Deep Learning Using R & TensorFlow



OC R User's Group March 26, 2019 April 29, 2019



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- Field of Expertise
 - Machine Learning, Deep Learning, Digital Image Processing, Database Management, CD-ROM/DVD
- Worked for
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Caltech Course

Caltech

CALIFORNIA INSTITUTE OF TECHNOLOGY

Center for Technology & Management Education



Division of Engineering & Applied Science

Deep Learning with TensorFlow

SCHEDULE

Classes are held Saturdays, 8:00 AM to 5:00 PM, on the Caltech campus in Pasadena, California.

	Spring 2019	Add to Cart
Deep Learning with TensorFlow	April 6, 13, 20	Register

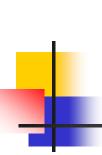
INSTRUCTOR

Ash Pahwa, PhD



Outline: Part 1 OC R User's Group: March 26, 2019

- What is Deep Learning
- Deep Learning Applications
- Tools for Deep Learning
- Misunderstanding about TensorFlow
- Availability of GPU
- TensorFlow Architecture
- R Code with TensorFlow



Outline: Part 2 OC R User's Group: April 29, 2019

- Title: Deep Learning Optimization Techniques
 - Gradient Descent
 - Momentum
 - Nesterov Momentum
 - AdaGrad
 - RMSProp
 - Adam: Adaptive Moments



What is Optimization Problem?

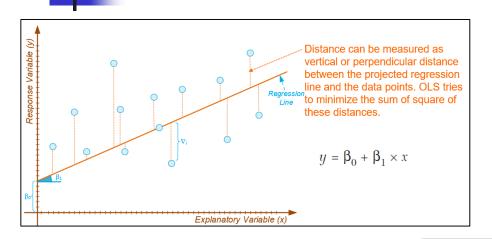
- Regression
 - Solution: Minimize the cost function
 - Closed form solution: Matrix Approach
 - Iterative Approach: Gradient Descent Algorithm
- Neural Networks: Deep Learning
 - Solution: Minimize the cost function
 - Iterative Approach: Gradient Descent Algorithm

Regression



Minimize Cost Function

Closed Form Solution: Matrix Approach



$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix} \quad X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \dots & \dots \\ 1 & x_n \end{bmatrix} \quad A = \begin{bmatrix} b \\ m \end{bmatrix} \quad E = \begin{bmatrix} e_1 \\ e_2 \\ \dots \\ e_n \end{bmatrix}$$

- Matrix Equation: Y = XA + E
- E = Y XA

Closed Form Solution Matrix Approach

Used by

- F
- Python
- Excel
- All other statistical software

$$RSS = (Y - XA)^T (Y - XA)$$

$$RSS = Y^TY - 2Y^TXA + AX^TXA$$

• Set
$$\frac{\partial RSS}{\partial A} = 0$$
,

• to compute the value of A for minimum RSS

$$A = (X^T X)^{-1} X^T Y$$

X	Y	
0	1	
1	3	
2	7	
3	13	
4	21	

•
$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

•
$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

• $A^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$

Solution for Least RSS =
$$A = (X^T X)^{-1} X^T Y$$

$$X^{T}X = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} = \begin{bmatrix} 5 & 10 \\ 10 & 30 \end{bmatrix}$$

$$(X^T X)^{-1} = \frac{1}{50} \begin{bmatrix} 30 & -10 \\ -10 & 5 \end{bmatrix} = \begin{bmatrix} 0.6 & -0.2 \\ -0.2 & 0.1 \end{bmatrix}$$

$$X^{T}Y = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \\ 7 \\ 13 \\ 21 \end{bmatrix} = \begin{bmatrix} 45 \\ 140 \end{bmatrix}$$

•
$$A = (X^T X)^{-1} X^T Y = \begin{bmatrix} 0.6 & -0.2 \\ -0.2 & 0.1 \end{bmatrix} \begin{bmatrix} 45 \\ 140 \end{bmatrix} = \begin{bmatrix} -1 \\ 5 \end{bmatrix}$$
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•
$$Y = \begin{bmatrix} 1\\3\\7\\13\\21 \end{bmatrix}$$
 $X = \begin{bmatrix} 1&0\\1&1\\1&2\\1&3\\1&4 \end{bmatrix}$

Regression Equation
$$y = 5x - 1$$

Who Invented Gradient Descent Algorithm?

