3. Multiple linear regression and Gradient descent

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14 August 2021

INDIAN INSTITUTE
OF TECHNOLOGY
PALAKKAD

Recap

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- Regression

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- Regression
  - dependent, independent variables

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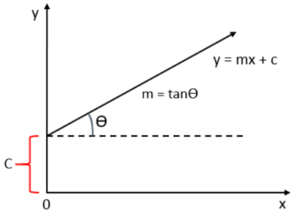
  - Ordinary least squares
  - Interpreting the regression coefficients

Revisiting simple linear regression



(a) A simple linear regression model

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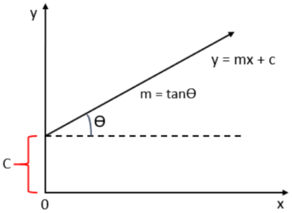

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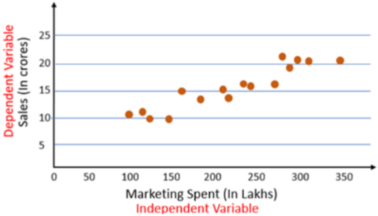

(b) Training dataset

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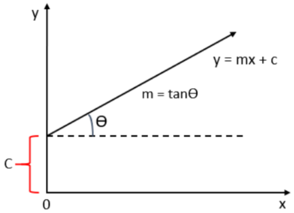

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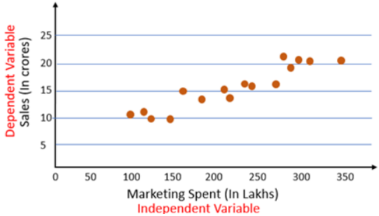

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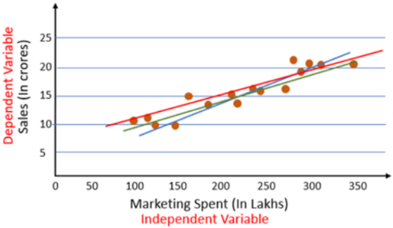

(c) Fitting a linear regression model

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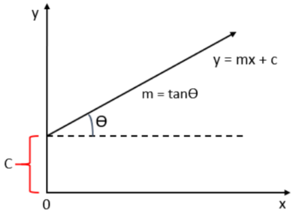

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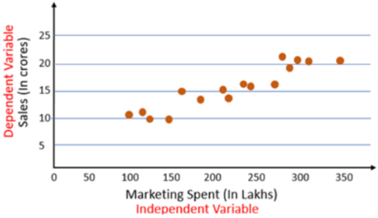

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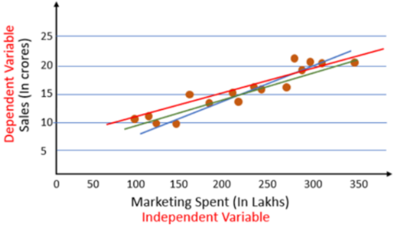

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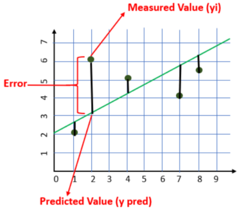

(d) Loss function for the model

Multiple regression

- more than one independent variable: $x_1, x_2, ..., x_D$

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- regression coefficient w_i measures the association between the predictor variable x_i and the outcome y
  - w_i represents the mean change in y corresponding to a unit increase in x_i when all other predictors are held fixed

Multiple regression

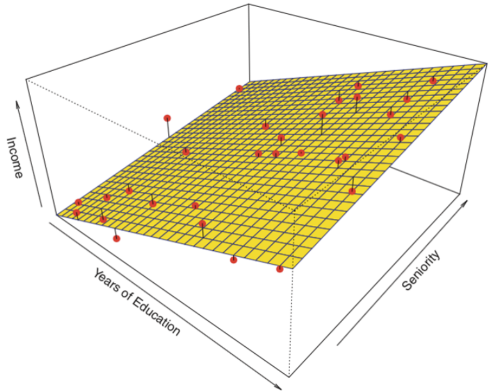

Figure: Visualizing the multiple regression model for predicting the response variable `Income` (y) based on the independent variables `Seniority` ($x1$) and `Years of Education` ($x2$)

Problem definition

Given: Training data set comprising N observations $(x_n, y_n)_{n=1}^{N}$, where $x_n = [x_{n1}, x_{n2}, ..., x_{nD}]$ is the input and y_n is the corresponding output

