[W207] Linear regression and “big data” optimization: gradient descent

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For today...

- Linear regression model and least squares.
- Parameter estimation – normal equations.
- Parameter estimation – gradient descent and stochastic gradient descent.

Introduction to linear regression

$$\mathbb{E}(Y|X) = \theta_0 + \theta_1 X_1 + \cdots + \theta_n X_n + \epsilon$$

- Linear regression model assumes that the regression $E(Y|X)$ function is linear in terms of the inputs $X_1, \cdots, X_n$.

Introduction to linear regression

$$Y = \theta_0 + \sum_{i=1}^{n} \theta_i X_i + \epsilon$$

$$\epsilon \sim N(0, 1)$$

- In other words the output Y can be thought of as a linear function of the inputs X

Introduction to linear regression

$$\% \text{ Republican}_s^g = \theta_0 + \sum_{i=1}^{n} \theta_i X_i + \epsilon$$

- In political science or other social science disciplines, you might encounter linear regression in models that attempt to predict elections.

Why learn about linear regression?

- It's uncommon to see linear regression applied in the machine learning context **BUT**...
- many nonlinear techniques (support vector machines, neural networks) are simply generalizations of linear regression.

Linear regression and least squares

$$Y = f(X) + \epsilon$$

$$f(X) = \theta_0 + \sum_{i=1}^{n} \theta_i X_i$$

- Recall from last time that the goal in machine learning is to find a function $f(\cdot)$ that does the best job of predicting outcomes.
- a **linear regression model** is a parametric model in which we assume that the inputs/predictors X are a linear function of Y.

Linear regression and least squares

$$Y = f(X) + \epsilon$$

$$f(X) = \theta_0 + \sum_{i=1}^{n} \theta_i X_i$$

- In linear regression models the output Y is usually a continuous outcome and the inputs X can be quantitative or qualitative (dummy variables etc).

Linear regression and least squares

$$\%\ \text{Rep.}_t^g = \theta_0 + \theta_1 \%\ \text{Rep.}_{t-1}^p + \theta_2 \text{Rep. Governor}_{t-1} + \theta_3 \text{Region} + \epsilon$$

$\%\ \text{Rep.}_t^g$ – is the Republican vote share for the president in the general election.

$\text{Rep. Governor}_{t-1}$ – is a dummy variable indicating whether the state had a Republican governor in $t-1$.

etc...

Linear regression and least squares

$$Y = \theta_0 + \theta_1 X_1 + \theta_2 X_1^2 + \theta_3 X_1^3 + \cdots$$

- X's can also be **basis expansions**, leading to an n^{th} order polynomial.
- what's important however is that the model is linear in the θ's.

Linear regression and least squares

$$\text{Training data: } (x_1, y_1), \cdots, (x_N, y_N)$$
$$x_i = (x_{i1}, \cdots, x_{ip})^T$$

- Consider some training data with N observations and p features.

Goal is to find θ's which minimize loss or cost function

$$\text{Goal is to estimate: } \theta = (\theta_0, \cdots, \theta_p)^T$$
$$\text{such that: } \arg\min_{\theta} J(\theta)$$

- Our goal is to find a set of θ's that minimize the cost function $J(\theta)$ or residual sum of squares (RSS) in the language of regression analysis.

Goal is to find θ's which minimize loss or cost function

Where...

$$J(\theta) = \sum_{i=1}^{N} (y_i - f(x_i))^2$$

$$= \sum_{i=1}^{N} \left(y_i - \theta_0 - \sum_{j=1}^{p} x_{ij}\theta_j \right)^2$$

Goal is to find θ's which minimize loss or cost function

Where...

