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A Bridge to Linear Regression

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PhD in Computer Science

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Objective

	Feature	Label
	area	price
	6.7	9.1
	4.6	5.9
	3.5	4.6
	5.5	6.7

House price data

Features			Label
TV	Radio	Newspaper	Sales
230.1	37.8	69.2	22.1
44.5	39.3	45.1	10.4
17.2	45.9	69.3	12
151.5	41.3	58.5	16.5
180.8	10.8	58.4	17.9

Advertising data

if area=6.0, price=?

if TV=55.0, Radio=34.0, and Newspaper=62.0, price=?

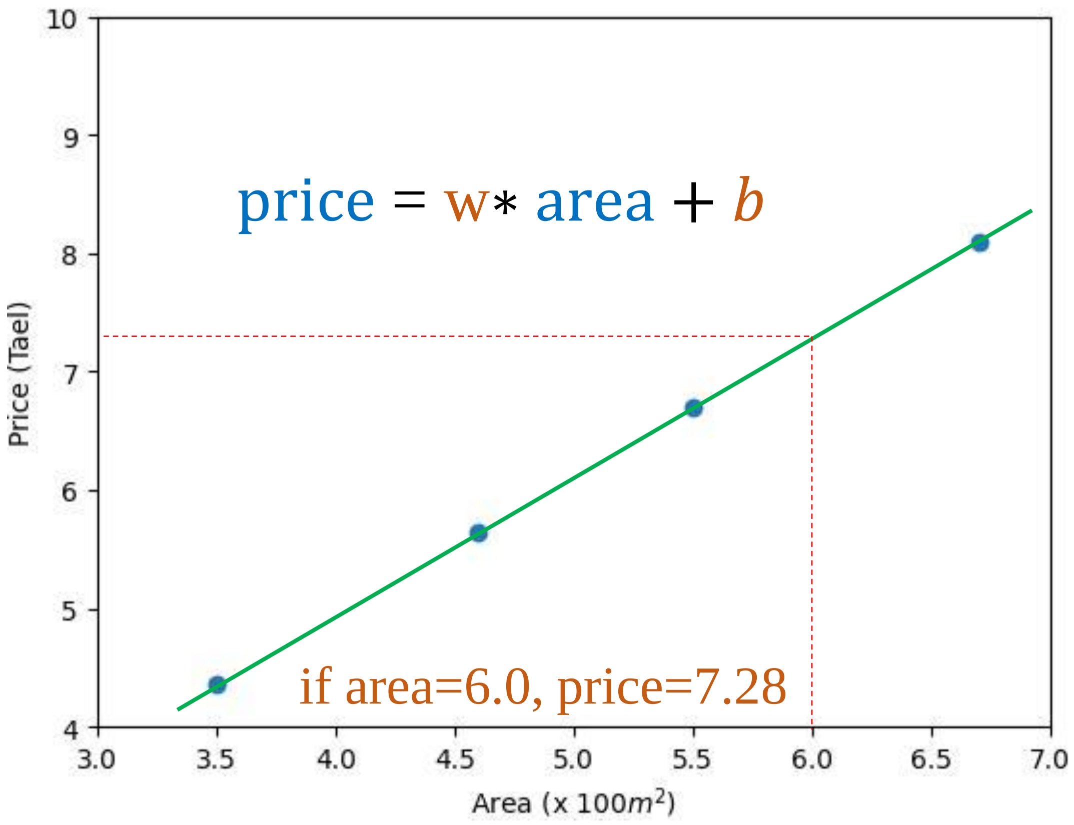
Features													Label
crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	black	lstat	medv
0.00632	18	2.31	0	0.538	6.575	65.2	4.09	1	296	15.3	396.9	4.98	24
0.02731	0	7.07	0	0.469	6.421	78.9	4.9671	2	242	17.8	396.9	9.14	21.6
0.03237	0	2.18	0	0.458	6.998	45.8	6.0622	3	222	18.7	394.63	2.94	33.4
0.06905	0	2.18	0	0.458	7.147	54.2	6.0622	3	222	18.7	396.9	5.33	36.2
0.08829	12.5	7.87	0	0.524	6.012	66.6	5.5605	5	311	15.2	395.6	12.43	22.9

Boston House Price Data

House Price Prediction

House price data

Feature	Label
area	price
6.7	8.1
4.6	5.6
3.5	4.3
5.5	6.7



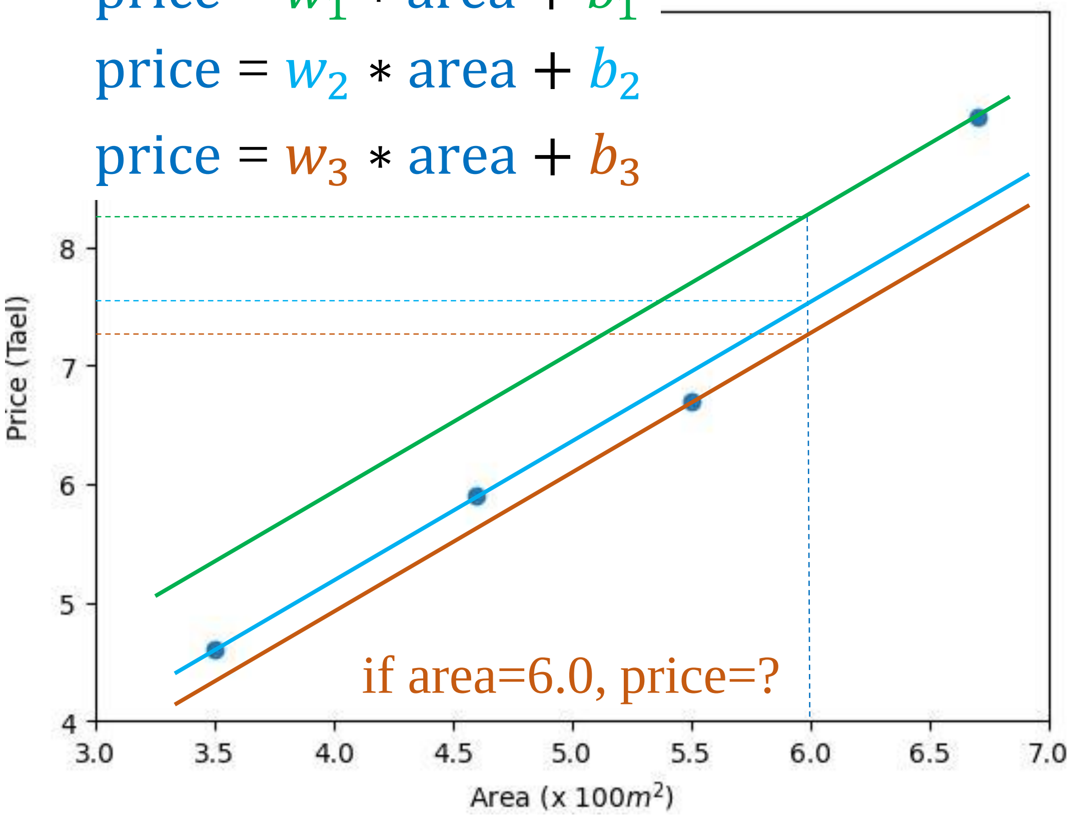
Feature	Label
area	price
6.7	9.1
4.6	5.9
3.5	4.6
5.5	6.7

House price data

$$\text{price} = w_1 * \text{area} + b_1$$

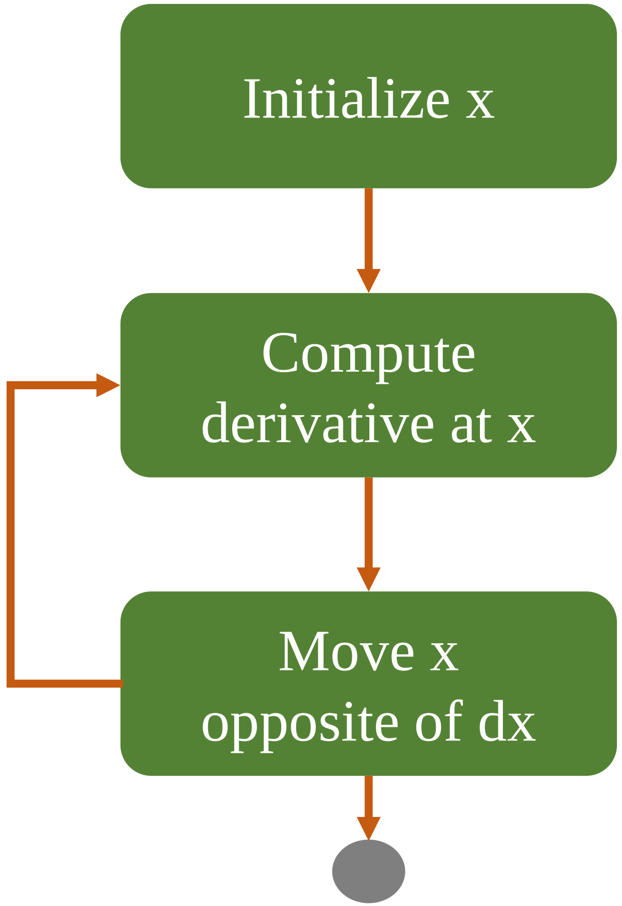
$$\text{price} = w_2 * \text{area} + b_2$$

$$\text{price} = w_3 * \text{area} + b_3$$



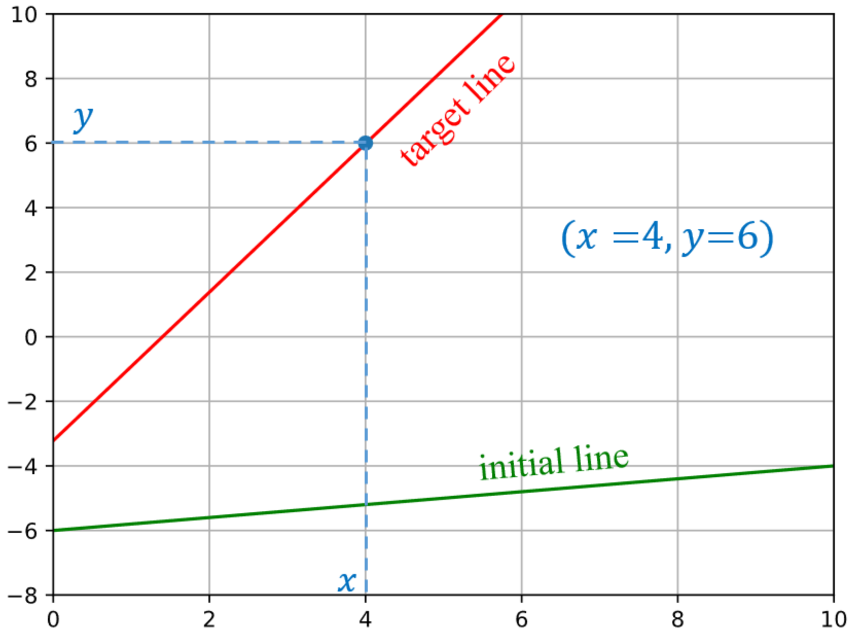
Objectives

Optimization

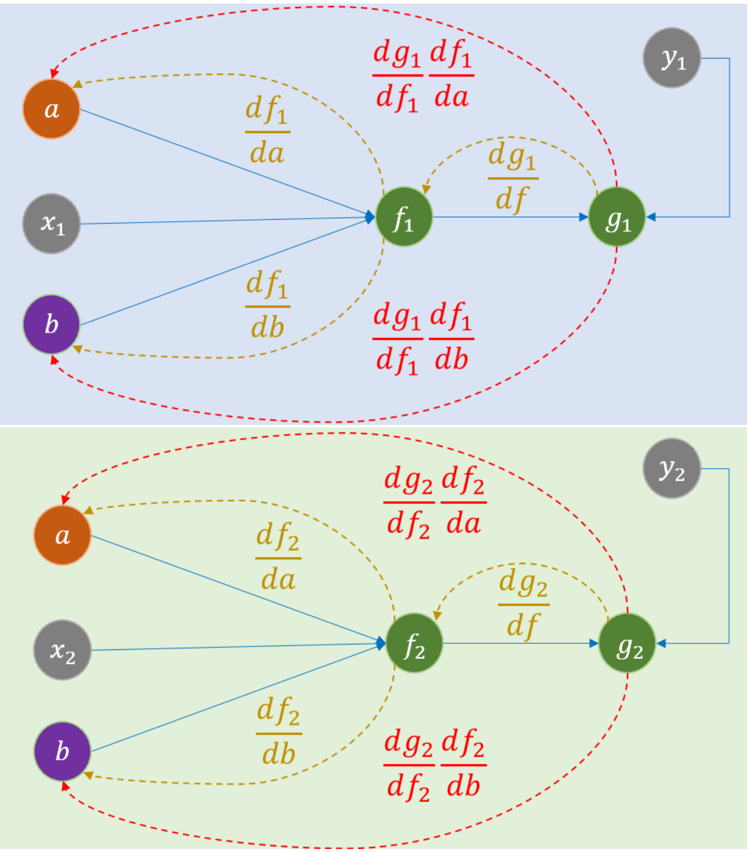


Problem Solving

$$f(x) = ax + b$$



Toward Linear Regression



Outline

SECTION 1

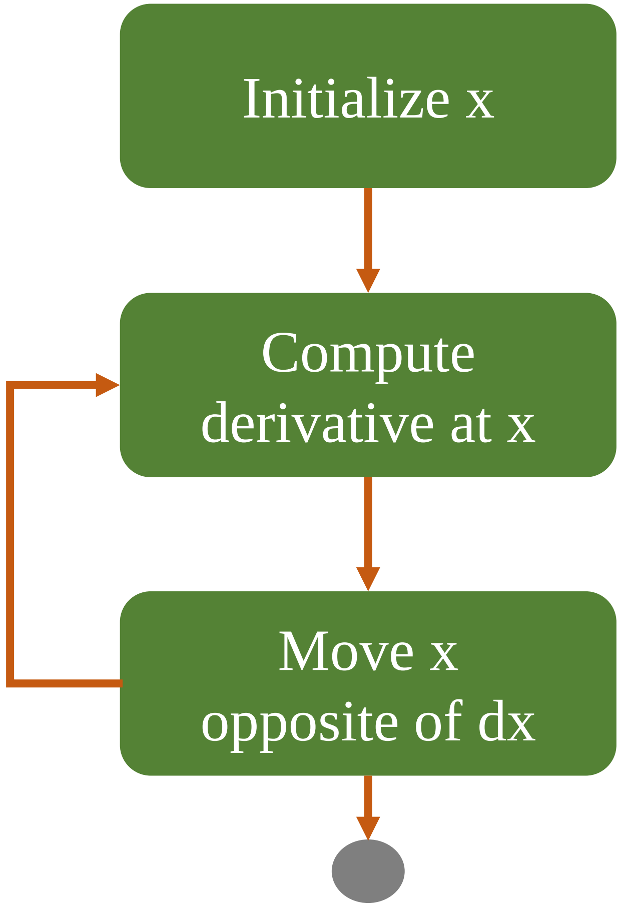
Optimization

SECTION 2

Problem Solving

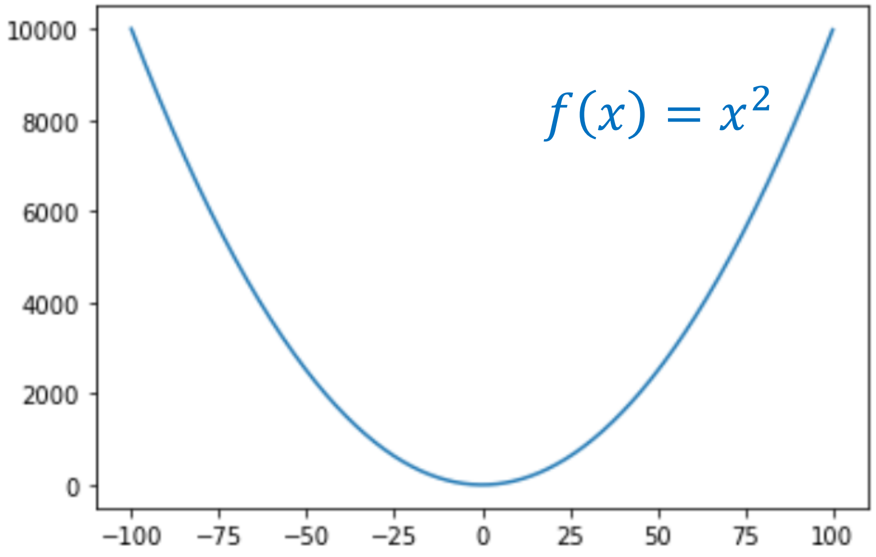
SECTION 3

Towards Linear Regression

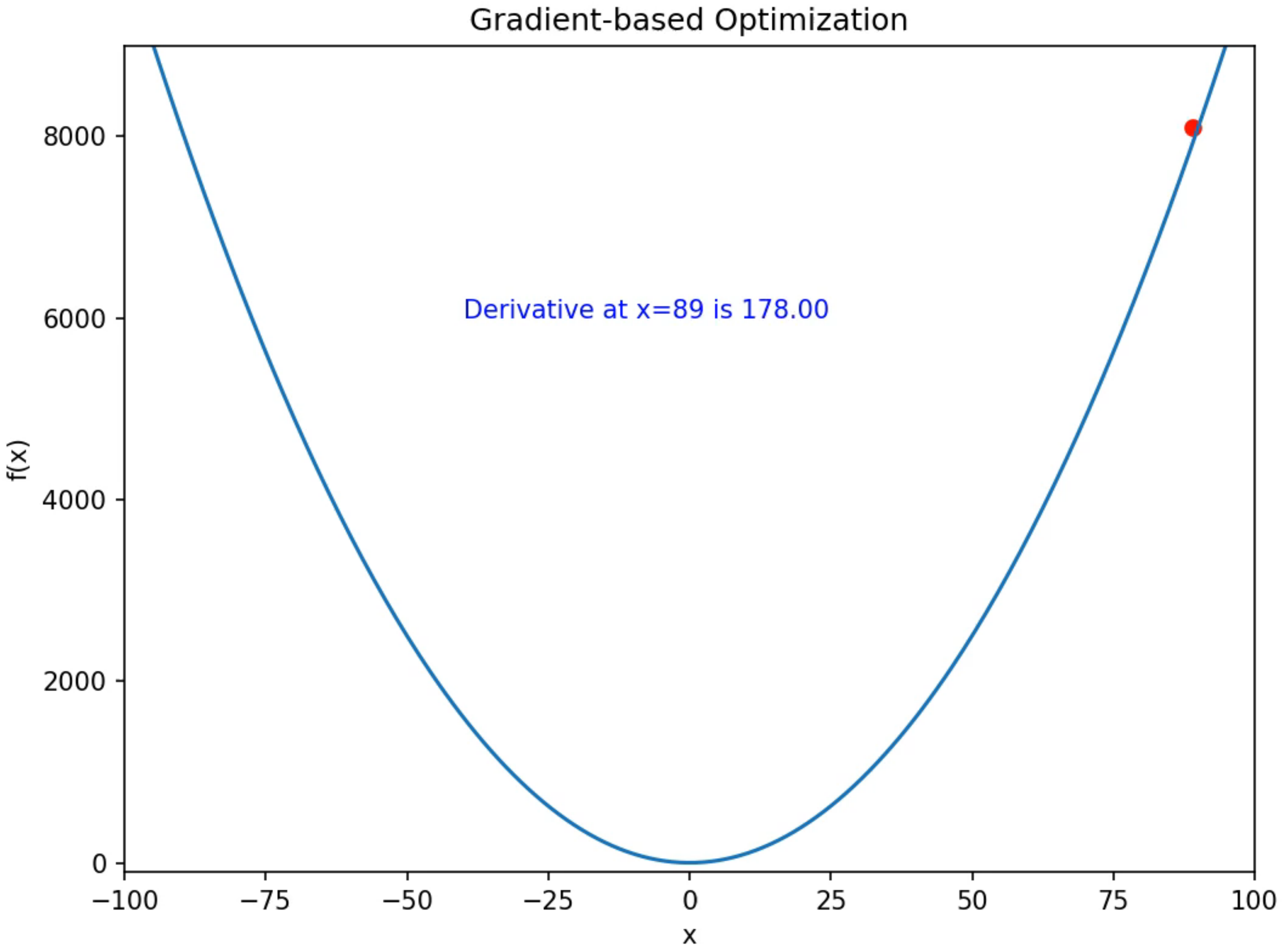


Optimization

❖ Square function

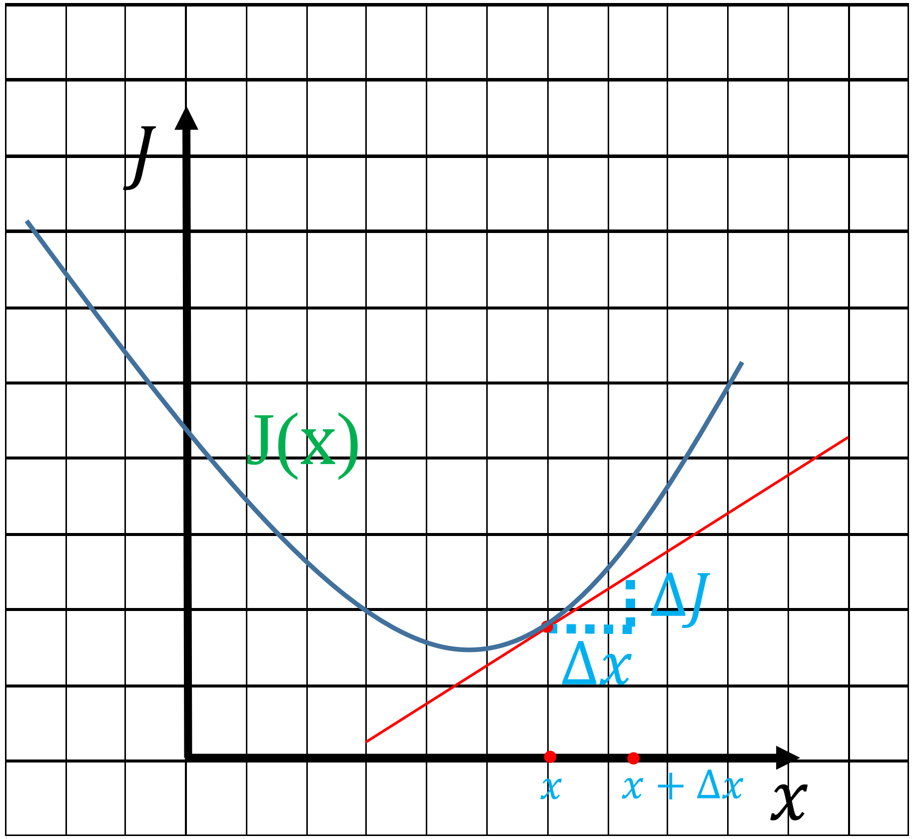


$$\frac{d}{dx} f(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

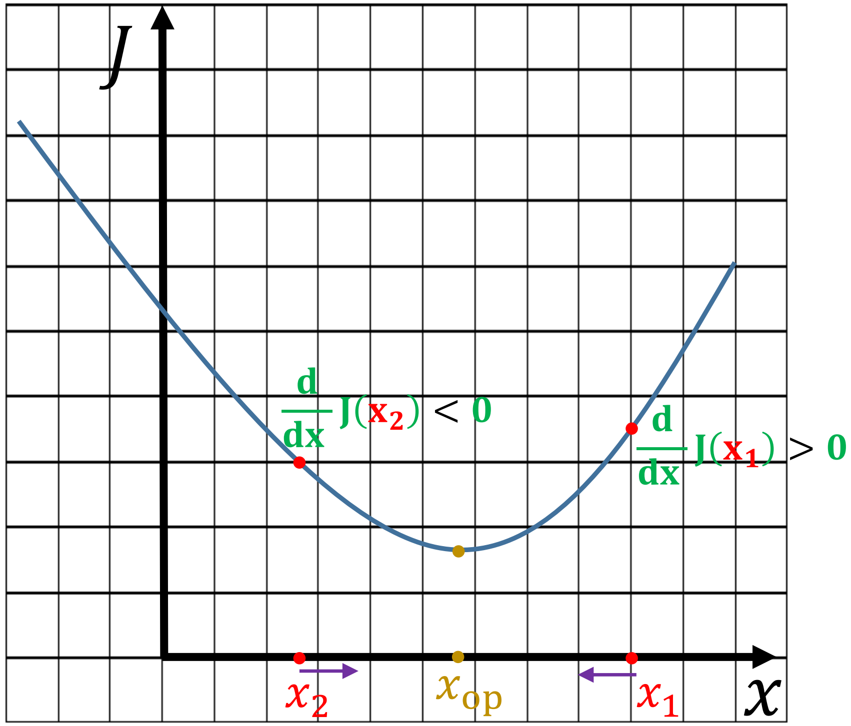


Optimization

❖ Gradient descent



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



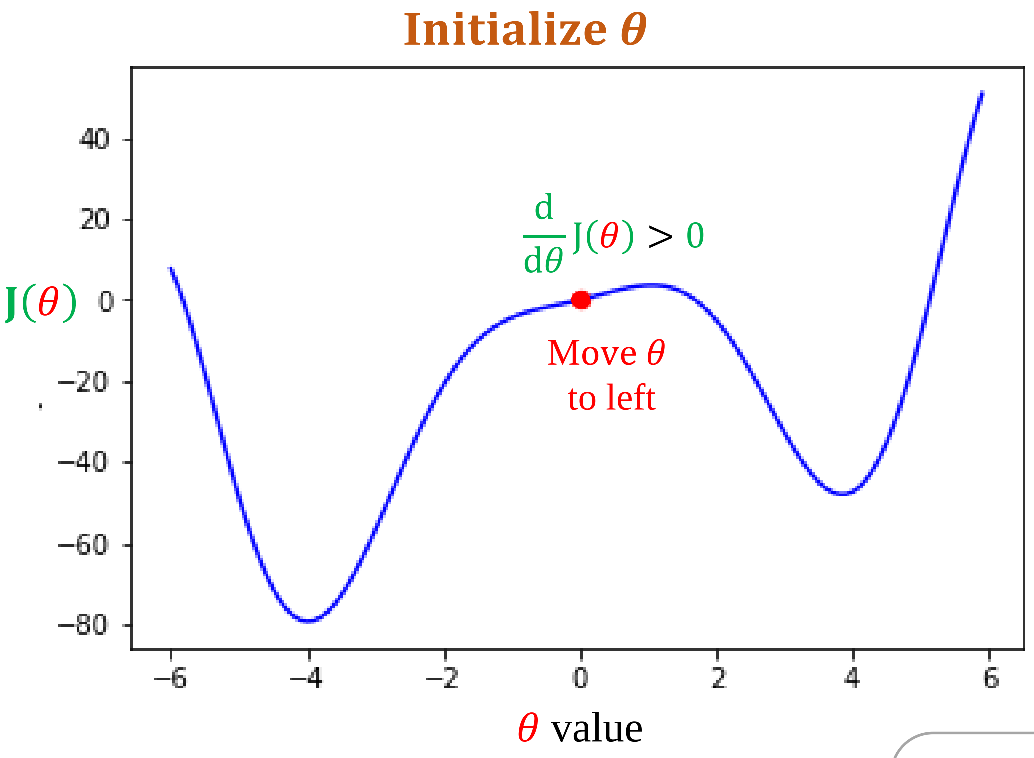
$$\mathbf{x}_{new} = \mathbf{x}_{old} - \eta \frac{\mathbf{d}}{\mathbf{dx}}\mathbf{J}(\mathbf{x}_{old})$$

