Gradient Descent

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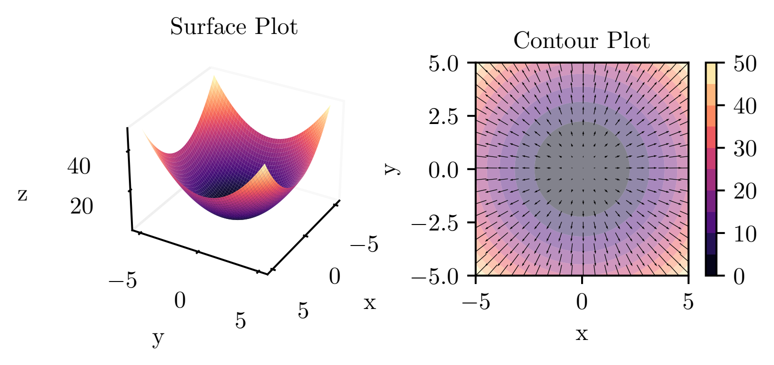
Revision

Contour Plot And Gradients

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



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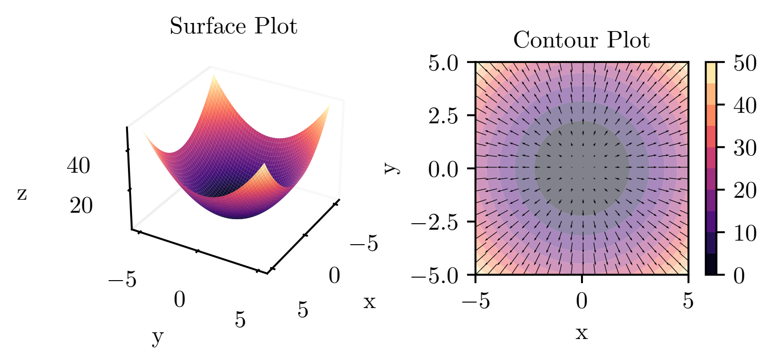

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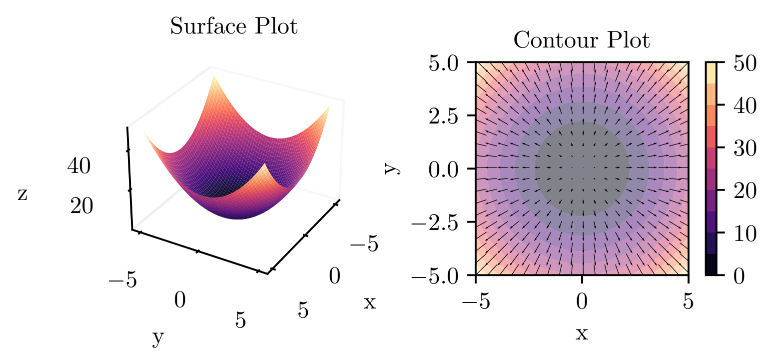

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$$\nabla f(x, y) = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

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- Goal:

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

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- It is a first order optimization algorithm
- It is a local search algorithm/greedy

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    - $\theta_i \leftarrow \theta_{i-1} - \alpha \nabla f(\theta_{i-1})$

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- The vector form of the above equation is given by:

$$f(\vec{x}) = f(\vec{x_0}) + \nabla f(\vec{x_0})^T(\vec{x} - \vec{x_0}) + \frac{1}{2}(\vec{x} - \vec{x_0})^T \nabla^2 f(\vec{x_0})(\vec{x} - \vec{x_0}) + \dots \quad (4)$$

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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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- First order Taylor's series approximation is given by:
- $f(x) = f(x_0) + f'(x_0)(x - x_0) = 6 + 4(x - 2) = 4x - 2$

Taylor's Series (Alternative form)

- We have:

$$f(x) = f(x_0) + \frac{f'(x_0)}{1!}(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \dots \quad (5)$$

