — square; $x_i^2 = x_i x_i$



Loss Function & Learning Model

- For polynomial regression (previous lectures)

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- Let $f(\mathbf{x}_i, \mathbf{w})$ be the prediction of target y_i from features $\mathbf{x}_i$ for i-th training sample. For example, suppose $f(\mathbf{x}_i, \mathbf{w}) = \mathbf{p}_i^T\mathbf{w}$, then above becomes

$$\mathbf{p}_i = \begin{bmatrix} x_{1,i} \\ x_{2,i} \end{bmatrix}$$

2 features affine model

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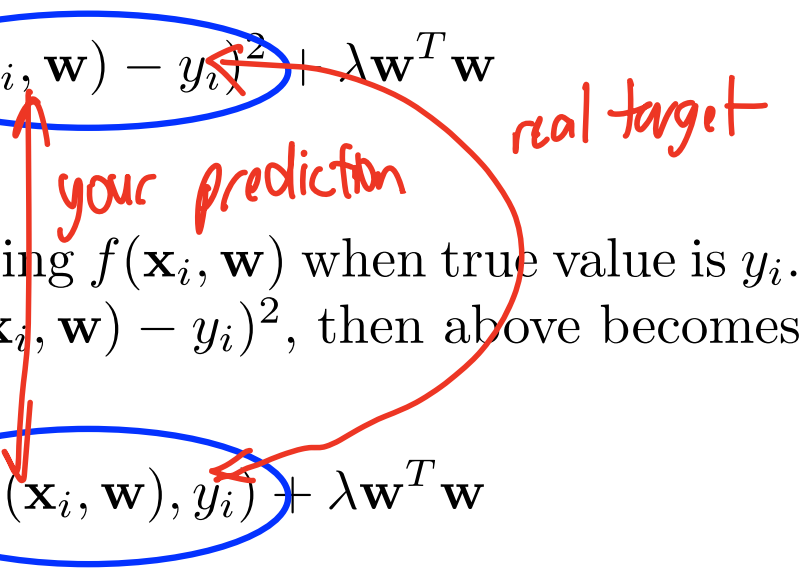

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$$\underset{\mathbf{w}}{\operatorname{argmin}} C(\mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{m} L(f(\mathbf{x}_i, \mathbf{w}), y_i) + \lambda \mathbf{w}^T\mathbf{w}$$

Loss Function & Learning Model

- From previous slide

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Loss function

regularization

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$$\underset{\mathbf{w}}{\operatorname{argmin}} C(\mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{m} L(f(\mathbf{x}_i, \mathbf{w}), y_i) + \lambda R(\mathbf{w})$$

Loss Function & Learning Model

- From previous slide

$$w^T w = \sum_{i=1}^{d} w_i^2$$

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Cost Function Loss Function Learning Model Regularization

Building Blocks of ML algorithms

- From previous slide

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$f(x_i, w) = \begin{bmatrix} 1 \\ x_{1,i} \\ x_{2,i} \end{bmatrix}$

believe affine r/s bet. x_i & y_i

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weight/waist length ↑ height

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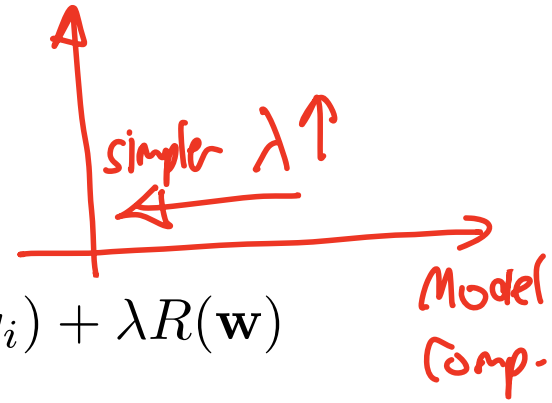

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- Regularization R encourages less complex models

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regularization param

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- Cost function C is the final optimization criterion we want to minimize

$\lambda \uparrow$: encourage simpler models.

Building Blocks of ML algorithms

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- Regularization R encourages less complex models
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- Optimization routine to find solution to cost function

Motivation for Gradient Descent

- Different learning function f, loss function L & regularization R give rise to different learning algorithms

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- In polynomial regression (previous lectures), optimal $\mathbf{w}$ can be written with the following "closed-form" formula (primal solution):

$$\hat{\mathbf{w}} = (\mathbf{P}_{train}^T \mathbf{P}_{train} + \lambda \mathbf{I})^{-1} \mathbf{P}_{train}^T \mathbf{y}_{train}$$

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closed-form

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easy

- For other learning function f, loss function L & regularization R, optimizing $C(\mathbf{w})$ might not be so easy
- Usually have to estimate $\mathbf{w}$ iteratively with some algorithm
- Optimization workhorse for modern machine learning is gradient descent

$f(w)$

Questions?

Gradient Descent Algorithm

- Suppose we want to minimize $C(\mathbf{w})$ with respect to $\mathbf{w} = [w_1, \cdots, w_d]^T$

Gradient Descent Algorithm

- Suppose we want to minimize $C(\mathbf{w})$ with respect to $\mathbf{w} = [w_1, \cdots, w_d]^T$
- Gradient $\nabla_{\mathbf{w}} C(\mathbf{w}) = \begin{pmatrix} \frac{\partial C}{\partial w_1} \\ \frac{\partial C}{\partial w_2} \\ \vdots \\ \frac{\partial C}{\partial w_d} \end{pmatrix} \in \mathbb{R}^d$

$w^* = \arg\min_{\underline{w}} C(\underline{w})$

$C(w)$ gradient $\frac{dC}{dw}$

$C(\underline{w})$

e.g. $C(\underline{w}) = C(w_1, w_2) = w_1^2 + 2w_1w_2 + w_2^3$

$\underline{w} = (w_1, w_2)$

$\nabla_{\underline{w}} C(\underline{w}) = \begin{bmatrix} \frac{\partial C}{\partial w_1} \\ \frac{\partial C}{\partial w_2} \end{bmatrix} = \begin{bmatrix} 2w_1 + 2w_2 \\ 2w_1 + 3w_2^2 \end{bmatrix}$

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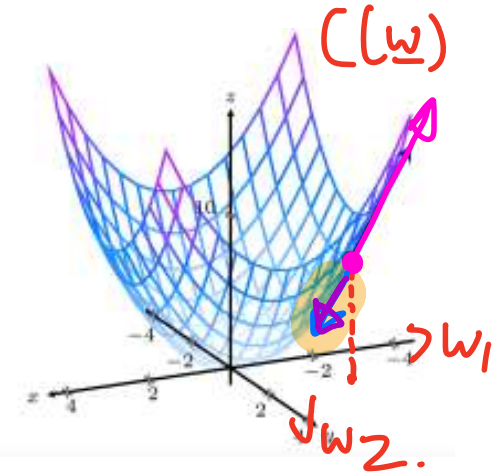

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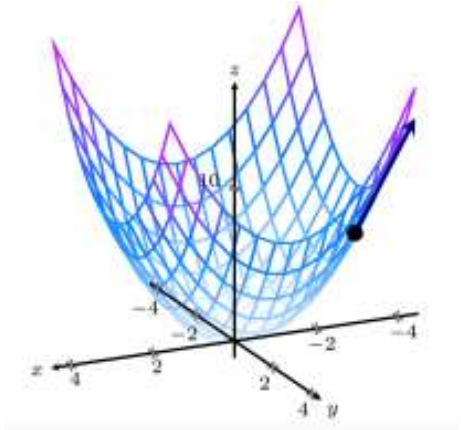

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  Initialize $\mathbf{w}_0$ and learning rate η;

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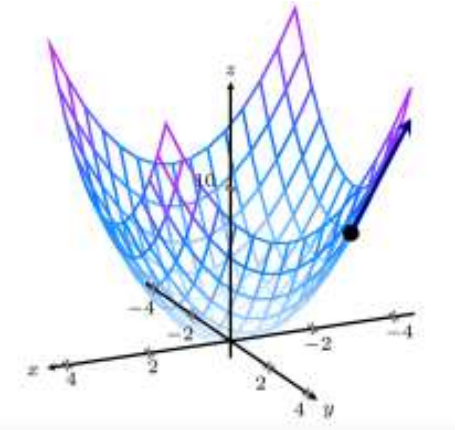

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while *true* **do**
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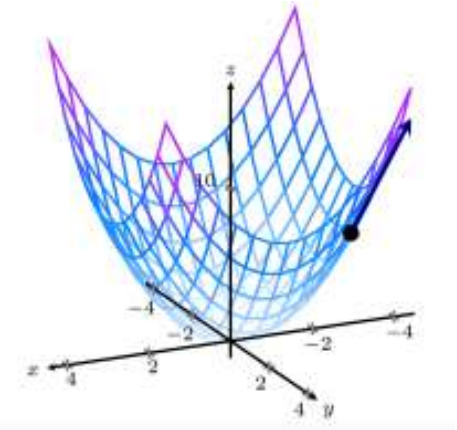

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- Gradient Descent:

Initialize $\mathbf{w}_0$ and learning rate η;
while *true* **do**
  Compute $\mathbf{w}_{k+1} \leftarrow \mathbf{w}_k - \eta \nabla_{\mathbf{w}} C(\mathbf{w}_k)$
end

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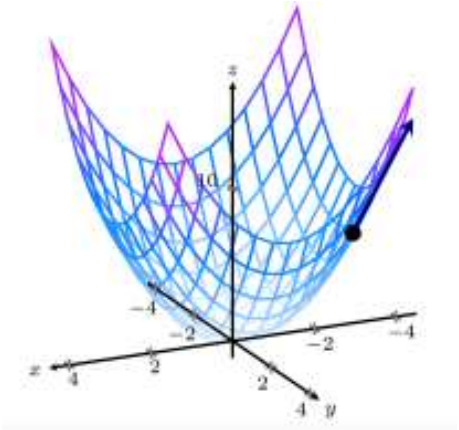
- Suppose we want to minimize $C(\mathbf{w})$ with respect to $\mathbf{w} = [w_1, \cdots, w_d]^T$
- Gradient $\nabla_{\mathbf{w}} C(\mathbf{w}) = \begin{pmatrix} \frac{\partial C}{\partial w_1} \\ \frac{\partial C}{\partial w_2} \\ \vdots \\ \frac{\partial C}{\partial w_d} \end{pmatrix}$



  - $\nabla_{\mathbf{w}} C(\mathbf{w})$ is vector & function of $\mathbf{w}$
  - $\nabla_{\mathbf{w}} C(\mathbf{w})$ is direction at $\mathbf{w}$ where C is increasing most rapidly, so $-\nabla_{\mathbf{w}} C(\mathbf{w})$ is direction at $\mathbf{w}$ where C is decreasing most rapidly

- Gradient Descent:

Initialize $\mathbf{w}_0$ and learning rate η;
while *true* **do**
  Compute $\mathbf{w}_{k+1} \leftarrow \mathbf{w}_k - \eta \nabla_{\mathbf{w}} C(\mathbf{w}_k)$
end

According to multi-variable calculus, if eta is not too big, then $C(\mathbf{w}_{k+1}) < C(\mathbf{w}_k)$ => we get better $\mathbf{w}$ after each iteration

Gradient Descent Algorithm

- Suppose we want to minimize $C(\mathbf{w})$ with respect to $\mathbf{w} = [w_1, \cdots, w_d]^T$
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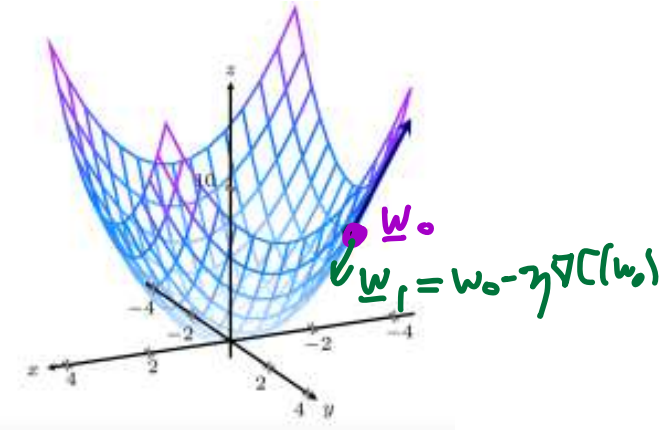

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  if *converge* **then**
    return $\mathbf{w}_{k+1}$
  end
end

step size / learning rate

k^{th} iterate

η

According to multi-variable calculus, if ~~eta~~ η is not too big, then $C(\mathbf{w}_{k+1}) < C(\mathbf{w}_k)$ => we get better $\mathbf{w}$ after each iteration

smaller cost

current cost.

Gradient Descent Algorithm

- Gradient Descent:

Initialize $\mathbf{w}_0$ and learning rate η;
while *true* **do**
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Gradient Descent Algorithm

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- Possible convergence criteria
  - Set maximum iteration k
  - Check percentage or absolute change in C below a threshold
  - Check percentage or absolute change in $\mathbf{w}$ below a threshold

Gradient Descent Algorithm

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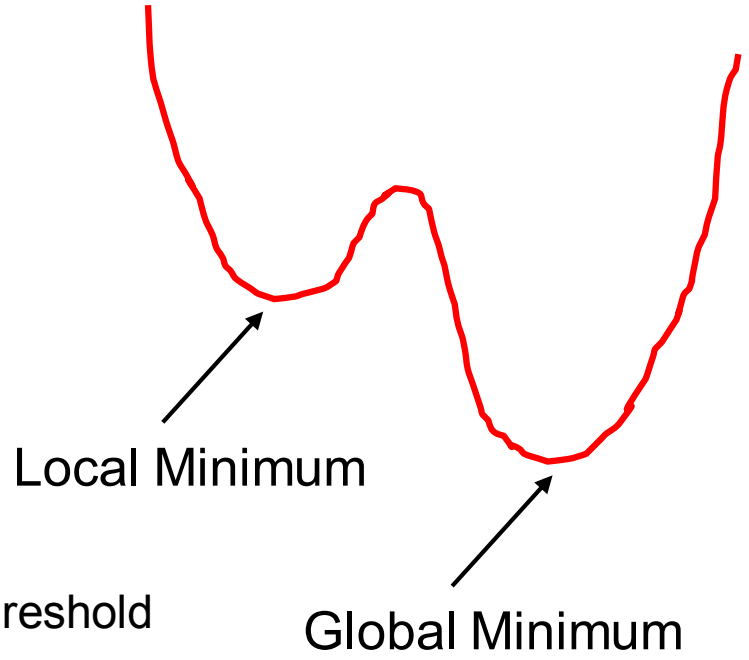
  end
end



- Possible convergence criteria
  - Set maximum iteration k
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  - Check percentage or absolute change in $\mathbf{w}$ below a threshold
- Gradient descent can only find local minimum
  - Because gradient = 0 at local minimum, so $\mathbf{w}$ won't change after that

Gradient Descent Algorithm

- Gradient Descent:

  Initialize $\mathbf{w}_0$ and learning rate η;
  while *true* **do**
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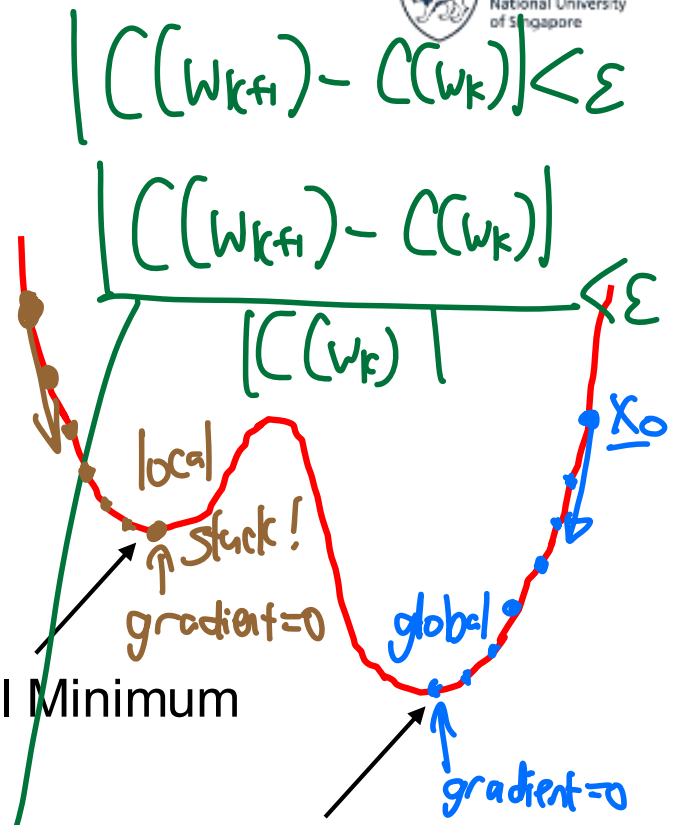
  end



- Possible convergence criteria
  - Set maximum iteration k (e.g. after 10^3 iterations)
  - Check percentage or absolute change in C below a threshold
  - Check percentage or absolute change in $\mathbf{w}$ below a threshold
- Gradient descent can only find a local minimum
  - Because gradient = 0 at local minimum, so $\mathbf{w}$ won't change after that
- Many variations of gradient descent, e.g., change how gradient is computed or learning rate η decreases with increasing k

Initial $\underline{w}_0$

while not Converged

$$\underline{w}_{k+1} = \underline{w}_k - \eta \nabla_{\underline{w}} C(\underline{w}_k)$$

Questions?

At $\underline{w}$, $\nabla C(\underline{w})$ points in the direction of steepest ascent.

