# Gradient Descent

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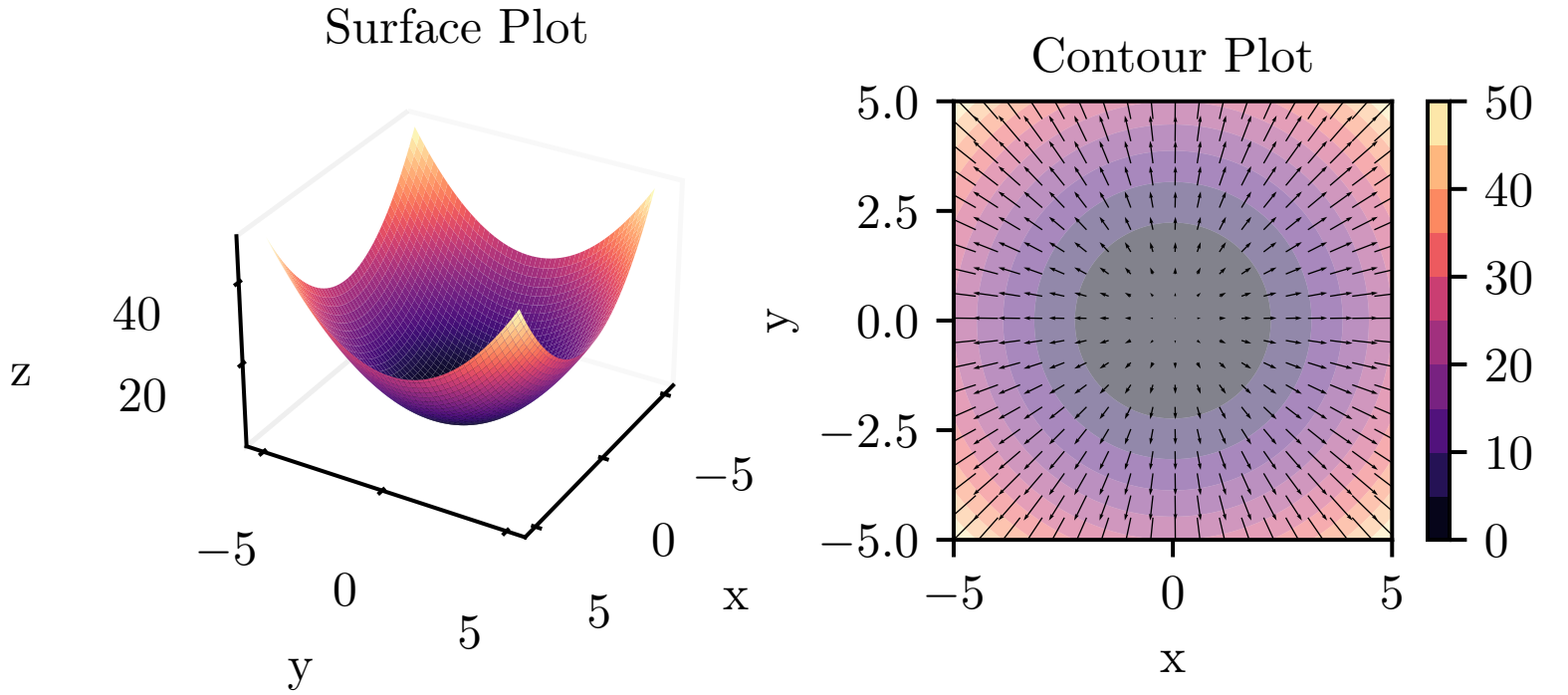
# Revision

# Contour Plot And Gradients

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



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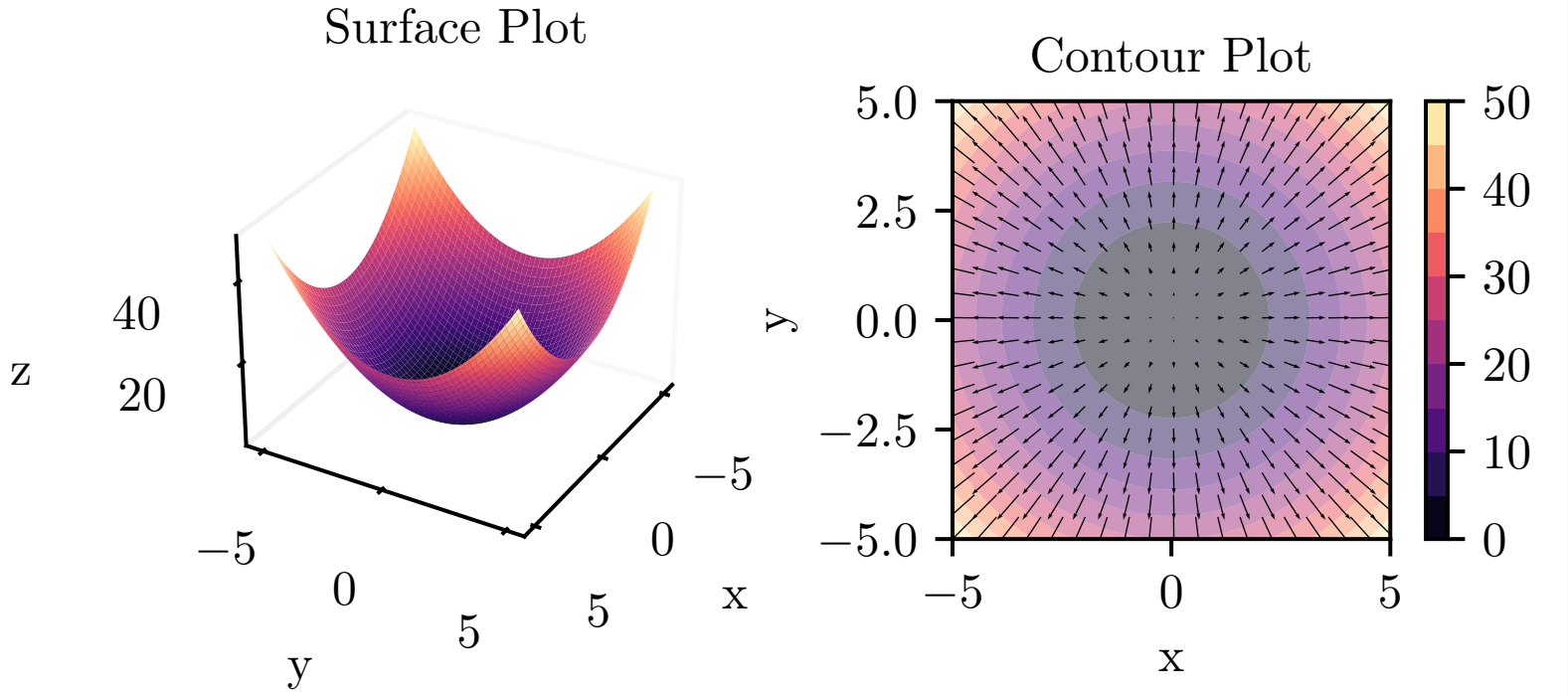


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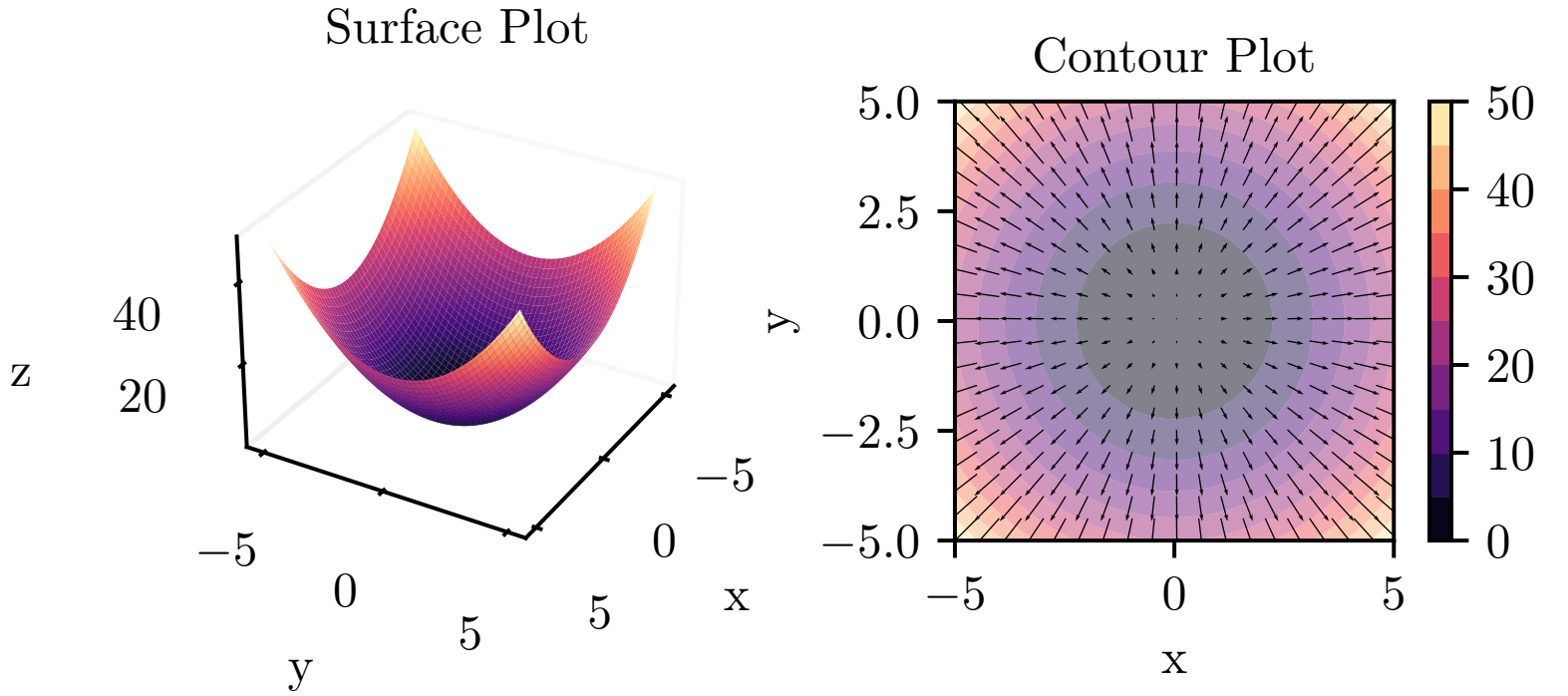


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$$\nabla f(x, y) = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

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- Note, here $\theta$ is the parameter vector

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- Goal:

$$\theta^* = \arg\min_{\theta} f(\theta) \tag{2}$$

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- It is a local search algorithm/greedy

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- where $\nabla^2 f(\vec{x_0})$ is the Hessian matrix and $\nabla f(\vec{x_0})$ is the gradient vector

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- $f(x) = 1 + 0(x - 0) + \frac{-1}{2!}(x - 0)^2 = 1 - \frac{x^2}{2}$

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- Question: How does the first order Taylor's series approximation look like?
- First order Taylor's series approximation is given by:
- $f(x) = f(x_0) + f'(x_0)(x - x_0) = 6 + 4(x - 2) = 4x - 2$

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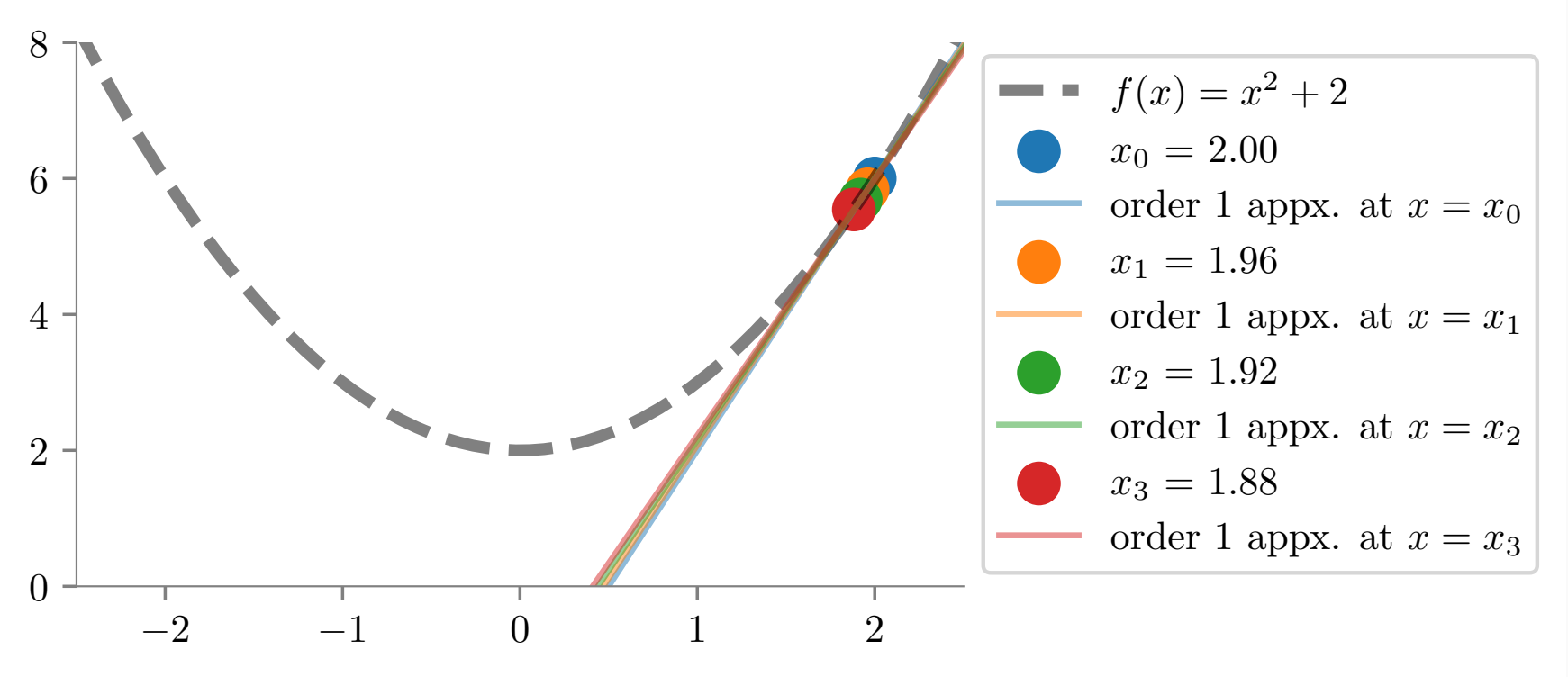
- This happens when $\Delta\vec{x} = -\alpha\nabla f(\vec{x_0})$ where $\alpha$ is a scalar
- This is the gradient descent algorithm: $\vec{x_1} = \vec{x_0} - \alpha\nabla f(\vec{x_0})$

