Numerical Optimization for ML&DL (NOFML&DL)

Information Technology Institute

Agenda

Why Numerical Optimization?

The Machine Learning Problem.

Analytic, Algebraic and Numerical Solutions.

Numerical Optimization.

Single Variable Linear Regression.

Vector Norms and Loss Function

Gradient

Gradient Descent (GD) Algorithm.

The Machine Learning Problem

Data at hand is just a sample data.

Definite solution does not generalize the model.

We need to find an approximate solution to generalize the model.

Learning is no more than finding the optimal model parameters that minimizing the prediction error.

Analytic Solution

- An analytic solution involves framing the problem in a well-understood form and calculating the exact solution. **(can be done by hand)**.
- We prefer the analytical method in general because it is faster and because the solution is exact.
- If our data matrix is square, we can find model parameters by solving system of linear equations $\boldsymbol{X\theta = y \Rightarrow \theta = X^{-1}y}$
- **However, this solution is not general. i.e., it is only available for the data at hand (training data).**

Approximate Solution

- In general, data matrix $(\boldsymbol{X}_{\boldsymbol{m}\times\boldsymbol{n}})$ is not square. i.e.;
  - $\boldsymbol{m} > \boldsymbol{n}$ (no solution)
  - or $\boldsymbol{m} < \boldsymbol{n}$ (infinite number of solutions exist)
- In this case we will not have a definite solution.
- In order to solve this problem, we use approximation. i.e., find an approximate solution.

Algebraic Solution

- In case of linear models (e.g., linear regression), we can obtain the approximate solution algebraically (find a closed-form solution).
- For $\boldsymbol{m} > \boldsymbol{n}$ (overdetermined system) we can use least-squares method

$$\boldsymbol{\theta} = \left(\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{X}\right)^{-\mathbf{1}}\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{y}$$

- However, if $\boldsymbol{n}$ is large $\left(\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{X}\right)^{-\mathbf{1}}$ will be computationally expensive.
- The computational burden stems from both forming $\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{X}$ and inverting an $n \times n$ matrix.
- (this approach can also be numerically unstable for large or ill-conditioned matrices)

Algebraic Solution

- For $\boldsymbol{m} < \boldsymbol{n}$ (underdetermined system) we can use the least-norm method

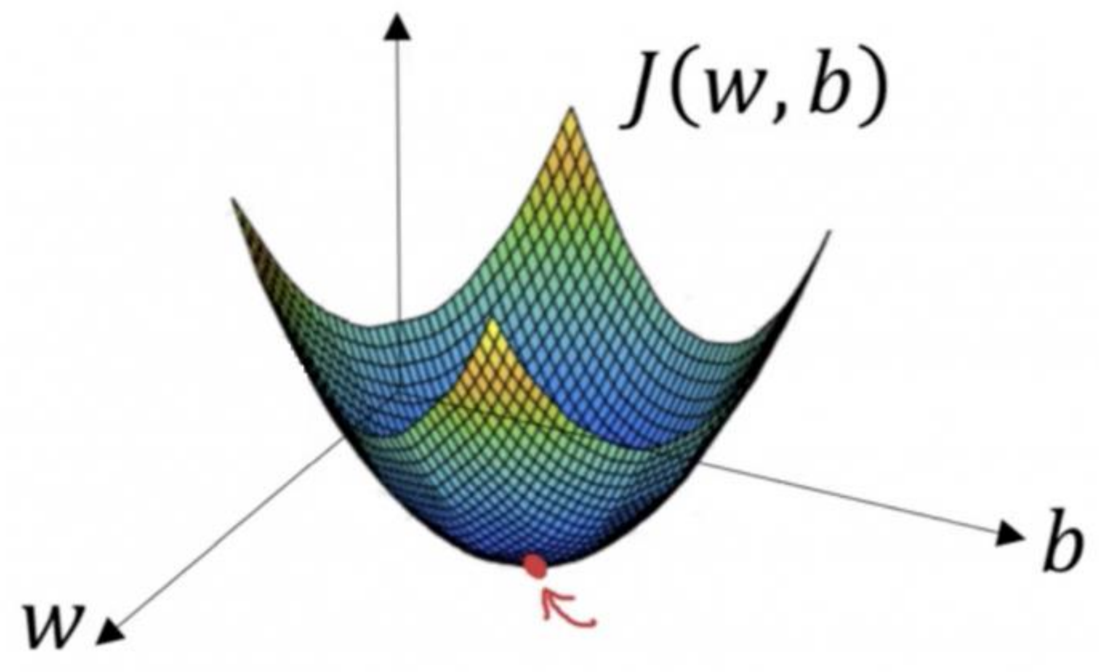
$$\boldsymbol{\theta} = \boldsymbol{X}^{\boldsymbol{T}}\left(\boldsymbol{X}\boldsymbol{X}^{\boldsymbol{T}}\right)^{-\mathbf{1}}\boldsymbol{y}$$

- However, if $\boldsymbol{m}$ is large $\left(\boldsymbol{X}\boldsymbol{X}^{\boldsymbol{T}}\right)^{-\mathbf{1}}$ will be computationally expensive.

- In addition, if the model is nonlinear in the parameters, algebraic (closed-form) solutions generally do not exist, and iterative numerical methods must be used. This is the case for artificial neural networks

Numerical Optimization

- Keep iterating until we reach the minimum error. i.e., finding the values of model parameters that minimizes/maximizes the loss/cost/error function.
- These parameters range from simple linear regression model to weights and biases for deep neural networks. The same concept is applied.



Numerical Solution

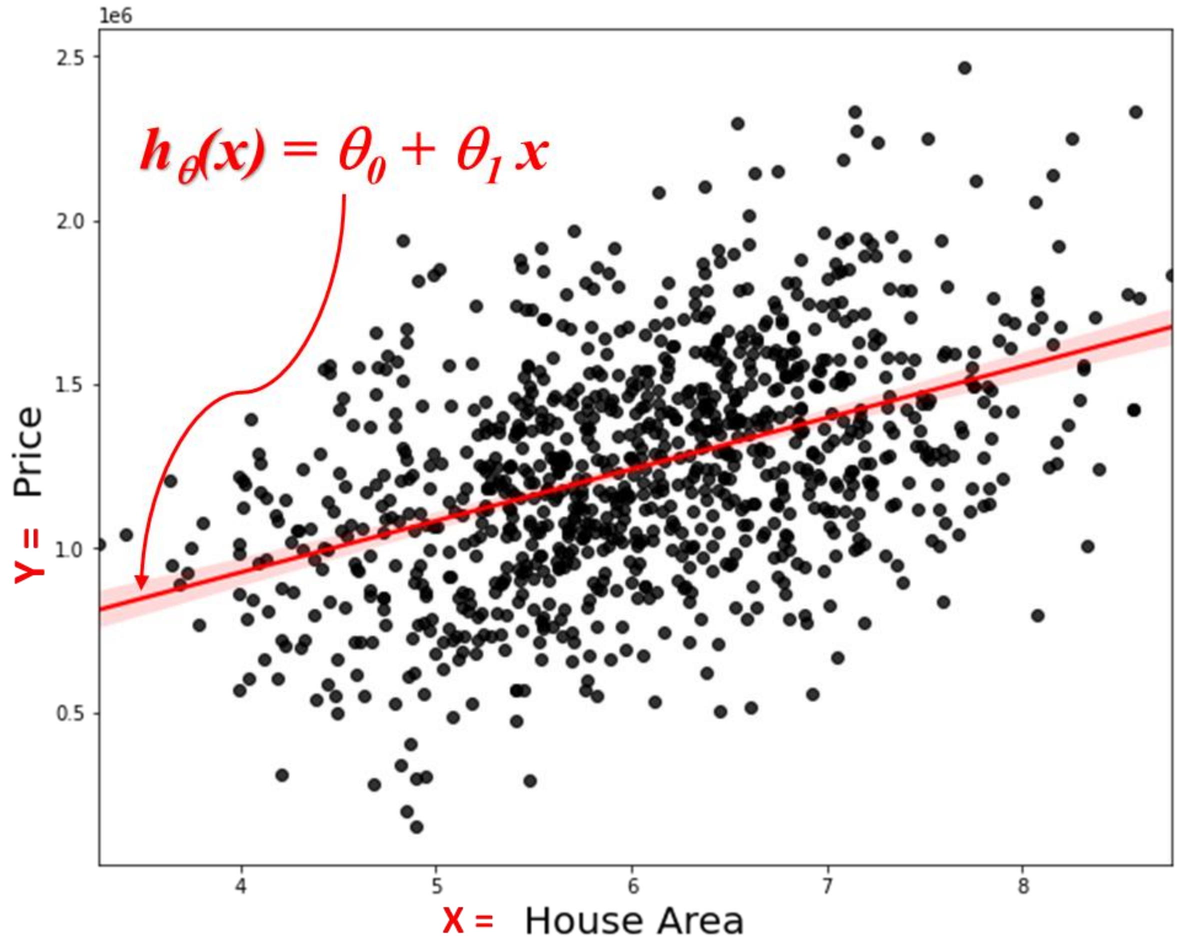
- Loosely speaking, after deciding the model (e.g., single-variable linear regression), and the objective function, numerical solution involves the following steps:

1. Parameters initialization (assume $\boldsymbol{\theta_0} = \boldsymbol{\theta_1} = \mathbf{0}$).
2. Predict the output using $\hat{\boldsymbol{y}} = \boldsymbol{\theta_0} + \boldsymbol{\theta_1 x}$.
3. Evaluate the prediction error using any error function e.g., $|\hat{\boldsymbol{y}} - \mathbf{y}|$.
4. Find the direction and magnitude of changing the model parameters $(\boldsymbol{\theta_0}, \boldsymbol{\theta_1})$ to decrease the error.
5. Update model parameters.
6. Go to step 2 (repeat until convergence).

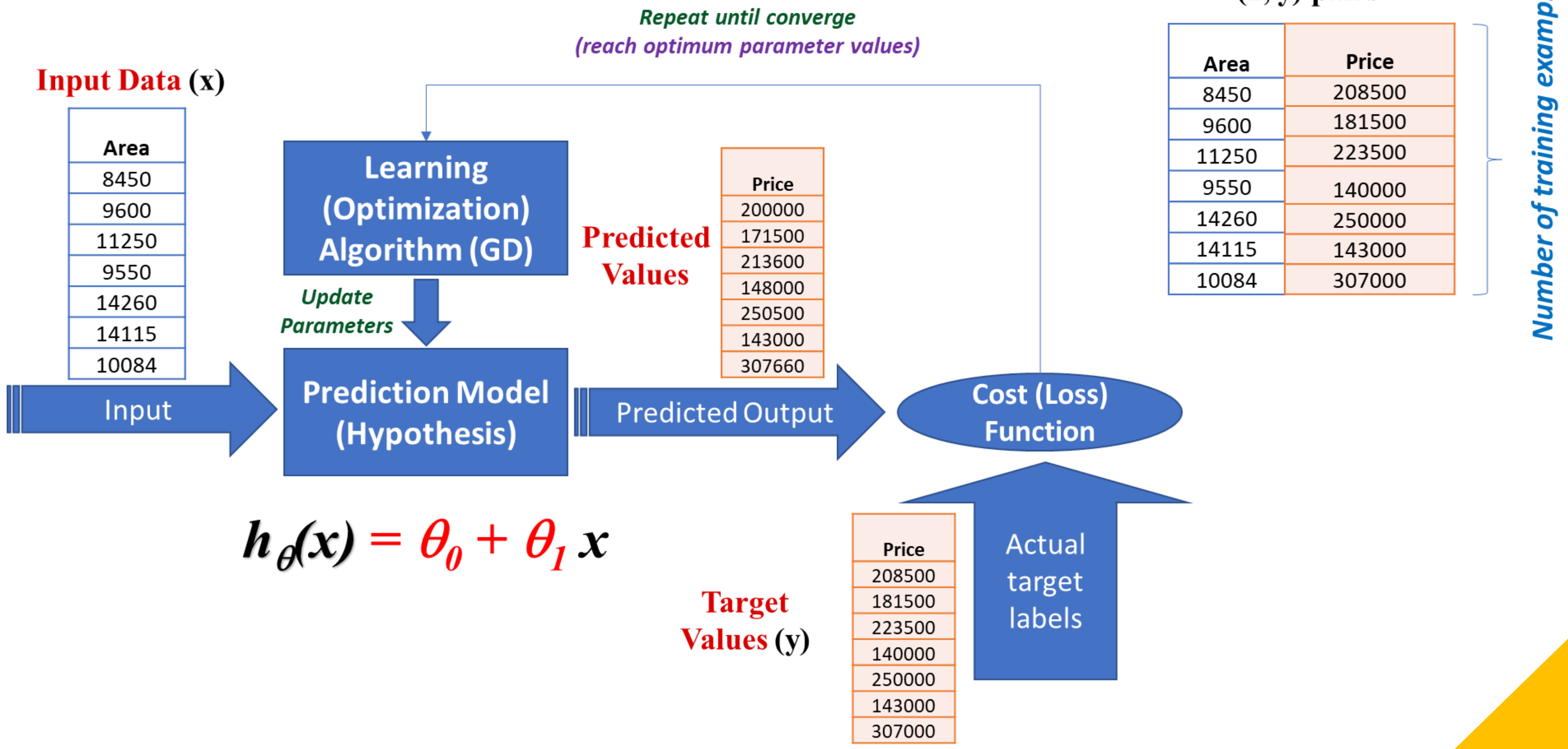
Single Variable Linear Regression (LR)

$h_\theta(x) = \theta_0 + \theta_1 x$

(hypothesis)



Single Variable Linear Regression (LR)



Input Data (x)

Area
8450
9600
11250
9550
14260
14115
10084

Predicted Values

Price
200000
171500
213600
148000
250500
143000
307660

Target Values (y)

Price
208500
181500
223500
140000
250000
143000
307000

Training Data
(x, y) pairs

Area	Price
8450	208500
9600	181500
11250	223500
9550	140000
14260	250000
14115	143000
10084	307000

$$h_\theta(x) = \theta_0 + \theta_1 x$$

Numerical Solution

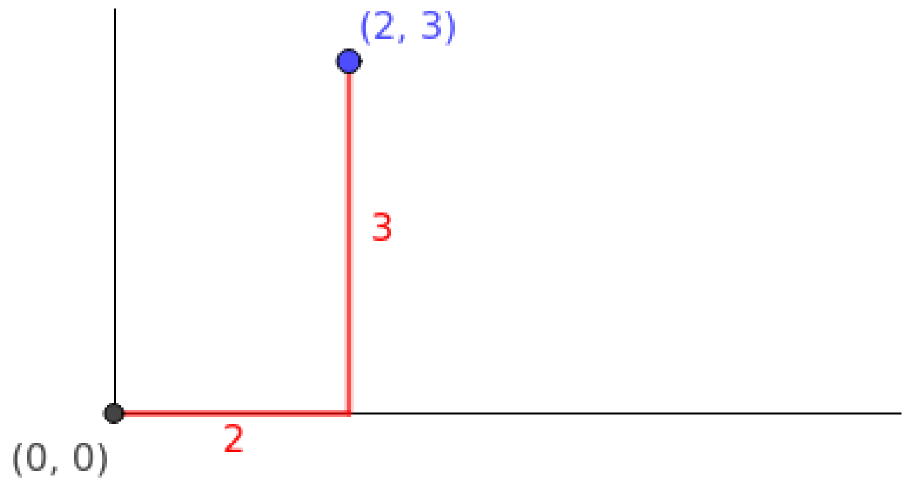
- Loosely speaking, after deciding the model (e.g., single-variable linear regression), and the objective function, numerical solution involves the following steps:

1. Parameters initialization (assume $\boldsymbol{\theta_0 = \theta_1 = 0}$).
2. Predict the output using $\boldsymbol{\hat{y} = \theta_0 + \theta_1 x}$.
3. **Evaluate the prediction error using any error function** e.g., $|\boldsymbol{\hat{y} - \mathrm{y}}|$.
4. Find the direction and magnitude of changing the model parameters (θ_0, θ_1) to decrease the error.
5. Update model parameters.
6. Go to step 2 (repeat until convergence).