Find x to minimize $g(x) = x^2$

$\underset{x \in \mathbb{R}}{\operatorname{argmin}}\ g(x) = 0.$

Find x to minimize $g(x) = x^2$

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Find x to minimize $g(x) = x^2$

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  - Gradient $\nabla_x g(x) = 2x$

$\frac{dg}{dx} = 2x$

Find x to minimize $g(x) = x^2$

- Obviously minimum corresponds to $x = 0$, but let's do gradient descent
  - Gradient $\nabla_x g(x) = 2x$
  - Initialize $x_0 = -1$, learning rate $\eta = 0.4$

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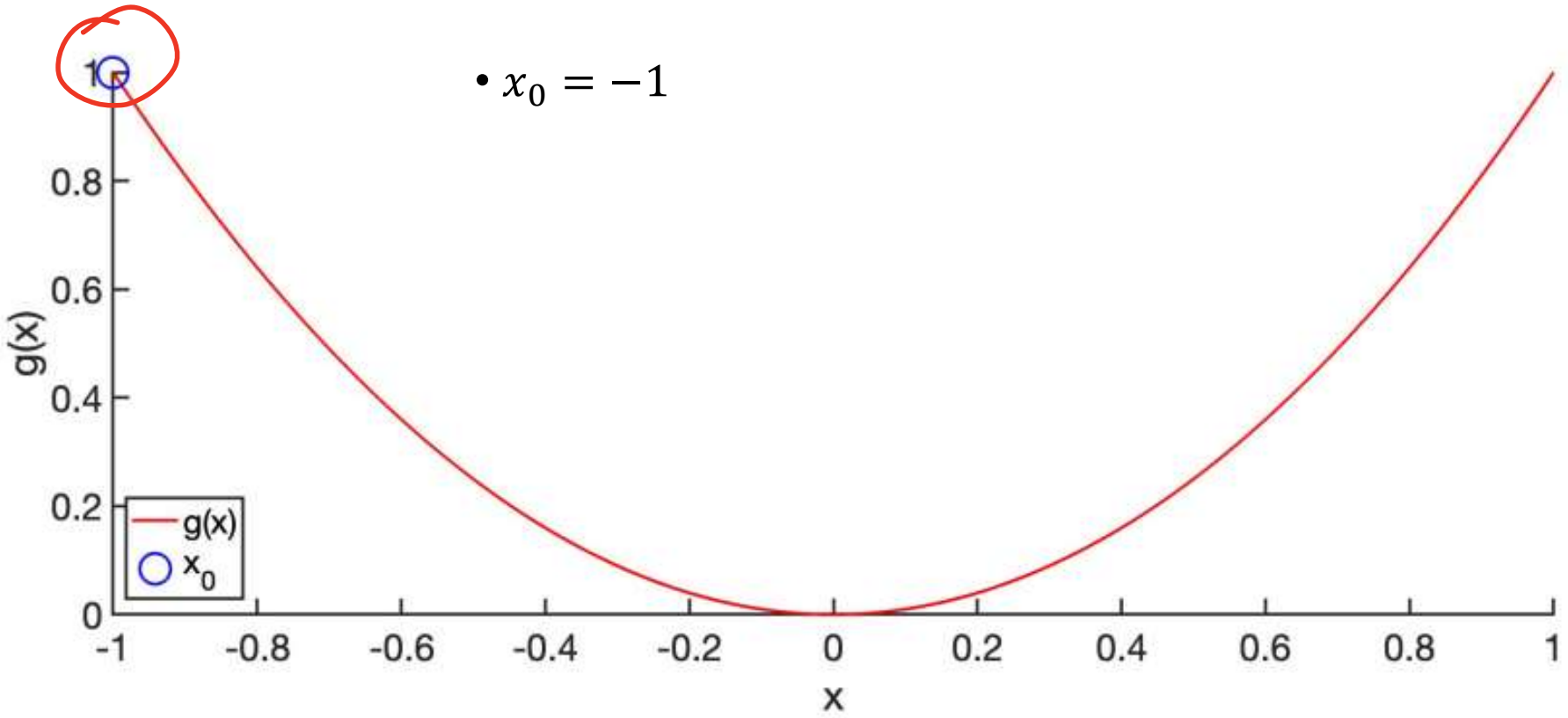

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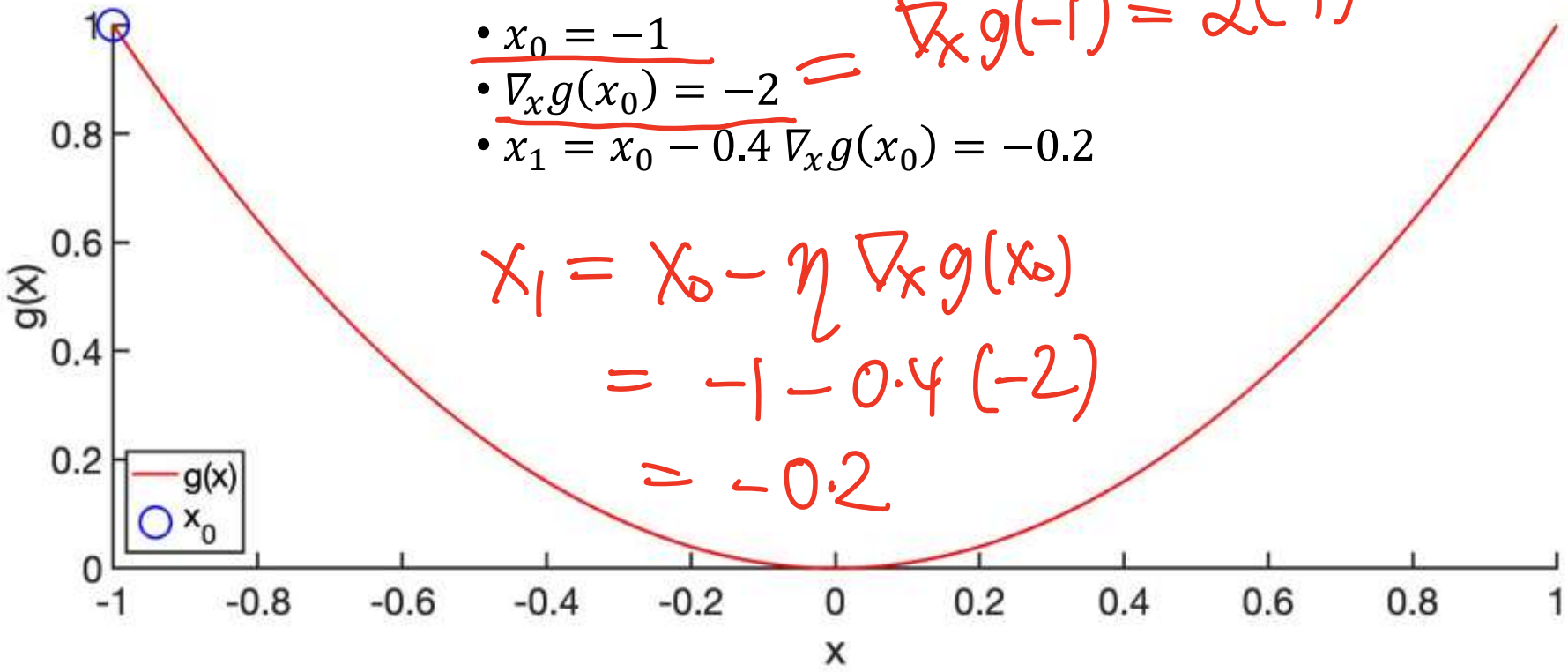

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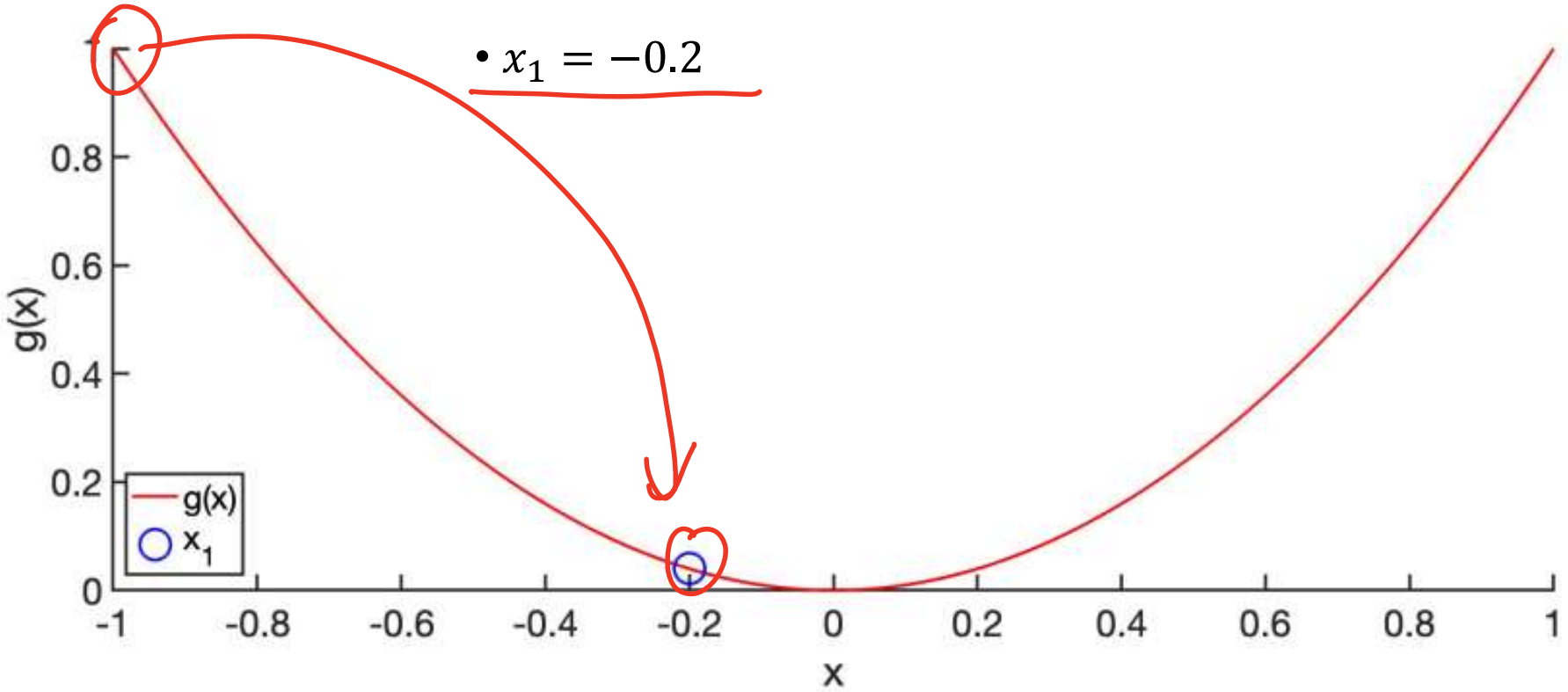

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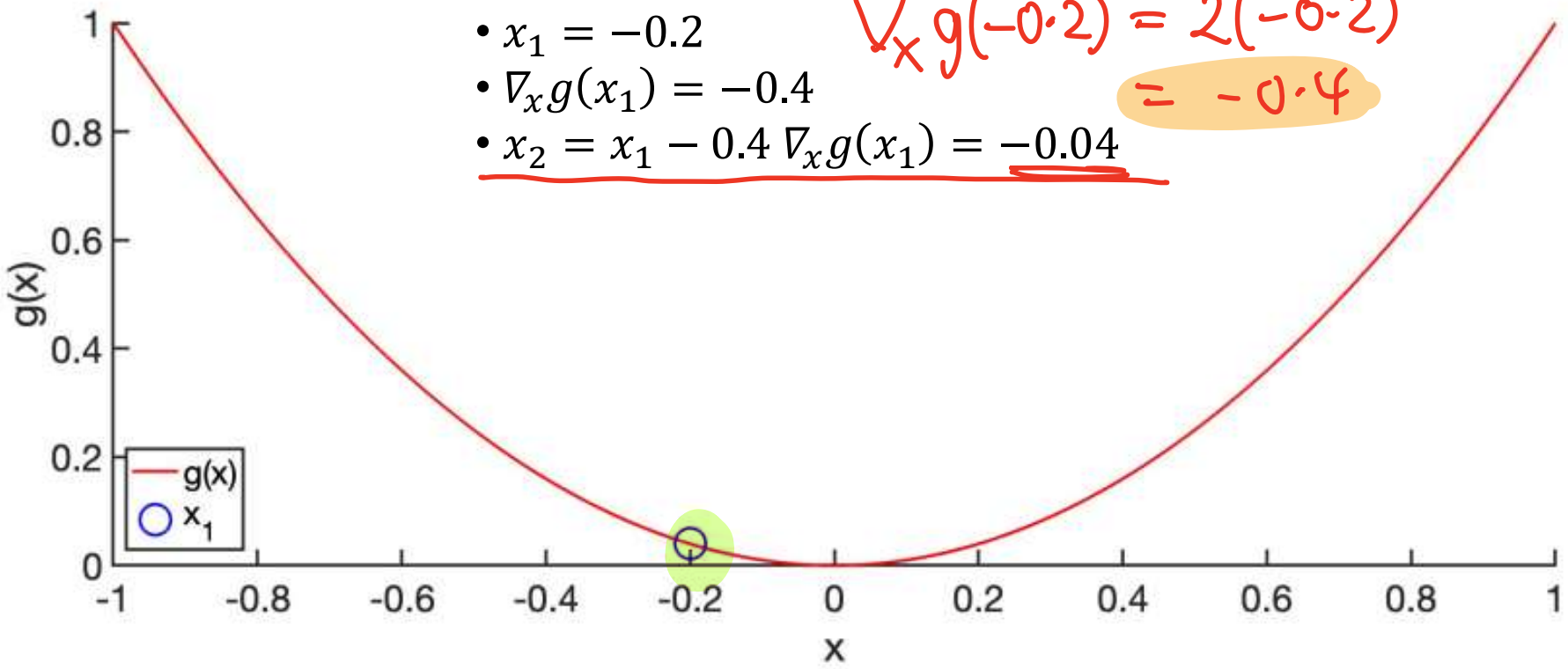
  - Initialize $x_0 = -1$, learning rate $\eta = 0.4$
  - At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$

$x_2 = x_1 - \eta \nabla_x g(x_1)$
$= -0.2 - 0.4(-0.4)$
$= -0.04$

$\nabla_x g(-0.2) = 2(-0.2)$
$= -0.4$

- $x_1 = -0.2$
- $\nabla_x g(x_1) = -0.4$
- $x_2 = x_1 - 0.4\, \nabla_x g(x_1) = -0.04$



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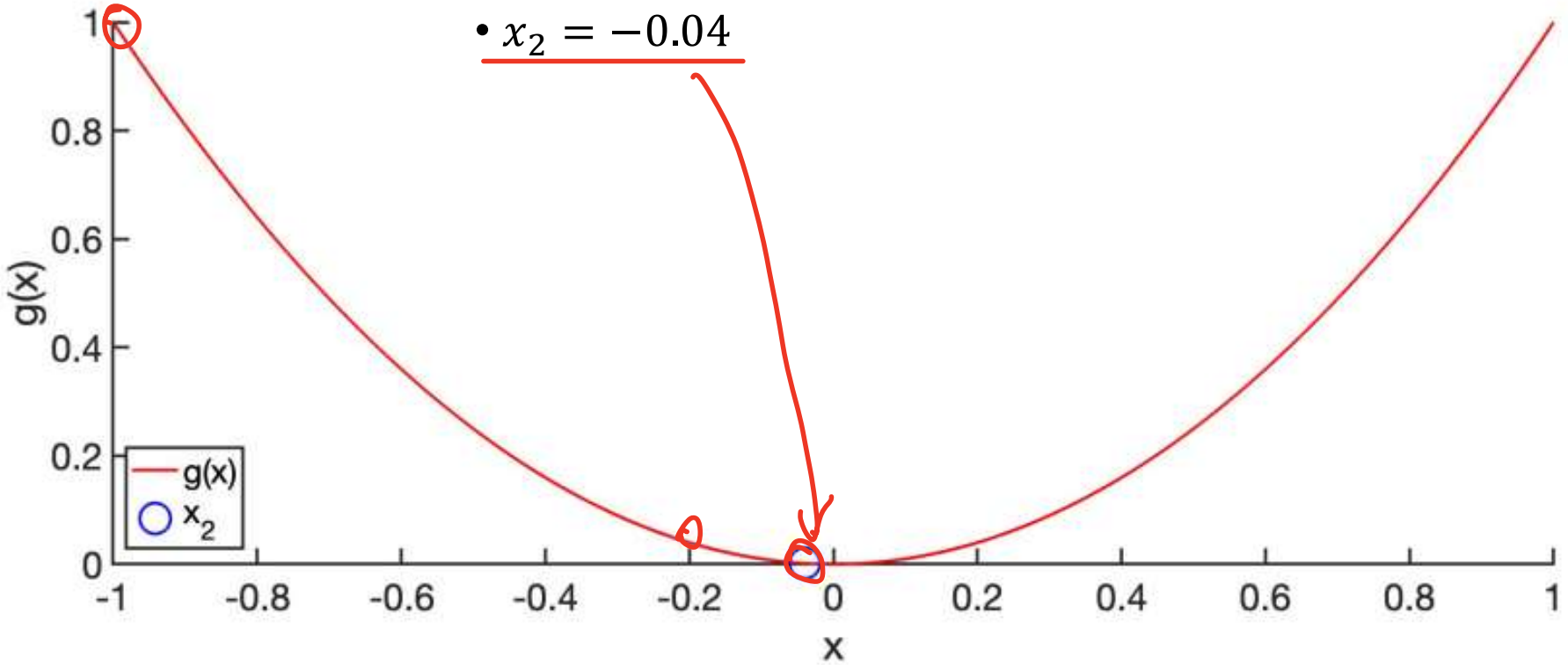