- Gradient Descent algorithm was invented by Cauchy in 1847
- Méthode générale pour la résolution des systèmes d'équations simultanées. pp. 536–538



What is Gradient Descent Algorithm?



- Gradient Descent algorithm allows us to find the values of 'x' where the 'y' value becomes minimum or maximum
- The Gradient Descent algorithm can be extended to any function with 2 or more variables z = f(x, y)
- Function y=f(x)
- Gradient Descent Algorithm: Minimum
 - Initialize the value of x
 - Learning rate = η
 - While NOT converged:
 - $x^{t+1} \leftarrow x^t \eta \frac{\partial y}{\partial x} \|_{x^t}$

- Function z=f(x,y)
- Gradient Descent Algorithm: Minimum
 - Initialize the value of x and y
 - Learning rate = η
 - While NOT converged:

$$x^{t+1} \leftarrow x^t - \eta \frac{\partial z}{\partial x} \|_{x^t, y^t}$$

$$y^{t+1} \leftarrow y^t - \eta \frac{\partial z}{\partial y} \parallel_{x^t, y^t}$$

Partial Derivatives of the RSS w.r.t. Intercept and Slope

- Residuals Sum of Squares = $(RSS) = \sum_{i=1}^{N} (y_i (mx_i + b))^2$
- To find the minimum point of this function,
 - we will take the partial derivative of RSS with respect to 'm' and 'b' and set that to zero.

•
$$RSS = \sum_{i=1}^{N} (y_i - (mx_i + b))^2$$

$$\frac{\partial RSS(m,b)}{\partial b} = \sum_{i=1}^{N} \frac{\partial}{\partial b} (y_i - (mx_i + b))^2$$

$$\frac{\partial RSS(m,b)}{\partial b} = -2\sum_{i=1}^{N} (y_i - (mx_i + b))$$

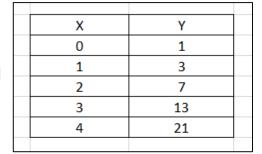
•
$$RSS = \sum_{i=1}^{N} (y_i - (mx_i + b))^2$$

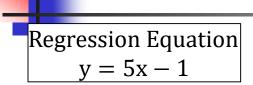
$$\frac{\partial RSS(m,b)}{\partial m} = \sum_{i=1}^{N} \frac{\partial}{\partial m} (y_i - (mx_i + b))^2$$

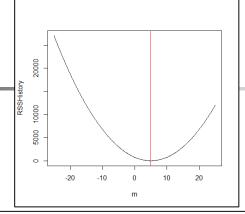
$$\frac{\partial RSS(m,b)}{\partial m} = -2\sum_{i=1}^{N} (y_i - (mx_i + b))x_i$$

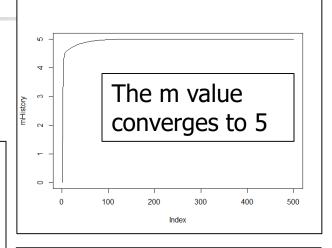
$$\nabla RSS(b,m) = \left| \frac{\partial RSS(m,b)}{\partial b} \atop \frac{\partial RSS(m,b)}{\partial m} \right| = \left| \begin{array}{c} -2\sum_{i=1}^{N} (y_i - (mx_i + b)) \\ -2\sum_{i=1}^{N} (y_i - (mx_i + b))x_i \end{array} \right| = 0$$

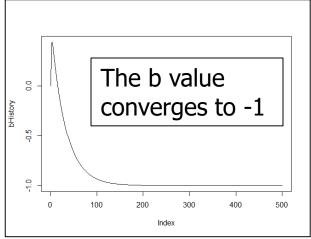
Regression Gradient Descent Algorithm Approach











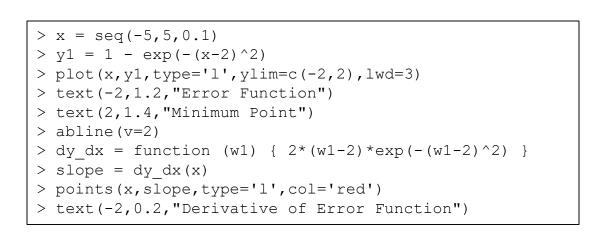
Problems with Gradient Descent Algorithm