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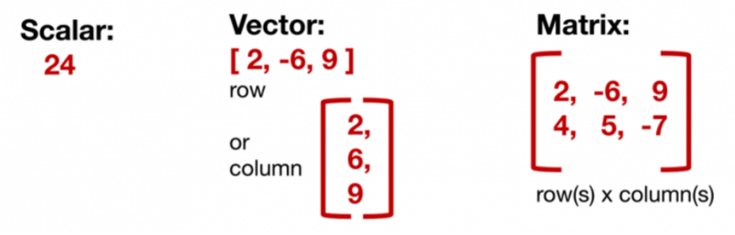
Estimate: The weights $w = [w_0, w_1, ..., w_D]$

Minimize: `Mean-squared error`: $l(w) = \frac{1}{N}\sum_{i=1}^N (y_i - \hat{y}_i)^2$
where $\hat{y}_i = f(w, x_i) = w_0 + w_1 x_1 + ... + w_D x_D$

A small mathematics refresher

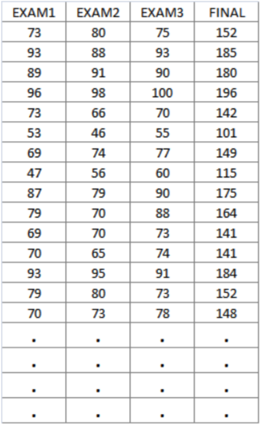


Scalar: a single number

Vector: an ordered array of numbers
can be in a row or a column
an index points to a specific value within the vector

Matrix: two dimensional array of numbers
each element identified by two numbers

Multiple regression



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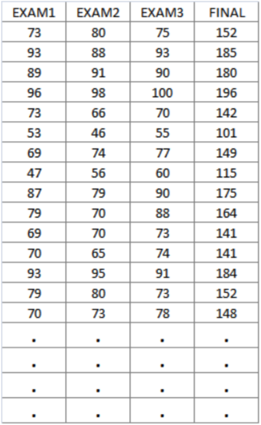
Multiple regression



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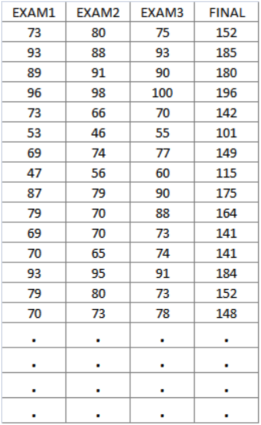
Consider the problem of predicting the Final exam score (y) based on the scores obtained in the first three exams (x_1, x_2, x_3)

Multiple regression



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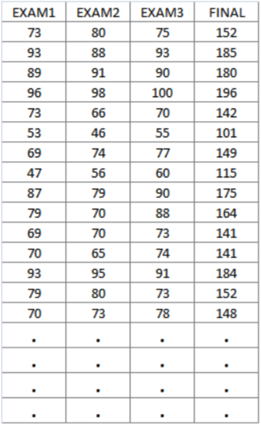

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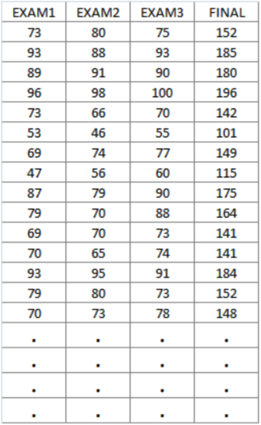

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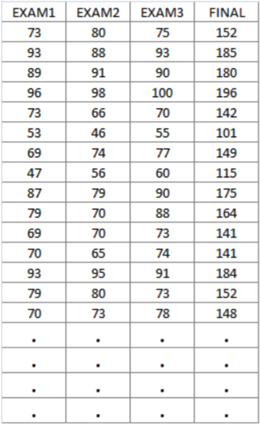
Multiple regression



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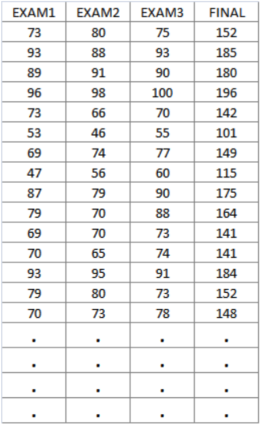
  - $x_{42} =$