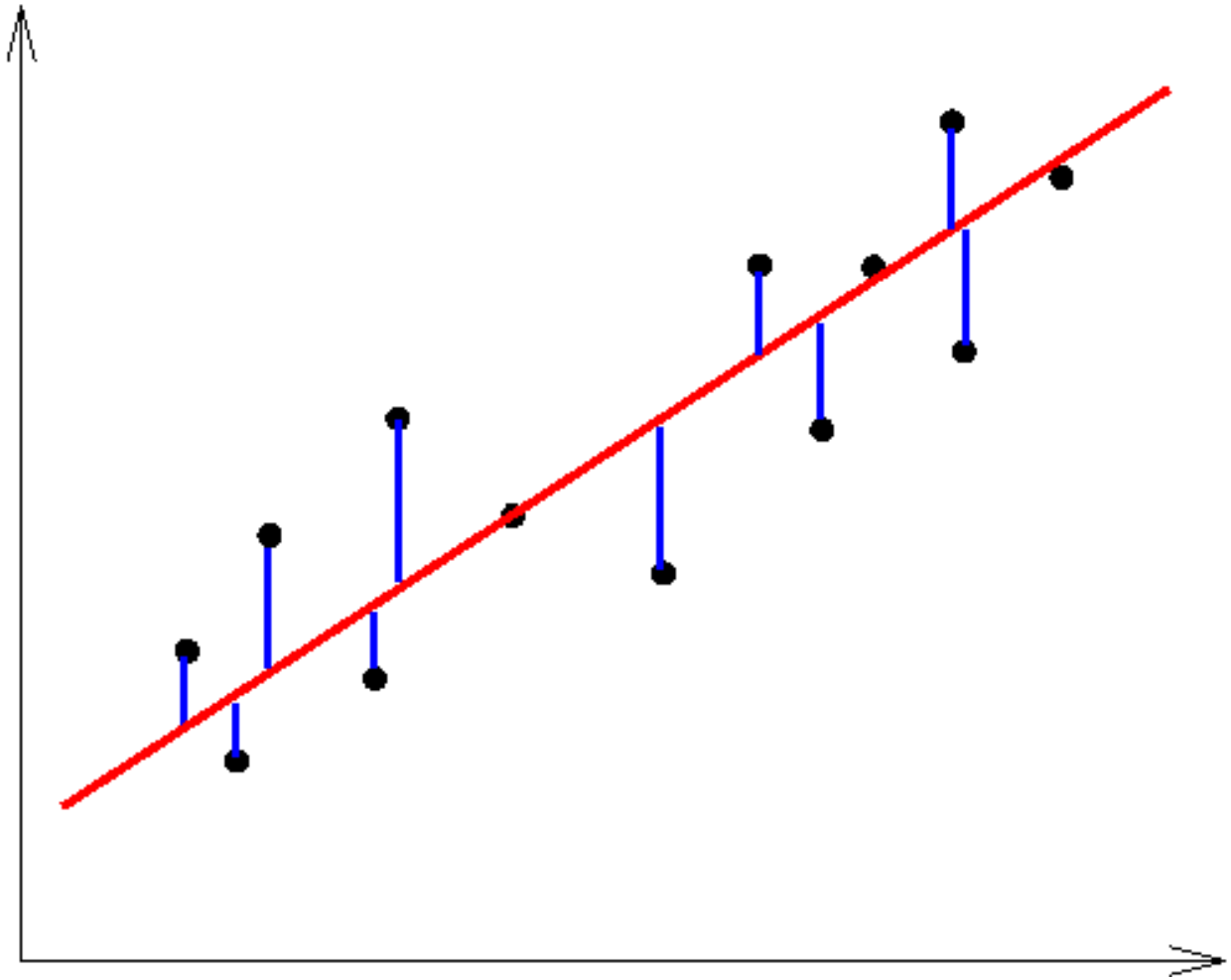
$$J(\theta) = \sum_{i=1}^{N} (y_i - f(x_i))^2$$
$$= \sum_{i=1}^{N} \left(y_i - \theta_0 - \sum_{j=1}^{p} x_{ij}\theta_j \right)^2$$

In words, we want to choose θ's which minimize the squared difference between the observed and predicted values.