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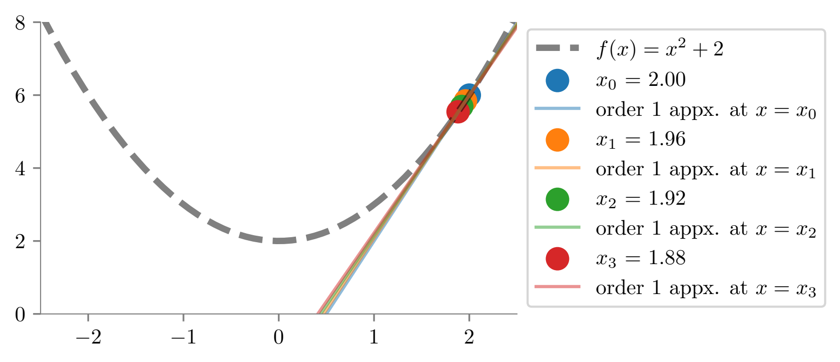
- This happens when $\Delta\vec{x} = -\alpha\nabla f(\vec{x_0})$ where α is a scalar
- This is the gradient descent algorithm: $\vec{x_1} = \vec{x_0} - \alpha\nabla f(\vec{x_0})$

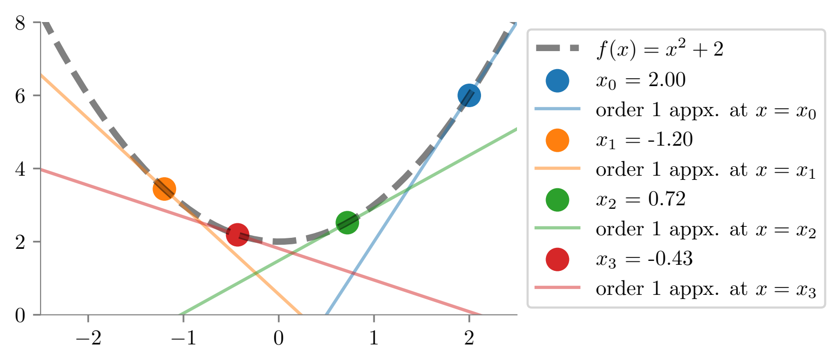
Effect of learning rate

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



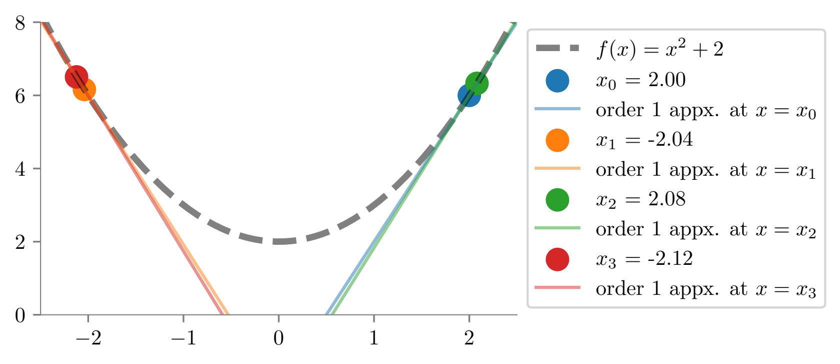
Effect of learning rate

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



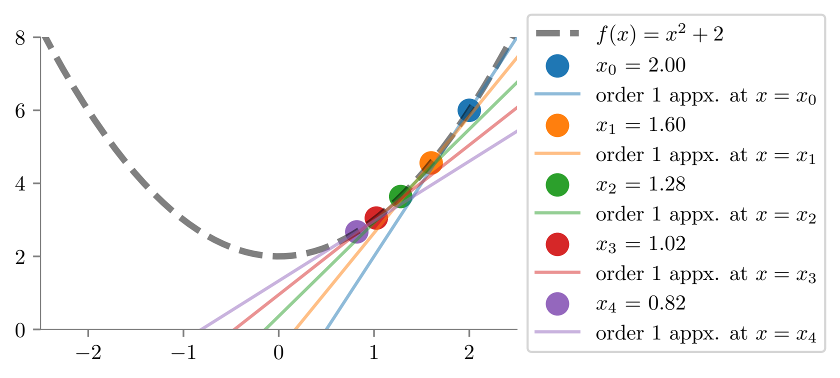
Effect of learning rate

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

$$\theta_1 = -0.67$$

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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Gradient Descent : Example