# Effect of learning rate

Low learning rate $\alpha = 0.01$ : Converges slowly



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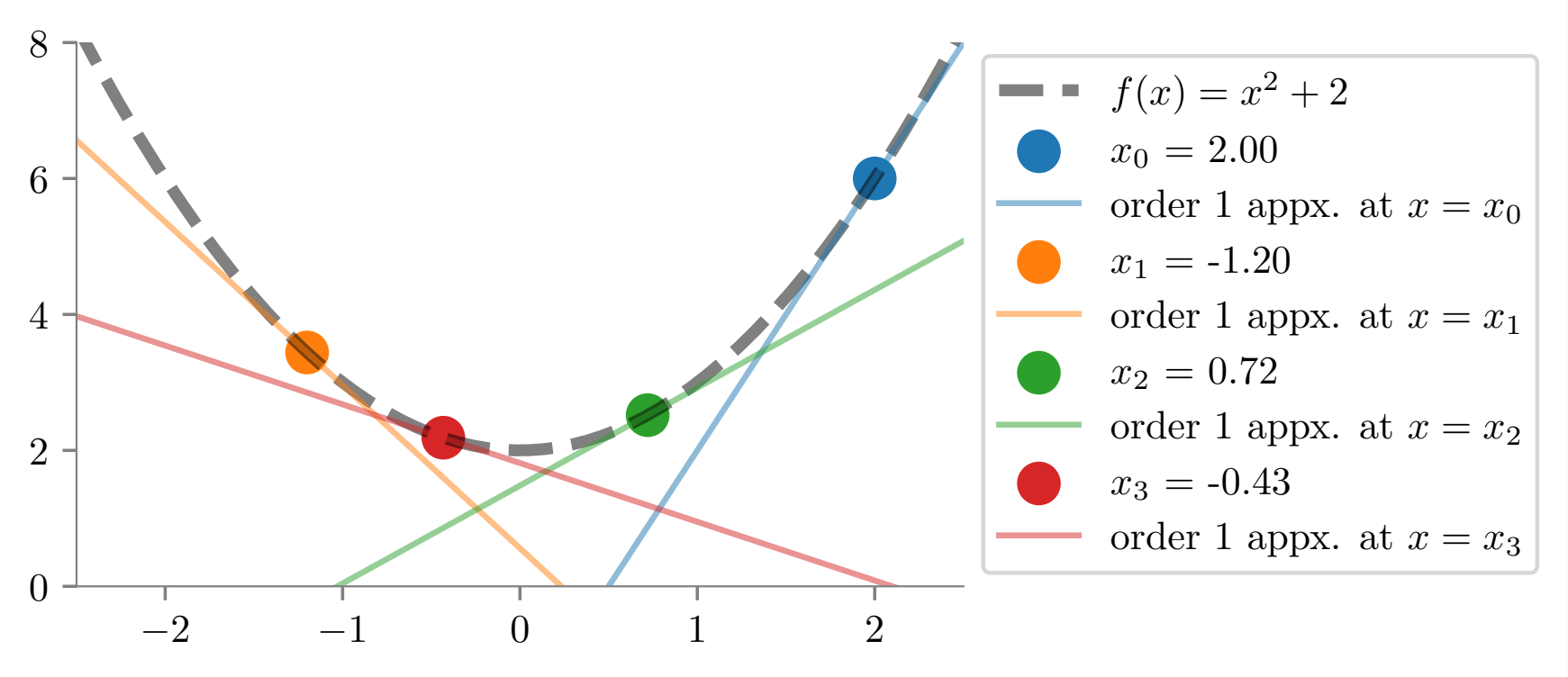
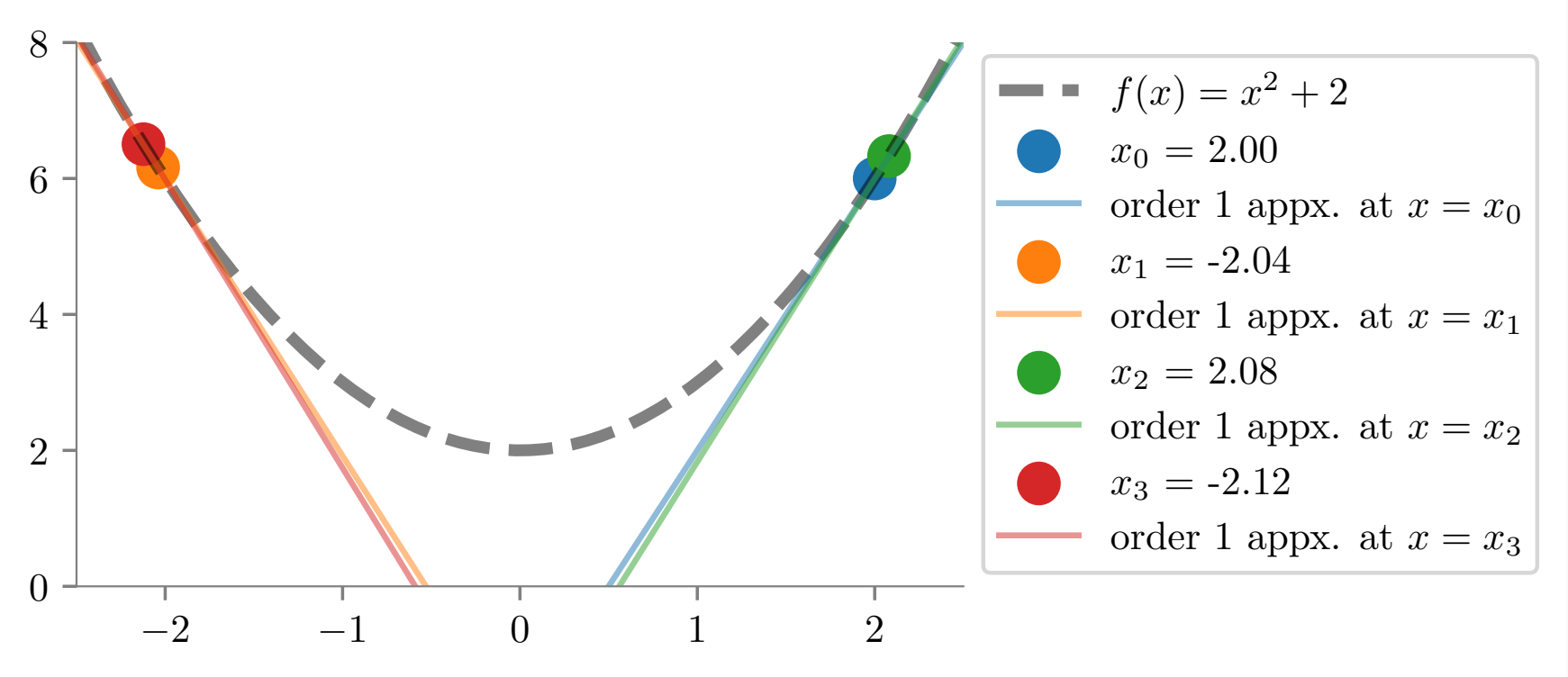
High learning rate $\alpha = 0.8$: Converges quickly, but might overshoot



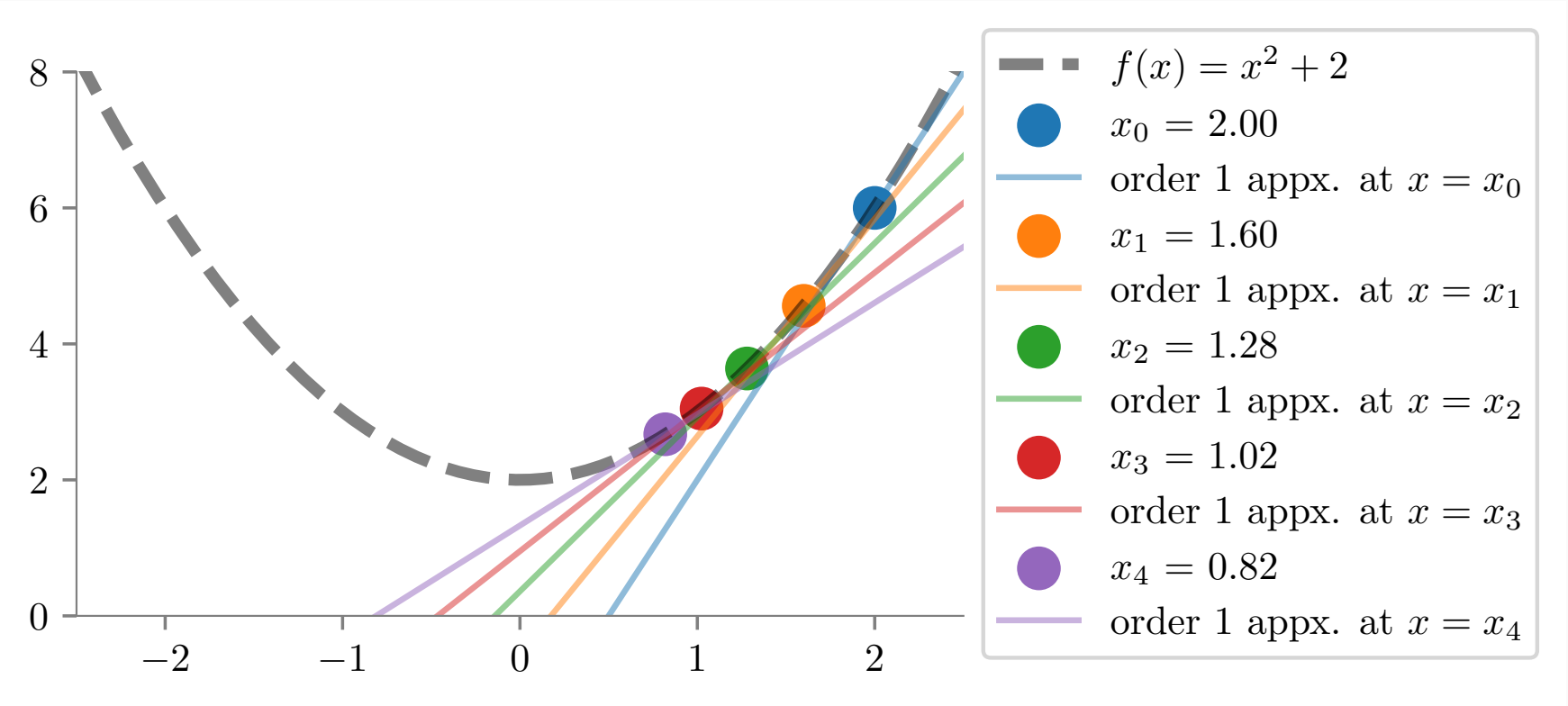
# Effect of learning rate

Very high learning rate $\alpha = 1.01$: Diverges



# Effect of learning rate

Appropriate learning rate $\alpha = 0.1$



# Gradient Descent for linear regression

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- Mean Squared Error $MSE(\theta) = \frac{1}{N}\sum_{i=1}^{N}\left(f\left(x_i|\theta\right) - y_i\right)^2$
- **Objective function** is the most general term for any function that you optimize during training.

# Gradient Descent : Example

Learn $y = \theta_0 + \theta_1 x$ on following dataset, using gradient descent where initially $(\theta_0, \theta_1) = (4, 0)$ and step-size, $\alpha = 0.1$, for 2 iterations.

| x | y |
|---|---|
| 1 | 1 |
| 2 | 2 |
| 3 | 3 |

# Gradient Descent : Example

Our predictor, $\hat{y} = \theta_0 + \theta_1 x$

Error for $i^{th}$ datapoint, $\epsilon_i = y_i - \hat{y}_i$

$\epsilon_1 = 1 - \theta_0 - \theta_1$

$\epsilon_2 = 2 - \theta_0 - 2\theta_1$

$\epsilon_3 = 3 - \theta_0 - 3\theta_1$

$$\text{MSE} = \frac{\epsilon_1^2 + \epsilon_2^2 + \epsilon_3^2}{3} = \frac{14 + 3\theta_0^2 + 14\theta_1^2 - 12\theta_0 - 28\theta_1 + 12\theta_0\theta_1}{3}$$

# Difference between SSE and MSE

$$\sum \epsilon_i^2 \textit{ increases as the number of examples increase}$$

So, we use MSE

$$MSE = \frac{1}{n} \sum \epsilon_i^2$$

Here $n$ denotes the number of samples

# Gradient Descent : Example

$$\frac{\partial MSE}{\partial \theta_0} = \frac{2\sum_i (y_i - \theta_0 - \theta_1 x_i)(-1)}{N} = \frac{2\sum_i \epsilon_i (-1)}{N}$$

$$\frac{\partial MSE}{\partial \theta_1} = \frac{2\sum_i (y_i - \theta_0 - \theta_1 x_i)(-x_i)}{N} = \frac{2\sum_i \epsilon_i (-x_i)}{N}$$

# Gradient Descent : Example

**Iteration 1**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

# Gradient Descent : Example

**Iteration 1**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 4 - 0.2 \frac{((1-(4+0))(-1)+(2-(4+0))(-1)+(3-(4+0))(-1))}{3}$$

$$\theta_0 = 3.6$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

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$$\theta_1 = 0 - 0.2 \frac{((1-(4+0))(-1)+(2-(4+0))(-2)+(3-(4+0))(-3))}{3}$$

$$\theta_1 = -0.67$$

# Gradient Descent : Example

**Iteration 2**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

# Gradient Descent : Example

## Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.6 - 0.2 \frac{((1-(3.6-0.67))(-1)+(2-(3.6-0.67\times 2))(-1)+(3-(3.6-0.67\times 3))(-1))}{3}$$