In the single feature case we need to solve:

$$\frac{\partial J}{\partial \theta_0} = 0$$
$$\frac{\partial J}{\partial \theta_1} = 0$$

Fitting a line with slope θ_1 and y-intercept θ_0



Starting with θ_0 we have:

$$\sum \frac{\partial J}{\partial \theta_0} (y_i - \theta_0 - \theta_1 x_1)^2 = 0$$

$$\implies \theta_0 = \bar{y} - \theta_1 \bar{x}$$

(Proof on the board)

Is θ_0 a minimum?

$$\frac{\partial^2 J}{\partial \theta_0^2} = 2N > 0$$

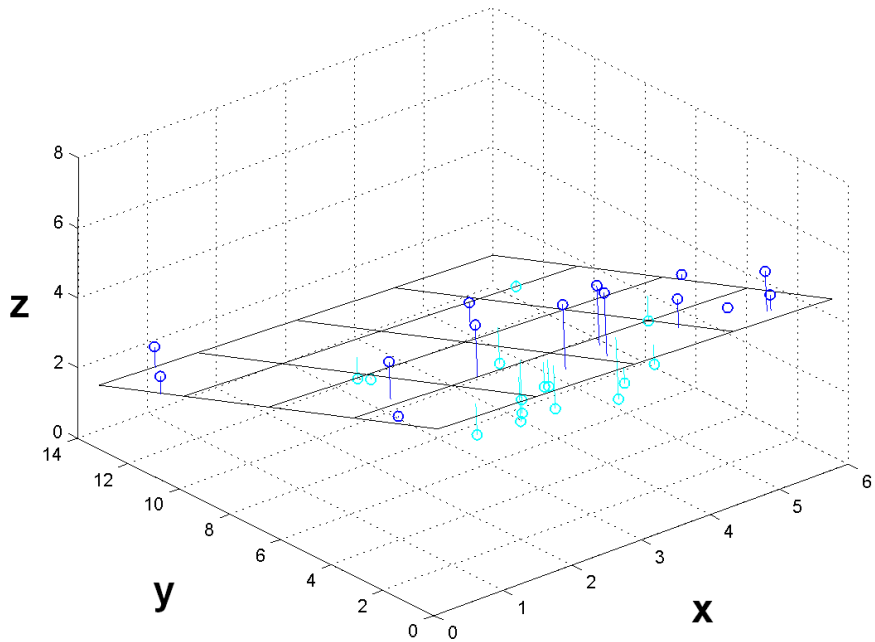
- Second derivative test guarantees that θ_0 is a local minimum when we set the first derivative to 0 and solve for θ_0.

For θ_1 we have:

$$\theta_1 = \frac{\sum y_i \sum x_i - N \sum x_i y_i}{(\sum x_i)^2 - N \sum x_i}$$

Prove it to yourself.

When we have more features we fit a plane or hyperplane to the data



What if we have multiple parameters?

$$J(\boldsymbol{\theta}) = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^T(\mathbf{y} - \boldsymbol{X}\boldsymbol{\theta})$$

$$\boldsymbol{X} \in \mathbb{R}^{nxp}, \boldsymbol{\theta} \in \mathbb{R}^{nx1}, \boldsymbol{y} \in \mathbb{R}^{nx1}$$

Need to find...

$$\frac{\partial J}{\partial \boldsymbol{\theta}} = 0$$
$$\frac{\partial J}{\partial \boldsymbol{\theta}} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta)$$
$$\hat{\boldsymbol{\theta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

Prove it to yourself.

Interpretation and prediction

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

- Once we estimate θ we might be interested both in *interpretations* of the parameters of the model and *prediction* using the model.

Interpretation

- Which features/feature sets do the best job of predicting **y** and why?

Interpretation

- To do so we need to:
  1. Learn about the *variance* of θ and;
  2. Make certain distributional and functional assumptions about the data and the errors.

Variance of θ

- It is useful to learn about the variance of θ because once we know this, we can conduct hypothesis tests for the parameters.

Assumptions for inference

- Need to assume that the linear model is indeed appropriate.
- That the error term has a mean of 0 and variance of 1.
- That the $\hat{\theta}$ follow a multivariate normal distribution with a mean equal to the true θ and variance equal to the estimated variance.

Hypothesis testing

- For each parameter, we might be interested in testing whether it contributes anything to the model (whether the true value is 0).
- To accomplish this we can do hypothesis testing with the t distribution or the normal distribution.

Prediction

- More often, we are interested in prediction and interpretability.

Prediction

- Remember, adding more features will always reduce the *training error* but will also reduce both interpretability AND tend to increase *test error* due to overfitting.

Model and variable selection

- In order to strike a good balance between the two, we can use the $F - test$ for two competing models or;
- Subset selection algorithms to choose which group of predictors should be included and excluded from the model.