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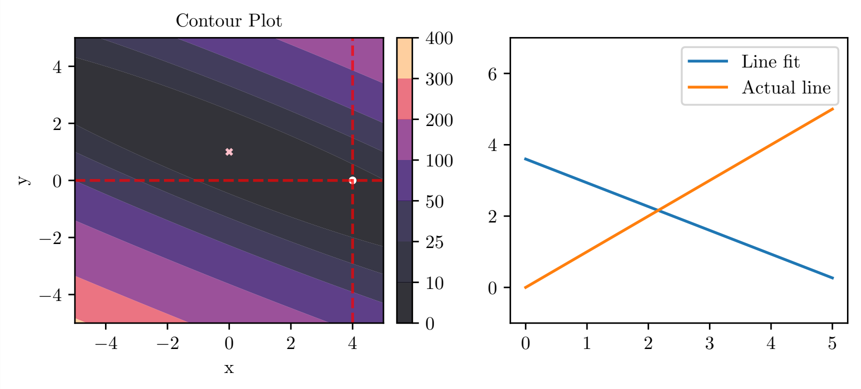
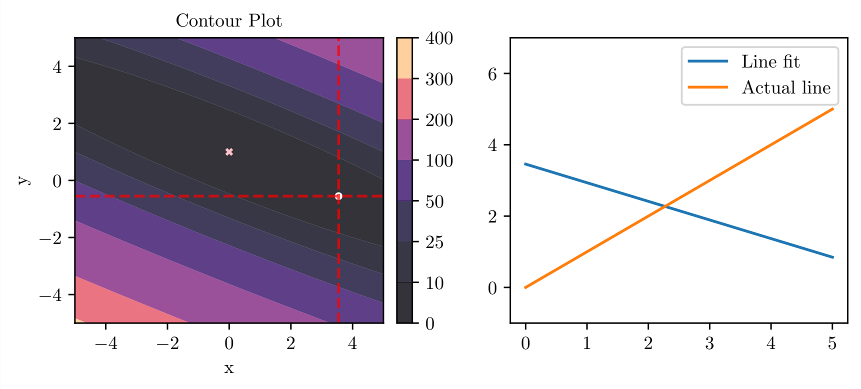
$$\theta_0 = -0.55$$

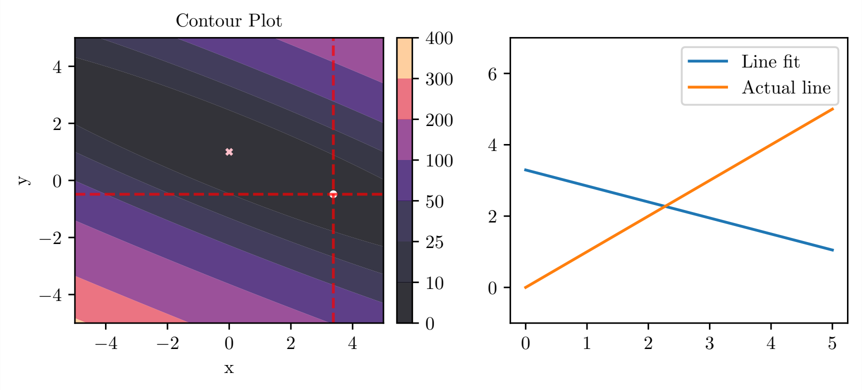
Gradient Descent : Example (Iteraion 0)



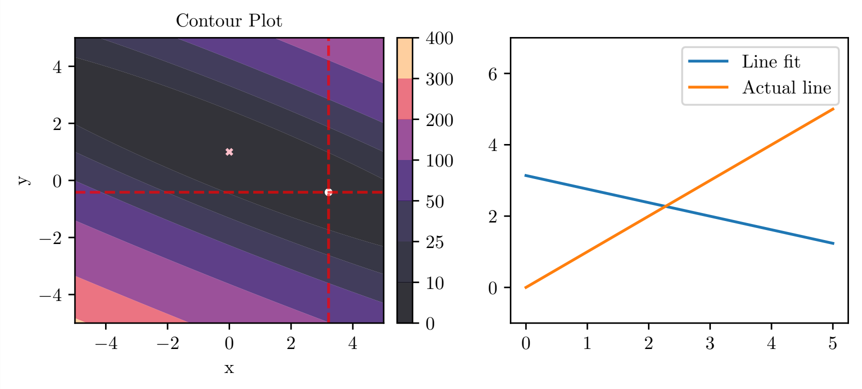
Gradient Descent : Example (Iteraion 2)