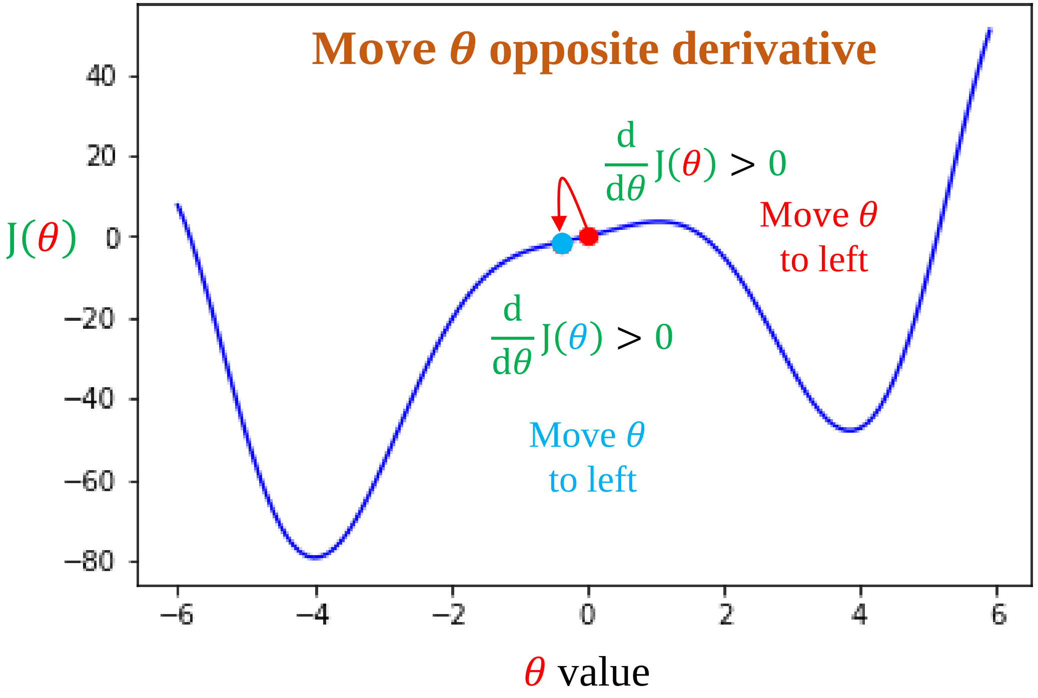
Derivate at x_{old}

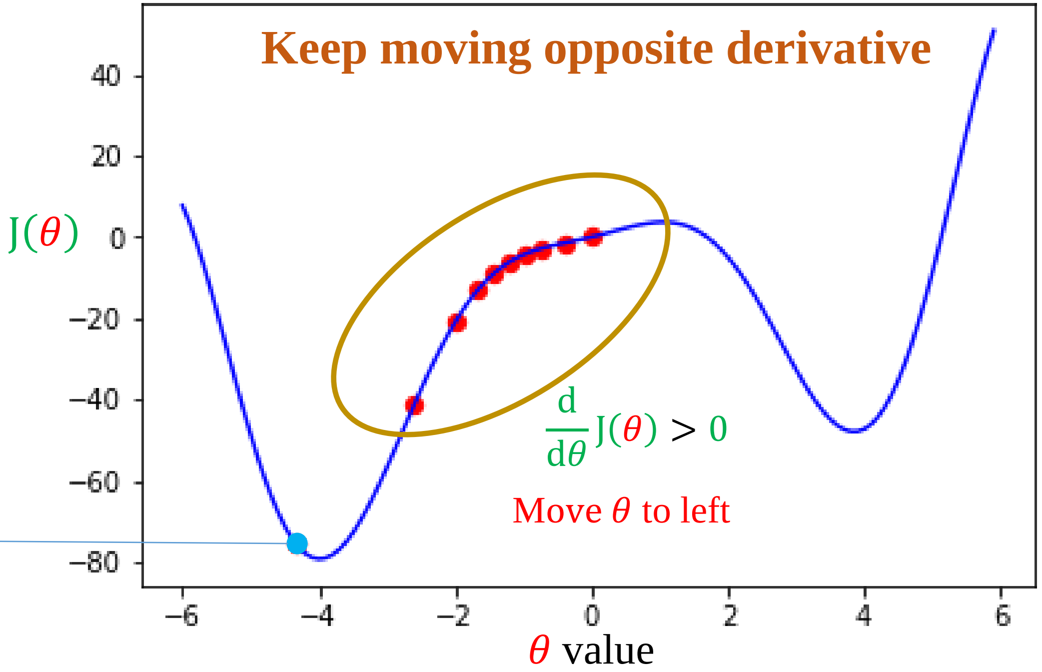
learning rate

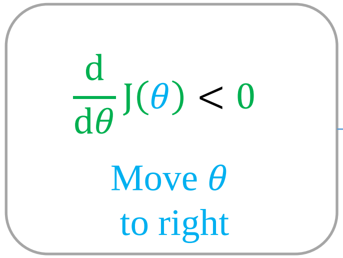
Optimization

❖ Gradient descent





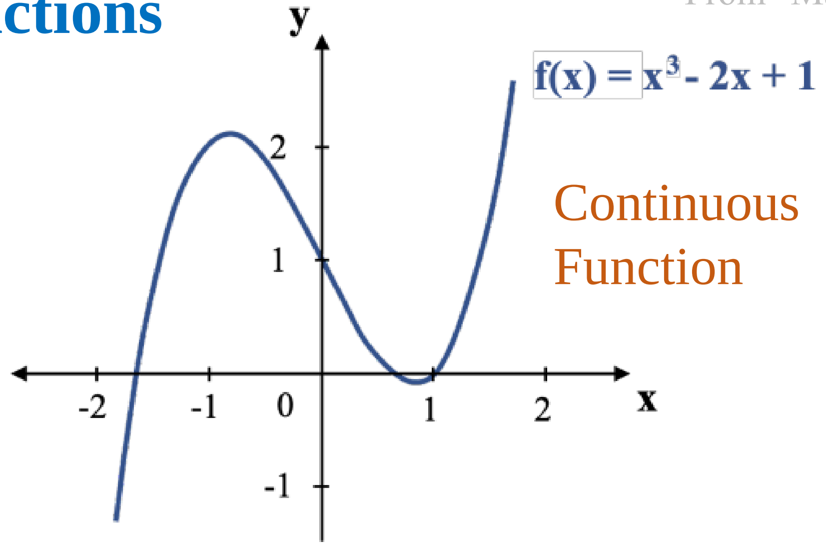




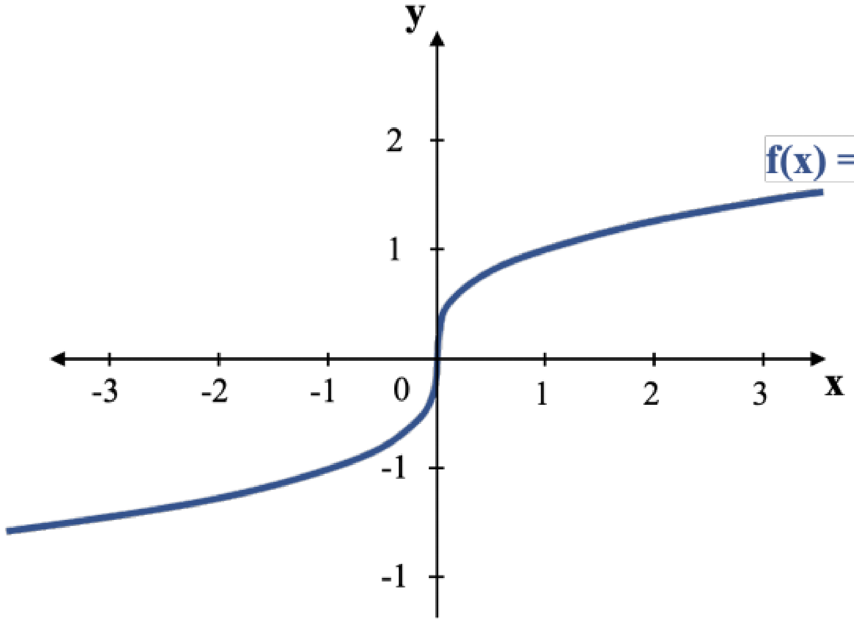
Optimization Algorithms

Loss functions

From "Machine Learning Simplified"

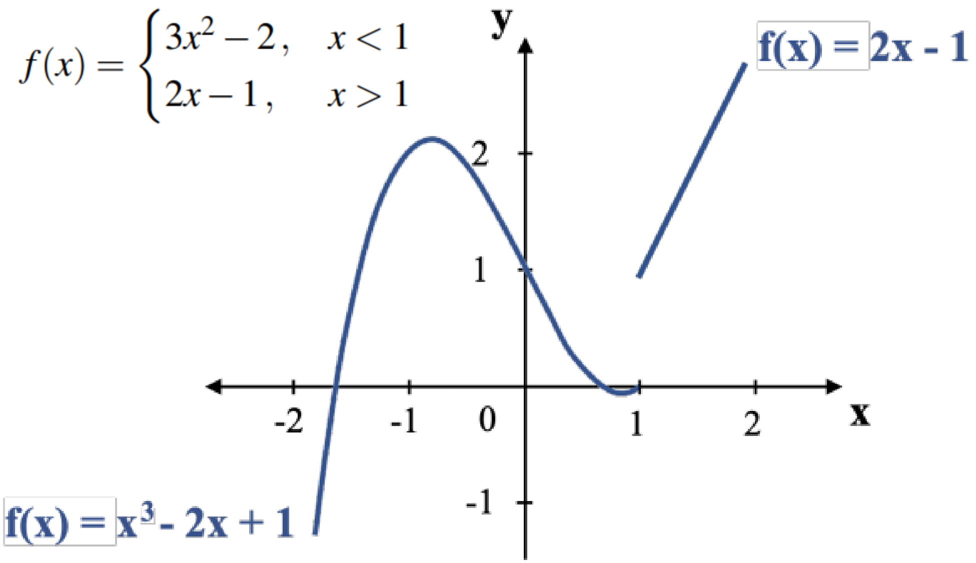


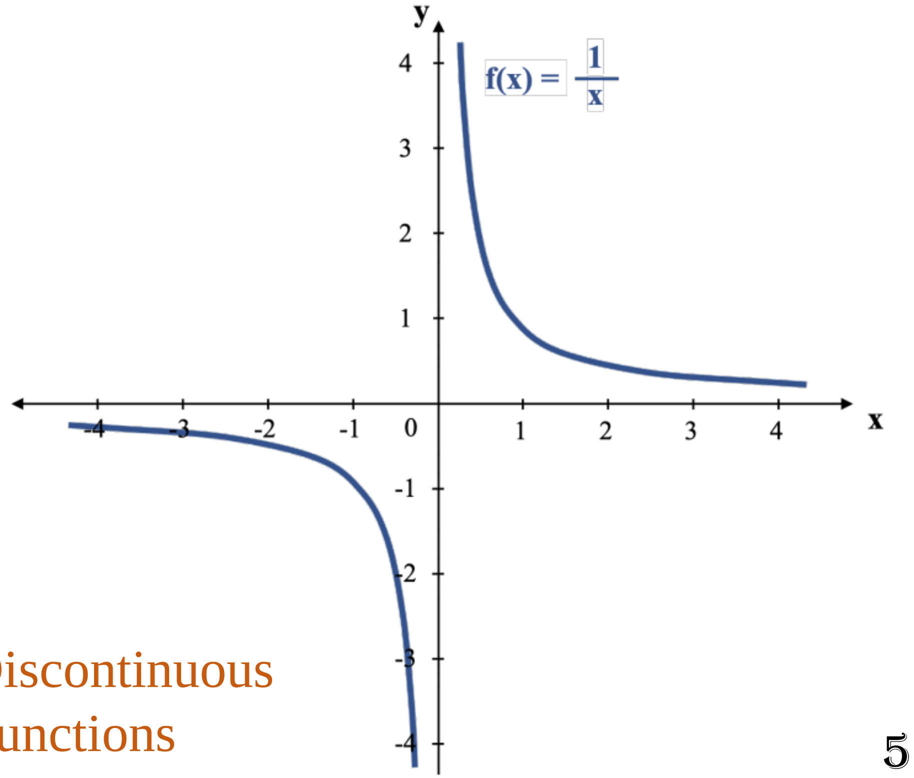
Continuous Function



Continuous non-differentiable functions

$$f(x) = \begin{cases} 3x^2 - 2, & x < 1 \\ 2x - 1, & x > 1 \end{cases}$$

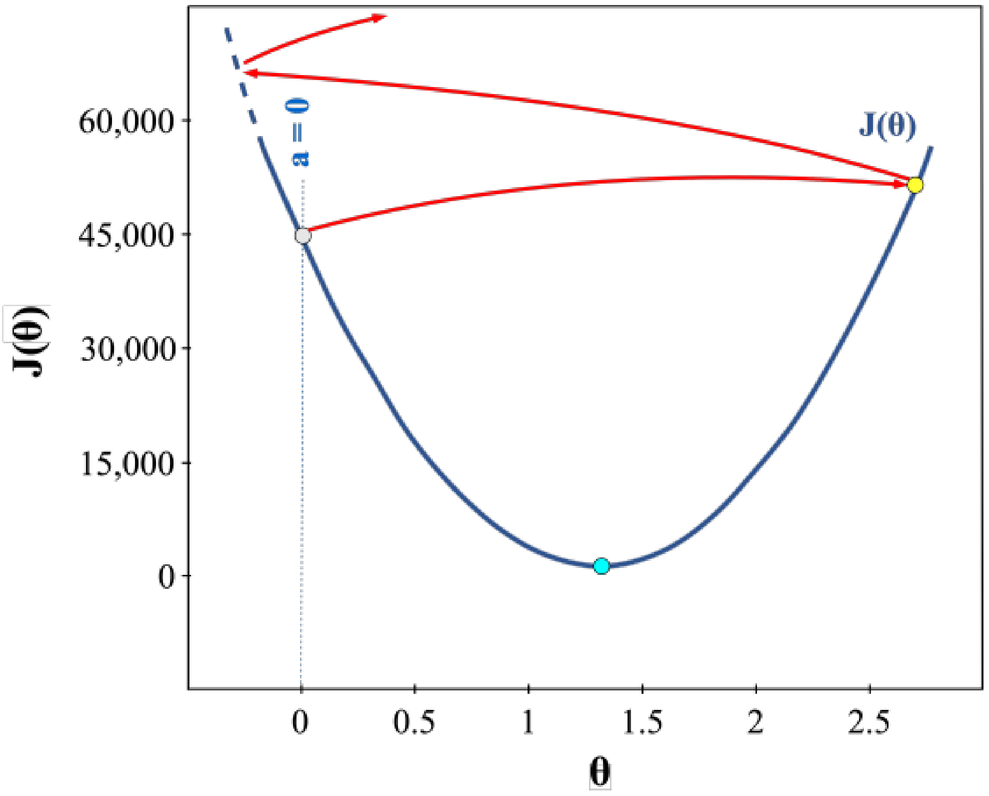




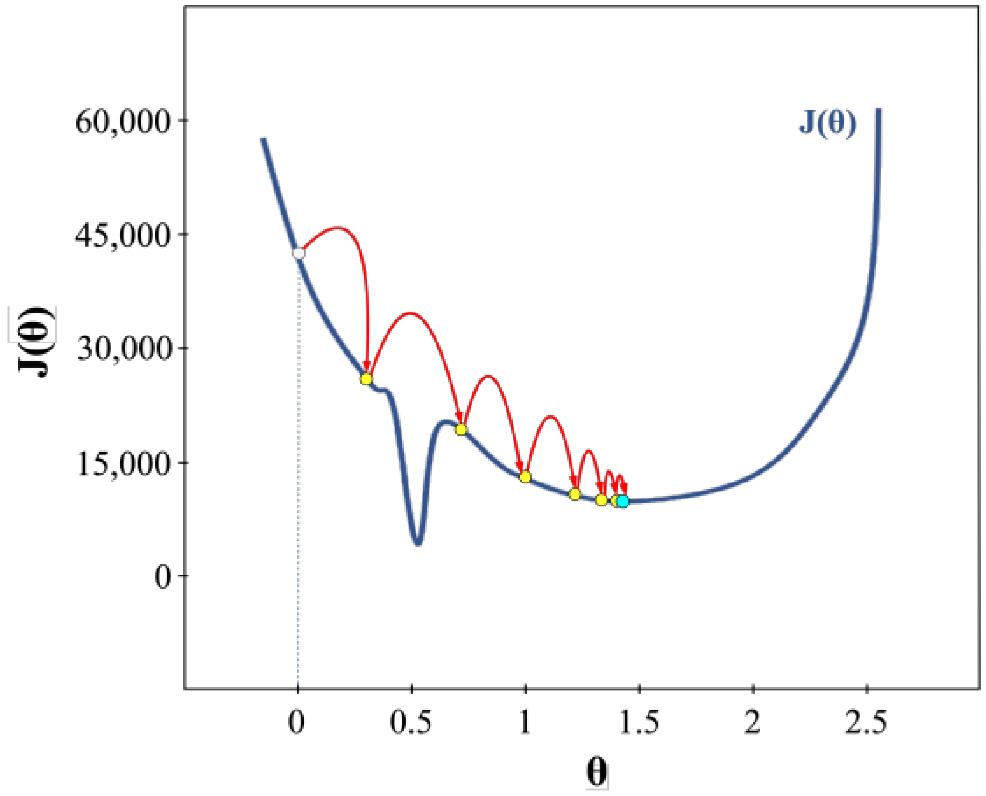
Discontinuous Functions

Optimization Algorithms

❖ Learning rate



(a) Gradient descent missing global minimum on a convex cost function due to a very large learning rate.



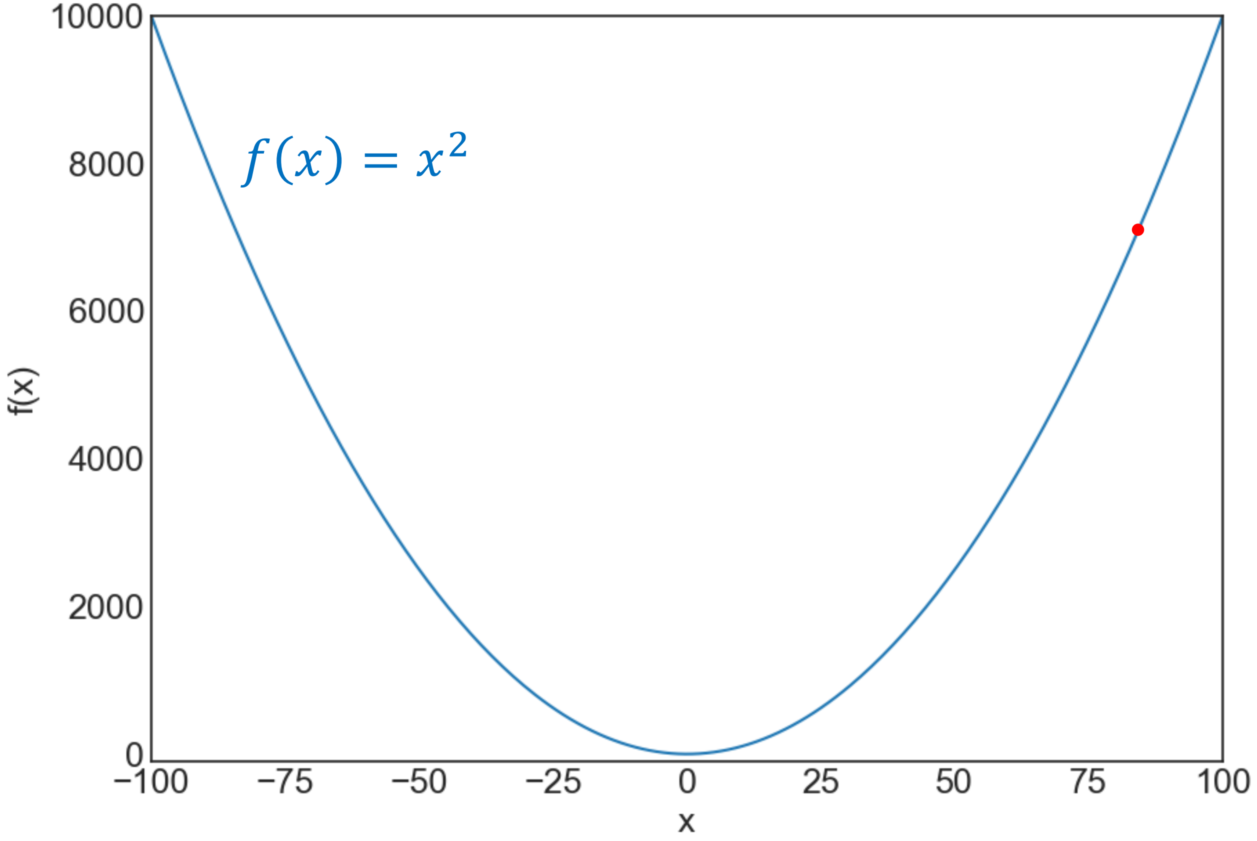
(b) Gradient Descent missing global minimum on a non-convex cost function due to a very large learning rate.

From “Machine Learning Simplified”

Observation 1

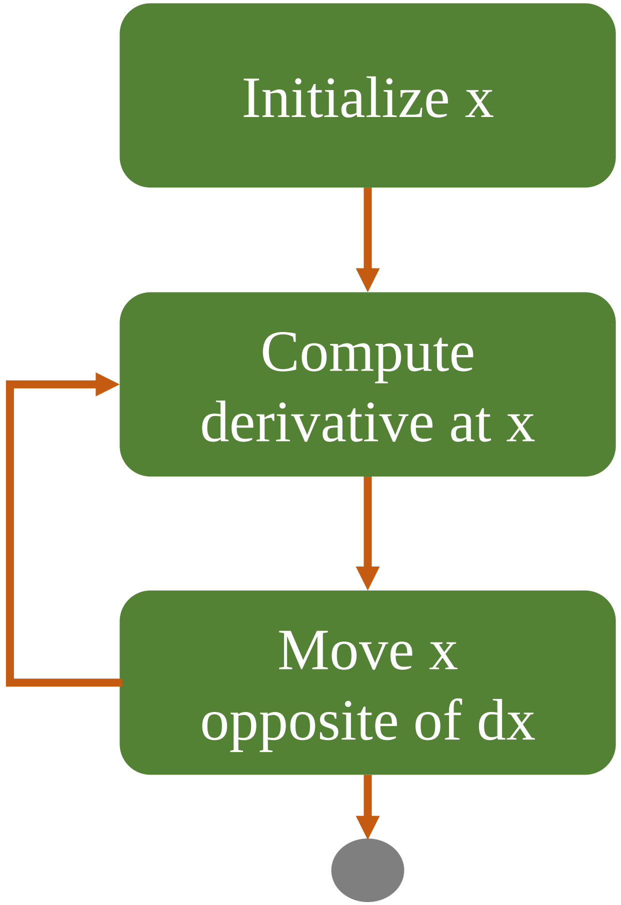
Optimization

❖ Square function



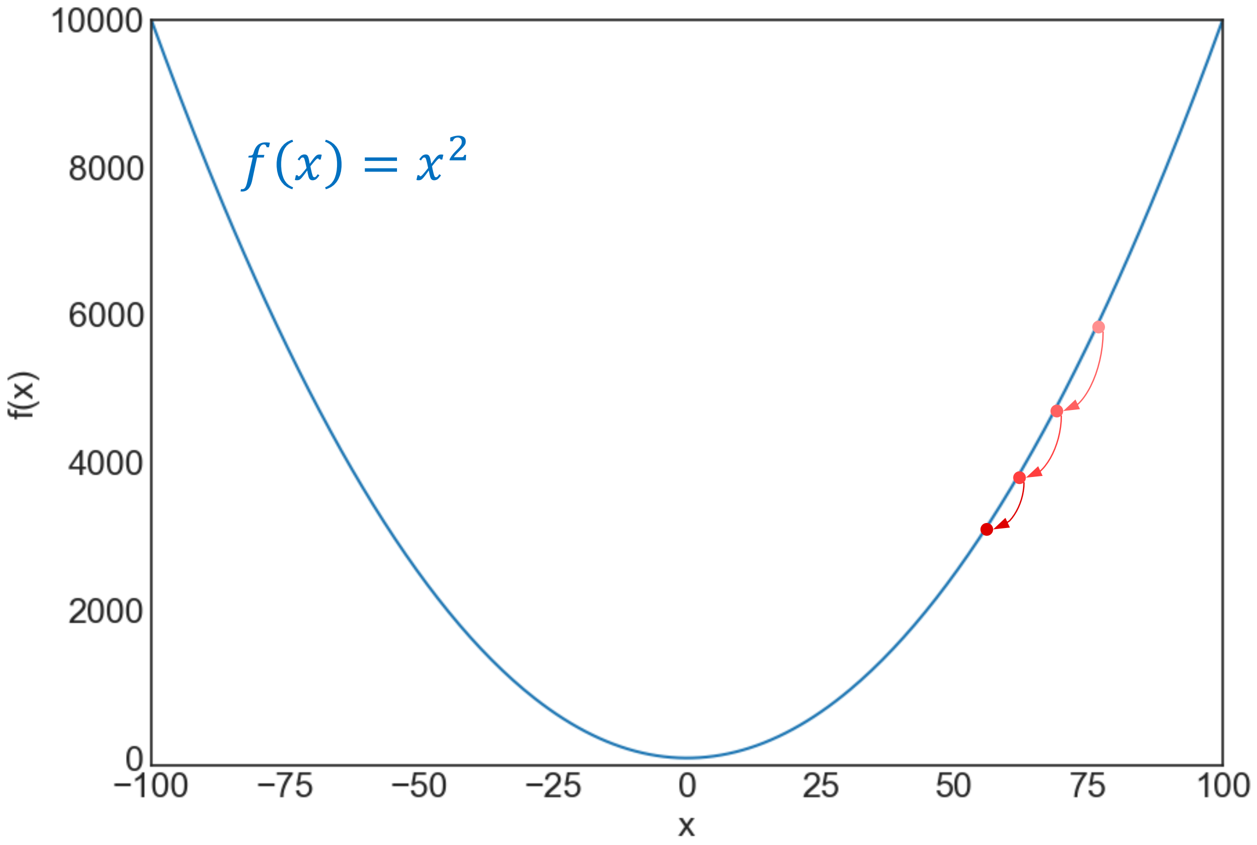
$$-100 \leq x \leq 100$$
$$x \in \mathbb{N}$$

