Machine Learning: Introduction to Linear Regression, Logistic Regression, and Neural Networks

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2.1 Linear Regression: Mathematical Foundations

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Linear Regression: Mathematical Foundations

Goal of this Section:

- Present the mathematical foundations for the machine learning approach for linear regression, including:
    - Format of training data
    - Function structure and parameters
    - Loss function
    - Training algorithm
    - Prediction algorithm

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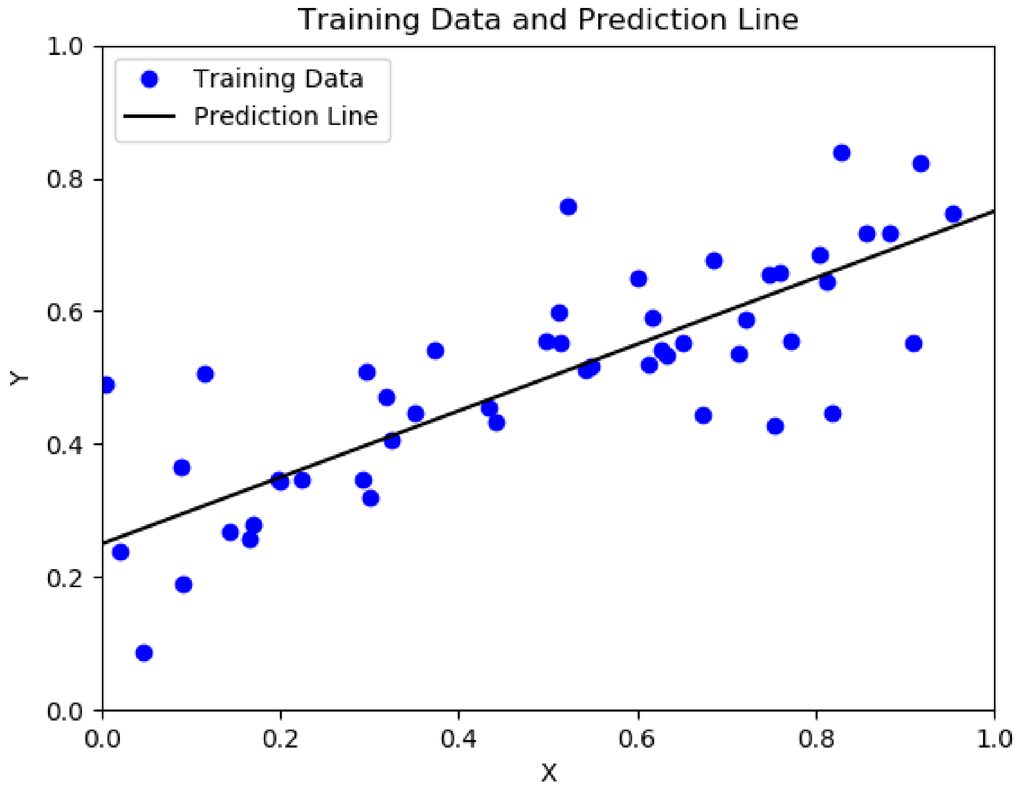
Linear Regression – Line Fitting

Training Data:
- Input information: X values
- Output information: Y values

Linear Regression Goal:
- Find straight line that best fits the training data

Prediction:
- Use line to predict Y values given new input X values

Why start with Linear Regression?
- Simple problem with well known solution
- This course will present a general approach that can also be applied to Logistic Regression and Neural Networks



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Least Squares Approach

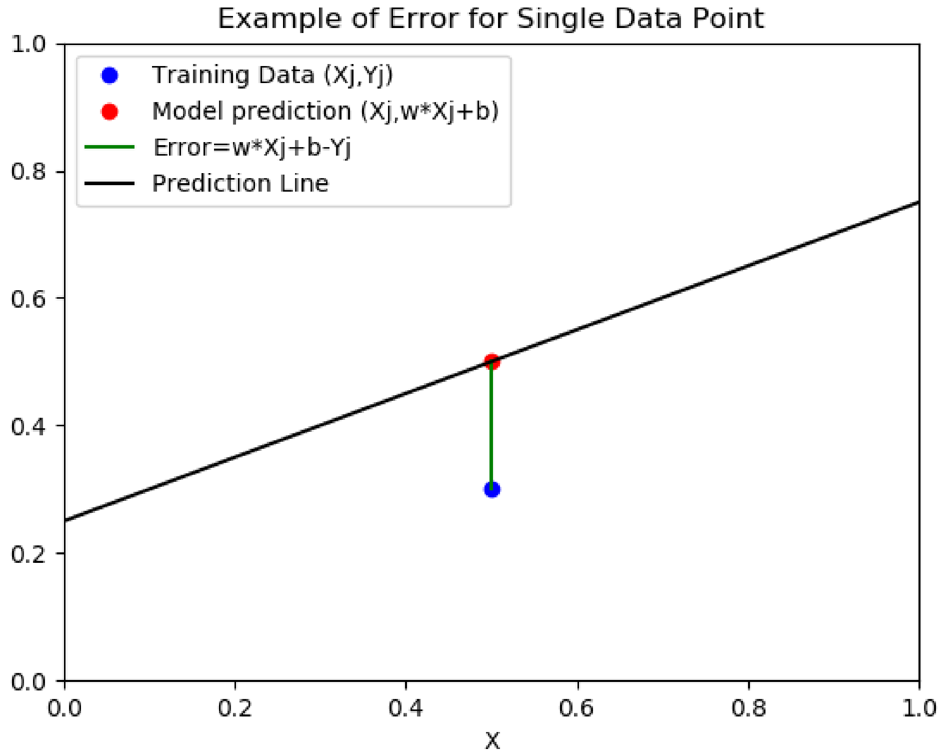
- Assume Y=WX+b

- Least squares approach: find W and b that minimizes sum of squared error:

$$L = \sum_{j=0}^{m-1} (WX_j + b - Y_j)^2$$

- Error for a single input/output information pair

- Loss is sum of squares of error



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Summary of Least Squares Approach

TRAINING DATA:

- Input/Output information pairs: (X_o,Y_o), (X_1,Y_1), …, (X_{m-1},Y_{m-1})

FUNCTION STRUCTURE

- Assume line Y = W*X + b (in this example W and b are scalars)

LOSS:

- Measure accuracy of function structure using Loss function: $L = \sum_{j=0}^{m-1}(WX_j + b - Y_j)^2$

TRAINING PHASE:

- Find slope W and intercept b that minimize squared error function
- W and b are solutions of the normal equations

FUNCTION PARAMETERS/RULES:

- These are the W and b that minimize the squared error

PREDICTION PHASE

- Given new input information X, use computed W and b to determine Y = W*X + b

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Normal Equations

- For the 1-dimensional problem input/output info: (X_o, Y_o), (X_1, Y_1), …, (X_{m-1}, Y_{m-1})
- Let us define:

$$\hat{X} = \begin{bmatrix} X_0 & X_1 & \dots & X_{m-1} \\ 1 & 1 & \dots & 1 \end{bmatrix} \text{ and } Y = \begin{bmatrix} Y_0 & Y_1 & \dots & Y_{m-1} \end{bmatrix}$$

- Define the parameter vector as:

$$\widehat{W} = \begin{bmatrix} W & b \end{bmatrix}$$

- The least squares normal equations solution is (T signifies transpose and -1 is the inverse)

$$\widehat{W} = \left(Y\hat{X}^T\right)\left(\hat{X}\hat{X}^T\right)^{-1}$$

(Note: this formula is different from what you have probably seen. In typical linear algebra courses, Y and w are column vectors. The above formula is the transpose of the typical formula from courses.)