Vector Norms

- The ***L^1 norm***, also known as the **Manhattan (Taxicab) norm**, is the sum of absolute vector components and forms the basis of MAE loss and LASSO regularization.

- Note that MAE is not the norm itself, but a **scaled L^1 loss**.



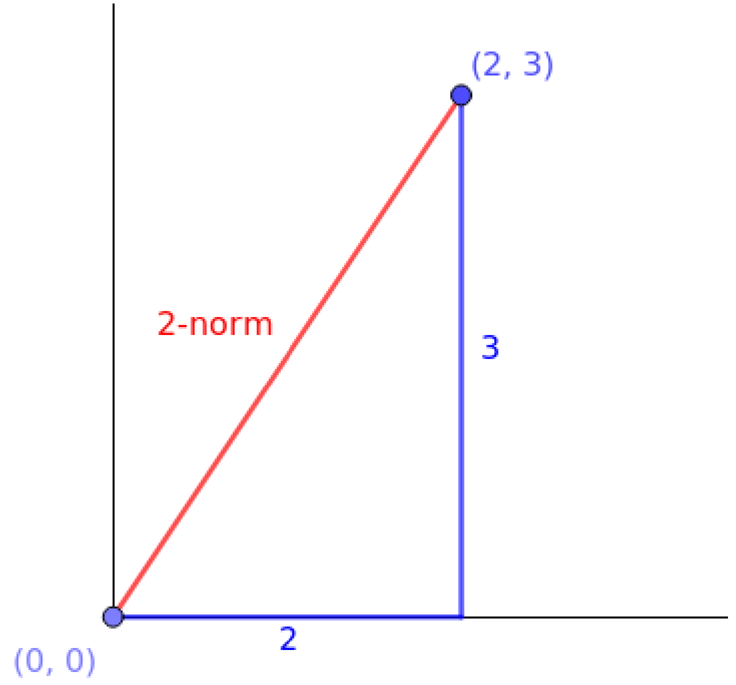
$$\|\mathbf{x}\|_1 = \sum_{i=1}^{N} |x_i| = |x_1| + |x_2| + \ldots + |x_N|$$

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n} |y_i - \hat{y}_i|$$

Vector Norms

- The ***L²* (*Euclidean*) *Norm*** is the square root of the sum of squared vector components and induces the straight-line (Euclidean) distance.

- In regression, the squared L² norm of the residual vector $(\mathbf{y} - \hat{\mathbf{y}})$ gives the **Sum of Squared Residuals (SSR)**,
- Dividing SSR by the number of samples m gives the **Mean Squared Error (MSE)**.



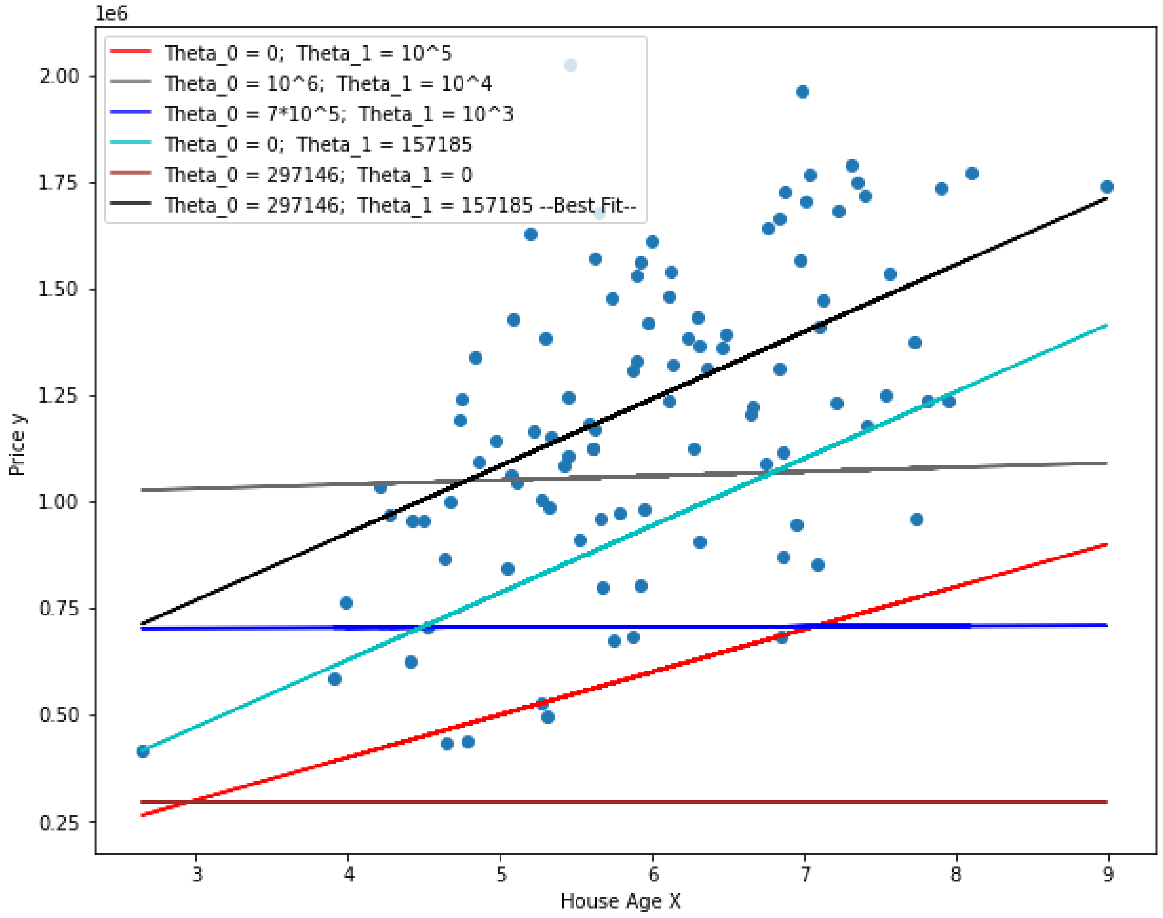
$$\|\mathbf{x}\|_2 = \left(\sum_{i=1}^{N} |x_i|^2\right)^{1/2} = \sqrt{x_1^2 + x_2^2 + \ldots + x_N^2}$$

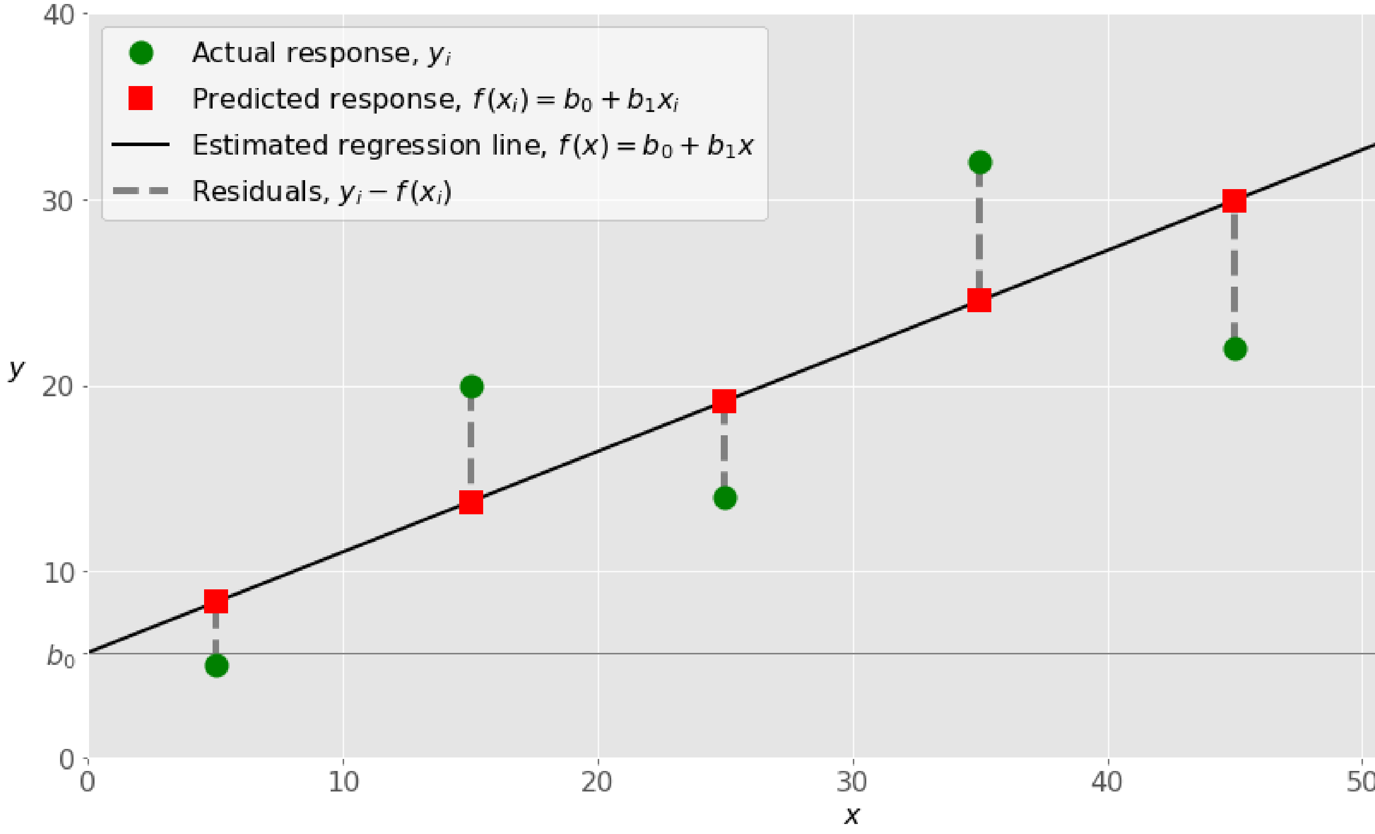
$$\mathrm{SSR} = \|\mathbf{y} - \hat{\mathbf{y}}\|_2^2 = \sum_{i=1}^{m} (y_i - \hat{y}_i)^2$$

$$\mathrm{MSE} = \frac{1}{m}\|\mathbf{y} - \hat{\mathbf{y}}\|_2^2$$

Loss (Cost) Function

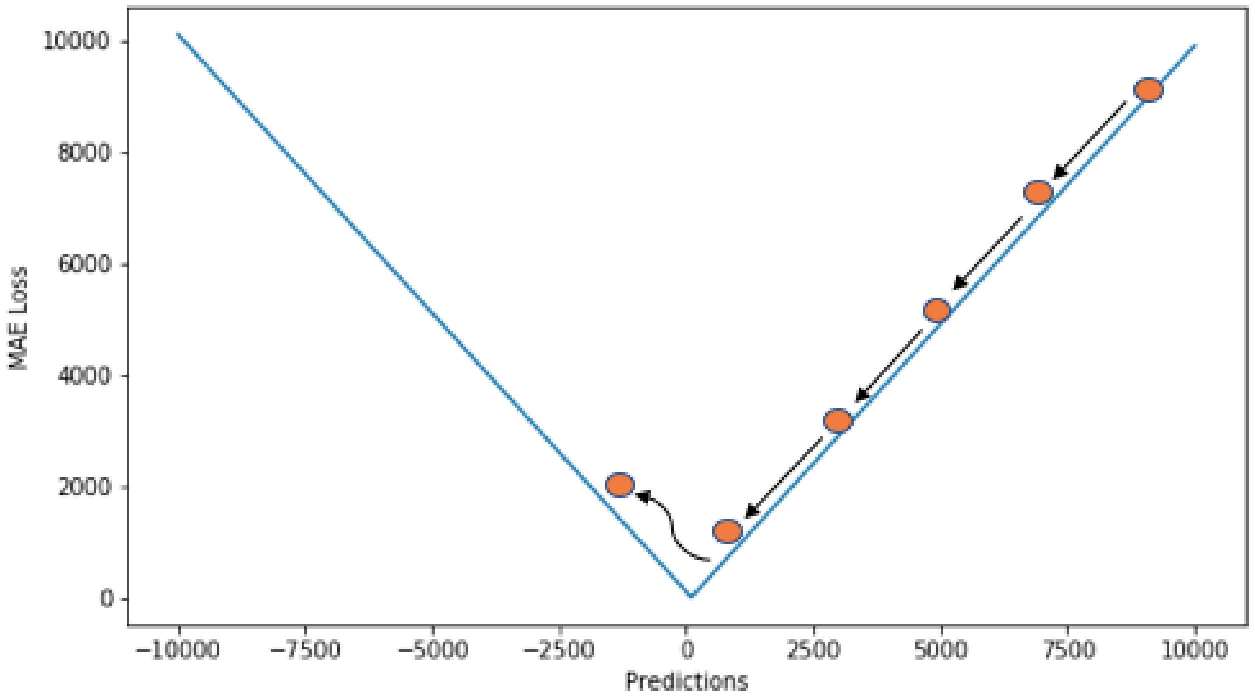
- Residual is a norm of two vectors subtraction.
- Each parameter pairs give different fit.