Multiple regression



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- x_{ij} - j^{th} feature of the i^{th} observation
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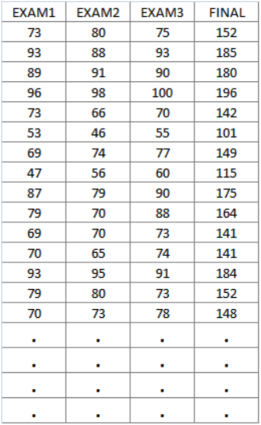
Multiple regression



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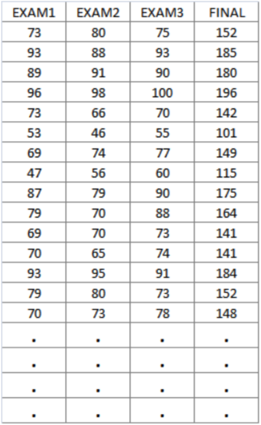
Multiple regression



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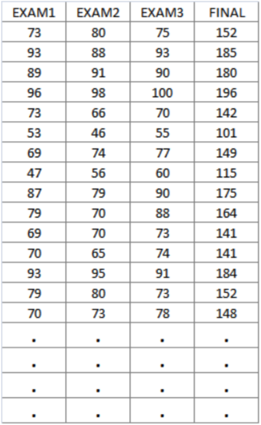

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- y_i - y value of the i^{th} observation
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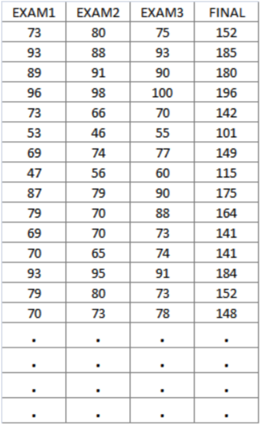
Multiple regression



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  - $x_{13} = 75$
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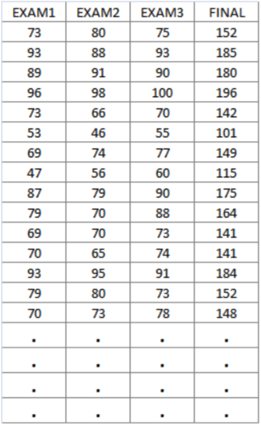
- y_i - y value of the i^{th} observation
  - $y_1 = 152$
  - $y_4 =$

Multiple regression



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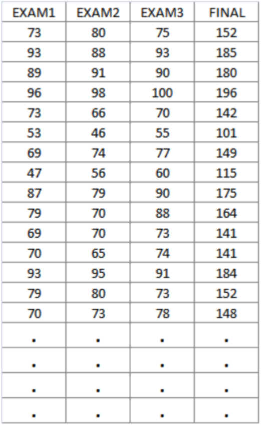
Multiple regression



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70	65	74	141
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.	.	.	.
.	.	.	.
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Multiple regression

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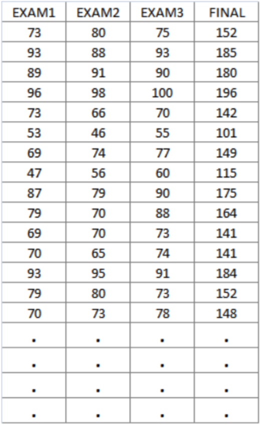
$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3$$



EXAM1	EXAM2	EXAM3	FINAL
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93	88	93	185
89	91	90	180
96	98	100	196
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53	46	55	101
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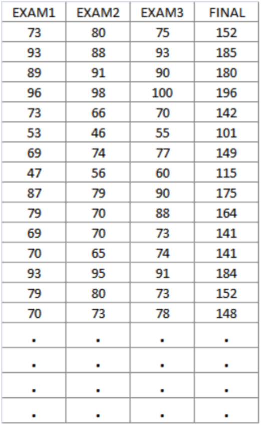

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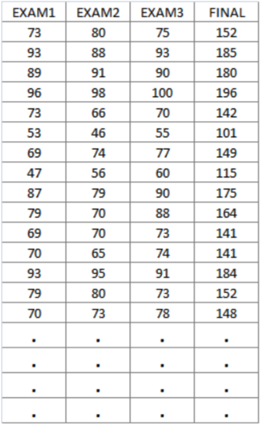

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The N equations can be written as:

$$y = Xw + e$$

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$$= \begin{bmatrix} e_1 & e_2 & \dots & e_N \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix} = e^T e = (y - Xw)^T (y - Xw)$$