- These ideas can be generalized to higher dimensions

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Linear Regression: General Approach

General approach has following components and phases:

(1) Training Data

(2) Function Structure

- Defines general form of the function with unknown parameters
- Process of applying function structure is called Forward Propagation

(3) Loss Function

- Used to measure effectiveness of function structure and choice of parameters

(4) Training Phase

- Uses optimization to determine function parameters that minimize loss function for training data
- Process of computing derivatives is called Back Propagation

(5) Prediction Phase

- Applies forward propagation using parameters determined in Training Phase to predict outputs when new input data is provided

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Training Data

- Consider more general regression problem where there are m data points, each consisting of a input information vector of length d and value Y:

- Data point j: input information (feature) vector: $\begin{bmatrix} X_{0,j} \\ X_{1,j} \\ \ldots \\ X_{d-1,j} \end{bmatrix}$ and output: Y_j

- Define the feature matrix (dxm) and output vector (1xm):

$$X = \begin{bmatrix} X_{00} & \ldots & X_{0,m-1} \\ \ldots & \ldots & \ldots \\ X_{d-1,0} & \ldots & X_{d-1,m-1} \end{bmatrix} \qquad Y = \begin{bmatrix} Y_0 & \ldots & Y_{m-1} \end{bmatrix}$$

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Training Data – Example Points in Plane

- For the 1-dimensional least squares problem in the motivating example, the training data consists of points in the plane: (X_o,Y_o), (X_1,Y_1), …, (X_{m-1},Y_{m-1})
- For example consider 4 samples in training set: (1,1), (0.5,2), (2,3), (4,2)
- In this case each data point has 1 feature (the X value)
- Feature matrix and output vector are:

$$X = \begin{bmatrix} 1 & 0.5 & 2 & 3 \end{bmatrix} \qquad Y = \begin{bmatrix} 1 & 2 & 3 & 2 \end{bmatrix}$$

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Training Data – Example Predicting House Prices

- Suppose we have input information (features) of a house and output information (price)

Feature 0: Lot area (in square feet)

Feature 1: House area (in square feet)

Feature 2: Number of bathrooms

Feature 3: Number of floors

Feature …:

Feature d-1: Size of garage (number of cars)

- Data point j: feature vector: $\begin{bmatrix} 5000 \\ 2000 \\ 3 \\ 2 \\ \dots \\ 2 \end{bmatrix}$ and output information (price): Y_j= 800,000
- Collect all feature vectors and output values to create feature matrix and output vector

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Function Structure - Forward Propagation

Forward Propagation is name applied to process of estimating output values using function structure

Input: feature matrix X (dxm d features and m data points)

Assign: parameter vector $W = [W_0 \quad W_1 \quad \ldots \quad W_{d-1}]$ and bias b

1. Linear part: for j=0,…,m-1

$$Z_j = W_o X_{oj} + W_1 X_{1j} + W_2 X_{2j} + \cdots + W_{d-1} X_{d-1j} + b$$

In vector form $Z = [Z_0 \quad Z_1 \quad \ldots \quad Z_{m-1}]$ and $Z = WX + b$

Function Structure

2. Activation: apply function f(z) to each component of Z:

$$A_j = f(Z_j) \qquad j = 0, \ldots, m-1$$

For Linear Regression f(z) = z, so $A_j = Z_j,\ j = 0, \ldots, m-1$

$[A_0 \ \ A_1 \quad \ldots \quad A_{m-1}]$ is estimate of output values

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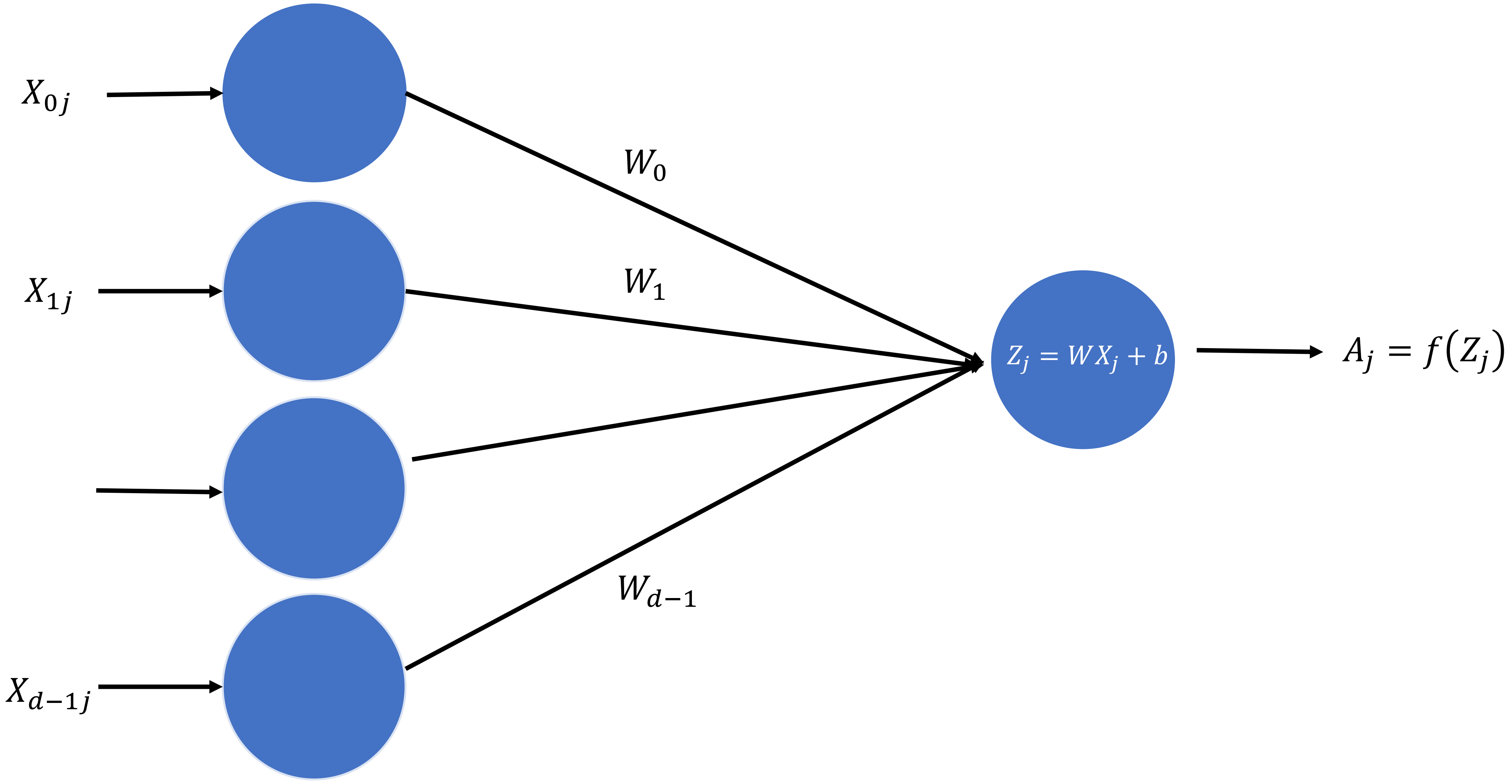
Forward Propagation Diagram



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Forward Propagation - Example