$$\theta_0 = 3.54$$

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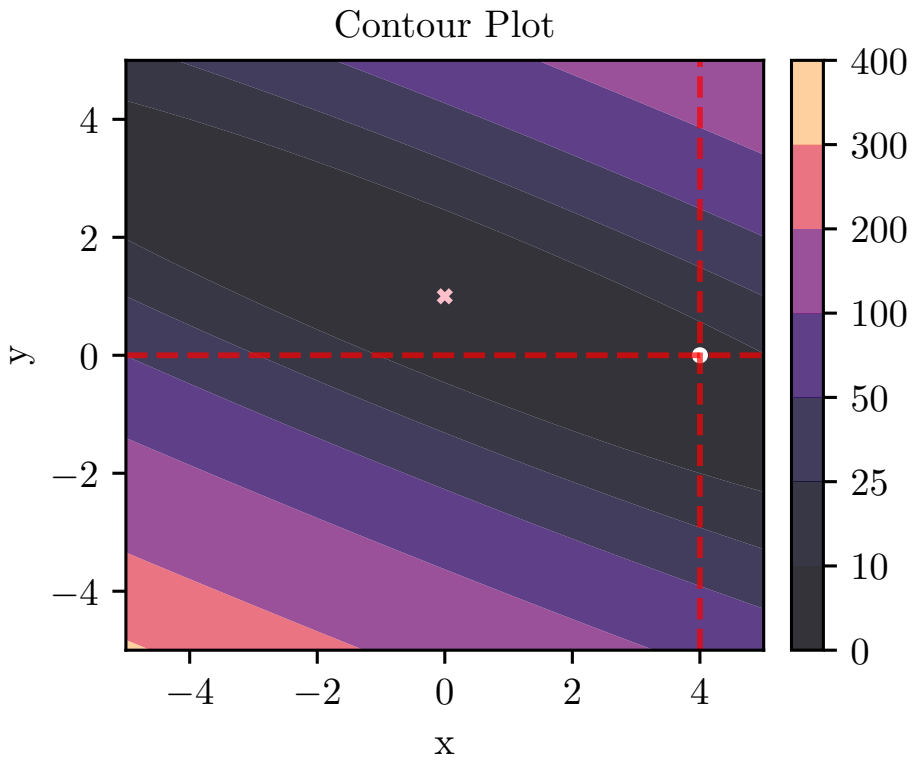
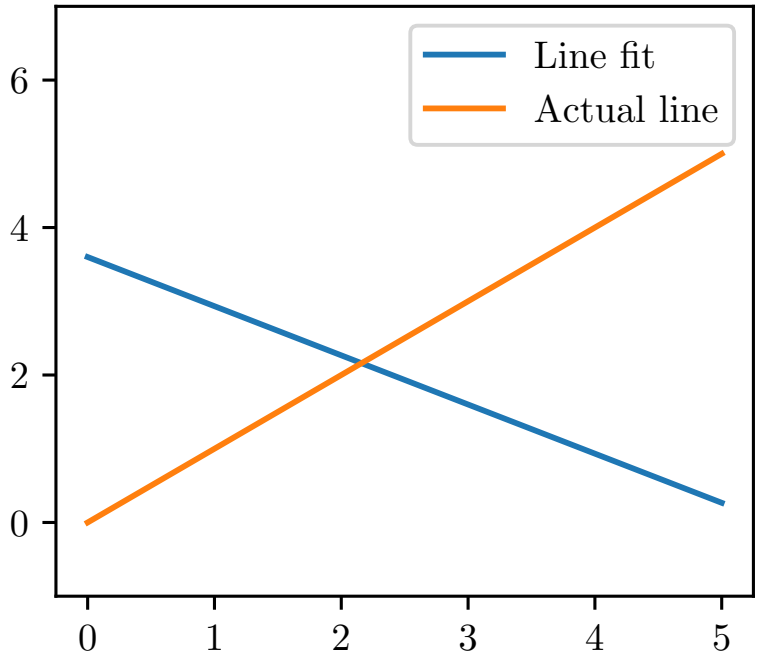
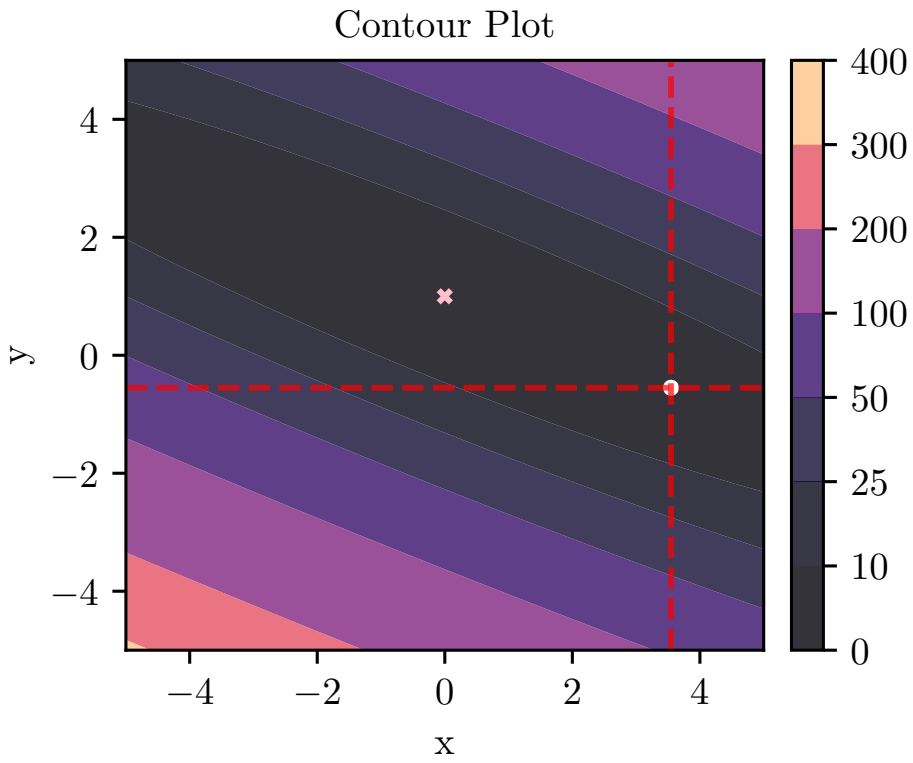
$$\theta_0 = -0.55$$

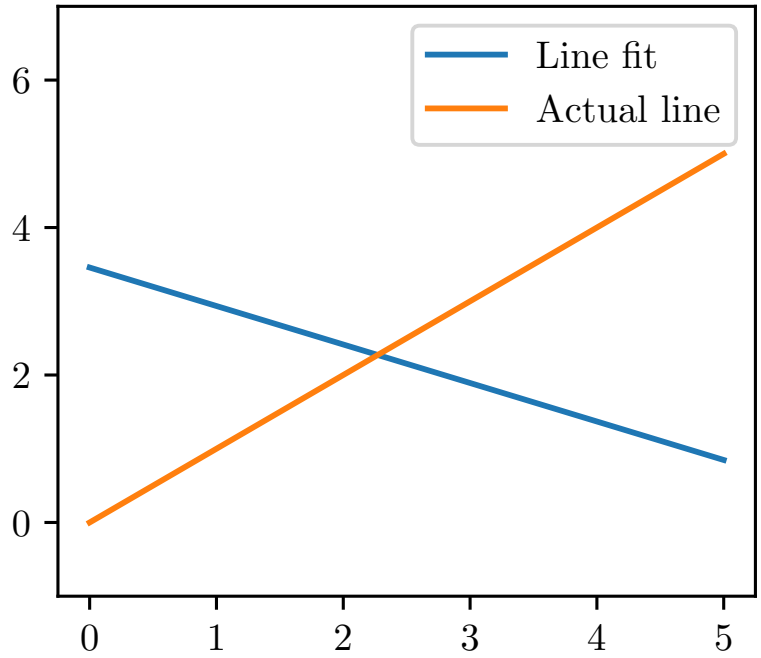
# Gradient Descent : Example (Iteraion 0)



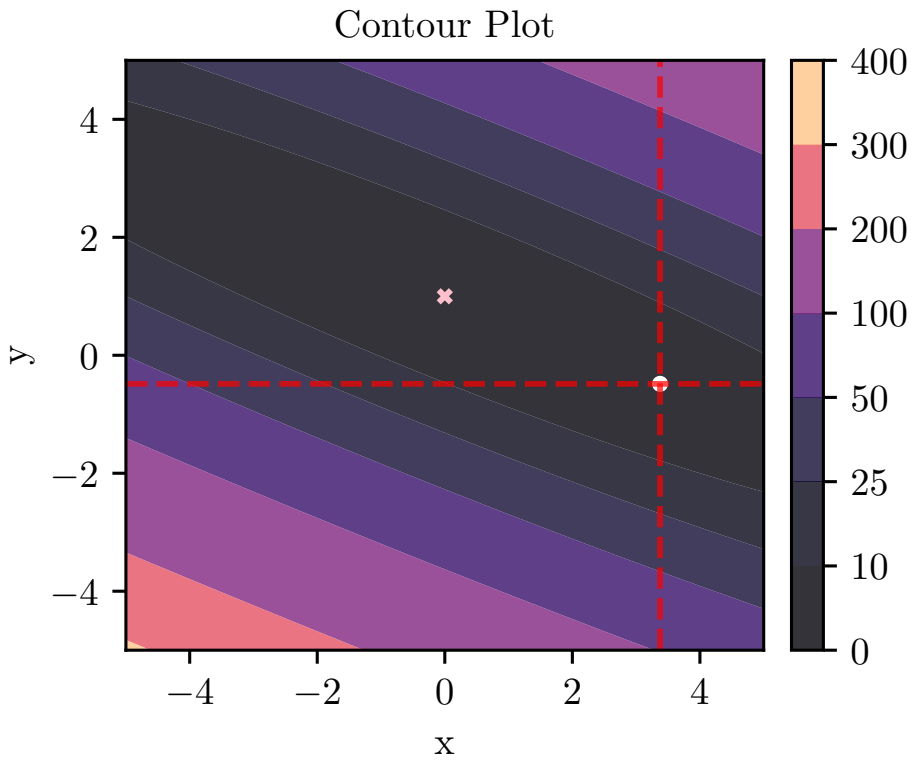



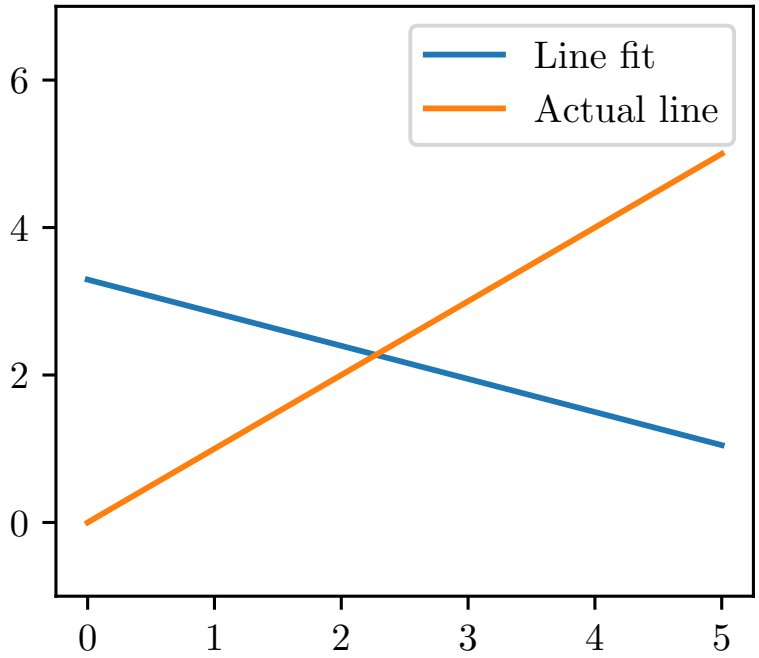
# Gradient Descent : Example (Iteraion 2)



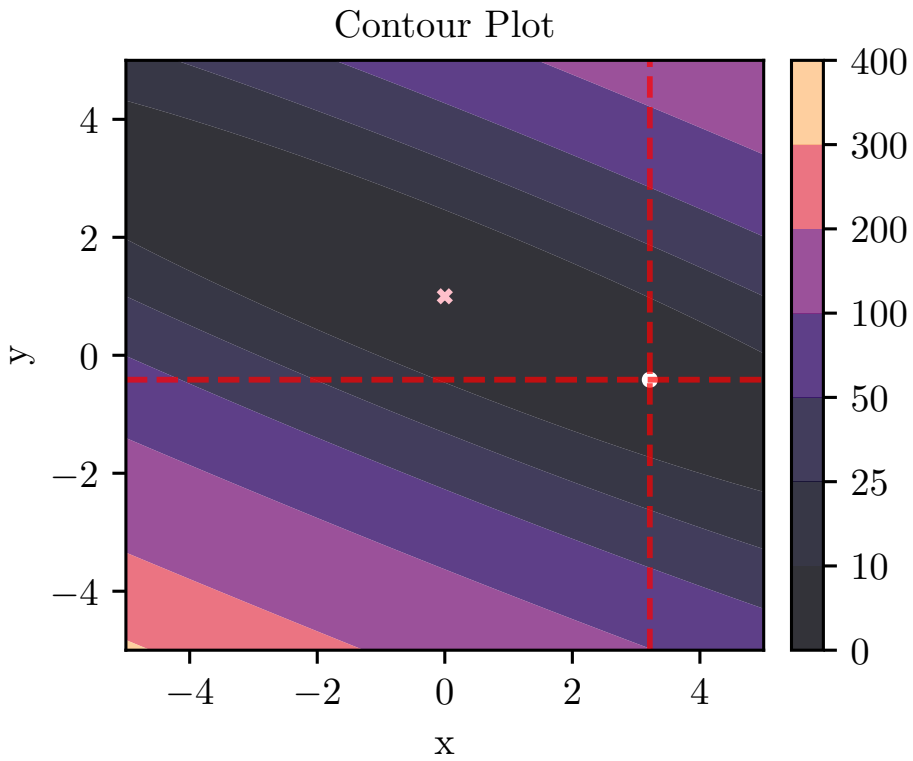



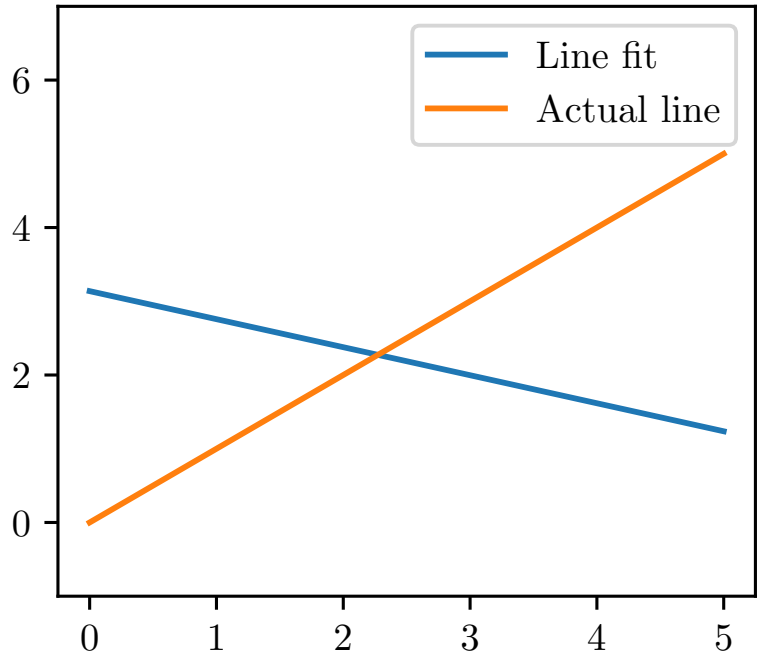
# Gradient Descent : Example (Iteraion 4)