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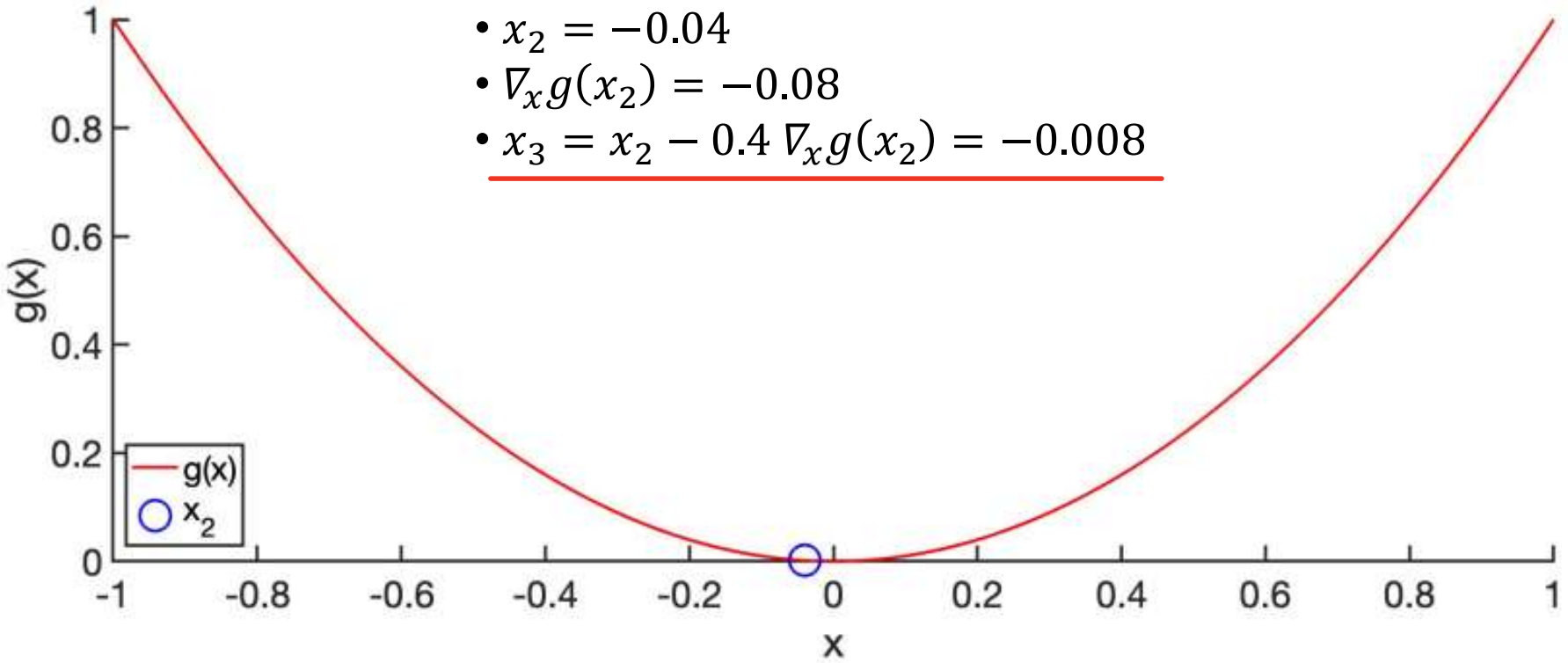
  - At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$

$x_3 = x_2 - \eta \nabla g(x_2)$

$= -0.04 - 0.4\,(2 \times (-0.04))$

$= -0.008$

- $x_2 = -0.04$
- $\nabla_x g(x_2) = -0.08$
- $x_3 = x_2 - 0.4\,\nabla_x g(x_2) = -0.008$



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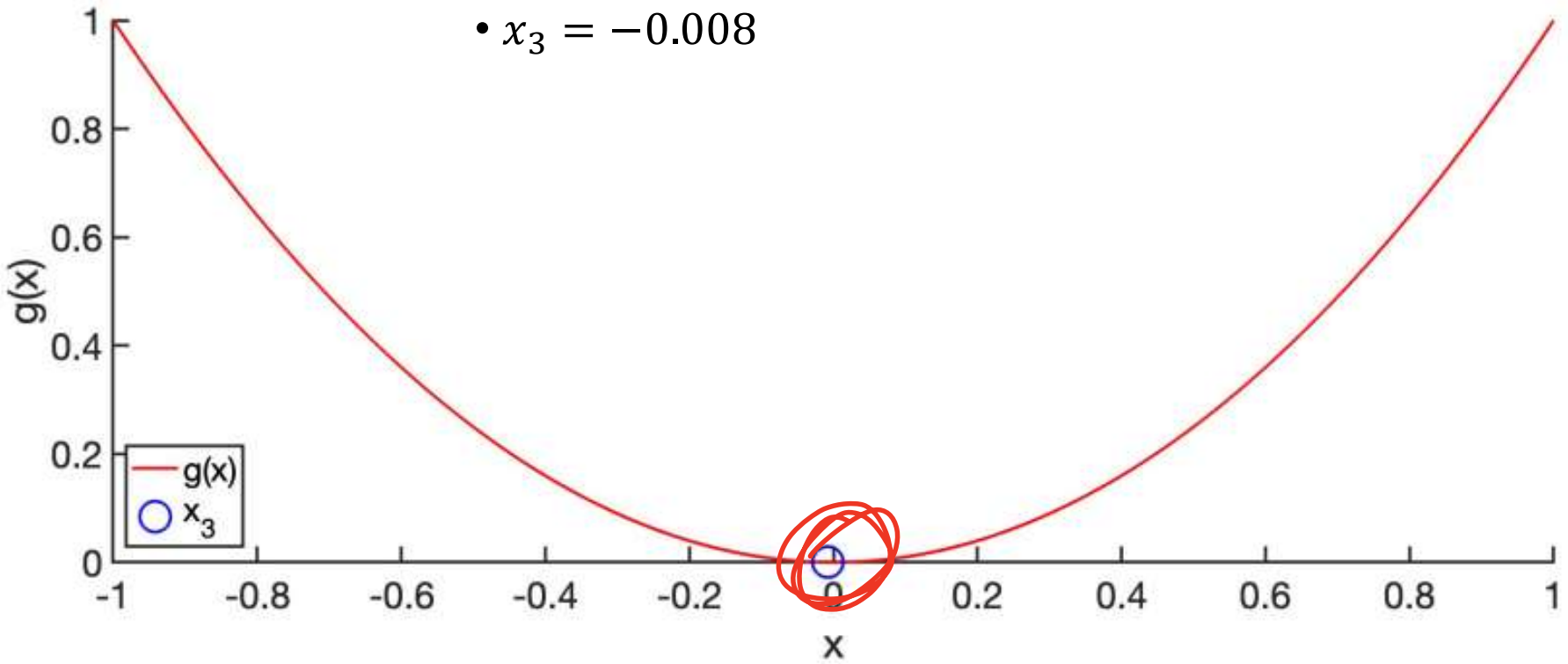

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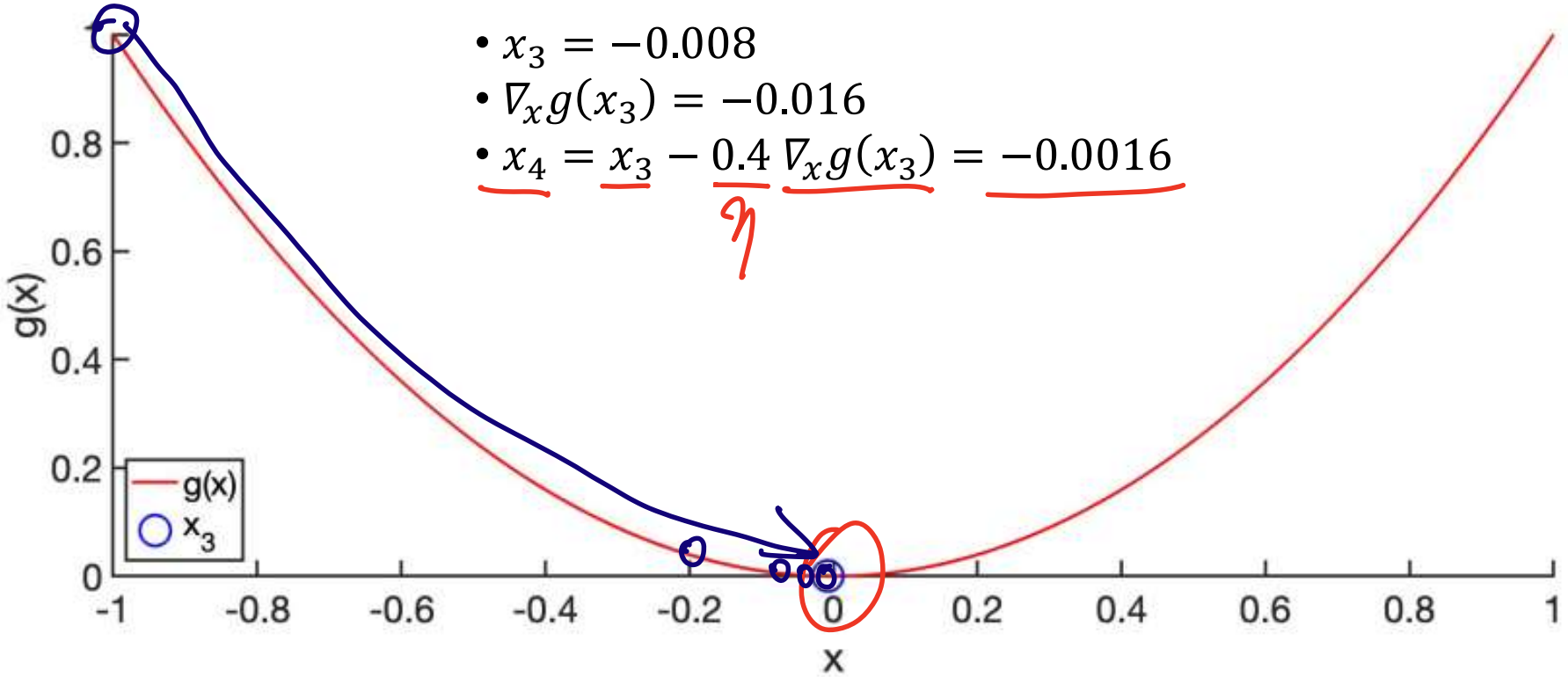

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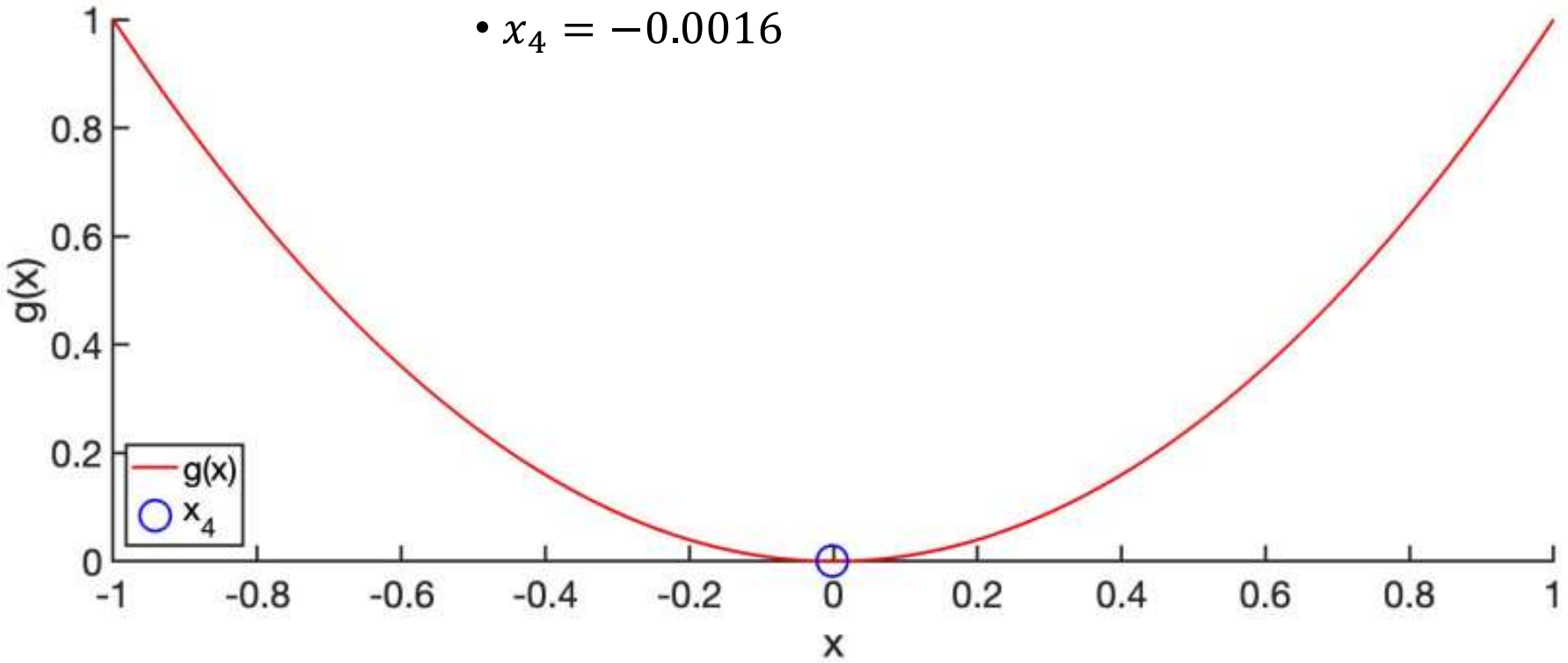
- $x_4 = -0.0016$



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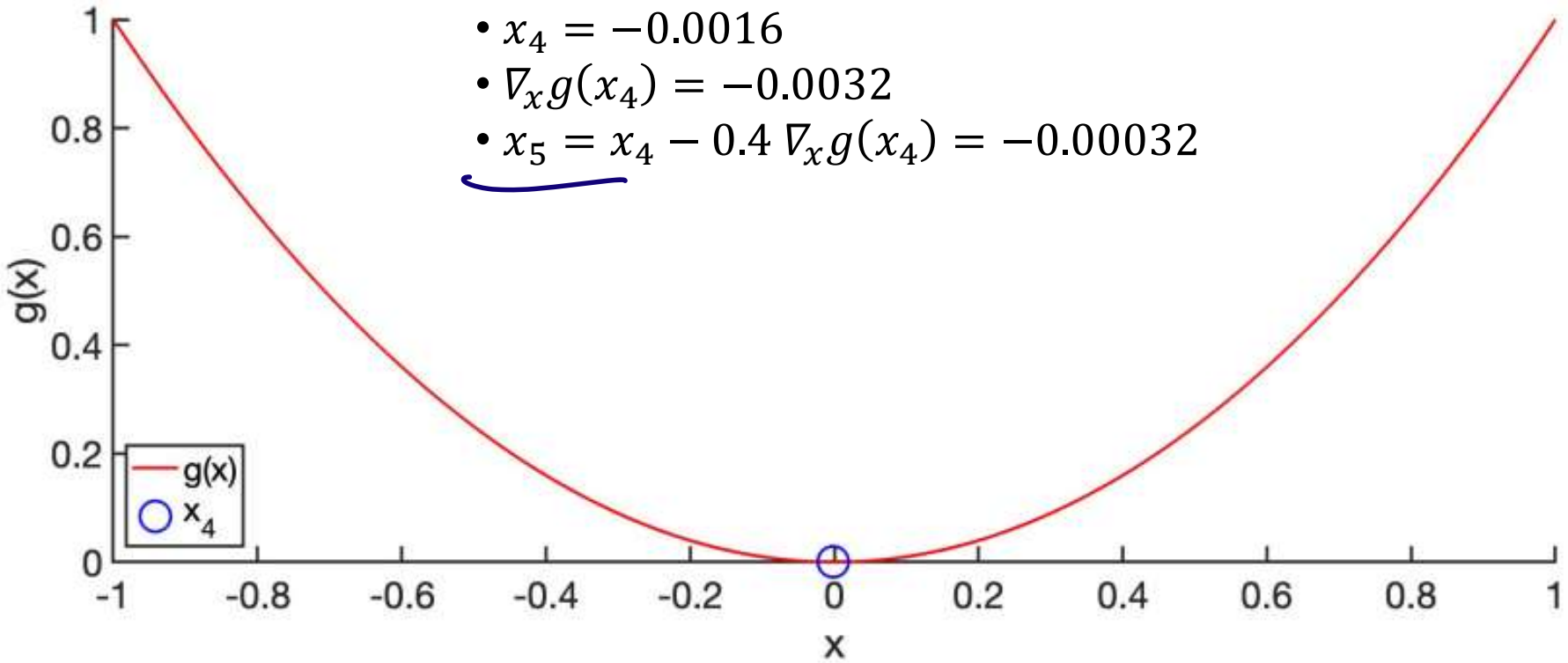
- $x_4 = -0.0016$
- $\nabla_x g(x_4) = -0.0032$
- $x_5 = x_4 - 0.4\, \nabla_x g(x_4) = -0.00032$