- Consider a case of 2 features and 3 data points (m=3)

$$X = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} \qquad Y = \begin{bmatrix} 8 & 6 & 10 \end{bmatrix}$$

- Assume that initial parameter values are:

$$W = \begin{bmatrix} 1 & 1 \end{bmatrix} \qquad \mathrm{b} = [2]$$

- Forward Propagation:

$$Z = WX + b = \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} + [2] = \begin{bmatrix} 5 & 9 & 13 \end{bmatrix}$$

$$A = Z = \begin{bmatrix} 5 & 9 & 13 \end{bmatrix}$$

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Loss Function

- Loss function used to measure effectiveness of choice W and b
- Standard approach for Linear regression is to use Mean Squared Error function:

$$Loss = L = \frac{1}{m}\sum_{j=0}^{m-1}(A_j - Y_j)^2$$

- A_j-Y_j is the error between the original training data point and the prediction based on the function structure and forward propagation
- Loss is mean of squares of errors for all training points

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Loss Function - Example

- Consider a case of 2 features and 3 data points (m=3)

$$X = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} \qquad Y = \begin{bmatrix} 8 & 6 & 10 \end{bmatrix}$$

- From the Forward Propagation Example

$$A = \begin{bmatrix} 5 & 9 & 13 \end{bmatrix}$$

- Loss function defined by

$$L = \frac{1}{m}\sum_{j=0}^{m-1}(A_j - Y_j)^2 = \frac{1}{3}\sum_{j=0}^{m-1}[(5-8)^2 + (9-6)^2 + (13-10)^2] = 9$$

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Training Phase

- Training phase attempts to find suitable coefficients W and b by minimizing loss function when applied to training data
- From multi-variable calculus, Loss function has a local minimum when the gradients are 0

$\nabla_W L = 0$ and $\nabla_b L = 0$

- Can solve these equations analytically for Linear Regression, but not in general case (Logistic Regression and Neural Networks)
- Use optimization algorithm (example: Gradient Descent) to minimize Loss function
    - Need to compute the above gradients

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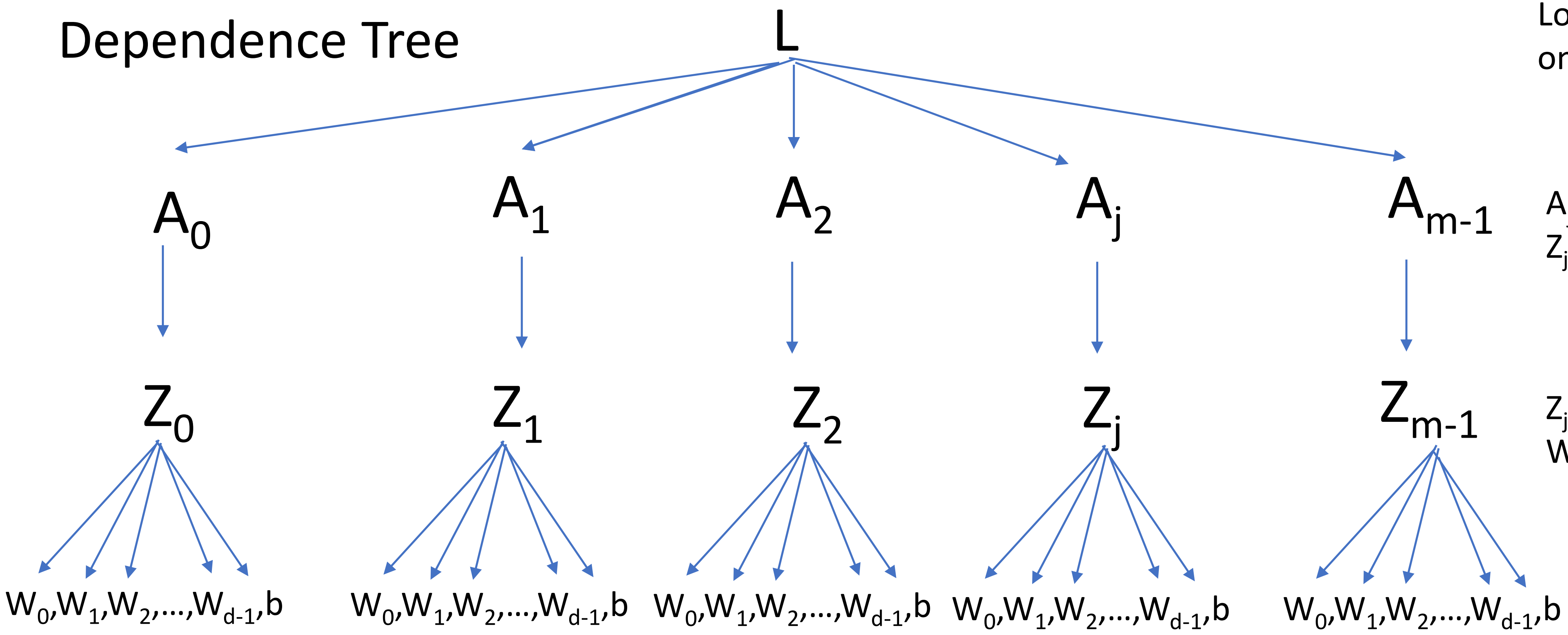
Computing Gradients

Apply Chain Rule of Calculus to determine $\nabla_W L$ and $\nabla_b L$.

Dependence Tree



Loss L depends on each A_j

A_j depends on Z_j only

Z_j depends on all W_i and b

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Multi-Variable Calculus – Chain Rule

Recall the chain rule lecture (Section 1.6)

- If L = L(Z_0,…,Z_{m-1}) and Z = WX + b, then

$\nabla_W L = \nabla_Z L X^T$ and $\nabla_b L = \sum_{j=0}^{m-1} \nabla_Z L_j$

- For linear regression, the loss function L depends on A_0 ,…,A_{m-1}
- A_0 depends exclusively on Z_0, A_1 depends exclusively on Z_1 and so on
- In fact $\frac{\partial A_j}{\partial Z_j} = 1$ since the activation function is the identity f(z)=z
- To compute the derivatives correctly, we need to again apply the chain rule

$$\nabla_Z L = \begin{bmatrix} \frac{\partial L}{\partial Z_0} & \dots \frac{\partial L}{\partial Z_{m-1}} \end{bmatrix} = \begin{bmatrix} \frac{\partial L}{\partial A_0}\frac{\partial A_0}{\partial Z_0} & \frac{\partial L}{\partial A_1}\frac{\partial A_1}{\partial Z_1} & \dots & \frac{\partial L}{\partial A_{m-1}}\frac{\partial A_{m-1}}{\partial Z_{m-1}} \end{bmatrix}$$

$$\nabla_Z L = \begin{bmatrix} \frac{\partial L}{\partial A_0} & \frac{\partial L}{\partial A_1} & \dots \frac{\partial L}{\partial A_{m-1}} \end{bmatrix} * \begin{bmatrix} \frac{\partial A_0}{\partial Z_0} & \frac{\partial A_1}{\partial Z_1} & \dots & \frac{\partial A_{m-1}}{\partial Z_{m-1}} \end{bmatrix} = \nabla_A L * \begin{bmatrix} 1 & 1 & \dots & 1 \end{bmatrix}$$

Here * means component-wise multiplication

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Gradient of Mean Squared Error Function