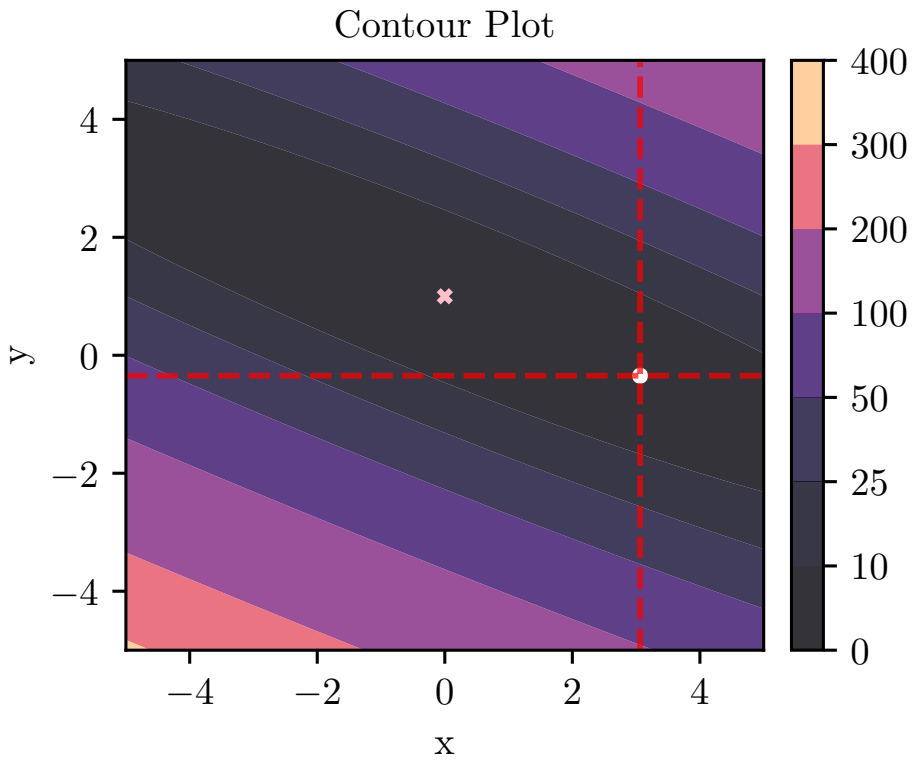



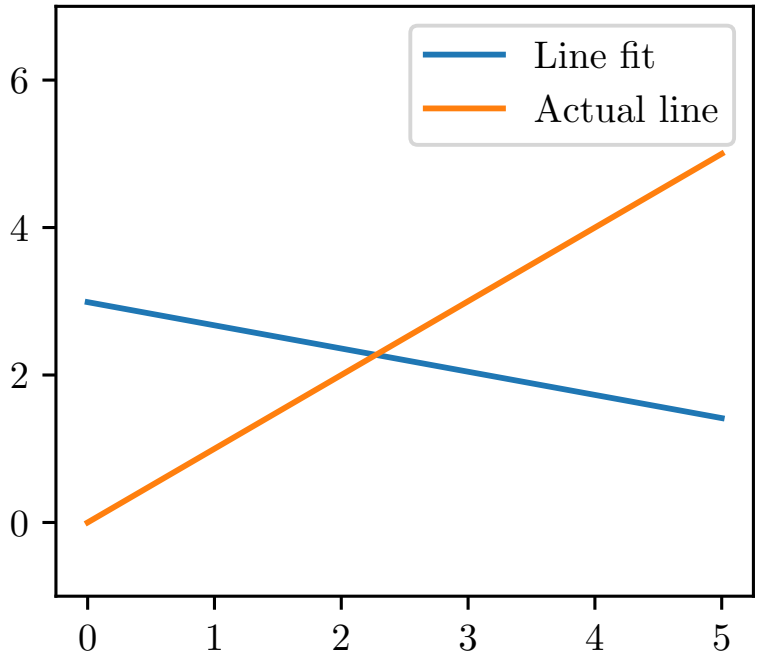
# Gradient Descent : Example (Iteraion 6)



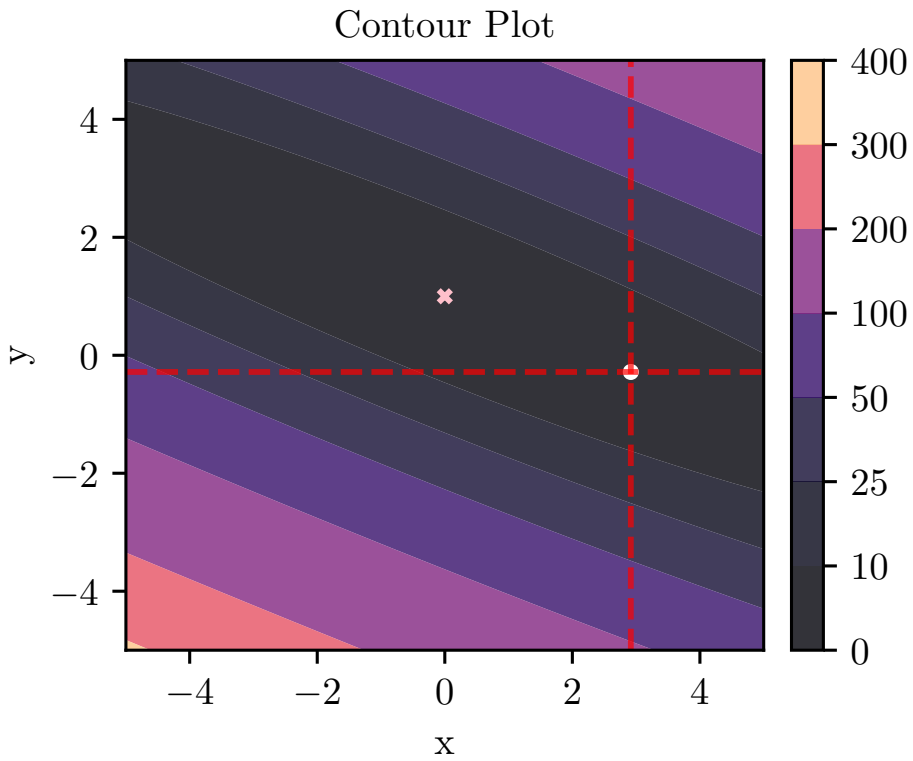



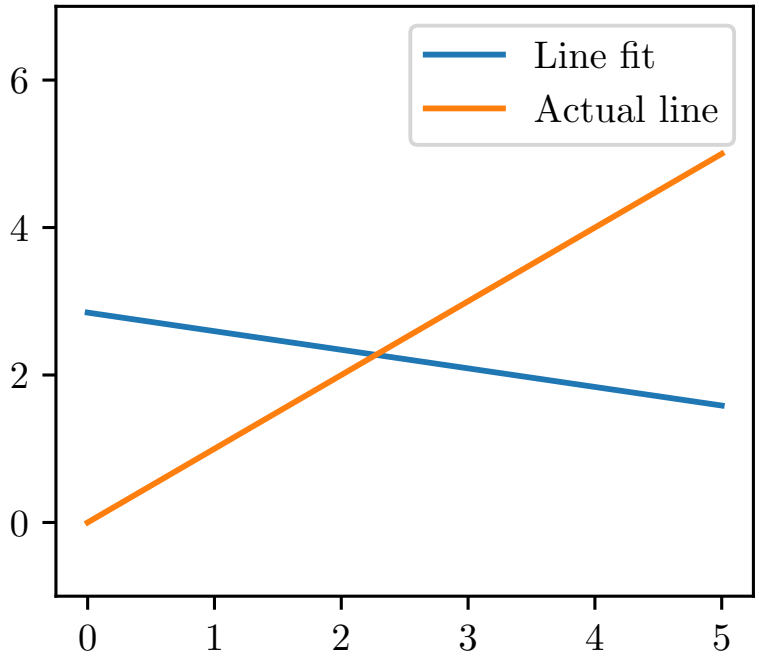
# Gradient Descent : Example (Iteraion 8)



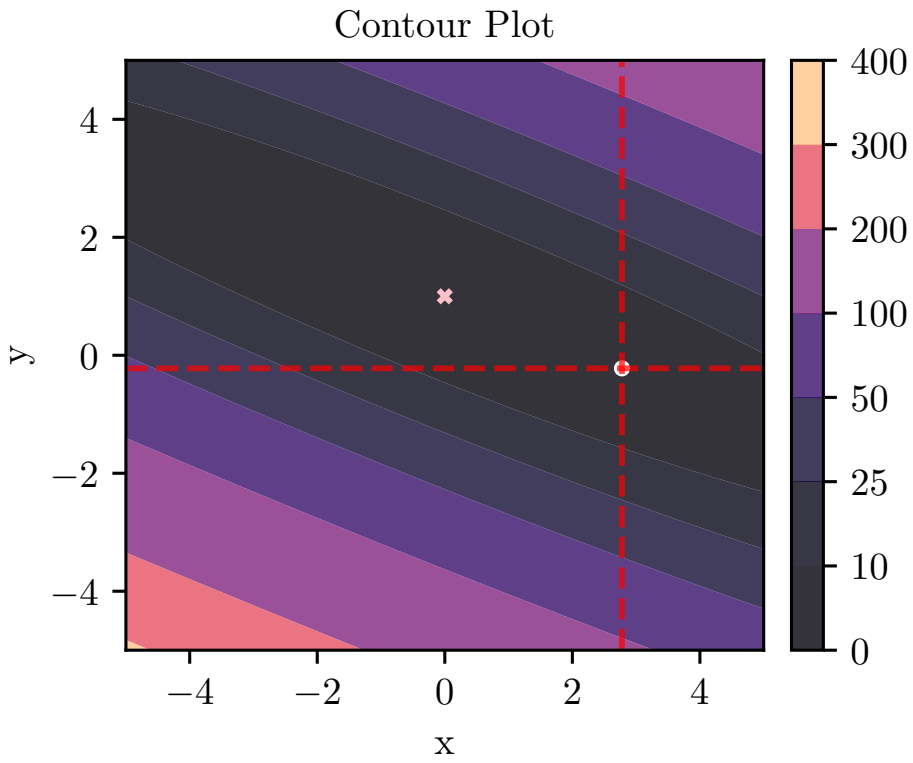



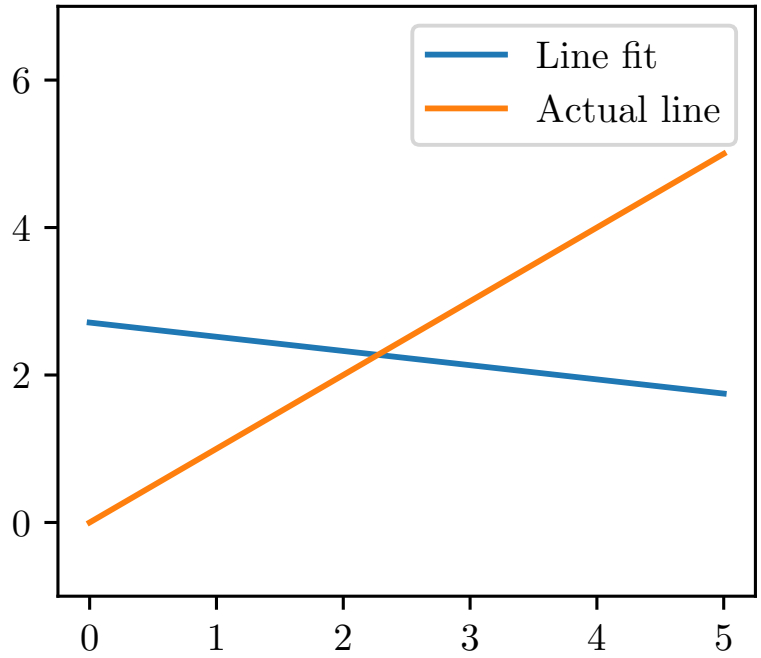
# Gradient Descent : Example (Iteraion 10)



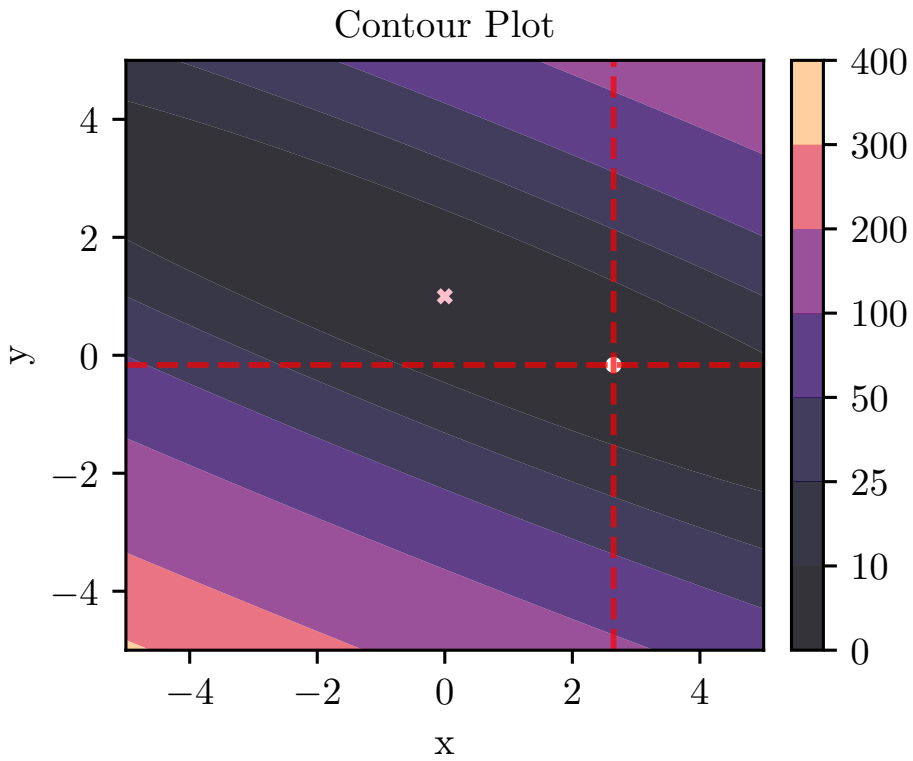



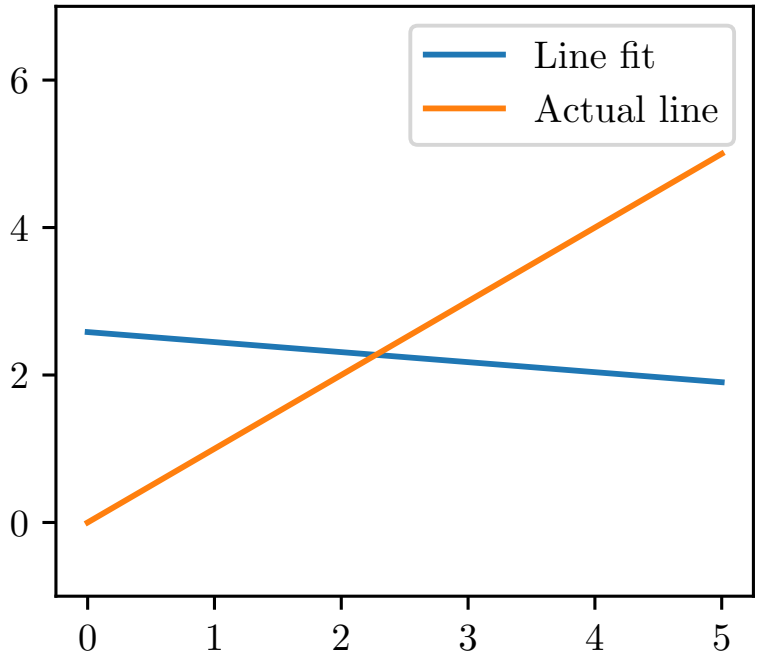
# Gradient Descent : Example (Iteraion 12)



