Aprendizado de Máquina e Reconhecimento de Padrões 2021.2

Linear Regression and Gradient Descent

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São Paulo
Campus Campinas

Notations

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These are the notations ˙ that we will use throughout this course:

housing median age	population	median income	housing price
10	546	76000.0	162500.0
7	6274	244970.0	90900.0
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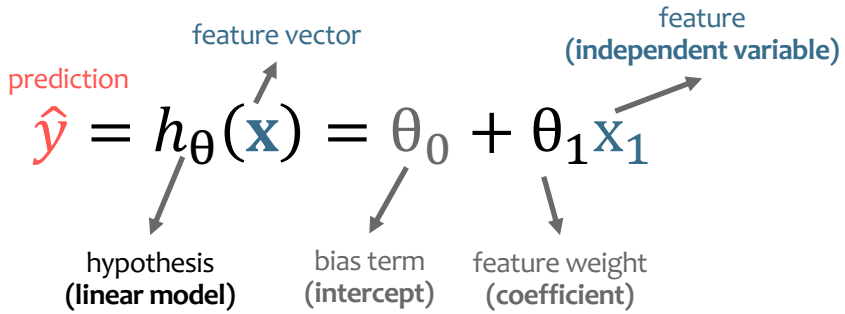
Remember that Python indexes **start at 0.**

Linear Regression

Linear Regression

- An **linear** approach for modeling the **relationship** between **independent (explanatory) variables** and a **numerical dependent variable** by fitting a **linear model** (*e.g.*,, a straight line) to the observations of a training set.
- Such a linear model is used **to predict** **numerical dependent variables** for new observations (unseen data).

Simple Linear Regression



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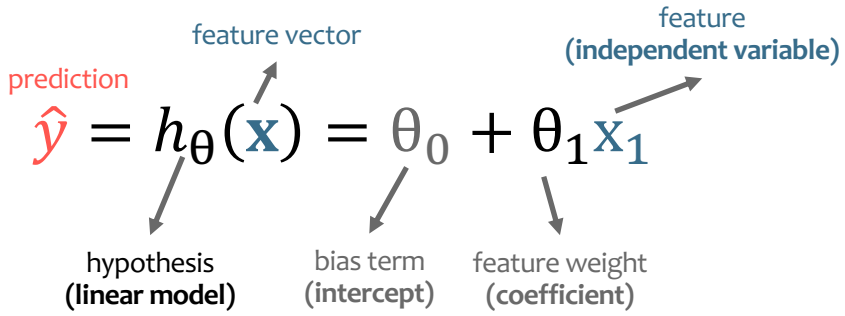

median income	housing price
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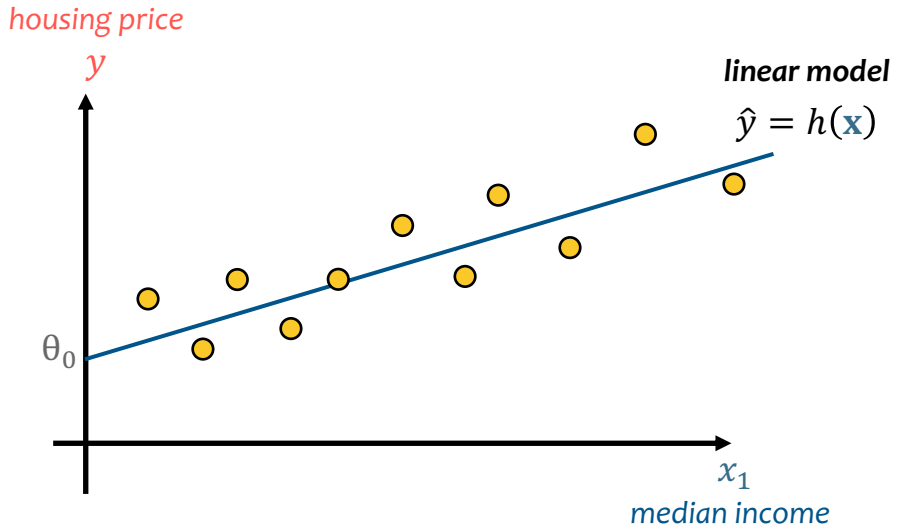
...	...



Simple Linear Regression

$$\hat{y} = h_{\theta}(\mathbf{x}) = \theta_0 + \theta_1 x_1$$

- $\hat{y}$: prediction
- $\mathbf{x}$: feature vector
- x_1: feature (independent variable)
- h_{θ}: hypothesis (linear model)
- θ_0: bias term (intercept)
- θ_1: feature weight (coefficient)

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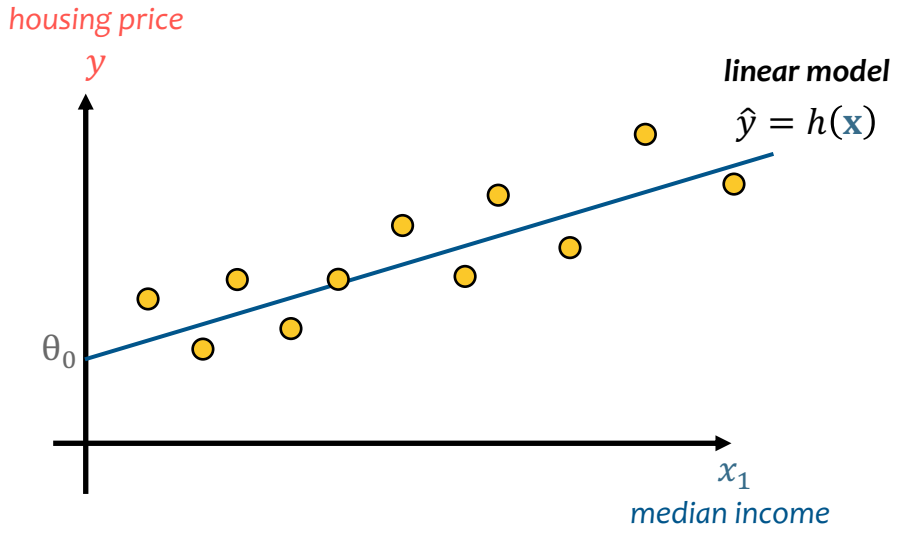

Multiple Linear Regression

$$\hat{y} = h_{\theta}(\mathbf{x}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

- $\hat{y}$: prediction
- $\mathbf{x}$: feature vector
- $x_1, x_2, \ldots, x_n$: features (independent variables)
- h_{θ}: hypothesis (linear model)
- θ_0: bias term (intercept)
- $\theta_1, \theta_2, \ldots, \theta_n$: feature weights (coefficients)

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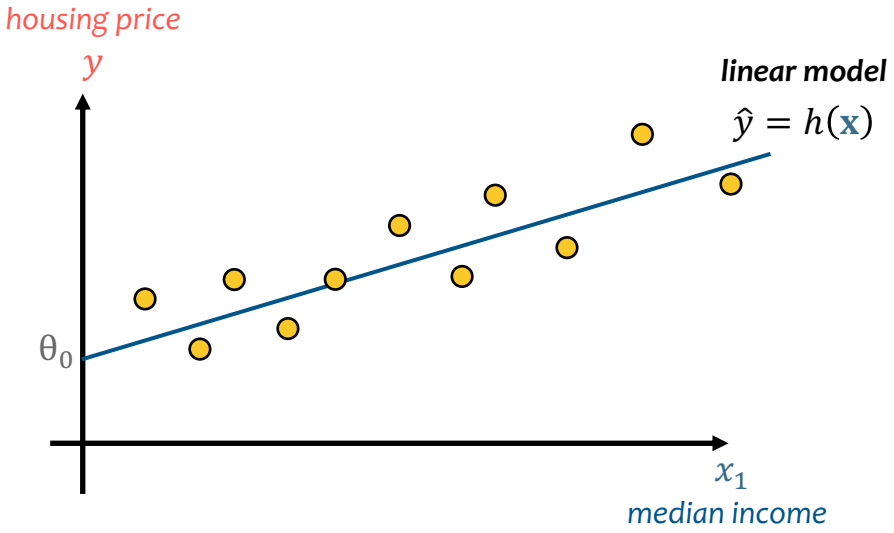

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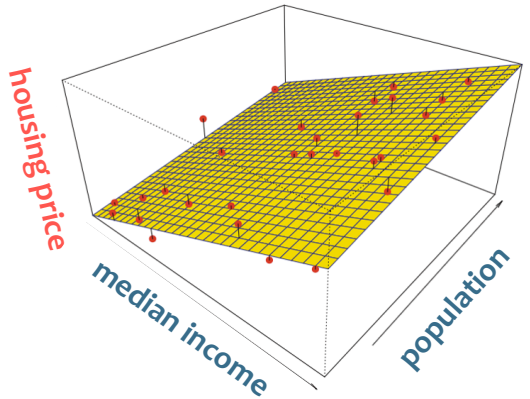


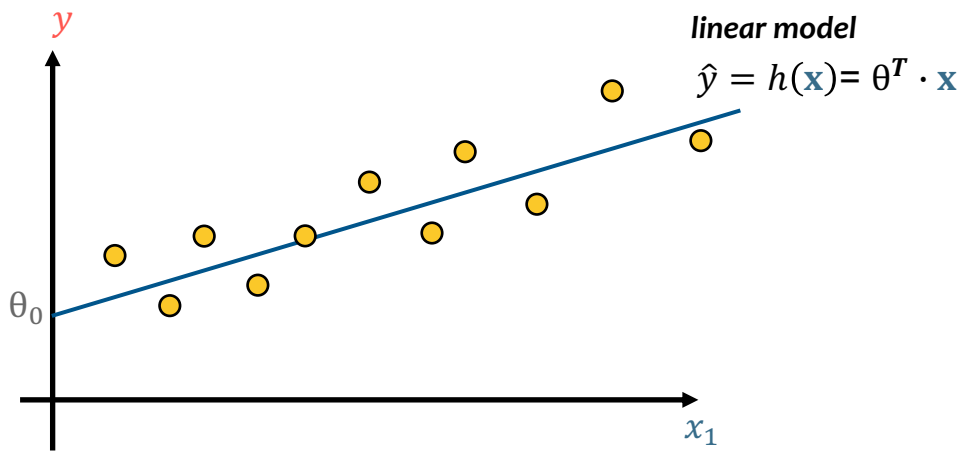
Linear Regression model (vectorized form)

$$\hat{y} = h_\theta(\mathbf{x}) = \theta^T \cdot \mathbf{x}$$

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n$$

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \cdots \\ \theta_n \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} 1 \\ x_1 \\ \cdots \\ x_n \end{bmatrix} \quad x_0$$

$$\theta^T = [\theta_0 \ \theta_1 \cdots \theta_n]$$



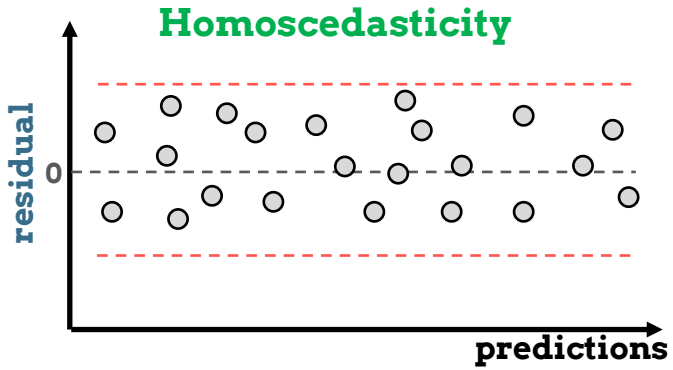
Assumptions of Linear Regression

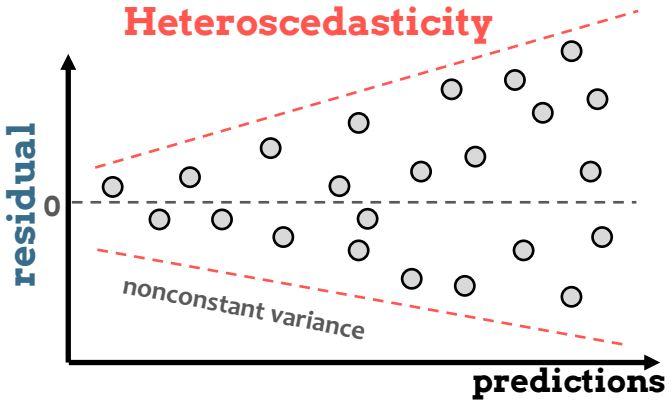
X = features (independent variables)

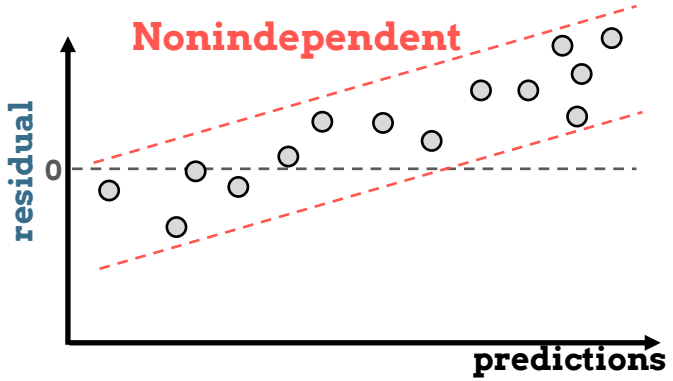
y = outcome (dependent variables)

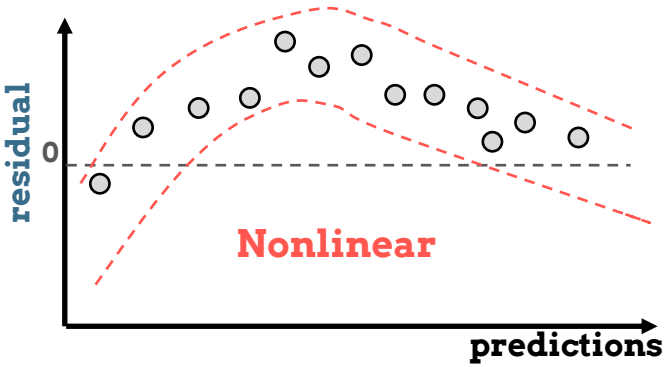
1. **Linearity:** The relationship between **X** and **y** is **linear**.
2. **Observations** are **independent** of each other.
3. No or little **multicollinearity** (the **independent variables** are **highly correlated** with each other).
4. **Residuals** **$(\hat{y} - y)$** are **normally** distributed.
5. **Homoscedasticity:** The **variance** of **residual** is the same for any value of **X**.

Checking Homoscedasticity Visually

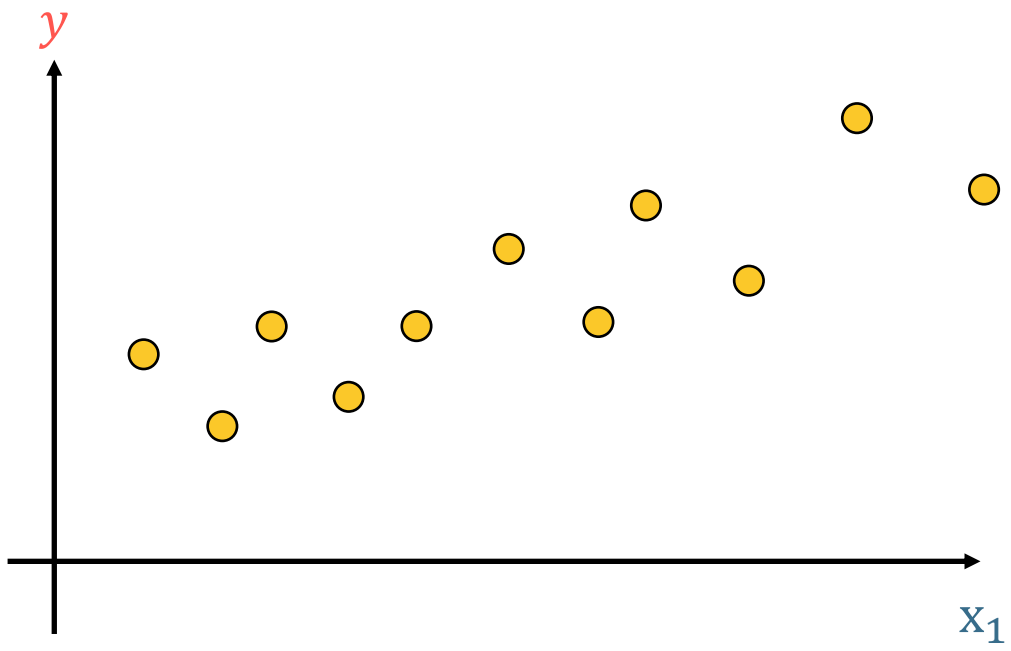








Which is the best linear model?