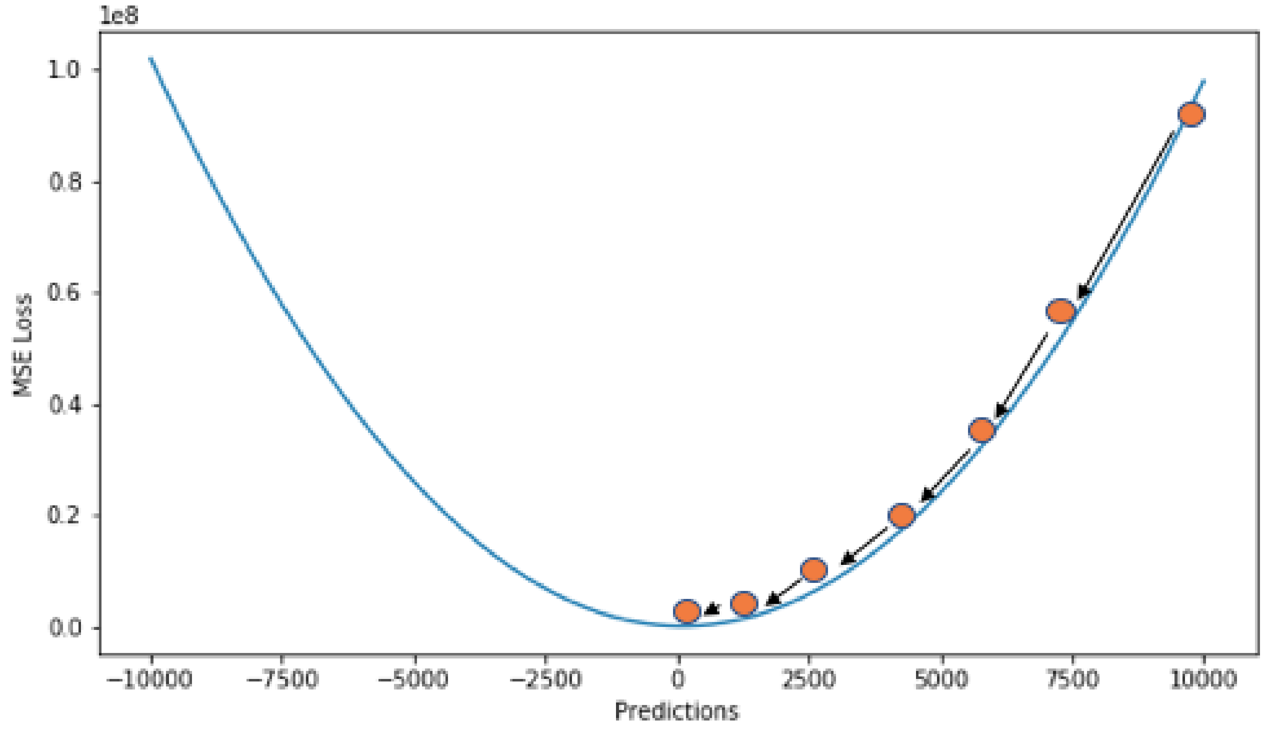
Loss (Cost) Function

- **Mean Absolute Error (MAE) (L1 Loss Function)** is used to minimize the error which is the sum of the all the **absolute** differences between the true value and the predicted value.
- $\boldsymbol{MAE = \frac{1}{m}\sum_{i=1}^{m}|\hat{y} - y|}$
- MAE is robust to outliers. However, it has a constant gradient, and the gradient is not defined at the minimum.



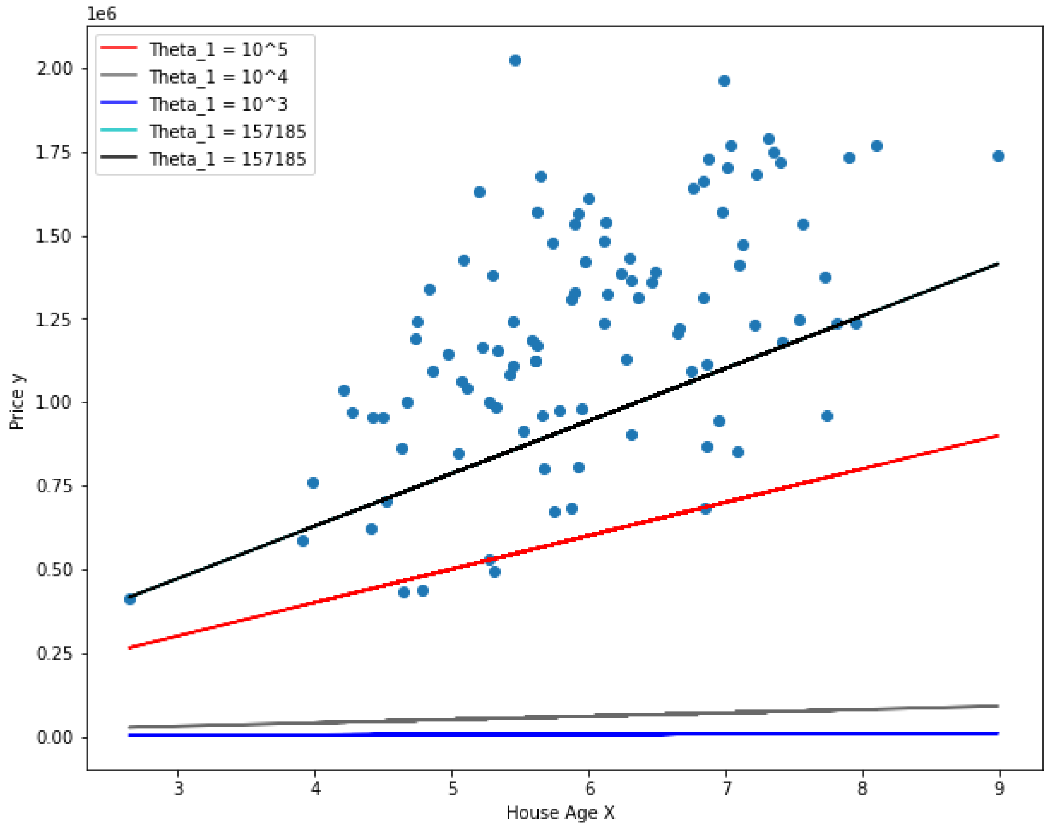
Loss (Cost) Function

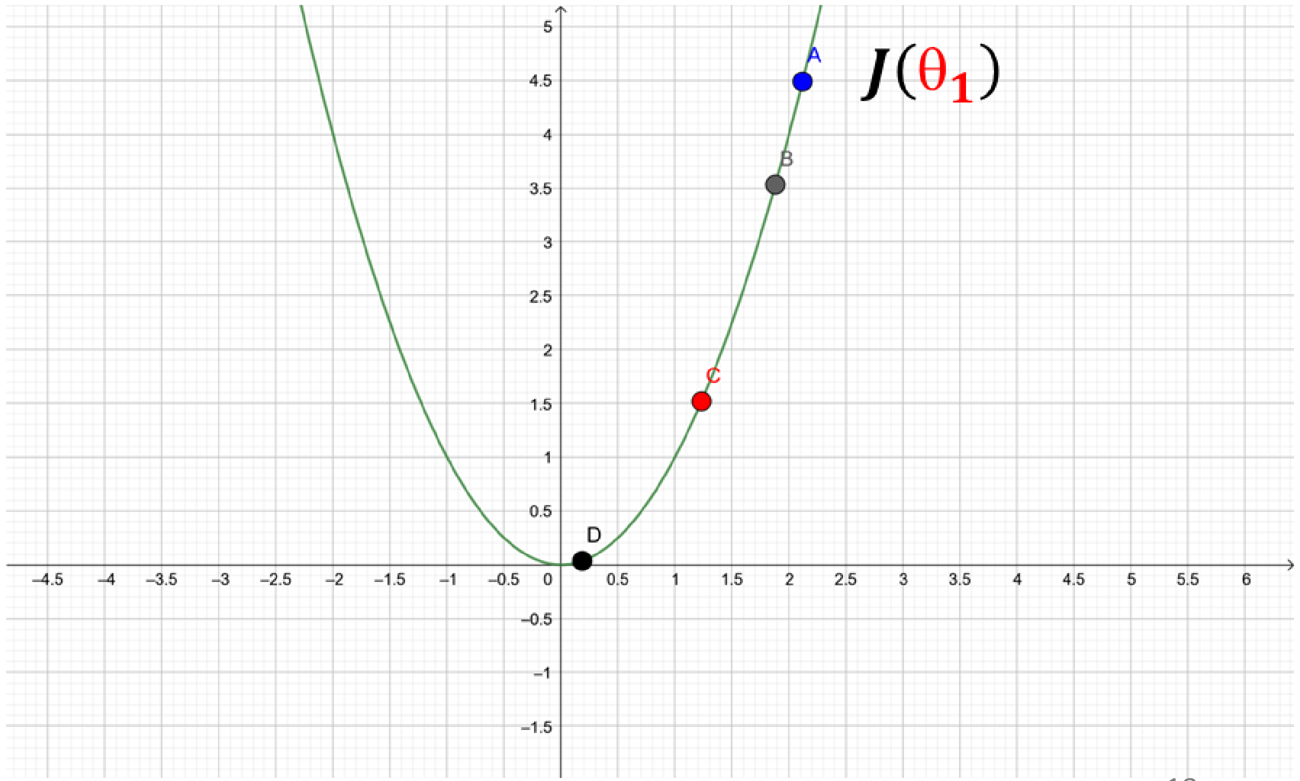
- **Mean Squared Error (MSE) (L2 Loss Function)** is used to minimize the error which is the sum of the all the **squared** differences between the true value and the predicted value.
- $\boldsymbol{MSE = \frac{1}{m}\sum_{i=1}^{m}(\hat{y} - y)^2}$
- MSE is not robust to outlier. However, it has a changing gradient that enables better learning.



Loss (Cost) Function

- For simplicity let $\theta_0 = \mathbf{0}$. *i.e.* $\boldsymbol{h}(\theta_1) = \theta_1 \boldsymbol{x}$
- We can plot loss as a function of θ_1 for different fits.
  $J(\theta_1) = \boldsymbol{predicted\ value - actual\ value}$

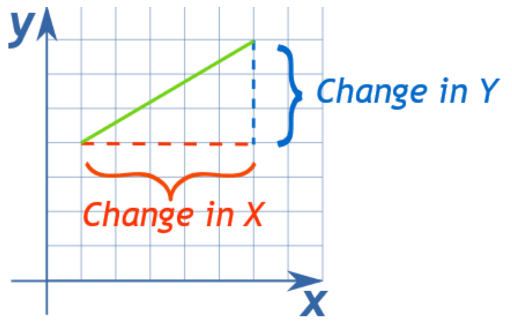


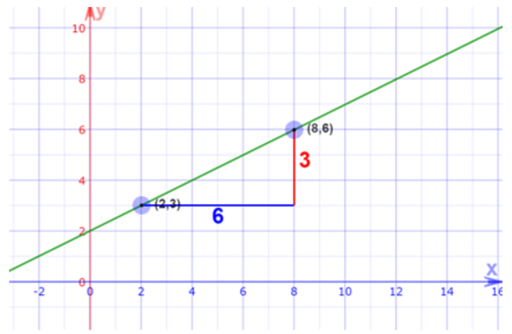


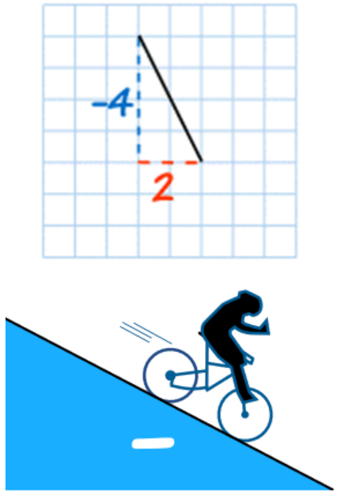
Numerical Solution

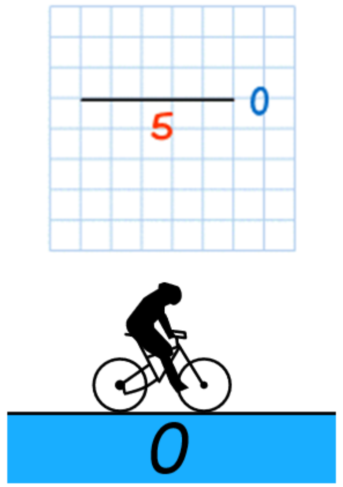
- Loosely speaking, after deciding the model (e.g., single-variable linear regression), and the objective function, numerical solution involves the following steps:

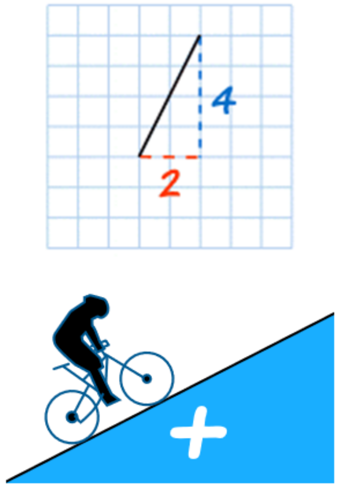
1. Parameters initialization (assume $\boldsymbol{\theta_0 = \theta_1 = 0}$).
2. Predict the output using $\boldsymbol{\hat{y} = \theta_0 + \theta_1 x}$.
3. Evaluate the prediction error using any error function e.g., $|\boldsymbol{\hat{y} - y}|$.
4. **Find the direction and magnitude of changing the model parameters $(\boldsymbol{\theta_0, \theta_1})$ to decrease the error.**
5. Update model parameters.
6. Go to step 2 (repeat until convergence).