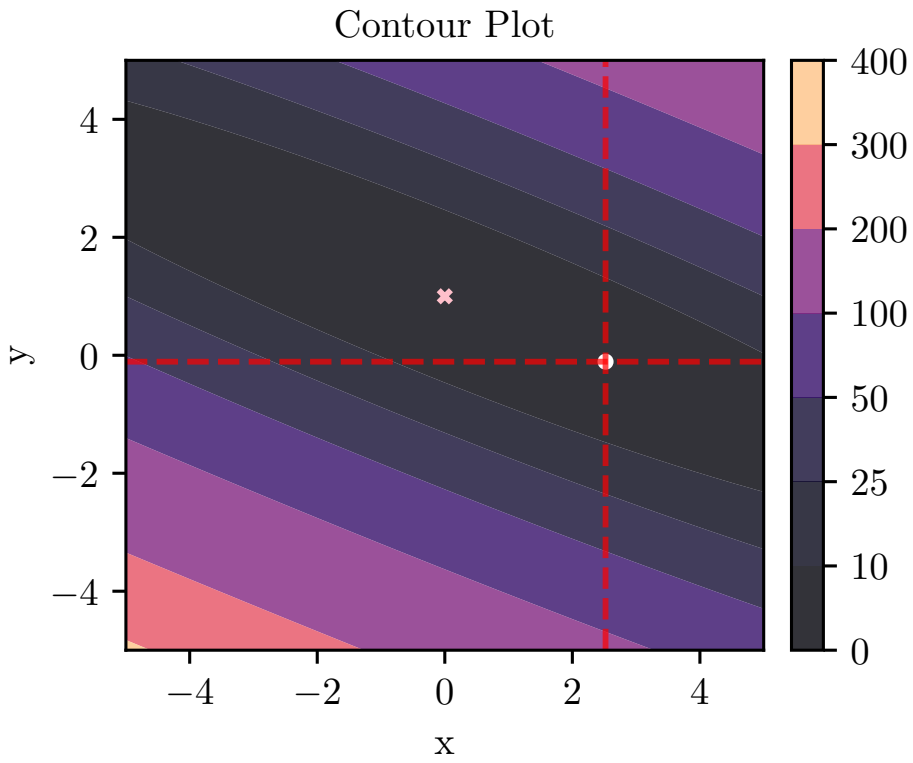



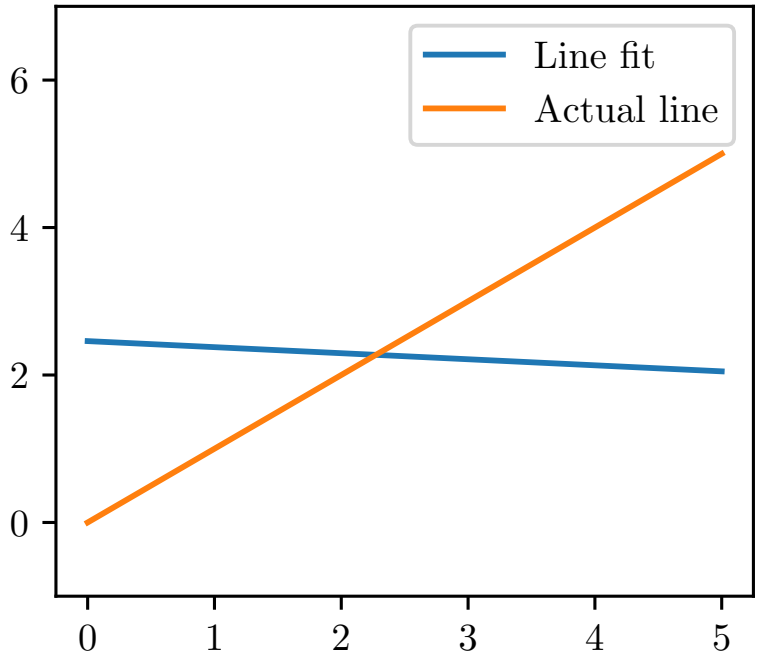
# Gradient Descent : Example (Iteraion 14)



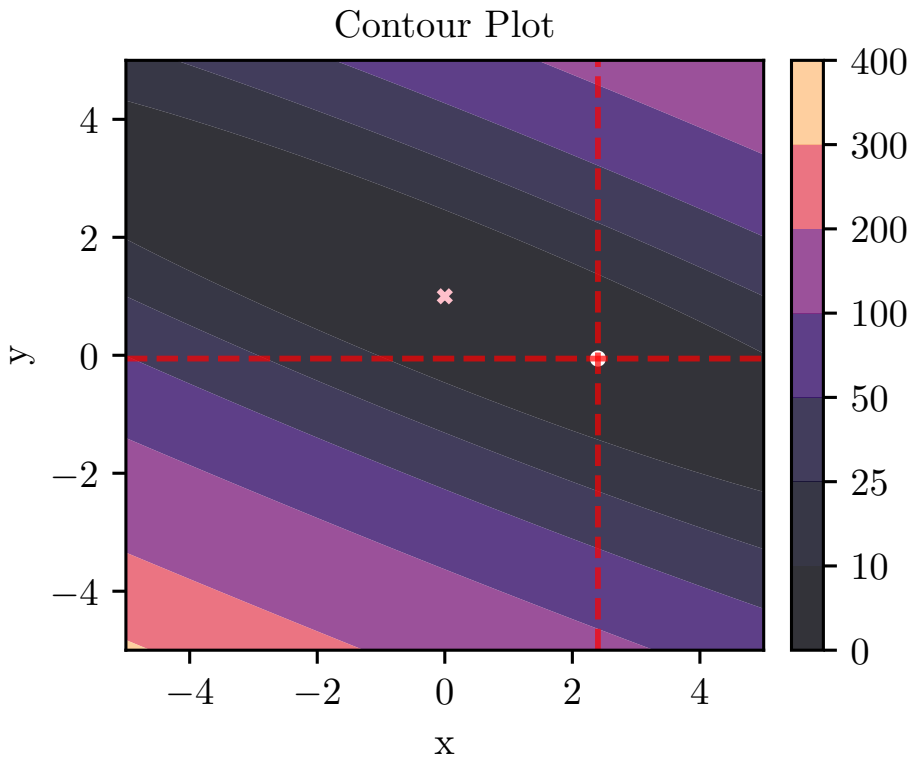



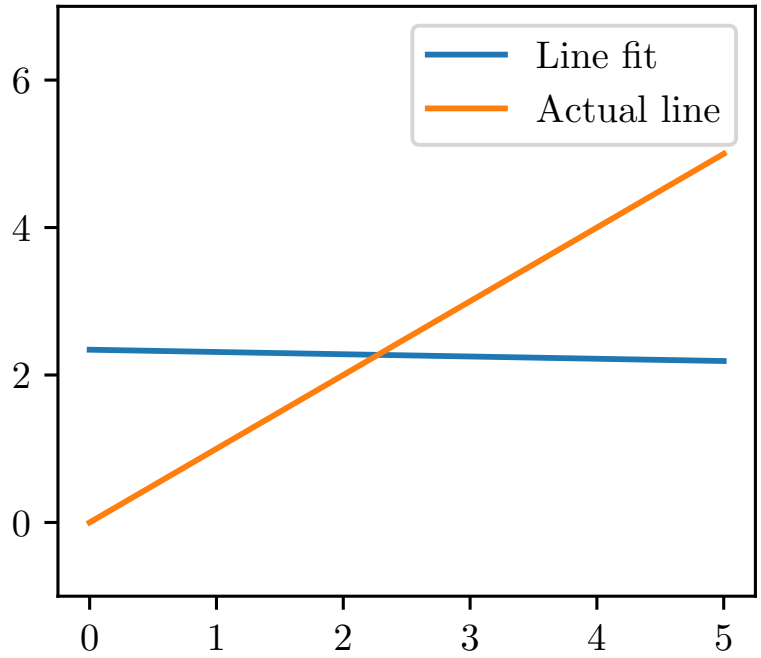
# Gradient Descent : Example (Iteraion 16)



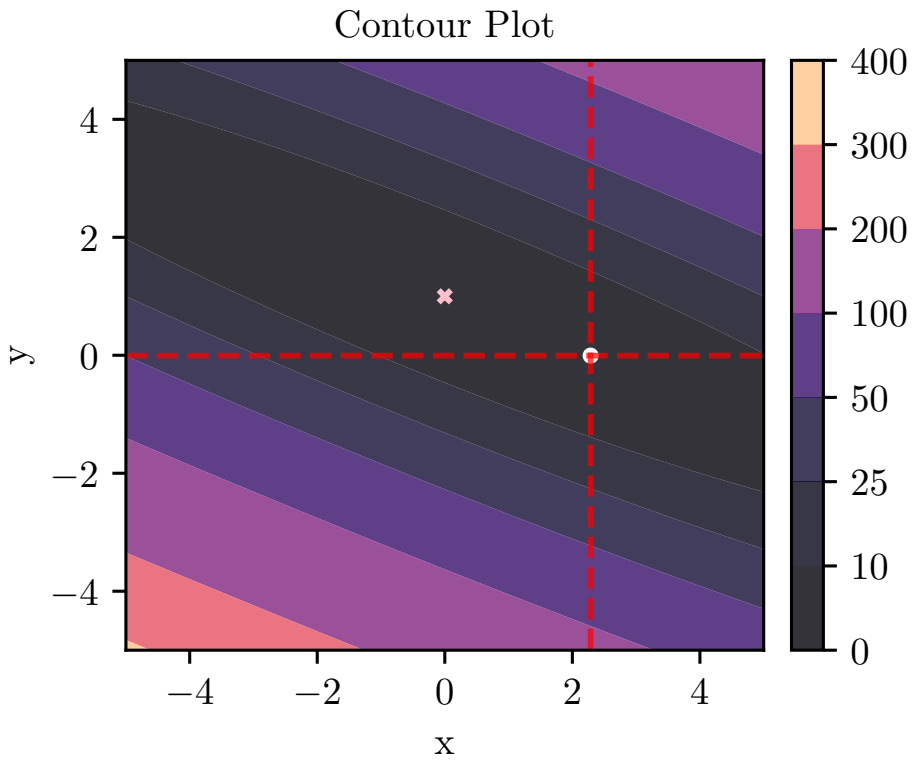



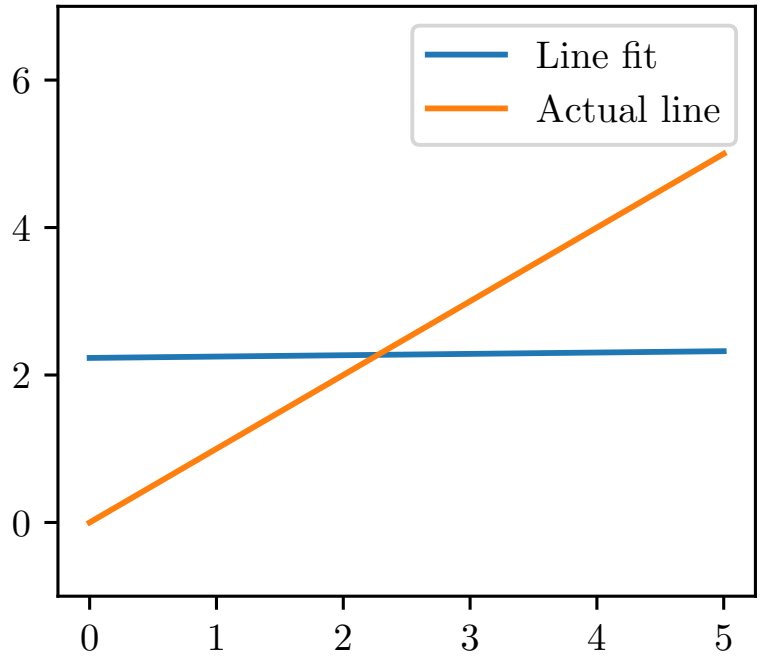
# Gradient Descent : Example (Iteraion 18)



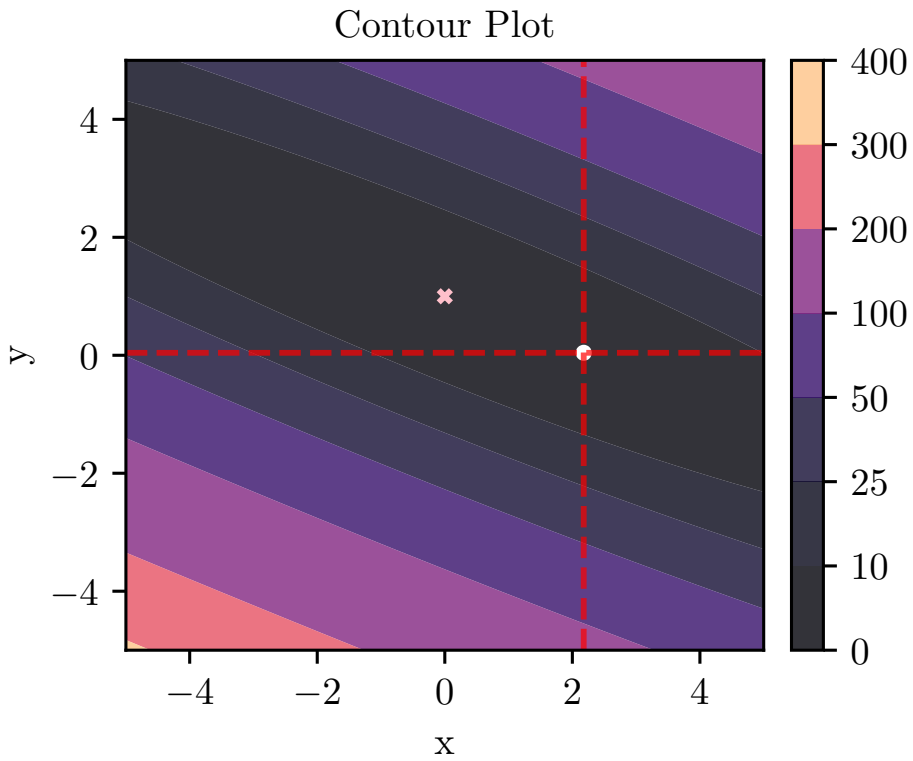



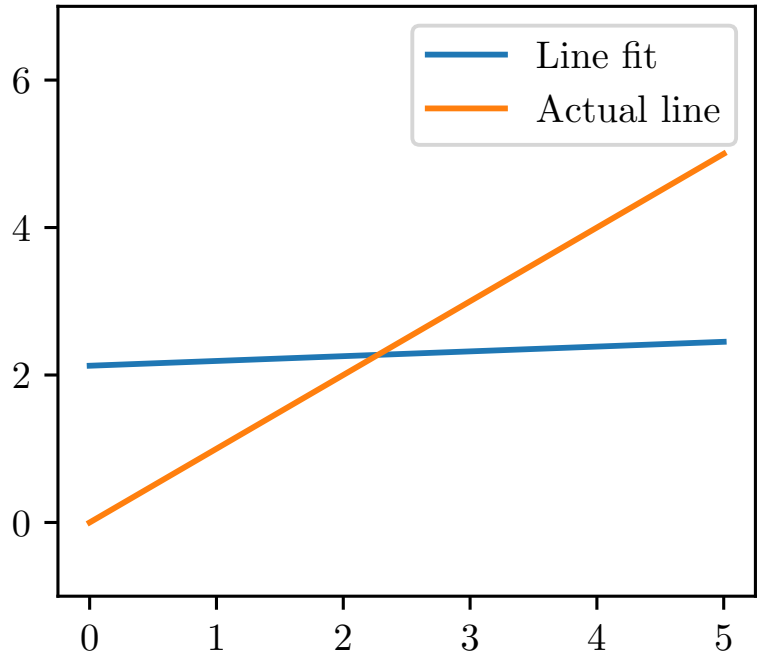
# Gradient Descent : Example (Iteraion 20)