- For the mean squared error function:

$$L = \frac{1}{m}\sum_{j=0}^{m-1}(A_j - Y_j)^2$$

- Gradient given by

$$\nabla_A L = \left[\frac{\partial L}{\partial A_0} \quad \frac{\partial L}{\partial A_1} \quad \ldots \frac{\partial L}{\partial A_{m-1}}\right]$$ where $\frac{\partial L}{\partial A_j} = \frac{2}{m}(A_j - Y_j)$ for j=0,…,m-1

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Back Propagation Algorithm

Back propagation is the process of computing $\nabla_W L$ and $\nabla_b L$

Assume that forward propagation has taken place so $[A_0 \;\; A_1 \;\; \ldots \;\; A_{m-1}]$ has been computed

Input: feature matrix X and value vector Y

1. Compute gradient of L with respect to A

$$\nabla_A L = \left[\frac{\partial L}{\partial A_0} \quad \frac{\partial L}{\partial A_1} \quad \ldots \quad \frac{\partial L}{\partial A_{m-1}}\right], \frac{\partial L}{\partial A_j} = \frac{2}{m}\left(A_j - Y_j\right), \quad j = 0, \ldots, m-1$$

2. Compute derivatives of A: $\dfrac{\partial A_j}{\partial Z_j} = 1, j = 0, \ldots, m-1$

3. Compute gradient L with respect to Z:

$$\nabla_Z L = \nabla_A L * \left[\frac{\partial A_0}{\partial Z_0} \quad \frac{\partial A_1}{\partial Z_1} \quad \ldots \quad \frac{\partial A_{m-1}}{\partial Z_{m-1}}\right]$$ (component-wise multiplication)

4. Compute gradient of L with respect to W and b:

$$\nabla_W L = \nabla_Z L X^T, \qquad \nabla_b L = \sum_{j=0}^{m-1} \nabla_Z L_j$$

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Back Propagation - Example

- Consider a case of 2 features and 3 data points (m=3)

$X = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} \qquad Y = \begin{bmatrix} 8 & 6 & 10 \end{bmatrix}$

- Assume that initial parameter values are:

$W = \begin{bmatrix} 1 & 1 \end{bmatrix} \qquad \mathrm{b} = [2]$

- From forward propagation example:

$A = Z = \begin{bmatrix} 5 & 9 & 13 \end{bmatrix}$

- Gradient of Loss with respect to A:

$\frac{\partial L}{\partial A_j} = \frac{2}{m}(A_j - Y_j)$ for j=0,…,m-1 $\quad \nabla_A L = \begin{bmatrix} \frac{2}{3}(5-8) & \frac{2}{3}(9-6) & \frac{2}{3}(13-10) \end{bmatrix} = \begin{bmatrix} -2 & 2 & 2 \end{bmatrix}$

$\begin{bmatrix} \frac{\partial A_0}{\partial Z_0} & \frac{\partial A_1}{\partial Z_1} & \frac{\partial A_2}{\partial Z_2} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$

$\nabla_Z L = \nabla_A L * \begin{bmatrix} \frac{\partial A_0}{\partial Z_0} & \frac{\partial A_1}{\partial Z_1} & \frac{\partial A_2}{\partial Z_2} \end{bmatrix} = \begin{bmatrix} -2 & 2 & 2 \end{bmatrix} * \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} -2 & 2 & 2 \end{bmatrix}$ (component-wise multiplication)

$\nabla_W L = \nabla_Z L X^T = \begin{bmatrix} -2 & 2 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 5 \\ 4 & 7 \end{bmatrix} = \begin{bmatrix} 10 & 20 \end{bmatrix}$

$\nabla_b L = \sum_{j=0}^{m-1} \nabla_Z L_j = 2$ (sum of entries of $\nabla_b L$)

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Training Algorithm

- Training algorithm uses Gradient Descent to find parameters W and b that minimize the Loss function
- At each step of gradient descent need to compute gradient of loss with respect to W and b
- Computation of gradient involves both forward and back propagation

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Training Algorithm

Input training data: feature matrix X and values Y

Make initial guess for parameters $W_{epoch=0}$ and $b_{epoch=0}$

Choose learning rate $\alpha > 0$

1. Loop for epoch i = 1, 2, …
   - Forward Propagate using X to compute $A_{epoch=i-1}$
   - Back Propagate using X, Y, and $A_{epoch=i-1}$ to compute $\nabla_W L_{epoch=i-1}, \nabla_b L_{epoch=i-1}$
   - Update parameters: (Gradient Descent)

     $W_{epoch=i} = W_{epoch=i-1} - \alpha \nabla_W L_{epoch=i-1}$

     $b_{epoch=i} = b_{epoch=i-1} - \alpha \nabla_b L_{epoch=i-1}$
   - Forward Propagate to compute $A_{epoch=i}$
   - Compute Loss at $A_{epoch=i}$

Loop for fixed number of epochs (or if Loss reduced sufficiently)

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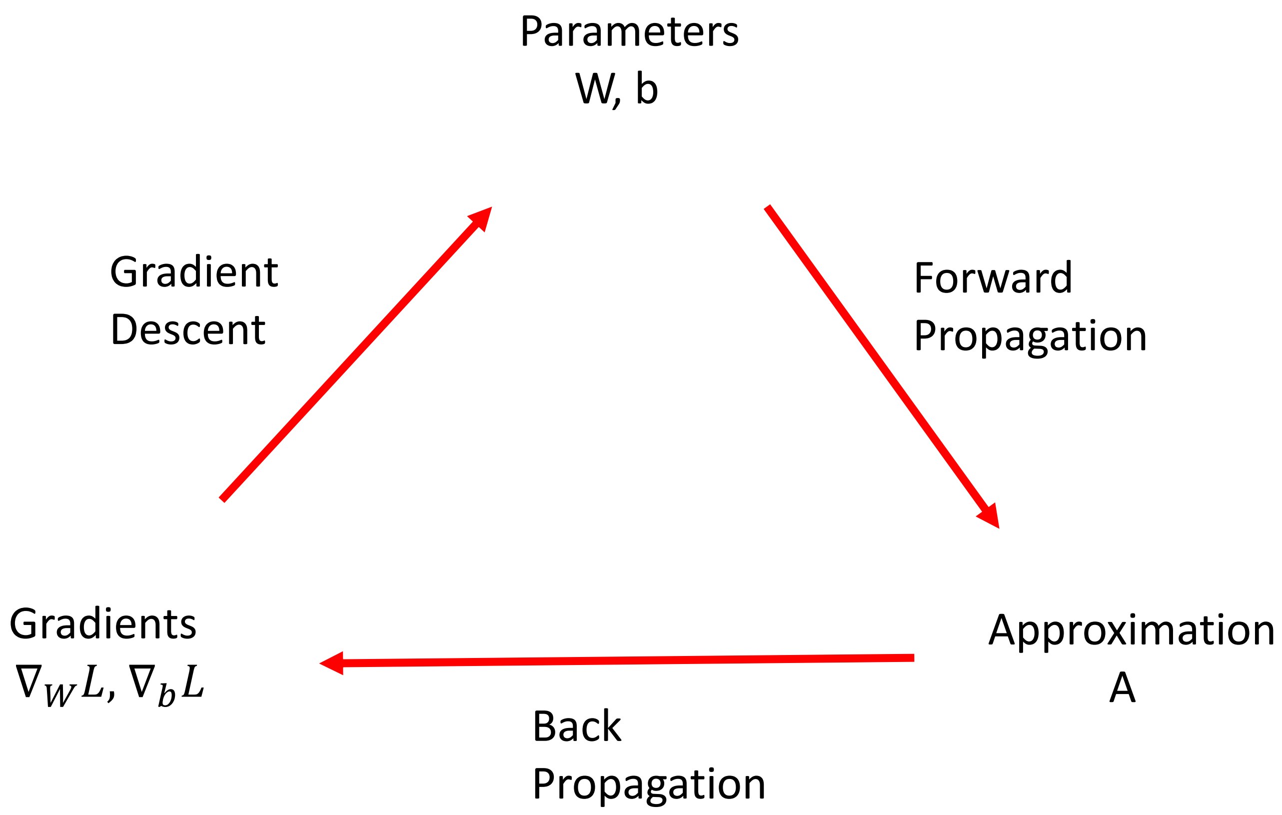
Training Algorithm