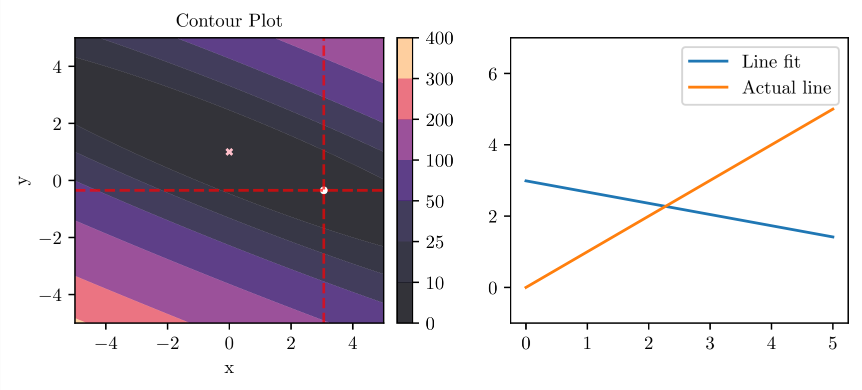
Gradient Descent : Example (Iteraion 4)



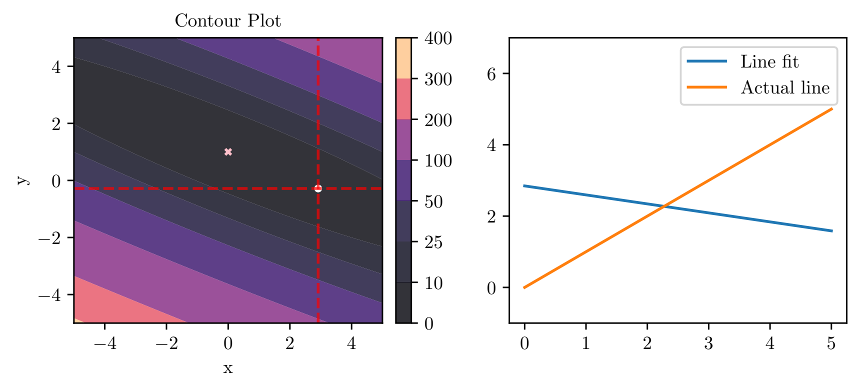
Gradient Descent : Example (Iteraion 6)



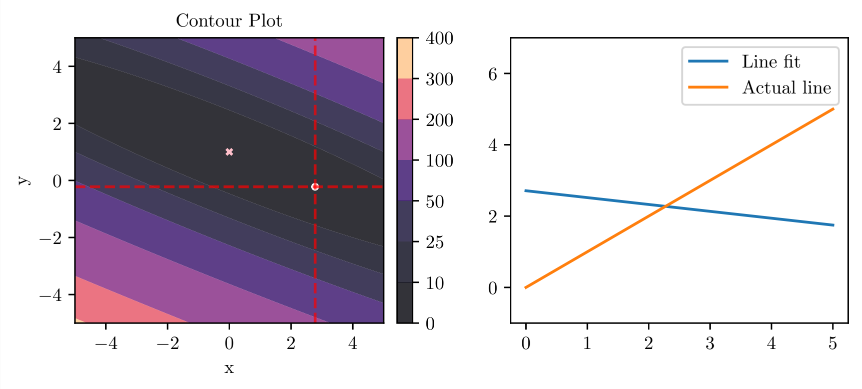
Gradient Descent : Example (Iteraion 8)



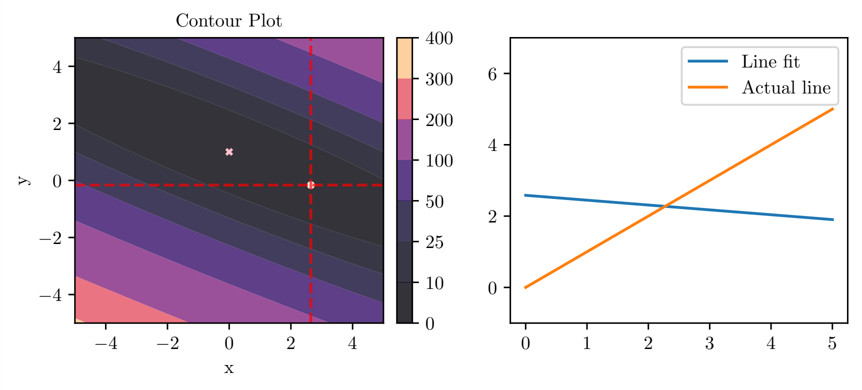
Gradient Descent : Example (Iteraion 10)