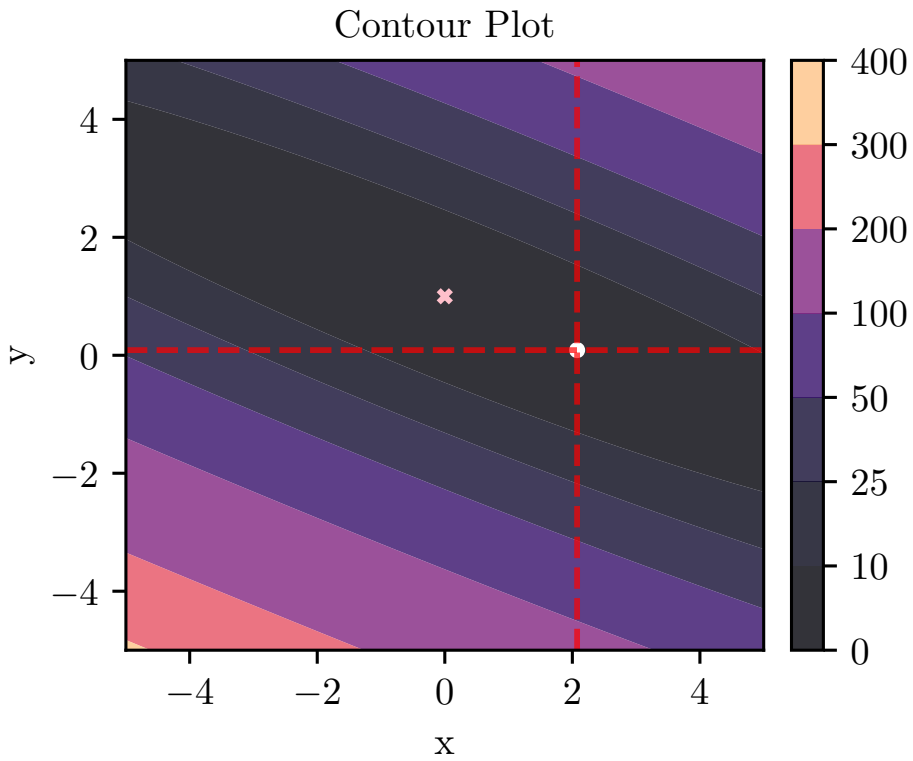



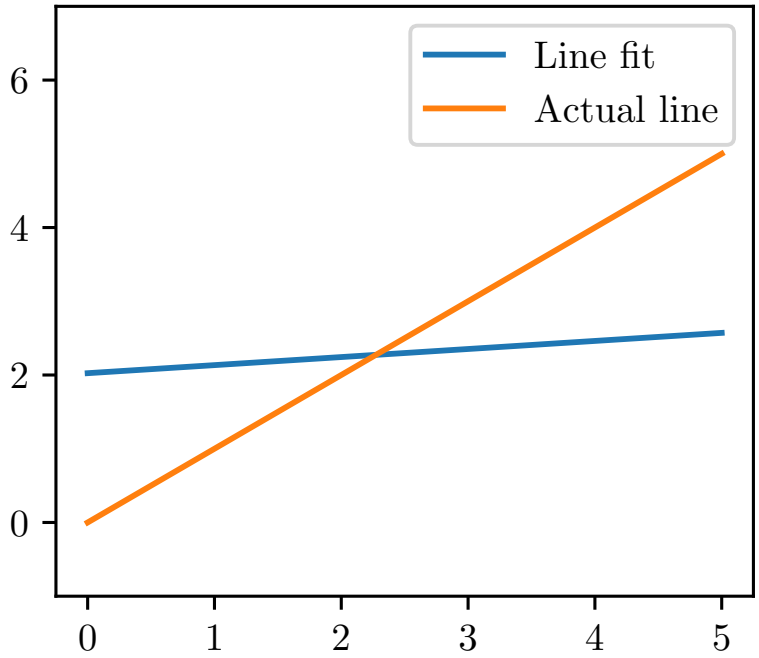
# Gradient Descent : Example (Iteraion 22)



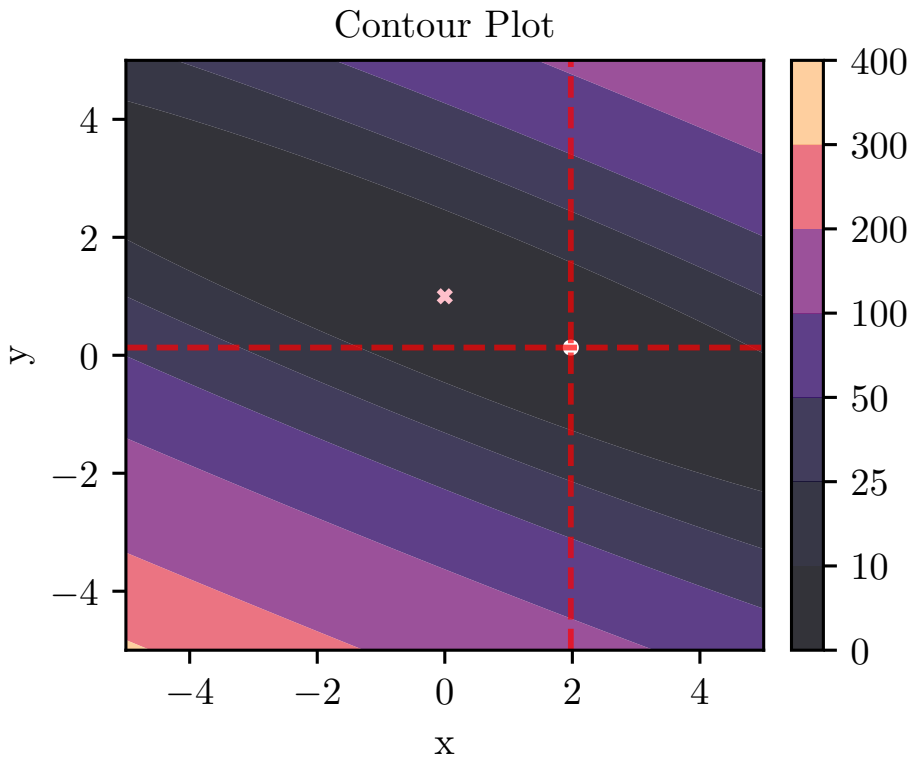



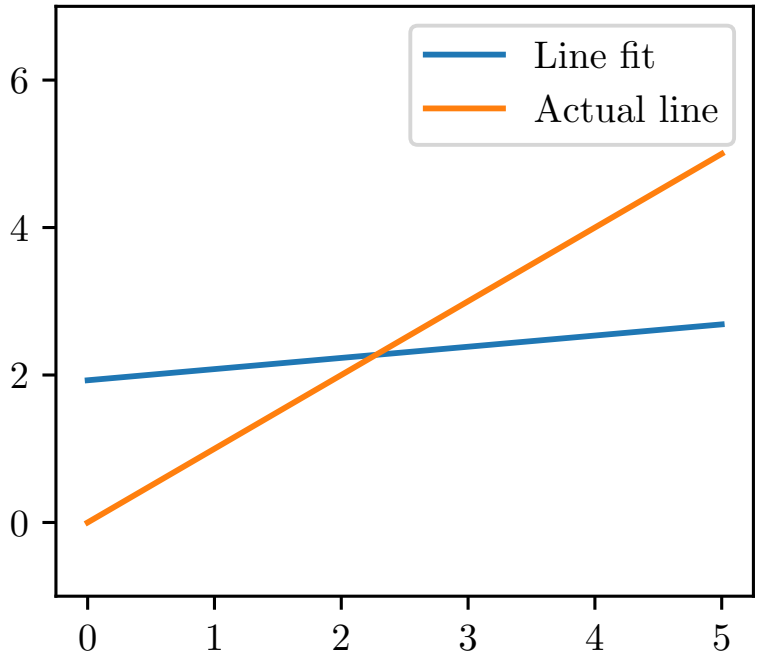
# Gradient Descent : Example (Iteraion 24)



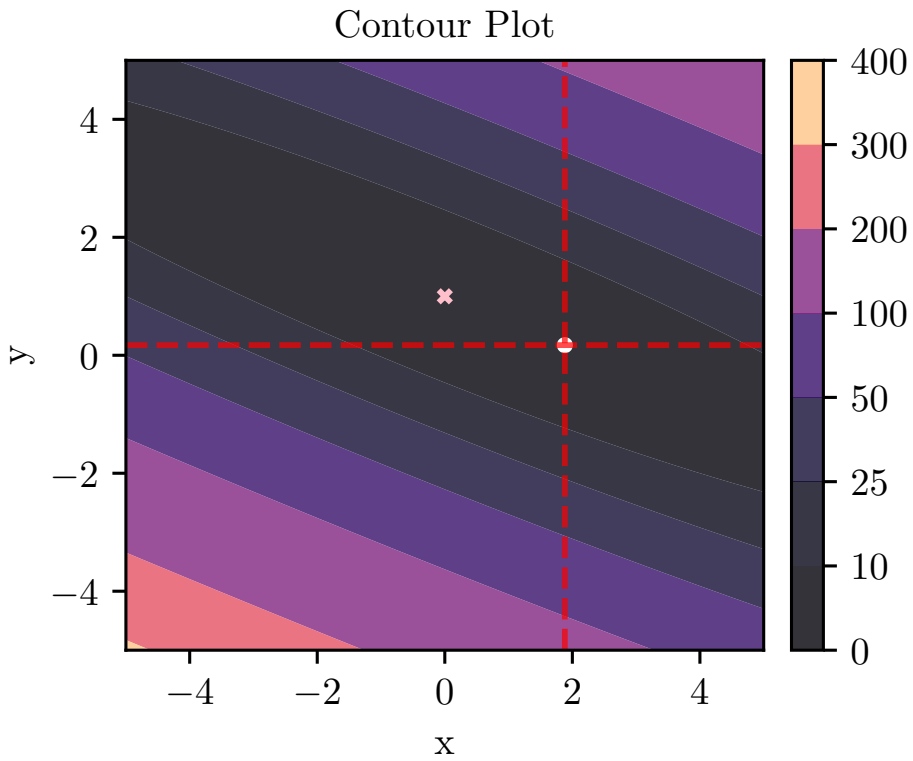



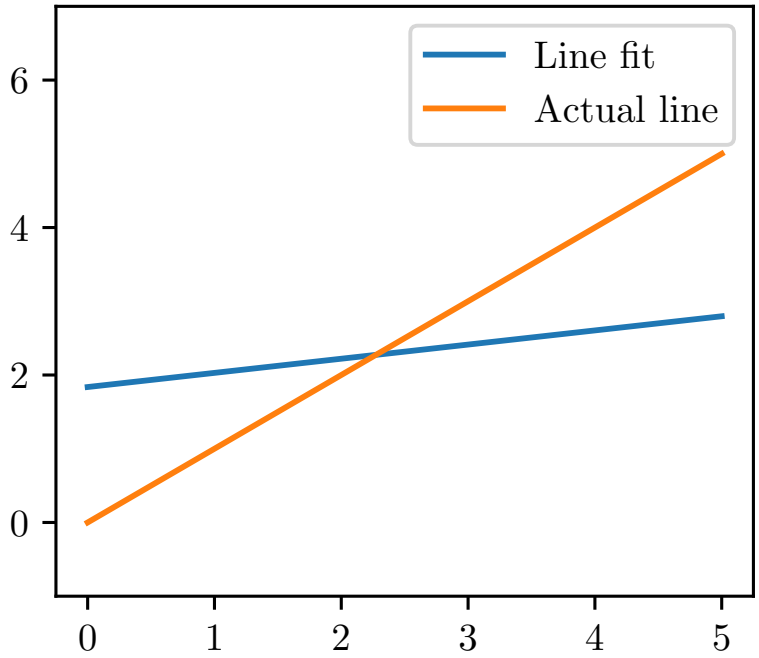
# Gradient Descent : Example (Iteraion 26)



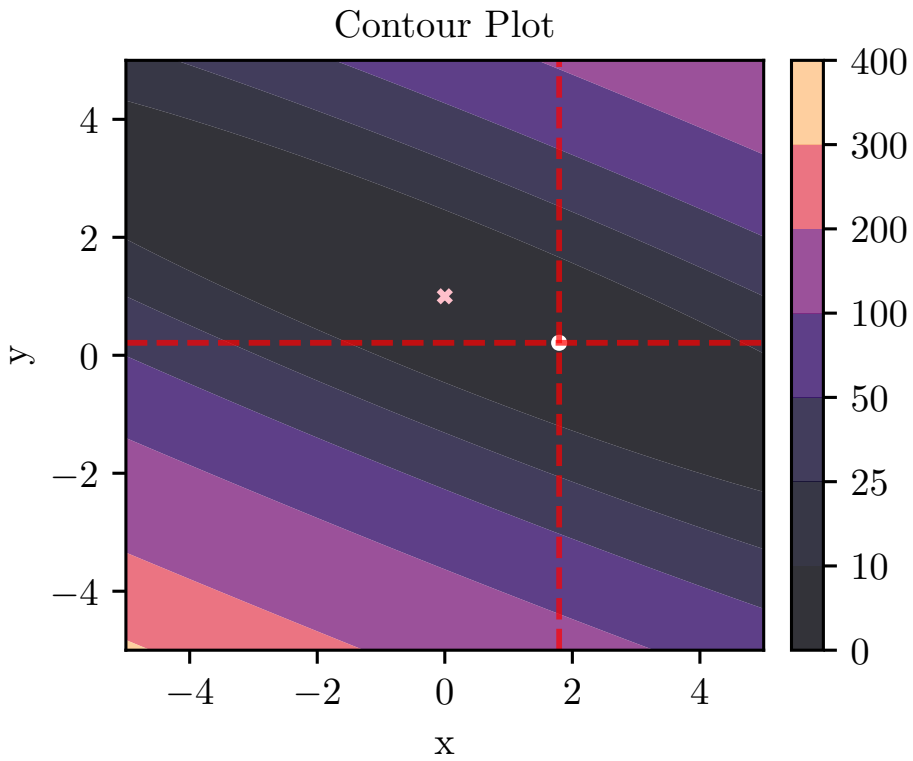



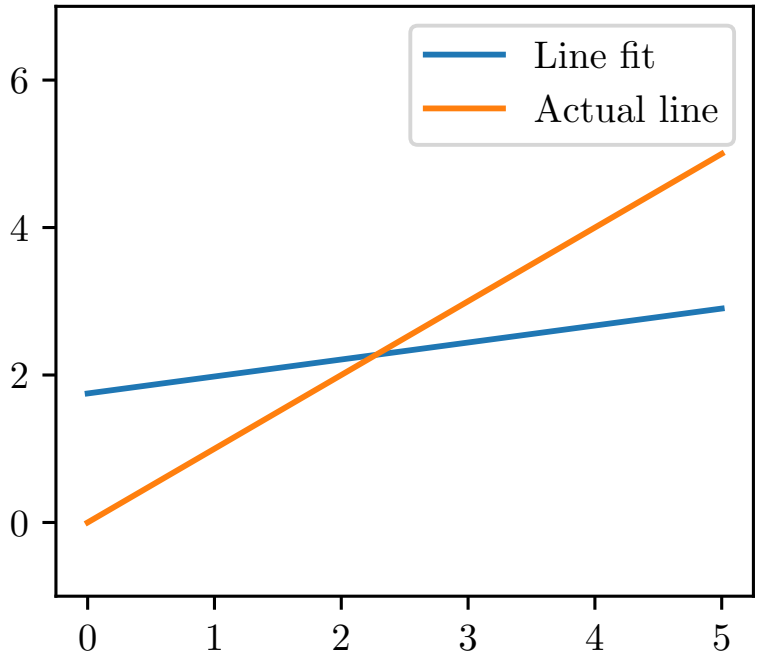
# Gradient Descent : Example (Iteraion 28)