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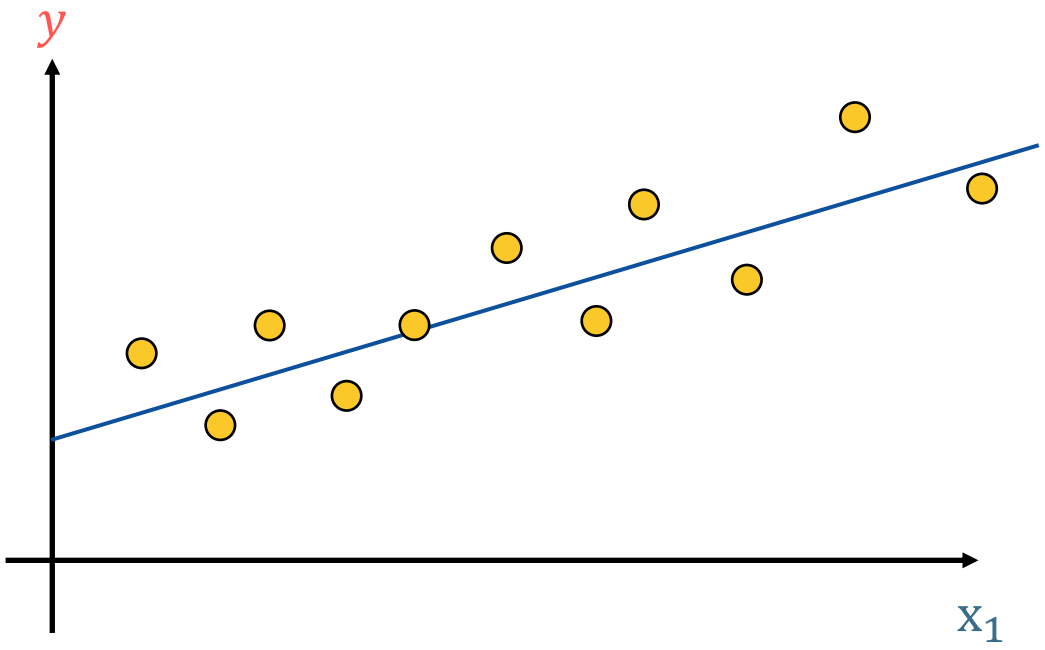

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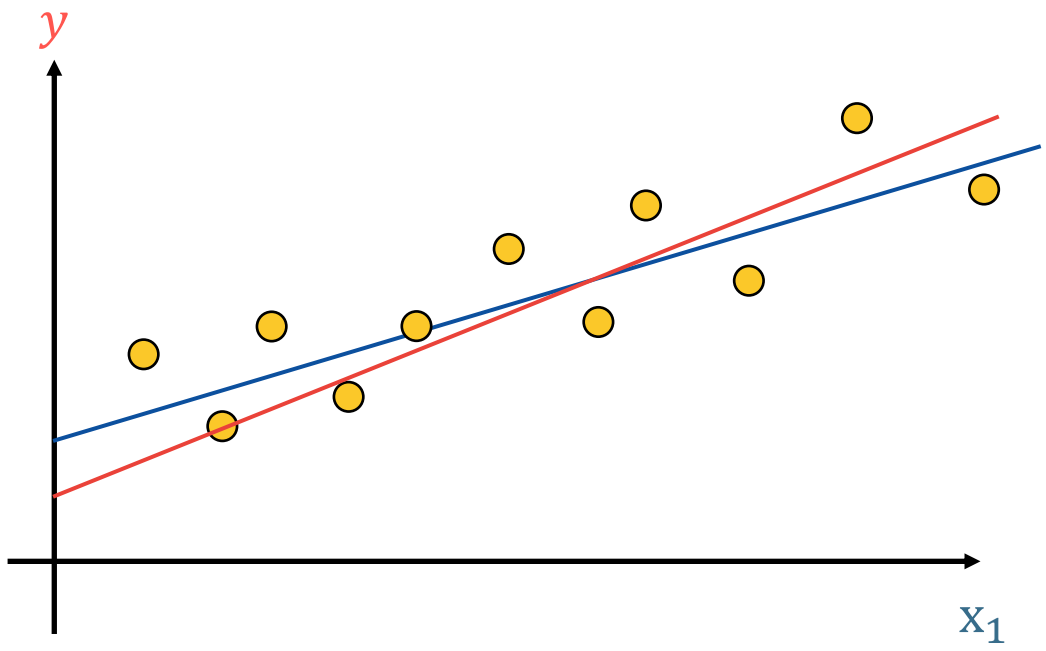

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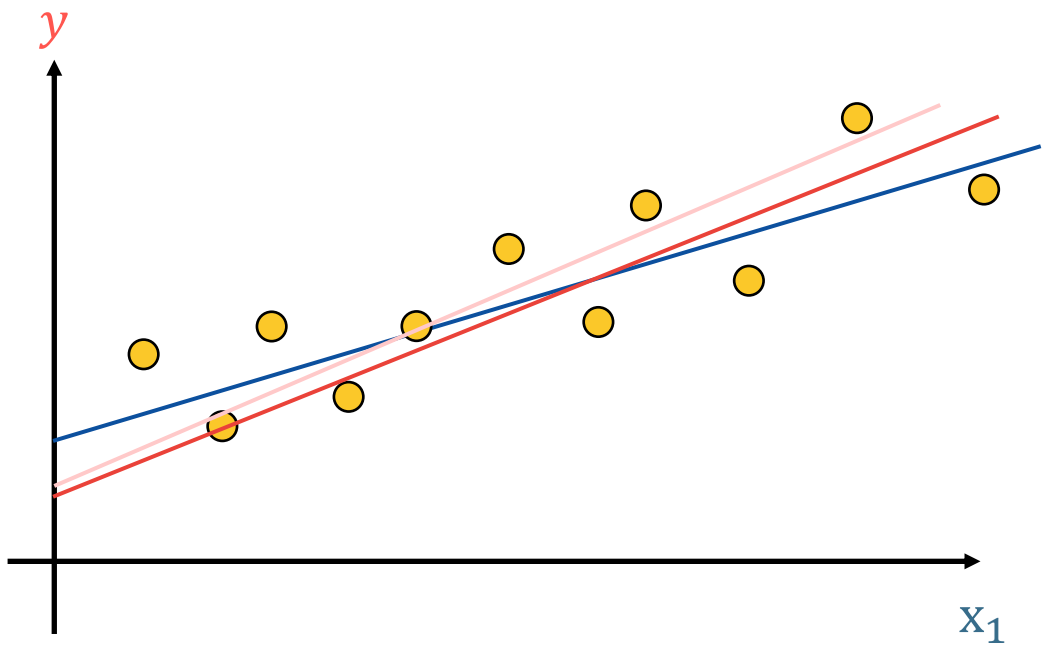

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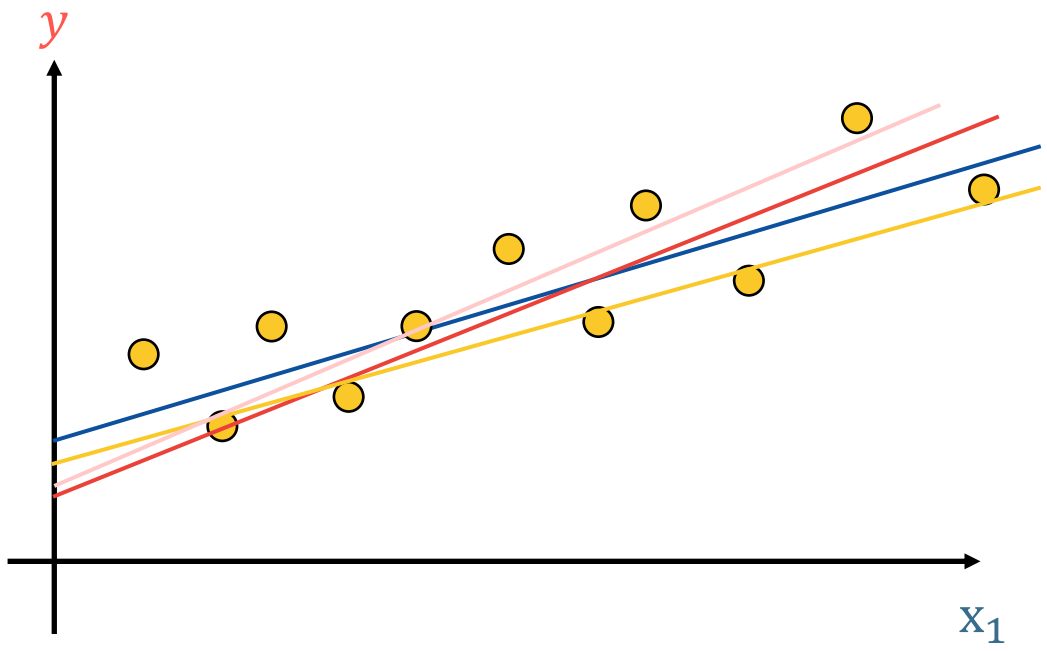
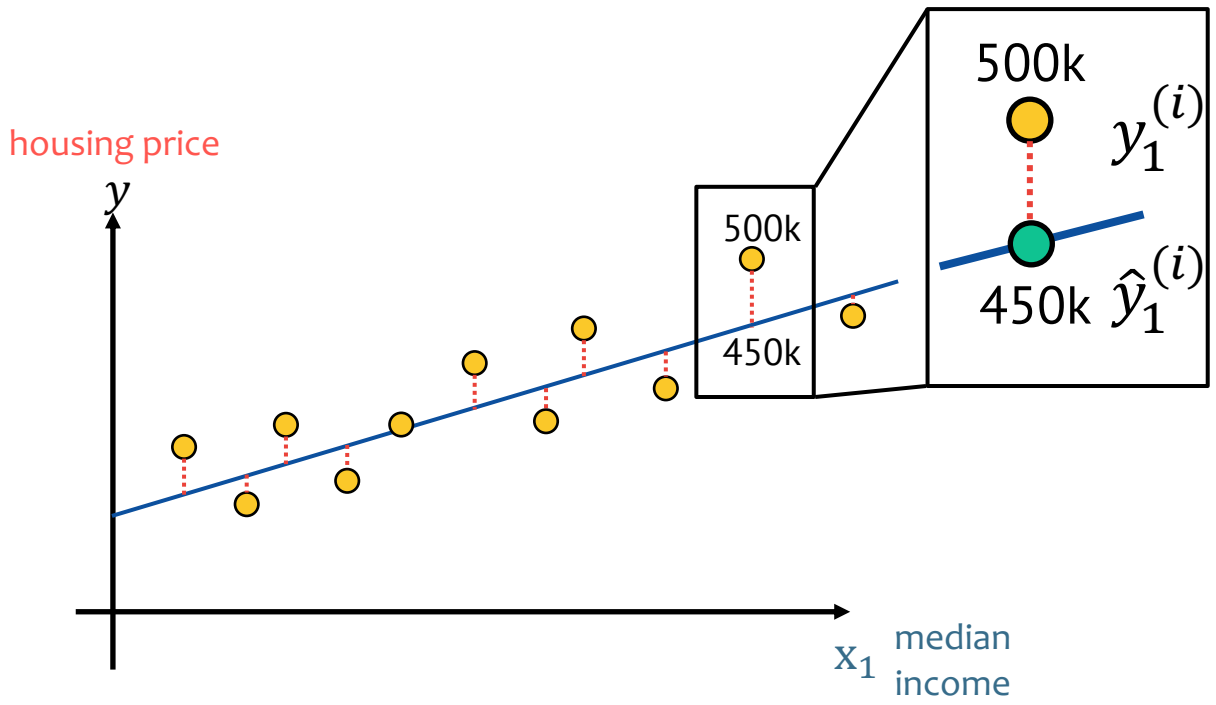


Cost Function / Error Function

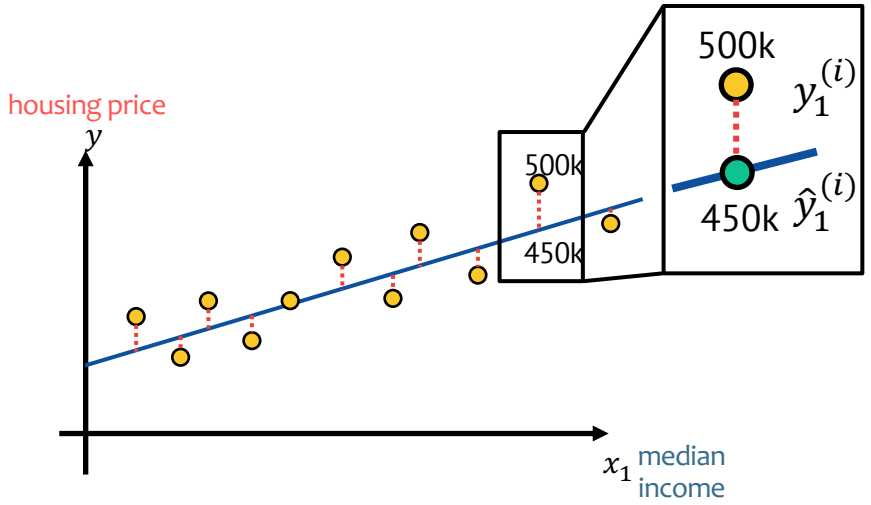


Cost Function / Error Function

Mean Square Error

$$J(\theta) = MSE(\mathbf{X}, h_\theta) = \frac{1}{m}\sum_{i=1}^{m}(\theta^{T} \cdot \mathbf{x}^{(i)} - y^{(i)})^2$$

$$h_\theta(\mathbf{x}^{(i)}) = \hat{y}^{(i)}$$



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training

Goal: Choose the parameters $\boldsymbol{\theta}$ (for simple regression, $\boldsymbol{\theta_0}, \boldsymbol{\theta_1}$) that **minimizes** the **cost function** $J(\theta)$ for the training data.

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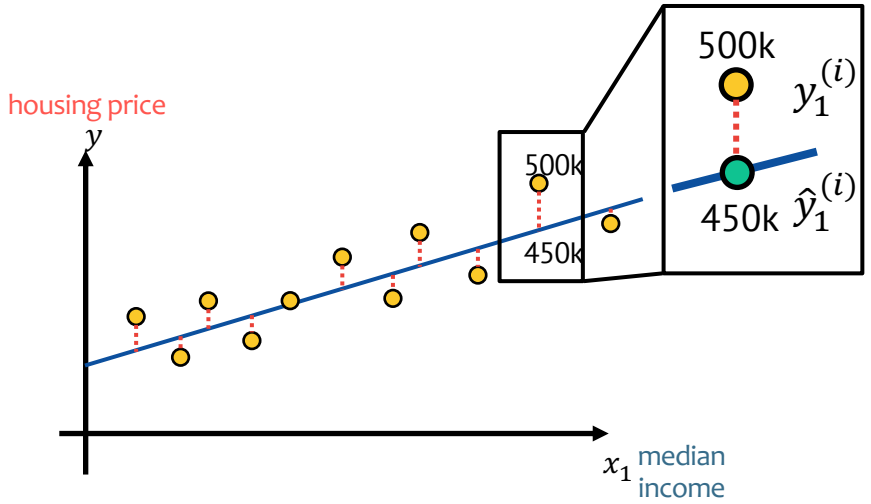


Linear Model

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1$$

Simplified Linear Model

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_1 x_1$$

simplifying: $\theta_0 = 0$

Cost Function

$$J(\theta) = J(\theta_0, \theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}^{(i)} - y^{(i)})^2$$

Goal: $\min_{\theta_0,\theta_1} J(\theta_0, \theta_1)$

Cost Function

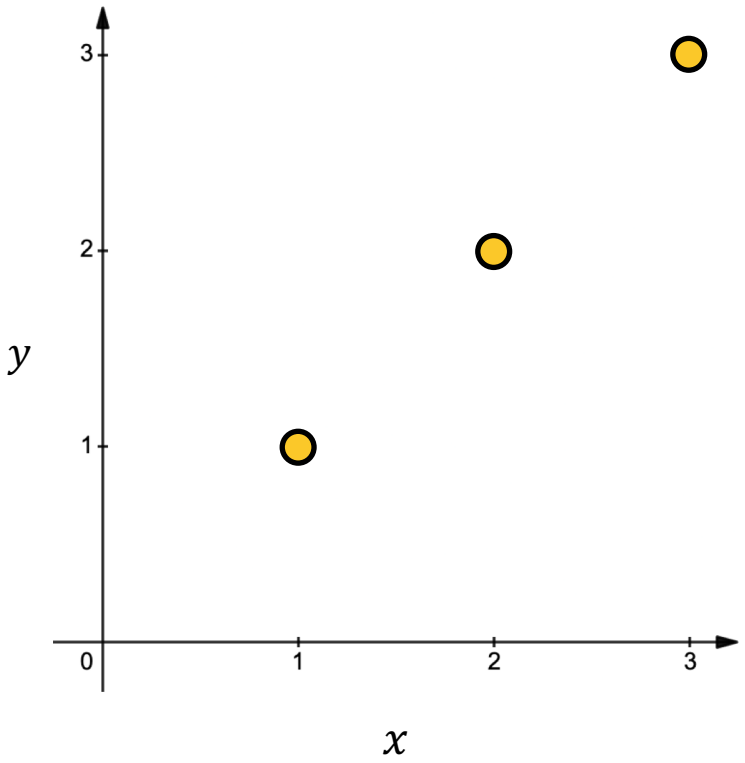
$$J(\theta) = J(\theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}^{(i)} - y^{(i)})^2$$