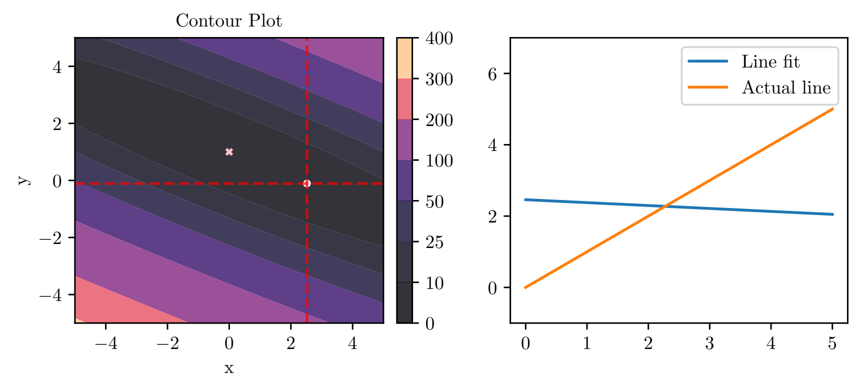
Gradient Descent : Example (Iteraion 12)



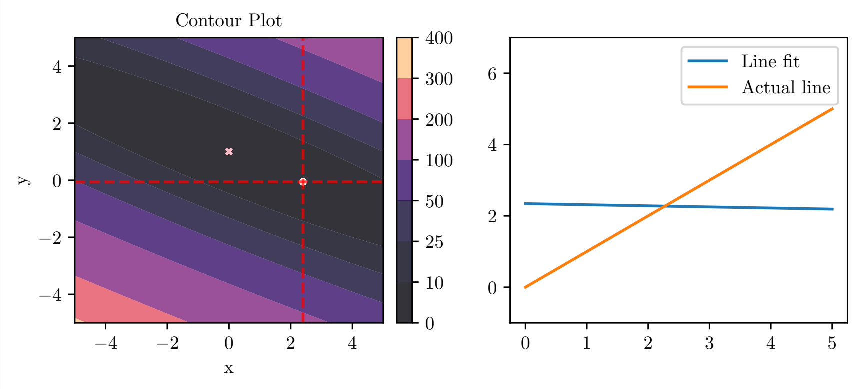
Gradient Descent : Example (Iteraion 14)



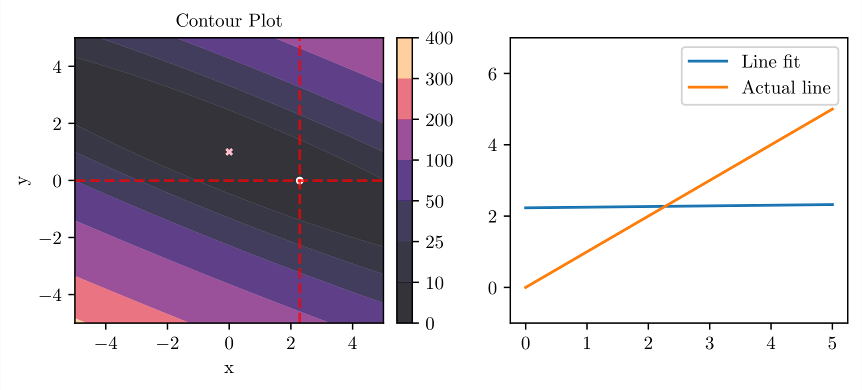
Gradient Descent : Example (Iteraion 16)