F-Test

- Two models, one simple and one more complex.
- F-test will tell you whether the more complex model is an improvement over the simple one.

F-Test Example

$$\text{Model 1: } Rep_s^g = \theta_0 + \theta_1 Rep_s^p + \theta_2 Pop_s + \epsilon$$
$$\text{Model 0: } Rep_s^g = \theta_0 + \theta_1 Rep_s^p + \epsilon$$

- Two models predicting Republican presidential vote share.
- Model 1 includes primary vote share and population of the state.
- Model 0 includes on the primary vote share.
- Which model should we use?

F-Test Example

$$H_0 : \text{Model 0 is better}$$

$$F = \frac{(J(\theta)_0 - J(\theta)_1)/(p_1 - p_0)}{J(\theta)_1/(N - p_1 - 1)}$$

$p_1 =$ parameters in Model 1.

$p_2 =$ parameters in Model 2.

Reject H_0 if...

$$\mathbb{P}(X > F_{p_1-p_0,N-p_1-1}) > 0.05$$

$p_1 =$ parameters in Model 1.

$p_2 =$ parameters in Model 2.

Optimization

- Often times in machine learning problems, the matrix $\boldsymbol{X}^T\boldsymbol{X}$ is very *sparse* in the case of linear regression or;
- In the case of non–linear models (neural networks etc), there is no closed form solution available to estimate the parameters.

Optimization

- In these cases iterative methods such as *gradient descent* or *stochastic gradient descent* can estimate model parameters much more quickly that normal equations.