$$x_t = x_{t-1} - \eta f'(x_{t-1})$$



Optimization

❖ Square function



$$-100 \le x \le 100$$
$$x \in \mathbb{N}$$

$$x_t = x_{t-1} - \eta f'(x_{t-1})$$

$x_0 = 70.0$ $\eta = 0.1$

$f'(x_0) = 140.0$

$x_1 = x_0 - \eta f'(x_0) = 56.0$

$\mathrm{f}'(\mathrm{x}_1) = 112.0$

$x_2 = x_1 - \eta f'(x_1) = 44.8$

$\mathrm{f}'(\mathrm{x}_2) = 89.6$

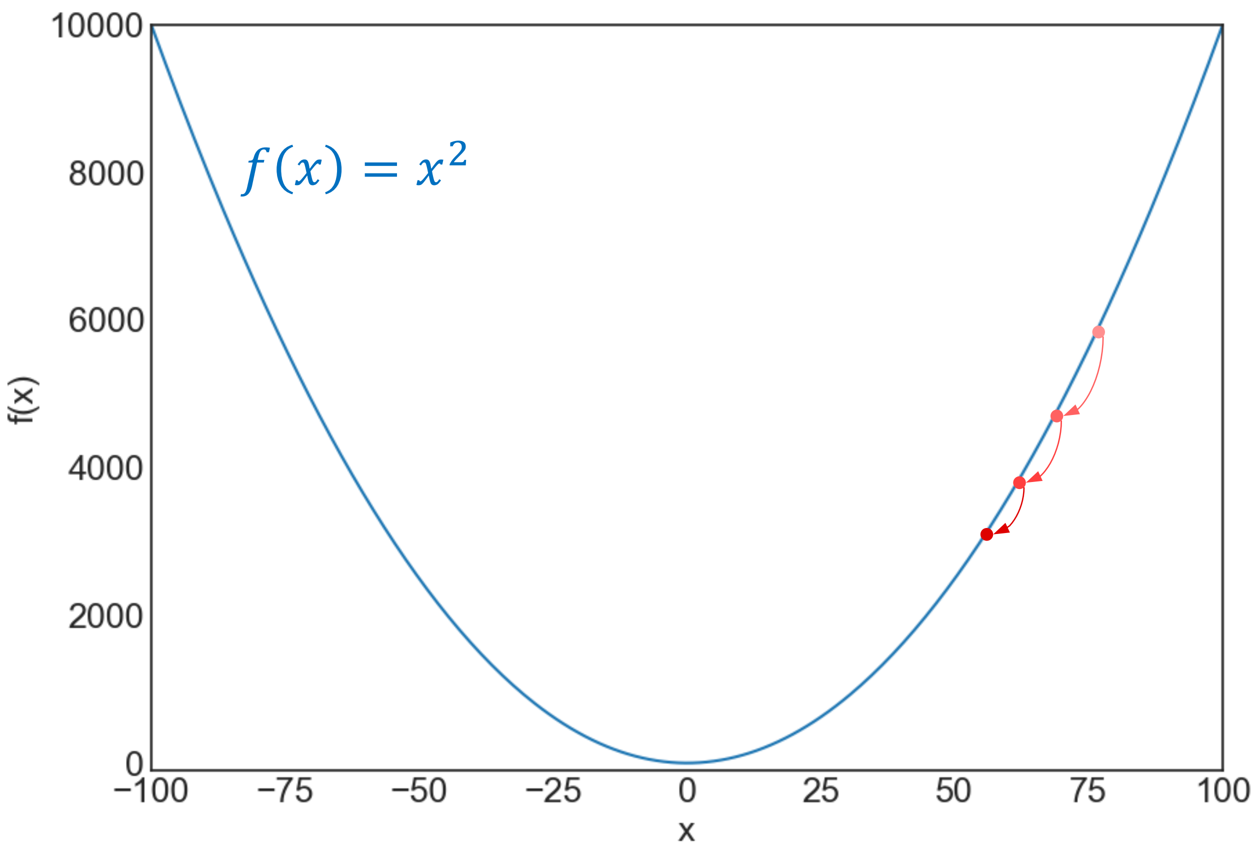
$x_3 = x_2 - \eta f'(x_2) = 35.84$

$\mathrm{f}'(\mathrm{x}_3) = 71.68$

$x_4 = x_3 - \eta f'(x_3) = 28.672$

Optimization

❖ **Square function**



Keep doing

$$x_t = x_{t-1} - \eta f'(x_{t-1})$$

$x_{10} = 6.012$ $\eta = 0.1$

$f'(x_{10}) = 12.02$

$x_{11} = x_{10} - \eta f'(x_{10}) = 4.81$

$\mathrm{f}'(\mathrm{x}_{11}) = 9.62$

$x_{12} = x_{11} - \eta f'(x_{11}) = 3.84$

$\mathrm{f}'(\mathrm{x}_{12}) = 7.69$

$x_{13} = x_{12} - \eta f'(x_{12}) = 3.078$

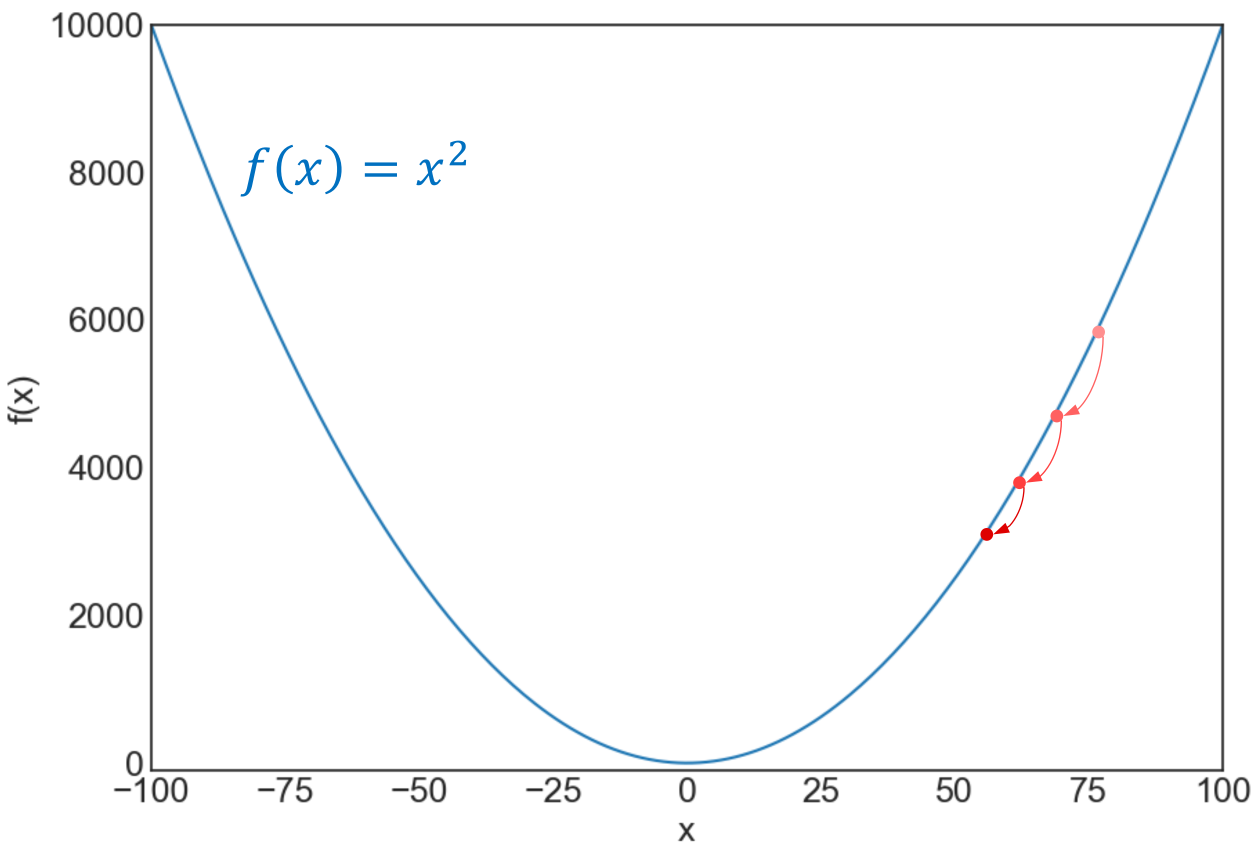
$\mathrm{f}'(\mathrm{x}_{13}) = 6.15$

$x_{14} = x_{13} - \eta f'(x_{13}) = 2.46$

Optimization

$$x_t = x_{t-1} - \eta f'(x_{t-1})$$

❖ Square function



$x_{30} = 0.069 \qquad \eta = 0.1$

$f'(x_{30}) = 0.138$

$x_{31} = x_{30} - \eta f'(x_{30}) = 0.055$

$f'(x_{31}) = 0.11$

$x_{32} = x_{31} - \eta f'(x_{31}) = 0.044$

$f'(x_{32}) = 0.88$

$x_{33} = x_{32} - \eta f'(x_{32}) = 0.035$

$f'(x_{34}) = 0.071$

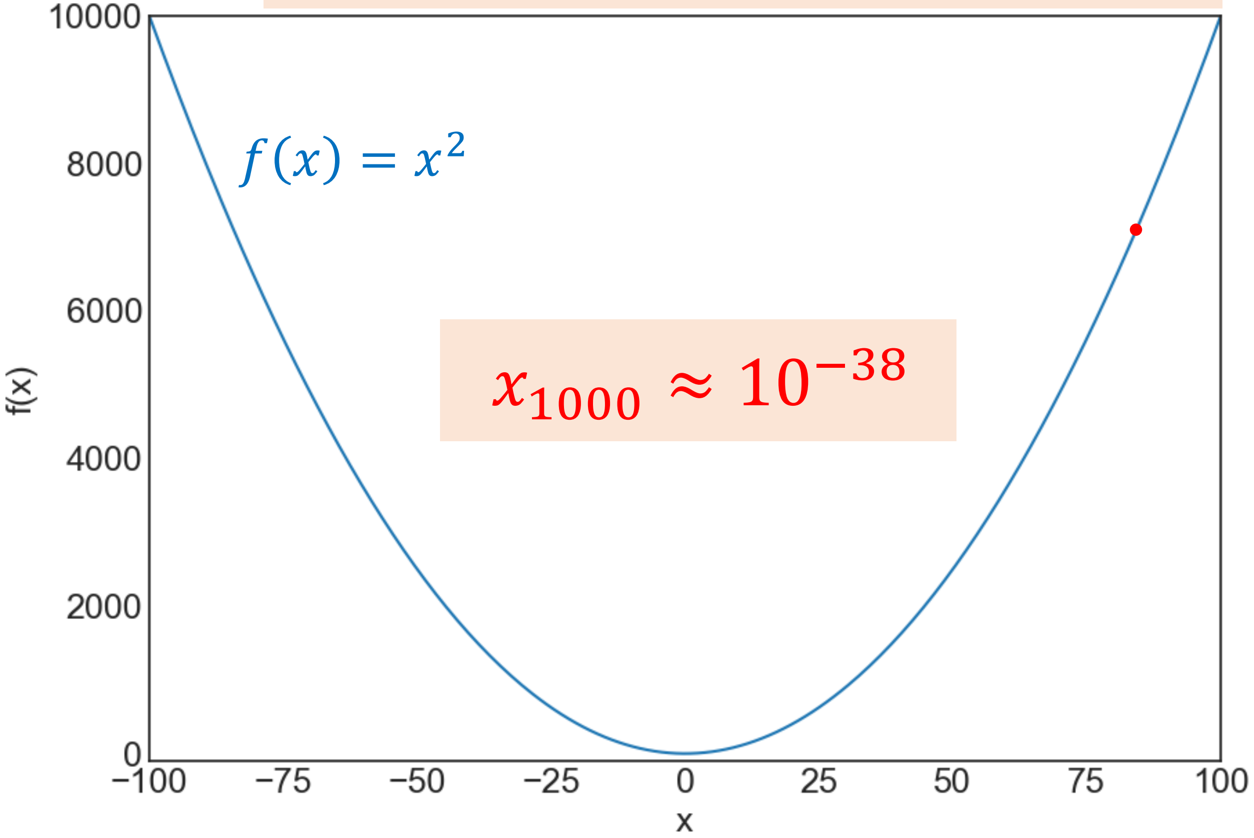
$x_{34} = x_{33} - \eta f'(x_{33}) = 0.028$

Keep doing

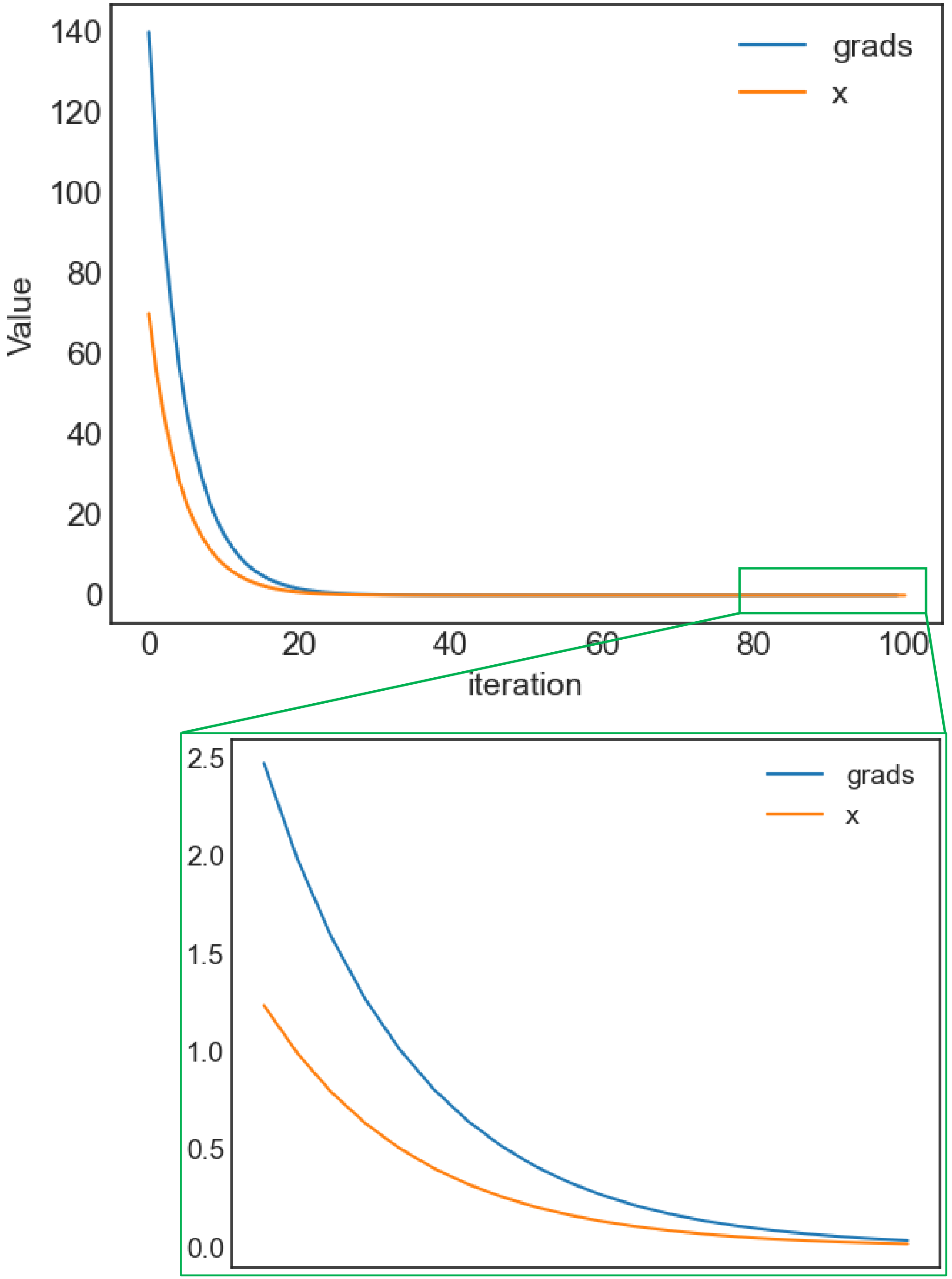
Optimization

❖ **Square function**

$$x_t = x_{t-1} - \eta f'(x)$$



$$x_{1000} \approx 10^{-38}$$



Optimized successfully!