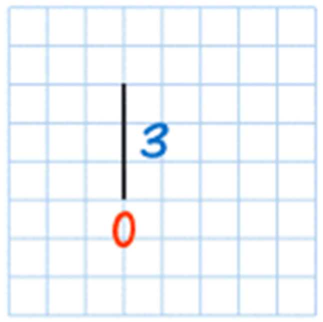












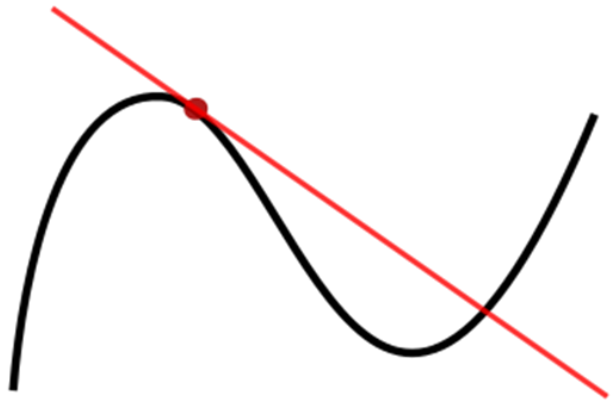
Undefined
Divide by zero

Gradient

- **What is the gradient?**
- **Gradient is the slope**
- $$\boldsymbol{Gradient = \frac{Change\ in\ Y}{Change\ in\ X} = \frac{Rise}{Run}}$$

Gradient

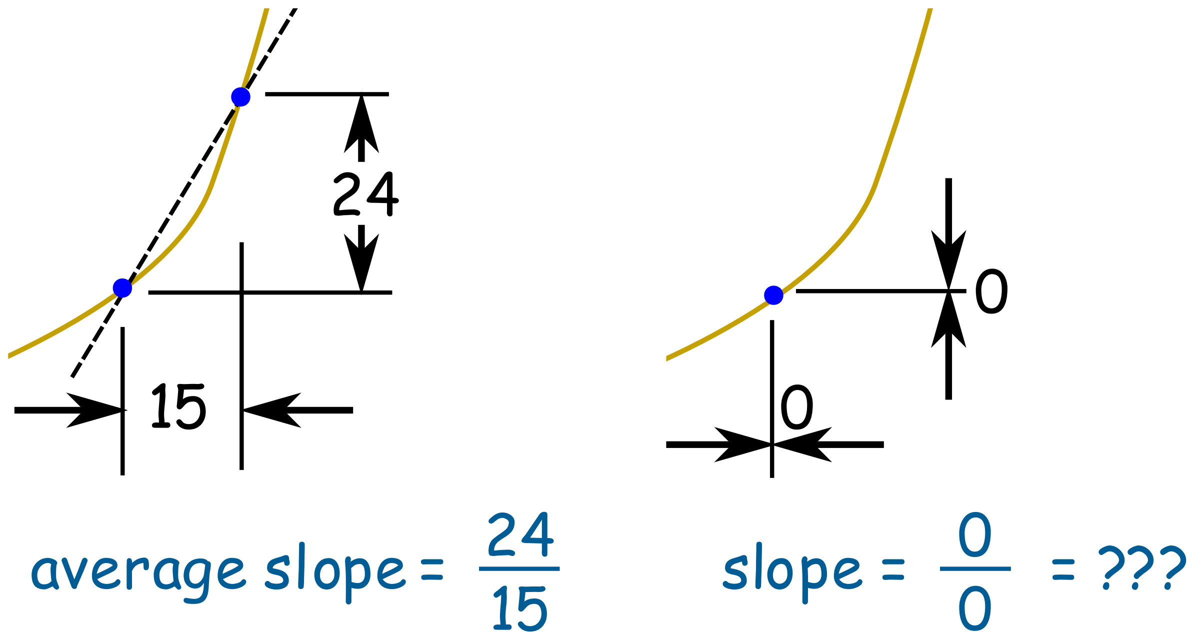
- The **derivative** of a function of a real variable measures the sensitivity to change of the function value (output value) with respect to a change in its argument (input value).
- For example, the derivative of the position of a moving object with respect to time is the object's velocity: this measures how quickly the position of the object changes when time advances.



The graph of a function, drawn in black, and a tangent line to that function, drawn in red. The slope of the tangent line is equal to the derivative of the function at the marked point.

Gradient

- We can find an average slope between two points.
- But how do we find the slope at a point?



average slope = $\frac{24}{15}$

slope = $\frac{0}{0}$ = ???

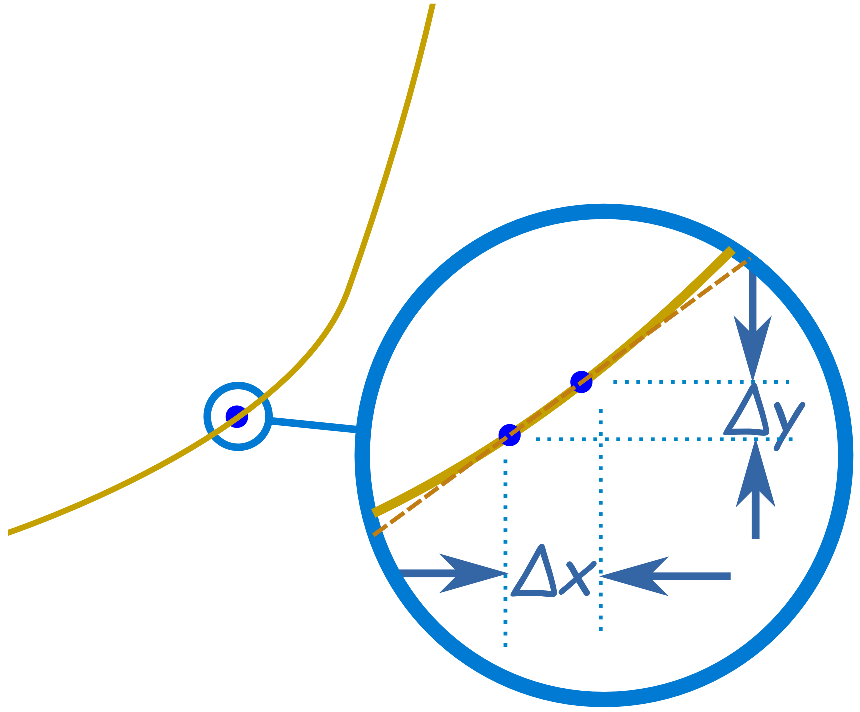
Gradient

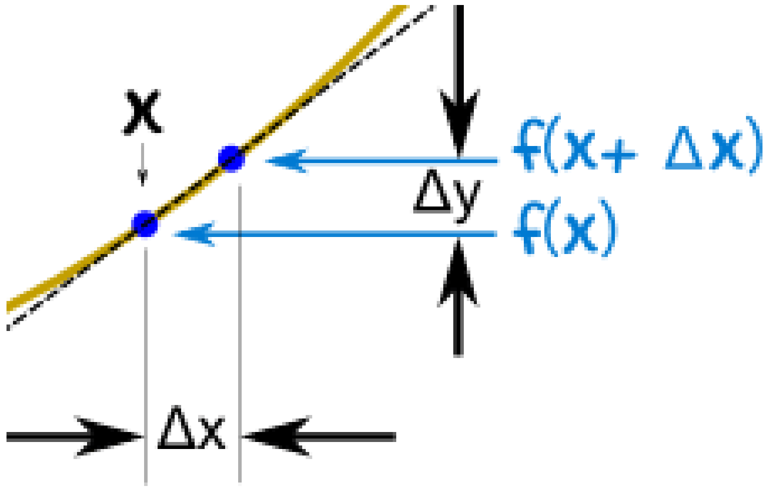
- But with derivatives we use a small difference then have it shrink towards zero

- $\frac{\Delta y}{\Delta x} = \frac{f(x+\Delta x) - f(x)}{\Delta x}$
- **Gradient at x = derivative at x**

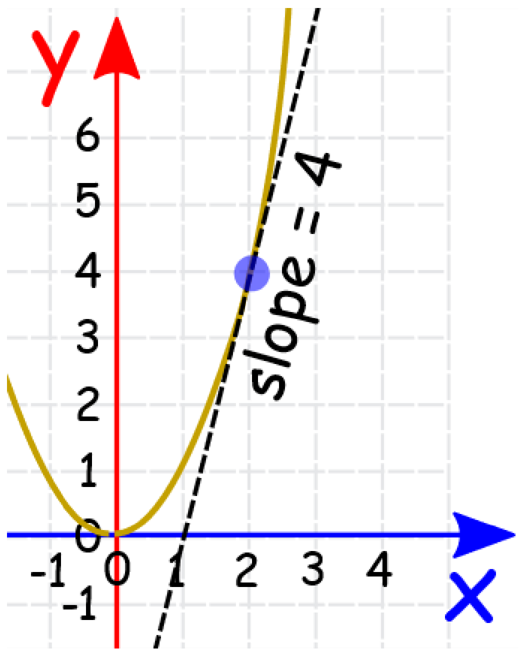
=

$$\lim_{\Delta x \to 0} \left(\frac{f(x+\Delta x) - f(x)}{\Delta x} \right)$$

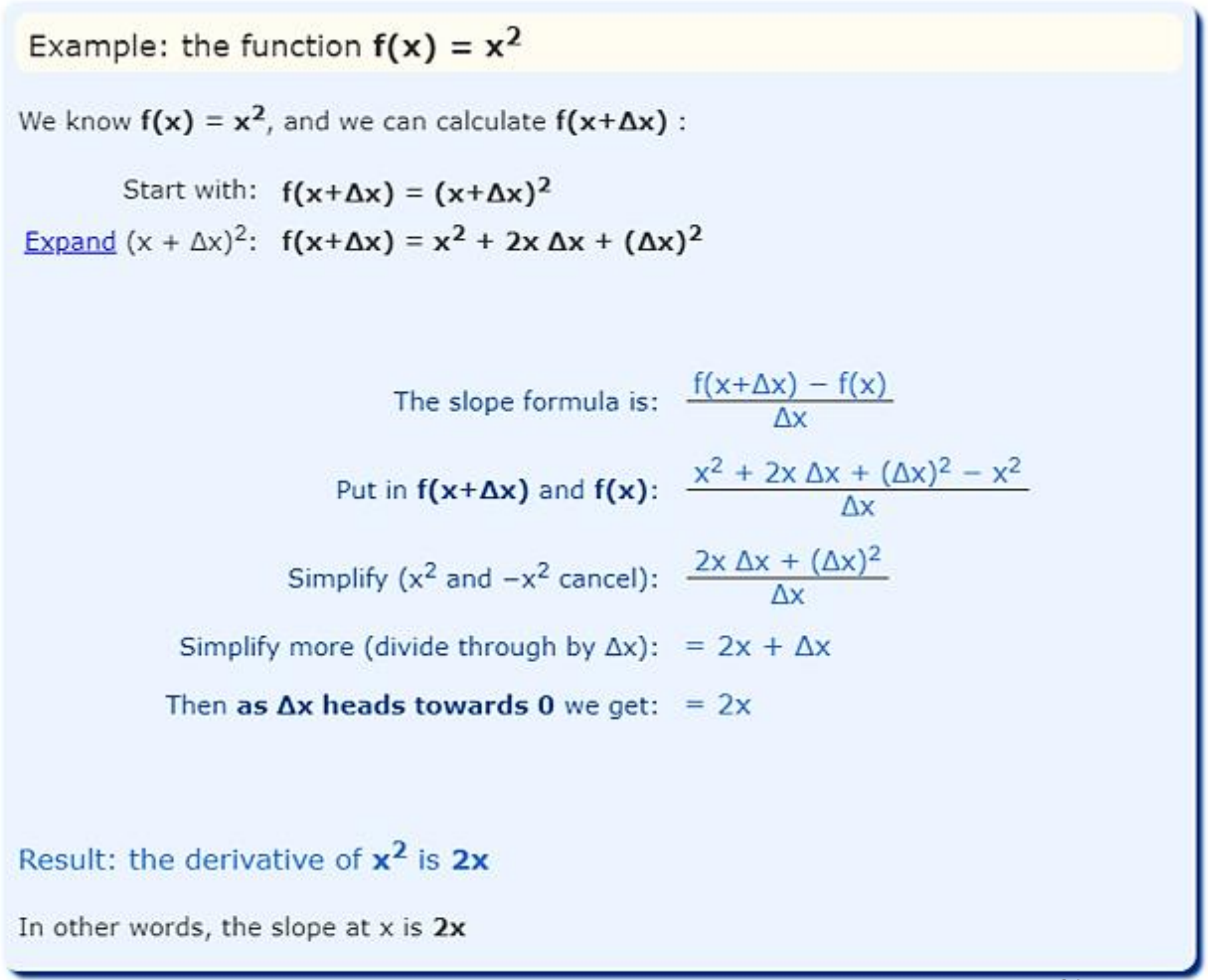




Gradient



$$f'(x) = \frac{d}{dx}(x^2) = 2x$$



Example: the function **f(x) = x^2**

We know **f(x) = x^2**, and we can calculate **f(x+Δx)** :

Start with: **f(x+Δx) = $(x+\Delta x)^2$**

Expand $(x + \Delta x)^2$: **f(x+Δx) = $x^2 + 2x\,\Delta x + (\Delta x)^2$**

The slope formula is: $\frac{f(x+\Delta x) - f(x)}{\Delta x}$

Put in **f(x+Δx)** and **f(x)**: $\frac{x^2 + 2x\,\Delta x + (\Delta x)^2 - x^2}{\Delta x}$