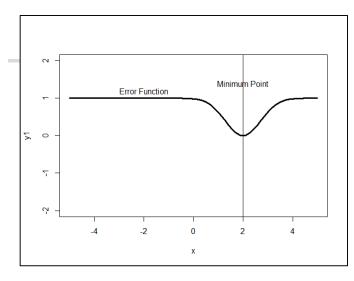
- When the gradient of the error function is low (flat)
 - It takes a long time for the algorithm to converge (reach the minimum point)
- If there are multiple local minima, then
 - There is no guarantee that the procedure will find the global minimum

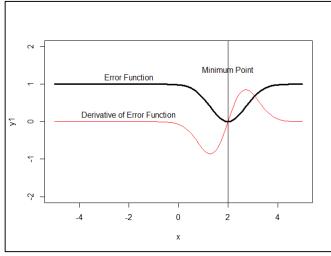
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Error Function

- *Error Function*: $y = f(x) = 1 e^{-(x-2)^2}$
- $\frac{dy}{dx} = 2(x-2)e^{-(x-2)^2}$
- The error function 'y' is almost flat
 - $f(x) = 0: -\infty < x < 0$ and
 - f(x) = 0: $4 < x < \infty$

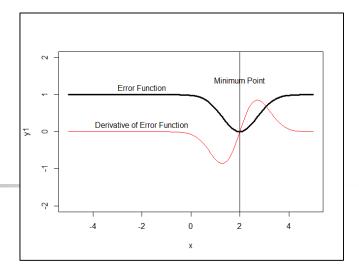


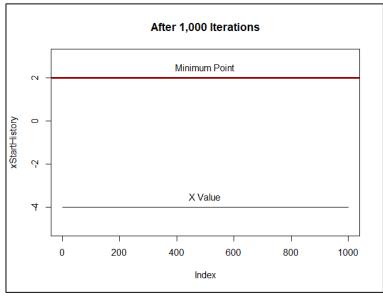




Gradient Descent Algorithm

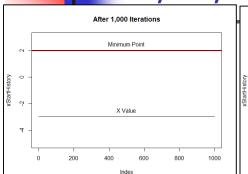
- Starting Point = -4
- Number of iteration = 1,000

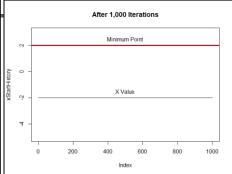


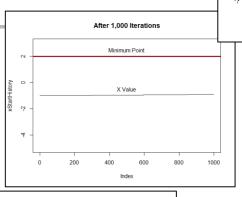


Starting Point = -4, DOES NOT CONVERGE

After 1,000 iteration Starting Point -3, -2, -1, -0.5



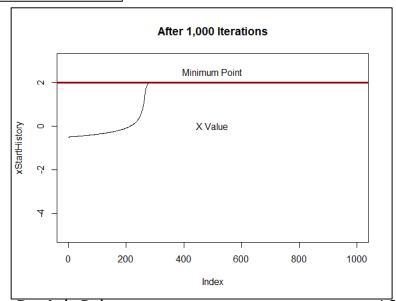




Starting Point = -3, -2, -1: 'x' value DOES NOT CONVERGE

Starting Point = -0.5,

'x' value CONVERGES AFTER 250 ITERATIONS



Error Function

Derivative of Error Function

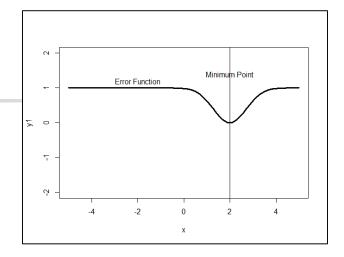
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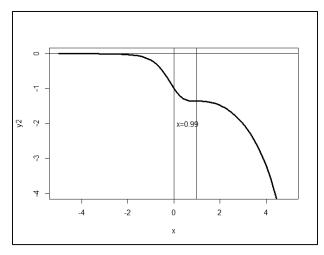
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Problems with Gradient Descent Algorithm