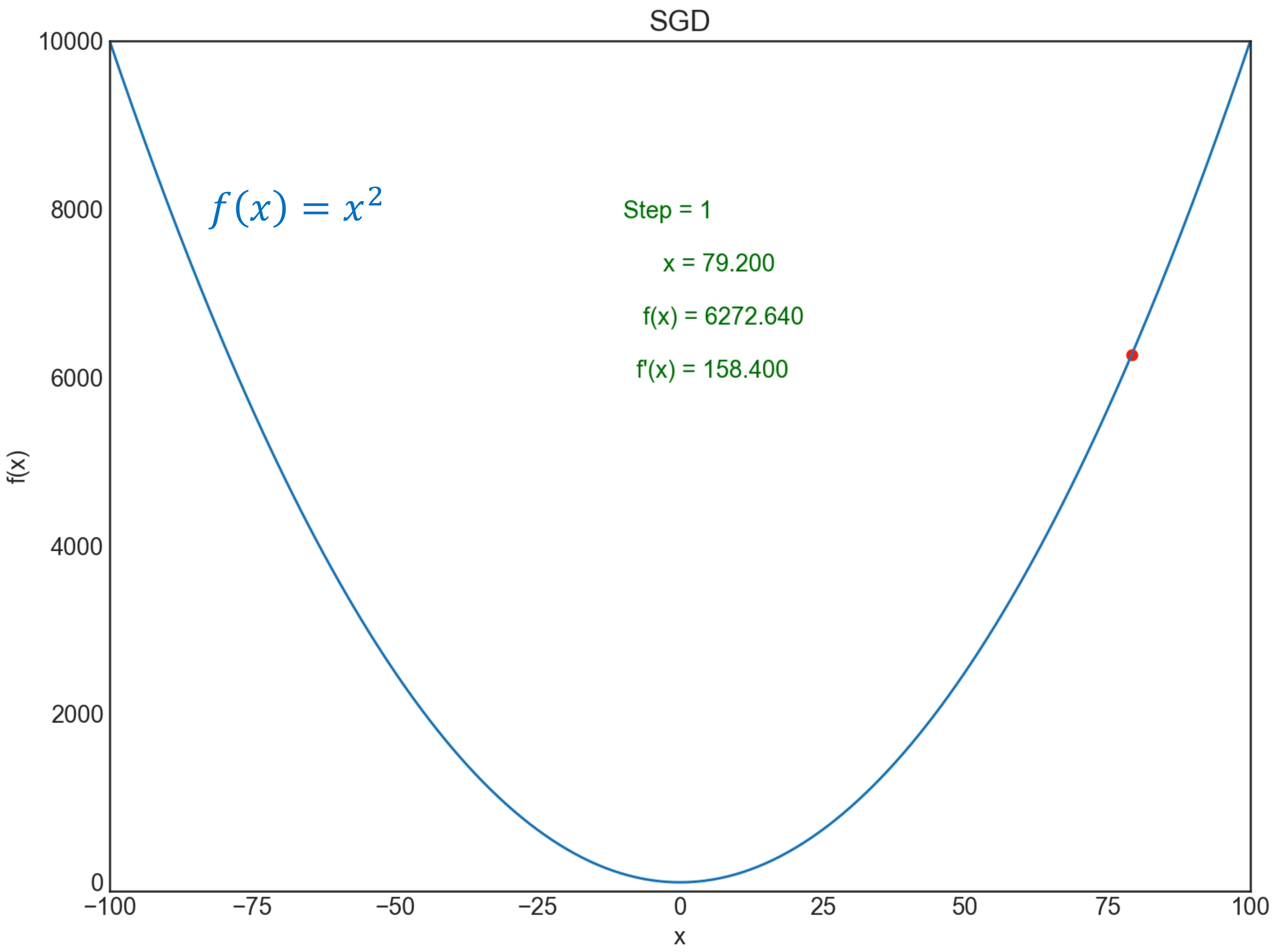
Optimization

❖ **Square function**

$$x_0 = 99.0$$

$$\eta = 0.1$$

$$x_t = x_{t-1} - \eta f'(x)$$



Optimization

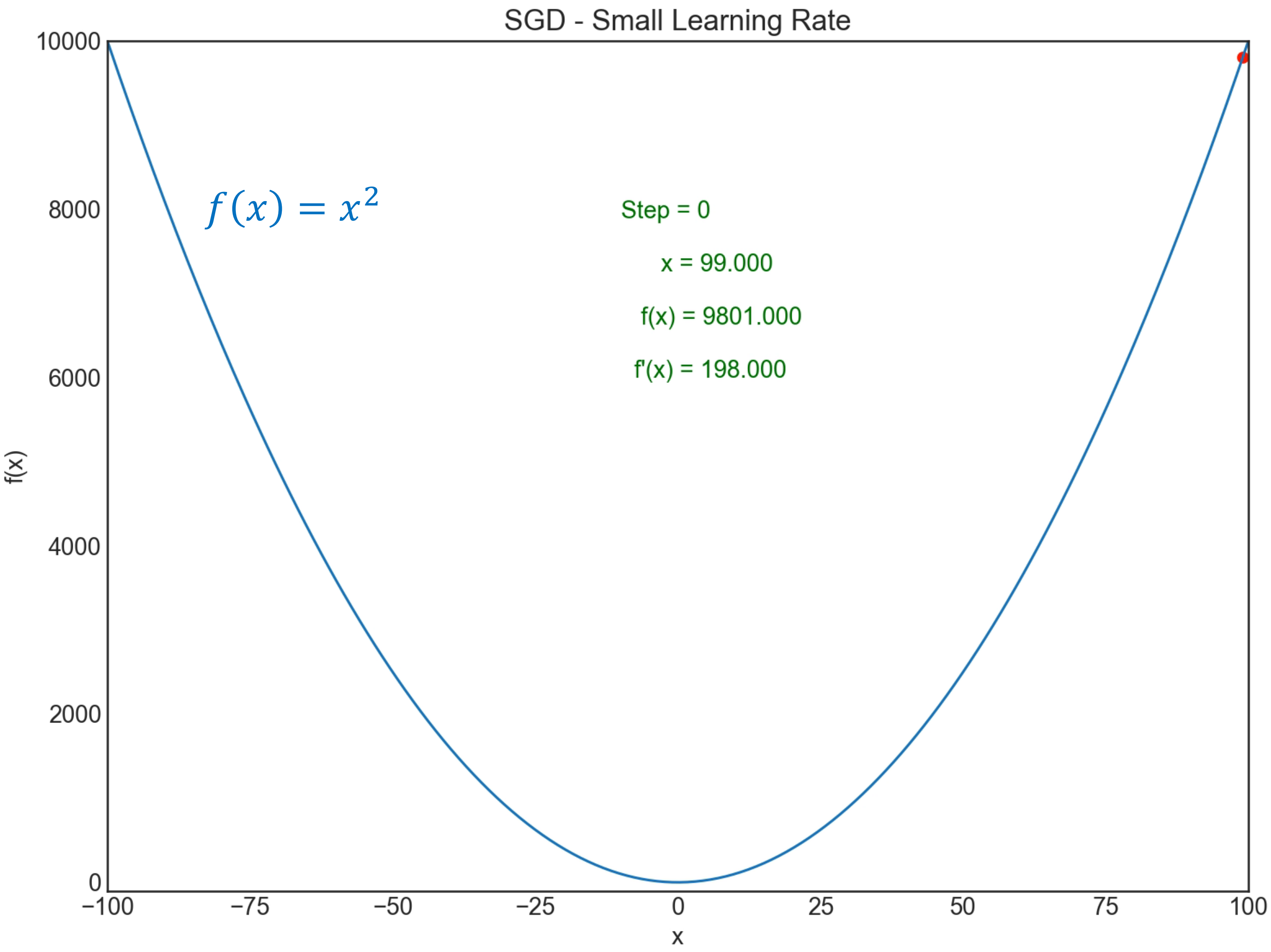
❖ **Square function**

Discussion

$$x_0 = 99.0$$

$$\eta = 0.001$$

$$x_t = x_{t-1} - \eta f'(x)$$



Optimization

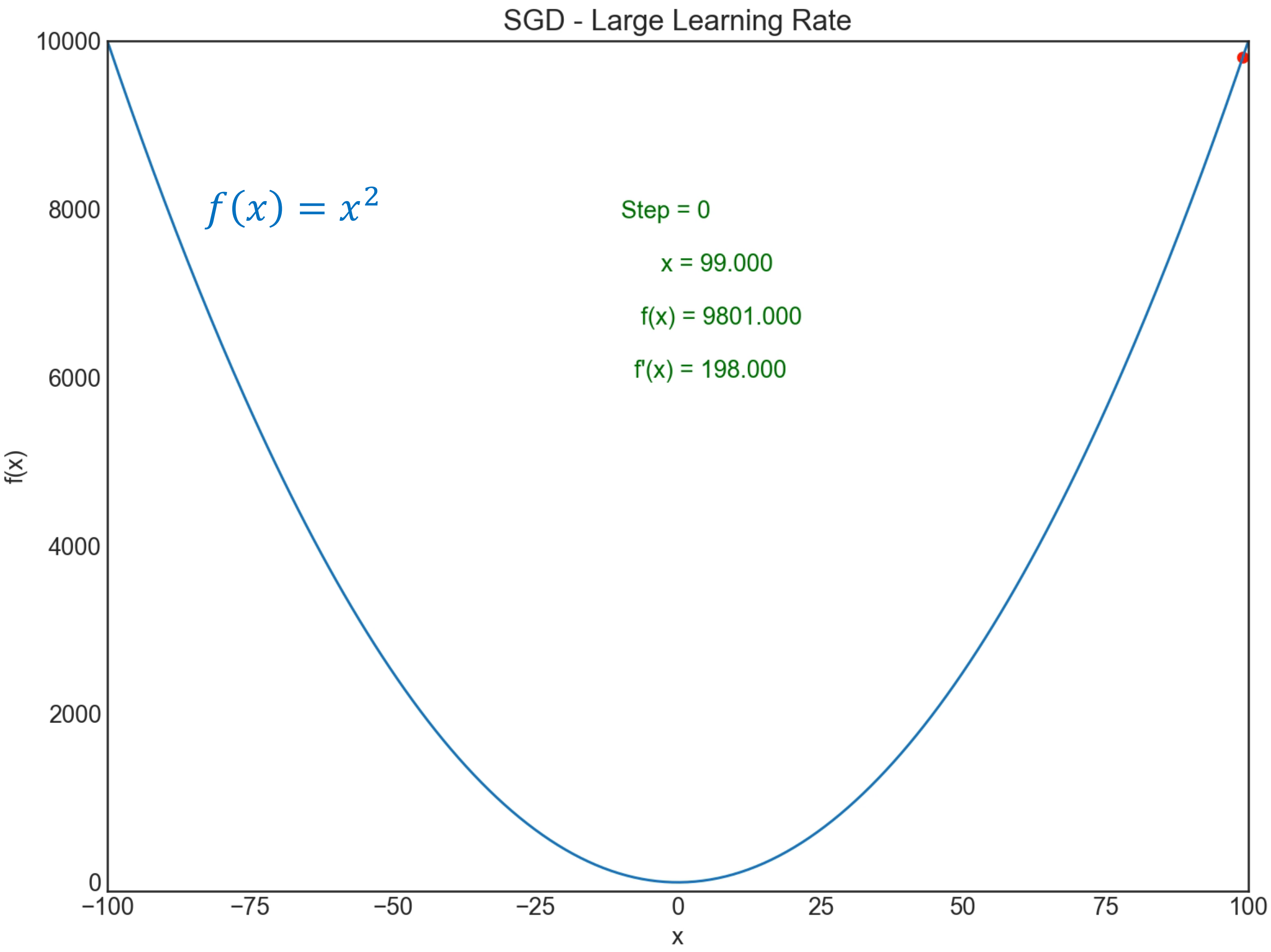
❖ **Square function**

Discussion

$$x_0 = 99.0$$

$$\eta = 0.8$$

$$x_t = x_{t-1} - \eta f'(x)$$



Optimization

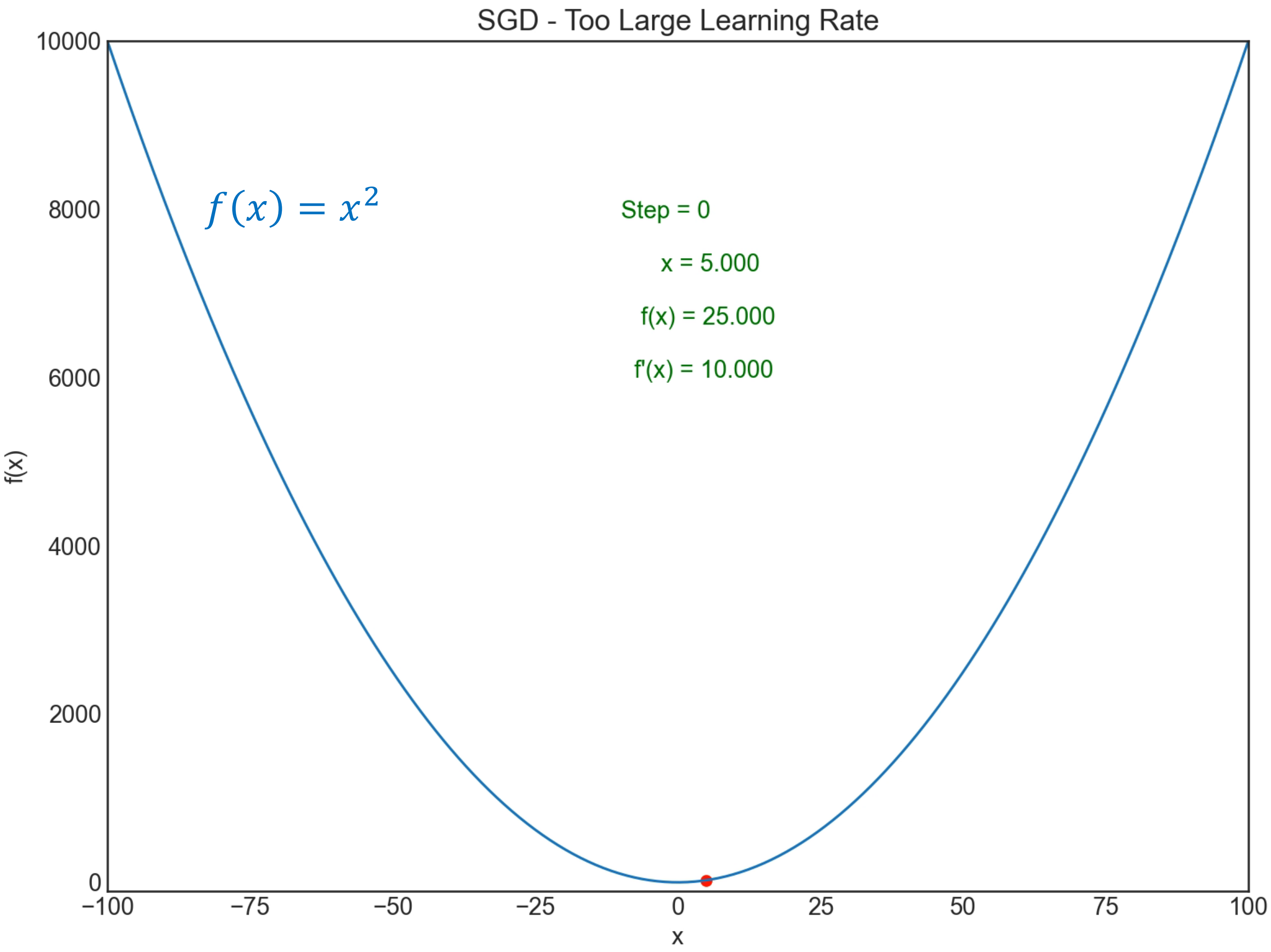
❖ **Square function**

Discussion

$$x_0 = 99.0$$

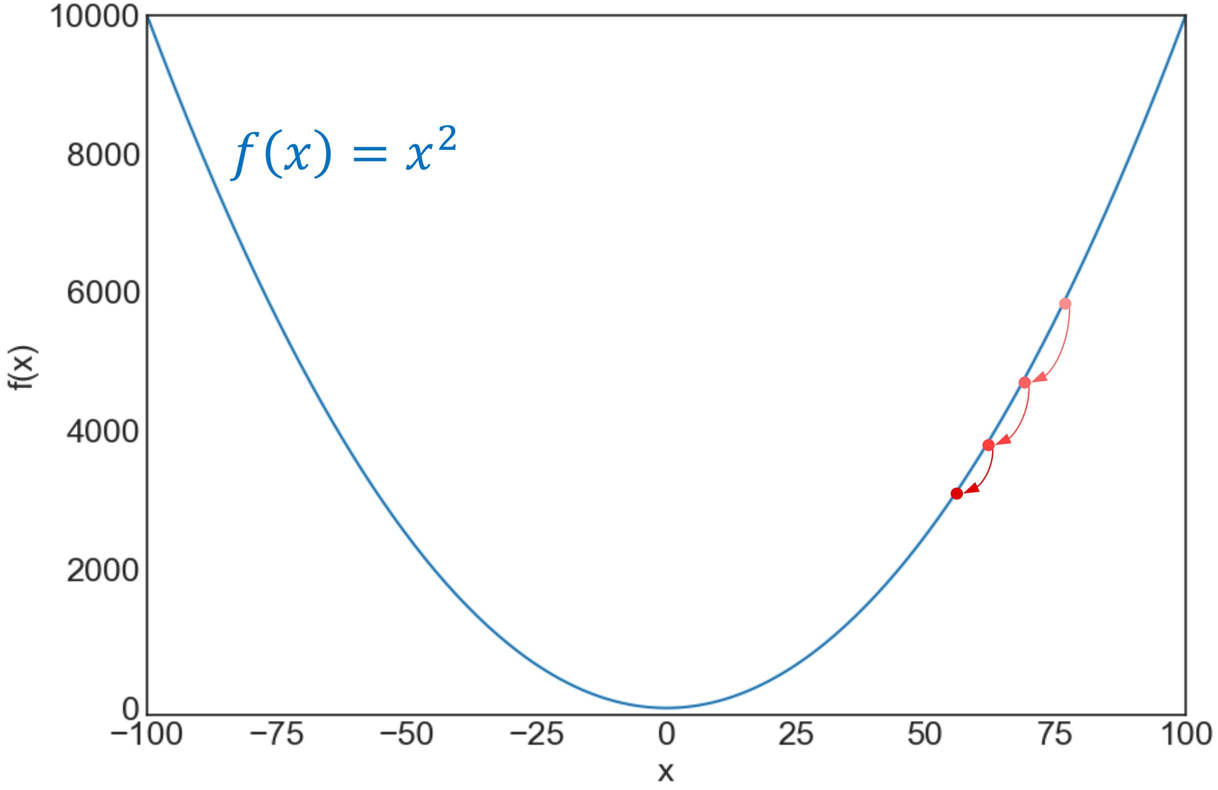
$$\eta = 1.1$$

$$x_t = x_{t-1} - \eta f'(x)$$



Optimization

❖ Square function: Summary



- Given a function f(x), find optimal x_{opt} so that $f(x_{opt})$ is minimum
- After an update, $f(x_{new}) \leq f(x_{old})$

$$x_t = x_{t-1} - \eta f'(x_{t-1})$$

$x_{30} = 0.069$ $\eta = 0.1$

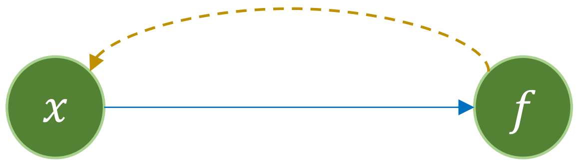
$f'(x_{30}) = 0.138$

$x_{31} = x_{30} - \eta f'(x_{30}) = 0.055$

$f'(x_{31}) = 0.11$

$x_{32} = x_{31} - \eta f'(x_{31}) = 0.044$

$\boxed{\frac{d}{dx} f(x)}$



what does f(x) mean?

Observation 2

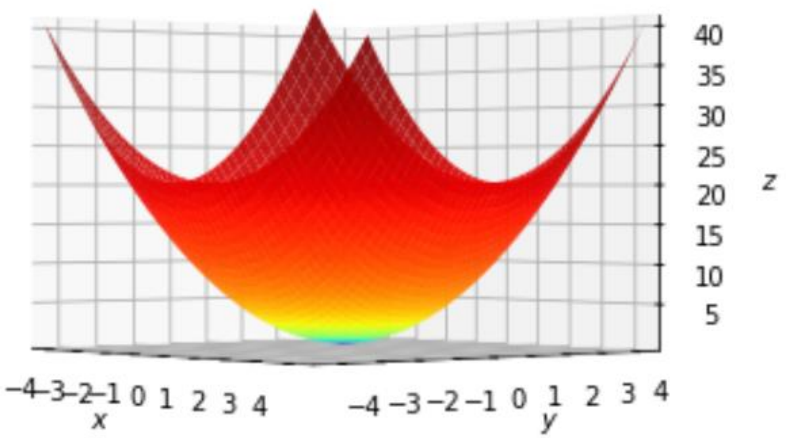
Optimization

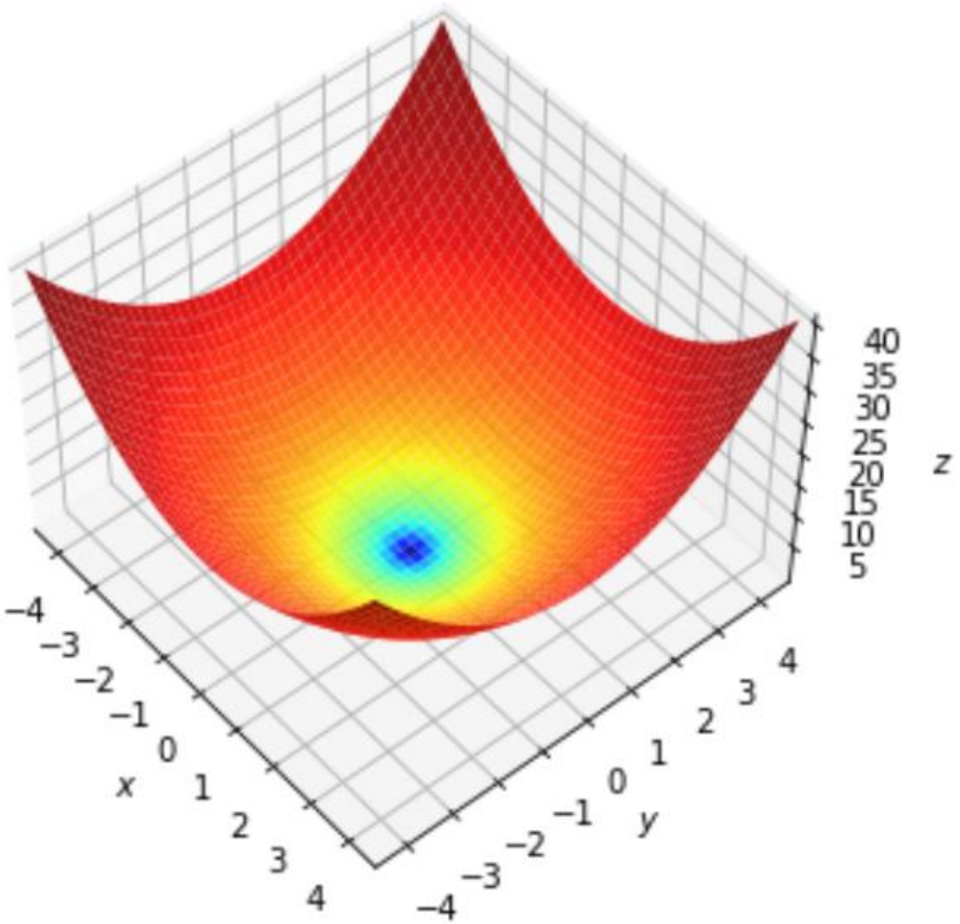
❖ Optimization: 2D function

$$f(x, y) = x^2 + y^2$$

$$-100 \leq x, y \leq 100$$

$$x, y \in \mathbb{N}$$





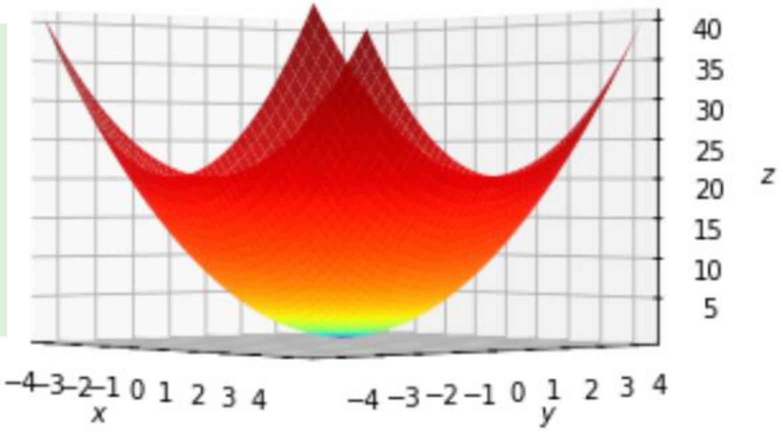
Optimization

- **Optimization: 2D function**

$$f(x,y) = x^2 + y^2$$

$$-100 \le x, y \le 100$$

$$x, y \in \mathbb{N}$$



$$x = x - \eta \frac{\partial f(x,y)}{\partial x}$$

$$y = y - \eta \frac{\partial f(x,y)}{\partial y}$$

$x_0 = 6.0 \quad y_0 = 9.0 \quad \eta = 0.1$

$$\frac{\partial f(x_0,y_0)}{\partial x} = 12 \qquad \frac{\partial f(x_0,y_0)}{\partial y} = 18$$

$$x_1 = 4.8 \qquad y_1 = 7.2$$

$$\frac{\partial f(x_1,y_1)}{\partial x} = 9.6 \qquad \frac{\partial f(x_1,y_1)}{\partial y} = 14.4$$

$$x_2 = 3.84 \qquad y_2 = 5.75$$

$$\frac{\partial f(x_2,y_2)}{\partial x} = 7.68 \qquad \frac{\partial f(x_2,y_2)}{\partial y} = 11.51$$

$$x_3 = 3.07 \qquad y_3 = 4.608$$

$$\frac{\partial f(x_3,y_3)}{\partial x} = 6.14 \qquad \frac{\partial f(x_3,y_3)}{\partial y} = 9.21$$

$$x_4 = 2.45 \qquad y_4 = 3.68$$

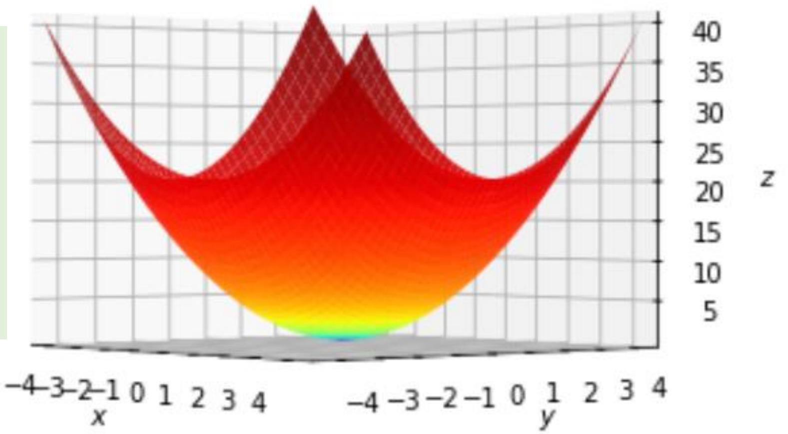
Optimization

❖ Optimization: 2D function

$$f(x, y) = x^2 + y^2$$

$$-100 \leq x, y \leq 100$$

$$x, y \in \mathbb{N}$$



$$\frac{\partial f(x_2, y_2)}{\partial x} = 7.68 \qquad \frac{\partial f(x_2, y_2)}{\partial y} = 11.51$$

$$x_3 = 3.07 \qquad y_3 = 4.608$$

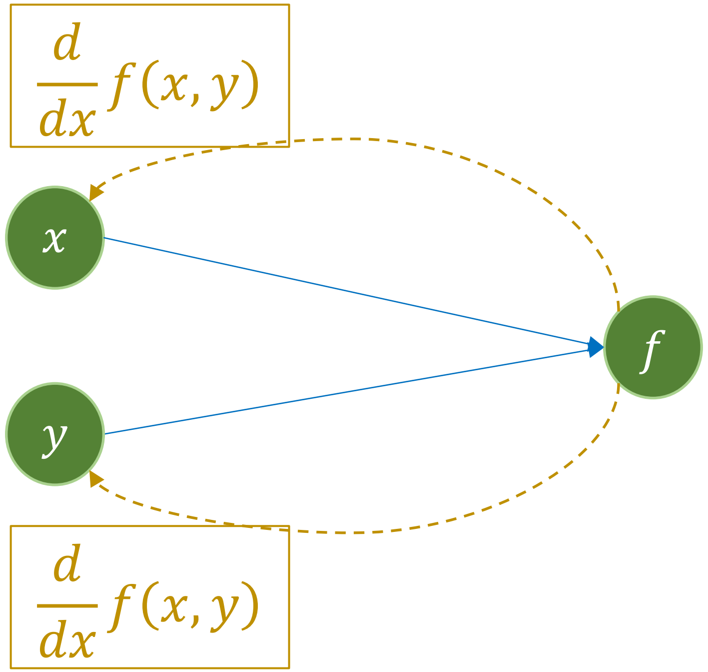
$$\frac{\partial f(x_3, y_3)}{\partial x} = 6.14 \qquad \frac{\partial f(x_3, y_3)}{\partial y} = 9.21$$

$$x_4 = 2.45 \qquad y_4 = 3.68$$

Summary:

- Given a function f(x, y), find optimal (x_{opt}, y_{opt}) so that f(x_{opt}, y_{opt}) is minimum

- After an update, f(x_{new}, y_{new}) ≤ f(x_{old}, y_{old})

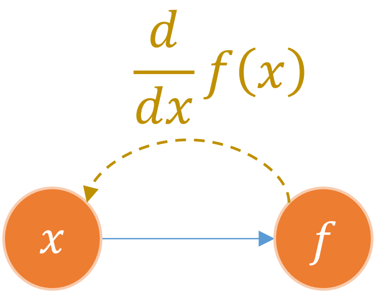


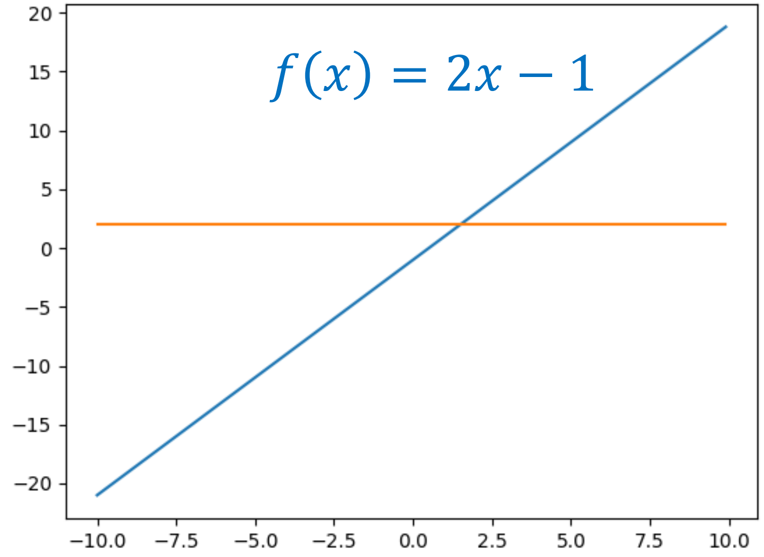
what does f(x,y) mean?

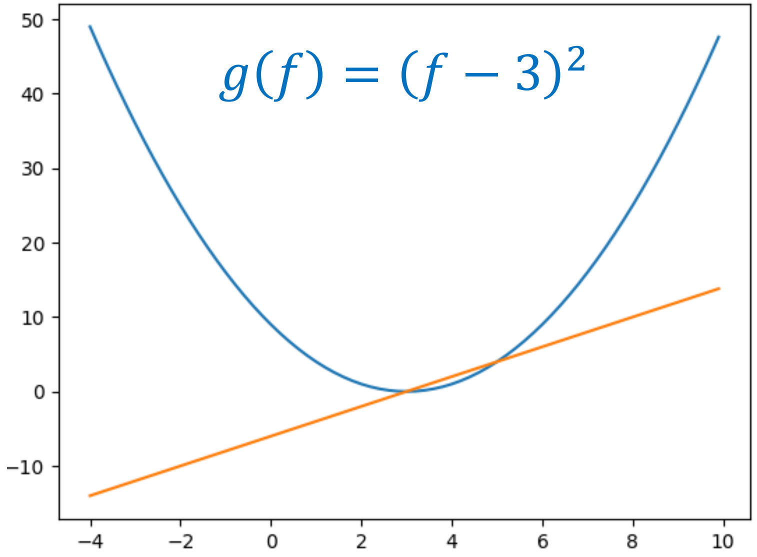
Observation 3

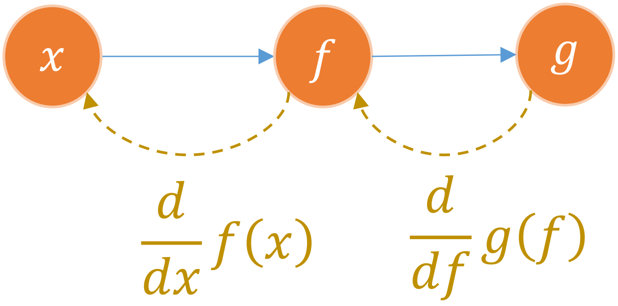
Gradient-based Optimization

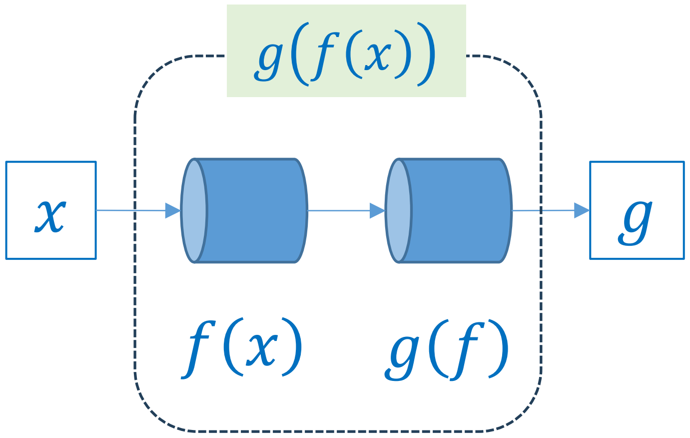
❖ For composite function

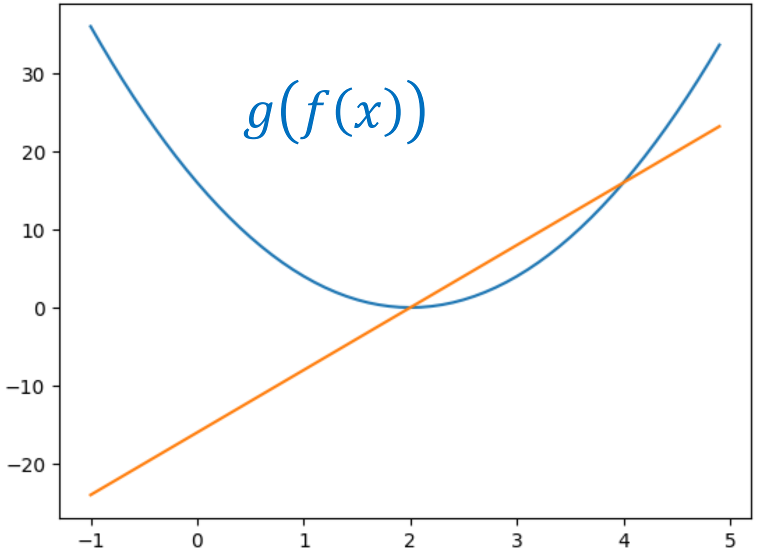








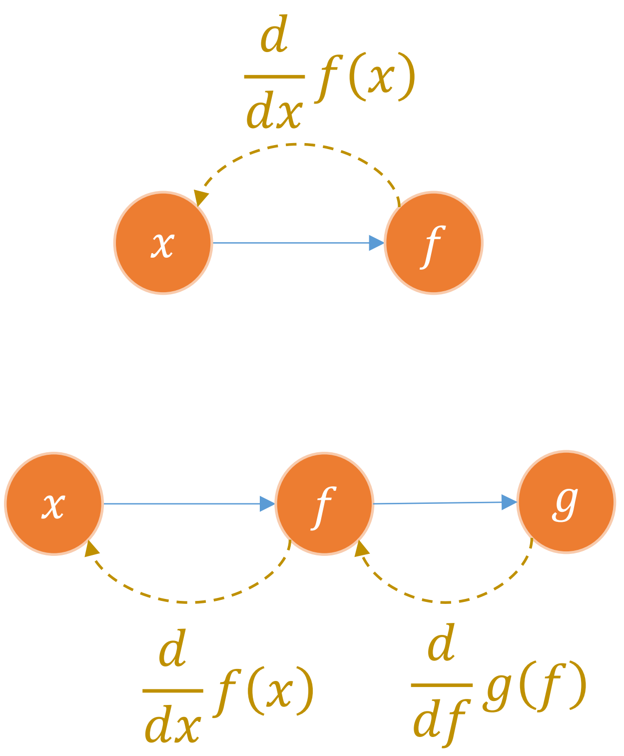




$$\frac{d}{dx}g(f(x)) = \left[\frac{d}{df}g(f)\right] * \left[\frac{d}{dx}f(x)\right]$$