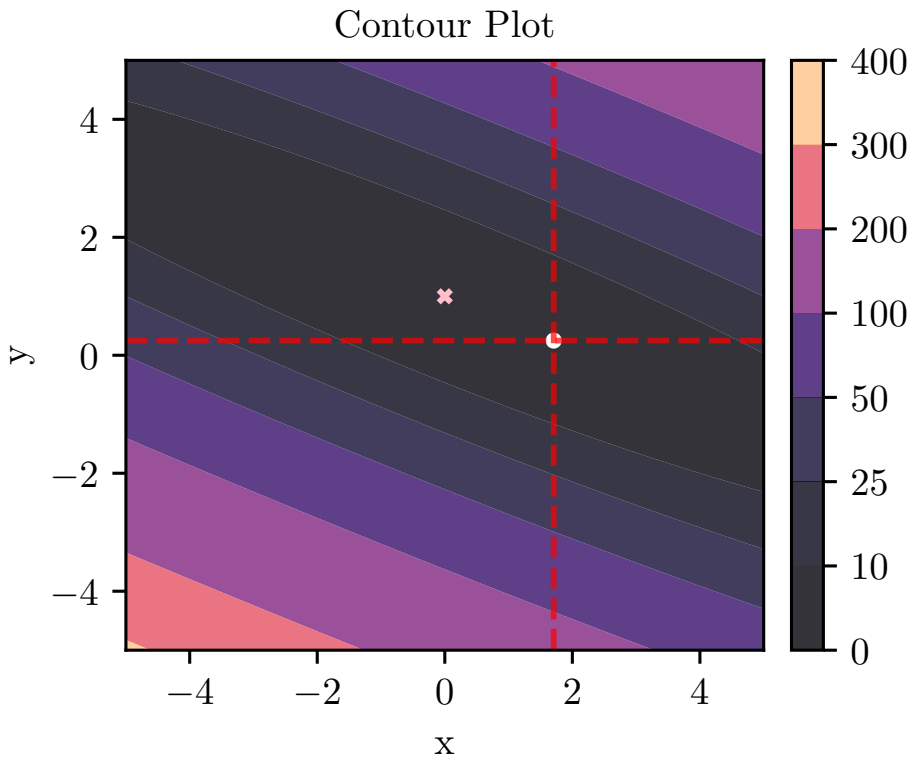



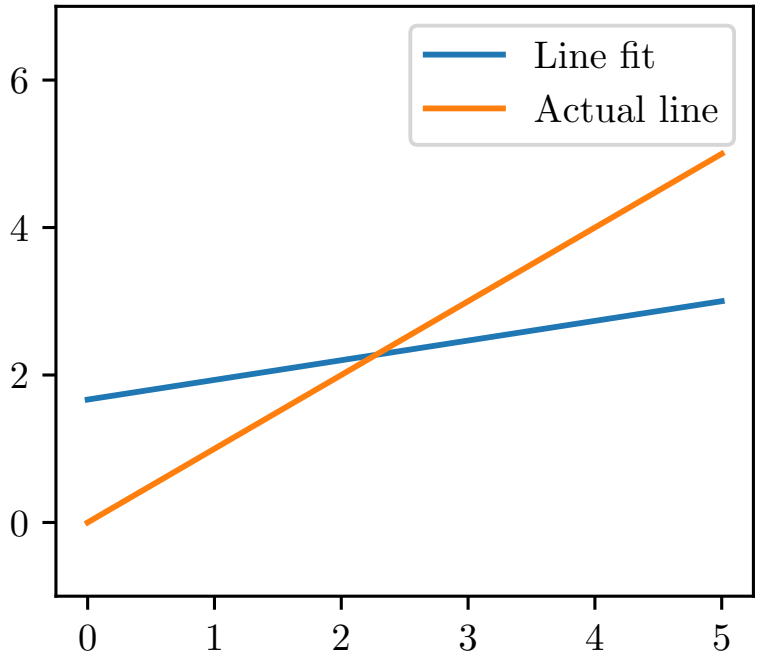
# Gradient Descent : Example (Iteraion 30)



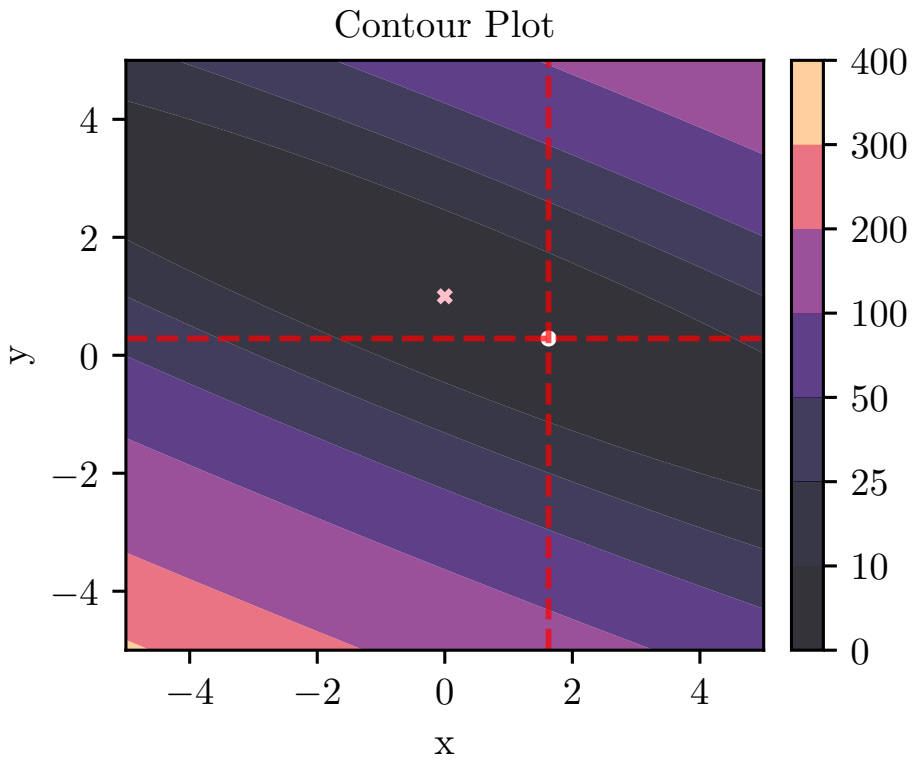



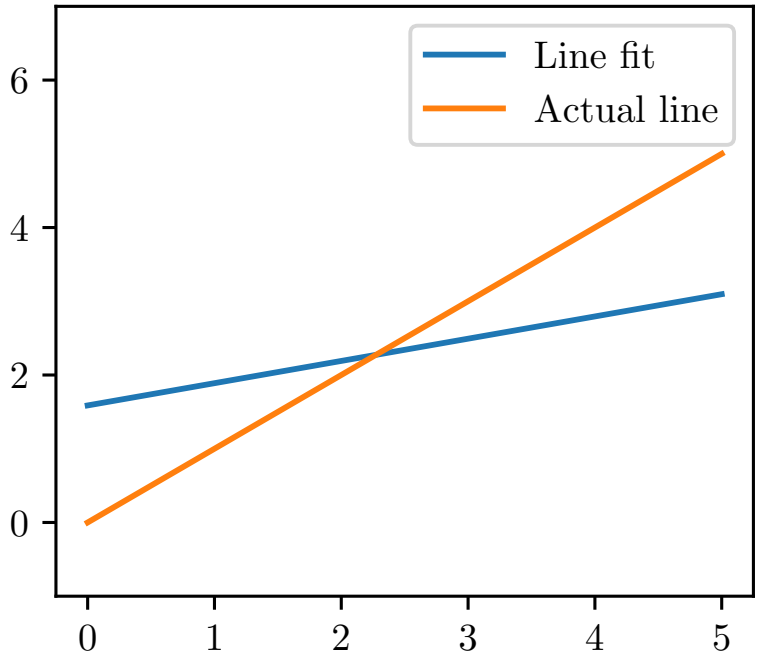
# Gradient Descent : Example (Iteraion 32)



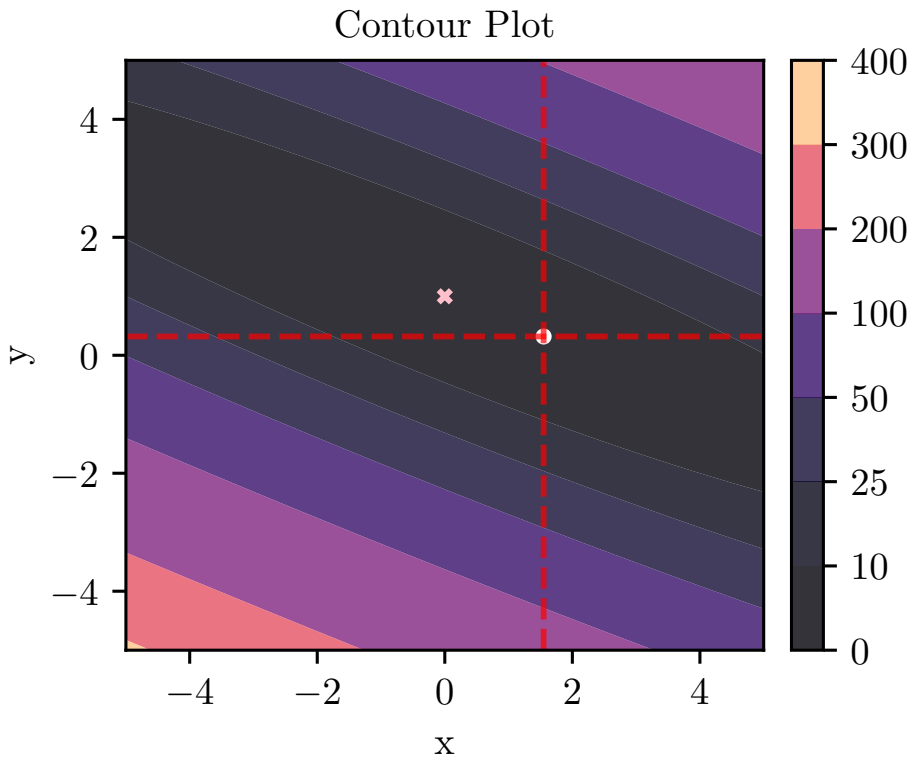



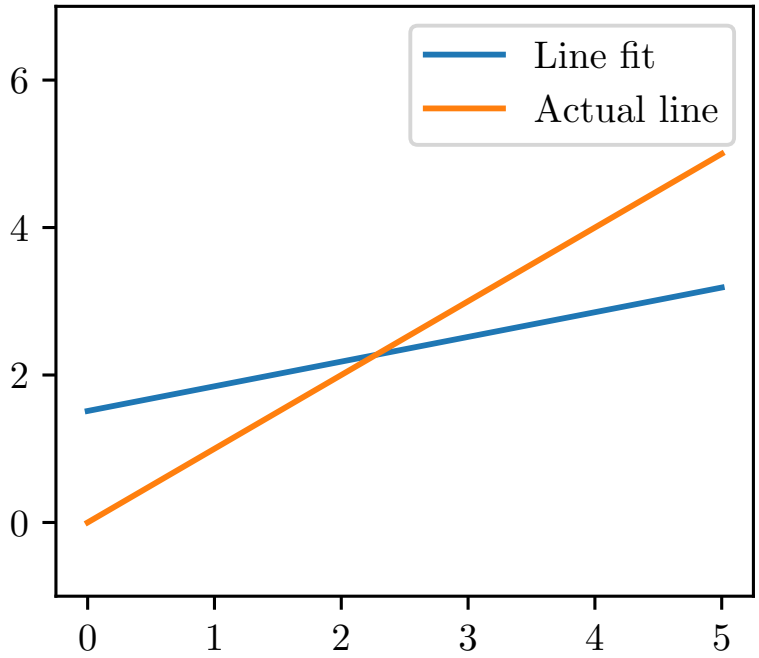
# Gradient Descent : Example (Iteraion 34)



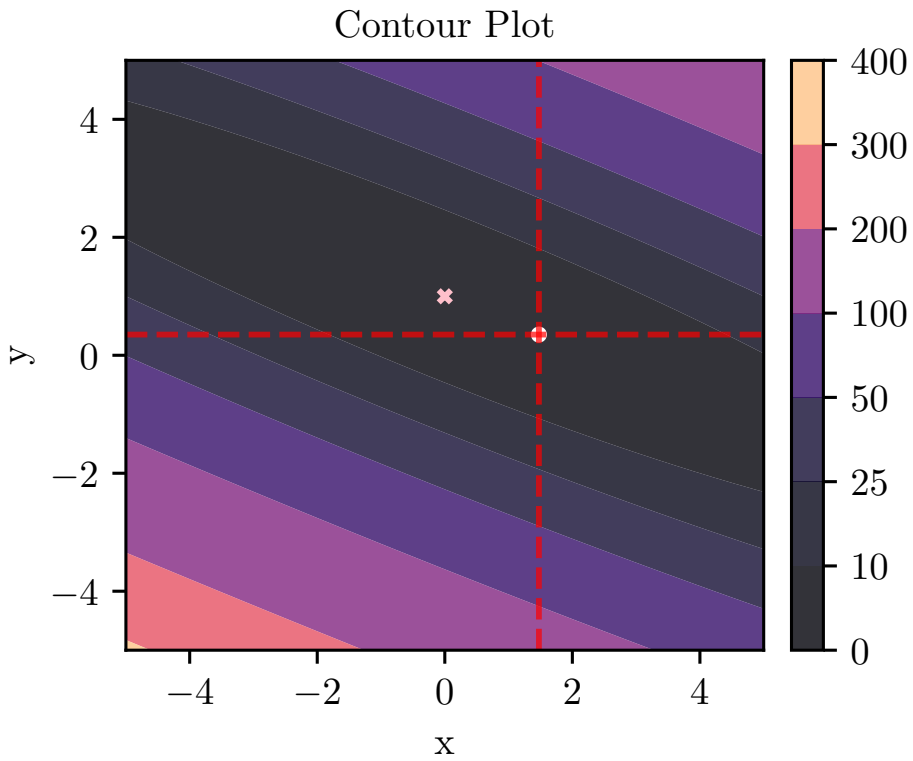



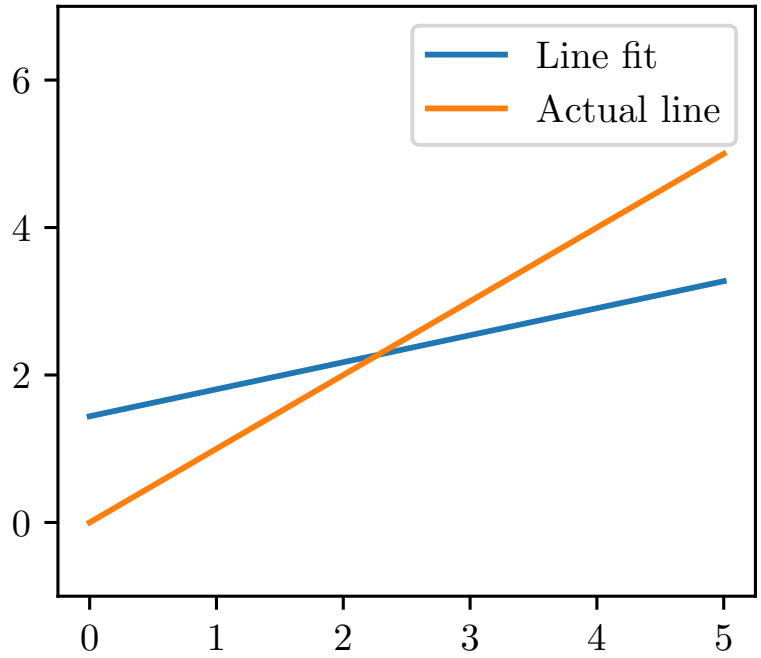
# Gradient Descent : Example (Iteraion 36)