Computing *w* using Ordinary Least Squares (OLS)

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Using OLS, the regression coefficients w are estimated by solving the following minimization problem:

$$\min_w \frac{1}{N}(y^T y - 2w^T X^T y + w^T X^T Xw)$$

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- cannot be easily parallelized

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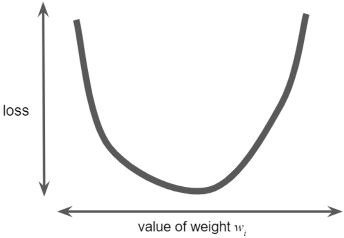

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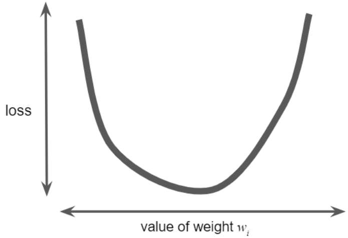

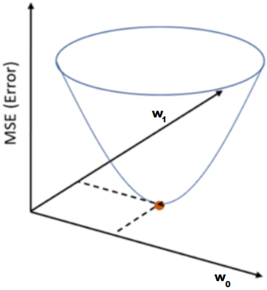

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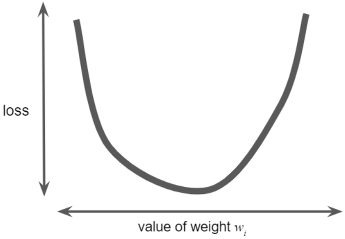

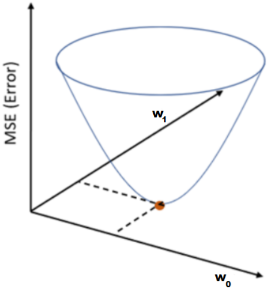

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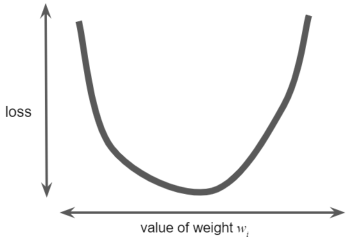

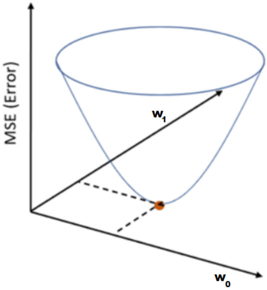

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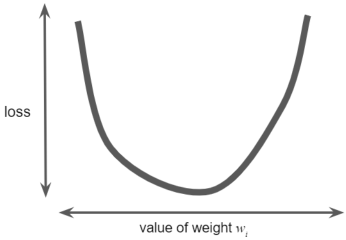

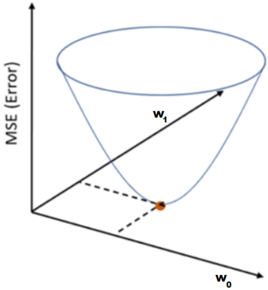

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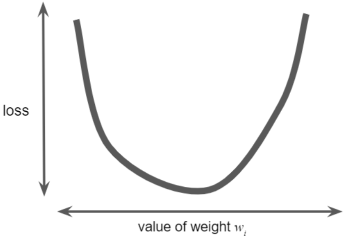

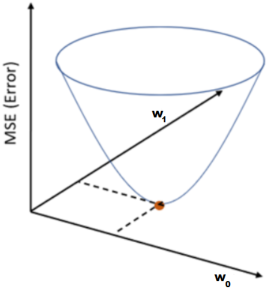

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Gradient descent

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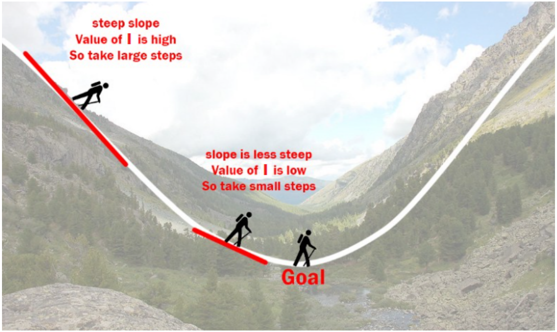