- If the error function has very small gradient
 - Starting point is on the flat surface
 - Gradient Descent Algorithm will take a long time to converge





Solutions to Gradient Descent Algorithm Problem

- Solution#1: Increase the step size
 - Momentum based GD
 - Nesterov GD
- Solution#2: Reduce the data points for approximate gradient
 - Stochastic Gradient Descent
 - Mini Batch Gradient Descent
- Solution#3: Adjust the Learning rate (η)
 - AdaGrad
 - RMSProp
 - Adam

- Function y=f(x)
- Gradient Descent Algorithm:Minimum
 - Initialize the value of x
 - Learning rate = η
 - While NOT converged:

•
$$x^{t+1} \leftarrow x^t - \eta \frac{\partial y}{\partial x} \|_{x^t}$$

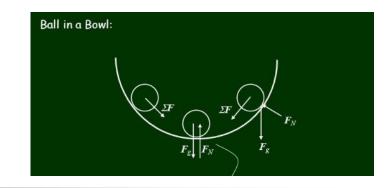


First Solution to the Gradient Descent Algorithm Problem

- When the gradient becomes zero
 - Find some way to move forward
- Step size is not only a function of current gradient at time 't'
 - But also previous gradient at time 't-1'
- Solution
 - Momentum
 - Exponentially Weighted Moving Average of Gradient

•
$$x_{t+1} = x_t - \eta \frac{\partial z}{\partial x} - (previous \ values \ of \ \frac{\partial z}{\partial x})$$

Momentum Based GD



Ball gains momentum while rolling down a slope

- Time t1
 - Ask for direction (Measure Gradient)
 - Take a small step in that direction
- Time t2
 - Ask for direction (Measure Gradient)
 - If the direction computed ay time 't2' is same as the direction at time 't1'
 - Take a bigger step in that direction
- Time t3
 - Ask for direction (Measure Gradient)
 - If the direction computed ay time 't3' is same as the direction at time 't1' and 't2'
 - Take a bigger step in that direction
- Momentum is building as we are moving along
- Speed at which we are moving will increase with time

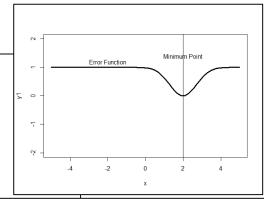
Exponentially Weighted Moving Averages (EWMA)

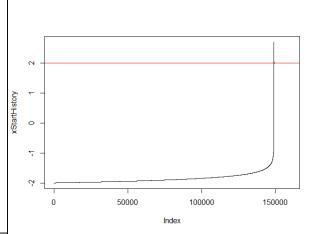
Exponentially Weighted Moving Average of Gradients

- $update_t = \gamma * update_{t-1} + \eta \frac{\partial z}{\partial x}|_t$
- $x_{t+1} = x_t update_t$
- _____
- $update_0 = 0$
- $update_1 = \gamma * update_0 + \eta \frac{\partial z}{\partial x}|_1$
- $update_2 = \gamma * update_1 + \eta \frac{\partial z}{\partial x}|_2 = (\gamma^2 * update_0) + (\gamma * \eta \frac{\partial z}{\partial x}|_1) + (\eta \frac{\partial z}{\partial x}|_2)$
- $update_3 = \gamma * update_2 + \eta \frac{\partial z}{\partial x}|_3 = (\gamma^3 * update_0) + (\gamma^2 * \eta \frac{\partial z}{\partial x}|_1) + (\gamma * \eta \frac{\partial z}{\partial x}|_2) + (\eta \frac{\partial z}{\partial x}|_3)$
- $update_4 = \gamma * update_3 + \eta \frac{\partial z}{\partial x}|_4 = (\gamma^4 * update_0) + (\gamma^3 * \eta \frac{\partial z}{\partial x}|_1) + (\gamma^2 * \eta \frac{\partial z}{\partial x}|_2) + (\gamma * \eta \frac{\partial z}{\partial x}|_3) + (\eta \frac{\partial z}{\partial x}|_4)$
- $update_t = \gamma * update_{t-1} + \eta \frac{\partial z}{\partial x}|_t = (\gamma^t * update_0) + \left(\gamma^{t-1} * \eta \frac{\partial z}{\partial x}|_1\right) + \left(\gamma^{t-2} * \eta \frac{\partial z}{\partial x}|_2\right) + \dots + \left(\eta \frac{\partial z}{\partial x}|_t\right)$