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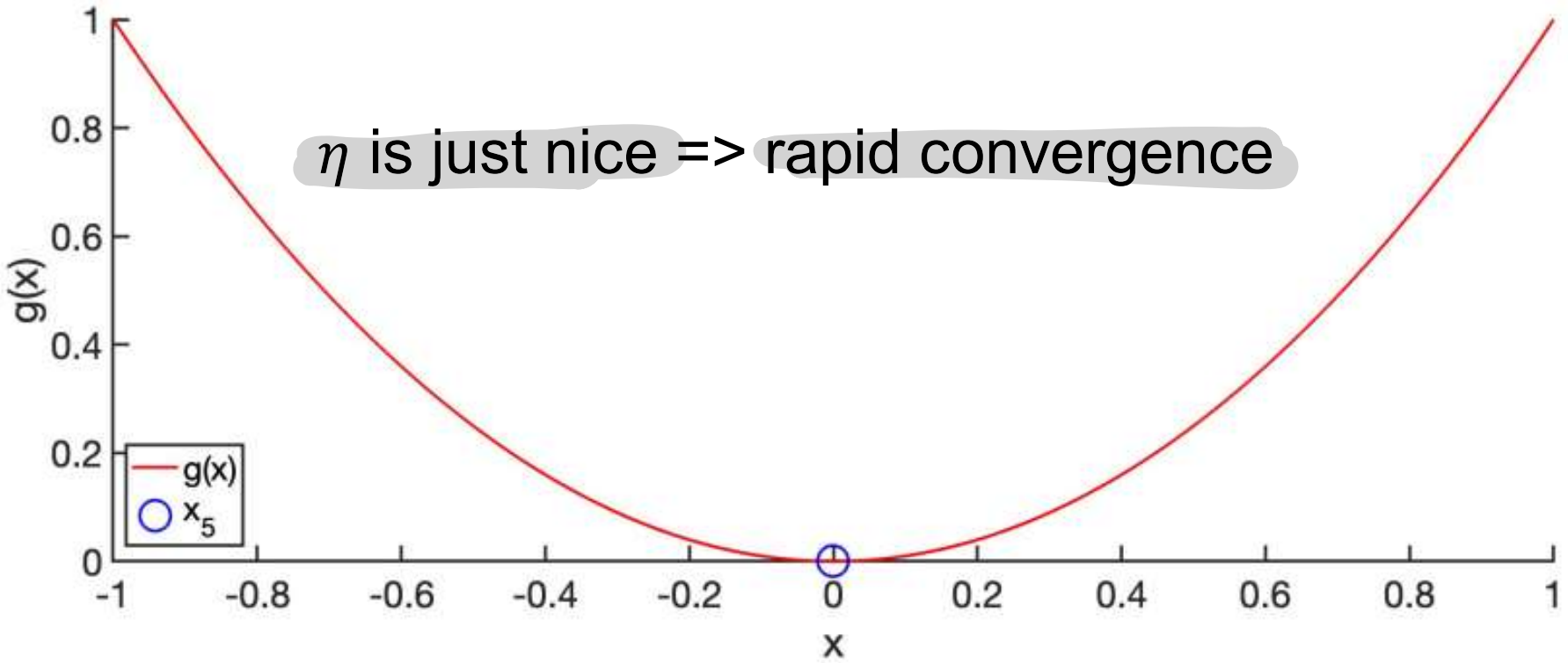
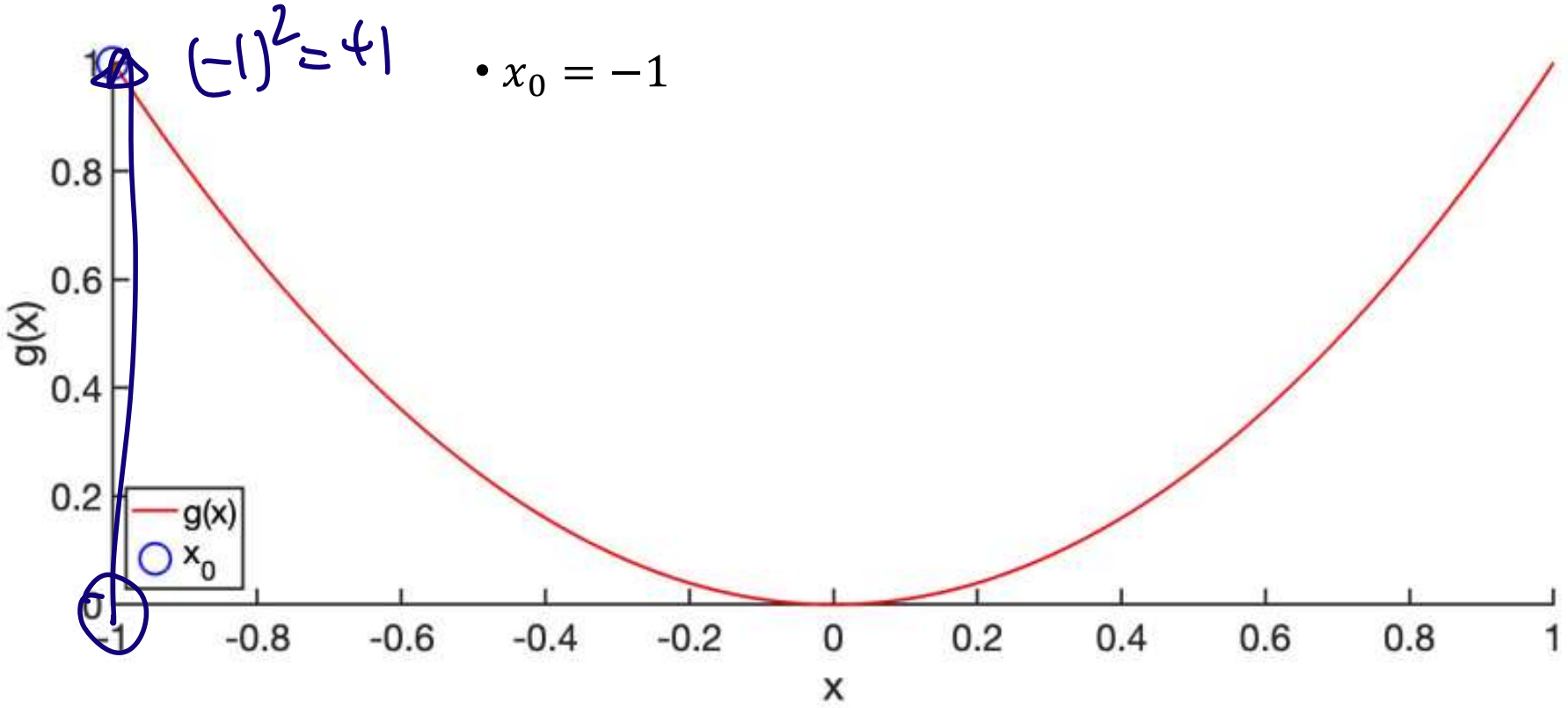


η is just nice => rapid convergence

What if learning rate η is too small?

- Obviously minimum corresponds to $x = 0$, but let's do gradient descent
  - Gradient $\nabla_x g(x) = 2x$
  - Initialize $x_0 = -1$, learning rate $\eta = 0.01$ (cf. $\eta = 0.4$)
  - At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$



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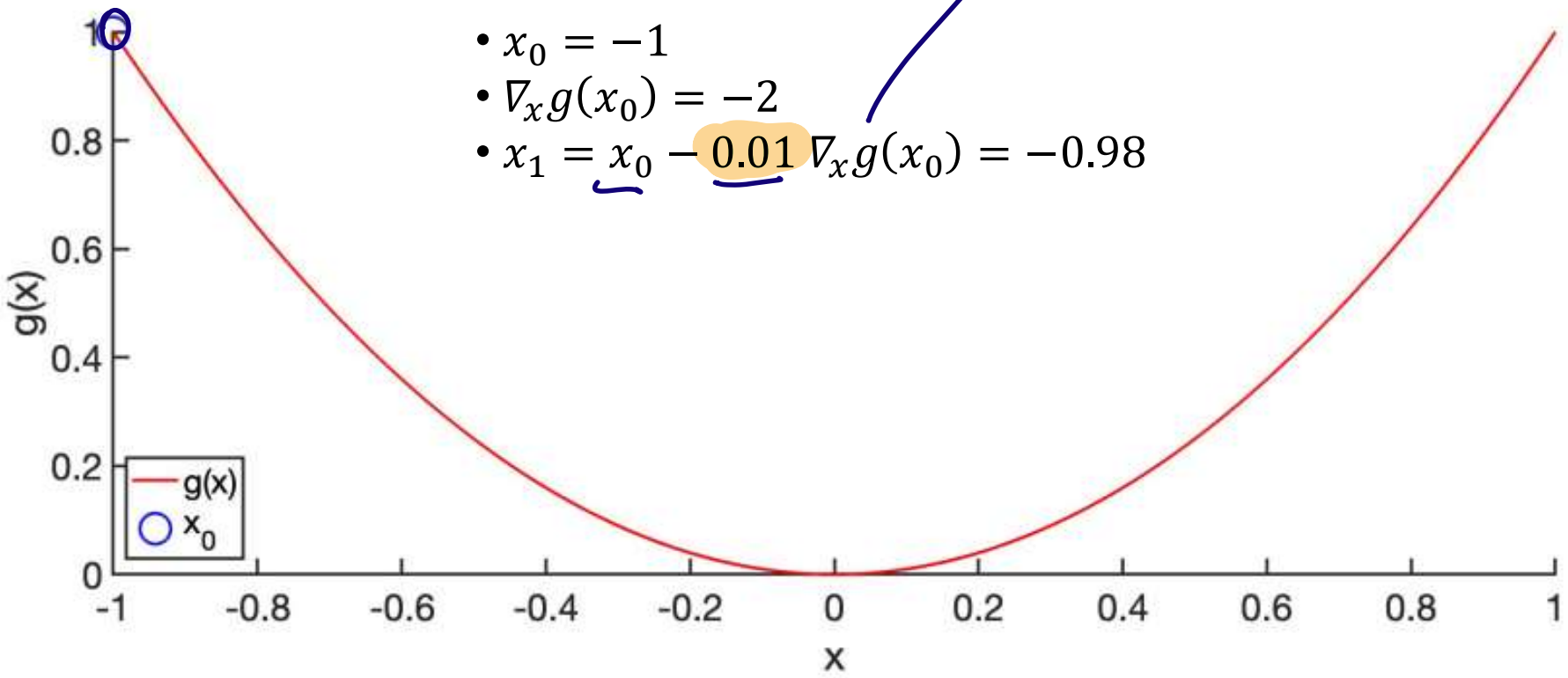
  - Gradient $\nabla_x g(x) = 2x$
  - Initialize $x_0 = -1$, learning rate $\eta = 0.01$
  - At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$

$-1 - 0.01(2\times(-1)) = -0.98$

- $x_0 = -1$
- $\nabla_x g(x_0) = -2$
- $x_1 = x_0 - 0.01\,\nabla_x g(x_0) = -0.98$



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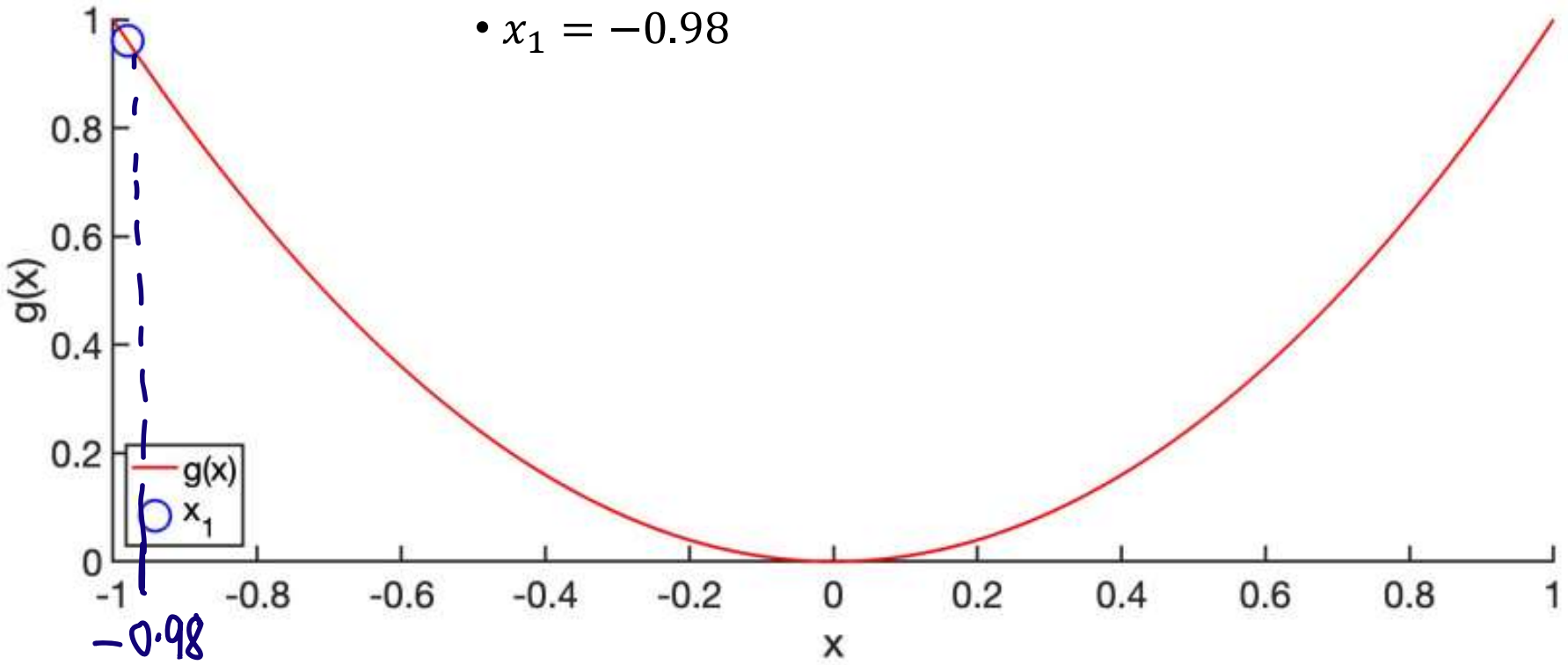

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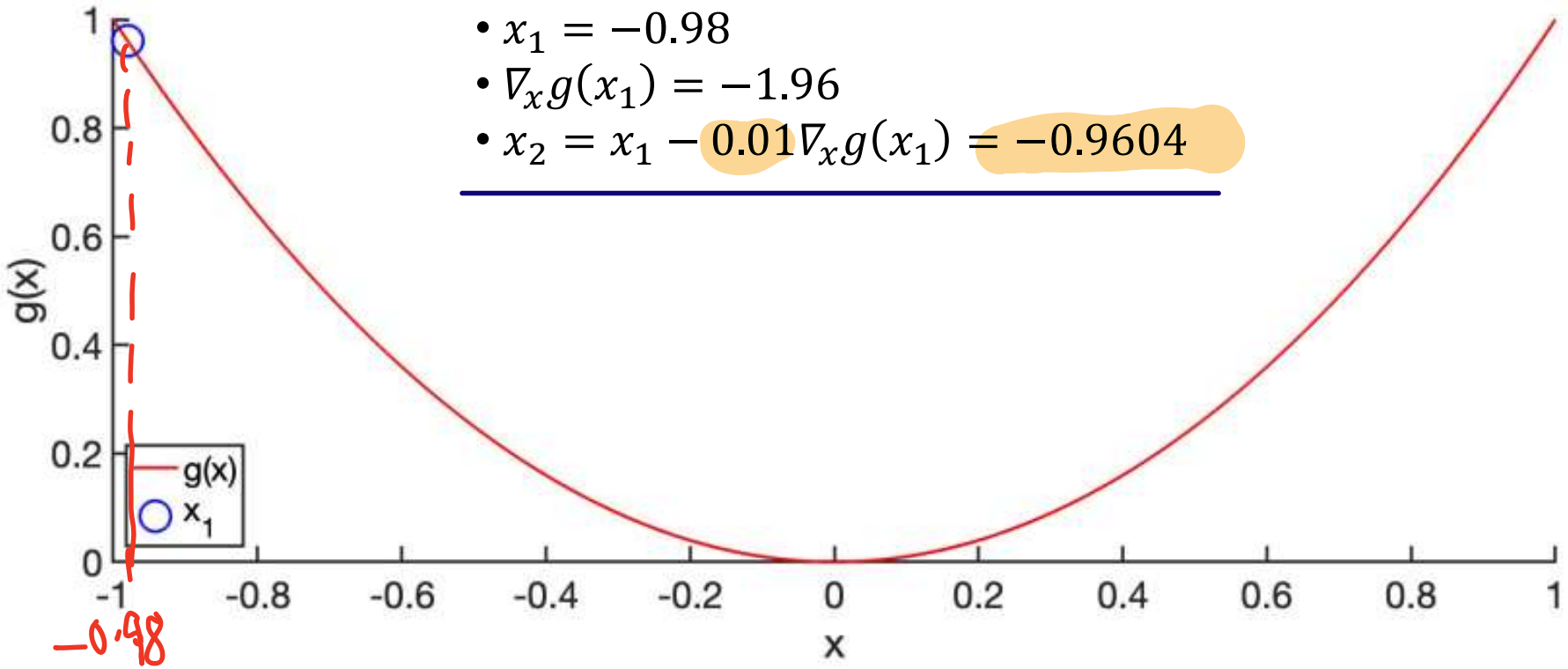
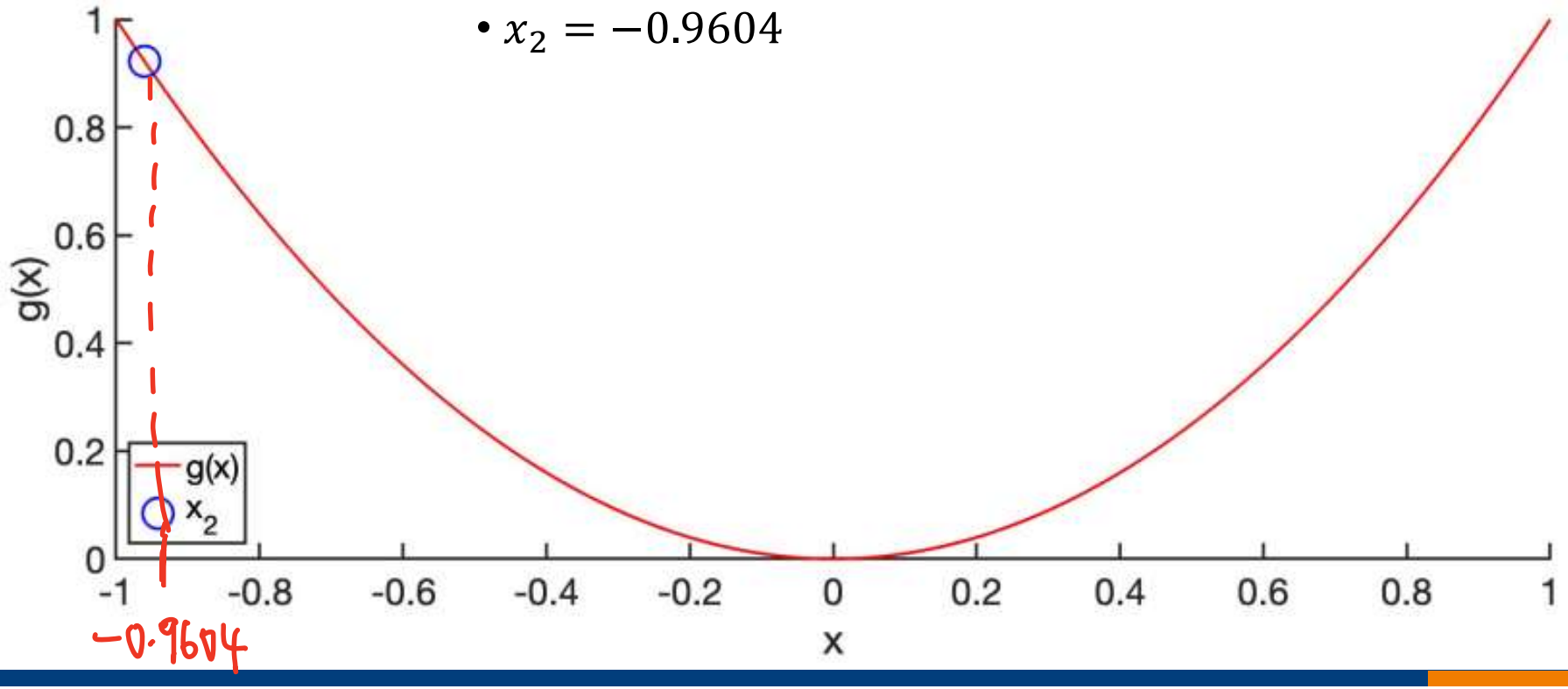


- $x_1 = -0.98$
- $\nabla_x g(x_1) = -1.96$
- $x_2 = x_1 - 0.01\nabla_x g(x_1) = -0.9604$

What if learning rate η is too small?