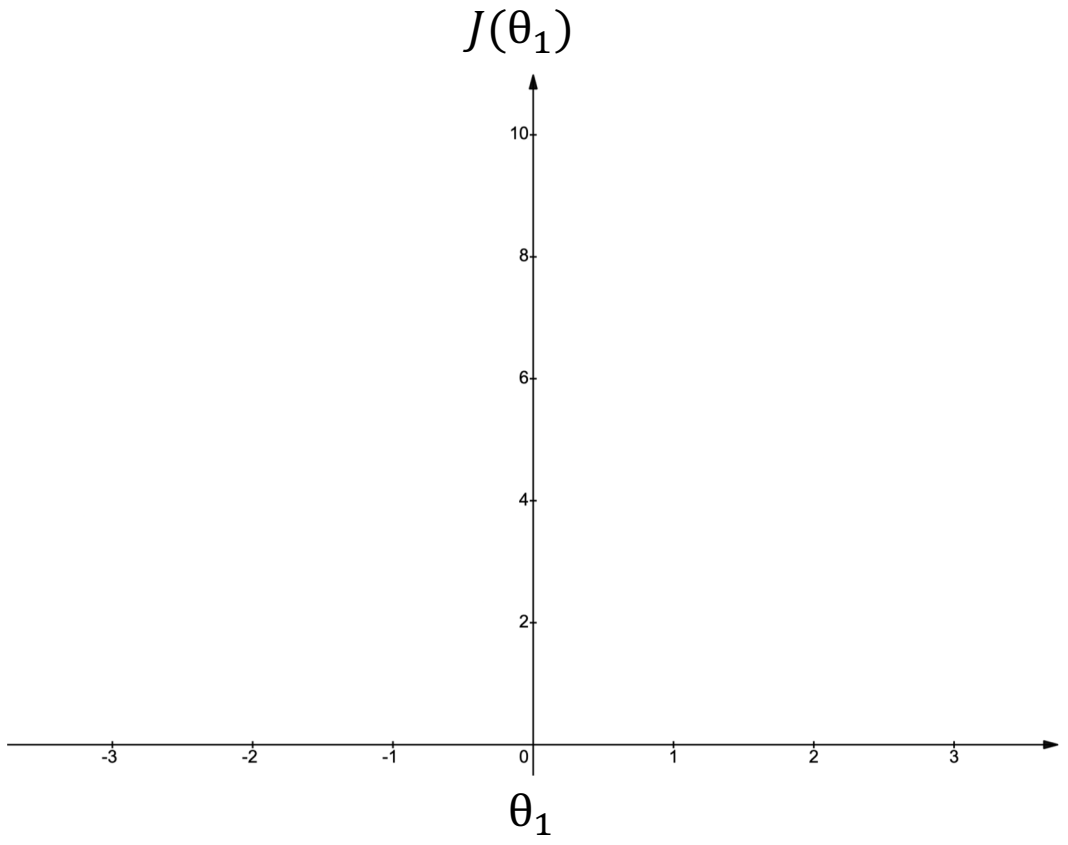
Goal: $\min_{\theta_1} J(\theta_1)$

Example

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_1 x_1$$

$$J(\theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\theta_1 x_1 - y^{(i)})^2$$





Example

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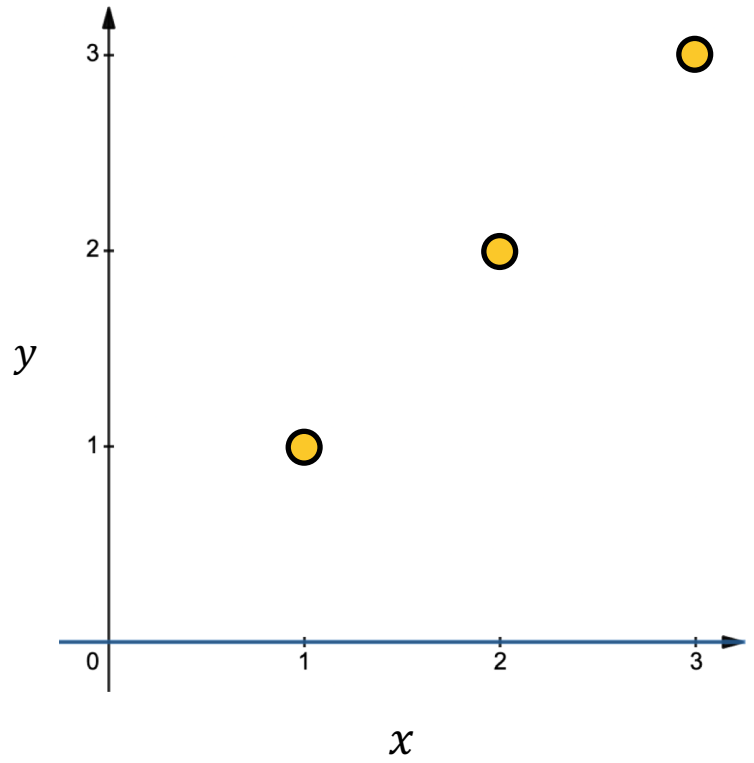
$$\theta_1 = 0$$



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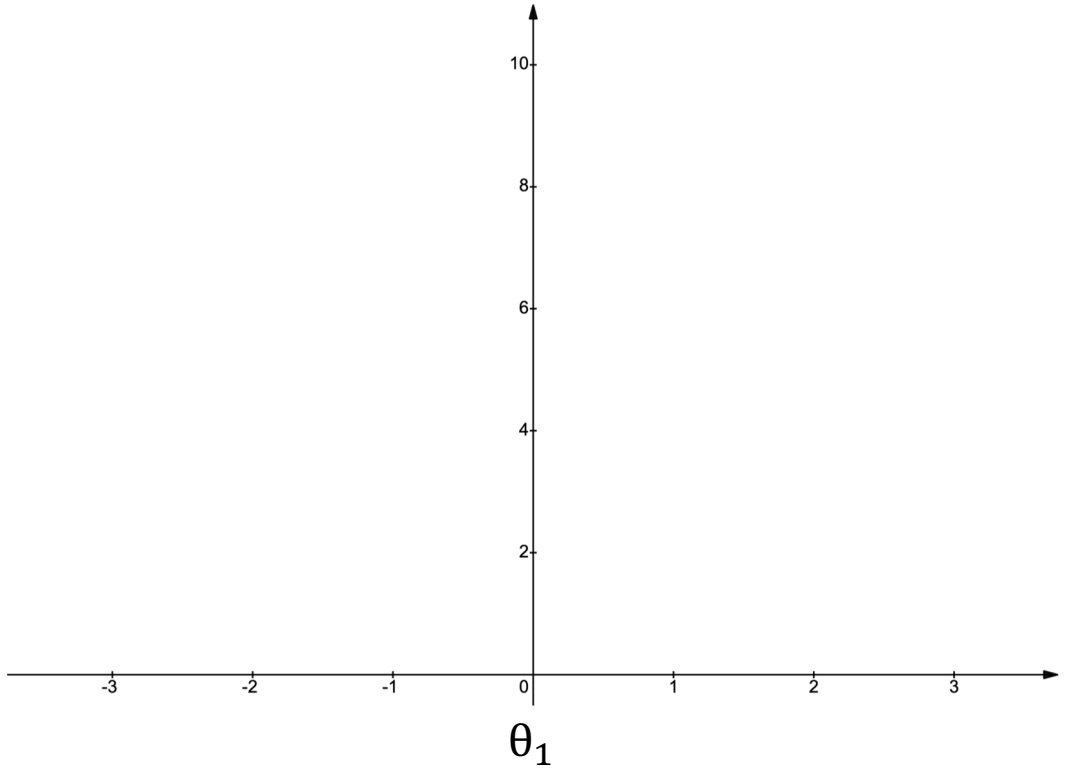
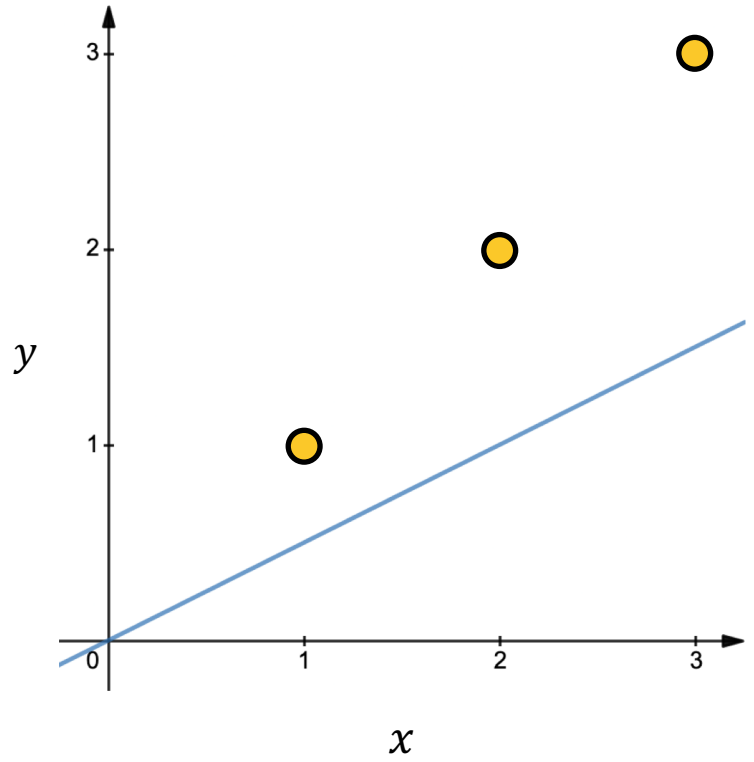
$J(\theta_1)$



Example

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_1 x_1$$

$$\theta_1 = 0.5$$



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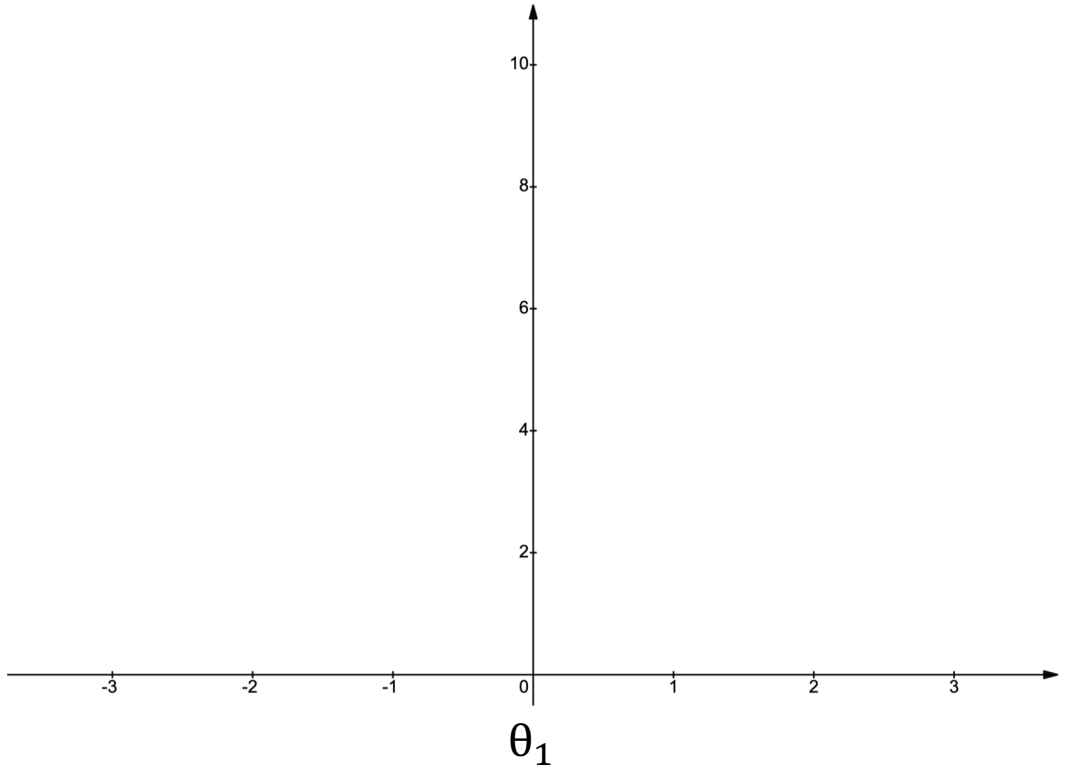
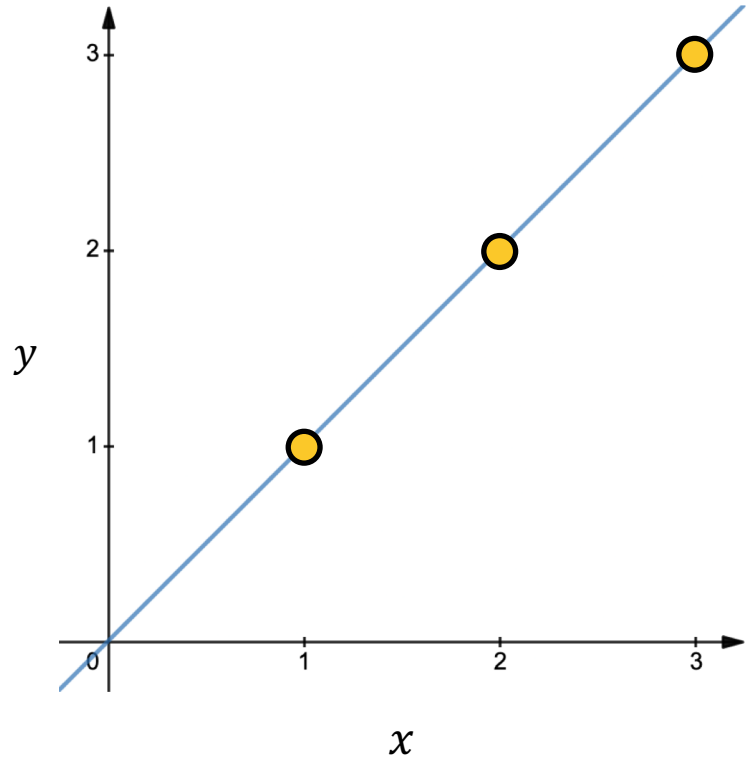


Example

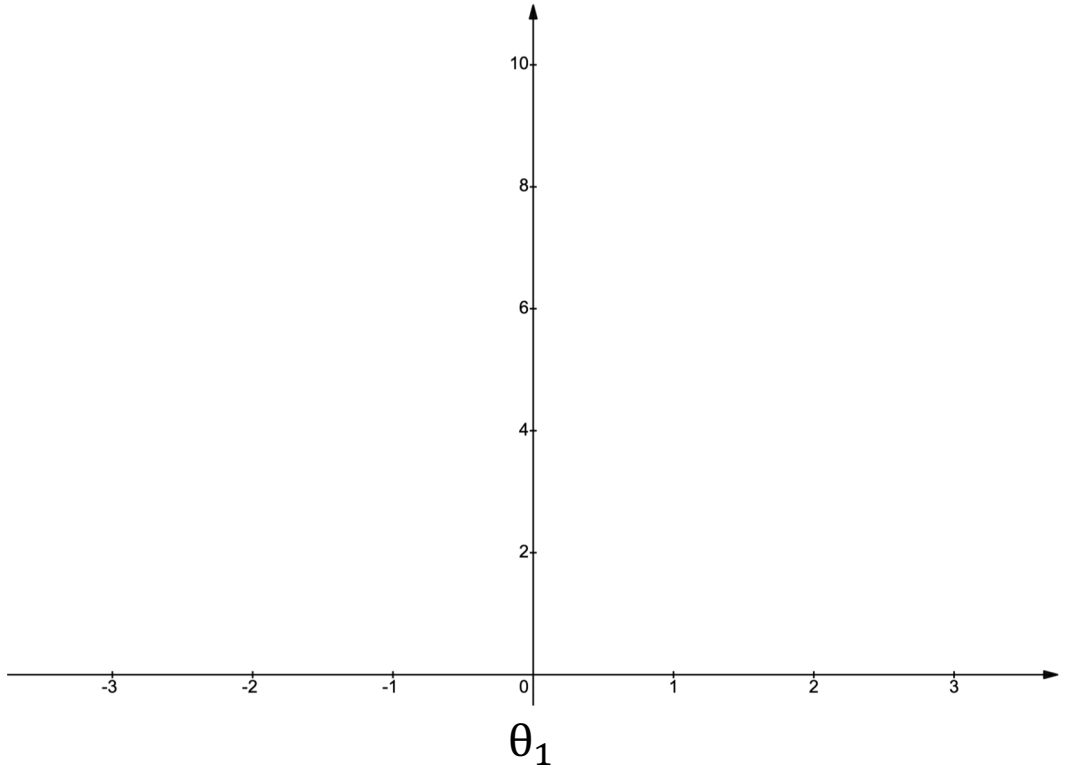
$$\hat{y} = h_\theta(\mathbf{x}) = \theta_1 x_1$$

$$\theta_1 = 1$$



$$J(\theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\theta_1 x_1 - y^{(i)})^2$$