Example#1: Gradient Descent with Momentum Converges after 150,000 Iterations

```
xStart = -2.0
learningRate = 0.1
# Momentum
maxLimit = 160000
xStartHistory = rep(0,maxLimit)
gamma = 0.9
update = 0
for ( i in 1:maxLimit ) {
 xStartHistory[i] = xStart
 gradient = dy dx(xStart)
 update = (gamma * update) + (learningRate * gradient)
 xStart = xStart - update
plot(xStartHistory, type='l')
abline (h=2, col='red')
```

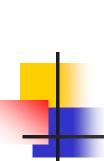




- $update_t = \gamma * update_{t-1} + \eta \frac{\partial z}{\partial x}|_t$
- $x_{t+1} = x_t update_t$
- $update_t = \gamma * update_{t-1} + \eta \frac{\partial z}{\partial x}|_t = \left(\gamma^{t-1} * \eta \frac{\partial z}{\partial x}|_1\right) + \left(\gamma^{t-2} * \eta \frac{\partial z}{\partial x}|_2\right) + \dots + \left(\eta \frac{\partial z}{\partial x}|_t\right)$

Example#1: Just Before Reaching the Minimum Point Oscillation

```
Expand when the values are converging
> xStartHistorySmall = xStartHistory[148500:149500]
 plot(xStartHistorySmall, type='l')
 abline (h=2, col='red')
 >
                                   xStartHistorySmall
                                             200
                                                  400
                                                       600
                                                            800
                                                                 1000
                                                    Index
```



Solution to Momentum Nesterov Momentum

- Before jumping to the next check the gradient at the next step also
- If the next step gradient forces to take a 'U' turn
 - Reduce the size of the step

Yurii Nesterov

- Nesterov is most famous for his work in convex optimization, including his 2004 book, considered a canonical reference on the subject
- His main novel contribution is an accelerated version of gradient descent that converges considerably faster than ordinary gradient descent (commonly referred as Nesterov momentum or Nesterov accelerated gradient, in short — NAG)

Yurii Nesterov



2005 in Oberwolfach

Born January 25, 1956 (age 63)

Moscow, USSR

Citizenship Russia

Alma mater Moscow State University (1977)

Awards Dantzig Prize, 2000

John von Neumann Theory Prize,

2009

EURO Gold Medal, 2016

Scientific career

Fields Convex optimization,

Semidefinite programming,

Nonlinear programming,

Numerical analysis,

Applied mathematics

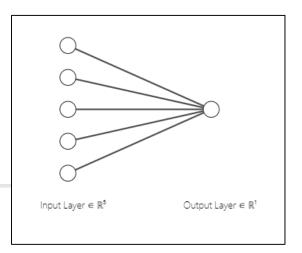
Learning Rate η

- Function y=f(x)
- Gradient Descent Algorithm:Minimum
 - Initialize the value of x
 - Learning rate = η
 - While NOT converged:

•
$$x^{t+1} \leftarrow x^t - \eta \frac{\partial y}{\partial x} \|_{x^t}$$

- How to decide the Learning Rate (LR)?
- If LR is small
 - Gradient will gently descend and we will get the optimum value of 'x' for which the error is minimum
 - But it may take a long time to converge
- If LR is large
 - NN will converge faster
 - But when we reach the destination "minimum" point of the error function we will see the 'x' values oscillation

AdaGrad Adaptive Gradient



- AdaGrad
 - It dynamically varies the learning rate
 - At each update
 - For each weight individually
- Learning rate decreases as the algorithm moves forward
- Every variable will have a separate learning rate
- In the above example
 - 5 weights from input to output layers
 - 5 separate learning rates which are decreasing as algorithm moves forward

AdaGrad Adaptive Gradient Algorithm

- Gradient Descent
 - While NOT converged:

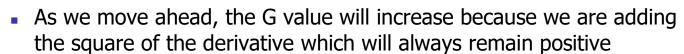
•
$$x^{t+1} \leftarrow x^t - \eta \frac{\partial y}{\partial x}|_{x^t}$$