Simplify (x^2 and $-x^2$ cancel): $\frac{2x\,\Delta x + (\Delta x)^2}{\Delta x}$

Simplify more (divide through by Δx): $= 2x + \Delta x$

Then **as Δx heads towards 0** we get: $= 2x$

Result: the derivative of **x^2** is **2x**

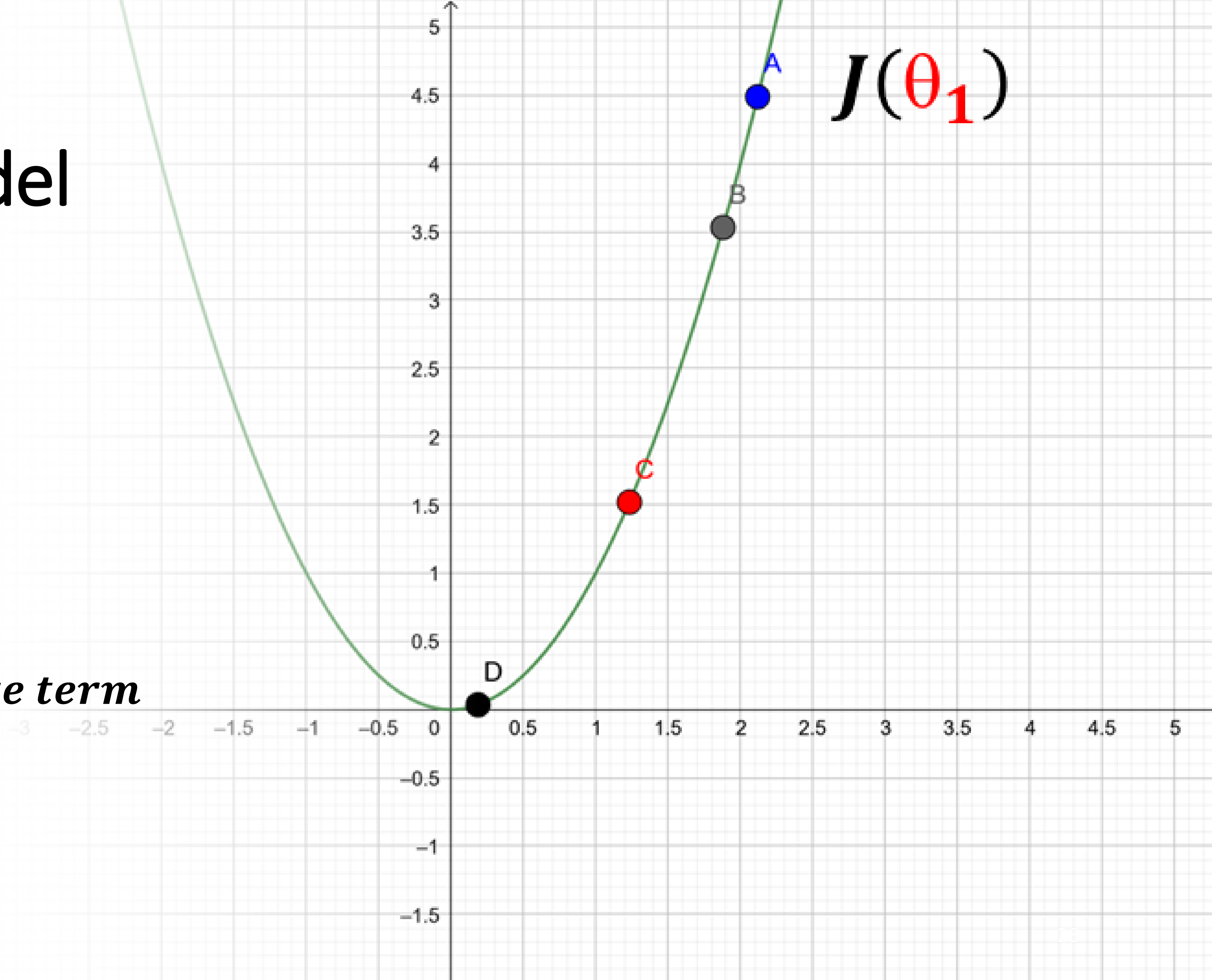
In other words, the slope at x is **2x**

Numerical Solution

- Loosely speaking, after deciding the model (e.g., single-variable linear regression), and the objective function, numerical solution involves the following steps:

1. Parameters initialization (assume $\boldsymbol{\theta_0 = \theta_1 = 0}$).
2. Predict the output using $\boldsymbol{\hat{y} = \theta_0 + \theta_1 x}$.
3. Evaluate the prediction error using any error function e.g., $|\hat{\mathbf{y}} - \mathbf{y}|$.
4. Find the direction and magnitude of changing the model parameters (θ_0, θ_1) to decrease the error.
5. **Update model parameters.**
6. Go to step 2 (repeat until convergence).

Update Model Parameters

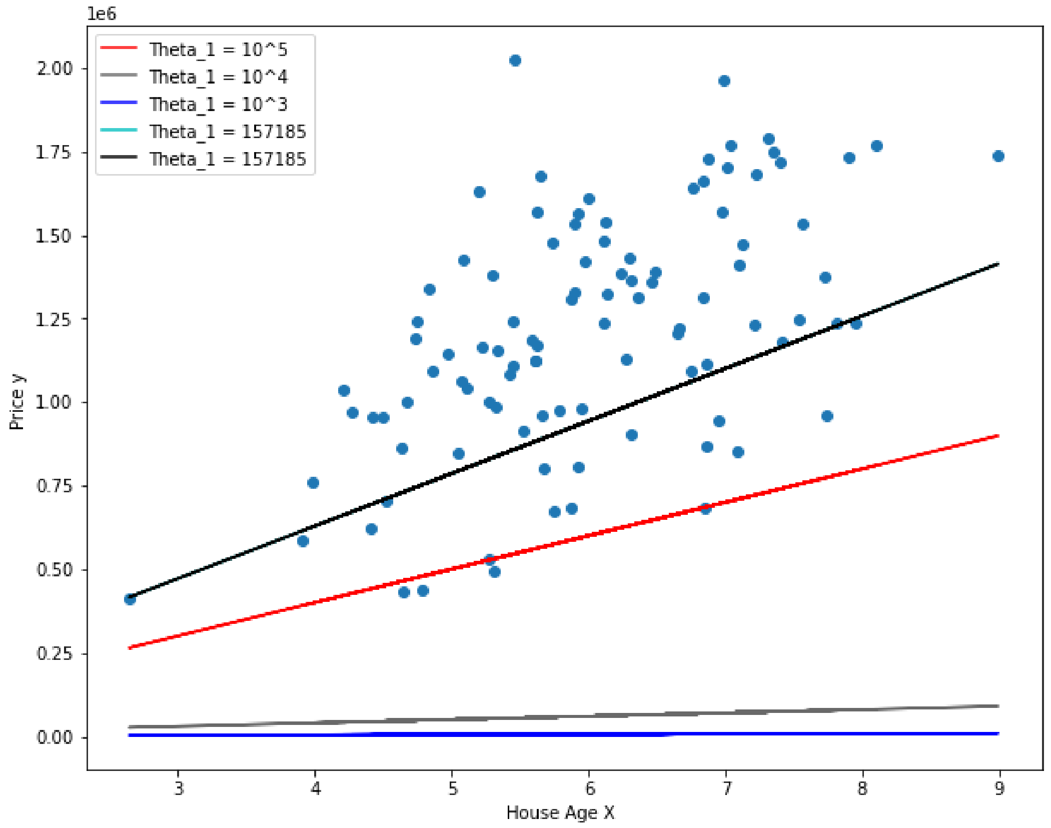


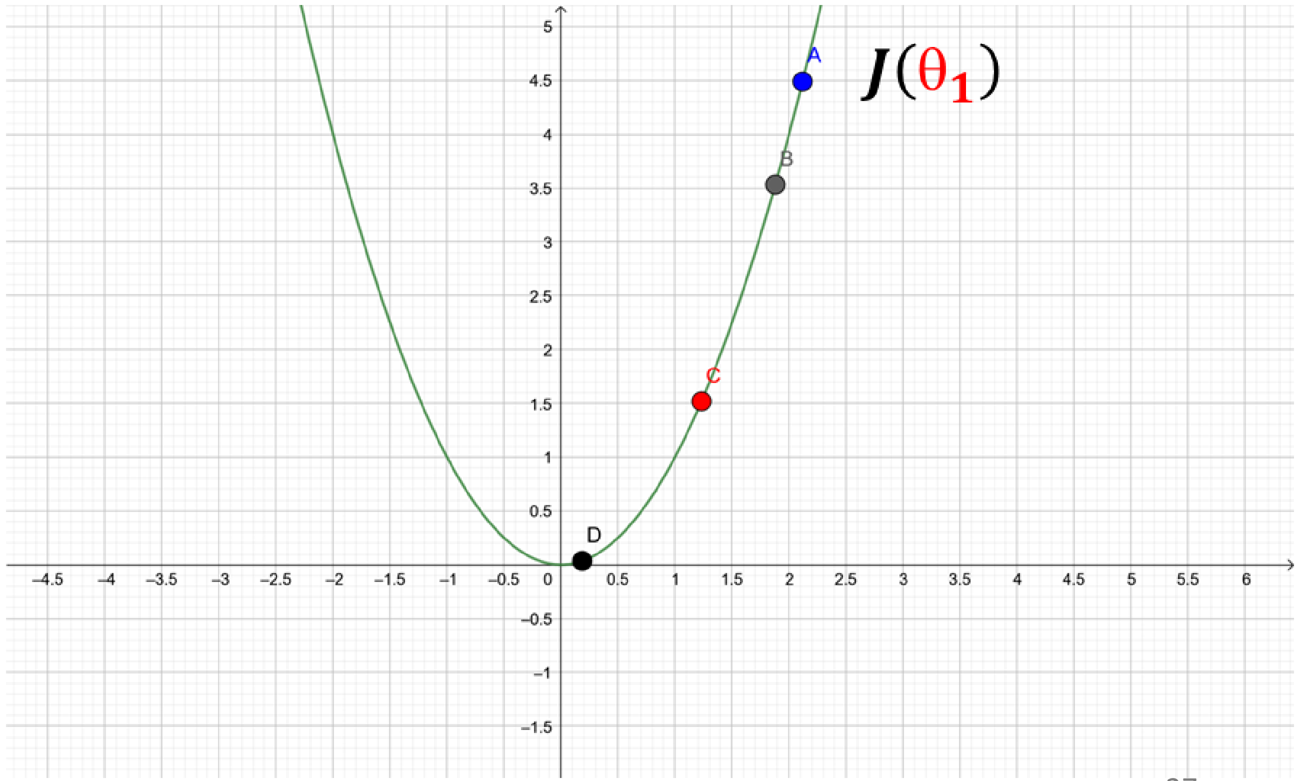
$$\theta_{t+1} = \theta_t - update\ term$$

Update Model Parameters

$$\theta_{\text{new}} = \theta_{\text{old}} - \boldsymbol{gradient}$$

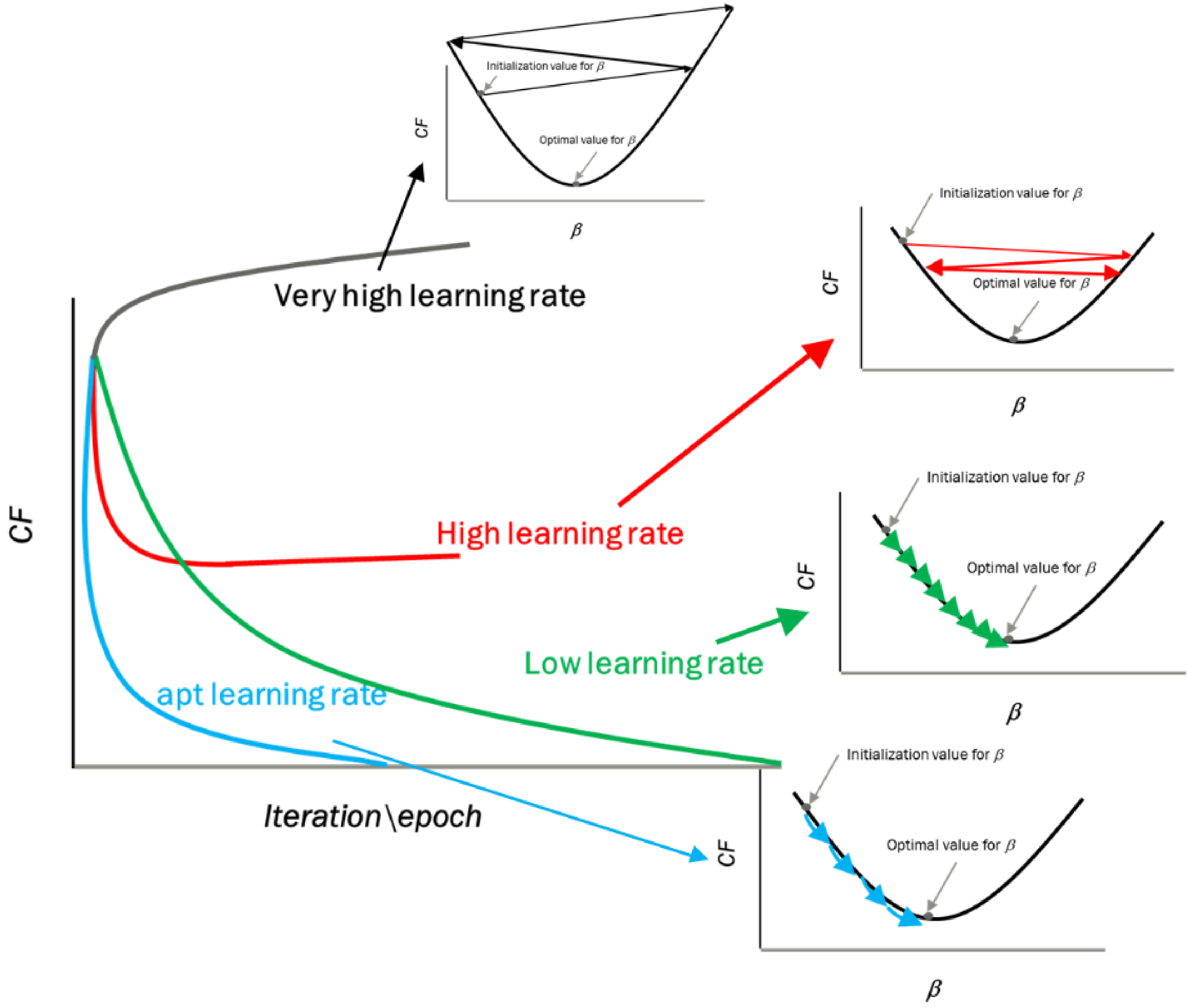
- If we have **+ve** gradient $\boldsymbol{\theta}$ will **increase**.
- If we have **–ve** gradient $\boldsymbol{\theta}$ will **decrease**.
- In both cases $\boldsymbol{\theta}$ approaches the value that **minimizes the cost function**.
- However, if we only use the gradient to update the parameter, $\boldsymbol{\theta}$ will **overshoot the minimum and diverge**.