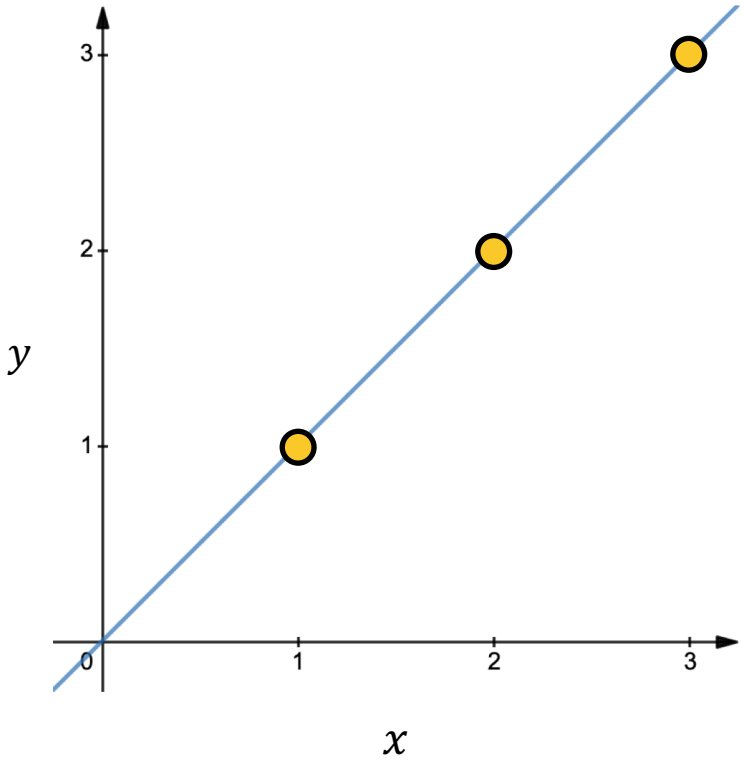
$$J(\theta_1)$$



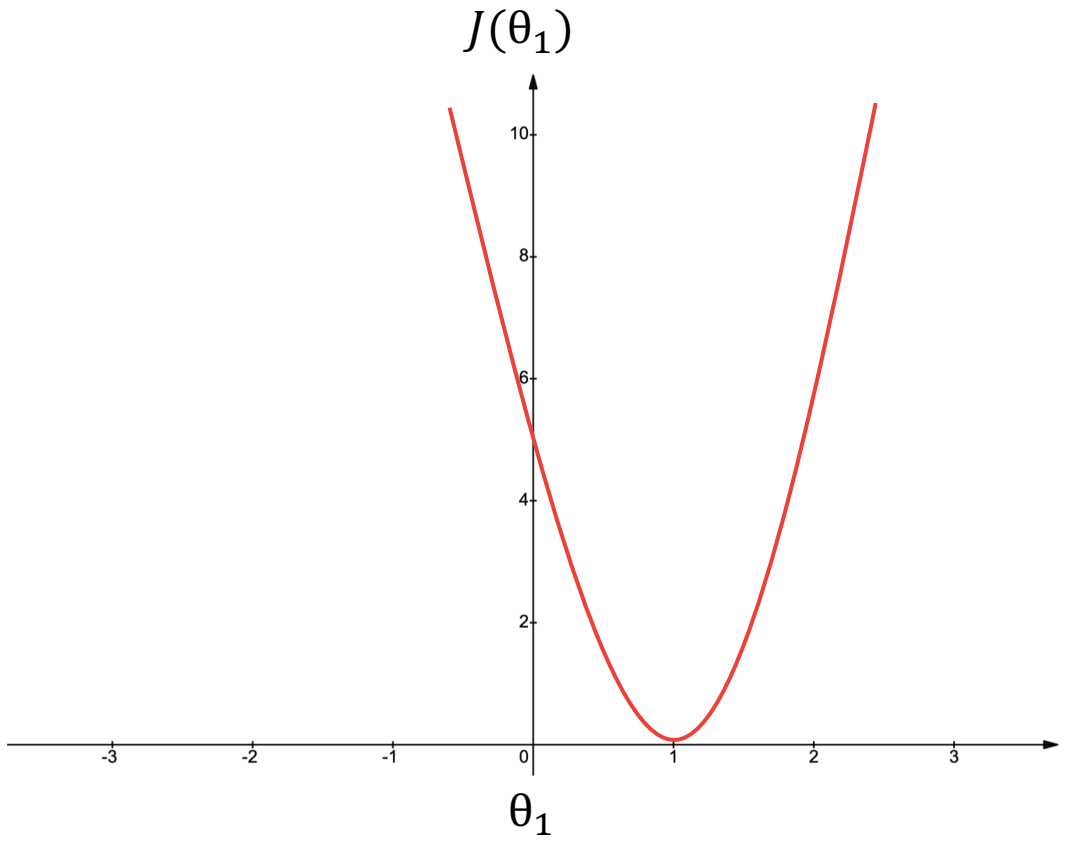
Example

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_1 x_1$$

$$\theta_1 = 1$$



$$J(\theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\theta_1 x_1 - y^{(i)})^2$$



Linear Model

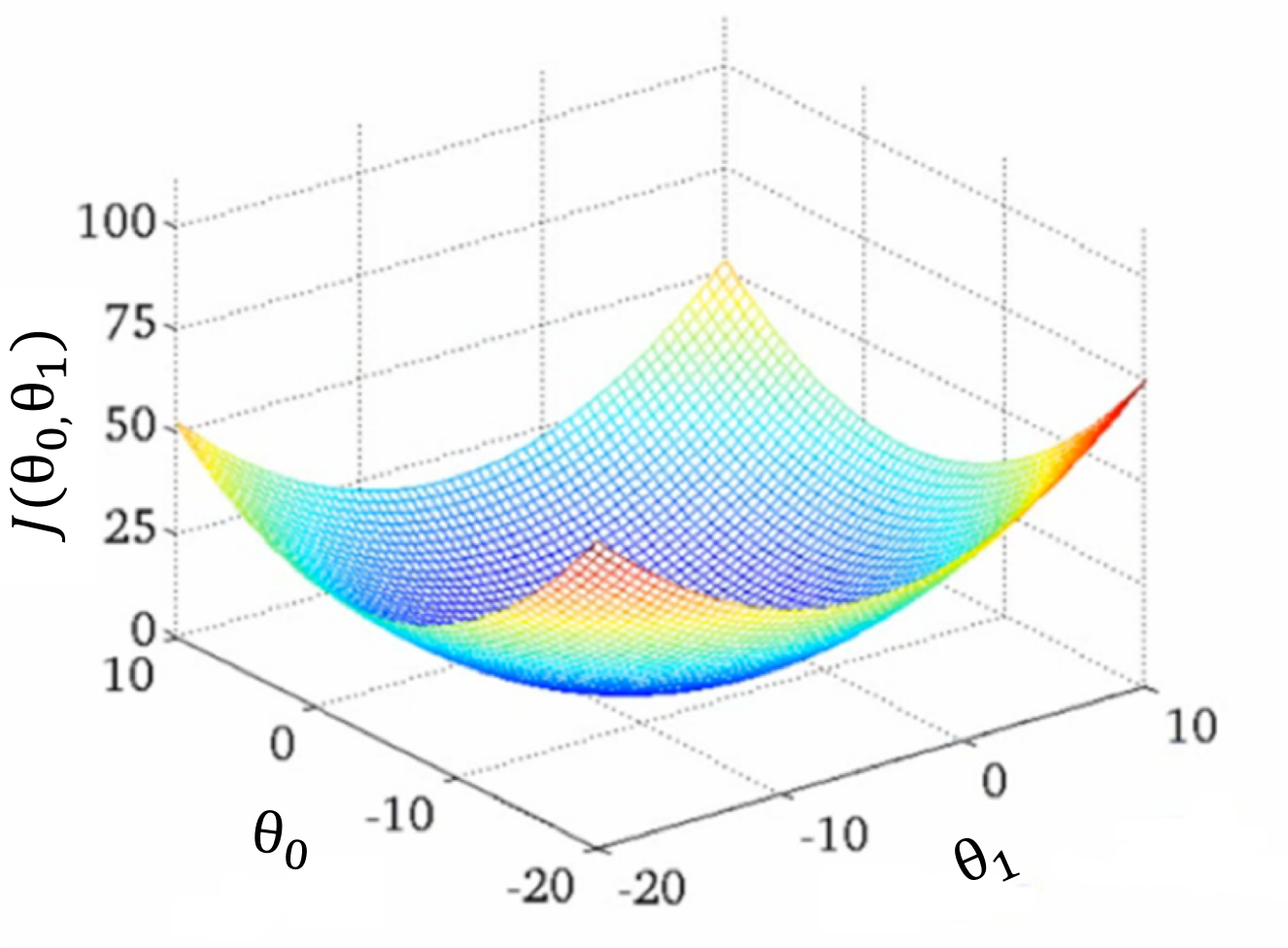
$$\hat{y} = h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1$$

Cost Function

$$J(\theta) = J(\theta_0, \theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}^{(i)} - y^{(i)})^2$$

Goal: $\min_{\theta_0,\theta_1} J(\theta_0, \theta_1)$

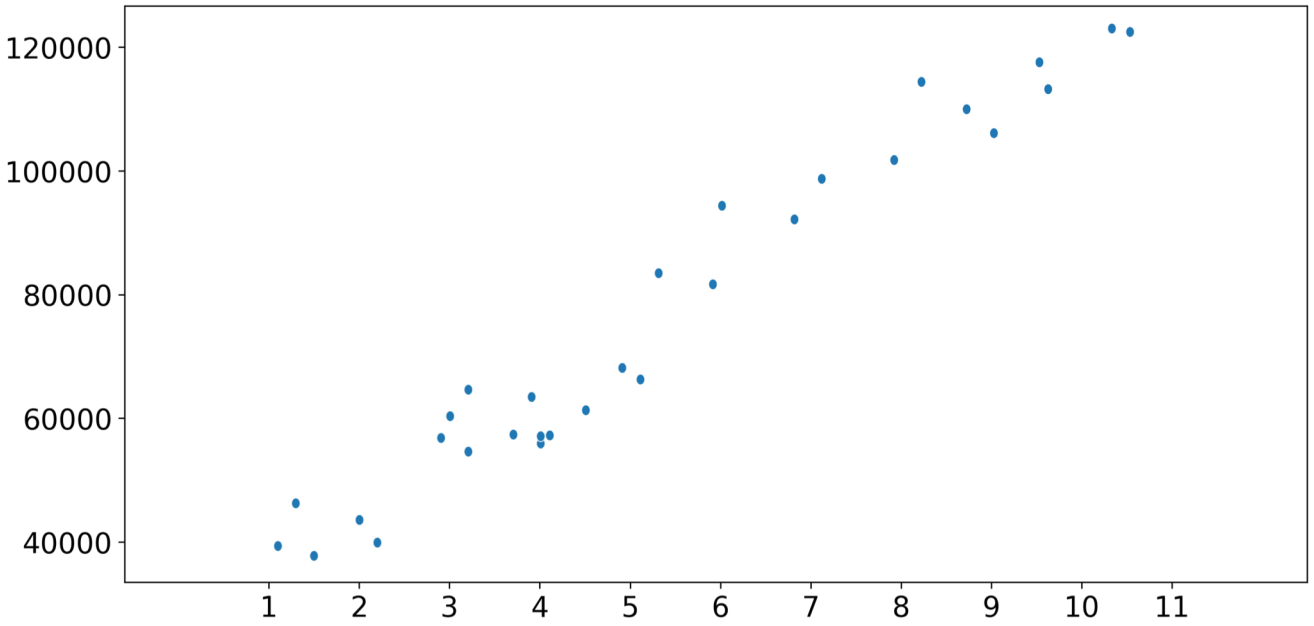
$$J(\theta_{0,}\theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\theta_0 + \theta_1 x_1 - y^{(i)})^2$$

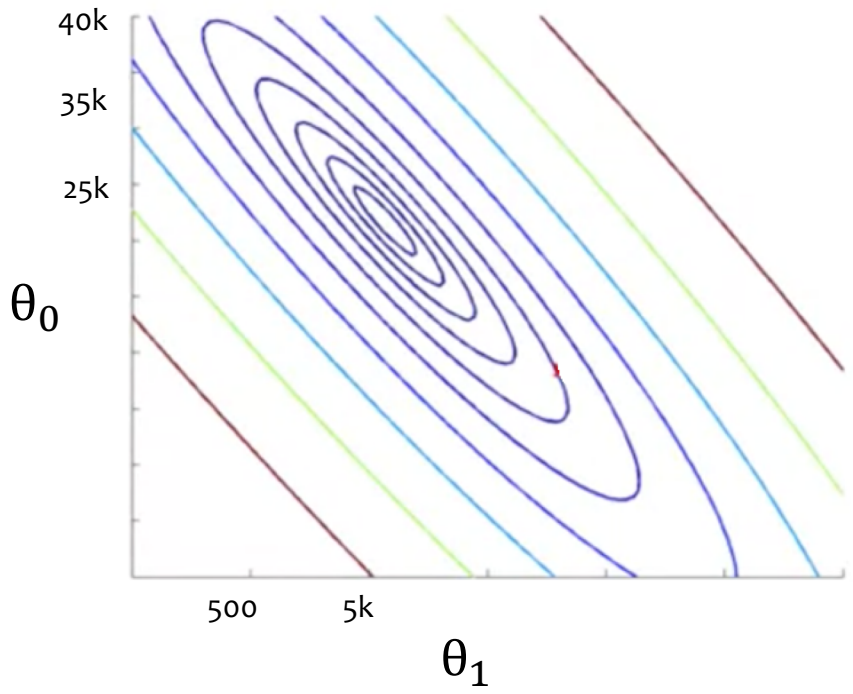


Example

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1$$

$$J(\theta_0,\theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\theta_0 + \theta_1 x_1 - y^{(i)})^2$$





Example

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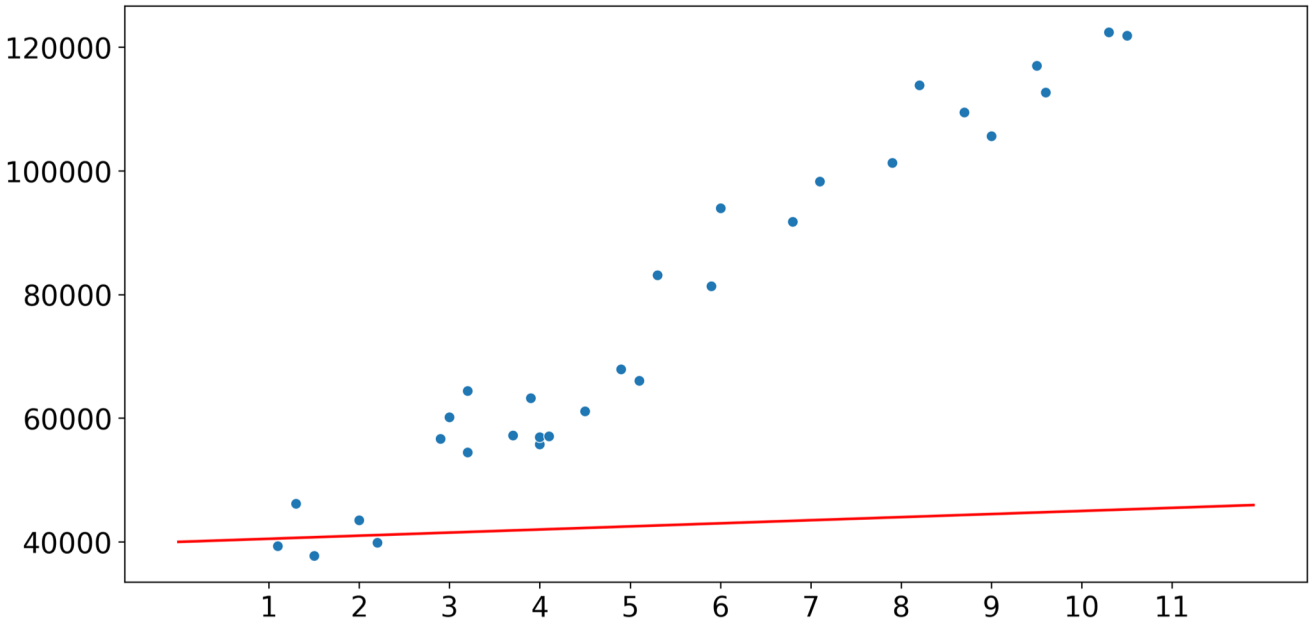
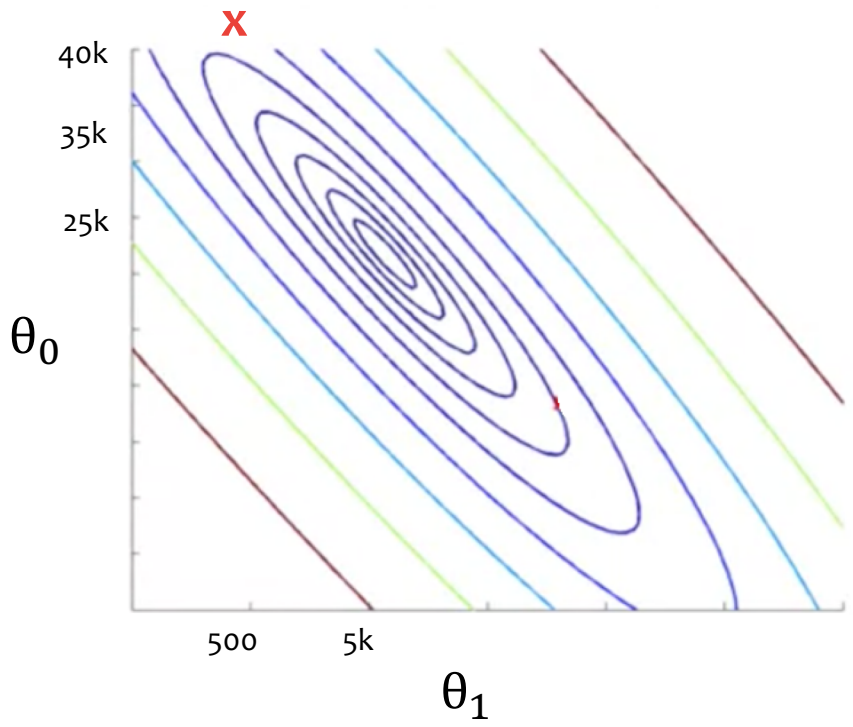