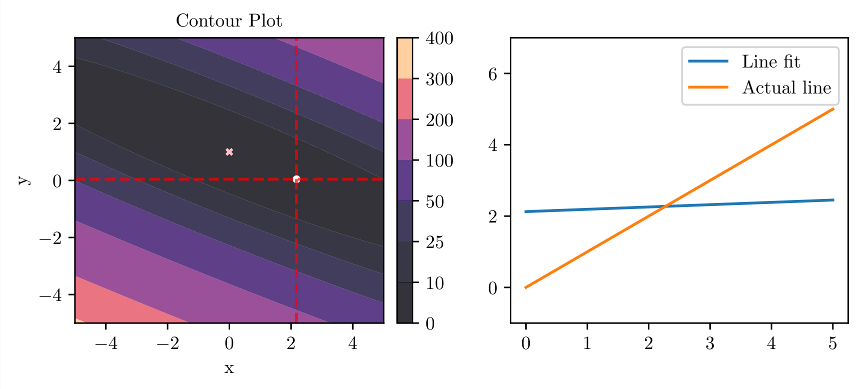
Gradient Descent : Example (Iteraion 18)



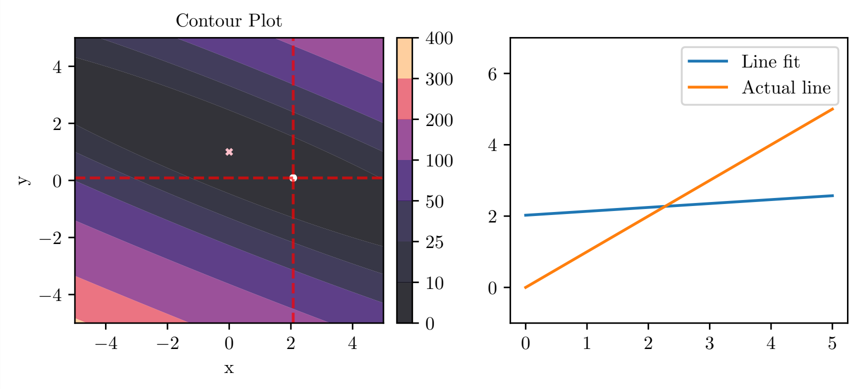
Gradient Descent : Example (Iteraion 20)



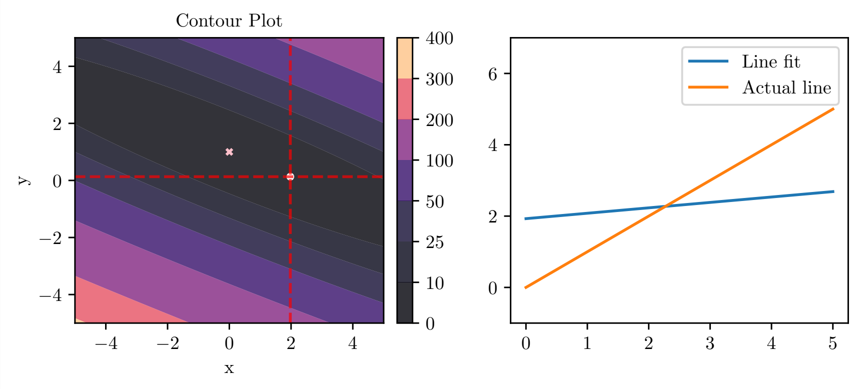
Gradient Descent : Example (Iteraion 22)



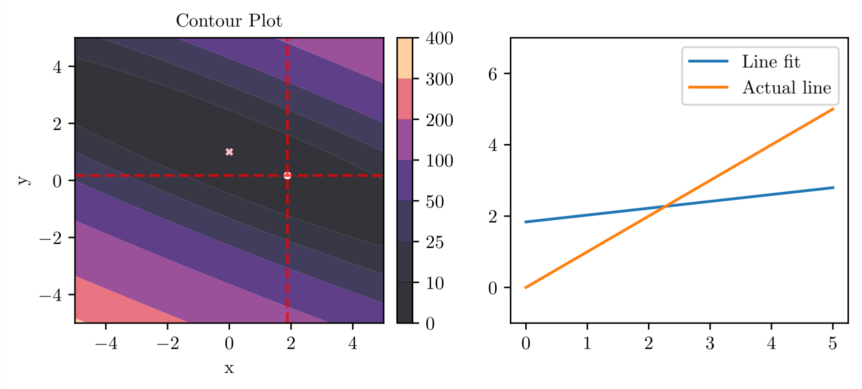
Gradient Descent : Example (Iteraion 24)