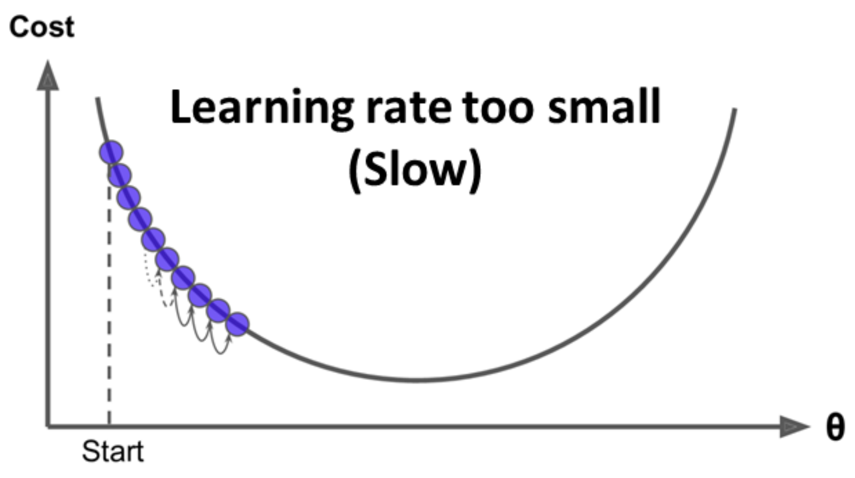
Learning Rate, α

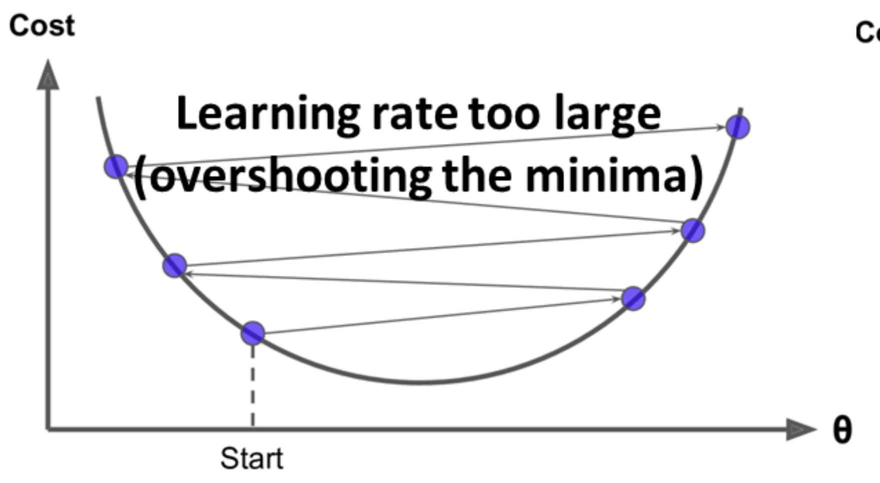
- $\theta_{\text{new}} = \theta_{\text{old}} - \alpha * gradient$

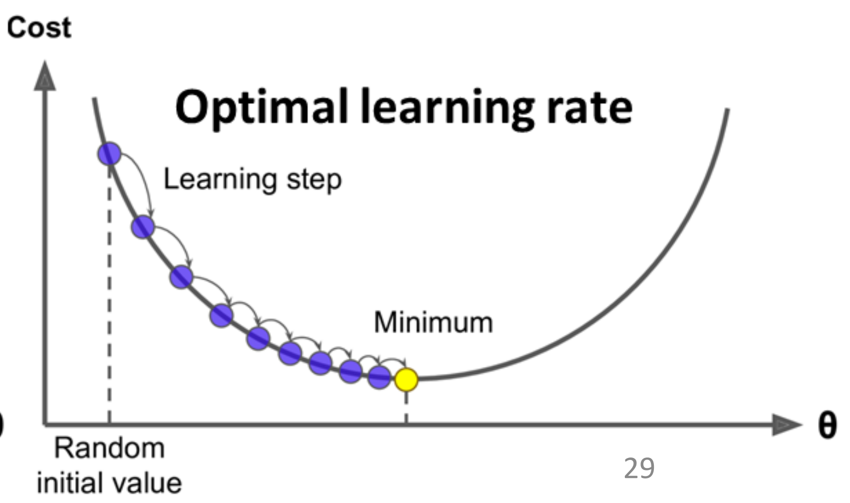

Initialization value for β
Optimal value for β
CF
β
Very high learning rate
Initialization value for β
Optimal value for β
CF
β
High learning rate
Initialization value for β
Optimal value for β
CF
β
Low learning rate
apt learning rate
CF
Iteration\epoch
Initialization value for β
Optimal value for β
CF
β

Learning Rate

- This size of steps taken to reach the minimum or bottom is called Learning Rate (***hyperparameter***). We can cover more area with larger steps/higher learning rate but are at the risk of overshooting the minima. On the other hand, small steps/smaller learning rates will consume a lot of time to reach the lowest point.
- **Example: Set a learning rate of (0.03), (1) , (0.1) on the slider:** https://developers.google.com/machine-learning/crash-course/fitter/graph

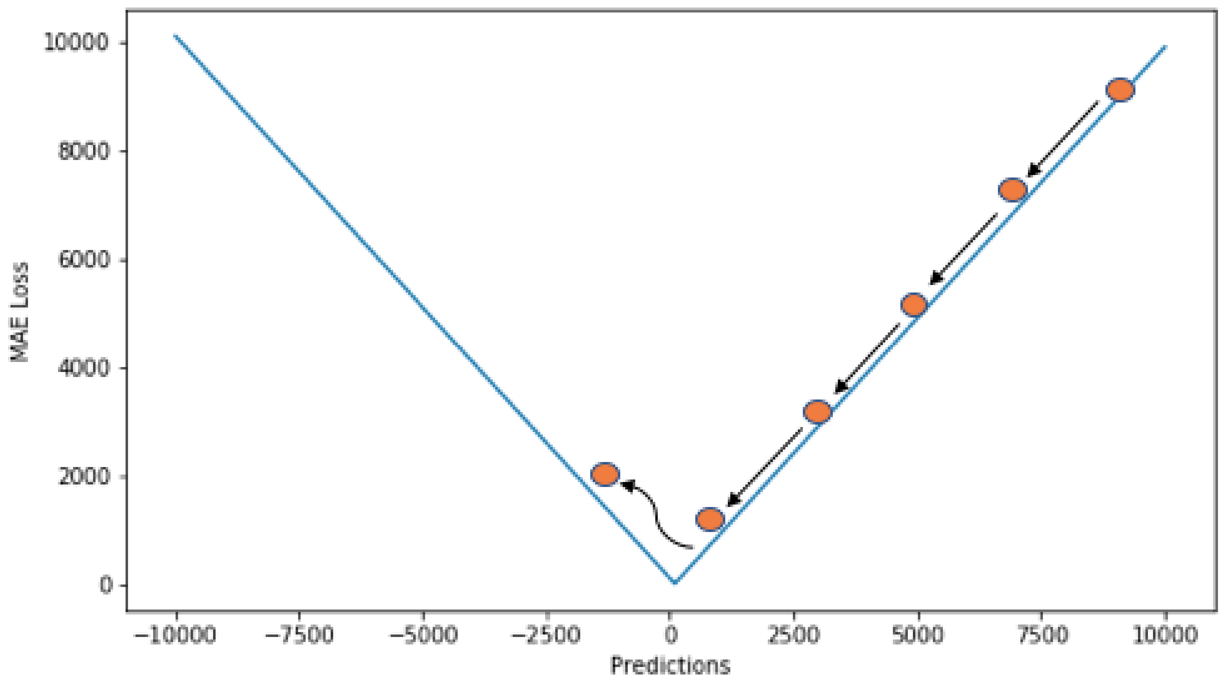


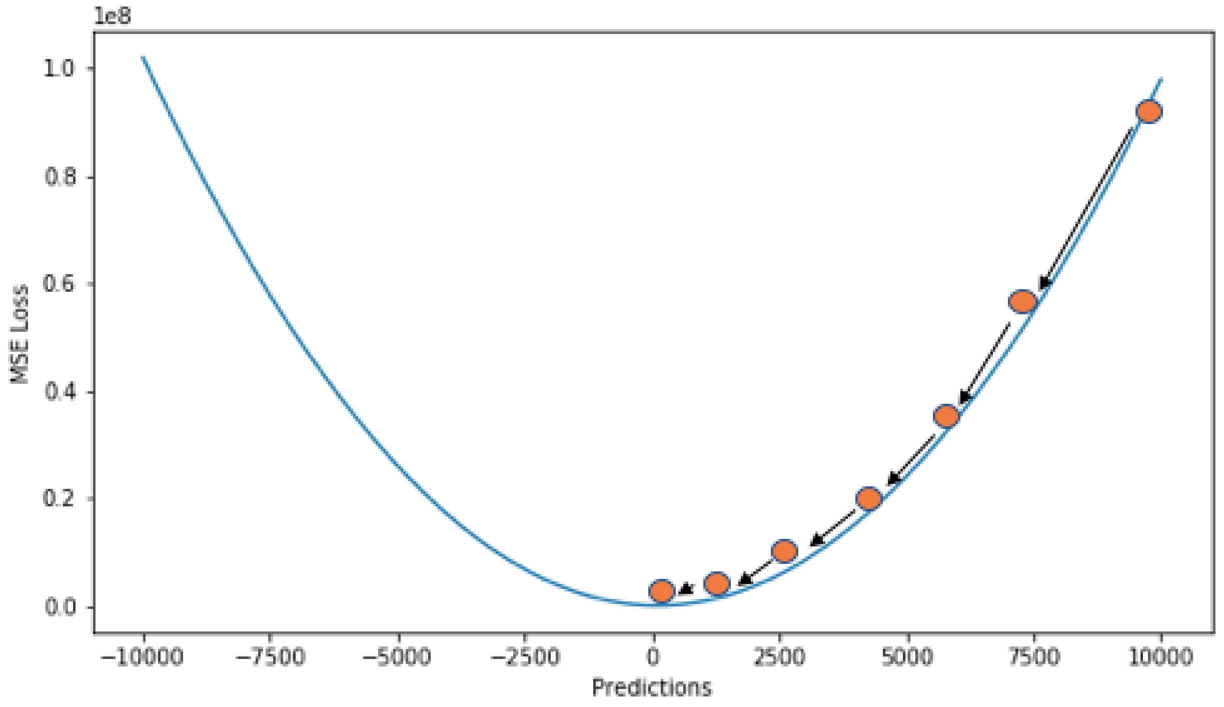




Loss Functions and Gradient

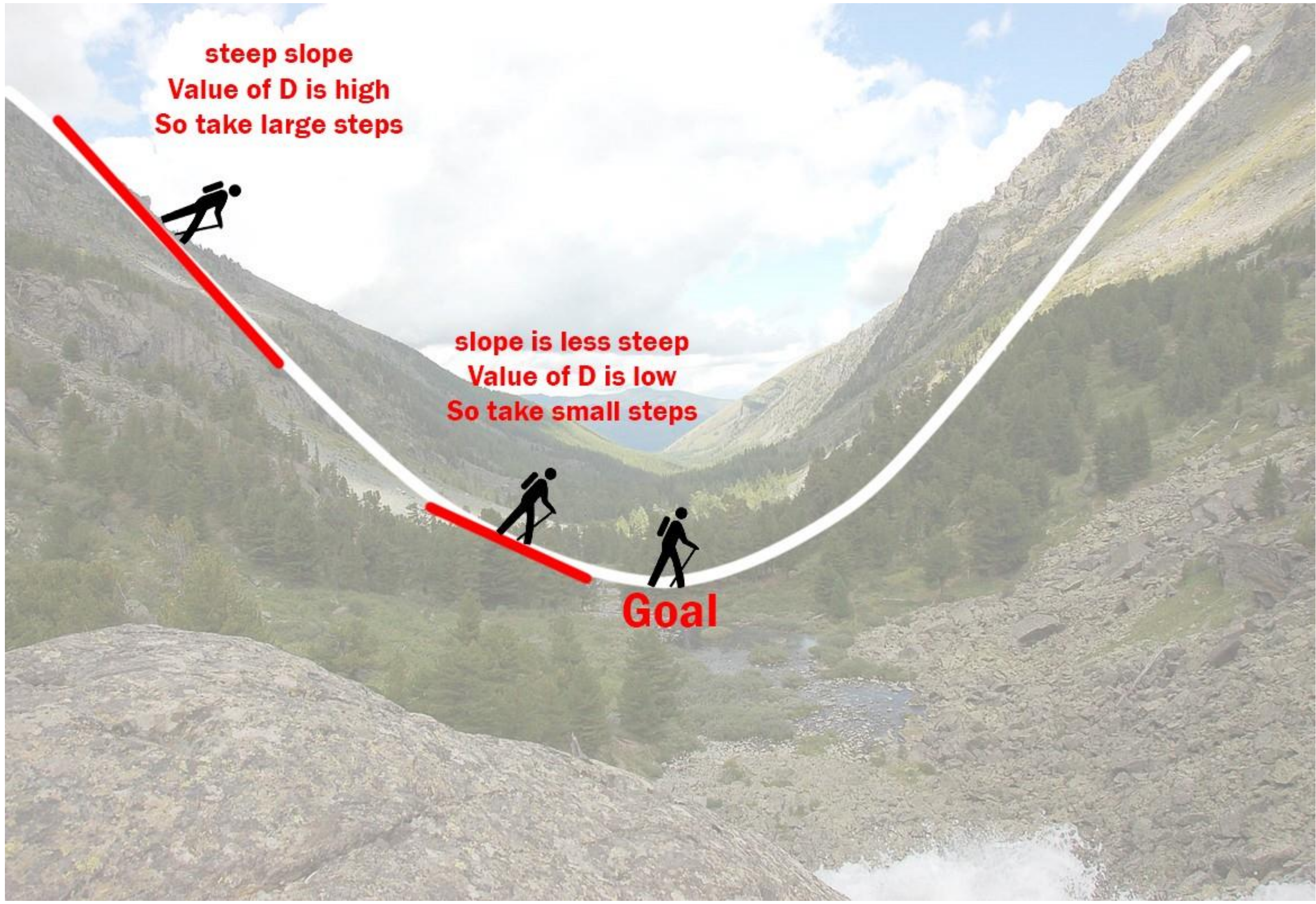
- **MAE** is robust to outlier. However, it has a constant gradient.
- **MSE** is not robust to outlier. However, it has a changing gradient that enables better learning.