AdaGrad: Update rule is for individual weight

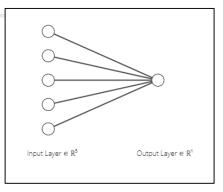
$$x_i^{t+1} = x_i^t - \frac{\eta}{\sqrt{G_i^t + \varepsilon}} * \frac{\partial y}{\partial x_i} |_t$$

$$G_i^t = G_i^{t-1} + \left(\frac{\partial y}{\partial x_i}|_t\right)^2$$

•
$$G_o^i = 0$$



- As the value of G increases, the value of learning rate η will decrease.
- The value of epsilon (an arbitrary small number) is added to the denominator to avoid a situation of dividing by zero

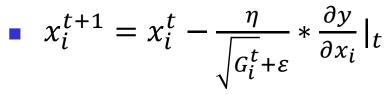


Adaptive Learning Rate Schedule for each weight

$$1 \le i \le n$$

Where n' = number of weights

Difference: AdaGrad and RMSProp



AdaGrad

$$G_i^t = G_i^{t-1} + \left(\frac{\partial y}{\partial x_i}|_t\right)^2$$

RMS Prop

$$G_i^t = \beta * G_i^{t-1} + (1 - \beta) * \left(\frac{\partial y}{\partial x_i}|_t\right)^2$$

- AdaGrad
 - Since the 'G' value will increase continuously
 - Learning rate will decrease continuously
 - Eventually learning rate will be very small
- RMS Prop
 - Since the 'G' value will NOT increase continuously
 - It will adjust to the data and decrease or increase the learning rate accordingly

Root Mean Square Propagation "RMS Prop" Algorithm



$$x_i^{t+1} = x_i^t - \frac{\eta}{\sqrt{G_i^t + \varepsilon}} * \frac{\partial y}{\partial x_i} |_t$$

$$G_i^t = G_i^{t-1} + \left(\frac{\partial y}{\partial x_i}|_t\right)^2$$

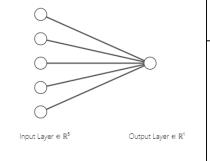
•
$$G_o^i = 0$$

RMS Prop

$$x_i^{t+1} = x_i^t - \frac{\eta}{\sqrt{G_i^t + \varepsilon}} * \frac{\partial y}{\partial x_i} |_t$$

$$G_i^t = \beta * G_i^{t-1} + (1-\beta) * \left(\frac{\partial y}{\partial x_i}|_t\right)^2$$

• Where β is another hyper parameter: typical value = 0.9



Adaptive Learning Rate Schedule for each weight

$$1 \le i \le n$$

Where n' = number of weights

What is Adam? Adaptive Moment Estimation

- Adam = RMS Prop + Momentum
- Adam takes the positive points of
 - Momentum &
 - RMS Prop algorithm
- Authors: Diederik Kingma and Jimmy Bai

D. P. Kingma and J. L. Bai. Adam: a method for stochastic optimization. *ICLR*, 2015.

Adam Adaptive Moment Estimation

- Adaptive Moment Estimation (Adam) combines ideas from both RMSProp and Momentum
- It computes adaptive learning rates for each parameter and works as follows

$$m_t = \beta_1 * m_{t-1} + (1 - \beta_1) \frac{\partial z}{\partial x} |_t$$

$$v_t = \beta_2 * v_{t-1} + (1 - \beta_2) \left(\frac{\partial z}{\partial x} |_t \right)^2$$

$$m_0 = 0$$

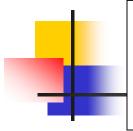
$$v_0 = 0$$

 Lastly, the parameters are updated using the information from the calculated averages

$$w_t = w_{t-1} - \eta \frac{m_t}{\sqrt{v_t} + \varepsilon}$$

- m_t : Exponentially weighted average of past gradients
- v_t : Exponentially weighted average of the past squares of gradients

Bias Correction



- The Adam works best when the
- Expectations (m_t) = Expectation(distribution of derivative)
- Expectation (v_t) = Expectation(distribution of square of derivative)
- After every update we adjust the value of m_t and v_t