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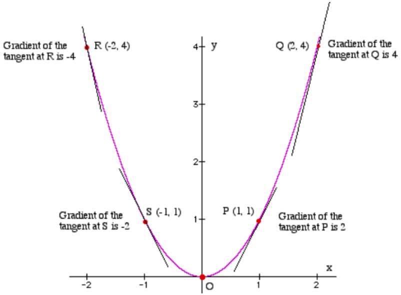

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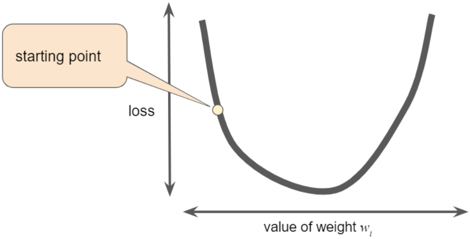

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   - gradient descent algorithm takes a step in the direction of the negative gradient in order to reduce loss as quickly as possible

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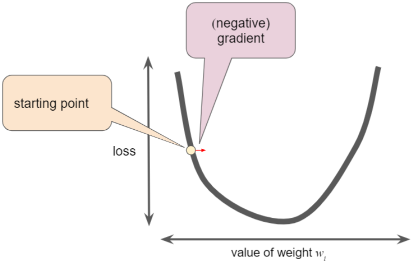

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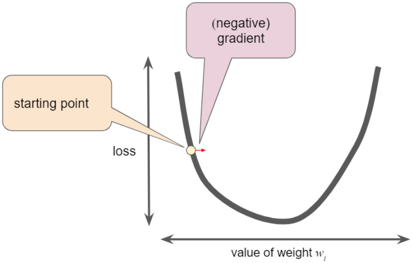

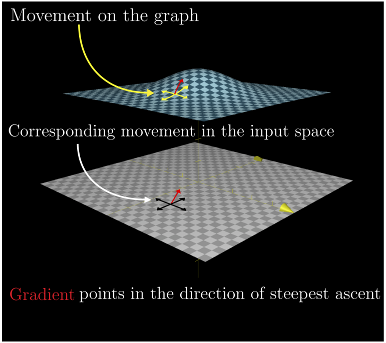
Movement on the graph
Corresponding movement in the input space
Gradient points in the direction of steepest ascent

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Gradient Descent: Determining the next value

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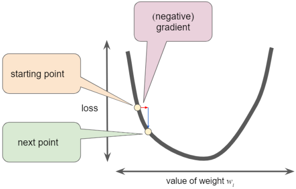

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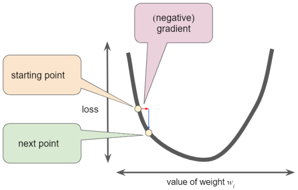
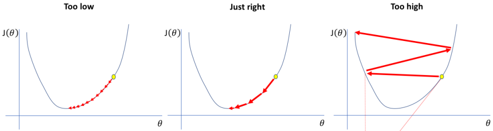


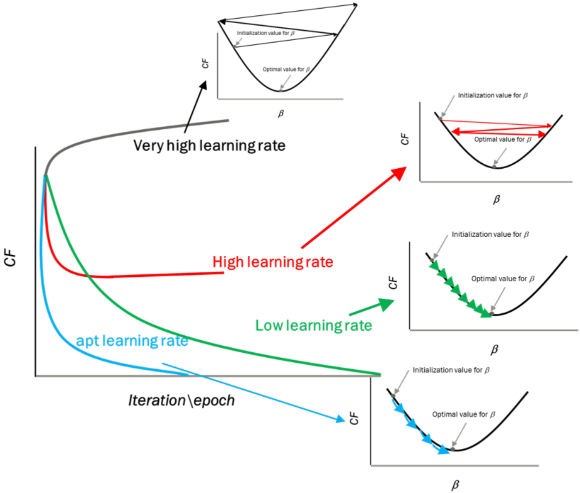


A small learning rate requires many updates before reaching the minimum point

The optimal learning rate swiftly reaches the minimum point

Too large of a learning rate causes drastic updates which lead to divergent behaviors

Choosing the learning rate



Gradient Descent for linear regression

Loss function: $l(w) = \frac{1}{N}\sum_{i=1}^{N}((\underbrace{w_0 + w_1 x_{i1} + ... + w_D x_{iD}}_{\hat{y}_i}) - y_i)^2$

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$$\vdots$$

$$w_D := w_D - \alpha * \frac{2}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i) * x_{iD}$$