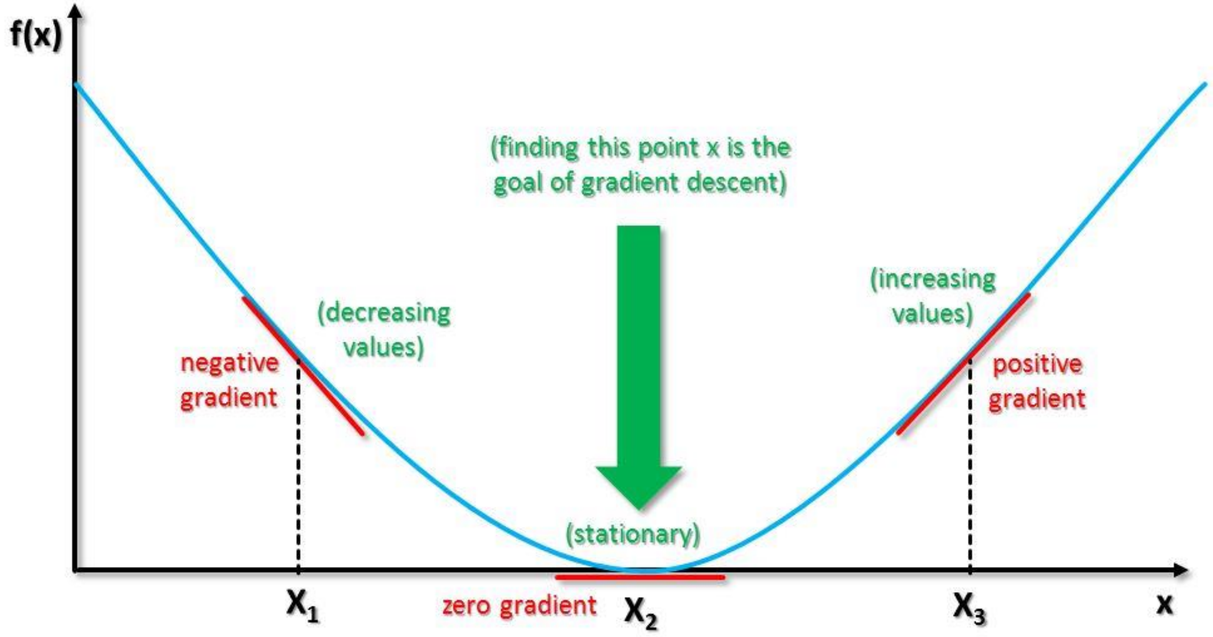
Gradient Descent Algorithm

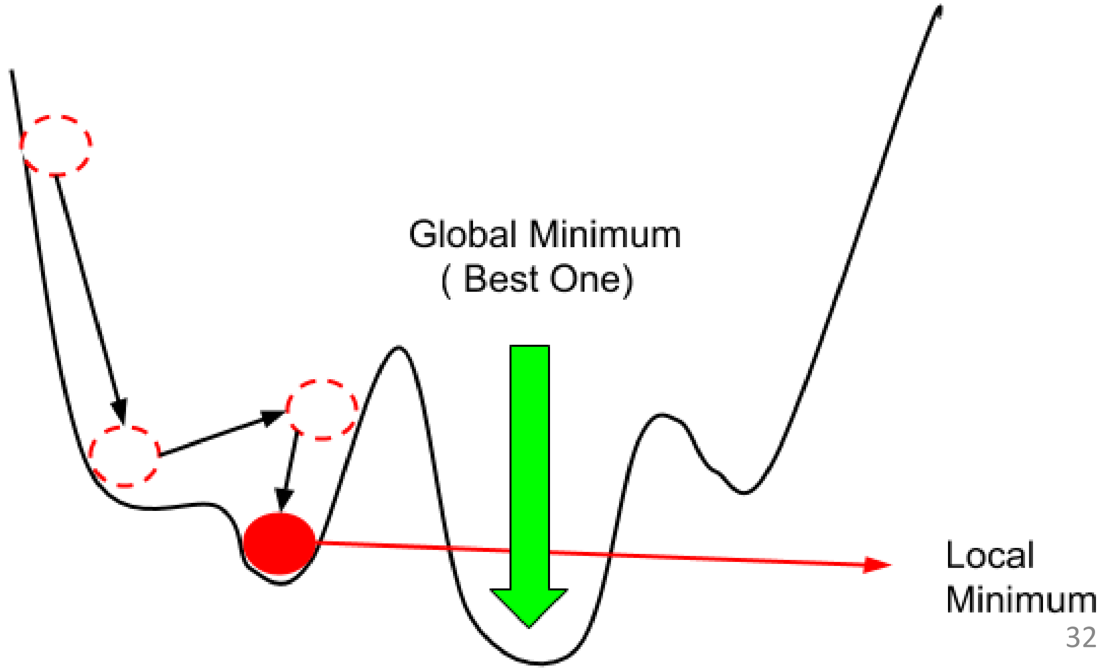
- **Intuition :** A person (blindly) trying to go down a hill when it is foggy. The idea is to make single step at a time, in the direction of the steepest descent.
- **GD** makes the same thing to find the min of a loss function.



Gradient Descent

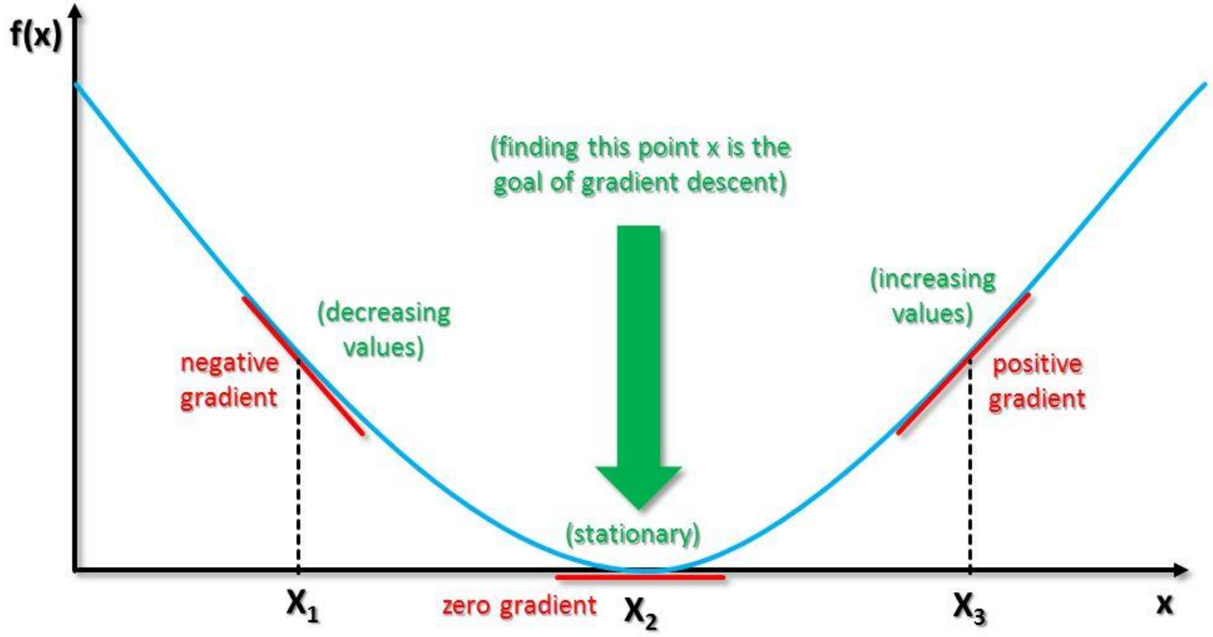
- **Gradient Descent** is a first-order iterative optimization algorithm for finding a **local** minimum of a **differentiable** function.
- The idea is to take repeated steps in the opposite direction of the gradient of the function at the current point, because this is the direction of steepest descent.

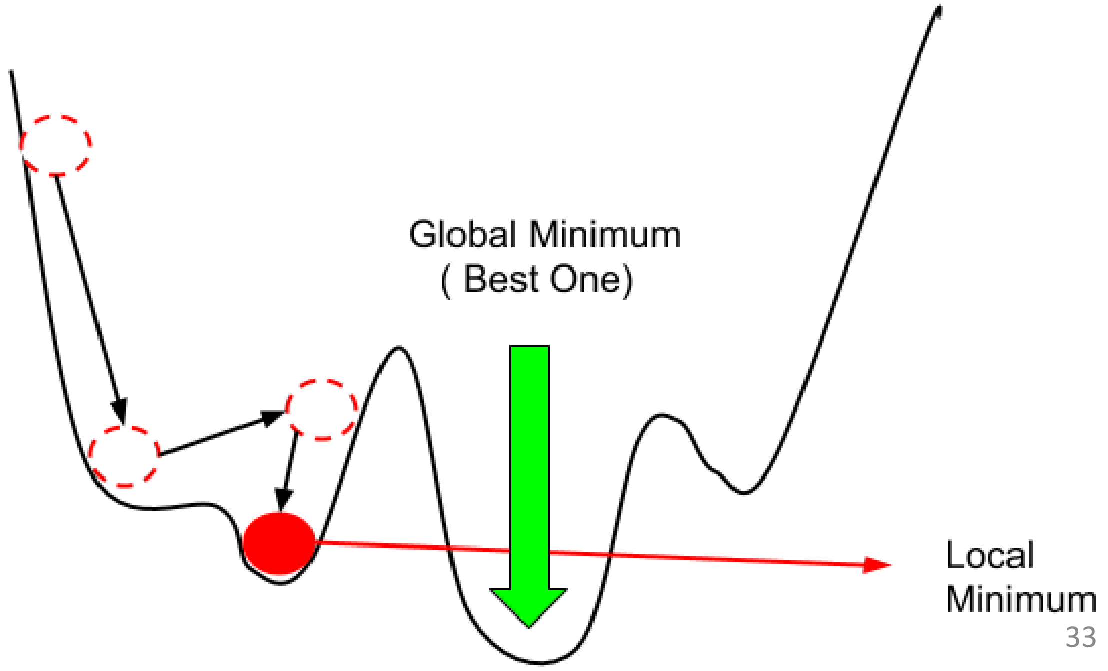




Gradient Descent

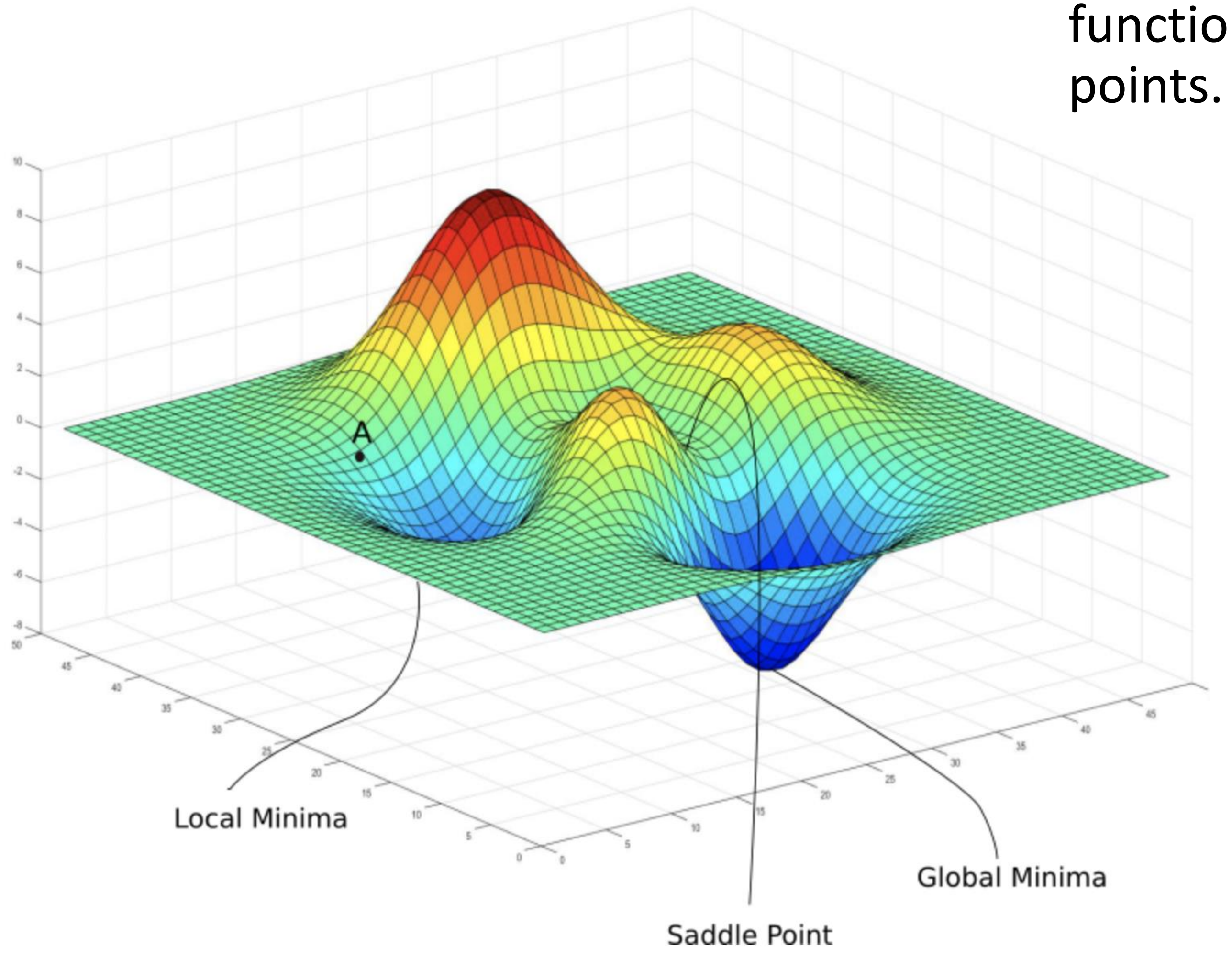
- This algorithm and its variants have been proven effective to solve data related problems, especially in the domain of neural networks. It's not the only algorithm or the best but it is seen as the « **hello world** » of ML.
- **Gradient descent (GD)** is an optimization algorithm that's used when training a machine learning model. It's based on a **convex** function and tweaks its parameters (coefficients) iteratively to **minimize** a given function as far as possible.