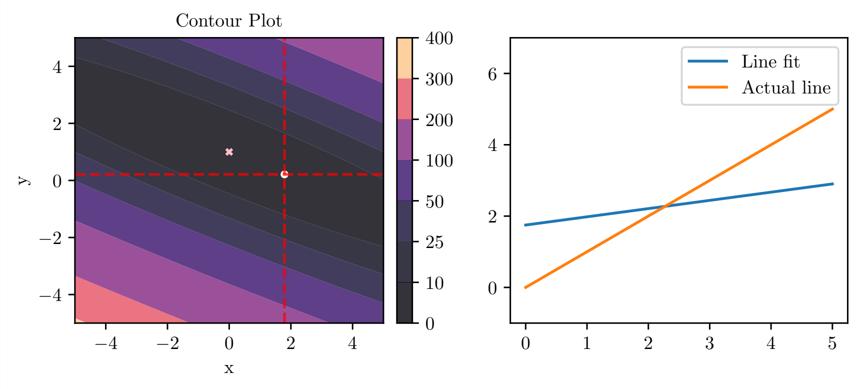
Gradient Descent : Example (Iteraion 26)



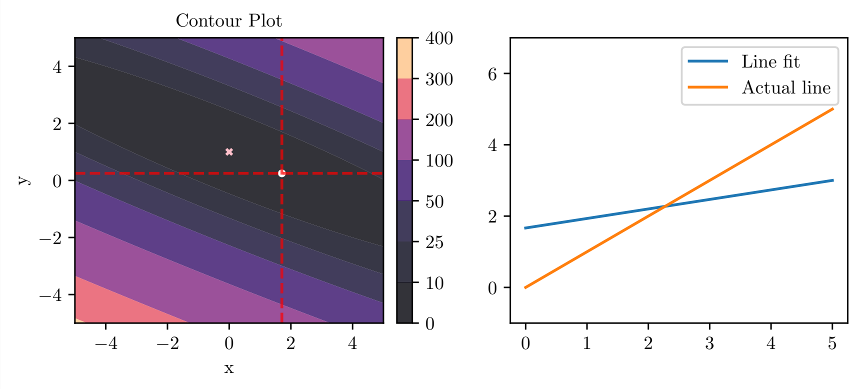
Gradient Descent : Example (Iteraion 28)



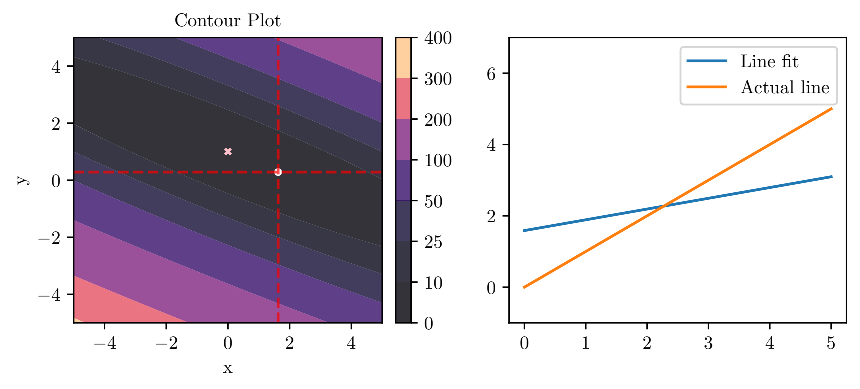
Gradient Descent : Example (Iteraion 30)



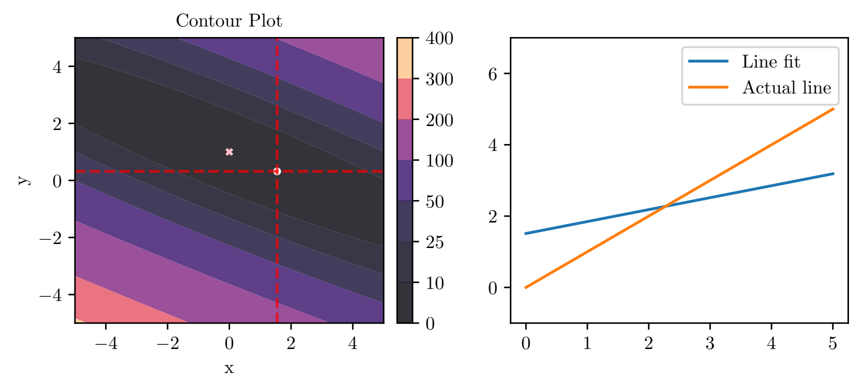
Gradient Descent : Example (Iteraion 32)