Gradient Descent for linear regression

repeat until convergence {

$$w_j = w_j - \alpha * \frac{2}{N} \sum_{i=1}^{N} (\hat{y}_i - y_i) * x_{ij} \qquad \text{for } j := 0...D \quad \}$$

Gradient Descent for linear regression

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Matrix notation: $w := w - \alpha \nabla l(w)$

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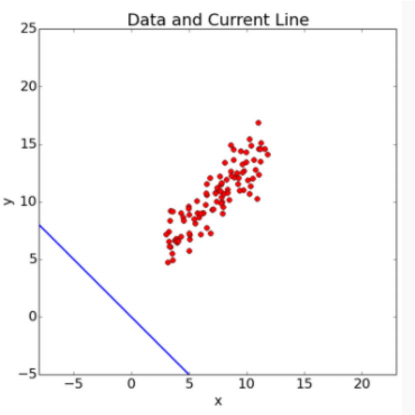
The matrix notation of the Gradient Descent rule is:

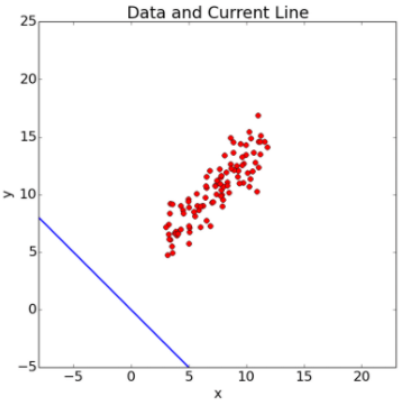
$$w := w - \frac{2\alpha}{N} X^T(Xw - y)$$

Gradient Descent: Demo



(a) Initial *w*

Gradient Descent: Demo



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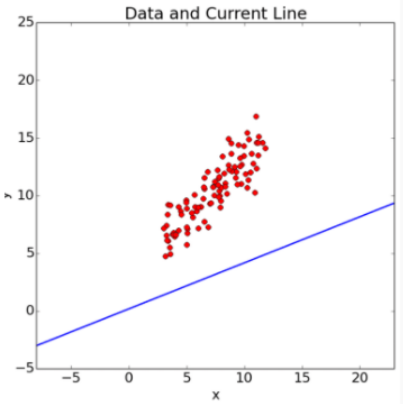
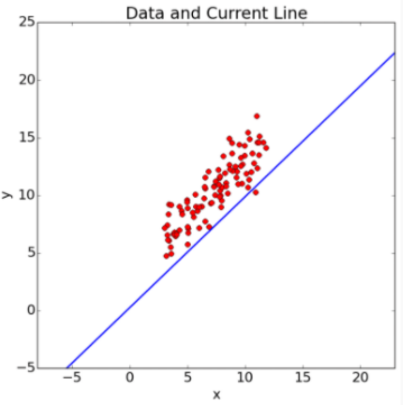


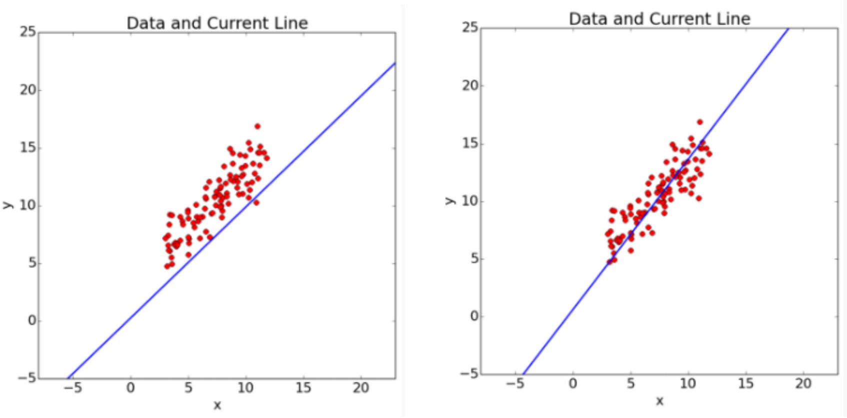
(b) After one iteration

Gradient Descent: Demo



(a) After 2 iterations

Gradient Descent: Demo



(a) After 2 iterations

(b) After 3 iterations

References

1. https://towardsdatascience.com/multiple-linear-regression-with-math-and-code-c1052f3c7446
2. https://developers.google.com/machine-learning/crash-course/reducing-loss/gradient-descent
3. https://www.coursera.org/learn/machine-learning/resources/QQx8l

Thanks Google for the pictures!