Gradient-based Optimization

❖ For composite function and chain rule



$$\frac{d}{dx}g(f(x)) = \left[\frac{d}{df}g(f)\right] * \left[\frac{d}{dx}f(x)\right]$$

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

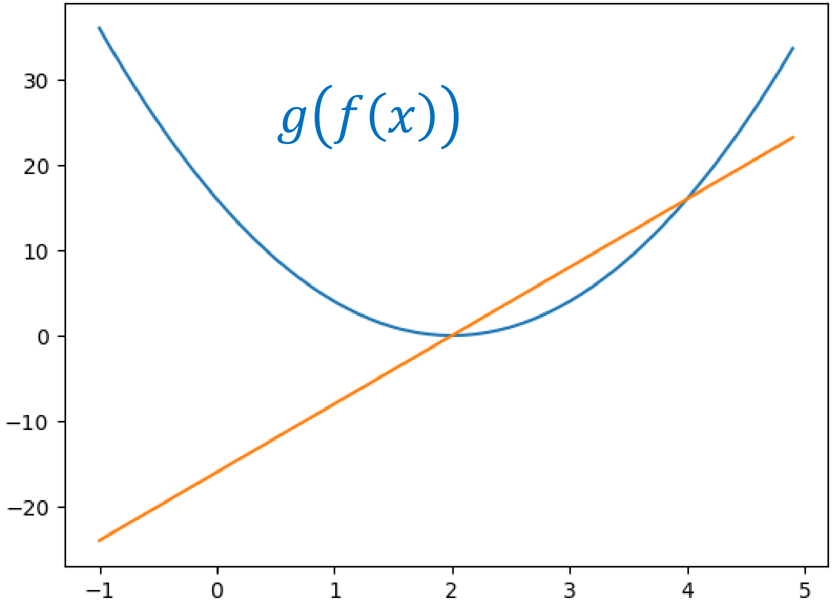
$$g(f) = (f - 3)^2$$

$$f'(x) = 2$$

$$g'(f) = 2(f - 3)$$

$$\begin{aligned}\frac{dg}{dx} &= \frac{dg}{df}\frac{df}{dx} \\ &= 2(f-3)2 \\ &= 4(2x-1-3) \\ &= 8x - 16\end{aligned}$$

Implementation



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

$$g(f) = (f - 3)^2$$

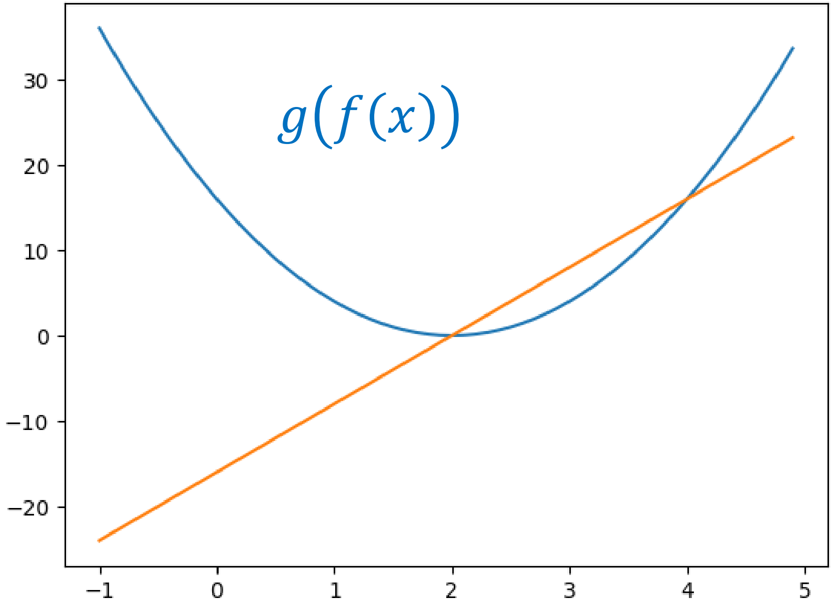
$$\frac{dg}{dx} = 8x - 16$$

```python
def fx(x):
    return 2*x - 1

def gf(f):
    return (f-3)**2

def dg_dx(x):
    return 8*x - 16
```

```python
import random

# parameters
lr = 0.1

# initialize x
x = 60

old_loss = gf(fx(x)) # logging
print(f'old_loss: {old_loss}')

# compute derivative
dg_dx_value = dg_dx(x)

# update
x = x - lr*dg_dx_value

new_loss = gf(fx(x)) # logging
print(f'new_loss: {new_loss}')
```

```
old_loss: 13456
new_loss: 538.2399999999994
```

Implementation



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

$$g(f) = (f - 3)^2$$

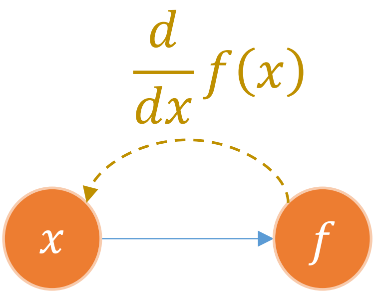
$$\frac{dg}{dx} = 8x - 16$$

```python
def fx(x):
    return 2*x - 1

def gf(f):
    return (f-3)**2

def dg_dx(x):
    return 8*x - 16
```

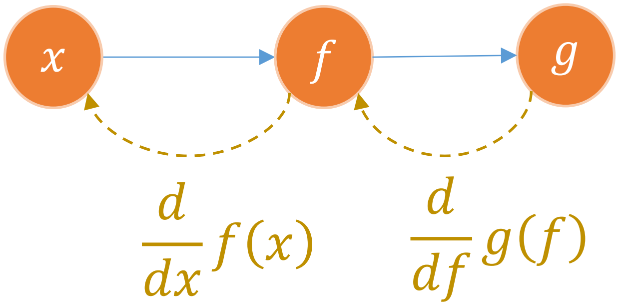
```python
import random

# parameters
num_steps = 5
lr = 0.1

# set x randomly
x = random.randint(-100, 100)

for _ in range(num_steps):
    # logging
    loss = gf(fx(x))

    # compute derivative
    dg_dx_value = dg_dx(x)

    # update
    x = x - lr*dg_dx_value
```

Gradient-based Optimization

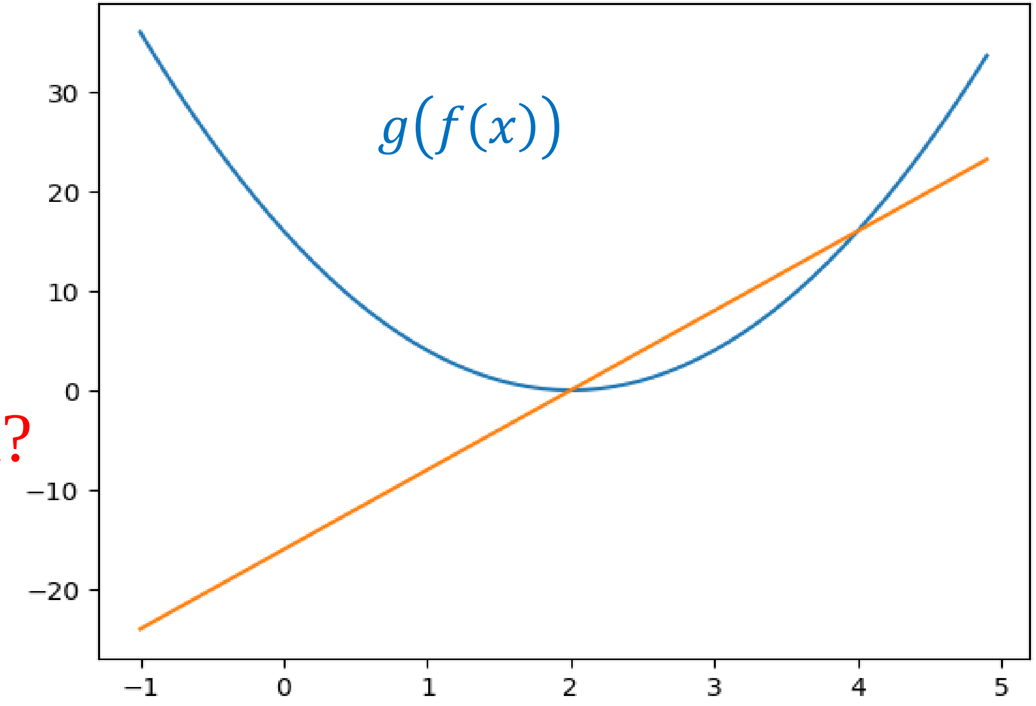
❖ For composite function: Summary



what does g(f(x)) mean?



$$\frac{d}{dx}g\big(f(x)\big) = \left[\frac{d}{df}g(f)\right] * \left[\frac{d}{dx}f(x)\right]$$



- Given a function g(f(x)), find optimal x_{opt} so that $f(x_{opt})$ is minimum

- After an update, $g(f(x_{new})) \leq g(f(x_{old}))$

Outline

SECTION 1

Optimization

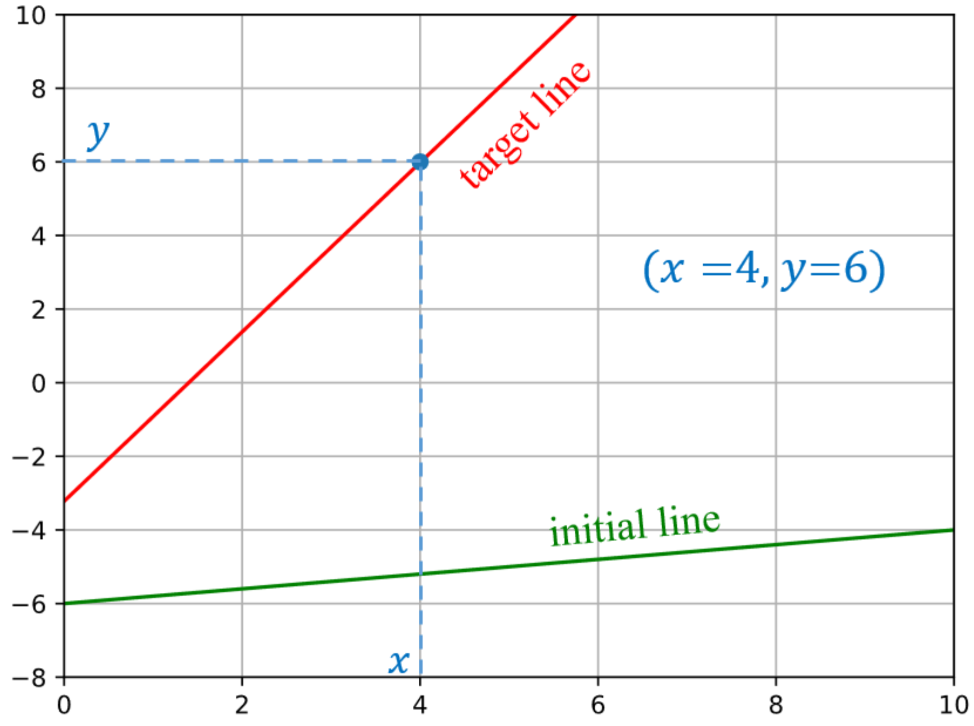
SECTION 2

Problem Solving

SECTION 3

Towards Linear Regression

$$f(x) = ax + b$$

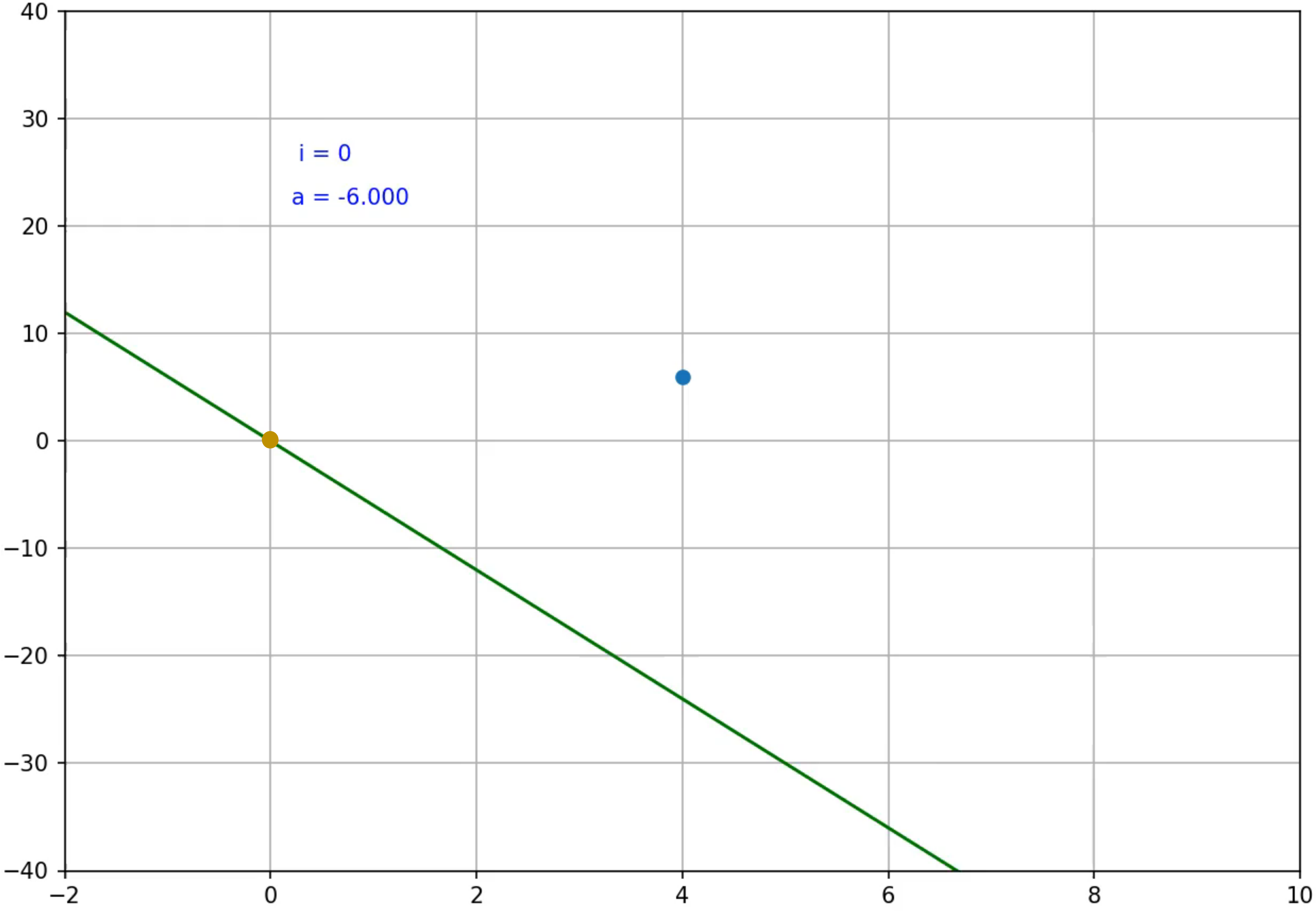


Gradient-based Optimization

❖ Problem 1

Given a line that is always through the origin

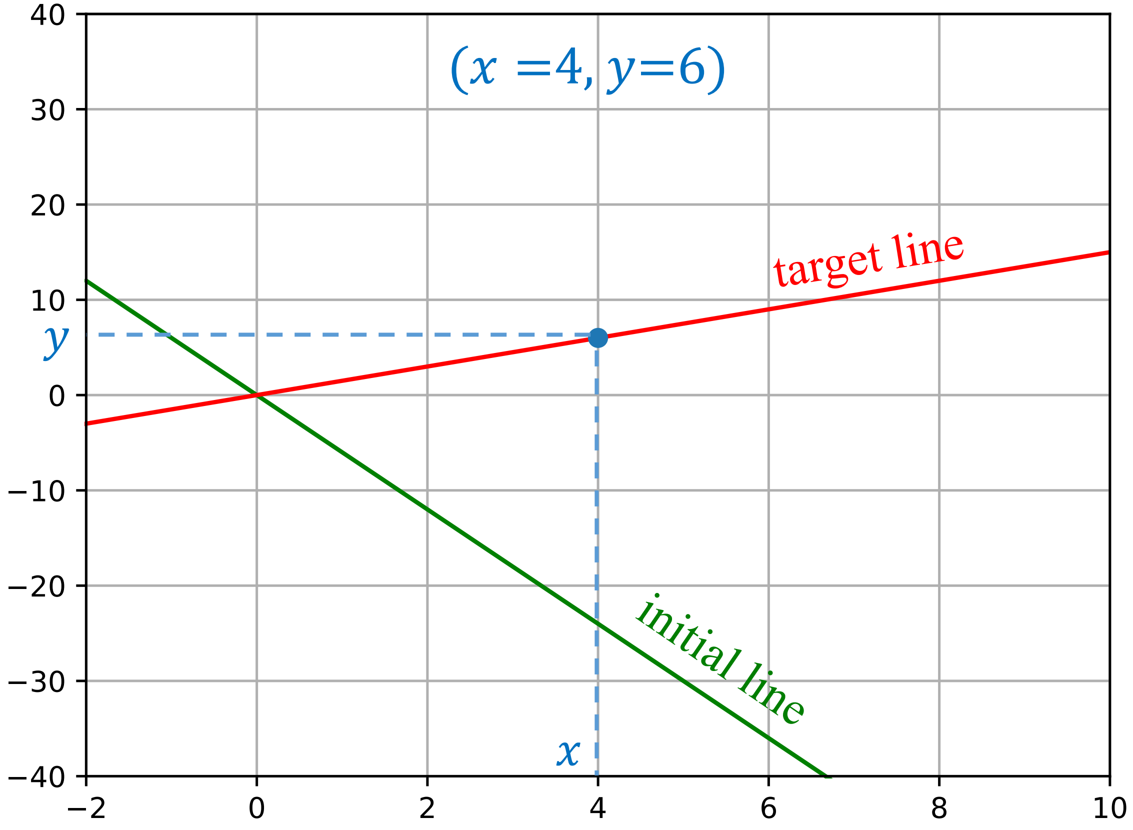
How to move the green line so that it is also through the blue point?



Gradient-based Optimization

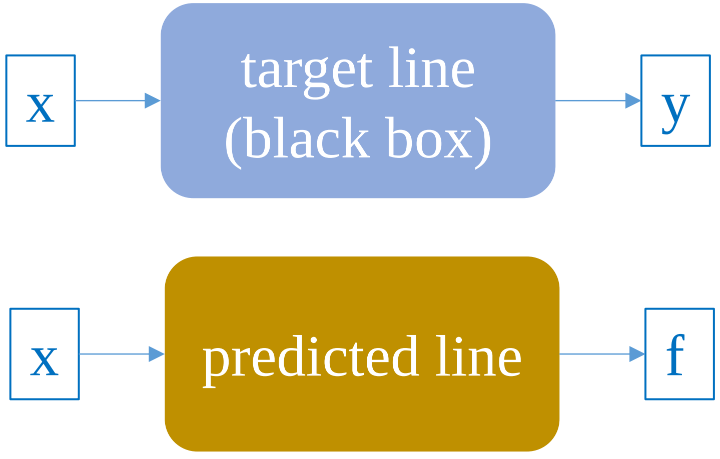
❖ Problem 1

$$f(x) = ax$$



❖ Constraints

$\eta = 0.1$

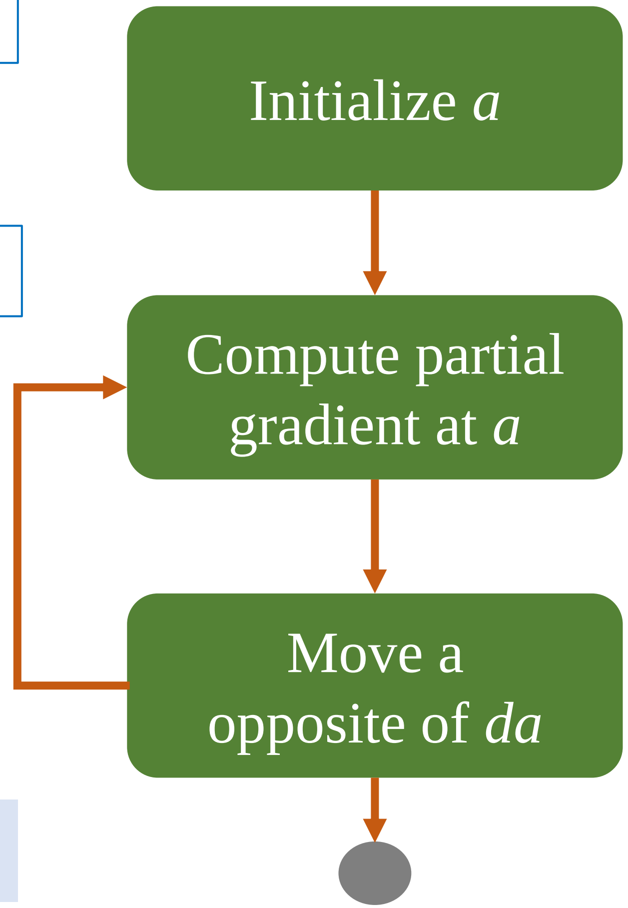


$$f(x) = ax$$

$$g(f) = (f - y)^2$$

$$g'(a) = 2x(f - y)$$

$$a_t = a_{t-1} - \eta g'(a_{t-1})$$



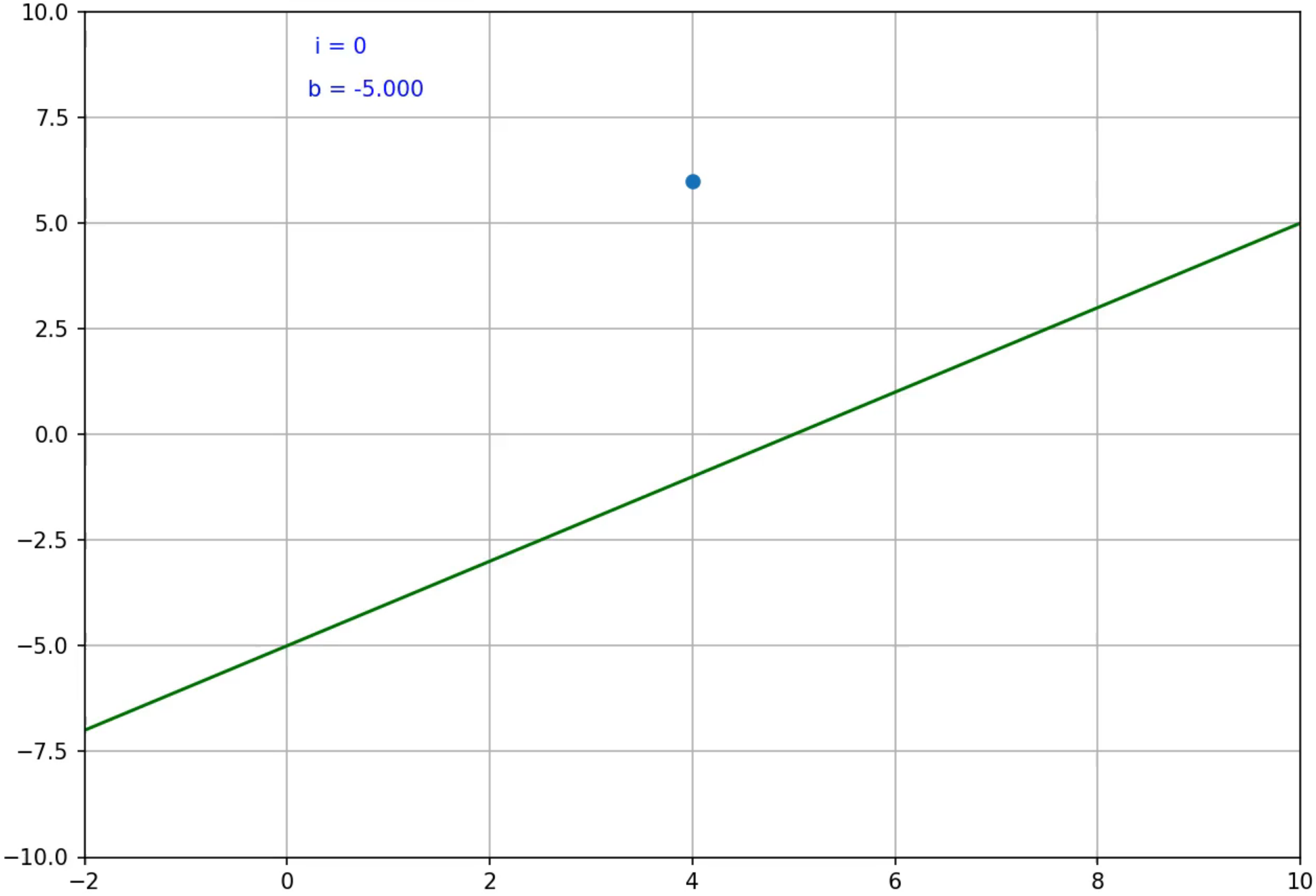
Gradient-based Optimization

❖ Problem 2

Given a line

$$f(x) = x + b$$

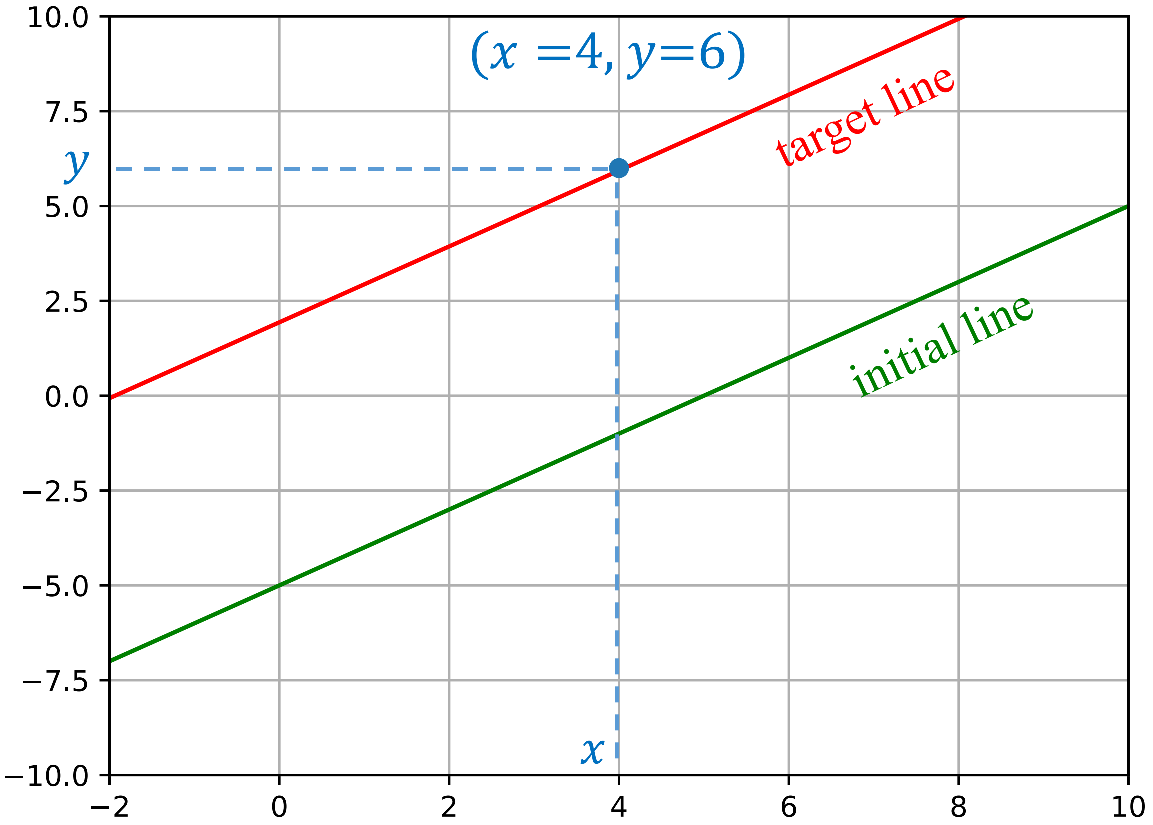
How to move the green line so that it is also through the blue point?