- With initial W and b use Forward Propagation to compute A
- Use Back Propagation to compute gradients
- Use Gradient Descent to update parameters
- Process is repeated

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Training Algorithm - Example

- Consider a case of 2 features and 3 data points (m=3)

$$X = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} \quad Y = \begin{bmatrix} 8 & 6 & 10 \end{bmatrix}$$

- Assume that initial parameter values are:

$$W_{epoch=0} = \begin{bmatrix} 1 & 1 \end{bmatrix} \quad b_{epoch=0} = [2]$$

- Choose learning rate α=0.01

EPOCH 1

- From Forward Propagation Example:

$$A_{epoch=0} = \begin{bmatrix} 5 & 9 & 13 \end{bmatrix}$$

- From Back Propagation Example:

$$\nabla_W L_{epoch=0} = \begin{bmatrix} 10 & 20 \end{bmatrix}, \; \nabla_b L_{epoch=0} = [2]$$

- Update:

$$\mathrm{W}_{epoch=1} = \mathrm{W}_{epoch=0} - \alpha \nabla_W L_{epoch=0} = \begin{bmatrix} 1 & 1 \end{bmatrix} - 0.01 * \begin{bmatrix} 10 & 20 \end{bmatrix} = \begin{bmatrix} 0.9 & 0.8 \end{bmatrix}$$

$$\mathrm{b}_{epoch=1} = \mathrm{b}_{epoch=0} - \alpha \nabla_b L_{epoch=0} = [2] - 0.01 * [2] = [1.98]$$

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Training Algorithm - Example

- Apply Forward Propagation with $\mathrm{W}_{epoch=1}$ and $\mathrm{b}_{epoch=1}$

$$A_{epoch=1} = Z_{epoch=1} = \mathrm{W}_{epoch=1}X + b_{epoch=1} = [0.9 \quad 0.8]\begin{bmatrix}1 & 2 & 4\\ 2 & 5 & 7\end{bmatrix} + [1.98] = [4.48 \quad 7.78 \quad 11.18]$$

$$Loss_{epoch=1} = \frac{1}{m}\sum_{j=0}^{m-1}(A_j - Y_j)^2 = \frac{1}{3}[(-3.52)^2 + 1.78^2 + 1.18^2] = 5.6504$$

EPOCH 2

- Forward propagation has been applied above to compute $\mathrm{A}_{guess=1}$
- Apply Back Propagation to compute $\nabla_W L_{epoch=1}, \nabla_b L_{epoch=1}$

$\frac{\partial L}{\partial A_j} = \frac{2}{m}(A_j - Y_j)$ for j=0,…,m-1 $\quad \nabla_A L = \left[\frac{2}{3}(4.48 - 8) \quad \frac{2}{3}(7.78 - 6) \quad \frac{2}{3}(11.18 - 10)\right] =$
$[-2.3467 \quad 1.1867 \quad 0.7867]$

$\left[\frac{\partial A_0}{\partial Z_0} \quad \frac{\partial A_1}{\partial Z_1} \quad \frac{\partial A_2}{\partial Z_2}\right] = [1 \quad 1 \quad 1]$

$$\nabla_Z L = \nabla_A L * \left[\frac{\partial A_0}{\partial Z_0} \quad \frac{\partial A_1}{\partial Z_1} \quad \frac{\partial A_2}{\partial Z_2}\right] = [-2.3467 \quad 1.1867 \quad 0.7867] * [1 \quad 1 \quad 1] = [-2.3467 \quad 1.1867 \quad 0.7867]$$

$$\nabla_W L = \nabla_Z L X^T = [-2.3467 \quad 1.1867 \quad 0.7867]\begin{bmatrix}1 & 2\\ 2 & 5\\ 4 & 7\end{bmatrix} = [3.1733 \quad 6.7467]$$

$$\nabla_b L = \sum_{j=0}^{m-1} \nabla_Z L_j = [-0.3733]$$

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Training Algorithm - Example

- Update:

$\mathrm{W}_{epoch=2} = \mathrm{W}_{epoch=1} - \alpha\nabla_W L_{epoch=1} = [0.9 \quad 0.8]$-0.01* $[3.1733 \quad 6.7467]$= $[0.8683 \quad 0.7325]$

$\mathrm{b}_{epoch=2} = \mathrm{b}_{epoch=1} - \alpha\nabla_b L_{epoch=1} = [1.98] - 0.01 * [-0.3733] = [1.9837]$

- Apply Forward Propagation with $\mathrm{W}_{epoch=2}$ and $\mathrm{b}_{epoch=2}$

$A_{epoch=2} = Z_{epoch=2} = \mathrm{W}_{epoch=2}X + b_{epoch=2} = [0.8686 \quad 0.7325]\begin{bmatrix}1 & 2 & 4\\ 2 & 5 & 7\end{bmatrix} + [1.9837]$
$= [4.3171 \quad 7.3829 \quad 10.5845]$

$Loss_{epoch=2} = \frac{1}{m}\sum_{j=0}^{m-1}(A_j - Y_j)^2 = \frac{1}{3}[(-3.6829)^2 + 1.3829^2 + 0.5845^2]$=5.2727

- Loss dropped from 5.6504 in EPOCH 1 to 5.2727 in EPOCH 2
- In general will use trial and error to adjust learning rate α

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Prediction Algorithm

Prediction algorithm makes use parameters computed in Training Algorithm

Input new input feature matrix $\tilde{X}$ (dxp - d features and p samples)

Use W and b computed by Training Algorithm

1. Perform Forward Propagation to compute output $\tilde{A}$

Prediction is $\tilde{A}$ (1xp values)

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Prediction Algorithm - Example

- From Training Algorithm Example:

$$X = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} \qquad Y = \begin{bmatrix} 8 & 6 & 10 \end{bmatrix}$$

- After 2 EPOCHs of Training Algorithm:

$$W_{epoch=2} = \begin{bmatrix} 0.8683 & 0.7325 \end{bmatrix} \quad b_{epoch=2} = \begin{bmatrix} 1.9837 \end{bmatrix}$$

- Prediction: Apply Forward Propagation with $\mathrm{W}_{epoch=2}$ and $\mathrm{b}_{epoch=2}$

$$A_{epoch=2} = Z_{epoch=2} = \mathrm{W}_{epoch=2}X + b_{epoch=2} = \begin{bmatrix} 0.8683 & 0.7325 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} + \begin{bmatrix} 1.9837 \end{bmatrix}$$
$$= \begin{bmatrix} 4.3170 & 7.3828 & 10.5844 \end{bmatrix}$$

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Accuracy Calculation

- Accuracy calculation compares value vector $\tilde{Y}$ to prediction
- Can use Mean Squared Error function to measure accuracy for regression
  - Mean Squared Error is not as informative for Classification as for Regression so a different measure will be introduced later in the chapter
- In this section, use Mean Absolute Error