Adam

$$m_t = \beta_1 * m_{t-1} + (1 - \beta_1) \frac{\partial z}{\partial x} |_t$$

$$v_t = \beta_2 * v_{t-1} + (1 - \beta_2) \left(\frac{\partial z}{\partial x}|_t\right)^2$$

$$w_t = w_{t-1} - \eta \frac{m_t}{\sqrt{v_t} + \varepsilon}$$

Adam Bias Correction

$$m_t = \beta_1 * m_{t-1} + (1 - \beta_1) \frac{\partial z}{\partial x} |_t$$

$$v_t = \beta_2 * v_{t-1} + (1 - \beta_2) \left(\frac{\partial z}{\partial x} |_t \right)^2$$

$$\widehat{m_t} = \frac{m_t}{1 - \beta_1^t} \qquad \widehat{v_t} = \frac{v_t}{1 - \beta_2^t}$$

Adam Algorithm Implementation in R

Adam Adaptive Moment Estimation

Define Adam Hyper Parameters

```
> # ADAM Hyper Parameters
> # learning Rate + epochs + epsilon
> learningRate <- 0.01
> epsilon <- 1e-8
> # EWMA: Exponentially Weighted Moving Average
> # Hyper parameters
> beta1 < - 0.9
> beta2 <- 0.999
> # Initial value of 'm' and 'v' is zero
> m < - 0
> v <- 0
> epochs <- 1000
> 1 < - nrow(Y)
> costHistory <- array(dim=c(epochs,1))</pre>
>
```

```
m_0 = 0v_0 = 0
```

TensorFlow default parameter values

- β_1 : Hyper parameter = 0.9
 - Exponential decay rate for the moment estimate
- β_2 : Hyper parameter = 0.999
 - Exponential decay rate for the second moment estimates
- η : Learning Rate = 0.01
- ε : Small value to avoid dividing by zero = 1e 08

Adam Implementation

```
> for(i in 1:epochs) {
      # 1. Computed output: h = x values * weight Matrix
      h = X % * % t(W)
      # 2. Loss = Computed output - observed output
      loss = h - Y
      error = (h - Y)^2
      costHistory[i] = sum(error)/(2*nrow(Y))
      # 3. gradient = loss * X
      gradient = (t(loss) %*% X)/1
      # 4. calculate new W weight values
      m = beta1*m + (1 - beta1)*gradient
      v = beta2*v + (1 - beta2)*(gradient^2)
      # 5. corrected values Bias Correcttion
      m hat = m/(1 - beta1^i)
      v hat = v/(1 - beta2^i)
      # 6. Update the weights
      W = W - learningRate*(m hat/(sqrt(v hat) + epsilon))
+ }
```

$$m_0 = 0$$
$$v_0 = 0$$

Adam

$$m_t = \beta_1 * m_{t-1} + (1 - \beta_1) \frac{\partial z}{\partial x} |_t$$

$$v_t = \beta_2 * v_{t-1} + (1 - \beta_2) \left(\frac{\partial z}{\partial x} |_t \right)^2$$

$$w_t = w_{t-1} - \eta \frac{m_t}{\sqrt{v_t} + \varepsilon}$$

Adam Bias Correction

$$\widehat{m_t} = \frac{m_t}{1 - \beta_1^t} \qquad \widehat{v_t} = \frac{v_t}{1 - \beta_2^t}$$

Pesults > print(W) [1,1] [,2] [,3] [,4] [1,] -0.0152272 0.696738 0.4110761 0.2406706 > plot(costHistory, type='l')

```
Regression Equation: R 'Im' function
```

strength = -0.01533 + 0.69688 * cement + 0.41118 * slag + 0.24075 * ash

```
Regression Equation: R Matrix Approach
```

strength = -0.01533 + 0.69688 * cement + 0.41118 * slag + 0.24075 * ash

Regression Equation: R Adam

strength = -0.01522 + 0.6967 * cement + 0.41107 * slag + 0.2406 * ash



Summary: Part 2 OC R User's Group: April 29, 2019

- Title: Deep Learning Optimization Techniques
 - Gradient Descent
 - Momentum
 - Nesterov Momentum
 - AdaGrad
 - RMSProp
 - Adam: Adaptive Moments