Gradient-based Optimization

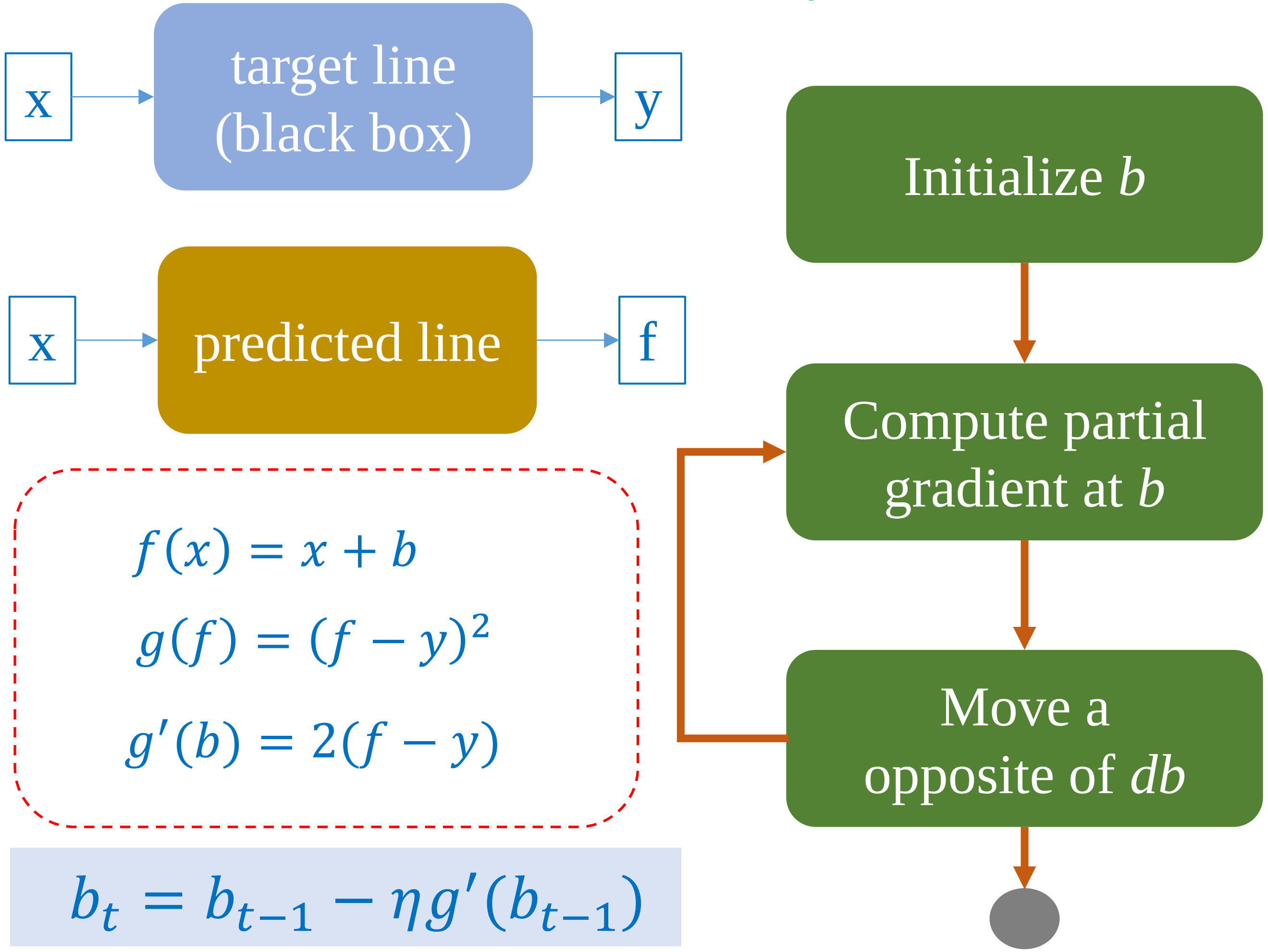
❖ Problem 2

$$f(x) = x + b$$



❖ Constraints

$\eta = 0.1$



$$f(x) = x + b$$

$$g(f) = (f - y)^2$$

$$g'(b) = 2(f - y)$$

$$b_t = b_{t-1} - \eta g'(b_{t-1})$$

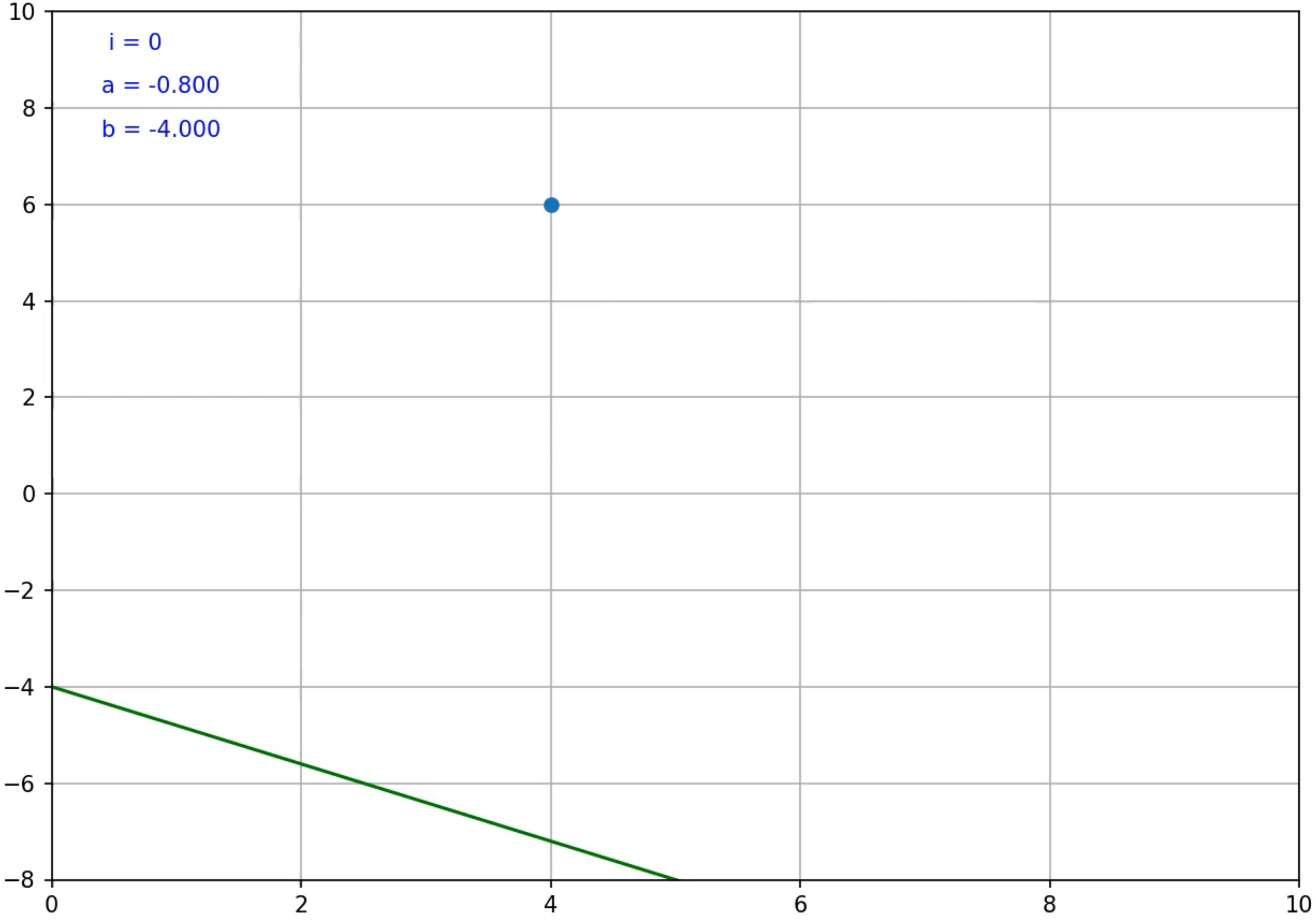
Gradient-based Optimization

❖ Problem 3

Given a line

$$f(x) = ax + b$$

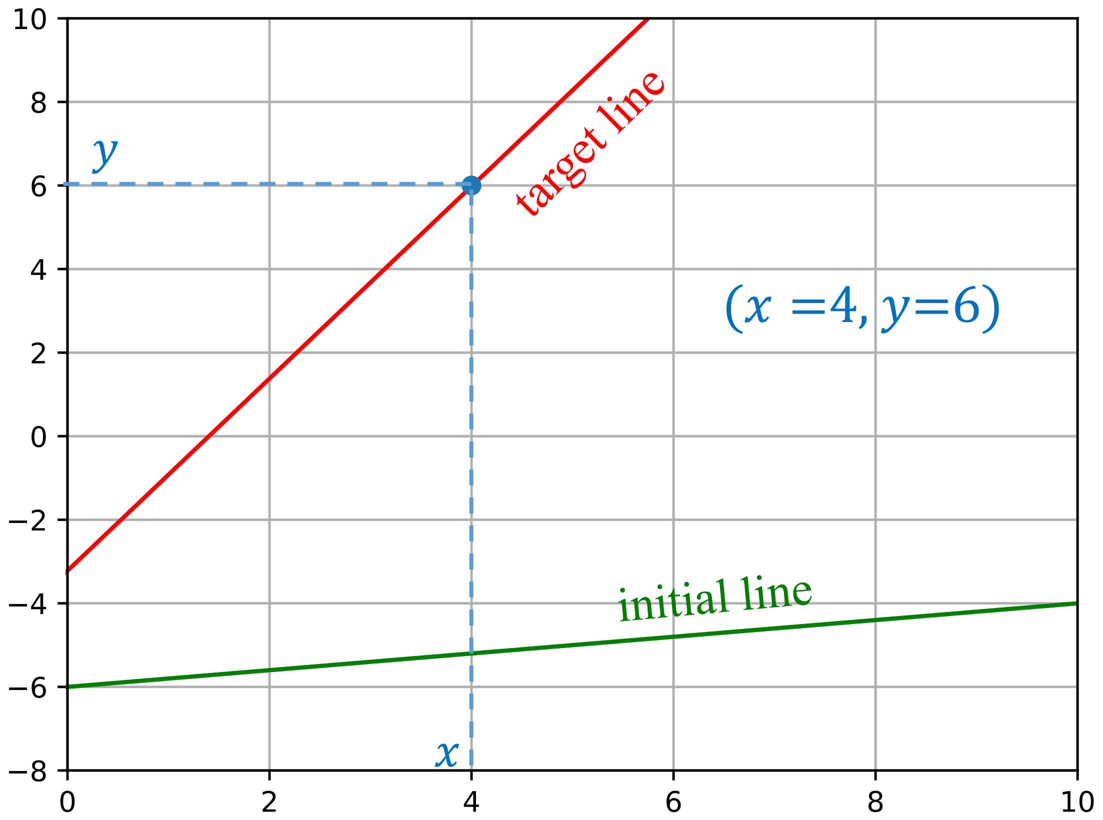
How to move the green line so that it is also through the blue point?



Gradient-based Optimization

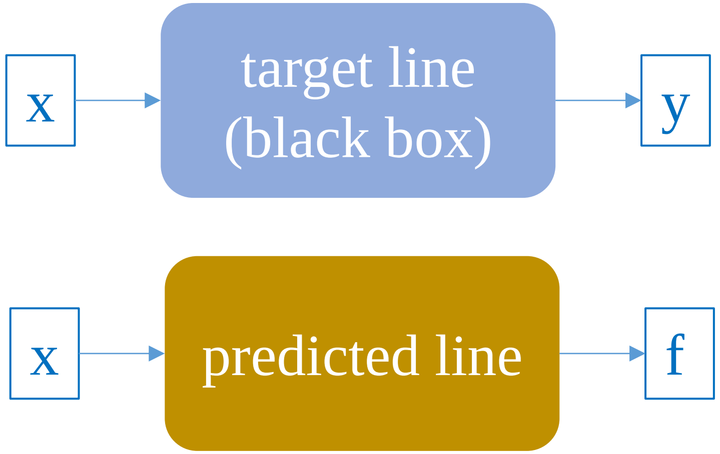
❖ Problem 3

$$f(x) = ax + b$$



❖ Constraints

$$\eta = 0.1$$



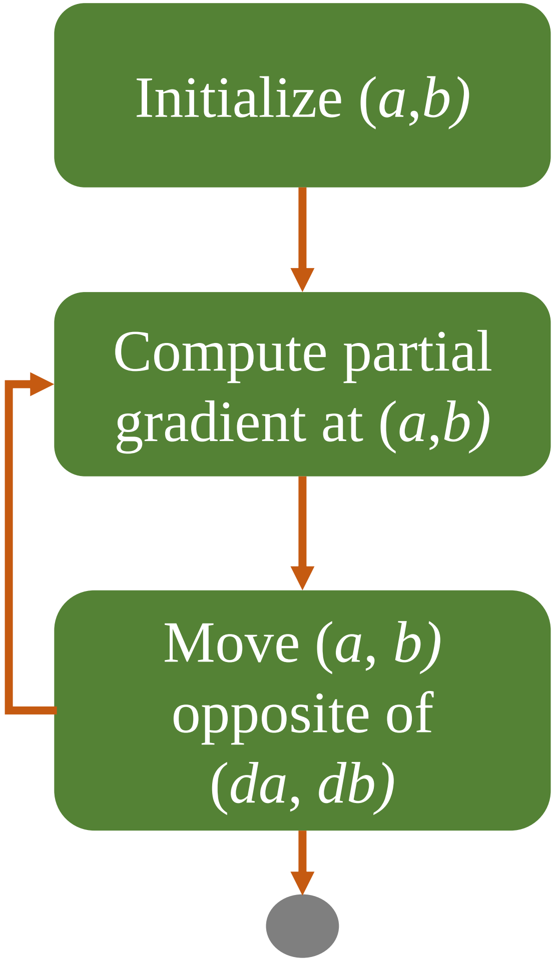
$$f(x) = ax + b$$

$$g(f) = (f - y)^2$$

$$g'(a) = 2x(f - y)$$

$$g'(b) = 2(f - y)$$

$$\theta_t = \theta_{t-1} - \eta g'(\theta_{t-1})$$



Outline

SECTION 1

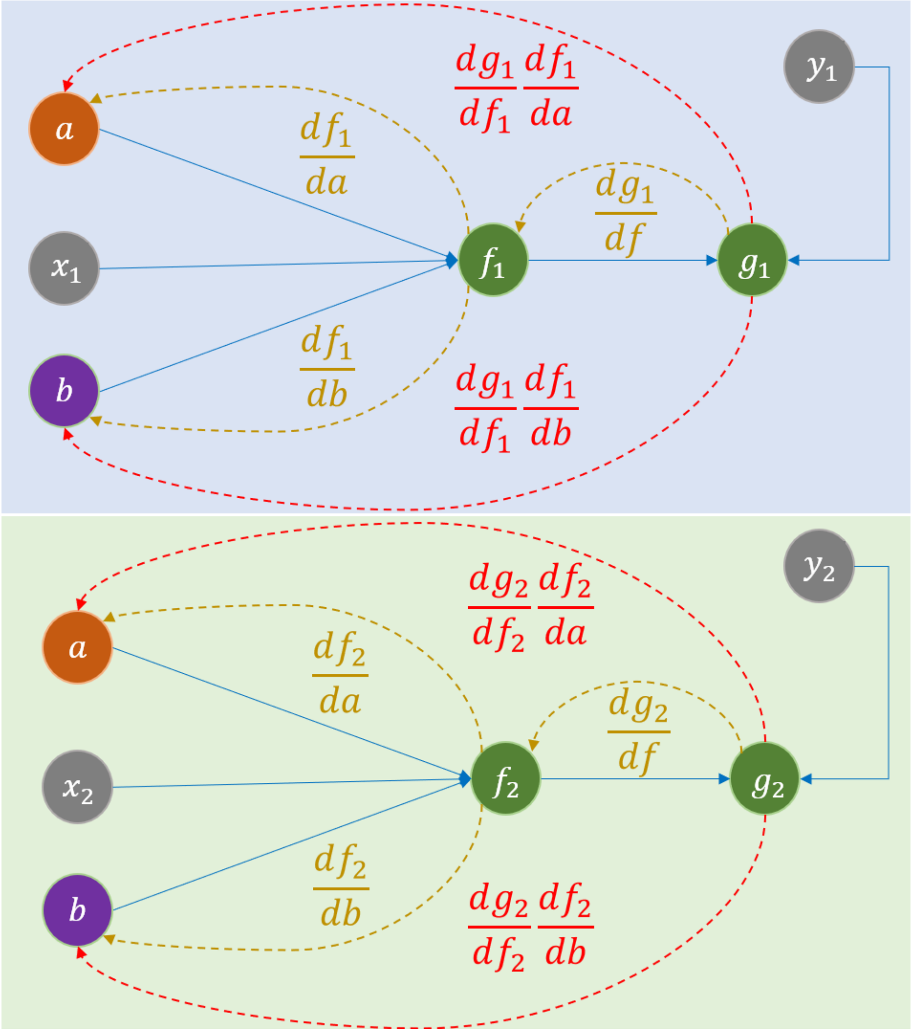
Optimization

SECTION 2

Problem Solving

SECTION 3

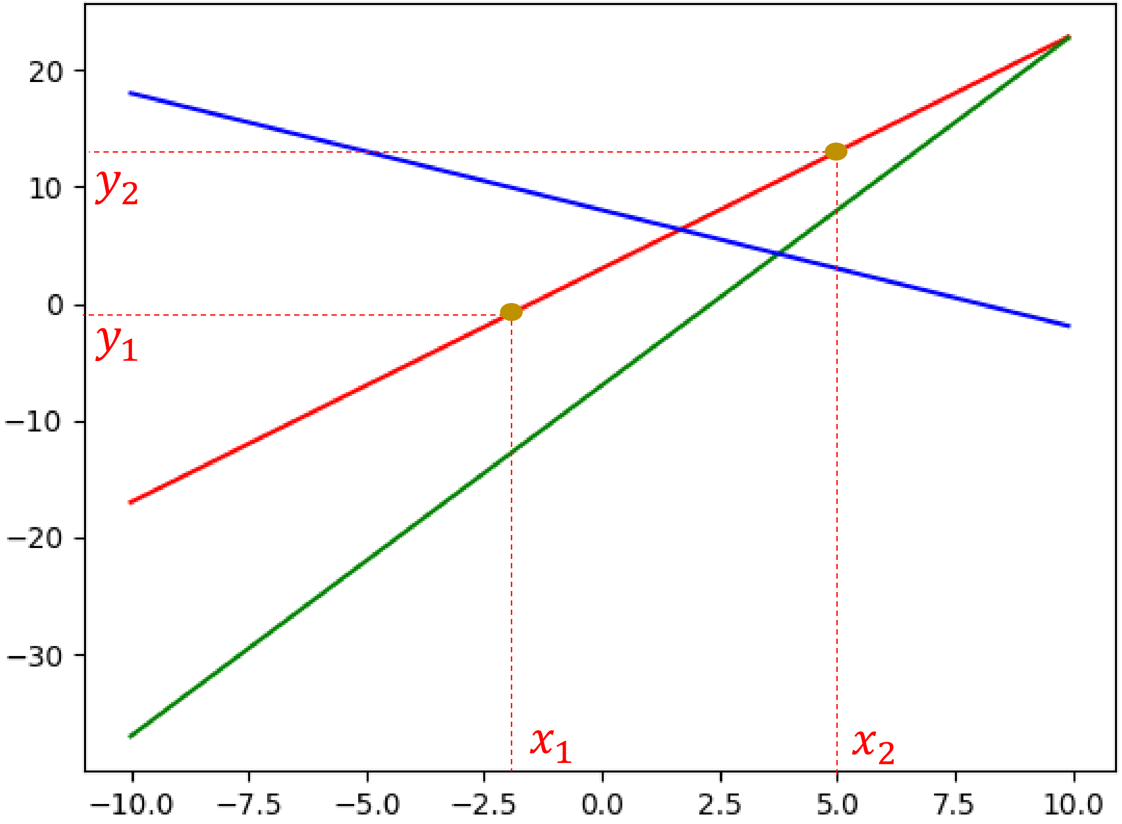
Towards Linear Regression



Gradient-based Optimization

❖ What about having two samples

$$f(x) = ax + b$$



❖ Constraints

$$\theta_t = \theta_{t-1} - \eta f'(\theta_{t-1})$$

x_i → The red line (Black box) → y_i

x_i → predicted line → f_i

(x_1=-2, y_1=-1)

(x_2=5, y_2=13)

$$g(f) = (f - y)^2$$

Initialize a, b

Compute partial gradient at a, b

Move a, b opposite of da, db

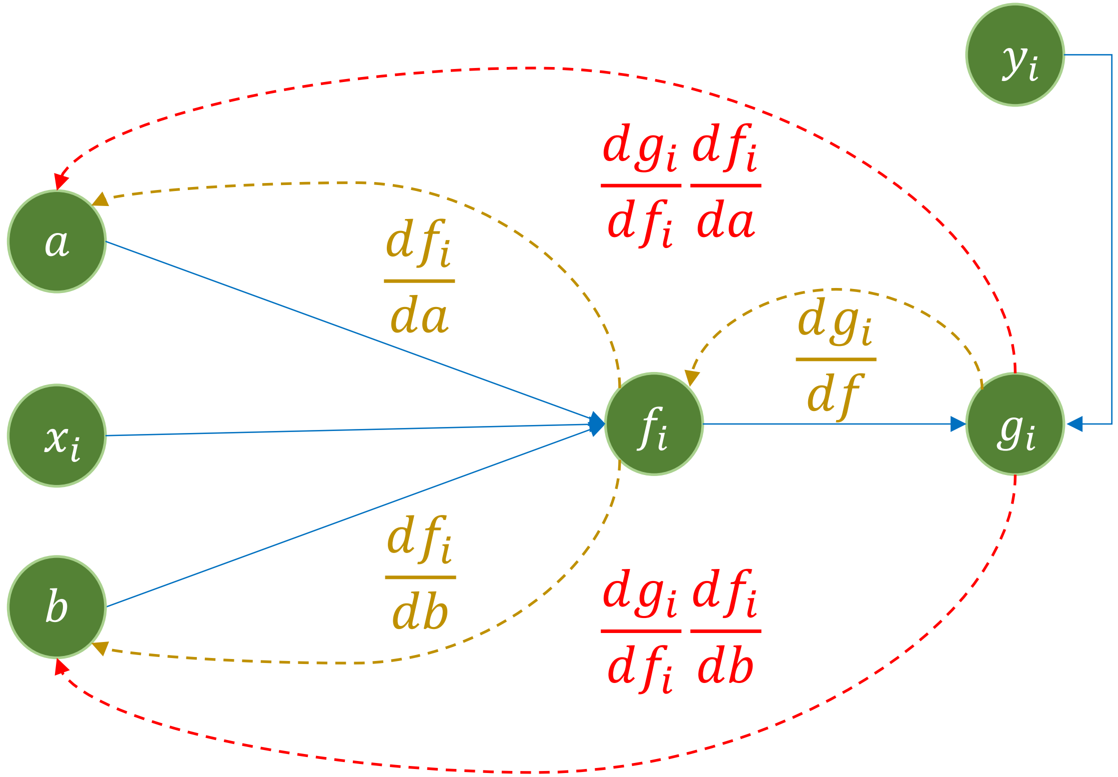
$\eta = 0.1$

Gradient-based Optimization

❖ Equations for partial gradients

$$f(x_i) = ax_i + b \qquad (x_1{=}1, y_1{=}5)$$

$$g(f_i) = (f_i - y_i)^2 \qquad (x_2{=}2, y_2{=}7)$$



$$\frac{df}{da} = x \qquad \frac{df}{db} = 1$$

$$\frac{dg}{df} = 2(f - y)$$

$$\frac{dg}{da} = \frac{dg}{df}\frac{df}{da} = 2x(f - y)$$

$$\frac{dg}{db} = \frac{dg}{df}\frac{df}{db} = 2(f - y)$$

During looking for optimal a and b, at a given time, a and b have concrete values