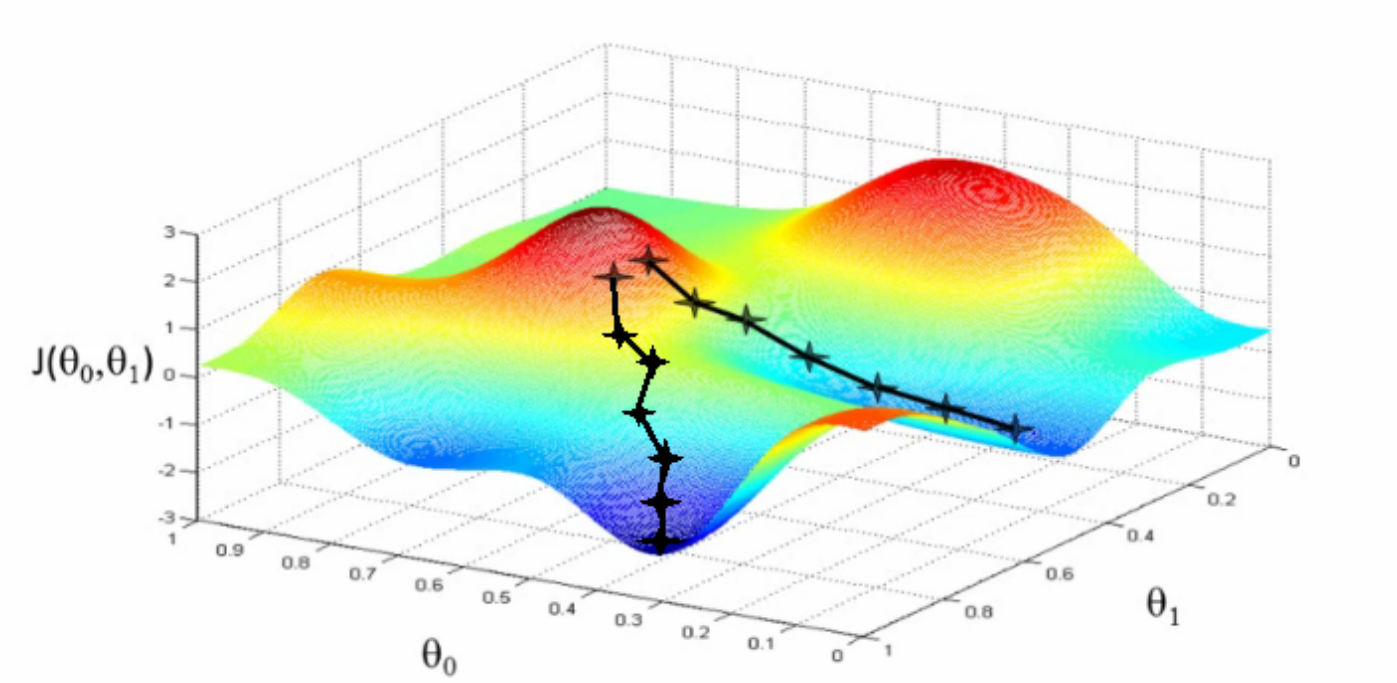
Gradient descent

$$\theta :\theta - \eta \nabla_\theta J(\theta)$$

$$\nabla J(\theta) = \left[\frac{\partial J}{\partial \theta_0}, \frac{\partial J}{\partial \theta_1}, \cdots, \frac{\partial J}{\partial \theta_p} \right]$$

- Gradient descent is an algorithm which starts with an initial guess for the θ's, calculates the cost function and updates θ in the direction of the gradient.
- $-\nabla_\theta J(\theta)$ is the direction of *steepest descent* of the cost function $J(\theta)$.
- η is the *step size.*

Gradient descent



- Thus $-\eta \nabla_\theta J(\theta)$ is taking a step of size η down in the direction of steepest descent.

For univariate regression

repeat while $(||\eta \nabla J(\theta)|| > \epsilon)$
{

$$\theta_j := \theta_j - \eta \frac{\partial J}{\partial \theta_j} J(\theta_0, \theta_1)$$

}

For univariate regression

repeat while $(||\eta \nabla J(\theta)|| > \epsilon)$
{

$$\theta_0 := \theta_0 - \eta \frac{\partial J}{\partial \theta_0} J(\theta_0, \theta_1)$$

$$\theta_1 := \theta_1 - \eta \frac{\partial J}{\partial \theta_1} J(\theta_0, \theta_1)$$

}

For univariate regression

$$\frac{\partial J}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{N} \sum_{i=1}^{N} (\theta_0 + \theta_1 x_i - y_i)$$

$$\frac{\partial J}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{1}{N} \sum_{i=1}^{N} (\theta_0 + \theta_1 x_i - y_i) x_i$$

For univariate regression

repeat while $(||\eta \nabla J(\theta)|| > \epsilon)$
{

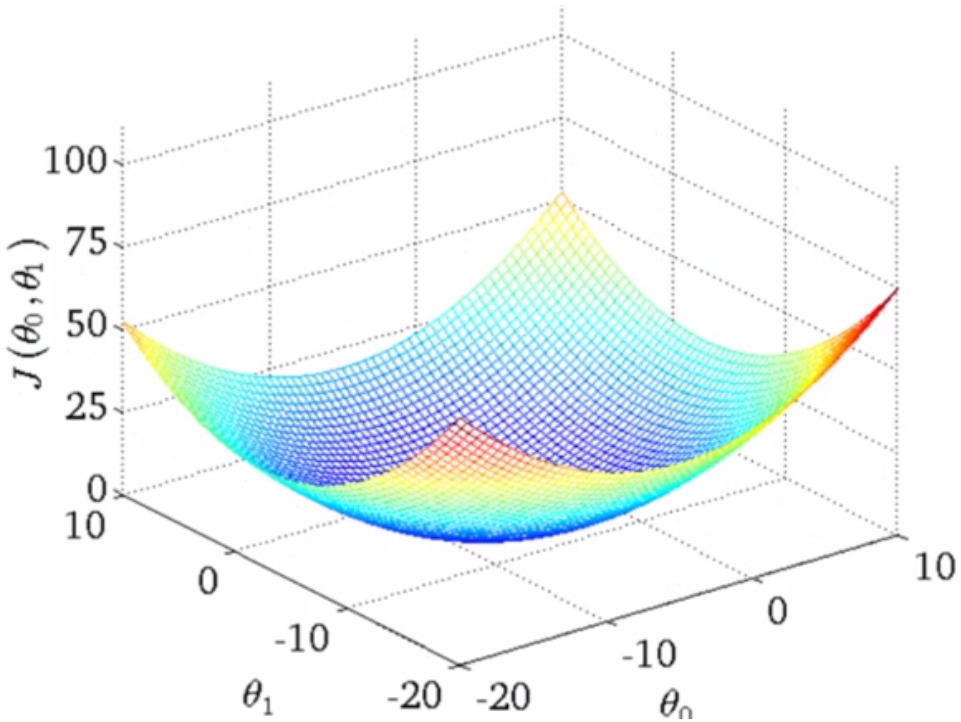
$$\theta_0 := \theta_0 - \eta \frac{1}{N} \sum_{i=1}^{N} (\theta_0 + \theta_1 x_i - y_i)$$

$$\theta_1 := \theta_1 - \eta \frac{1}{N} \sum_{i=1}^{N} (\theta_0 + \theta_1 x_i - y_i) x_i$$