- Obviously minimum corresponds to $x = 0$, but let's do gradient descent
  - Gradient $\nabla_x g(x) = 2x$
  - Initialize $x_0 = -1$, learning rate $\eta = 0.01$
  - At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$

- $x_2 = -0.9604$



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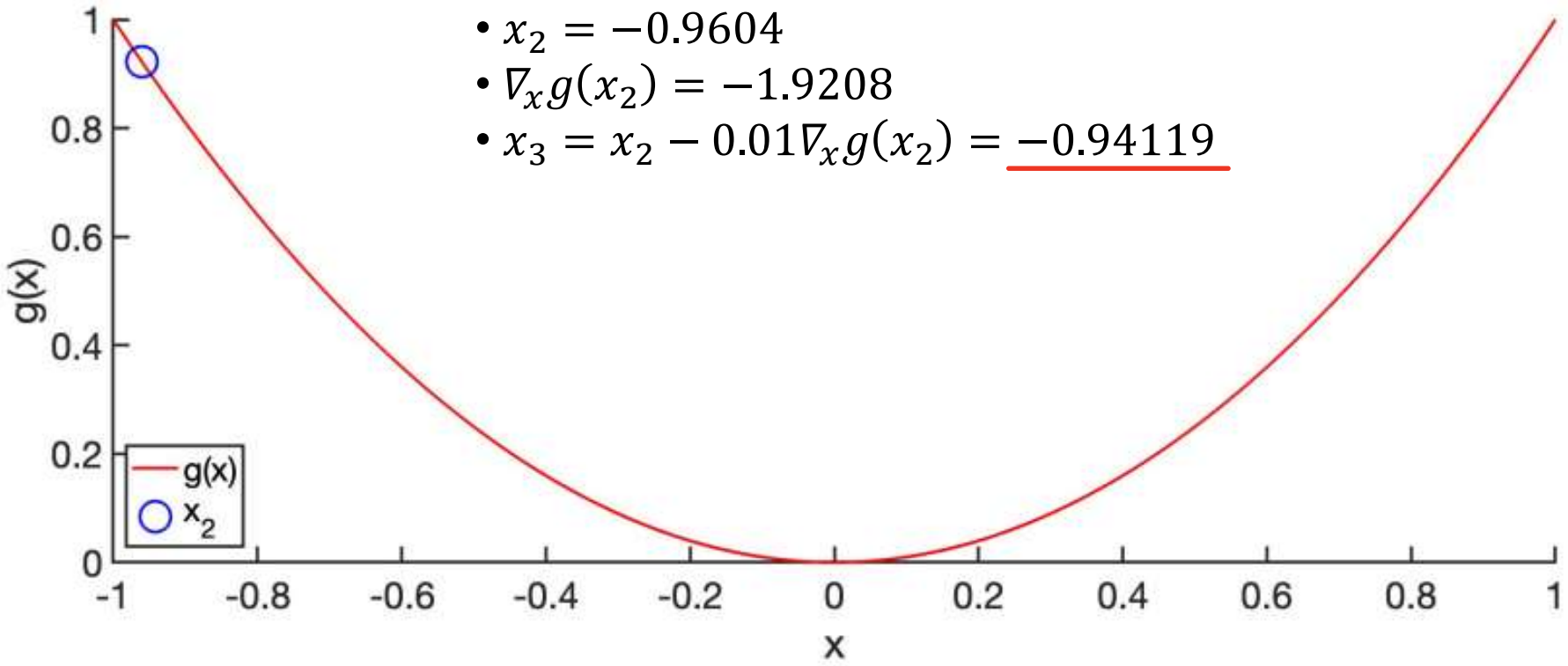
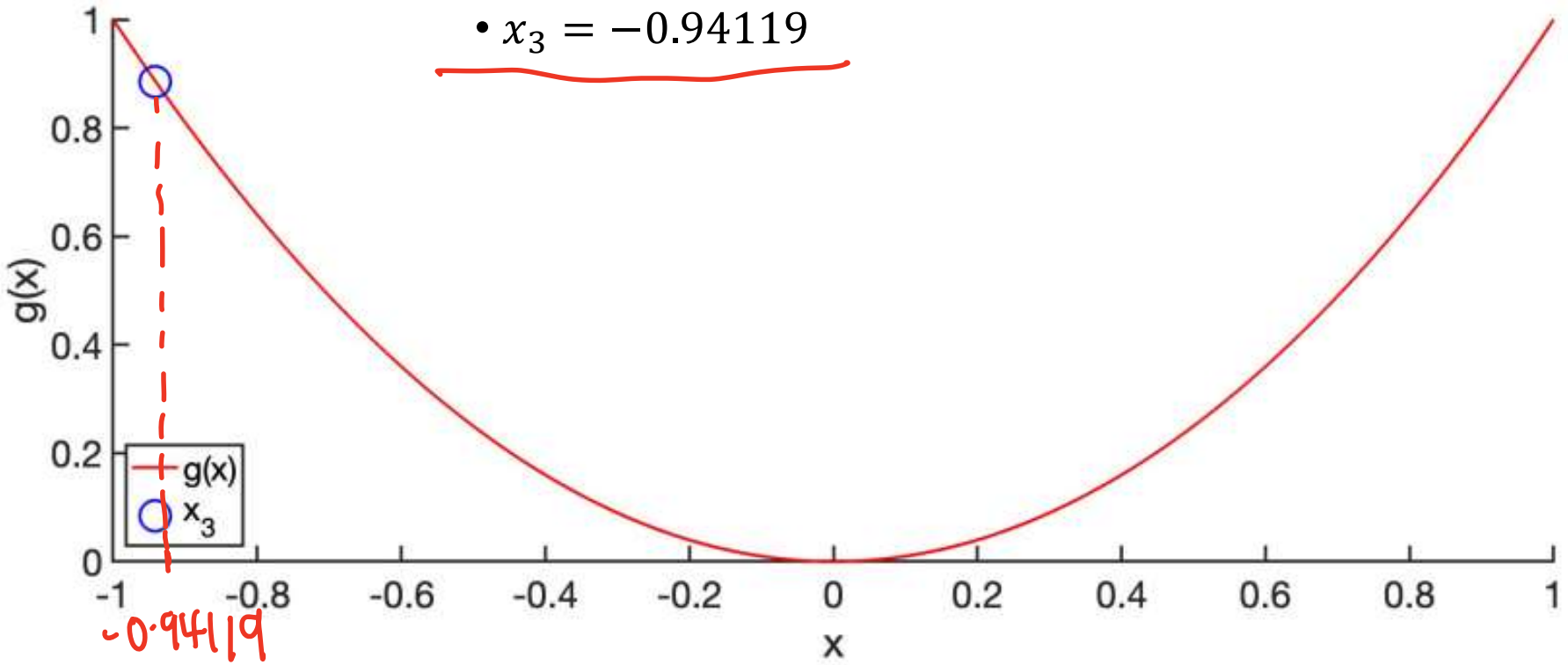


- $x_2 = -0.9604$
- $\nabla_x g(x_2) = -1.9208$
- $x_3 = x_2 - 0.01 \nabla_x g(x_2) = -0.94119$

What if learning rate η is too small?

- Obviously minimum corresponds to $x = 0$, but let's do gradient descent
  - Gradient $\nabla_x g(x) = 2x$
  - Initialize $x_0 = -1$, learning rate $\eta = 0.01$
  - At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$

- $x_3 = -0.94119$



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  - Gradient $\nabla_x g(x) = 2x$
  - Initialize $x_0 = -1$, learning rate $\eta = 0.01$
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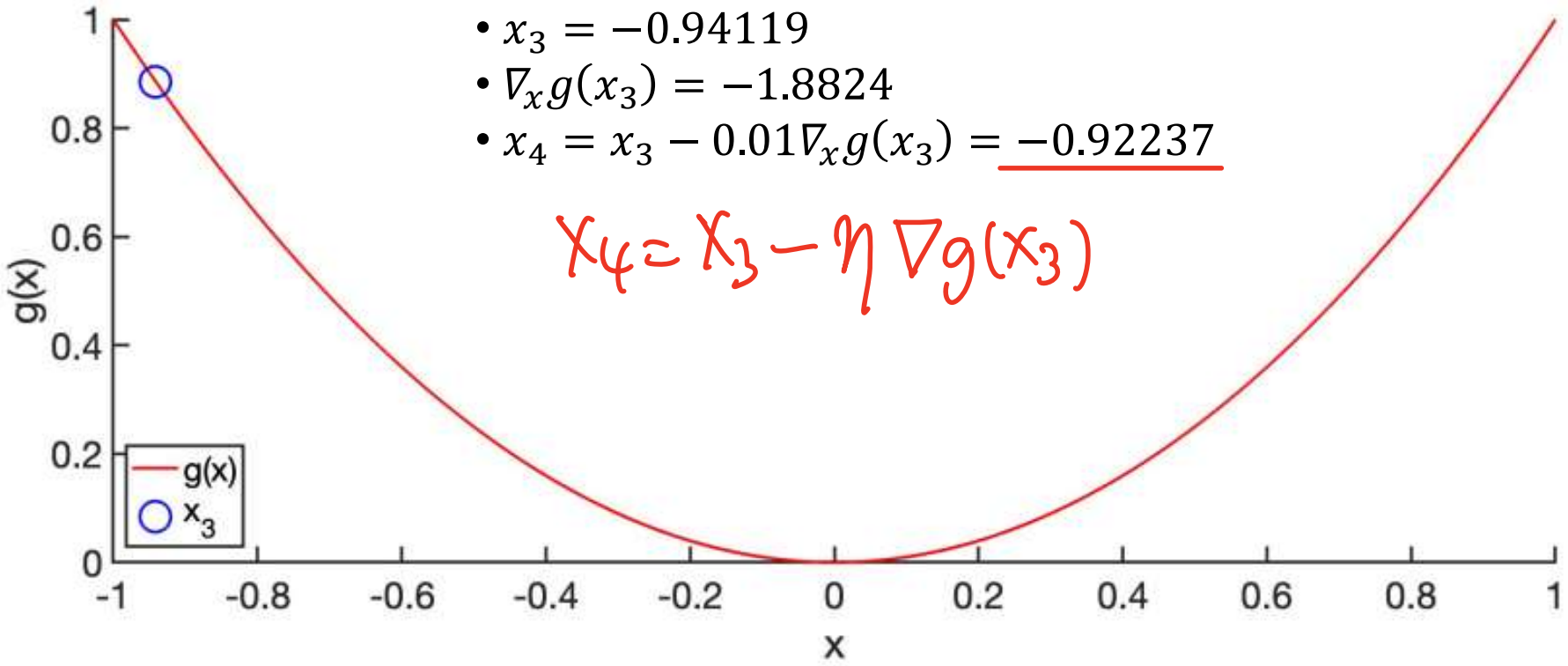

- $x_3 = -0.94119$
- $\nabla_x g(x_3) = -1.8824$
- $x_4 = x_3 - 0.01\nabla_x g(x_3) = -0.92237$

$x_4 = x_3 - \eta \nabla g(x_3)$

What if learning rate η is too small?

- Obviously minimum corresponds to $x = 0$, but let's do gradient descent
  - Gradient $\nabla_x g(x) = 2x$
  - Initialize $x_0 = -1$, learning rate $\eta = 0.01$
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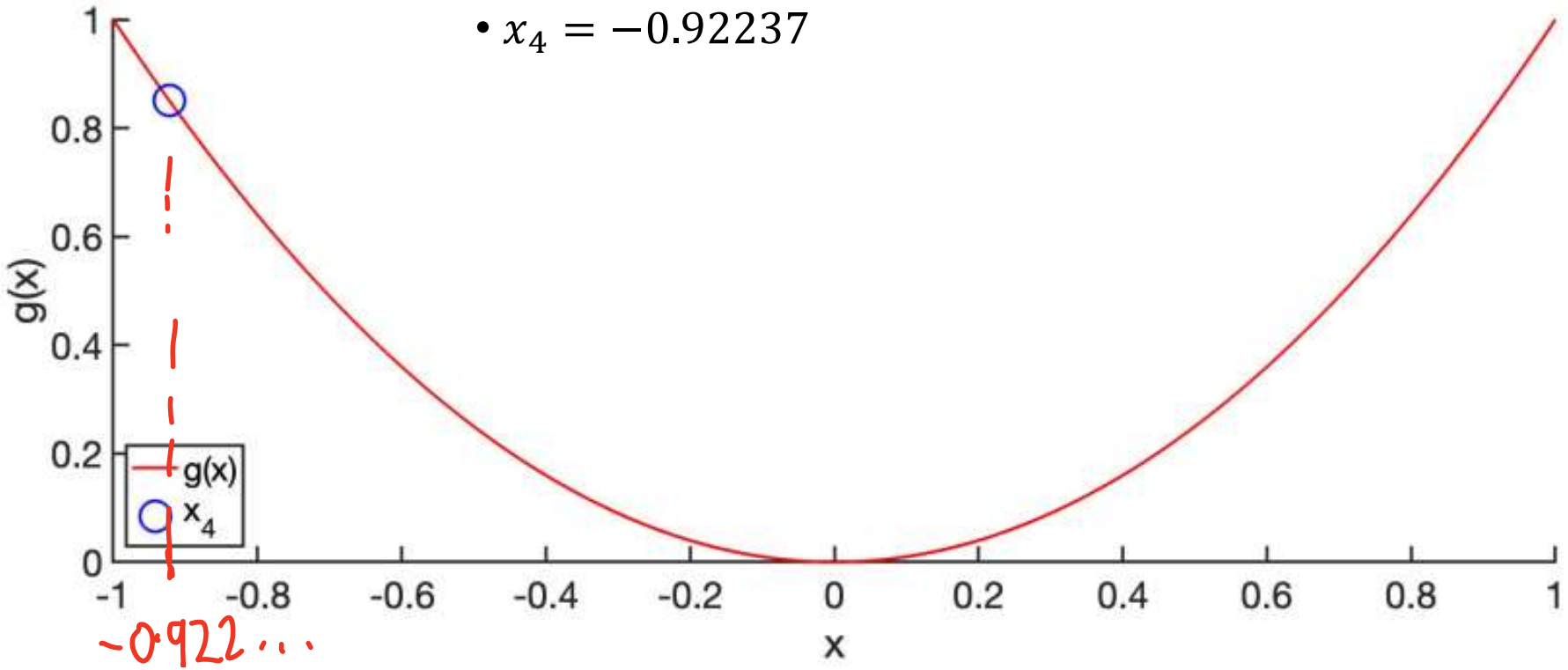
- $x_4 = -0.92237$