❖ Optimization for a composite function

Find a and b so that g(f(x)) is minimum

$f(x_i) = ax_i + b$ $(x_1{=}1, y_1{=}5)$

$g(f_i) = (f_i - y_i)^2$ $(x_2{=}2, y_2{=}7)$

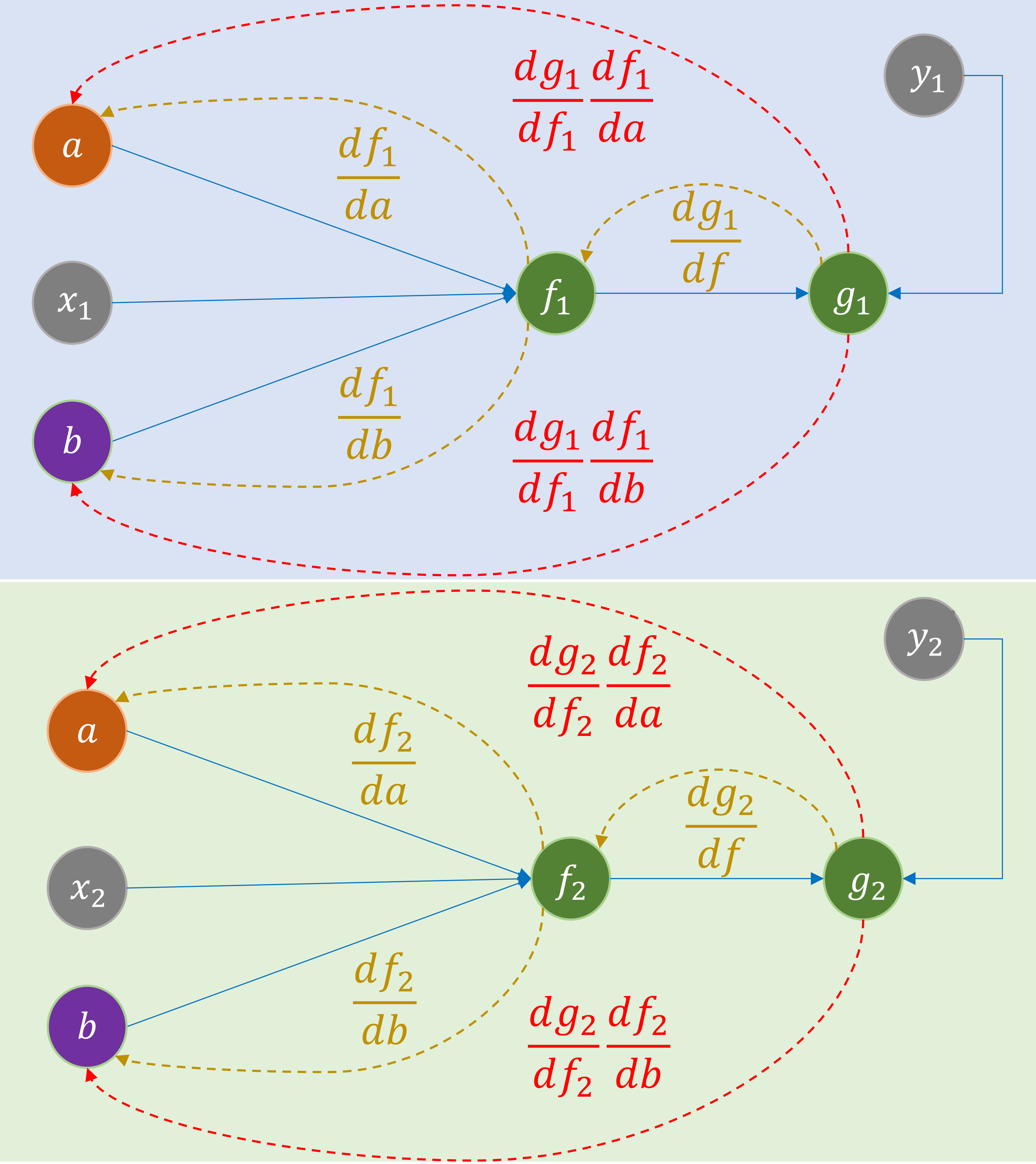
Partial derivative functions

$$\frac{dg}{da} = \frac{dg}{df}\frac{df}{da} = 2x(f-y)$$

$$\frac{dg}{db} = \frac{dg}{df}\frac{df}{db} = 2(f-y)$$

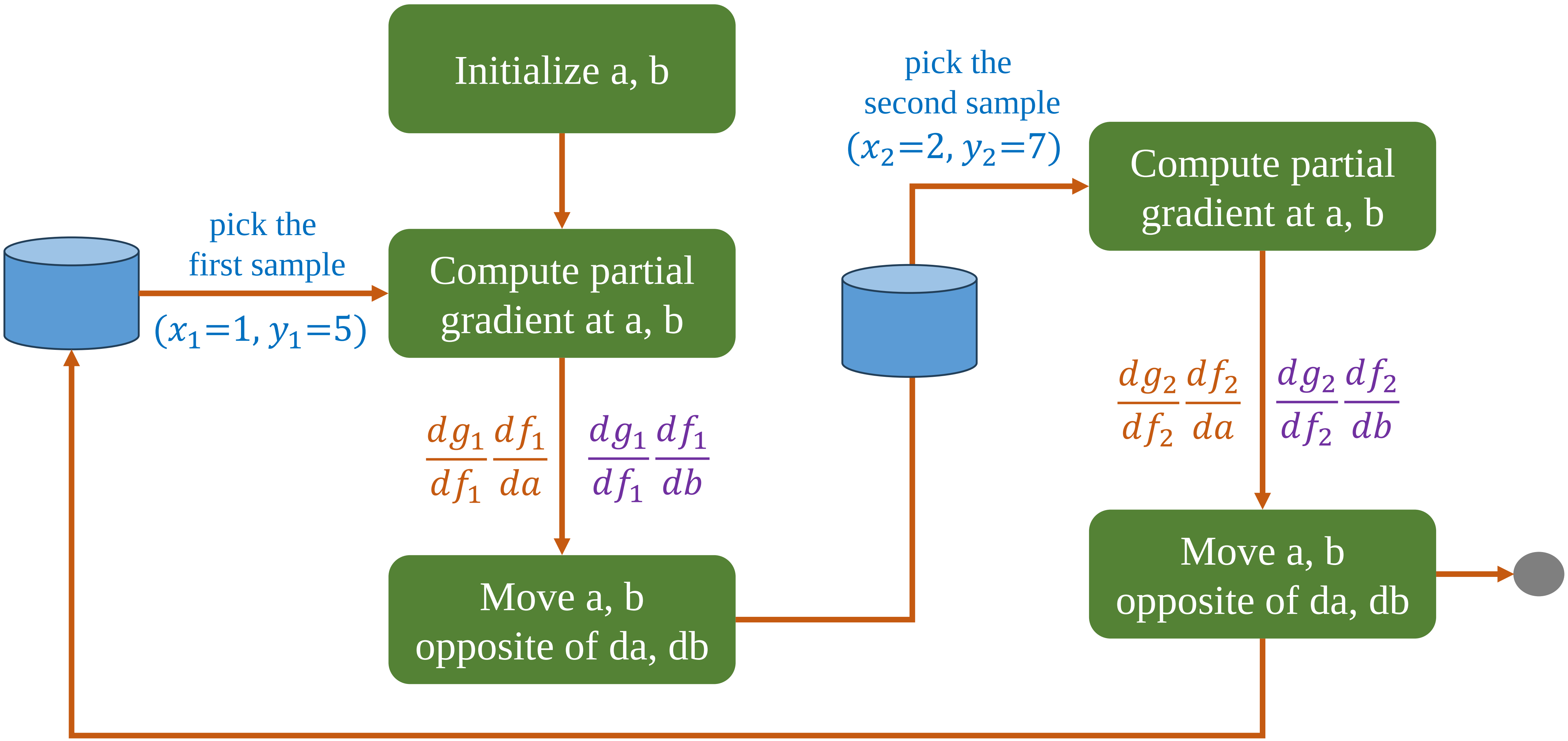
$$\boxed{\frac{dg_1}{df_1}\frac{df_1}{da}} \quad \boxed{\frac{dg_2}{df_2}\frac{df_2}{da}}$$

$$\boxed{\frac{dg_1}{df_1}\frac{df_1}{db}} \quad \boxed{\frac{dg_2}{df_2}\frac{df_2}{db}}$$



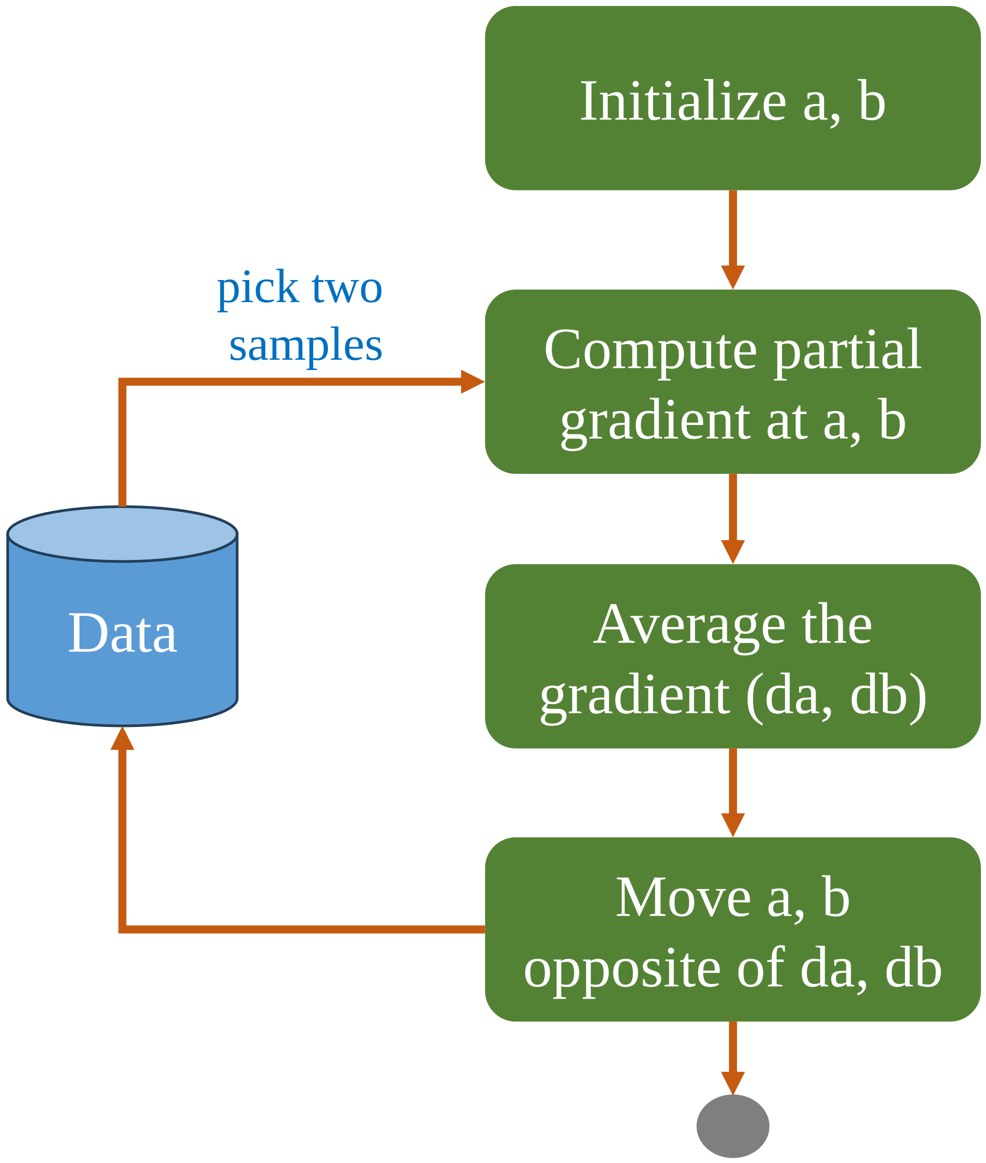
Gradient-based Optimization

❖ Discussion: Approach 1



Gradient-based Optimization

❖ Discussion: Approach 2

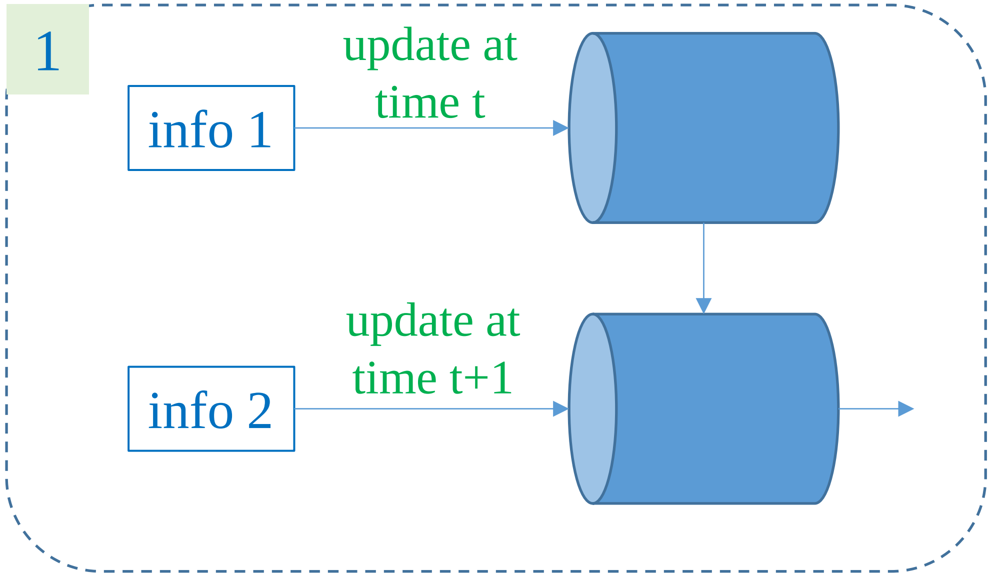


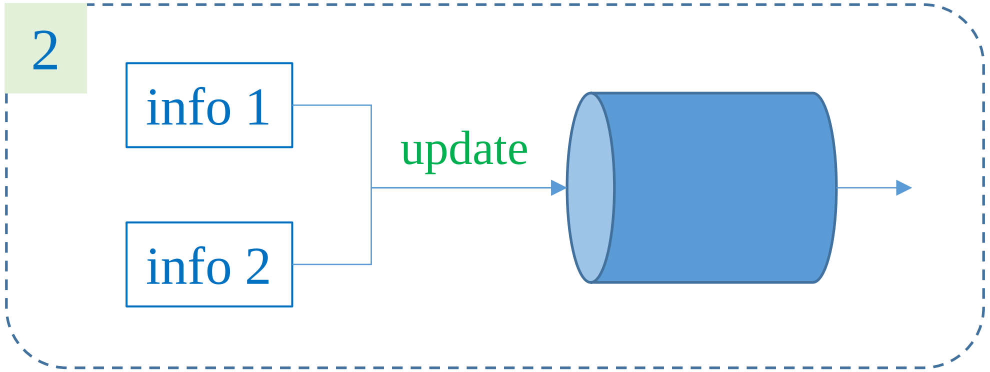
$$\frac{1}{2}\sum_i \frac{dg_i}{da} = \frac{1}{2}\left(\frac{dg_1}{df_1}\frac{df_1}{da} + \frac{dg_2}{df_2}\frac{df_2}{da}\right)$$

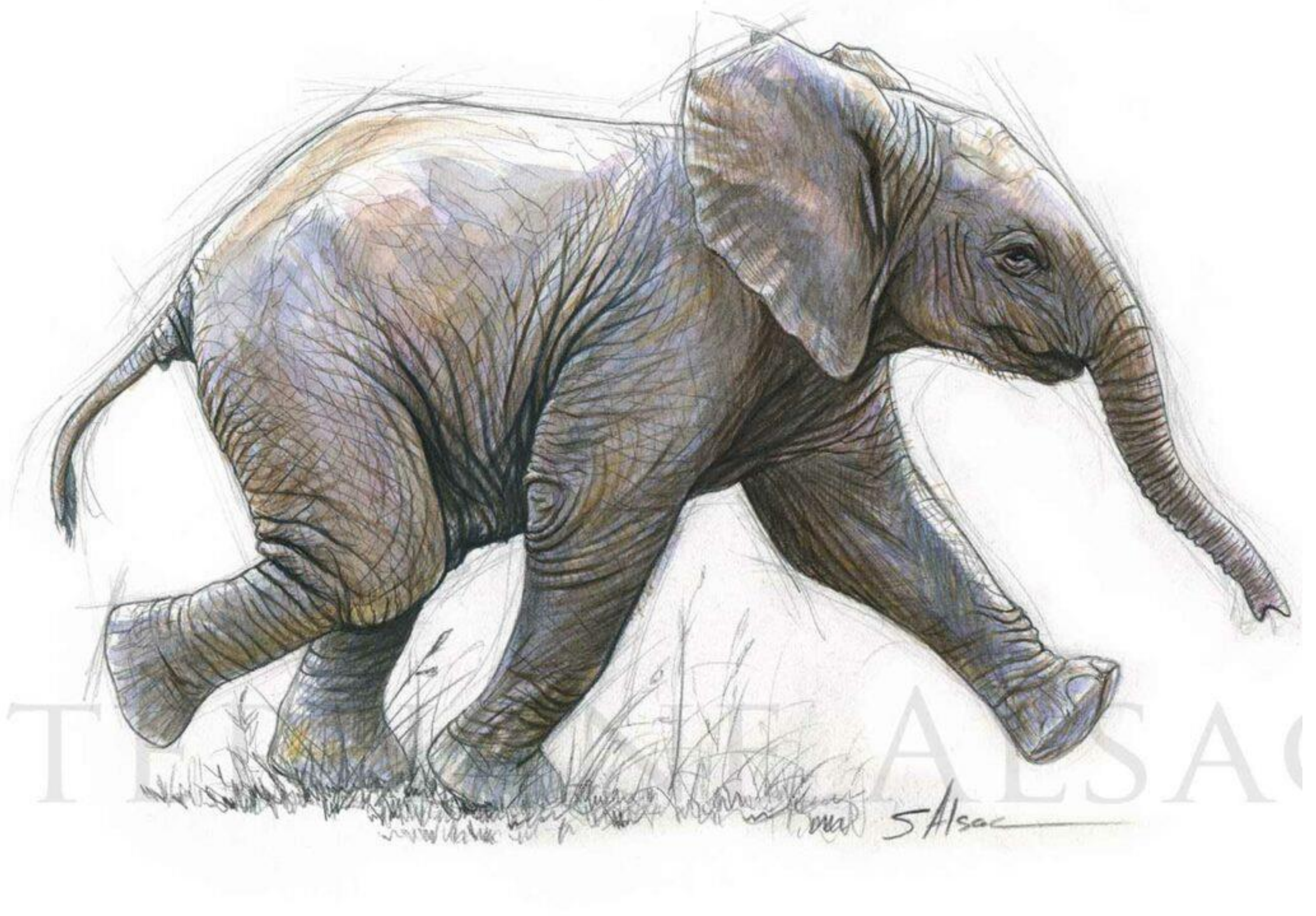
$$\frac{1}{2}\sum_i \frac{dg_i}{db} = \frac{1}{2}\left(\frac{dg_1}{df_1}\frac{df_1}{db} + \frac{dg_2}{df_2}\frac{df_2}{db}\right)$$

Gradient-based Optimization

❖ How to use gradient information



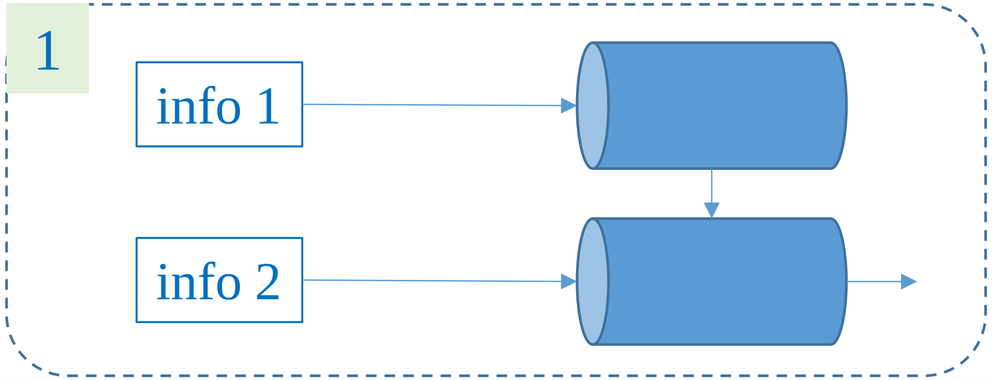




```python
import random

# predict function
def predict_func(x, a, b):
    return a*x + b

# parameters
num_steps = 100
lr = 0.01

# given data
data = [[-2, -1],
        [5, 13]]

# 1. set a, b randomly
a = random.random()*10.0 - 5.0
b = random.random()*10.0 - 5.0
```

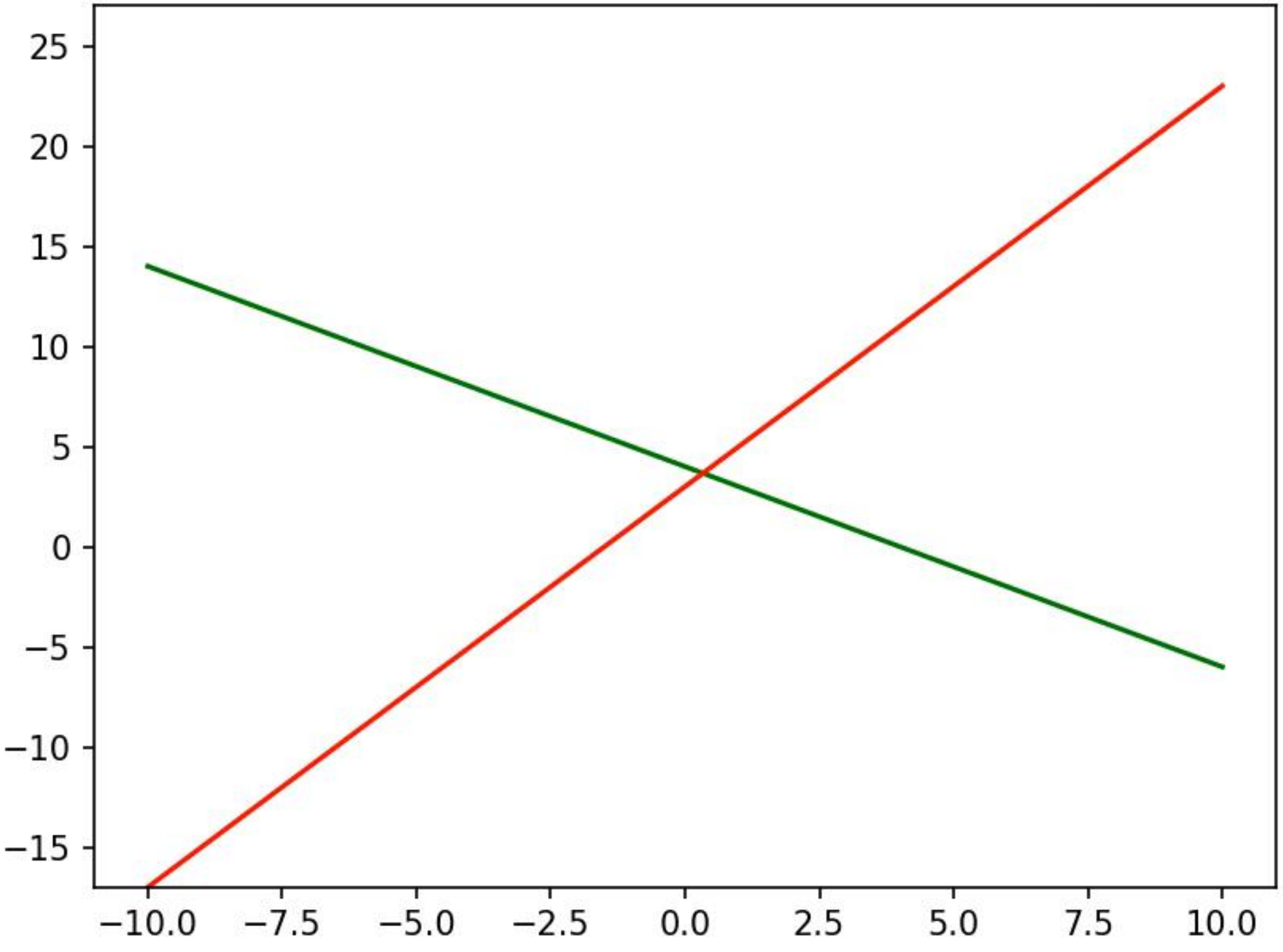
```python
for i in range(num_steps):
    for sample in data:
        x_value, y_value = sample

        # compute predicted_y
        predicted_y = predict_func(x_value, a, b)

        # compute g
        g_value = (predicted_y - y_value)**2

        # compute partial gradients for a and b
        dg_da = 2*x_value*(predicted_y - y_value)
        dg_db = 2*(predicted_y - y_value)

        # update
        a = a - lr*dg_da
        b = b - lr*dg_db
```

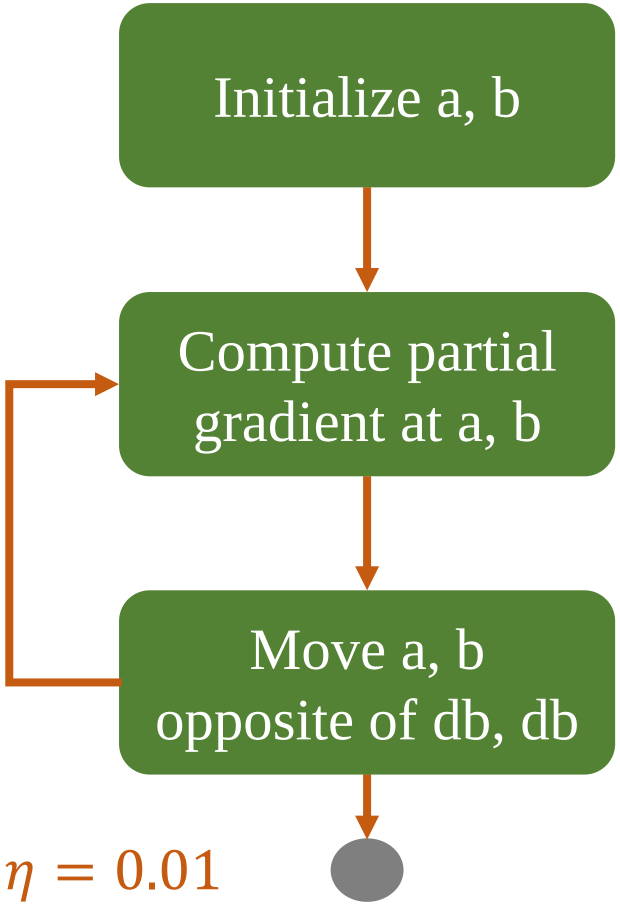
Summary



$$\frac{dg}{da} = \frac{dg}{df}\frac{df}{da} = 2x(f-y)$$

$$\frac{dg}{db} = \frac{dg}{df}\frac{df}{db} = 2(f-y)$$



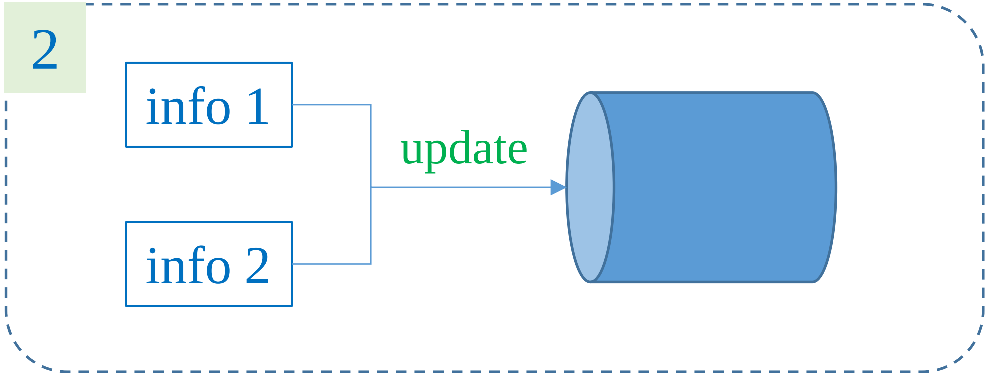


$\eta = 0.01$

```python
import random

# predict function
def predicted_func(x, a, b):
    return a*x + b

# parameters
num_steps = 100
lr = 0.01

# given data
x1 = -2
y1 = -1

x2 = 5
y2 = 13

# 1. set a, b randomly
a = random.random()*10.0 - 5.0
b = random.random()*10.0 - 5.0
```