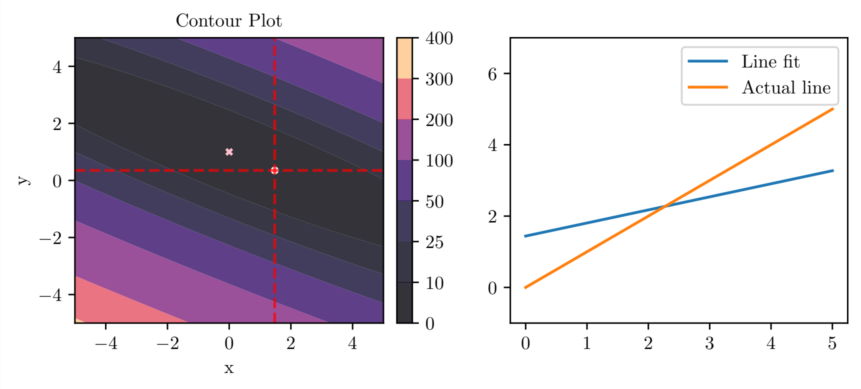
Gradient Descent : Example (Iteraion 34)



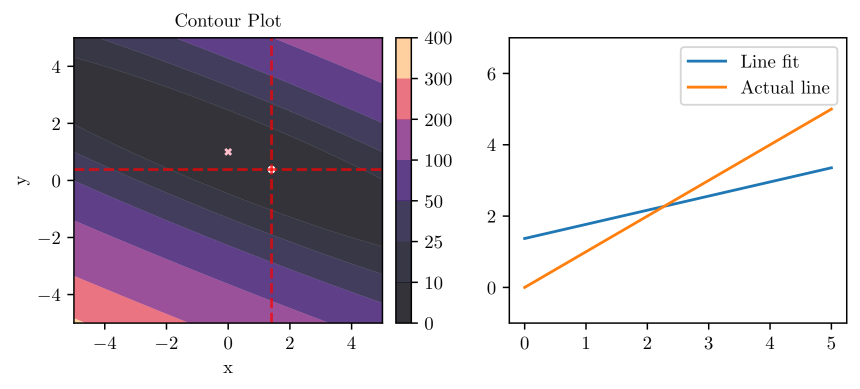
Gradient Descent : Example (Iteraion 36)



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

Stochastic Gradient Descent (SGD)

- Dataset: $D = \{(X, y)\}$ of size N
- Initialize θ
- 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 θ
- 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

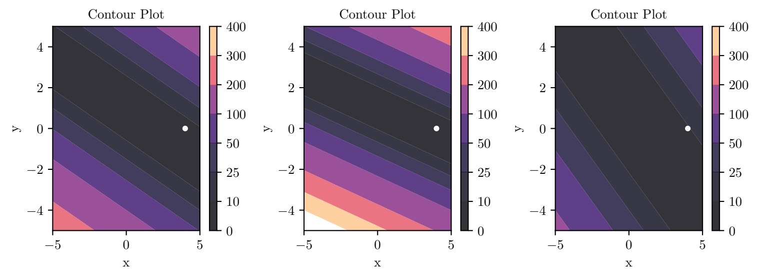
Our predictor, $\hat{y} = \theta_0 + \theta_1 x$

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 ϵ_1^2 for iteration 1 and ϵ_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

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

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

$$\theta_0 = 3.6$$

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

Stochastic Gradient Descent : Example

Iteration 1

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

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

$$\theta_0 = 3.6$$

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

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

$$\theta_1 = -0.8$$

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

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

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

$$\theta_0 = 3.96$$

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

Stochastic Gradient Descent : Example

Iteration 2

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

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

$$\theta_0 = 3.96$$

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

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

$$\theta_1 = 0.28$$

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

Iteration 3

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

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

$$\theta_0 = 3.312$$

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

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

$$\theta_1 = -0.368$$