Assume Training has been performed

Assume Prediction Algorithm has been applied to yield value vector $\tilde{A}$

1. Accuracy defined by mean absolute error

$$Accuracy = \frac{1}{m}\sum_{j=0}^{m-1}\left|\tilde{A}_j - \tilde{Y}_j\right|$$

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Accuracy Calculation - Example

- From example prediction example:

$$X = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} \qquad Y = \begin{bmatrix} 8 & 6 & 10 \end{bmatrix}$$

- Prediction:

$$A_{epoch=2} = \begin{bmatrix} 4.3170 & 7.3828 & 10.5844 \end{bmatrix}$$

- Accuracy:

$$Accuracy = \frac{1}{m}\sum_{j=0}^{m-1}\left|A_j - Y_j\right| = \frac{1}{3}[|-3.6830| + |1.3828| + |0.5844|] = 1.8834$$

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Linear Regression – Summary

Component	Algorithm	Details
Training Data		Input m data points: X (dxm-dimensional feature matrix) Y vector of values (1xm)
Function Structure	Forward Propagation	Linear: $Z = WX + b$ (Z is row vector of length m, W is row vector of length d, b is scalar) Activation function: $f(z) = z$ $\mathrm{A} = f(Z)$ (1xm)
Loss Function		Mean Squared Error: $L = \frac{1}{m}\sum_{j=0}^{m-1}(A_j - Y_j)^2$
Derivative	Back Propagation	Compute gradients $\nabla_W L$ and $\nabla_b L$
Training	Fitting using Gradient Descent to minimize Loss	Find W, b that minimizes loss Initial guess: $W_{epoch=0}, b_{epoch=0}$ Choose Learning Rate: α>0 For epoch=1,2,3… (for fixed number of epochs or until Loss reduced sufficiently) apply forward and back propagation to compute $\nabla_W L_{epoch=i-1}, \nabla_b L_{epoch=i-1}$ $W_{epoch=i} = W_{epoch=i-1} - \alpha\nabla_W L_{epoch=i-1}$ $b_{epoch=i} = b_{epoch=i-1} - \alpha\nabla_b L_{epoch=i-1}$
Prediction	Apply Forward Propagation	Using computed W and b from Training Algorithm Given new input feature matrix $\tilde{X}$ Perform Forward Propagation to compute $\tilde{A}$, the prediction for values

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Linear Regression – Jupyter Notebook Demo

- Open file IntroML/Examples/Chapter1/Chapter2.1_LinearRegresson.ipynb
- Has examples of
  - Forward Propagation
  - Loss Function
  - Backward Propagation
  - Training Algorithm
  - Prediction Algorithm
  - Accuracy Calculation

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2.2 Derivative Testing

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Derivative Testing

Goal of this Section:

- Present testing algorithm for comparing gradients computed using forward/back propagation with approximate estimates

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Motivation for Derivative Testing

- The forward/back propagation approach for computing gradients described in the previous section has a number of steps
- The formulas for neural networks presented in the next chapter are more complicated
- To gain confidence in a machine learning training system, it is useful to provide a check of the gradients produced by forward/back propagation

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Difference Formula for Derivatives

- Let L = L(p_0,p_1,p_2 ,…, p_d). Definition of partial derivative is:

$$\frac{\partial L}{\partial p_i} = \lim_{\varepsilon \to 0} \frac{L(p_0, p_1, \dots, p_i + \varepsilon, \dots, p_d) - L(p_0, p_1, \dots, p_i, \dots, p_d)}{\varepsilon}$$

- Forward difference formula: pick small ε (eg: 10^{-5}) - error proportional to ε or better as $\varepsilon \to 0$)

$$\frac{\partial L}{\partial p_i} \approx \frac{L(p_0, p_1, \dots, p_i + \varepsilon, \dots, p_d) - L(p_0, p_1, \dots, p_i, \dots, p_d)}{\varepsilon}$$

- Centered differences formula: (error is proportional to ε^2 or better as $\varepsilon \to 0$ – this is more accurate!)

$$\frac{\partial L}{\partial p_i} \approx \frac{L(p_0, p_1, \dots, p_i + \varepsilon, \dots, p_d) - L(p_0, p_1, \dots, p_i - \varepsilon, \dots, p_d)}{2\varepsilon}$$

- Apply centered differences approach for each variable (apply d+1 times)

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Derivative Testing - Example

- Consider Backpropagation Example in Section 2.1

$X = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} \quad Y = \begin{bmatrix} 8 & 6 & 10 \end{bmatrix} \quad W = \begin{bmatrix} 1 & 1 \end{bmatrix} \quad \text{b} = [2]$

- From the Back Propagation example of Section 2.1, we have

$\frac{\partial L}{\partial W_0} = 10, \frac{\partial L}{\partial W_1} = 20, \frac{\partial L}{\partial b} = 2$

- Approximate $\frac{\partial L}{\partial W_0}$ by bumping W_0 by plus +ε and –ε (choose ε=0.1)
- ε=0.1 case:

$Z = WX + b = \begin{bmatrix} 1.1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} + [2] = \begin{bmatrix} 5.1 & 9.2 & 13.4 \end{bmatrix} \quad A = Z$

$L_+ = \frac{1}{m} \sum_{j=0}^{m-1} (A_j - Y_j)^2 = \frac{1}{3}\left((-2.9)^2 + 3.2^2 + 3.4^2\right) = 10.07$

- ε=–0.1 case:

$Z = WX + b = \begin{bmatrix} 0.9 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} + [2] = \begin{bmatrix} 4.9 & 8.8 & 12.6 \end{bmatrix} \quad A = Z$

$L_- = \frac{1}{m} \sum_{j=0}^{m-1} (A_j - Y_j)^2 = \frac{1}{3}\left((-3.1)^2 + 2.8^2 + 2.6^2\right) = 8.07$

Hence:

$\frac{\partial L}{\partial W_0} \approx \frac{L_+ - L_-}{2\varepsilon} = \frac{10.07 - 8.07}{2(0.1)} = 10$ (this matches back propagation derivative exactly)

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Derivative Testing - Example

- Approximate $\frac{\partial L}{\partial W_1}$ by bumping W_1 by plus +ε and –ε (choose ε=0.1)
- ε=0.1 case:

$$Z = WX + b = \begin{bmatrix} 1 & 1.1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} + [2] = \begin{bmatrix} 5.2 & 9.5 & 13.7 \end{bmatrix} \quad A = Z$$

$$L_+ = \frac{1}{m} \sum_{j=0}^{m-1} (A_j - Y_j)^2 = \frac{1}{3}\left((-2.8)^2 + 3.5^2 + 3.7^2\right) = 11.26$$

- ε=–0.1 case:

$$Z = WX + b = \begin{bmatrix} 1 & 0.9 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} + [2] = \begin{bmatrix} 4.8 & 8.5 & 12.3 \end{bmatrix} \quad A = Z$$

$$L_- = \frac{1}{m} \sum_{j=0}^{m-1} (A_j - Y_j)^2 = \frac{1}{3}\left((-3.2)^2 + 2.5^2 + 2.3^2\right) = 7.26$$

Hence:

$\frac{\partial L}{\partial W_1} \approx \frac{L_+ - L_-}{2\varepsilon} = \frac{11.26 - 7.26}{2(0.1)} = 20$ (this matches back propagation derivative exactly)

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Derivative Testing - Example