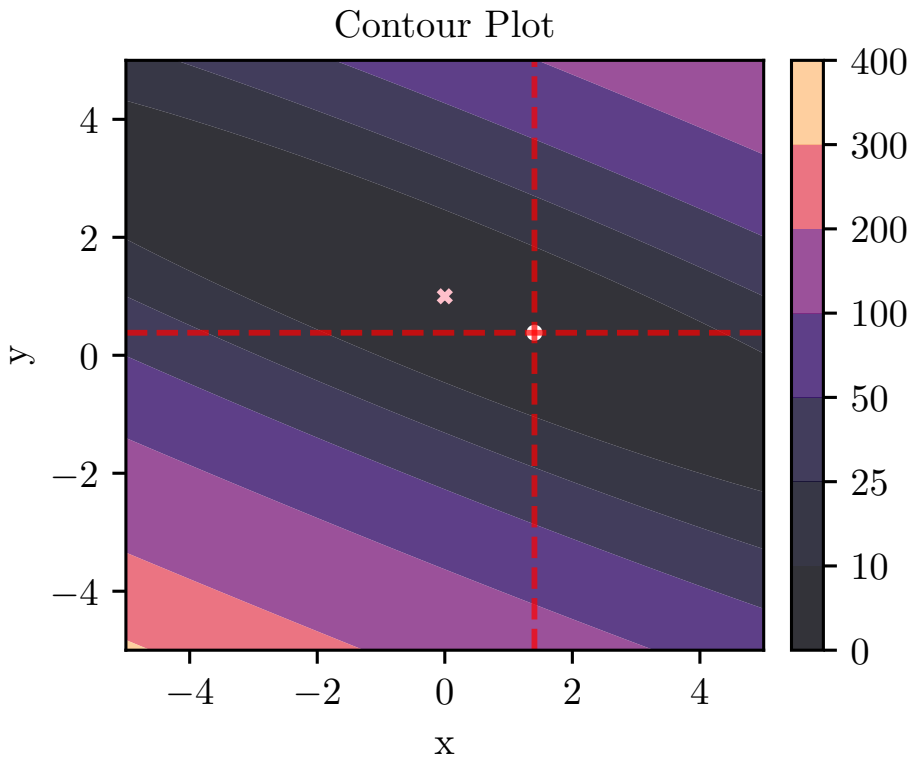



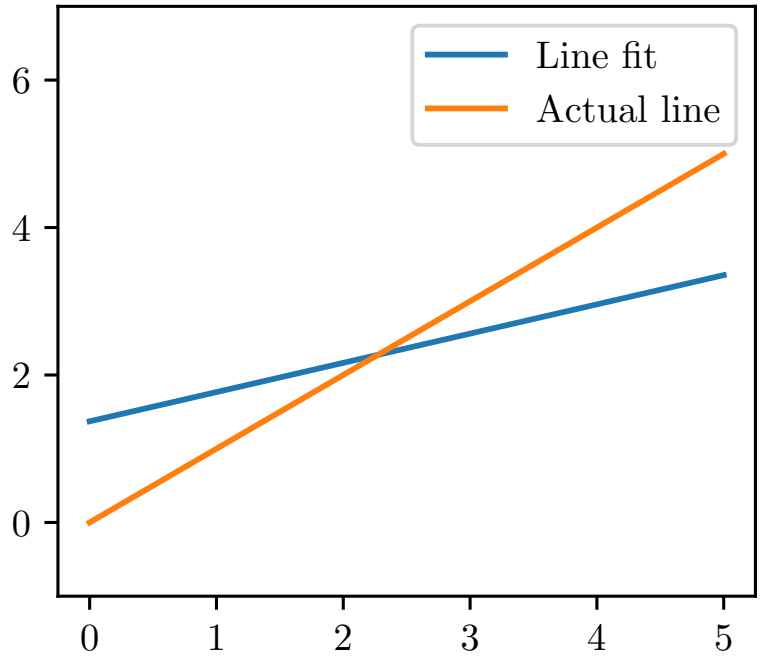
# Gradient Descent : Example (Iteraion 38)



# Gradient Descent : Example (Iteraion 40)



# Iteration v/s Epcohs for gradient descent

- Iteration: Each time you update the parameters of the model

# Iteration v/s Epcohs for gradient descent

- Iteration: Each time you update the parameters of the model
- Epoch: Each time you have seen all the set of examples

# Gradient Descent (GD)

- Dataset: $D = \{(X, y)\}$ of size $N$
- Initialize $\theta$
- For epoch $e$ in $[1, E]$
  - Predict $\hat{y} = \mathit{pred}(X, \theta)$
  - Compute loss: $J(\theta) = \mathit{loss}(y, \hat{y})$
  - Compute gradient: $\nabla J(\theta) = \mathit{grad}(J)(\theta)$
  - Update: $\theta = \theta - \alpha \nabla J(\theta)$

# Stochastic Gradient Descent (SGD)

- Dataset: $D = \{(X, y)\}$ of size $N$
- Initialize $\theta$
- For epoch $e$ in $[1, E]$
  - Shuffle $D$
  - For $i$ in $[1, N]$
    - Predict $\hat{y}_i = \mathit{pred}(X_i, \theta)$
    - Compute loss: $J(\theta) = \mathit{loss}(y_i, \hat{y}_i)$
    - Compute gradient: $\nabla J(\theta) = \mathit{grad}(J)(\theta)$
    - Update: $\theta = \theta - \alpha \nabla J(\theta)$

# Mini-Batch Gradient Descent (MBGD)

- Dataset: $D = \{(X, y)\}$ of size $N$
- Initialize $\theta$
- For epoch $e$ in $[1, E]$
  - Shuffle $D$
  - $Batches = make\_batches(D, B)$
  - For b in $Batches$
    - $X\_b, y\_b = b$
    - Predict $\hat{y\_b} = pred(X\_b, \theta)$
    - Compute loss: $J(\theta) = loss(y\_b, \hat{y\_b})$
    - Compute gradient: $\nabla J(\theta) = grad(J)(\theta)$
    - Update: $\theta = \theta - \alpha \nabla J(\theta)$

# Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data

# Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost

# Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost
- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

# Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost
- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

# Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost
- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

Stochastic Gradient Descent

- In SGD, we update parameters after seeing each each point

# Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost
- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

Stochastic Gradient Descent

- In SGD, we update parameters after seeing each each point
- Noisier curve for iteration vs cost

# Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost
- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

Stochastic Gradient Descent

- In SGD, we update parameters after seeing each each point
- Noisier curve for iteration vs cost
- For a single update, it computes the gradient over one example. Hence lesser time

# Stochastic Gradient Descent : Example

Learn $y = \theta_0 + \theta_1 x$ on following dataset, using SGD where initially $(\theta_0, \theta_1) = (4, 0)$ and step-size, $\alpha = 0.1$, for 1 epoch (3 iterations).

| x | y |
|---|---|
| 2 | 2 |
| 3 | 3 |
| 1 | 1 |

# Stochastic Gradient Descent : Example

Our predictor, $\hat{y} = \theta_0 + \theta_1 x$

Error for $i^{th}$ datapoint, $e_i = y_i - \hat{y}_i$

$\epsilon_1 = 2 - \theta_0 - 2\theta_1$

$\epsilon_2 = 3 - \theta_0 - 3\theta_1$

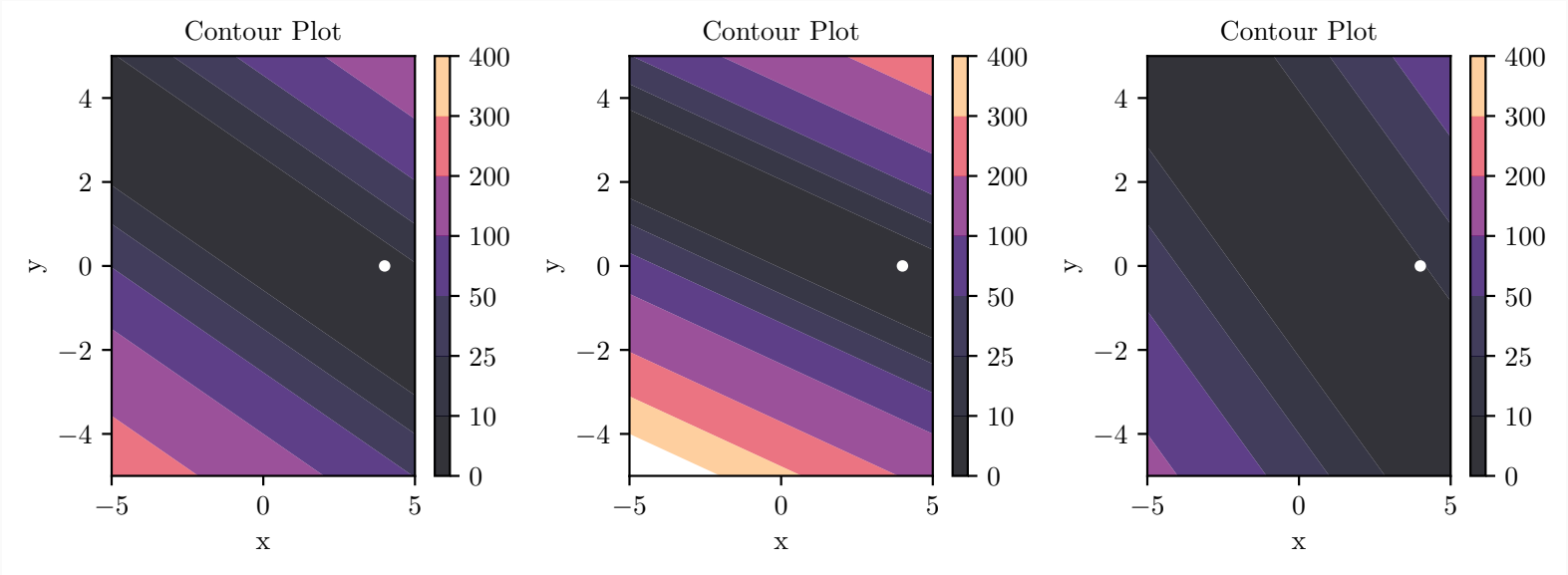
$\epsilon_3 = 1 - \theta_0 - \theta_1$

While using SGD, we compute the MSE using only 1 datapoint per iteration.

So MSE is $\epsilon_1^2$ for iteration 1 and $\epsilon_2^2$ for iteration 2.

# Stochastic Gradient Descent : Example

Contour plot of the cost functions for the three datapoints



# Stochastic Gradient Descent : Example

**For Iteration** $i$

$$\frac{\partial MSE}{\partial \theta_0} = 2\left(y_i - \theta_0 - \theta_1 x_i\right)(-1) = 2\epsilon_i\,(-1)$$

$$\frac{\partial MSE}{\partial \theta_1} = 2\left(y_i - \theta_0 - \theta_1 x_i\right)(-x_i) = 2\epsilon_i\,(-x_i)$$

# Stochastic Gradient Descent : Example

**Iteration 1**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

# Stochastic Gradient Descent : Example

**Iteration 1**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 4 - 0.1 \times 2 \times (2 - (4 + 0))\,(-1)$$

$$\theta_0 = 3.6$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

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$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

$$\theta_1 = 0 - 0.1 \times 2 \times (2 - (4 + 0))(-2)$$

$$\theta_1 = -0.8$$

# Stochastic Gradient Descent : Example

**Iteration 2**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

# Stochastic Gradient Descent : Example

**Iteration 2**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.6 - 0.1 \times 2 \times (3 - (3.6 - 0.8 \times 3))(-1)$$

$$\theta_0 = 3.96$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

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$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

$$\theta_0 = -0.8 - 0.1 \times 2 \times (3 - (3.6 - 0.8 \times 3))(-3)$$

$$\theta_1 = 0.28$$

# Stochastic Gradient Descent : Example

**Iteration 3**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

# Stochastic Gradient Descent : Example

**Iteration 3**

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.96 - 0.1 \times 2 \times (1 - (3.96 + 0.28 \times 1))(-1)$$

$$\theta_0 = 3.312$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

# Stochastic Gradient Descent : Example

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$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

$$\theta_0 = 0.28 - 0.1 \times 2 \times (1 - (3.96 + 0.28 \times 1))(-1)$$

$$\theta_1 = -0.368$$

# Stochastic gradient is an unbiased estimator of the true gradient

# True Gradient

Based on Estimation Theory and Machine Learning by Florian Hartmann

- Let us say we have a dataset $\mathcal{D}$ containing input output pairs $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$

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$$L(\theta) = \frac{1}{N} \sum_{i=1}^{N} loss(f(x_i, \theta), y_i)$$

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- loss can be any loss function such as squared loss, cross-entropy loss etc.

$$loss(f(x_i, \theta), y_i) = (f(x_i, \theta) - y_i)^2$$

# Time Complexity: Gradient Descent v/s Normal Equation for Linear Regression

# Normal Equation

- Consider $X \in \mathcal{R}^{N \times D}$

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- $N$ examples and $D$ dimensions

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- Consider $X \in \mathcal{R}^{N \times D}$
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- Scales cubic in the number of columns/features of $X$

# Gradient Descent

Start with random values of $\theta_0$ and $\theta_1$

Till convergence

- $\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} (\sum \epsilon_i^2)$

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- Question: Can you write the above for $D$ dimensional data in vectorised form?
- $\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} (y - X\theta)^\top (y - X\theta)$
  $\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} (y - X\theta)^\top (y - X\theta)$
  $\vdots$
  $\theta_D = \theta_D - \alpha \frac{\partial}{\partial \theta_D} (y - X\theta)^\top (y - X\theta)$

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- $\theta = \theta - \alpha \frac{\partial}{\partial \theta} (y - X\theta)^\top (y - X\theta)$

# Gradient Descent

$$
\begin{aligned}
&\frac{\partial}{\partial \theta}(y - X\theta)^\top (y - X\theta) \\
&= \frac{\partial}{\partial \theta}\left(y^\top - \theta^\top X^\top\right)(y - X\theta) \\
&= \frac{\partial}{\partial \theta}\left(y^\top y - \theta^\top X^\top y - y^\top x\theta + \theta^\top X^\top X\theta\right) \\
&= -2X^\top y + 2X^\top x\theta \\
&= 2X^\top (X\theta - y)
\end{aligned}
$$

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All of the above need only be calculated once!

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For each of the $t$ iterations, we now need to first multiply $\alpha X^\top X$ with $\theta$ which is matrix multiplication of a $D \times D$ matrix with a $D \times 1$, which is $\mathcal{O}(D^2)$

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$\mathcal{O}(tD^2) + \mathcal{O}(D^2N) = \mathcal{O}((t+N)D^2)$

# Gradient Descent (Alternative)

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If we do not rewrite the expression $\theta = \theta - \alpha X^\top (X\theta - y)$

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$\mathcal{O}(NDt)$