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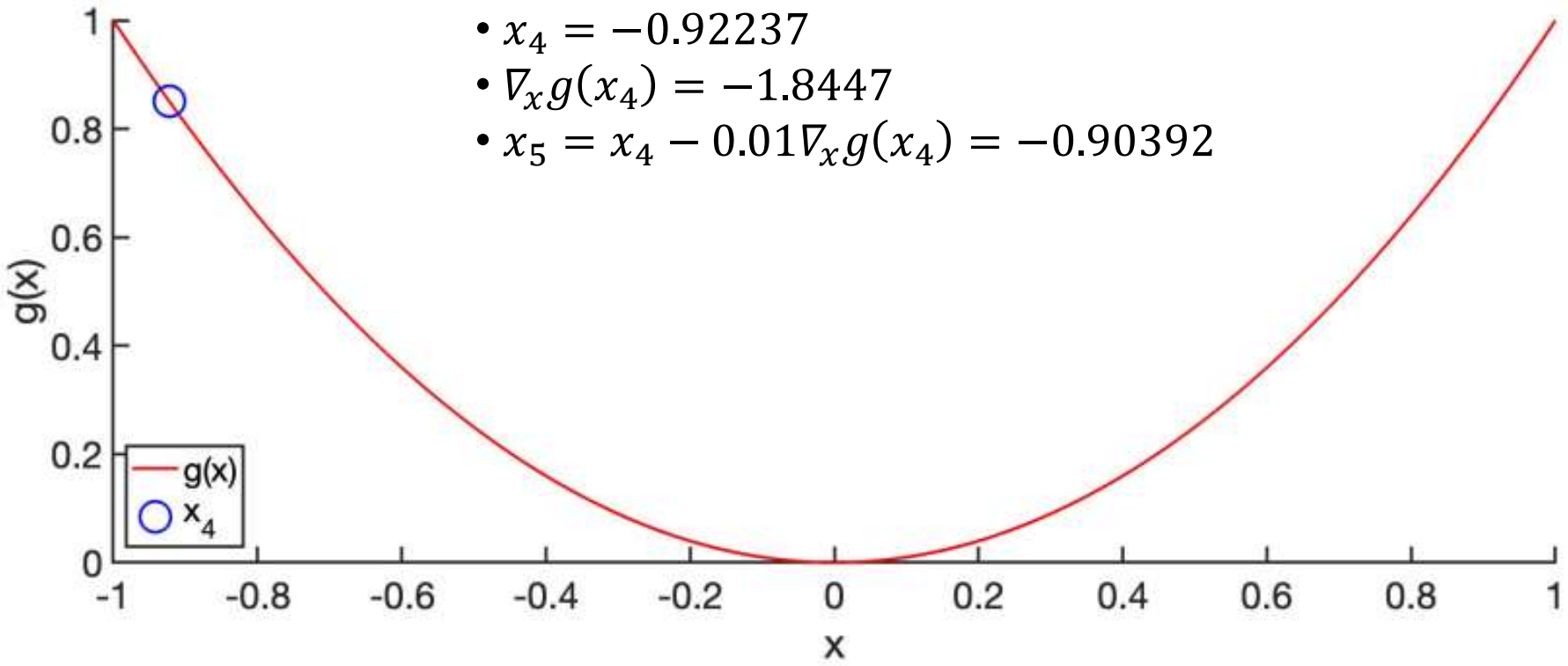
- Obviously minimum corresponds to $x = 0$, but let's do gradient descent
  - Gradient $\nabla_x g(x) = 2x$
  - Initialize $x_0 = -1$, learning rate $\eta = 0.01$
  - At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$



- $x_4 = -0.92237$
- $\nabla_x g(x_4) = -1.8447$
- $x_5 = x_4 - 0.01 \nabla_x g(x_4) = -0.90392$

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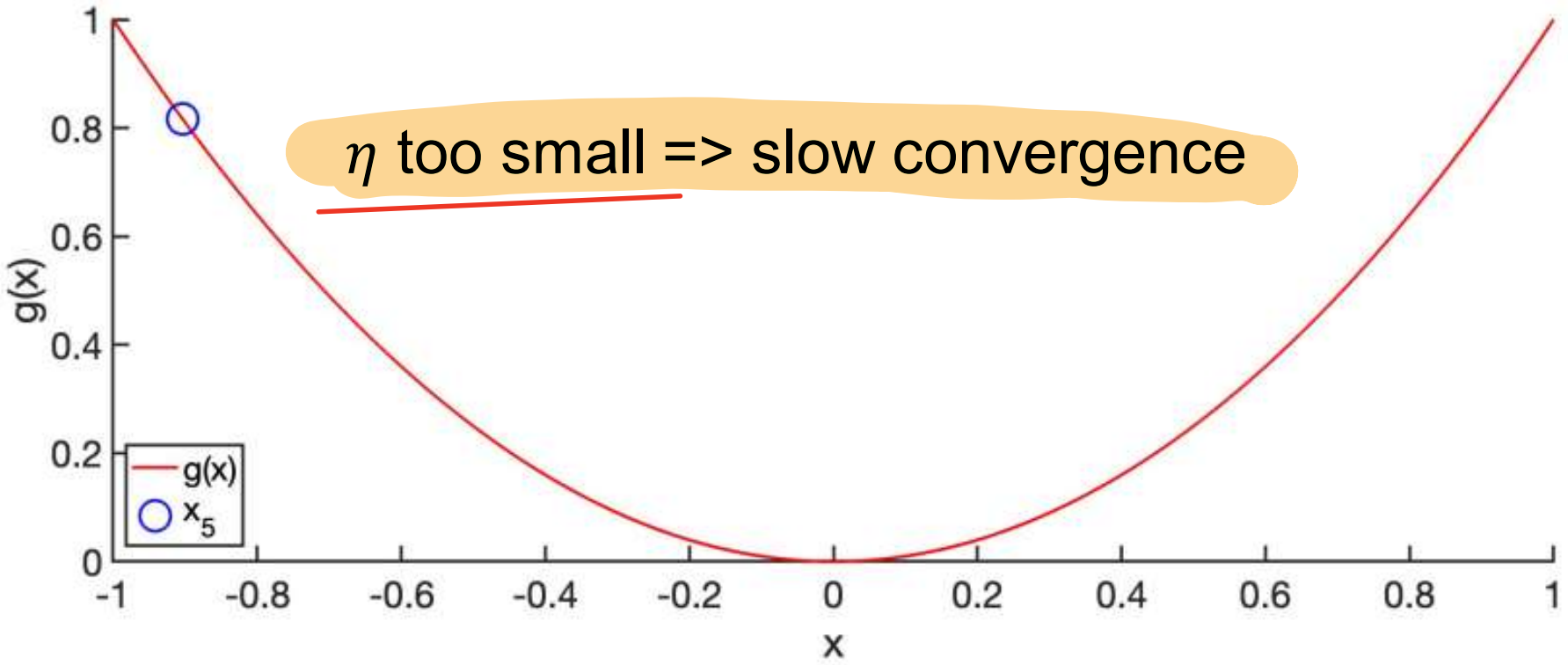
primal

$(P^T P + \lambda I)^{-1} P^T y = P^T (PP^T + \lambda I)^{-1} y$.

dual

iterative



η too small => slow convergence

What if learning rate η is too big?

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$\eta > 0$.

> 0.4

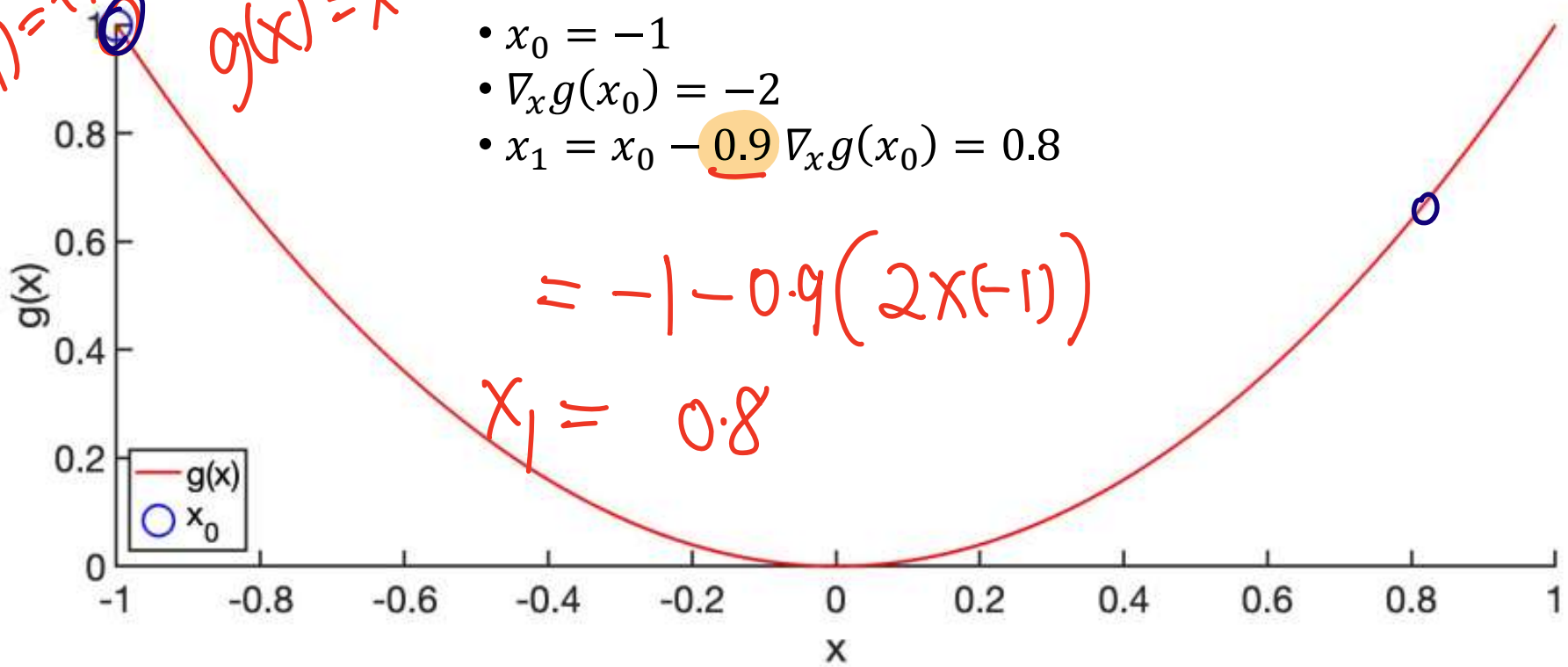
$g(-1) = +1$

$g(x) = x^2$

- $x_0 = -1$
- $\nabla_x g(x_0) = -2$
- $x_1 = x_0 - 0.9\,\nabla_x g(x_0) = 0.8$

$= -1 - 0.9(2 \times (-1))$

$x_1 = 0.8$



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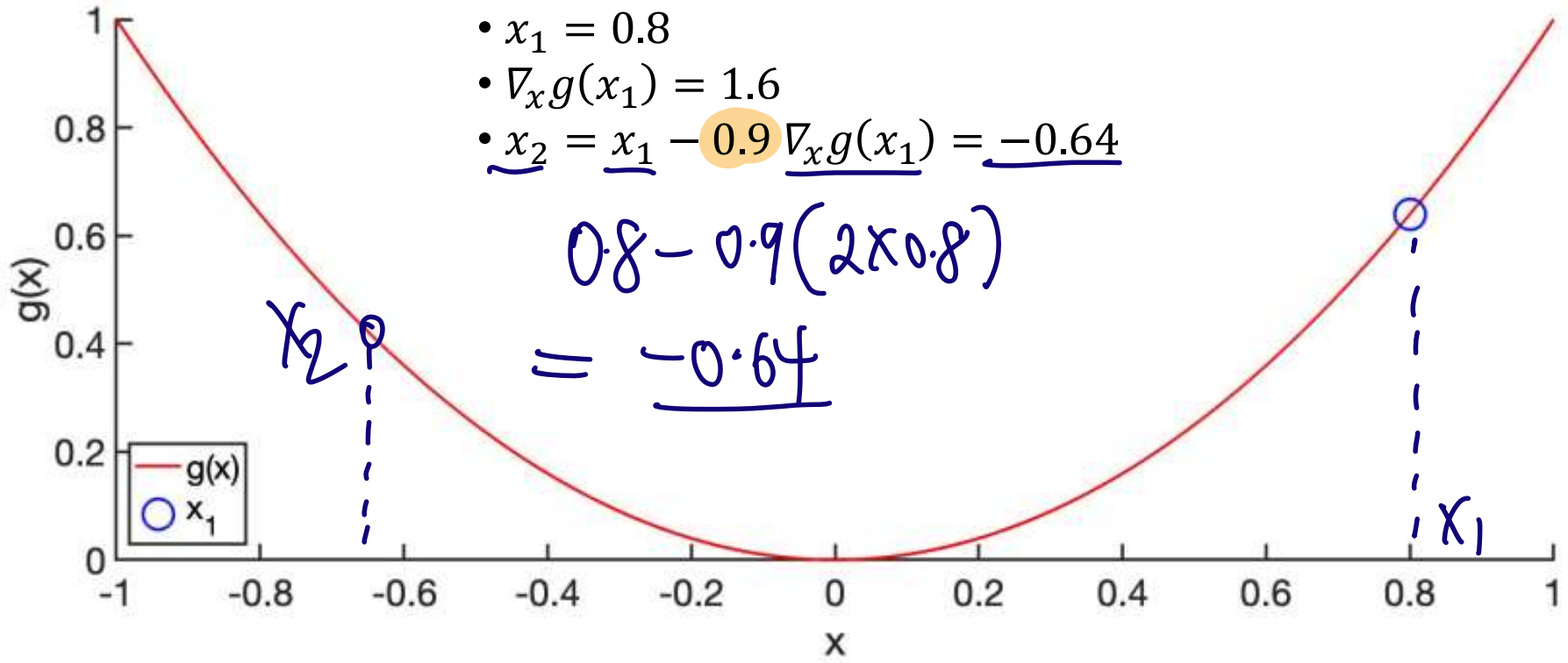

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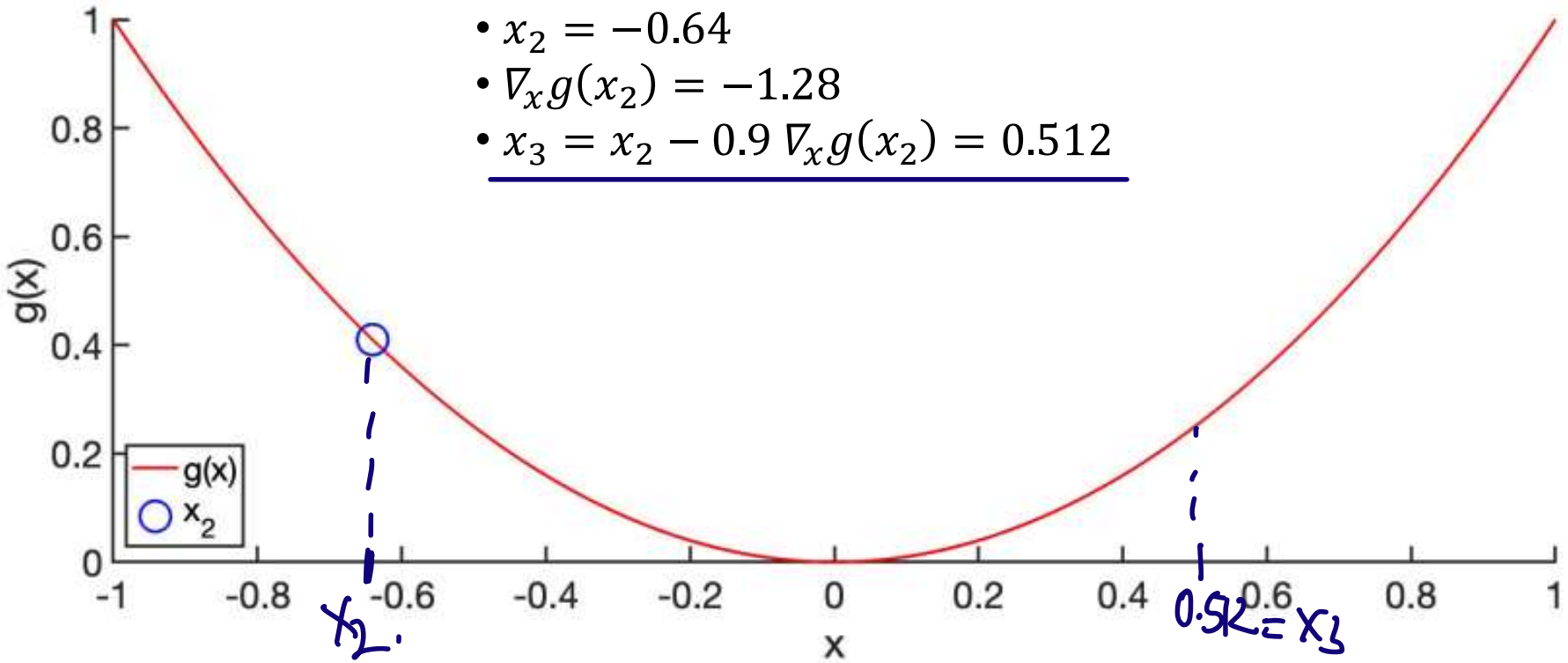
- $x_2 = -0.64$
- $\nabla_x g(x_2) = -1.28$
- $x_3 = x_2 - 0.9\, \nabla_x g(x_2) = 0.512$



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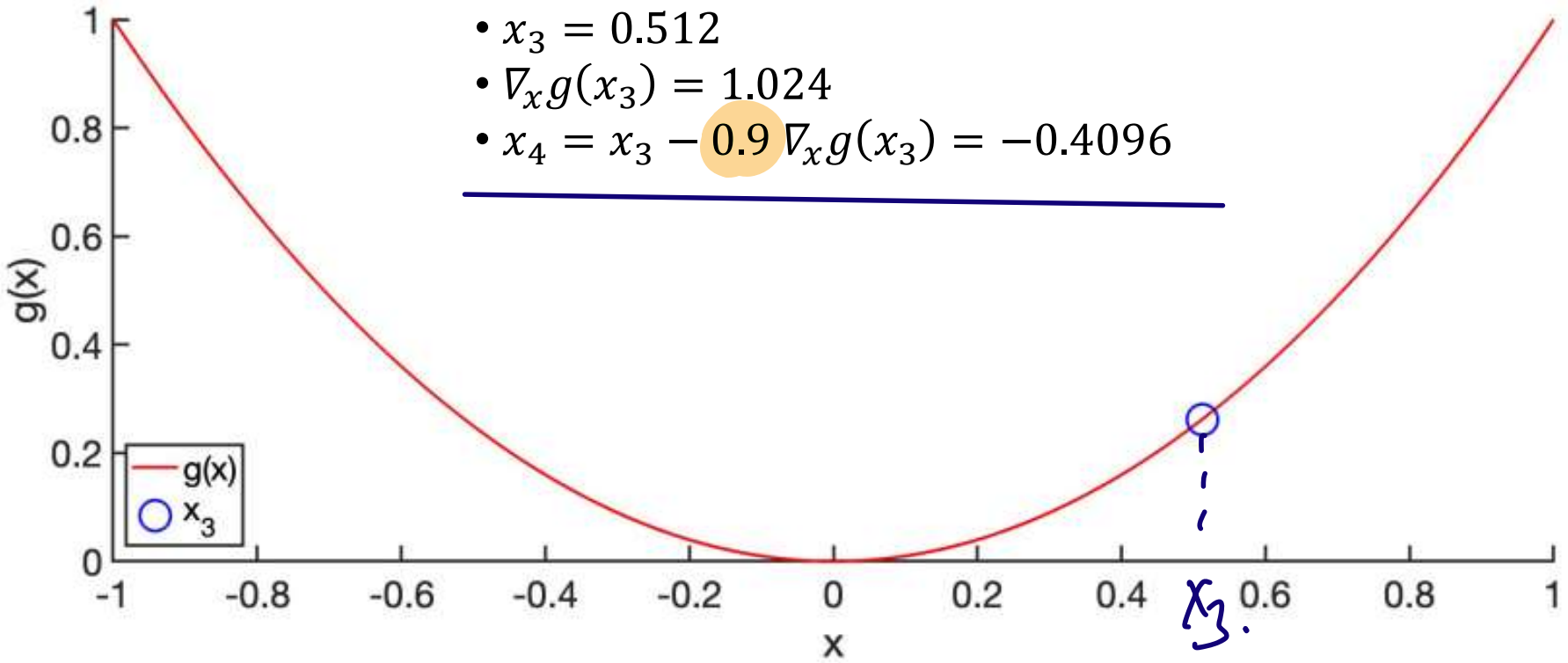
- $x_3 = 0.512$
- $\nabla_x g(x_3) = 1.024$
- $x_4 = x_3 - 0.9\,\nabla_x g(x_3) = -0.4096$