- Approximate $\frac{\partial L}{\partial b}$ by bumping b by plus +ε and –ε (choose ε=0.1)
- ε=0.1 case:

$$Z = WX + b = \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} + \begin{bmatrix} 2.1 \end{bmatrix} = \begin{bmatrix} 5.1 & 9.1 & 13.1 \end{bmatrix} \quad A = Z$$

$$L_{+} = \frac{1}{m} \sum_{j=0}^{m-1} (A_j - Y_j)^2 = \frac{1}{3}\left((-2.9)^2 + 3.1^2 + 3.1^2\right) = 9.21$$

- ε=–0.1 case:

$$Z = WX + b = \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 5 & 7 \end{bmatrix} + \begin{bmatrix} 1.9 \end{bmatrix} = \begin{bmatrix} 4.9 & 8.9 & 12.9 \end{bmatrix} \quad A = Z$$

$$L_{-} = \frac{1}{m} \sum_{j=0}^{m-1} (A_j - Y_j)^2 = \frac{1}{3}\left((-3.1)^2 + 2.9^2 + 2.9^2\right) = 8.81$$

Hence:

$$\frac{\partial L}{\partial b} \approx \frac{L_{+} - L_{-}}{2\varepsilon} = \frac{9.21 - 8.81}{2(0.1)} = 2$$ (this matches back propagation derivative exactly)

- Derivatives match approximations exactly – this occurs for linear regression as Loss depends quadratically on parameters W and b, but will not occur for Logistic Regression and Neural Network, in general, because activation and loss functions are more complicated

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Concatenating and Loading Parameters

- To efficiently bump each parameter it is convenient to store all parameter in a single vector
- Concatenation combines all parameters:

Original format: $W = [W_0 \;\; W_1 \;\; \ldots \;\;\; W_{d-1}]$ and scalar b

Concatenated format: $[W_0 \;\; W_1 \;\; \ldots \;\;\; W_{d-1} \;\; b]$ (vector with all parameters)

- Process of loading takes parameters in concatenated form and puts parameters back into original format (separate W and b)
- Testing approach:
    - Use concatenated form to bump parameters
    - Put back into original format to perform forward propagate and compute Loss after parameters are bumped

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Derivative Testing Algorithm

Assign W and b

Input Training Data: feature matrix X and values Y

1. Perform Forward and Back Propagation to compute $\nabla_W L, \nabla_b L$
2. Concatenate original parameters W, b and gradient vectors $\nabla_W L, \nabla_b L$
3. Loop over i = 0,1, .. d (d+1 parameters in W and b)

- Add ε to parameter i in original concatenated parameter list
- Load parameters back into W and b
- Forward propagate and compute Loss $L(p_i+\varepsilon)$
- Subtract ε from parameter i in original concatenated parameter list
- Load parameters back into W and b
- Forward propagate and compute Loss $L(p_i -\varepsilon)$
- Estimate partial derivative with respect to i'th parameter is $(L(p_i +\varepsilon) - L(p_i -\varepsilon))/2\varepsilon$

4. Compare estimated partial derivatives to those computed in Steps 1,2

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Derivative Testing – Jupyter Notebook Demo

- Open file IntroML/Examples/Chapter2/Chapter2.2_DerivativeTesting.ipynb
- Has example of
  - Derivative Testing

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2.3 Code Design Review

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Coding Design Review

Goal of this Section:

- Present overview of code design, including
  - Principal classes employed
  - Format of numpy arrays

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Coding Overview

- Code employs object-oriented approach
  - Two principal classes
    - NeuralNetwork_Base Class
    - Optimizer_Base Class (used to compute update in training algorithm)
- Additional codes
  - Activation functions
  - Loss functions
  - Plotting functions
  - Unit test
  - Drivers
  - Load Data functions
- Design considerations:
  - Numpy array is key building block
  - Use interfaces for framework Tensorflow as a rough guide

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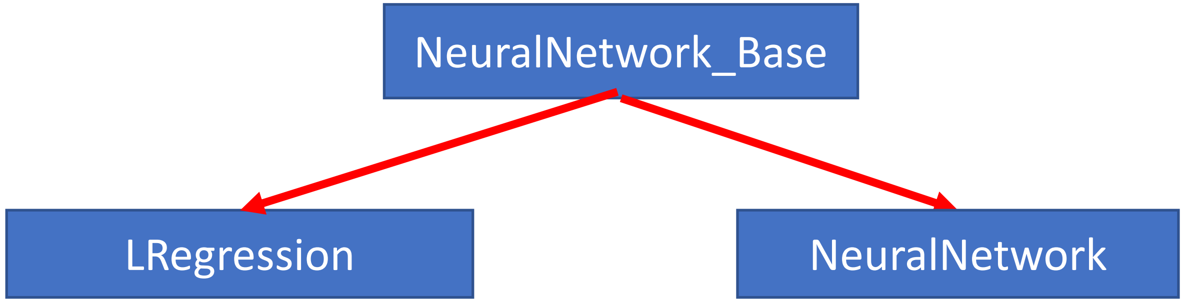
NeuralNetwork_Base Class

Linear/Logistic Regression



General Neural Networks (multiple layers)

Key Methods
- Forward Propagation
- Back Propagation
- Compute Loss
- Fit (for training)
- Predict
- Test Derivative
- Concatenate Parameters
- Load Parameters
- Compute accuracy

Will attempt to put as many methods as possible in NeuralNetwork_Base to handle both Linear/Logistic Regression and Neural Networks

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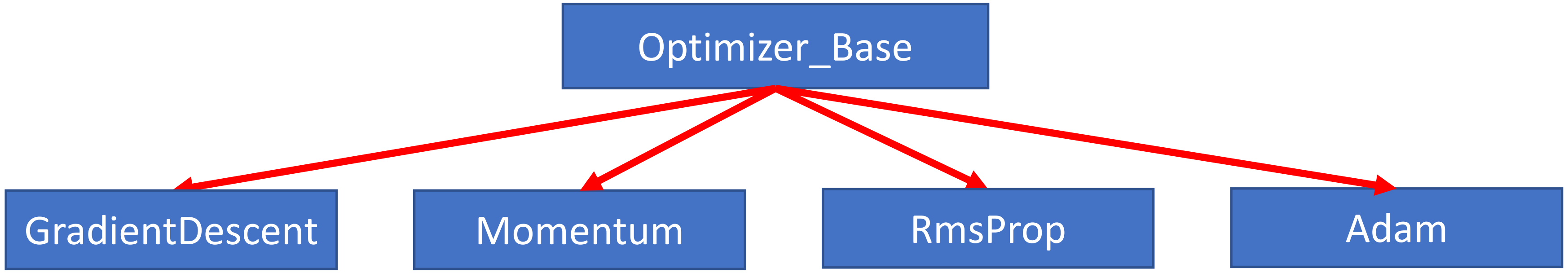
Optimizer_Base Class



Key Methods

- Update

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Code Design - Arrays

All relevant arrays will be defined explicitly as 2d numpy arrays

- Feature Matrix X
  - This naturally is a 2d object (dxm) (number of features x number of samples)
- Value Vector Y
  - This is a row vector – will be explicitly made to have dimensions (1 x m)
- Parameters W and b and gradients
  - For Linear/Logistic regression, W and $\nabla_W L$ are row vectors of length d (number of features)– will be explicitly made to have dimensions (1 x d)
  - b is a scalar – will be explicitly made to have dimensions (1 x 1)
  - For neural networks W and $\nabla_W L$ will naturally be 2d objects
  - For neural networks, in general, b and $\nabla_b L$ will be column vectors – will be explicitly made to be column vectors – dimensions (n x 1)
- Computed Values A and Z
  - For Linear/Logistic Regression, A and Z are row vectors – will have dimensions (1 x m)
  - For neural networks, A and Z will naturally be 2d objects