}

Gradient descent

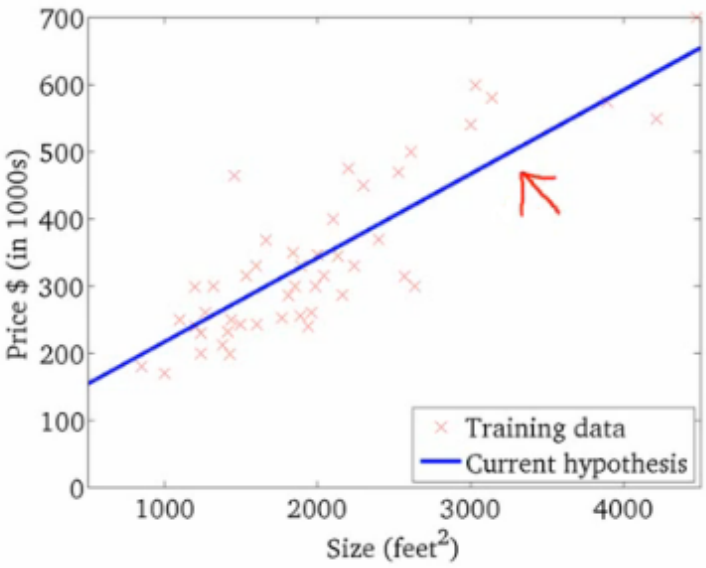
Because the cost function is convex it will have a global minimum



Gradient descent will fit the best least squares line

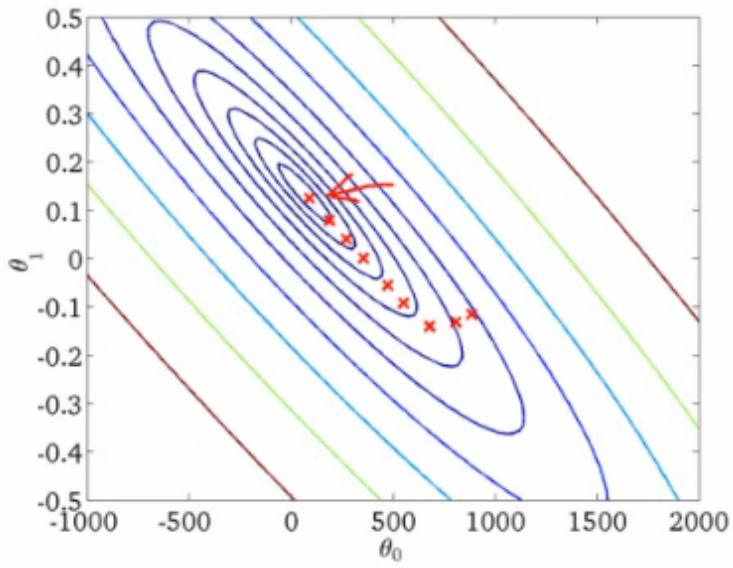
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



For multivariate regression

$$\theta = [\theta_0, \cdots, \theta_p]$$
$$y = [y_1, \cdots, \theta_N]$$
$$X \in \mathbb{R}^{Nx(p+1)}$$

repeat while $(||\eta \nabla J(\theta)|| > \epsilon)$
{

$$\theta := \theta - \eta \nabla J(\theta)$$

}

For multivariate regression

$$\nabla J(\theta) = \frac{1}{N}(y^T - \theta X^T)X$$

repeat while $(||\eta \nabla J(\theta)|| > \epsilon)$
{

$$\theta := \theta - \eta \frac{1}{N}(y^T - \theta X^T)X$$

}