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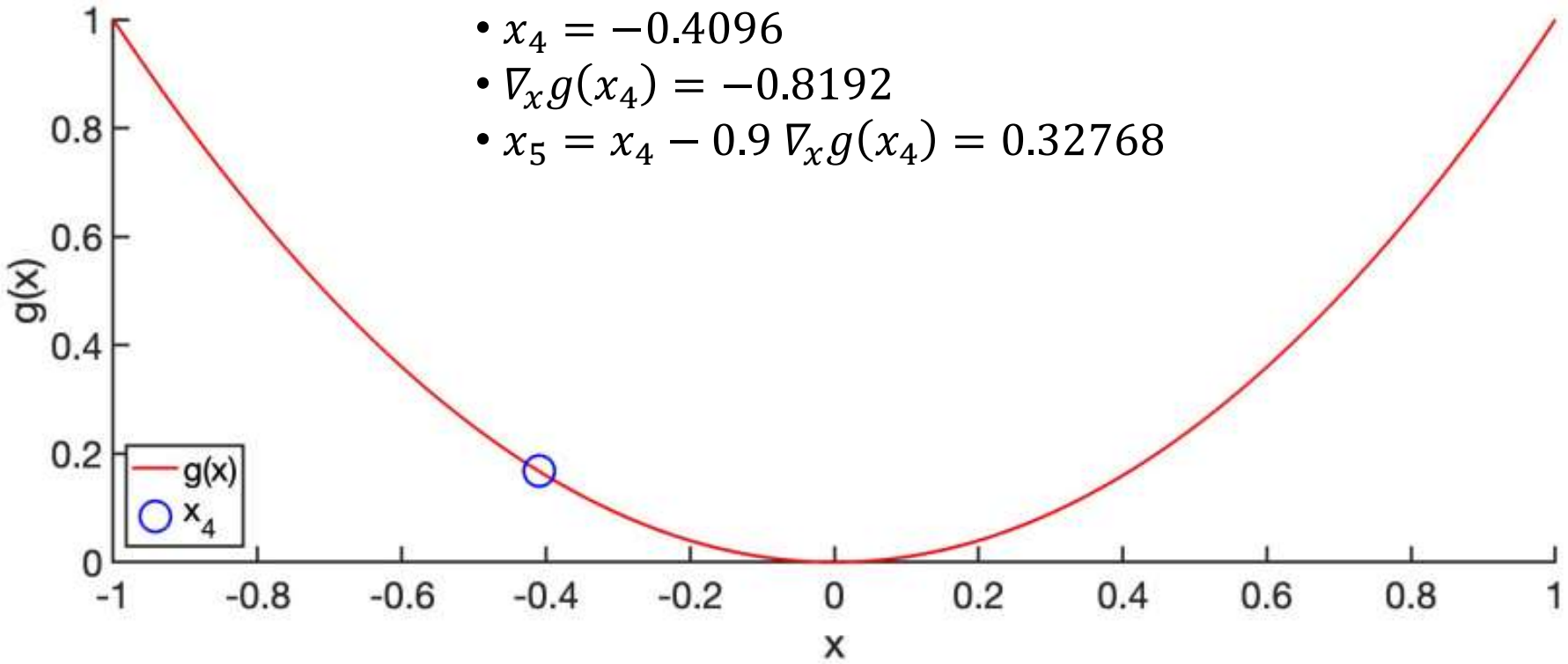
- $x_4 = -0.4096$
- $\nabla_x g(x_4) = -0.8192$
- $x_5 = x_4 - 0.9\, \nabla_x g(x_4) = 0.32768$



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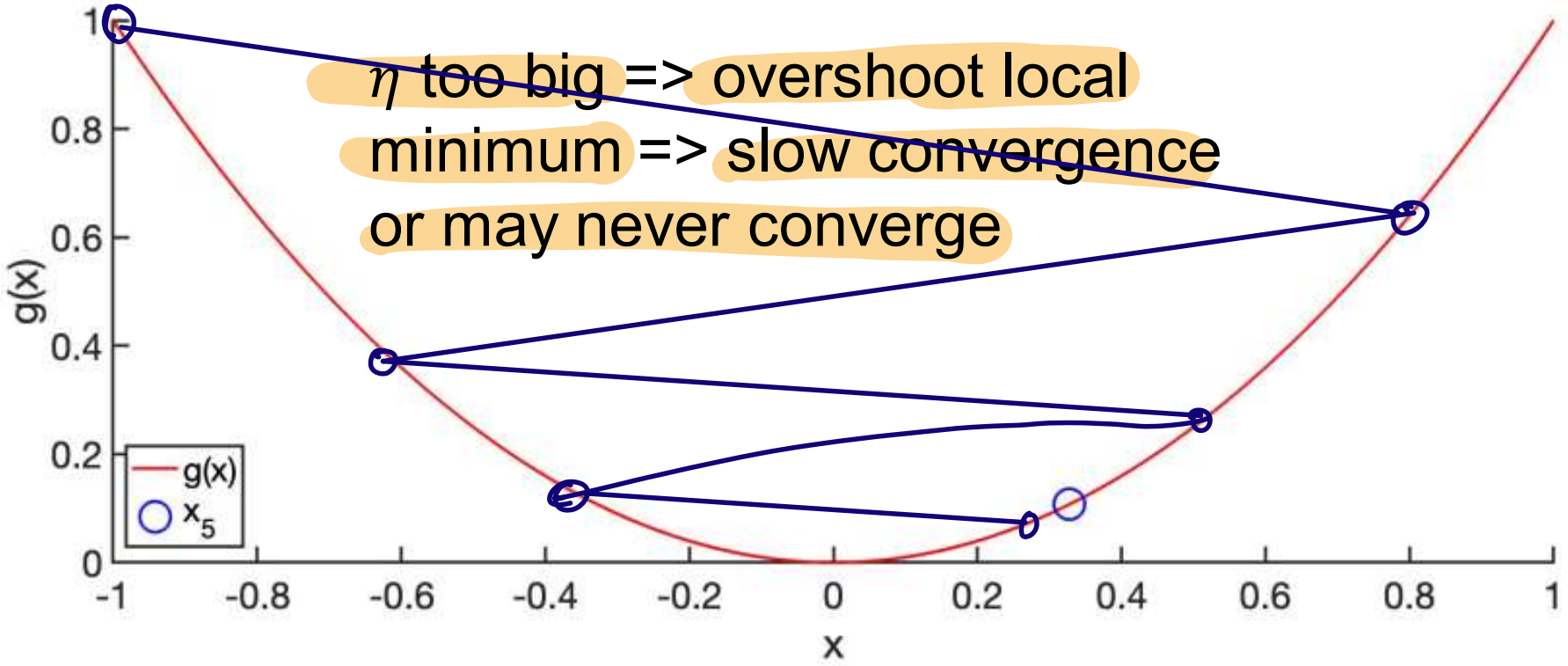


Gradient

$g \xrightarrow[\text{you compute}]{} \text{gradient } g.$

$g(x_1, x_2) = x_1^2 + x_2^5 + 3x_1^4 x_2$

η : given!

ReLU

Questions?

Closed-form

primal

$\hat{y} = (w^*)^T \begin{bmatrix} 1 \\ x \end{bmatrix}$

$w^* = (P^T P + \lambda I)^{-1} P^T y$

Python Demo on a Quadratic Function

```python
import numpy as np
from mpl_toolkits.mplot3d import Axes3D  # noqa: F401 unused import
import matplotlib.pyplot as plt
from matplotlib import cm
from matplotlib.ticker import LinearLocator, FormatStrFormatter
```

```python
Q = np.array([[1, 0], [0, 3]])

[x1,x2] = np.meshgrid(np.linspace(-10,10,1001),np.linspace(-10,10,1001))

x_vals = np.linspace(-10, 10, 1001)
y_vals = np.linspace(-10, 10, 1001)
X, Y = np.meshgrid(x_vals, y_vals)

Z = 0.5*(Q[0,0]*X**2 + Q[1,1]*Y**2 + 2*Q[0,1]*X*Y)

x_iter = np.array([[5], [3]]);
notConverged = 1;

lambdas, v = np.linalg.eig(Q)

eta = 2/(np.max(lambdas)+np.min(lambdas))
```

Here, we are defining a quadratic function

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{Q}\mathbf{x}$$

Finding the optimal step size (don't need to know)

Python Demo on a Quadratic Function

```
iter = 0
x = np.zeros([2,1000])

while notConverged and iter < 1e3:
    plt.plot(x_iter[0],x_iter[1],'gx')
    x[:,iter] = x_iter.T
    x_iter = x_iter - eta*Q.dot(x_iter)

    if (np.linalg.norm(x_iter) < 1e-5):
        notConverged = 0

    iter = iter + 1

cp = plt.contour(X, Y, Z, np.linspace(0,200,10))
plt.plot(x[0,0:iter-1],x[1,0:iter-1],'b--')
#plt.savefig('well_conditioned.eps', format='eps')
```

Running gradient descent.

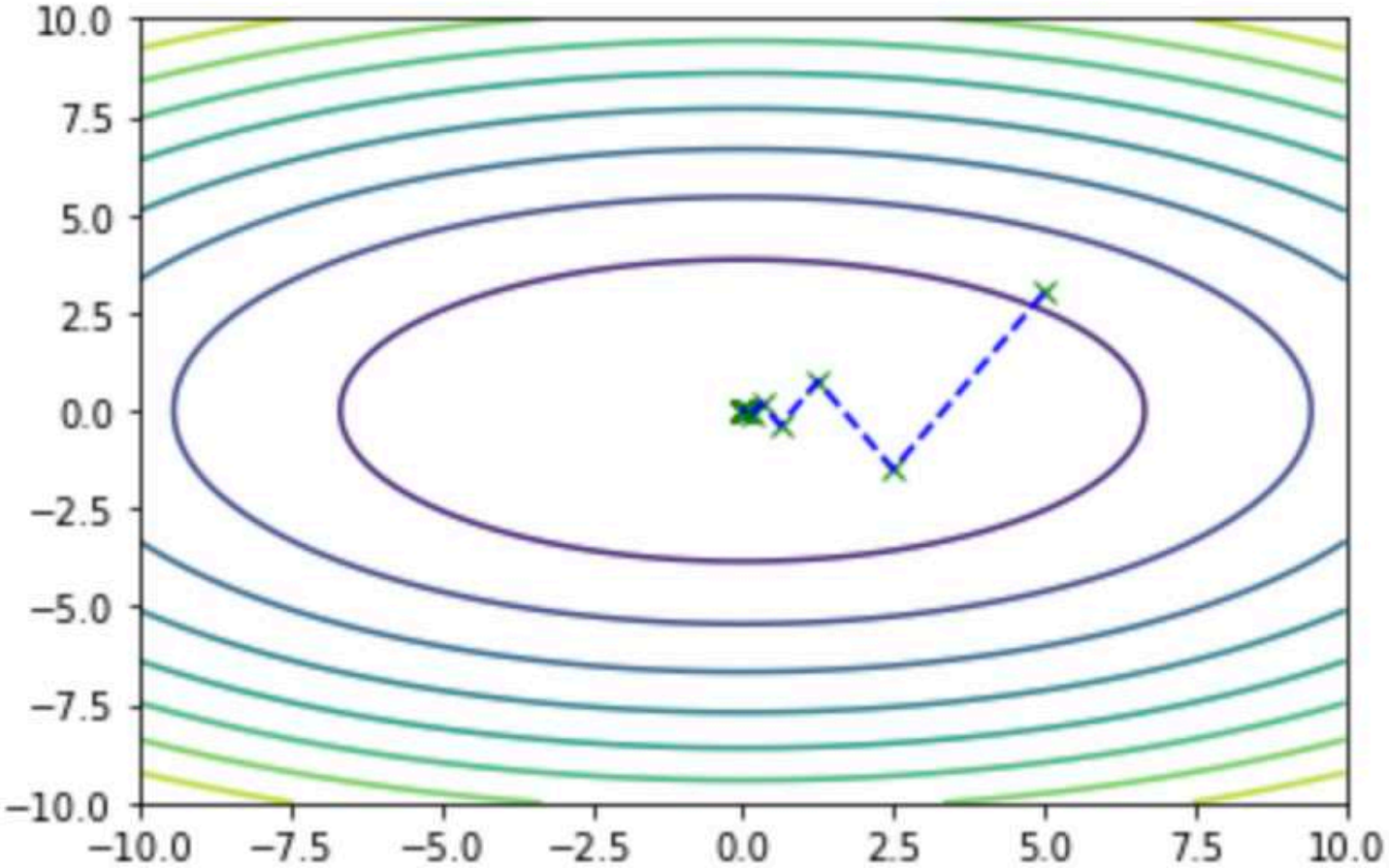
Note that the gradient of f is

$$\nabla f(\mathbf{x}) = \mathbf{Q}\mathbf{x}$$

Plotting contours (don't need to know)

Automatic saving

Python Demo



Convergence to the foot of the valley. Experiment with different values of the step size!

Questions?

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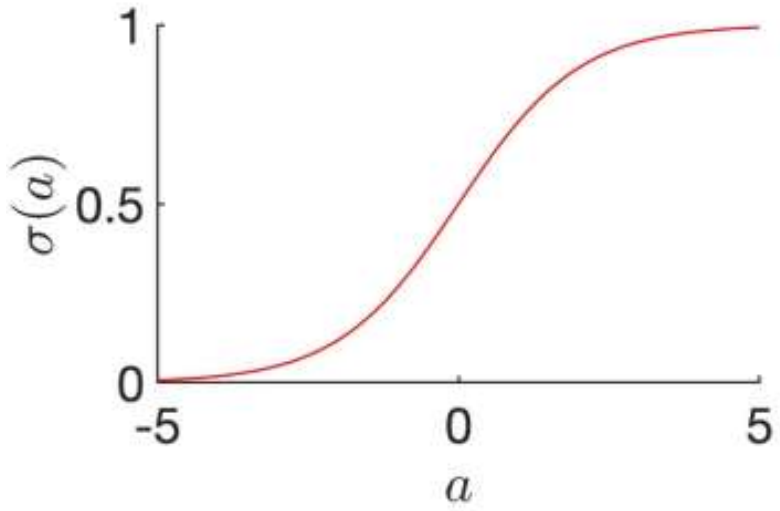
  - Can use sigmoid function to map $\mathbf{p}_i^T \mathbf{w}$ to between 0 and 1:

$$f(\mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{p}_i^T \mathbf{w})$$

$$\sigma(a) = \frac{1}{1 + e^{-a}}$$



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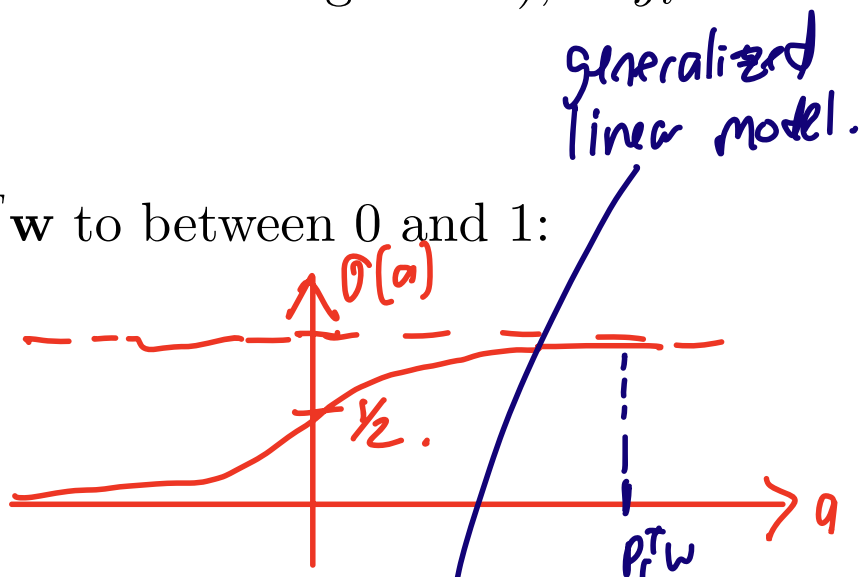

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- More generally, in one layer neural network: $f(\mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{p}_i^T \mathbf{w})$, where activation function σ can be sigmoid or some other functions & $\mathbf{p}$ is linear