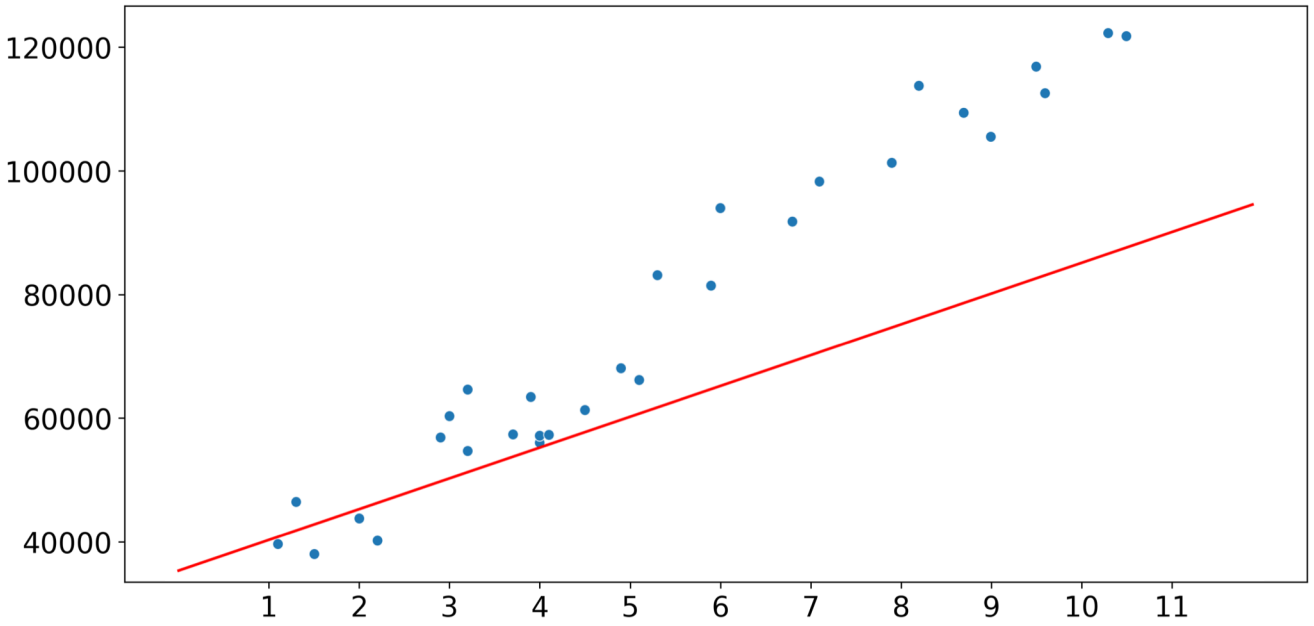


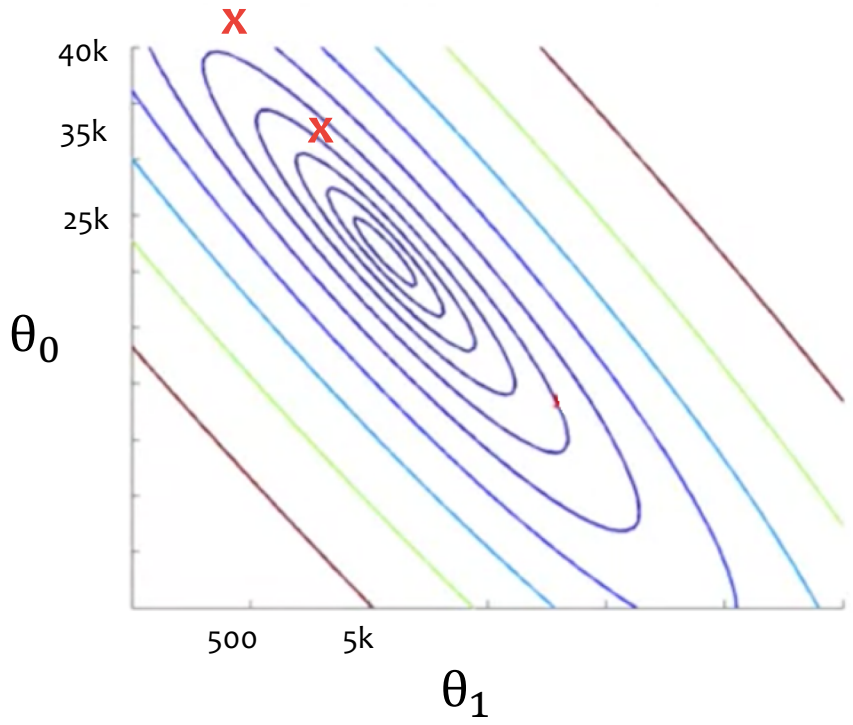
$\theta_0 = 40000$
$\theta_1 = 500$

Example

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1$$

$$J(\theta_0,\theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\theta_0 + \theta_1 x_1 - y^{(i)})^2$$



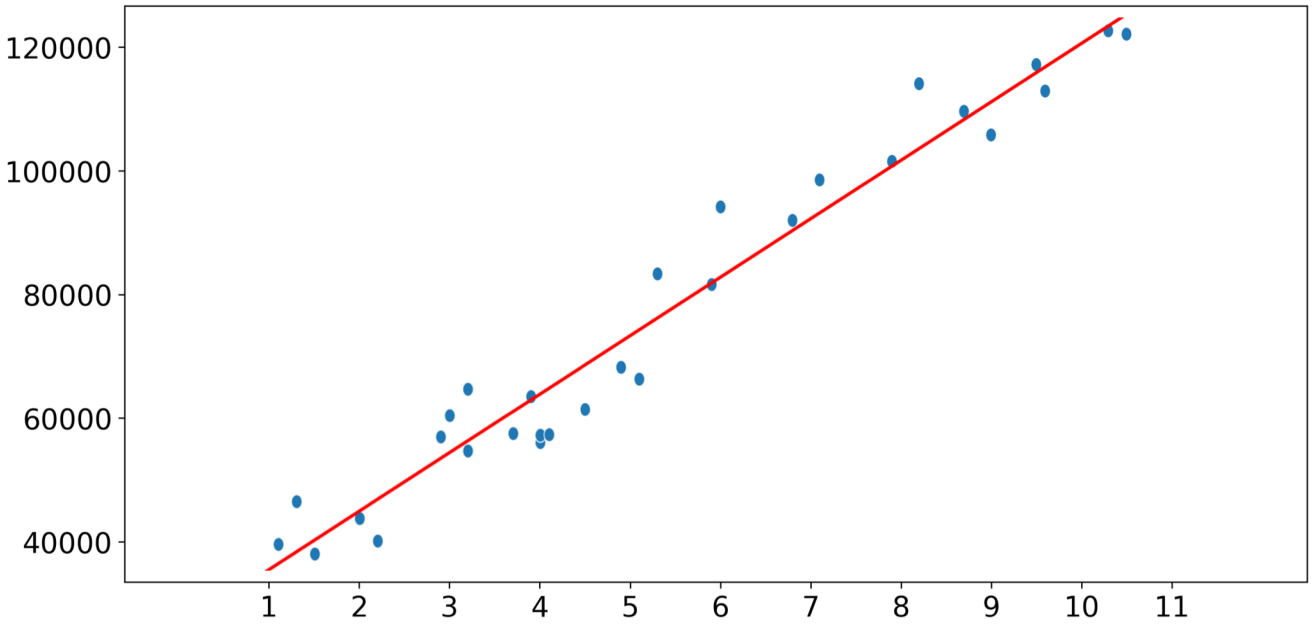


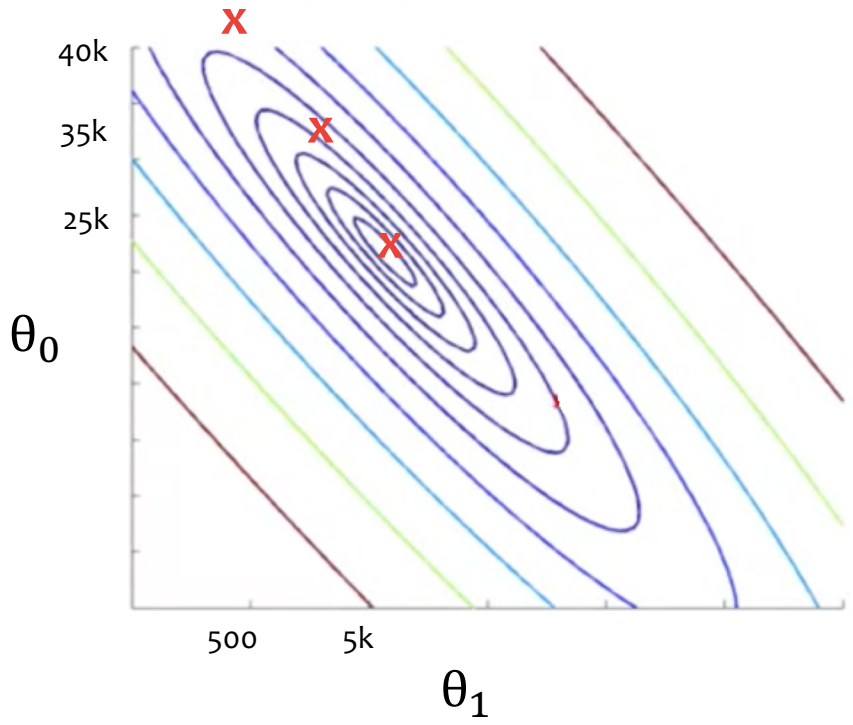
$\theta_0 = 35000$
$\theta_1 = 5000$

Example

$$\hat{y} = h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1$$

$$J(\theta_0,\theta_1) = \frac{1}{m}\sum_{i=1}^{m}(\theta_0 + \theta_1 x_1 - y^{(i)})^2$$





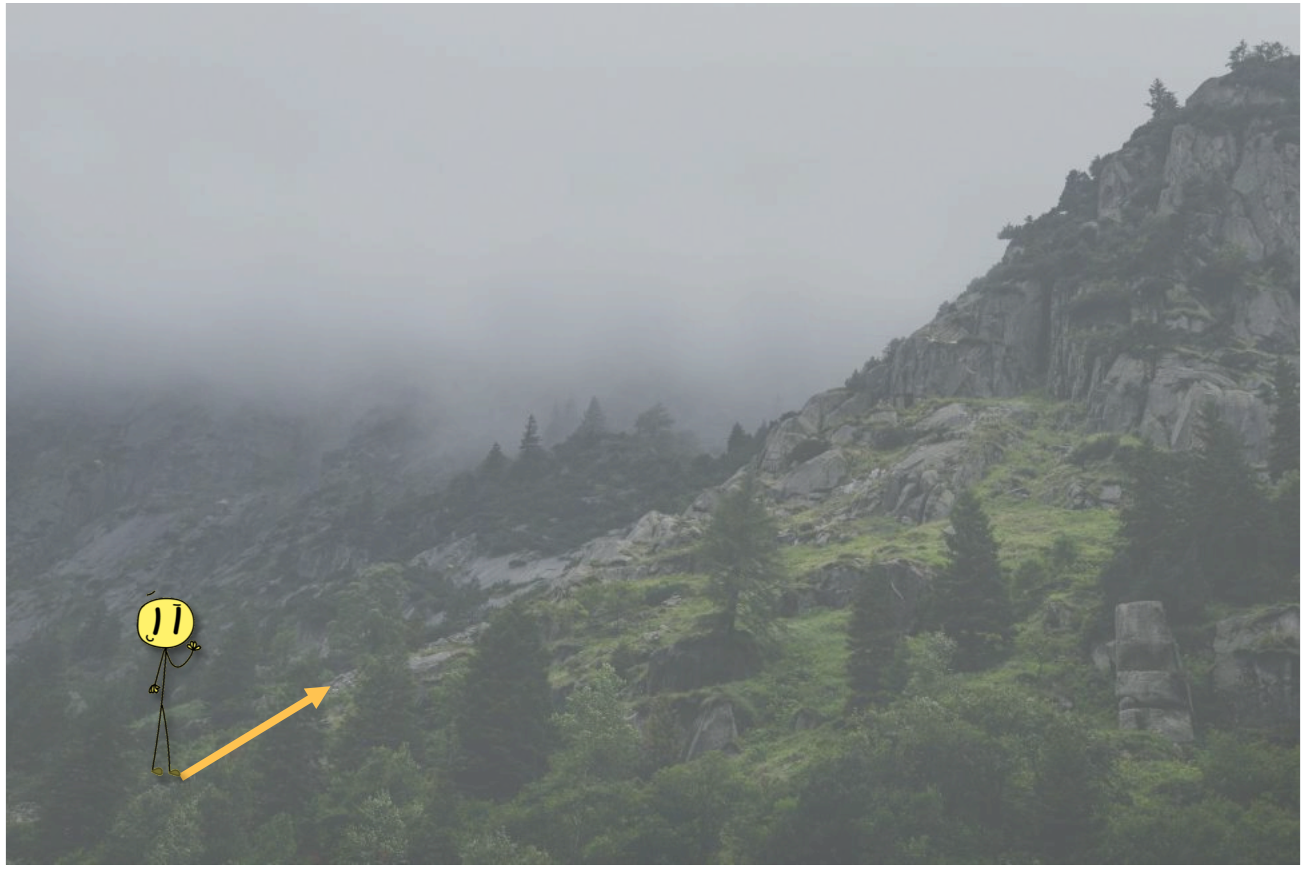
$$\theta_0 = 25000$$
$$\theta_1 = 9000$$

How to train a Linear Regression Model?