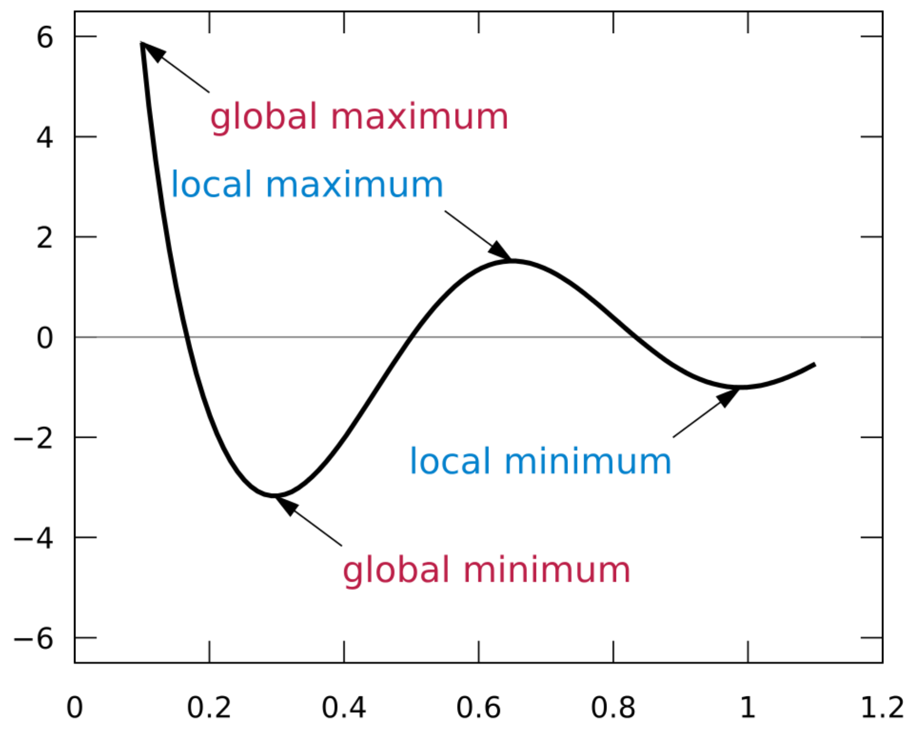




Local vs. Global Minimum

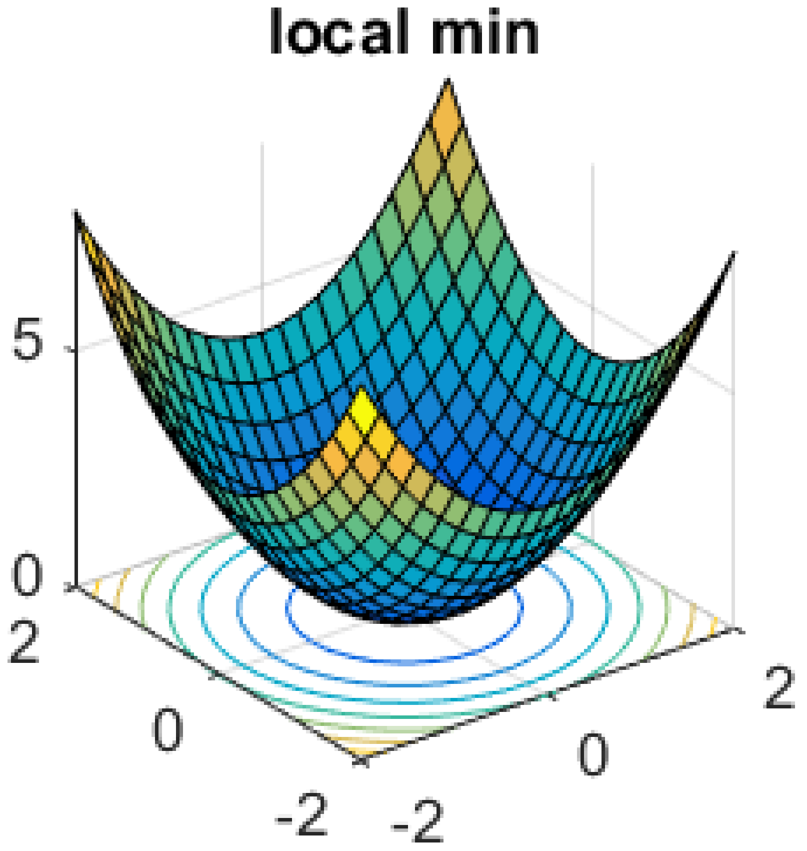
- A local minimum (or optimum) of a function is a point where the function value is smaller than at nearby points, but possibly greater than at a distant point.
- A global minimum (or optimum) is a point where the function value is smaller than at all other feasible points.

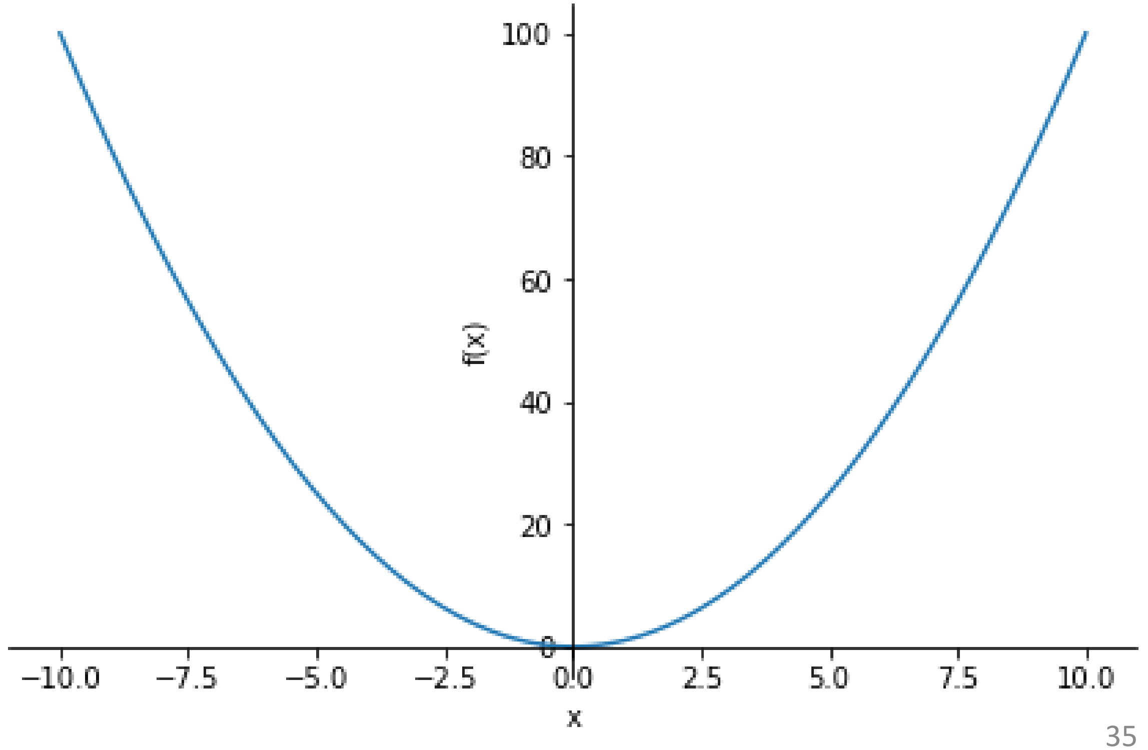




Convex Function

- Has one local minimum which also is its global minimum.





Convex Problem

- “We **try to** choose the formula for the cost function that makes it **convex**.”
- While we often aim to design convex cost functions to ensure a unique global minimum, it is not always possible. Nonlinear models, complex constraints, and custom loss functions often lead to non-convex optimization problems.

Logistic Regression

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} Cost(h_\theta(x^{(i)}), y^{(i)})$$

$$J(\theta) = \frac{1}{m}[\sum_{i=1}^{m} -y^{(i)} log(h_\theta(x^{(i)})) + (1 - y^{(i)}) log(1 - h_\theta(x^{(i)}))]$$

$m = number\ of\ samples$

Linear Regression

Cost Function: $J(\theta_0, \theta_1) = \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$

Goal: $\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$

Resources

- https://www.coursera.org/learn/machine-learning
- https://machinelearningmastery.com/analytical-vs-numerical-solutions-in-machine-learning/
- https://www.youtube.com/watch?v=e6kf6DDQVYA&ab_channel=TreeSoftMatterTheory
- https://en.wikipedia.org/wiki/Mathematical_optimization
- https://builtin.com/data-science/gradient-descent
- https://towardsdatascience.com/k-means-clustering-algorithm-applications-evaluation-methods-and-drawbacks-aa03e644b48a
- https://math.stackexchange.com/questions/2202545/why-using-squared-distances-in-the-cost-function-linear-regression
- https://towardsdatascience.com/optimization-loss-function-under-the-hood-part-ii-d20a239cde11
- https://www.mathsisfun.com/gradient.html
- https://en.wikipedia.org/wiki/Derivative
- https://www.mathsisfun.com/calculus/derivatives-introduction.html
- https://math.libretexts.org/Bookshelves/Calculus/Map%3A_Calculus__Early_Transcendentals_(Stewart)/14%3A_Partial_Derivatives/14.01%3A_Functions_of_Several_Variables
- https://slideplayer.com/slide/4753135/
- https://en.wikipedia.org/wiki/Gradient
- https://www.khanacademy.org/math/multivariable-calculus/multivariable-derivatives/partial-derivative-and-gradient-articles/a/the-gradient
- https://la.mathworks.com/help/matlab/ref/meshc.html
- http://www.adeveloperdiary.com/data-science/how-to-visualize-gradient-descent-using-contour-plot-in-python/
- https://rpubs.com/mgswiss15/M6C_7Multivariate
- https://stats.stackexchange.com/questions/354046/coordinate-descent-with-constraints
- https://www.mathworks.com/help/optim/ug/local-vs-global-optima.html#:~:text=A%20local%20minimum%20of%20a,at%20all%20other%20feasible%20points.
- https://en.wikipedia.org/wiki/Maxima_and_minima
- https://wngaw.github.io/linear-regression/
- http://www.cheerml.com/saddle-points
- https://towardsdatascience.com/understand-convexity-in-optimization-db87653bf920
- https://towardsdatascience.com/understand-convexity-in-optimization-db87653bf920
- https://www.sciencedirect.com/topics/engineering/convex-function
- https://www.math24.net/convex-functions#example2
- https://tutorial.math.lamar.edu/Classes/CalcI/NewtonsMethod.aspx
- https://en.wikipedia.org/wiki/Newton's_method
- https://tutorial.math.lamar.edu/Classes/CalcI/NewtonsMethod.aspx

Resources

- https://realpython.com/linear-regression-in-python/
- https://towardsdatascience.com/linear-regression-using-python-b136c91bf0a2
- https://towardsdatascience.com/why-norms-matters-machine-learning-3f08120af429
- https://towardsdatascience.com/why-norms-matters-machine-learning-3f08120af429
- https://machinelearningmastery.com/vector-norms-machine-learning/
- https://medium.com/linear-algebra/part-18-norms-30a8b3739bb
- https://heartbeat.fritz.ai/5-regression-loss-functions-all-machine-learners-should-know-4fb140e9d4b0
- Andrew Ng, Machine Learning, Stanford University, Coursera
- https://heartbeat.fritz.ai/5-regression-loss-functions-all-machine-learners-should-know-4fb140e9d4b0
- https://medium.com/data-science-365/linear-regression-with-gradient-descent-895bb7d18d52
- https://www.holehouse.org/mlclass/17_Large_Scale_Machine_Learning.html
- https://towardsdatascience.com/machine-learning-fundamentals-via-linear-regression-41a5d11f5220
- https://towardsdatascience.com/machine-learning-fundamentals-via-linear-regression-41a5d11f5220
- https://www.analyticsvidhya.com/blog/2019/08/detailed-guide-7-loss-functions-machine-learning-python-code/
- https://builtin.com/data-science/gradient-descent
- https://www.mltut.com/stochastic-gradient-descent-a-super-easy-complete-guide/
- https://towardsdatascience.com/linear-regression-using-gradient-descent-97a6c8700931
- https://kaigangi72.medium.com/stochastic-gradient-descent-demystified-part-1-8e4b897079b7
- https://medium.datadriveninvestor.com/gradient-descent-algorithm-b4c5afb4eb98
- https://medium.com/mindorks/an-introduction-to-gradient-descent-7b0c6d9e49f6
- https://medium.com/@venkatavinay222/at-the-end-machine-learning-is-all-about-optimization-ft-gradient-descent-e1588b7d95d2
- “Hands-on Machine Learning with Scikit-Learn, Keras, and TensorFlow” by Aurélien Géron
- https://laptrinhx.com/feature-scaling-why-and-how-3308094292/
- https://towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3