Different Learning Models

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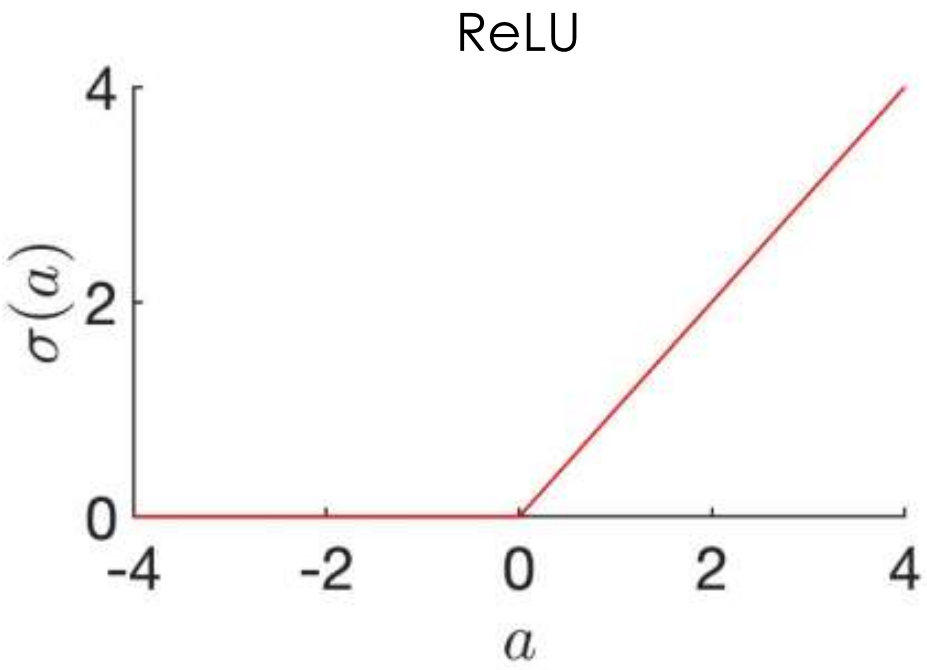

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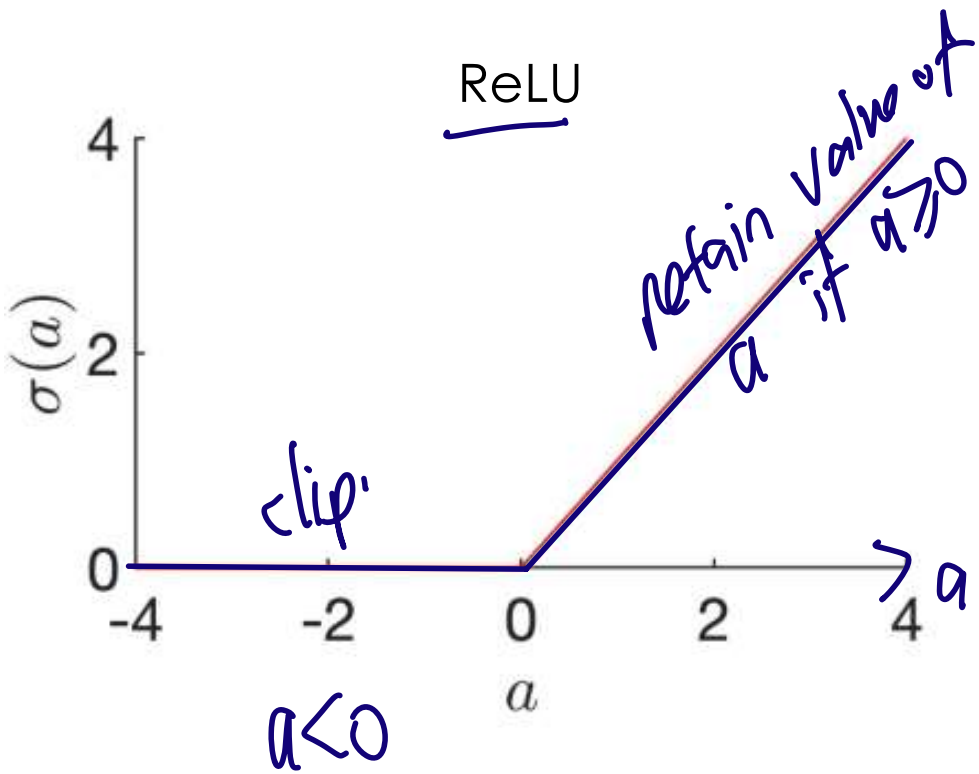
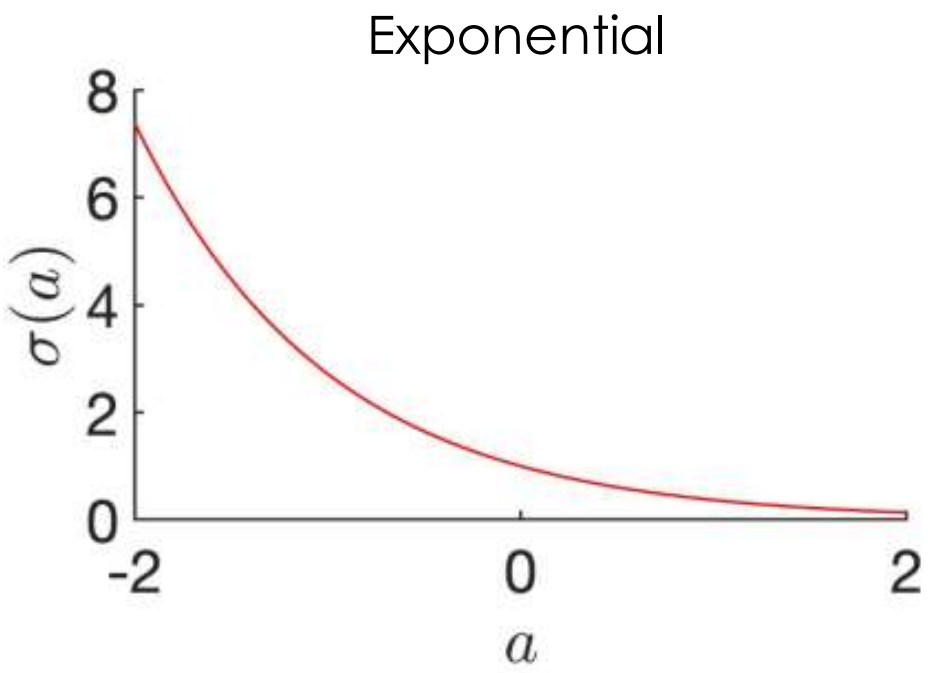
- Exponential: $\sigma(a) = \exp(-a)$





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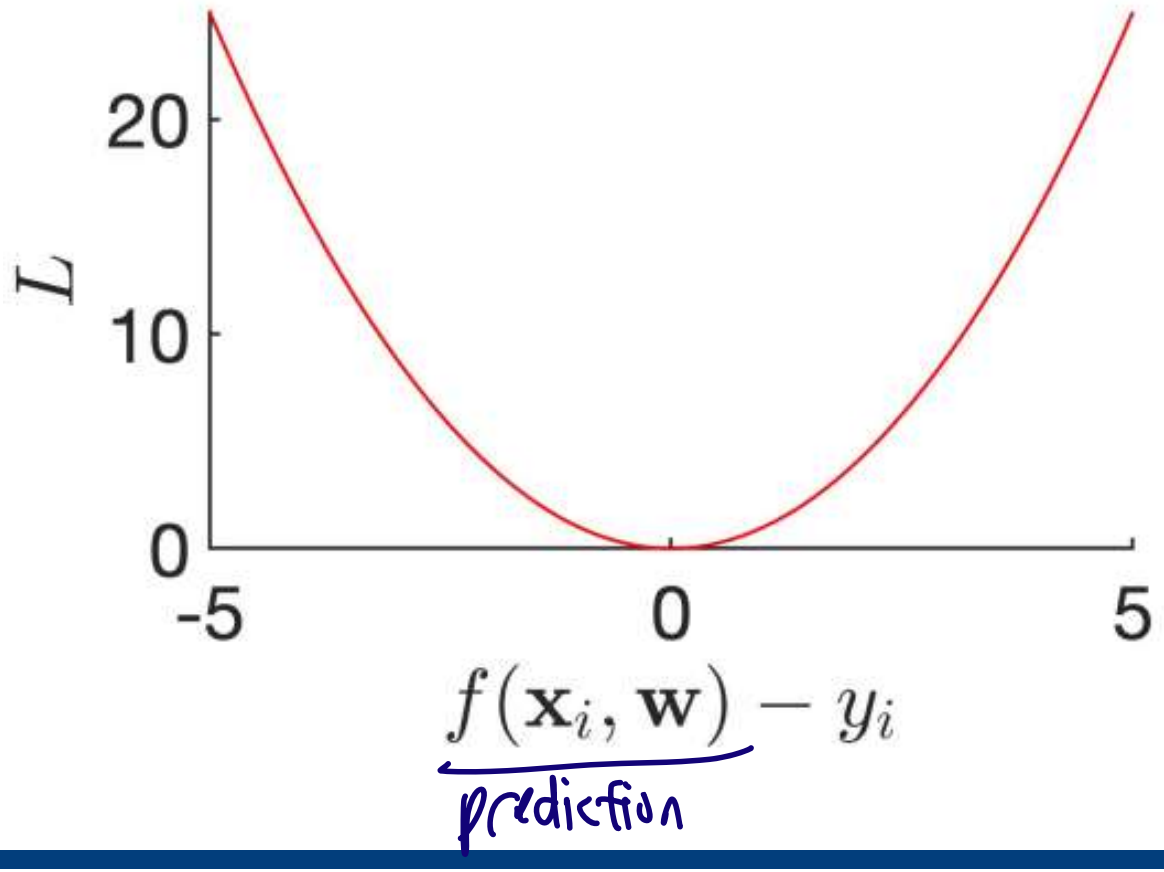

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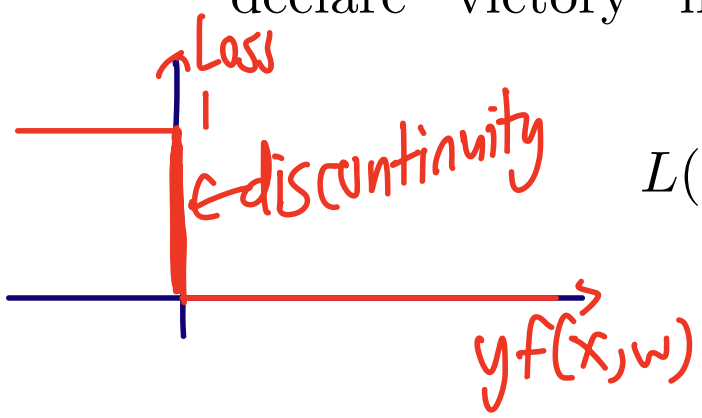

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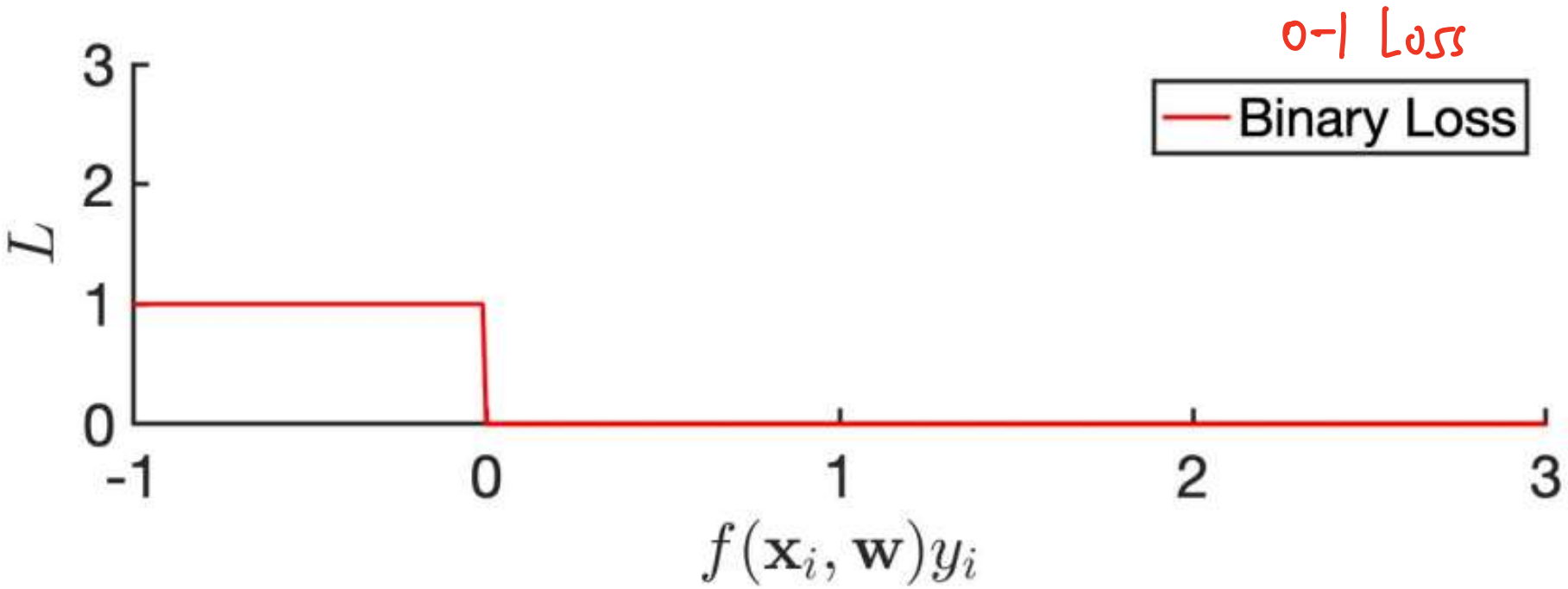

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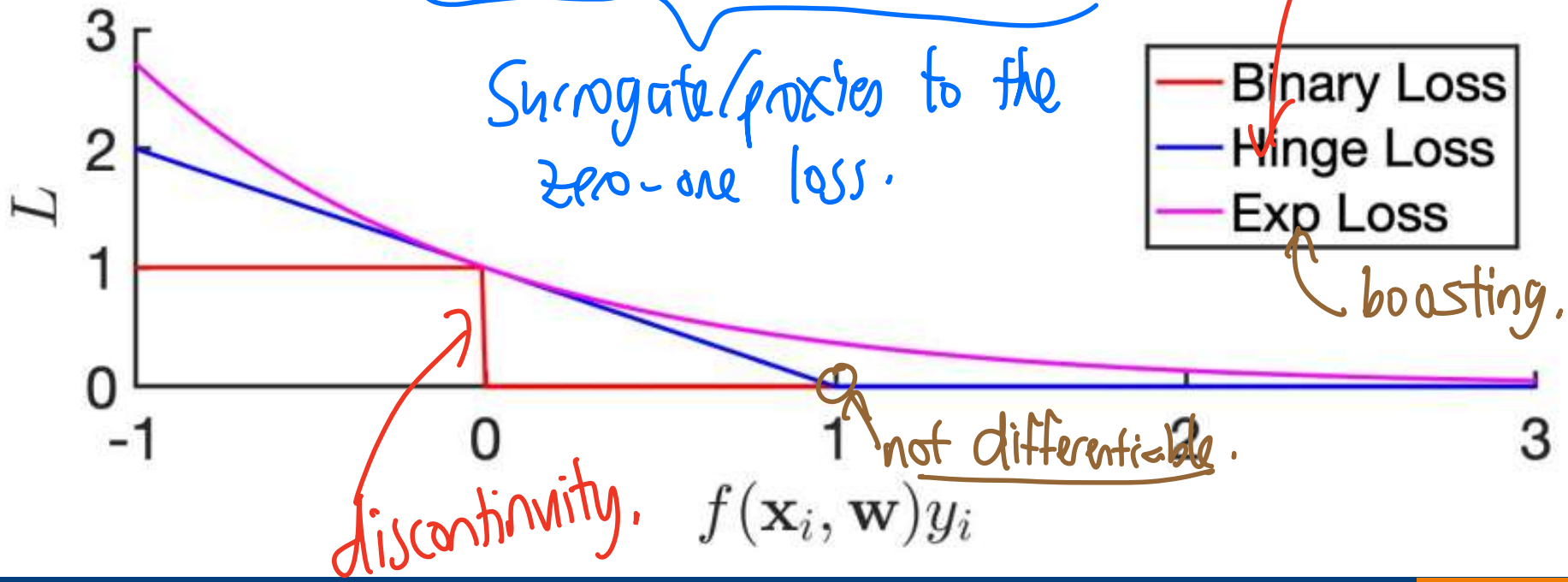
- Binary loss not differentiable, so two other possibilities
  - Hinge loss: $L(f(\mathbf{x}_i, \mathbf{w}), y_i) = \max(0, 1 - f(\mathbf{x}_i, \mathbf{w}) y_i)$
  - Exponential loss: $L(f(\mathbf{x}_i, \mathbf{w}), y_i) = \exp(-f(\mathbf{x}_i, \mathbf{w}) y_i)$



Questions?

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- Different loss functions, e.g., square error, binary, logistic, etc

Modelling: Choosing a model $f(\underline{x}, \underline{w})$,
Choosing a loss function (e.g. sq. error loss)
Choosing a regularization function ($\underline{w}^T\underline{w}$).

fixed

Separate

def

Loss / Cost / Objective function.

Optimization

$\underline{w}$

Choice of λ, choice of model $\Rightarrow$ Lecture 11.

Many ways to choose η.

$$\text{Cost}(\underline{w}) = \overbrace{(\underline{P}\underline{w} - \underline{y})^T (\underline{P}\underline{w} - \underline{y})}^{\text{Loss}(\underline{w})} + \overbrace{\lambda \underline{w}^T \underline{w}}^{\text{regularization}}.$$

$$\underline{w}^* = \underset{\underline{w}}{\text{argmin}} \ \text{Cost}(\underline{w})$$

$$\underline{w}^* = (\underline{P}^T\underline{P} + \lambda \underline{I})^{-1} \underline{P}^T \underline{y} = \underline{P}^T (\underline{P}\underline{P}^T + \lambda \underline{I})^{-1} \underline{y}$$

primal

dual.

$Reg(\underline{w}) = w^T w$ (Vanilla)

$Reg(\underline{w}) = \underline{w}^T R \underline{w}$