Gradient Descent

https://freerangestock.com/photos/123019/foggy-mountains-.html

Gradient Descent



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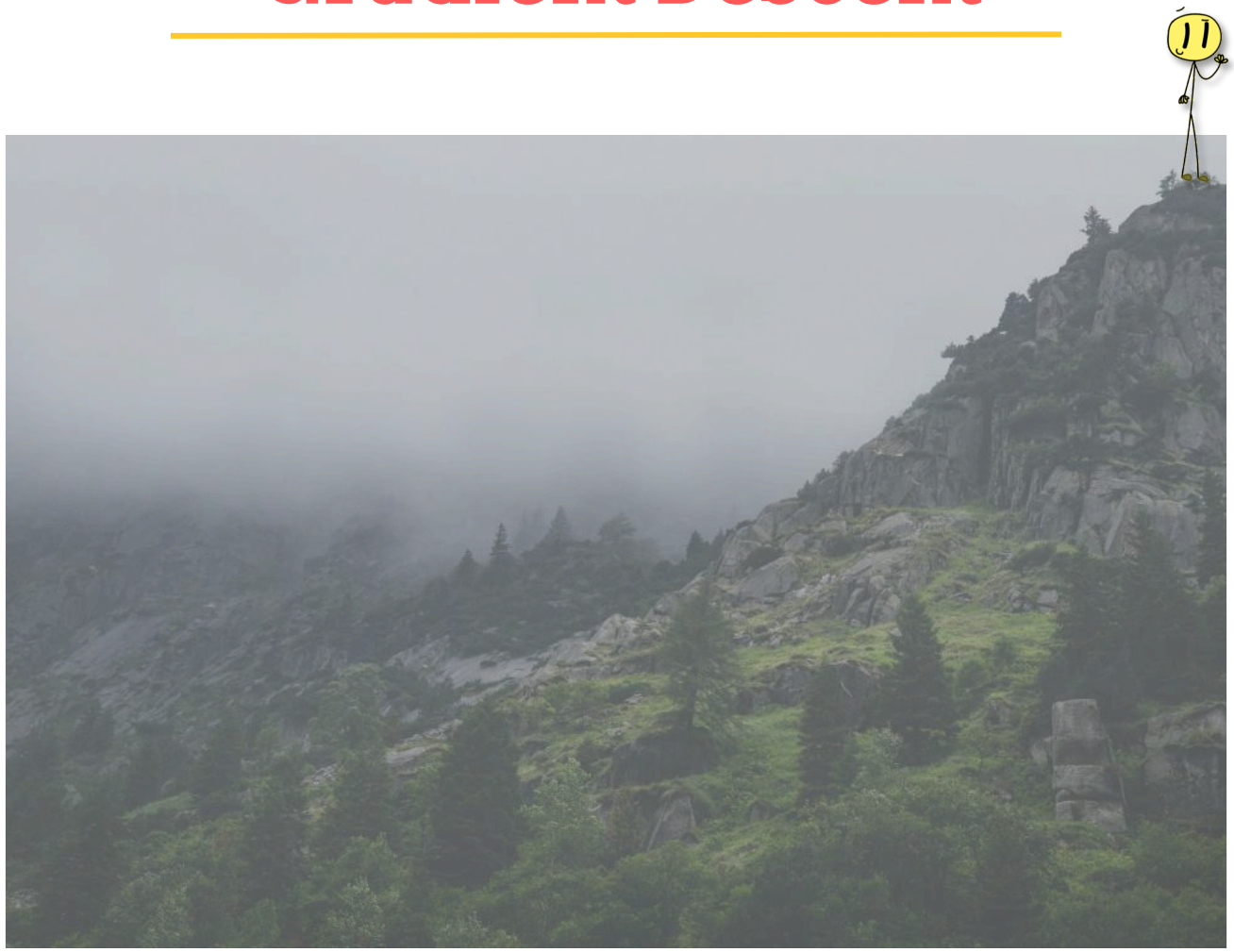
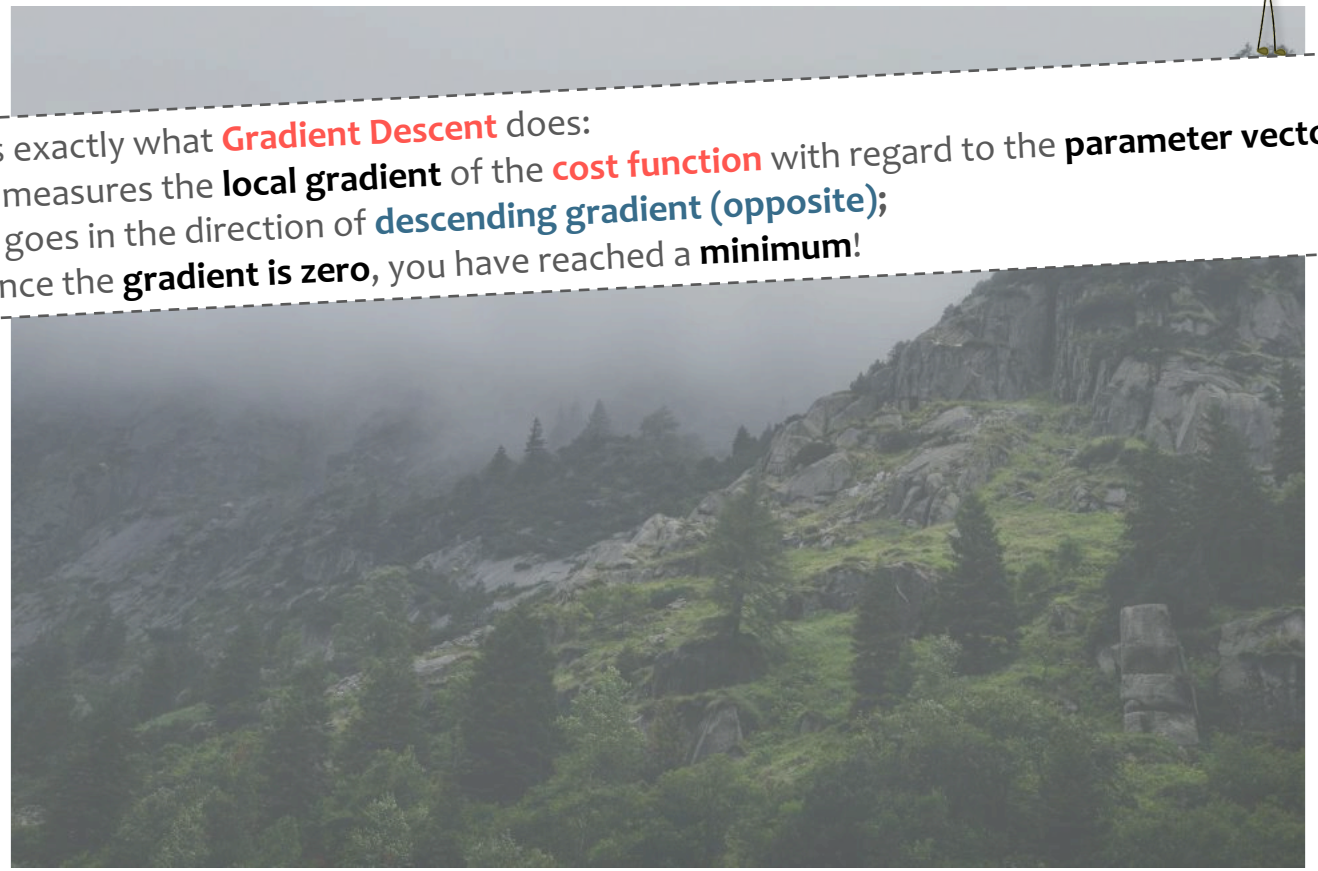


https://freerangestock.com/photos/123019/foggy-mountains-.html

Gradient Descent

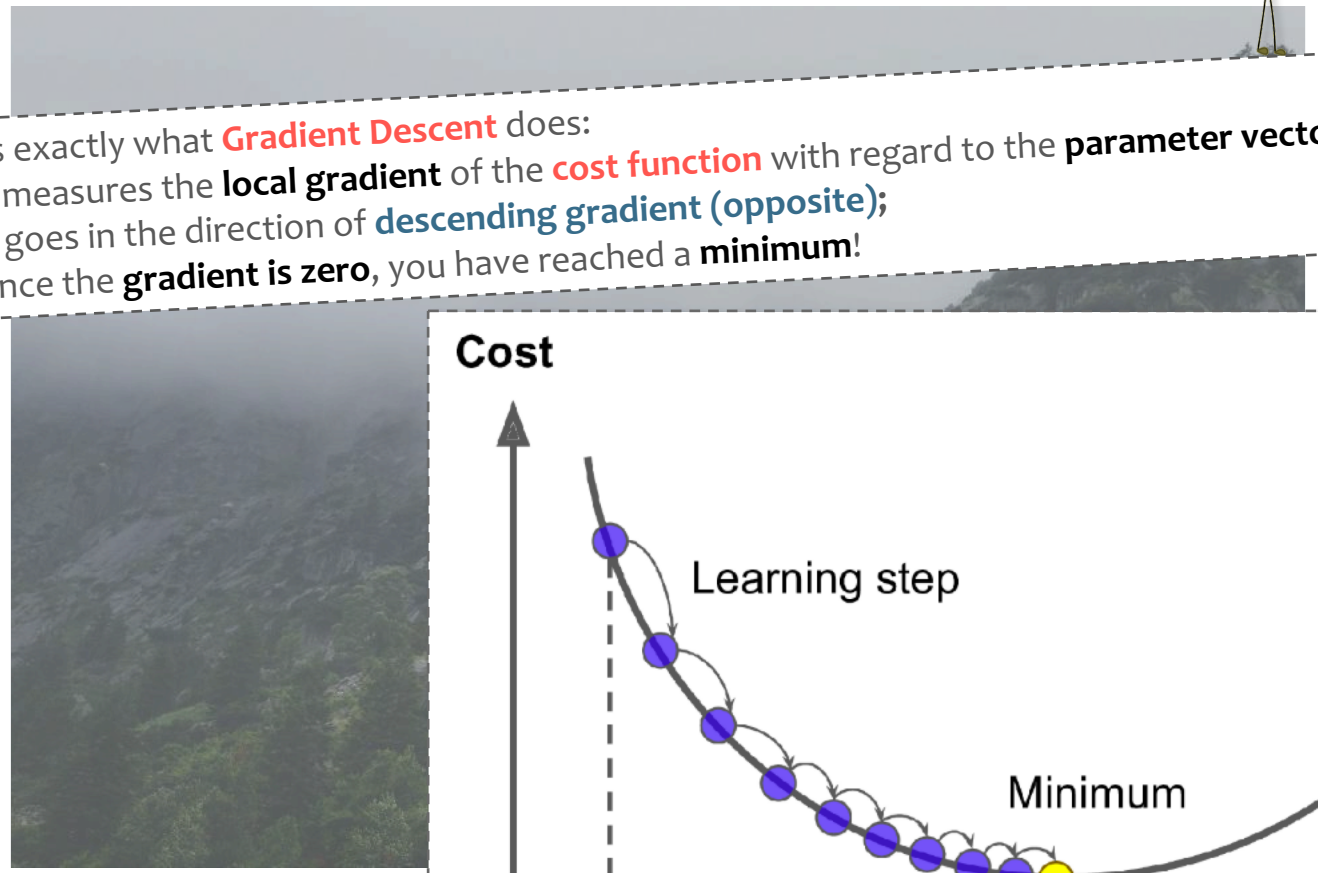


This is exactly what **Gradient Descent** does:

- it measures the **local gradient** of the **cost function** with regard to the **parameter vector θ**, and
- it goes in the direction of **descending gradient (opposite);**
- once the **gradient is zero**, you have reached a **minimum**!

https://freerangestock.com/photos/123019/foggy-mountains-.html

Gradient Descent



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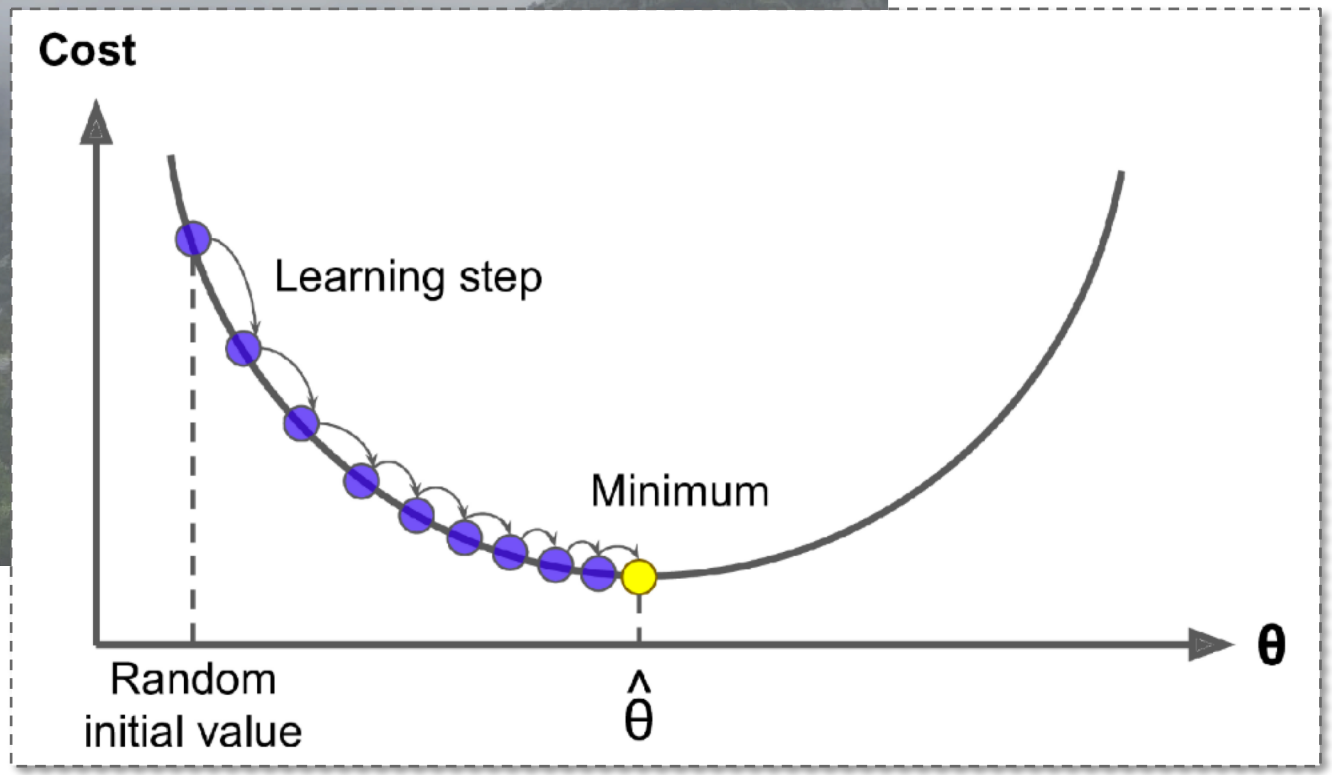
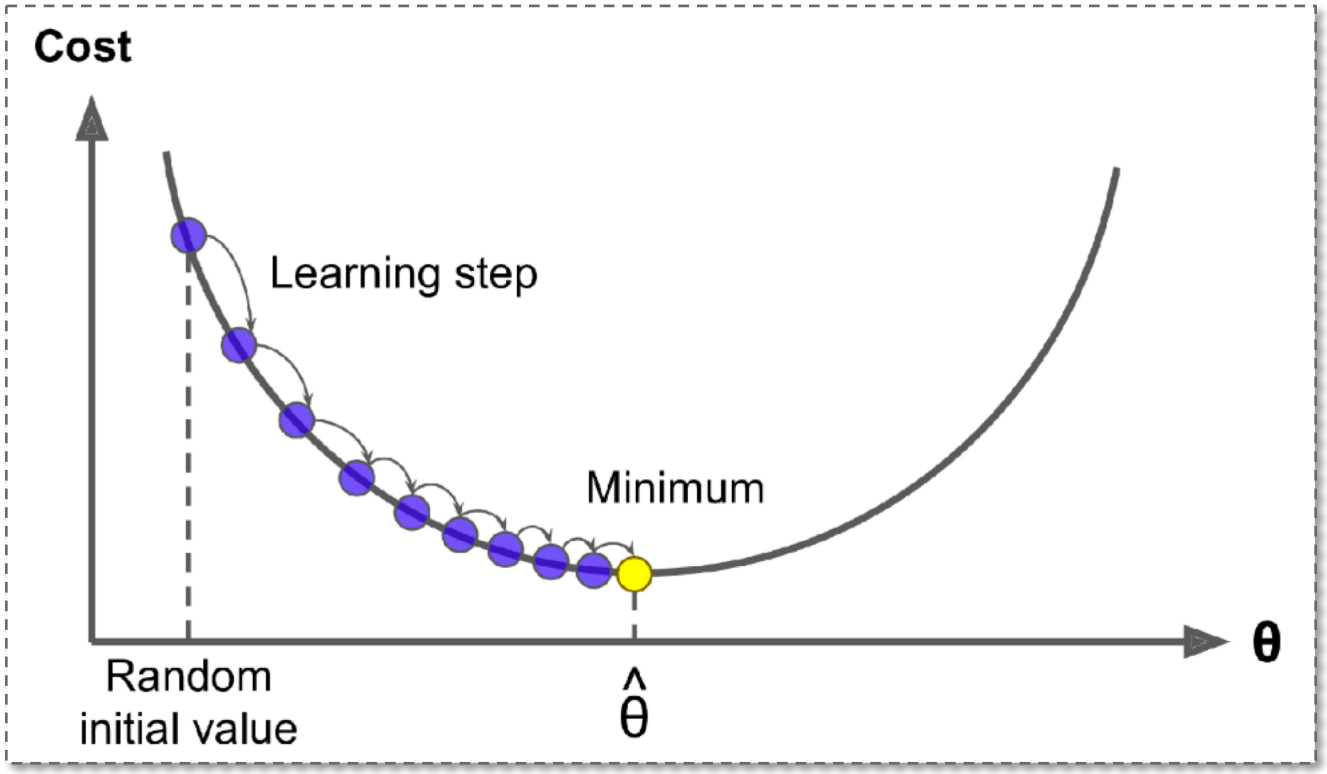


https://freerangestock.com/photos/123019/foggy-mountains-.html

Gradient Descent

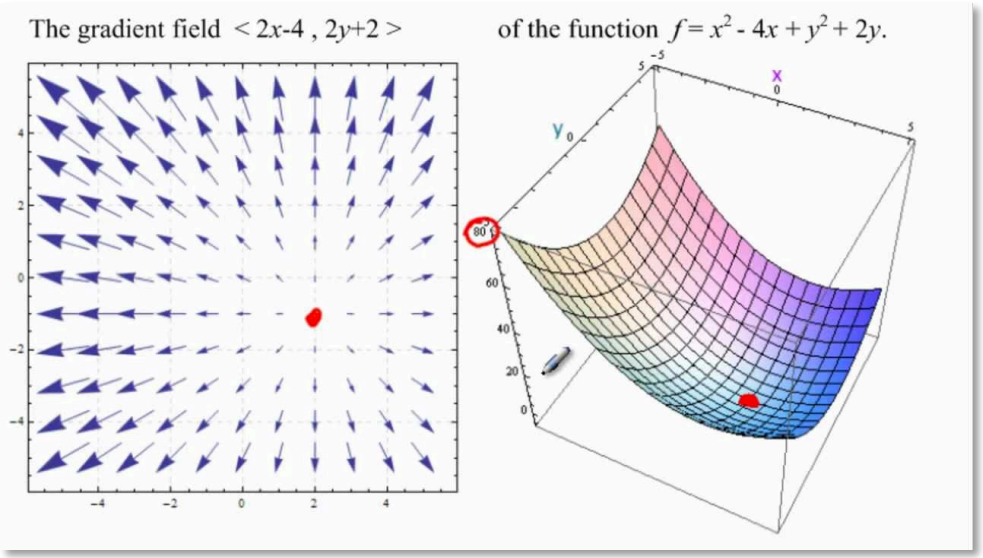
- A generic **optimization algorithm** capable of finding optimal solutions (e.g., **parameters**) to a wide range of problems.
- Its general idea is **to tweak parameters iteratively** in order **to minimize** a **cost function**.