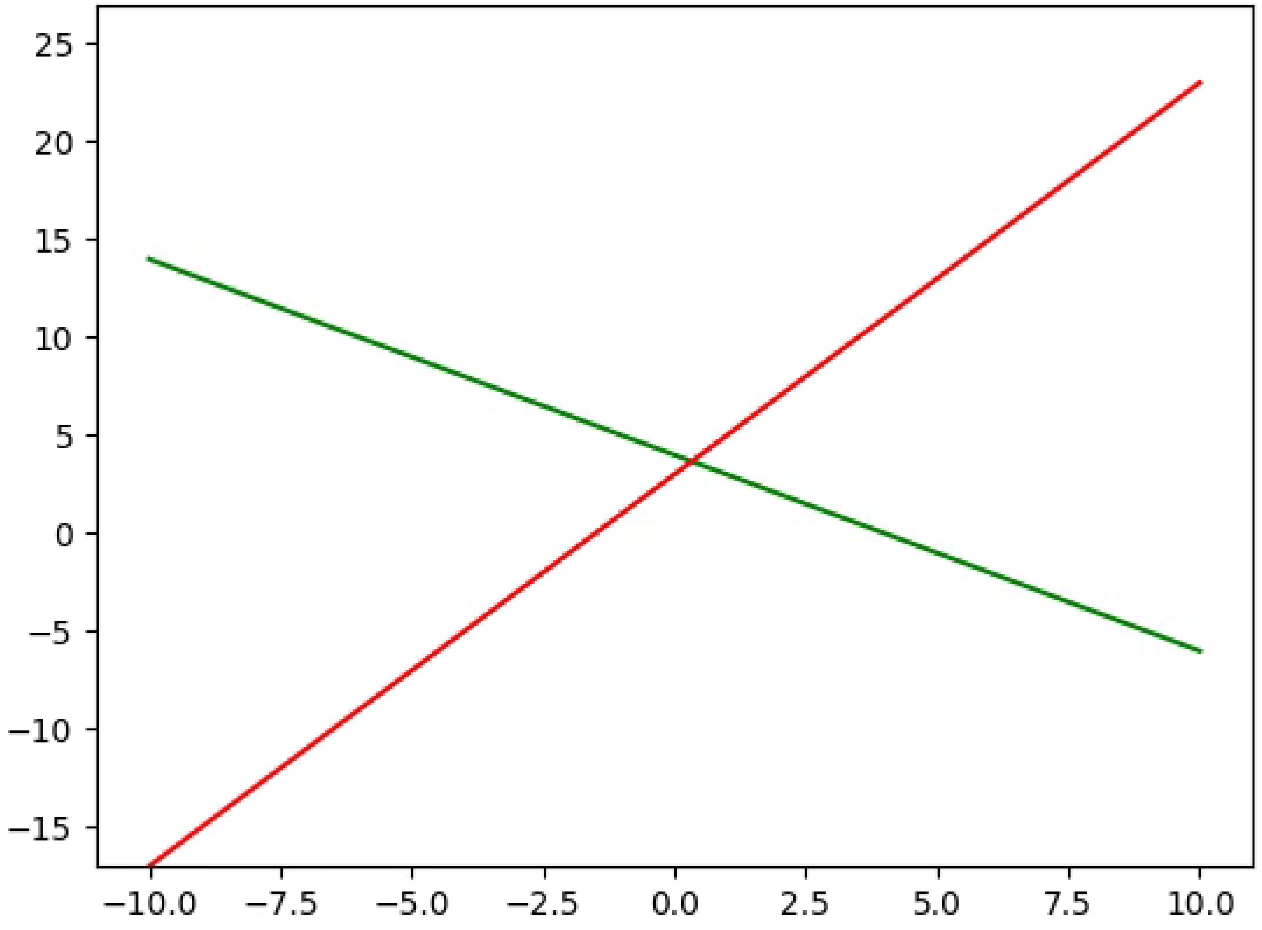
```python
for i in range(num_steps):
    # 2. compute predicted_y1 and predicted_y2
    predicted_y1 = predicted_func(x1, a, b)
    predicted_y2 = predicted_func(x2, a, b)

    # 3. compute g
    g_value_1 = (predicted_y1 - y1)**2
    g_value_2 = (predicted_y2 - y2)**2

    # logging
    # ...

    # 4. compute partial gradients for a and b
    dg_da = 2*x1*(predicted_y1 - y1) + 2*x2*(predicted_y2 - y2)
    dg_db = 2*(predicted_y1 - y1) + 2*(predicted_y2 - y2)

    # 5. update
    a = a - lr*dg_da/2
    b = b - lr*dg_db/2
```

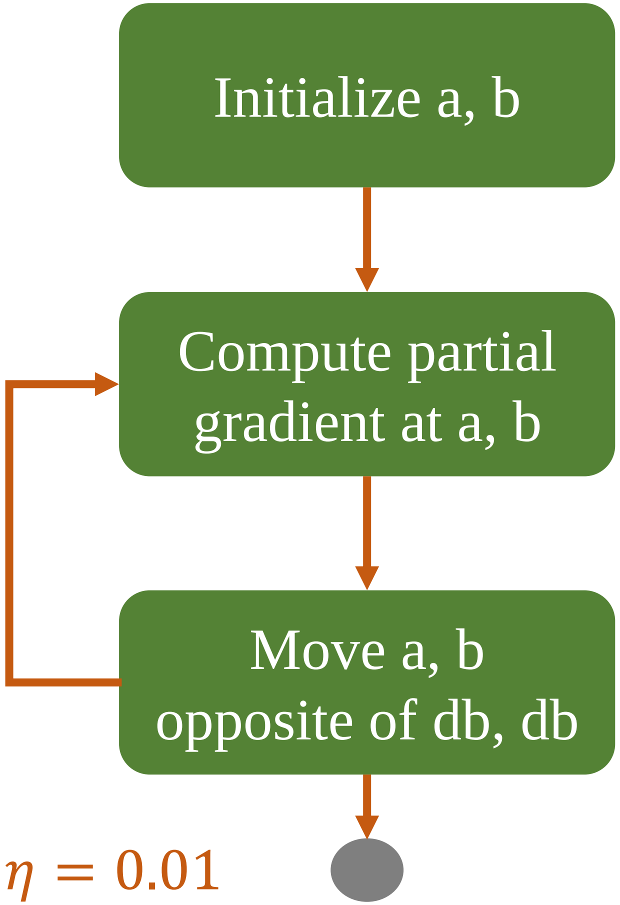
Summary



$$\frac{dg}{da} = \frac{dg}{df}\frac{df}{da} = 2x(f-y)$$

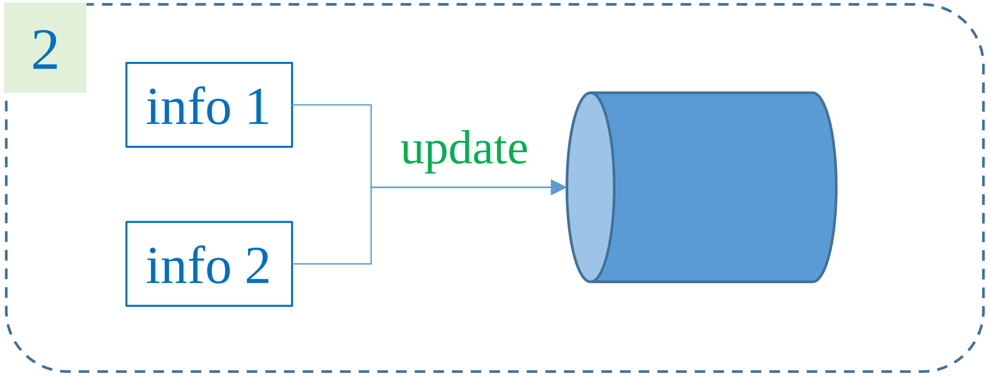
$$\frac{dg}{db} = \frac{dg}{df}\frac{df}{db} = 2(f-y)$$





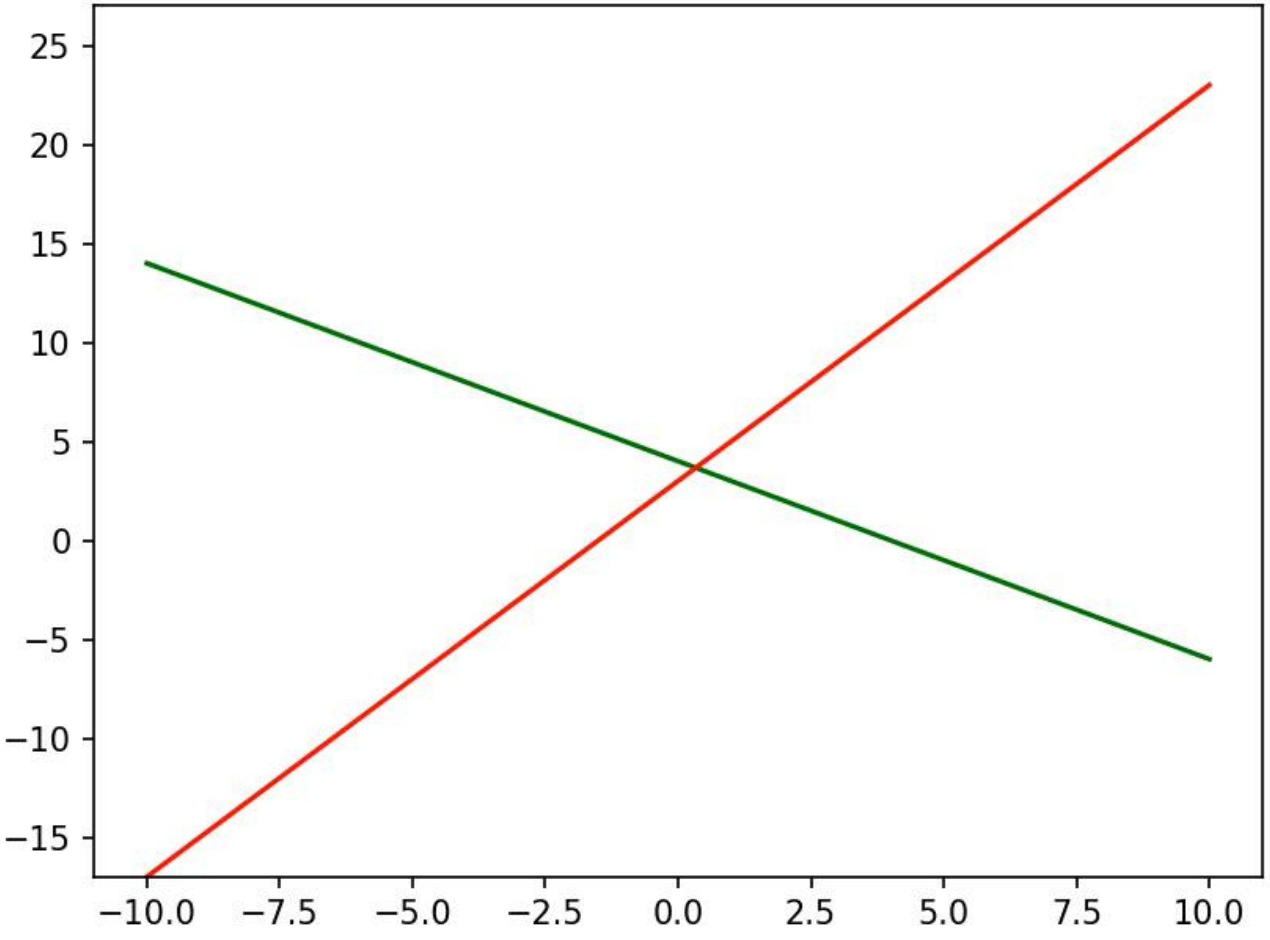
$\eta = 0.01$

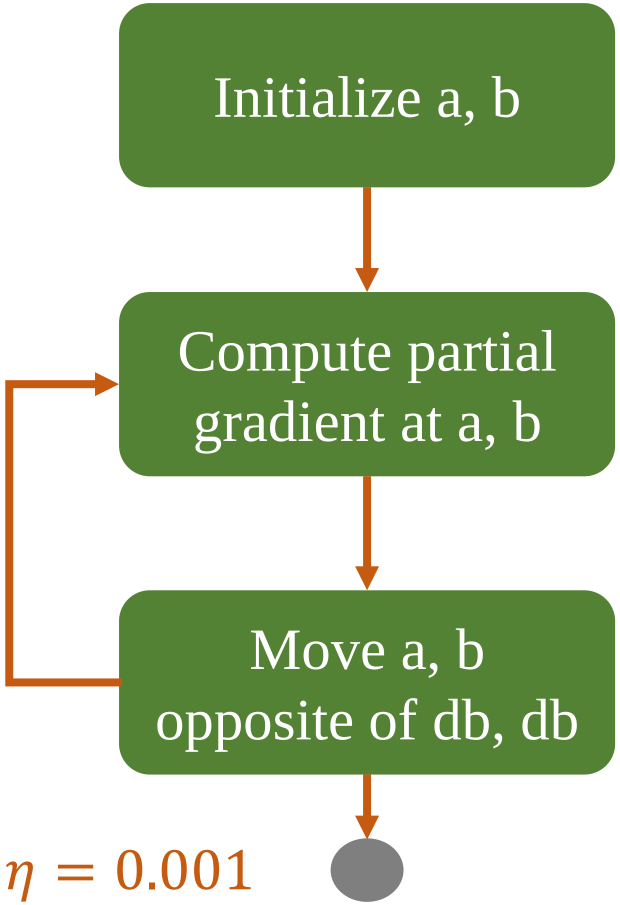
Summary



$$\frac{dg}{da} = \frac{dg}{df}\frac{df}{da} = 2x(f-y)$$

$$\frac{dg}{db} = \frac{dg}{df}\frac{df}{db} = 2(f-y)$$

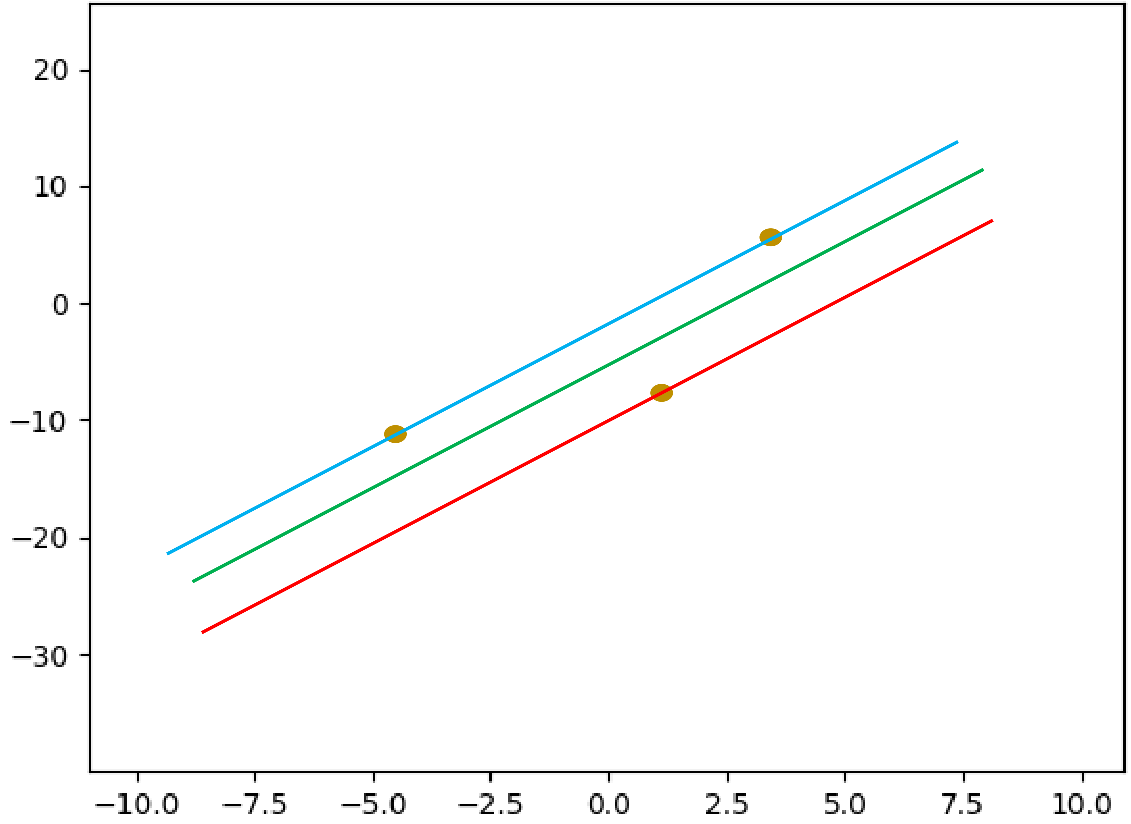




$\eta = 0.001$

Discussion

❖ What about this given samples?



Which line is the best representation of these three points?

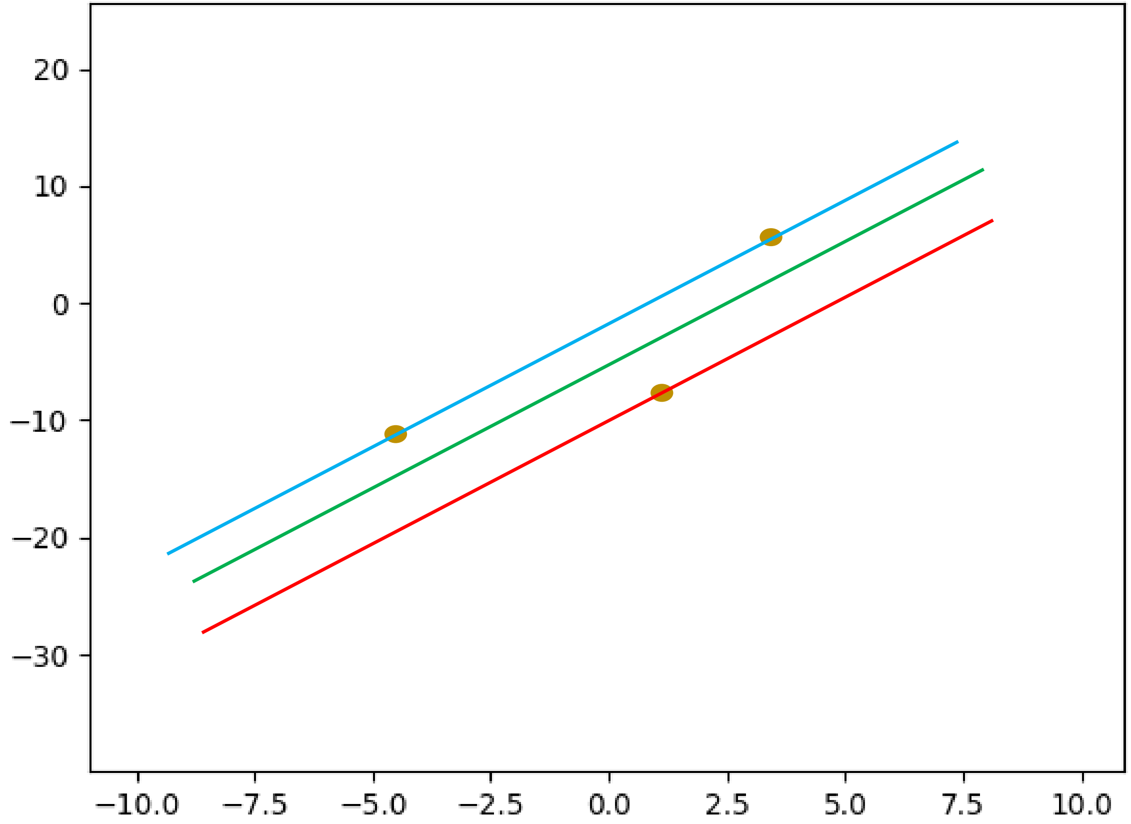
Line 1: go through two points

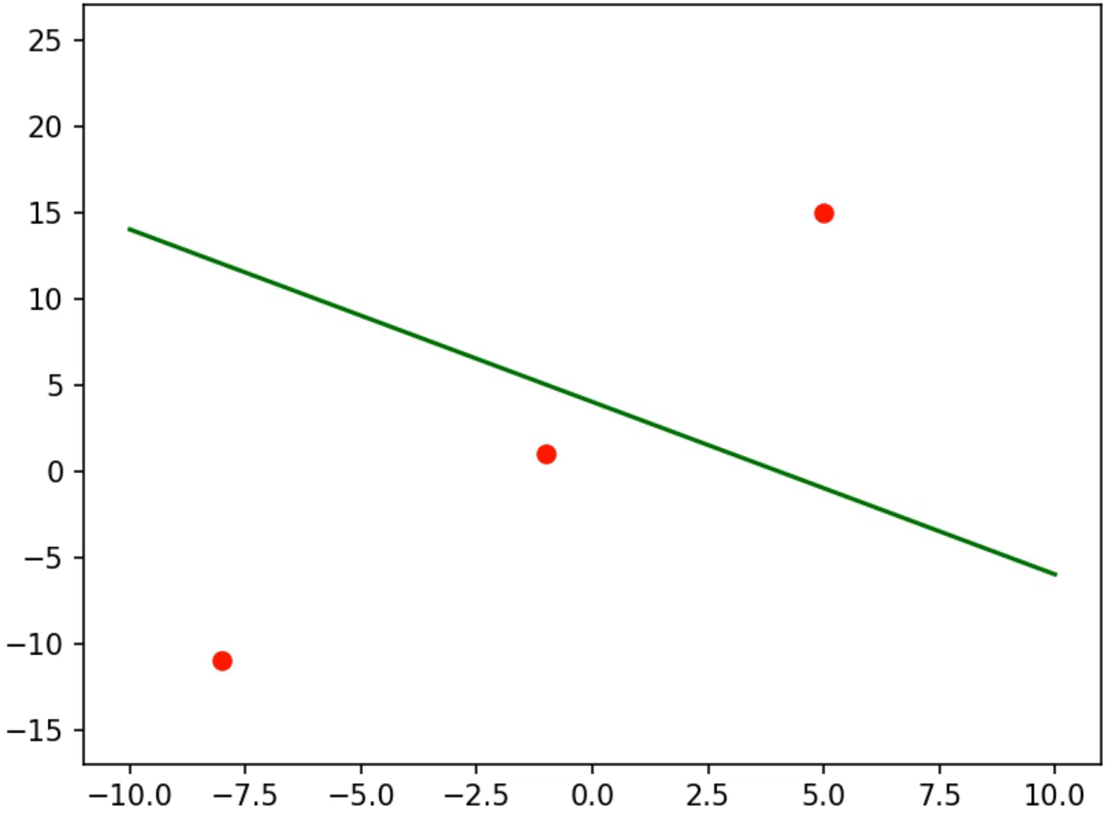
Line 2: smallest summation of distances

Line 3: go through one point

Discussion

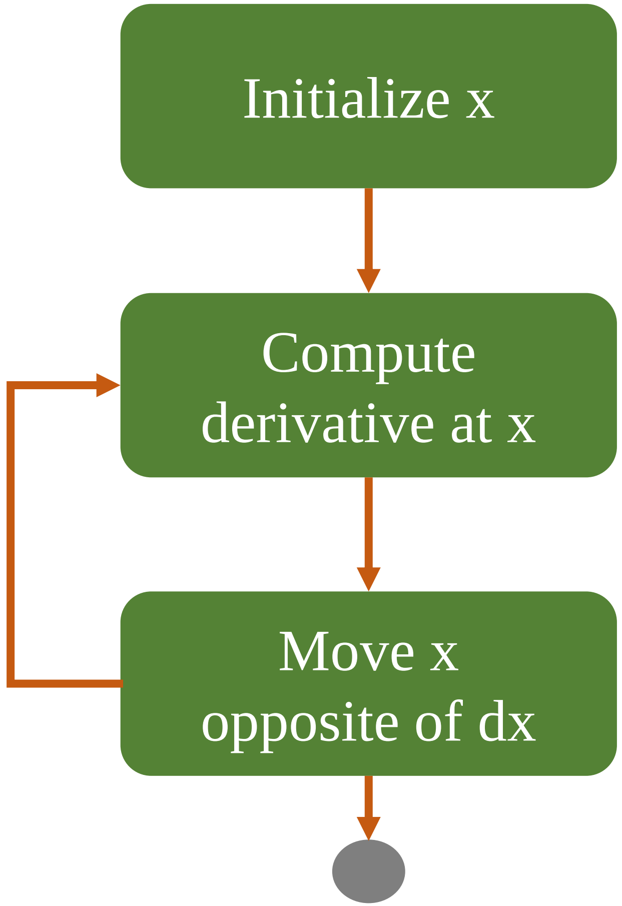
❖ **What about the given samples?**





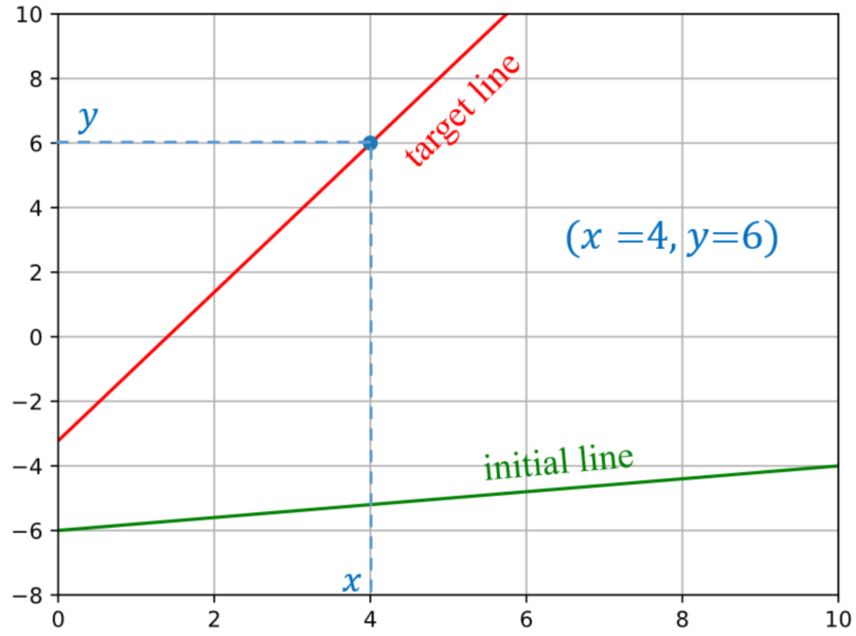
Objectives

Optimization



Problem Solving

$$f(x) = ax + b$$



Toward Linear Regression