Gradient Vector

- The **gradient vector**, or simply **gradient**, is a vector that points to **the direction of greatest increase** with a given **increase rate**, for any function points.
- It is formed by the **partial derivative** of each variable in the function.

$$\nabla f = \begin{bmatrix} \frac{\partial}{\partial x} f \\ \frac{\partial}{\partial y} f \\ \vdots \end{bmatrix} \qquad \nabla J(\theta) = \begin{bmatrix} \frac{\partial}{\partial \theta_0} J(\theta) \\ \frac{\partial}{\partial \theta_1} J(\theta) \\ \vdots \end{bmatrix}$$



Algorithm

Given some cost function: $J(\theta) = J(\theta_0, \theta_1, \cdots, \theta_n)$

Algorithm parameter: learning rate $\alpha \in (0, 1]$

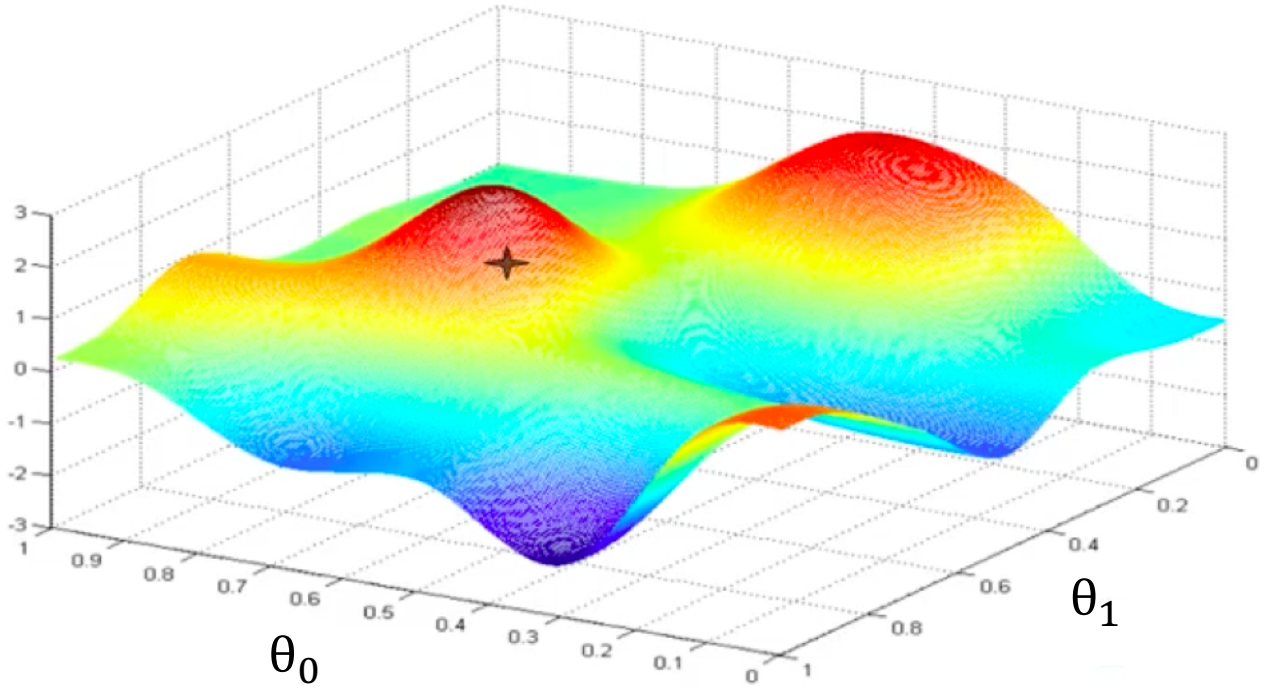
Goal: $\min_{\theta_0, \theta_1, \cdots, \theta_n} J(\theta_0, \theta_1, \cdots, \theta_n)$

Algorithm:

1. Initialize $\theta_0, \theta_1, \cdots, \theta_n$ arbitrarily (*e.g.*, $\theta_0 = 0, \theta_1 = 0, \cdots, \theta_n = 0$)
2. **repeat until convergence** (*e.g., for a given number of epochs/iterations):*
3. $\hat{y}$ = make predictions
4. Compute $J(\theta_0, \theta_1, \cdots, \theta_n)$
5. Change $\theta_0, \theta_1, \cdots, \theta_n$ **to reduce** $J(\theta_0, \theta_1, \cdots, \theta_n)$

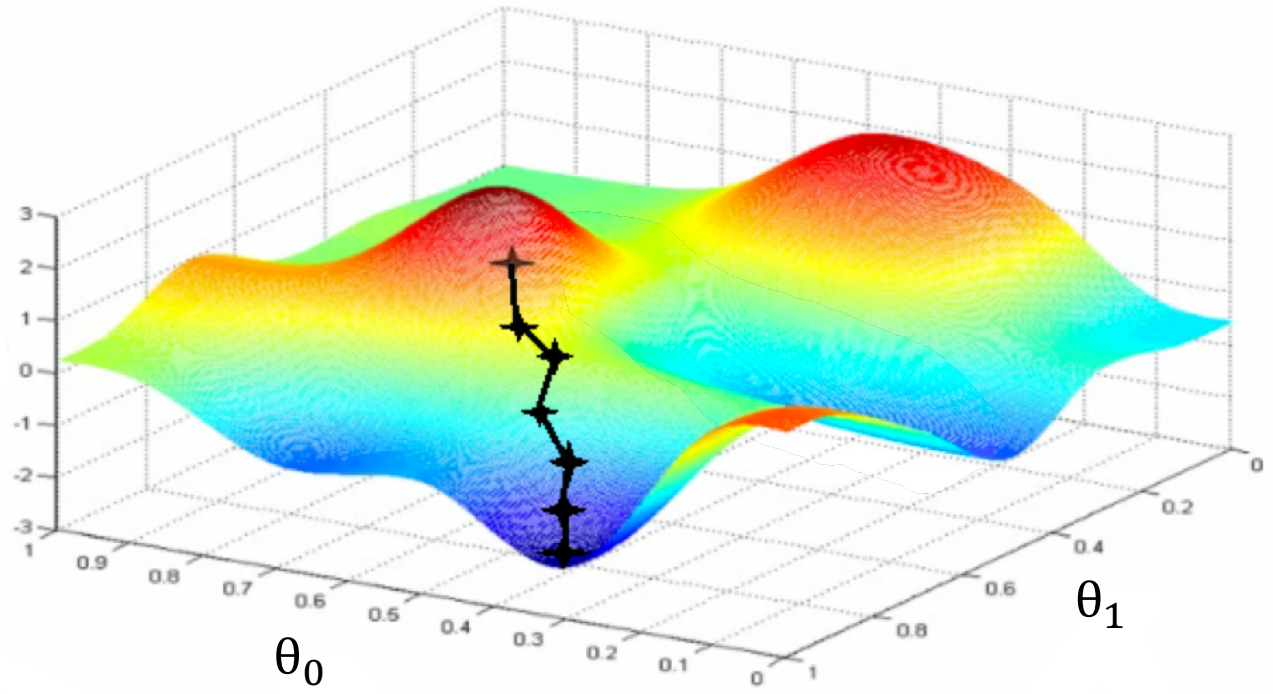
Algorithm

$J(\theta_0, \theta_1)$



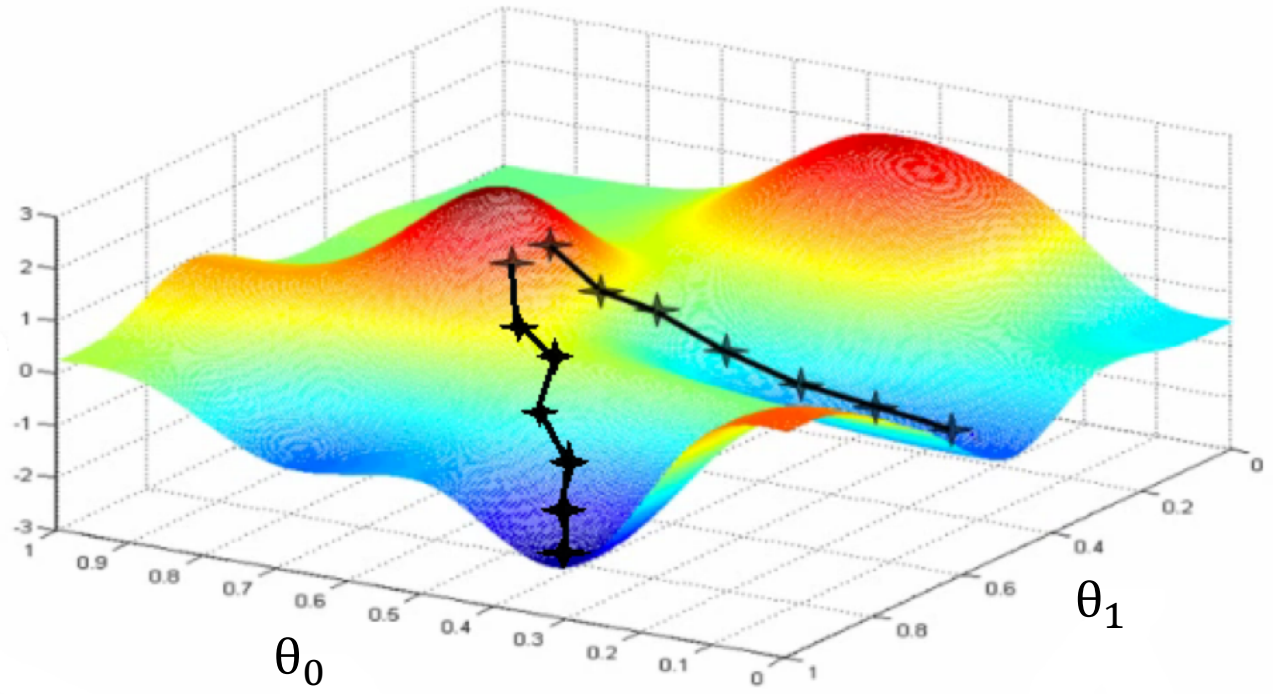
Algorithm

$J(\theta_0, \theta_1)$



Algorithm

$J(\theta_0, \theta_1)$



Algorithm

learning rate

for a given number of epochs/iterations

repeat until convergence {

$$temp_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

$$temp_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

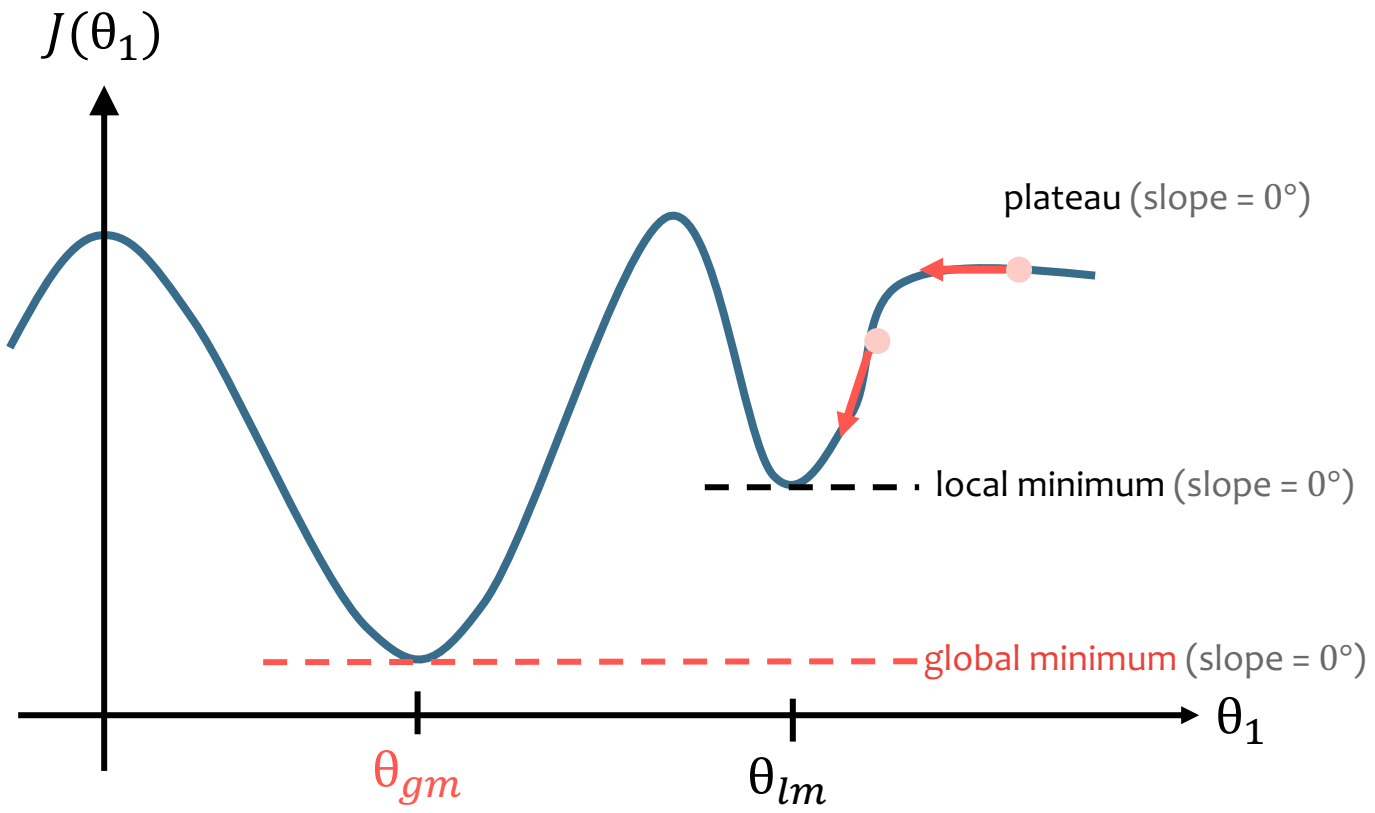
$$\theta_0 = temp_0$$

$$\theta_1 = temp_1$$

}

Local and global minima

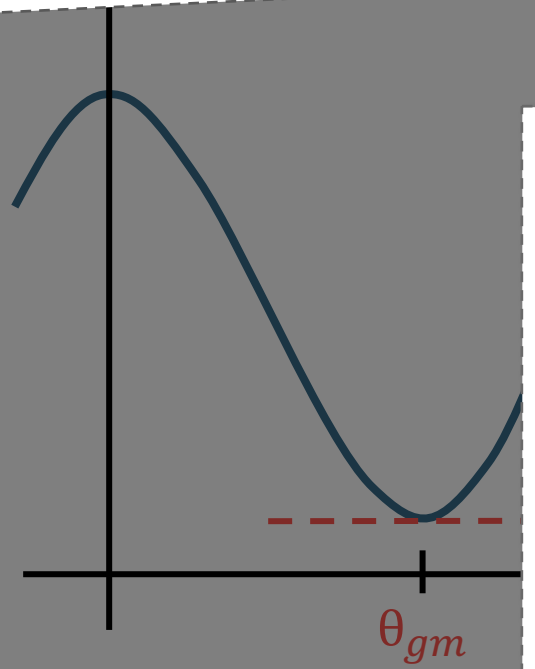
- **Gradient descent** approach usually presents some pittfals like local **minimum** or **plateaus**.



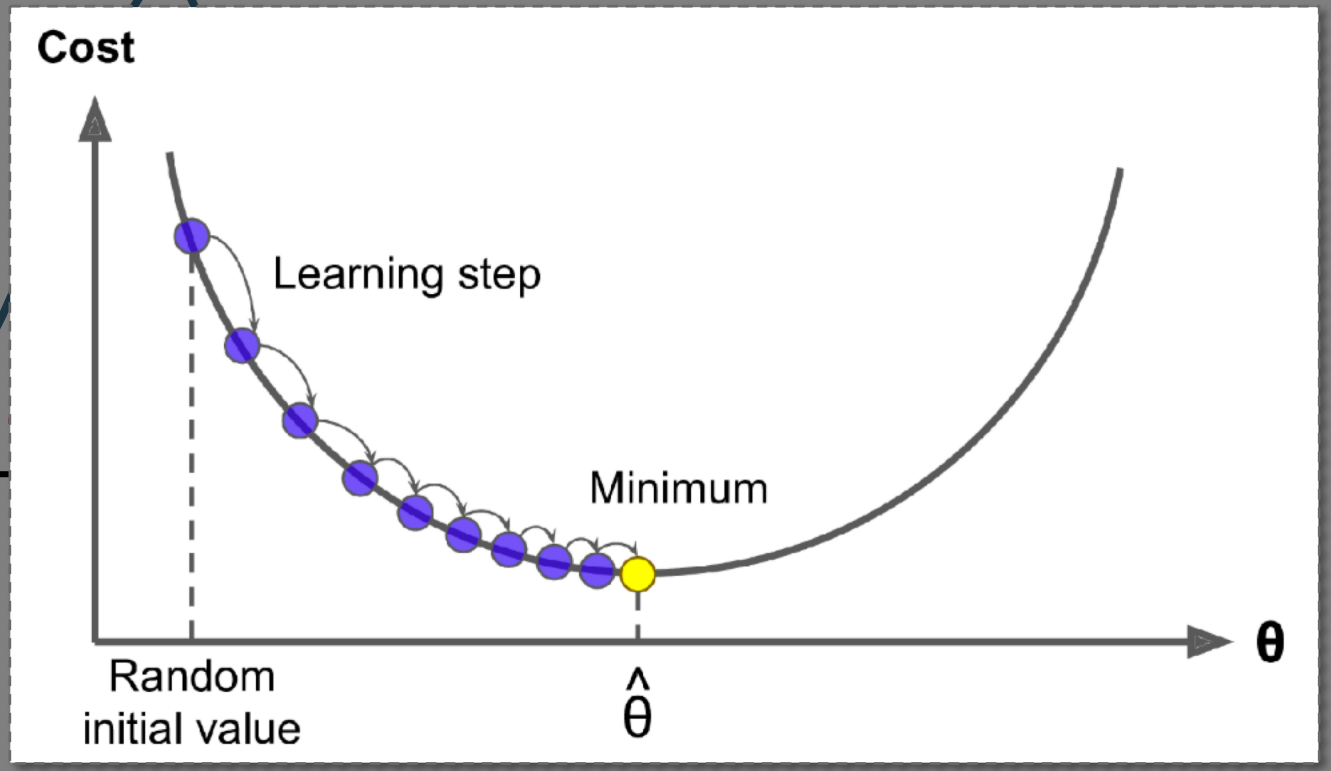
Local and global minima

- **Gradient descent** approach usually presents some pitfals like local **minima** and **plateaus**.

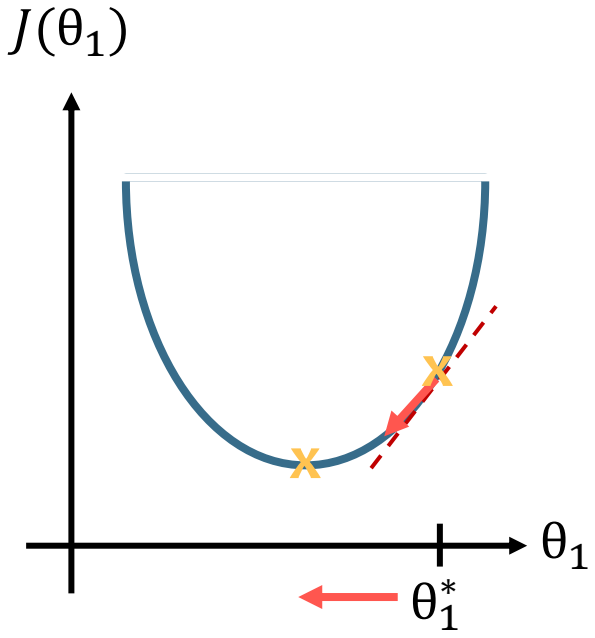
Fortunately, the **MSE** cost function for a Linear Regression is a **convex functions.**
This means that:
- There are no local minima, **just the global minimum**;
- Function never changes abruptly.



plateau (slope = 0°)

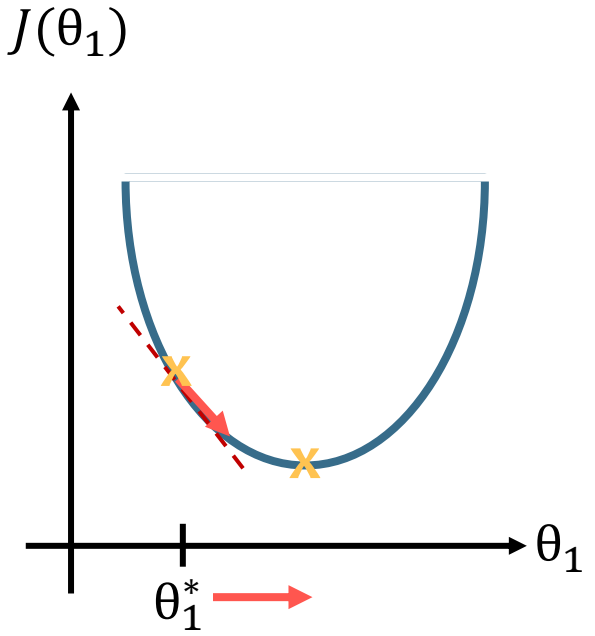


Updates



$$\theta_1 = \theta_1 - \alpha \boxed{\frac{\partial}{\partial \theta_1} J(\theta_1)}$$

≥ 0



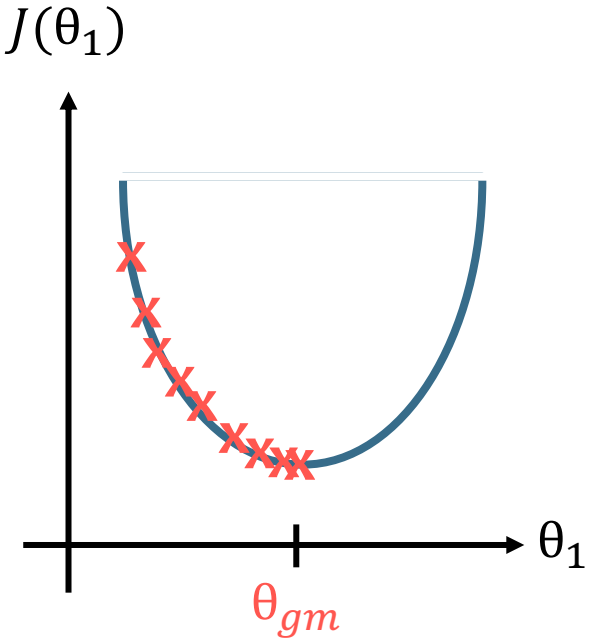
$$\theta_1 = \theta_1 - \alpha \boxed{\frac{\partial}{\partial \theta_1} J(\theta_1)}$$

≤ 0

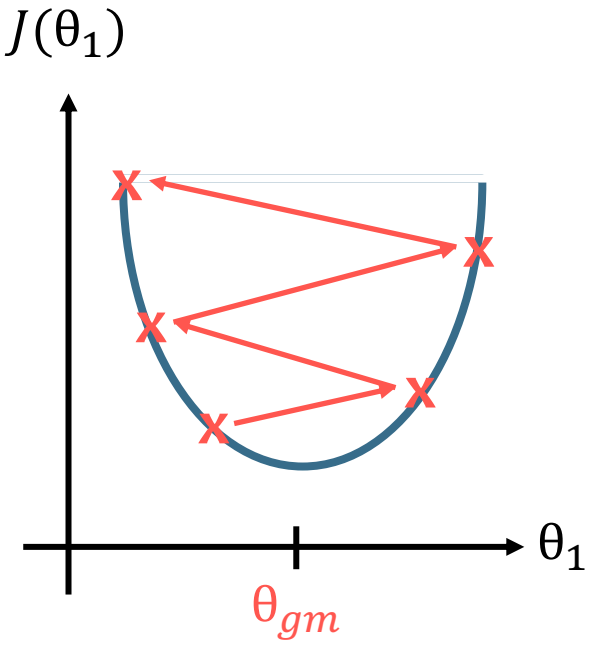
Learning rate

$$\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

If α is **too small**, gradient descent can be slow.



If α is **too large**, gradient descent can be overshoot the minimum, fail to converge, or even diverge.



Implementation Strategies for GD

Batch Gradient Descent

- Each iteration of the gradient descent (GD) training uses **all samples** of the **training set X**:

Algorithm:

1. Initialize $\theta_0, \theta_1, \cdots, \theta_n$ arbitrarily (*e.g.*, $\theta_0 = 0, \theta_1 = 0, \cdots, \theta_n = 0$)
2. **repeat until convergence**: *// (e.g., for a given number of epochs/iterations)*
3. $\hat{y} = h_\theta(\mathbf{X})$ *// predict all samples in* $\boldsymbol{X}$
4. Compute $J(\theta_0, \theta_1, \cdots, \theta_n)$ *// based on* y *and* $\hat{y}$
5. Change $\theta_0, \theta_1, \cdots, \theta_n$ **to reduce** $J(\theta_0, \theta_1, \cdots, \theta_n)$

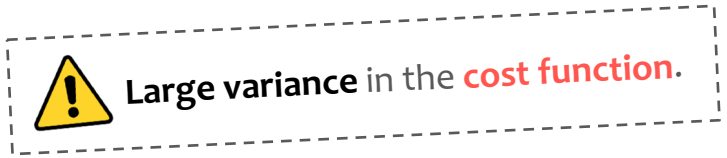
Impractical for **large training set.**

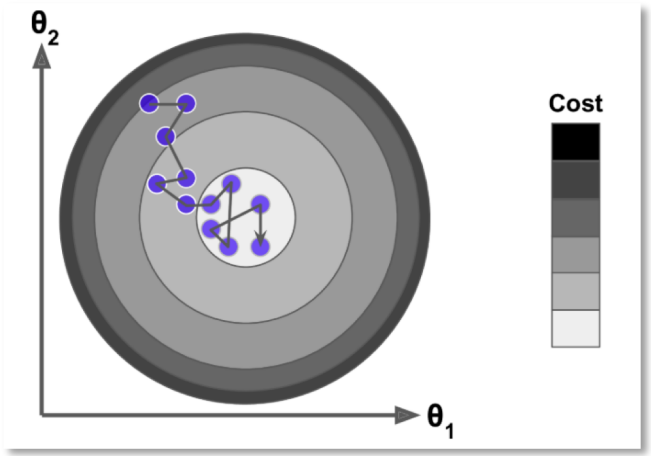
Stochastic Gradient Descent (SGD)

- Each iteration of the GD training uses **only one sample** of the **training set** chosen **randomly**.

Algorithm:

1. Initialize $\theta_0, \theta_1, \cdots, \theta_n$ arbitrarily (*e.g.*, $\theta_0 = 0, \theta_1 = 0, \cdots, \theta_n = 0$)
2. **repeat until convergence**: *// (e.g., for a given number of epochs/iterations)*
3. Shuffle $\langle \mathbf{X}, \boldsymbol{y} \rangle$
4. for each sample $\boldsymbol{x}^{(i)}$ in shuffled $\mathbf{X}$:
5. $\hat{y}^{(i)} = h_\theta(\boldsymbol{x}^{(i)})$ *// predict* $\boldsymbol{x}^{(i)}$
6. Compute $J(\theta_0, \theta_1, \cdots, \theta_n)$ *// based on shuffled* y *and* $\hat{y}$
7. Change $\theta_0, \theta_1, \cdots, \theta_n$ **to reduce** $J(\theta_0, \theta_1, \cdots, \theta_n)$





Mini-batch Gradient Descent

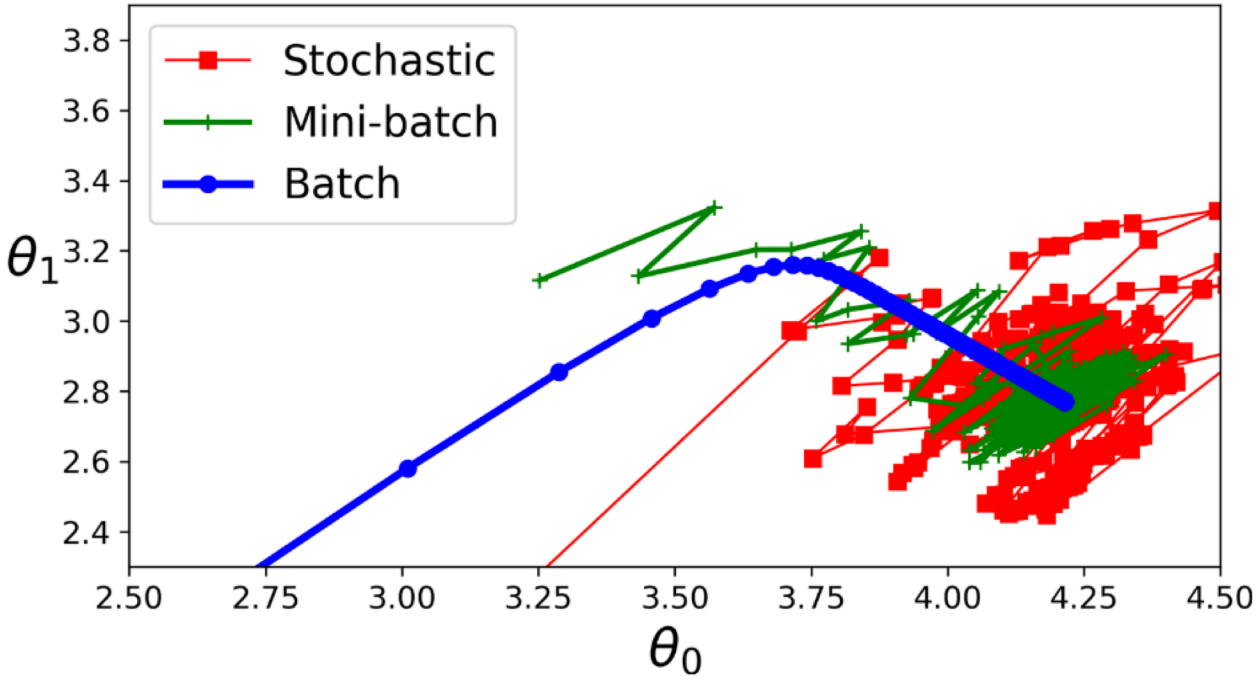
- Each iteration of the GD training uses k (min-batch size) samples of the training set chosen **randomly**.

Algorithm:

1. Initialize $\theta_0, \theta_1, \cdots, \theta_n$ arbitrarily (*e.g.*, $\theta_0 = 0, \theta_1 = 0, \cdots, \theta_n = 0$)
2. **repeat until convergence**: *// (e.g., for a given number of epochs/iterations)*
3. for each batch iteration: *// based on the batch size and training set size*
4. $\mathbf{X_b}, y_b$ = draw **k random samples** with replacement in $\langle \mathbf{X}, \boldsymbol{y} \rangle$
5. $\hat{y}_b = h_\theta(\mathbf{X_b})$ *// predict the mini batch* $\mathbf{X_b}$
6. Compute $J(\theta_0, \theta_1, \cdots, \theta_n)$ *// based on* y_b *and* $\hat{y}_b$
7. Change $\theta_0, \theta_1, \cdots, \theta_n$ **to reduce** $J(\theta_0, \theta_1, \cdots, \theta_n)$

It requires an additional **"mini-batch size"** hyperparameter for the learning algorithm.

Convergence



Closed-form solutions to train a Linear Regressor Model

Normal Equation

- It is an analytical approach to Linear Regression to find out the parameters $\boldsymbol{\theta}$.
- In other words, it is a mathematical equation that gives the result directly.

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(\mathbf{x}^{(i)}) - y^{(i)})^2$$

$$\frac{\partial}{\partial \theta_j}J(\theta) = \cdots = \mathbf{0}, \text{ solve for } \theta_0, \theta_1, \ldots, \theta_n$$

$$\hat{\theta} = (X^T X)^{-1} X^T y$$

not always *invertible*

SVD strategy

- $\hat{\theta} = X^{+} y$
- Strategy that uses the Singular Value Decomposition (SVD) to compute a pseudoinverse matrix to find the parameters $\boldsymbol{\theta}$.

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$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(\mathbf{x}^{(i)}) - y^{(i)})^2$$

$$\frac{\partial}{\partial \theta_j} J(\theta) = \cdots = \mathbf{0}, \text{ so } \theta_0, \theta_1, \ldots, \theta_n$$

The Normal Equation and the SVD approach get **very slow** when **the number of features grows large** (e.g., 100,000).

$$\hat{\theta} = (\mathrm{X}^T \mathrm{X})^{-1}\ \mathrm{X}^T y$$

not always *invertible*

On the positive side, both are **linear** with regard to the number of **training instances** (they are O(m)), so **they handle large training sets efficiently**, provided they can fit in memory

SVD strategy

- $\hat{\theta} = \mathrm{X}^{+} y$
- Strategy that uses the Singular Value Decomposition (SVD) to compute a pseudoinverse matrix to find the parameters $\boldsymbol{\theta}$.

There is almost **no difference** after **training**:
all these algorithms end up with very **similar models**
and **make predictions** in exactly **the same way**.

Table 4-1. Comparison of algorithms for Linear Regression

Algorithm	Large *m*	Out-of-core support	Large *n*	Hyperparams	Scaling required	Scikit-Learn
Normal Equation	Fast	No	Slow	0	No	N/A
SVD	Fast	No	Slow	0	No	`LinearRegression`
Batch GD	Slow	No	Fast	2	Yes	`SGDRegressor` ????
Stochastic GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`
Mini-batch GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor` ????

To check manual implementations of those algorithms, we refer to this GitHub repository.

Aprendizado de Máquina e Reconhecimento de Padrões 2021.2

Linear Regression and Gradient Descent

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