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2.4 Code Walkthrough
Version 1.1

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Coding Walkthrough: Version 1.1

Goal of this Section:

- Walkthrough of code necessary to perform unit test of forward/back propagation for Linear Regression

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Coding Walkthrough: Version 1.1 To Do

File/Component	To Do
NeuralNetwork_Base	Create NeuralNetwork_Base class and methods to be used for both Logistic/Linear Regression and Neural Networks
LRegression	Create class derived from NeuralNetwork_Base with methods specific to Linear and Logistic Regression
functions_loss	Create functions for mean square error loss function and its derivative
functions_activation	Create functions for linear activation and its derivative
unittest_forwardbackprop	Create functions for performing test of derivative calculation

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NeuralNetwork_Base Class – Attributes

<table>
<tr><th>Variable</th><th>Type</th><th>Description</th></tr>
<tr><td>nlayer</td><td>integer</td><td>Number of layers
• Equals 1 for Linear and Logistic Regression
• In general greater than 1 for Neural Networks</td></tr>
<tr><td>info</td><td>list
indices:
0,1,…,nlayer-1</td><td>info[k] is a dictionary containing information for layer = k
Keys:
• nIn: (integer) number of unit in previous layer (number of features for layer 0)
• nOut: (integer) number of units in current layer
• activation: (string) activation function type
• A: (numpy array) result after activation for current layer
• param: (dictionary) parameter matrices (keys W, b)
• param_der: (dictionary) derivatives of parameter matrices (keys W, b)
• optimizer: (dictionary) optimizer class objects (keys W,b)</td></tr>
<tr><td>loss_fun</td><td>string</td><td>Name of loss function</td></tr>
</table>

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NeuralNetwork_Base Class – Methods

Method	Input	Description
get_A	layer (integer)	Return: A, the result of Forward Propagation for specified layer
get_param	layer (integer) order (string): “param” or “param_der” label (string): “W” or “b”	Return: parameters W or b or gradients $\nabla_W L$, $\nabla_b L$ for specified layer, order, and label
compile	optimizer (dictionary) loss_fun (string)	Takes in loss function and optimizer information and constructs optimizer object for each parameter and layer Return: nothing
compute_loss	Y (numpy array)	Return: loss for output (label) vector Y assuming forward propagation has been performed
test_derivative	X (numpy array) Y (numpy array) eps (float)	Return: difference between exact (computed using forward/back propagation) and approximate (computed using centered differences with bump eps) gradients $\nabla_W L$, $\nabla_b L$

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LRegression – Methods

Method	Input	Description
__init__	nfeature (integer) activation (sting)	Initialization routine that takes in the number of features and the activation function ("linear" for regression) Return: nothing
forward_propagation	X (numpy array)	Performs forward propagation using feature matrix X to compute approximation A and updates info variable for key "A" Returns: nothing
back_propagation	X (numpy array) Y (numpy array)	Performs back propagation using feature matrix X and label vector Y Returns: nothing
concatenate_param	order (string): "param" or "param_der"	Concatenates all entries in W and b or in the their gradient into a single row vector
load_param	flat (numpy array) order (string): "param" or "param_der"	Takes values from flat (row vector) and puts them back into W or b or gradient objects

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Activation and Loss Functions

Function	Input	Description
functions_activation. activation	activation_fun (string) Z (numpy array)	Applies activation function f(z) to entries in Z for specified function Return: f(Z)
functions_activation. activation_der	activation_fun (string) Z (numpy array)	Applies derivative of activation function to entries in Z for specified function Return: f'(Z)
functions_loss. loss	loss_fun (string) A (numpy array) Y (numpy array)	Computes loss function given activation A, label vector Y, and specified function Return: Loss
functions_loss. loss_der	loss_fun (string) A (numpy array) Y (numpy array)	Computes gradient of loss function with respect to elements of A for activation A, label vector Y, and specified function Return: $\nabla_A L$

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Unit Test Functionality

```
In [1]: import unittest

        class Test(unittest.TestCase):
            def test1(self):
                x = 7
                y = 8
                z1 = (x+y)*(x+y)
                z2 = x*x + 2*x*y + y*y
                error = abs(z1-z2)
                self.assertLessEqual(error,1e-7)

        if __name__ == "__main__":
            #this is command in python when running in command window
            #unittest.main()
            # this is command in the jupyter notebook
            unittest.main(argv=['first-arg-is-ignored'], exit=False)

        .
        ----------------------------------------------------------------------
        Ran 1 test in 0.016s

        OK
```

- Use functionality in unittest package
- Documentation at https://docs.python.org/3.7/index.html
- Create a class derived from unittest.TestCase
- Individual unit tests are set up as methods of the class
- Test should have “assert” command which determines pass or fail
- Use unittest.main to run tests
- Will get OK if test passes

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Unit Test for Forward/Back Propagation

Unit test method has following components:

1. Preparation of Data
   - Create random X and Y
2. Creation of LRegression object
   - Create instance of the LRegression class
3. Compilation
   - Specify loss function and optimizer (None)
4. Run test_derivative method of LRegression object
   - This will compare forward/back propagation derivatives to approximations
5. Assert
   - Check if error less than or equal to tolerance (will use 10^{-7})

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Unit Test – Jupyter Notebook Demo

- Open file IntroML/Examples/Chapter2/Chapter2.4_UnittestExample.ipynb
- Has example of
  - Unit test

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Code Version 1.1 Walkthrough

- Code for walkthrough located at:

IntroML/Code/Version1.1

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2.5 Code Walkthrough
Version 1.2

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Coding Walkthrough: Version 1.2

Goal of this Section:

- Walkthrough creation of code to perform linear regression training and prediction

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Coding Walkthrough: Version 1.2 To Do

File/Component	To Duo
NeuralNetwork_Base	Add methods for training, prediction, updating parameters, and computing accuracy of prediction
Optimizer_Base	Create Optimizer_Base class and a constructor to create optimizer objects
GradientDescent	Create GradientDescent class derived from Optimizer_Base
Plotting	Create function to plot training data, normal equations result, and linear regression prediction as well as accuracy and loss versus epoch
Driver	Create driver for linear regression

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NeuralNetwork_Base Class – Methods

Method	Input	Description
update_param		Applies optimizer to update parameters Return: nothing
fit	X (numpy array) Y (numpy array) epochs (integer)	Applies training algorithm for specified number of epochs using feature matrix X and output information vector Y. Uses approach defined in optimizer input in compile method to compute updates. Return: history dictionary containing loss and accuracy at each epoch
predict	X (numpy array)	Applies prediction algorithm to compute output vector Y for input feature/information matrix X Return: predicted output values
accuracy	Y (numpy array) Y_pred (numpy array)	Computes accuracy comparing label vector Y to predicted results Y_pred Return: accuracy (float)

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GradientDescent – Methods

Method	Input	Description
__init__	learning_rate (float)	Takes relevant parameters Return: nothing
update	gradient (numpy array)	Computes update to be used by optimization algorithm. Input is gradient Return: update

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Linear Regression Driver

Driver has following components:

1. Preparation of Data
    - Create data or load from external file or create in external program
2. Creation of Model Object
    - Create instance of the LRegression class
3. Compilation
    - Specify optimizer object and loss function
4. Training
    - Input training data X and Y and specify number of epochs
5. Prediction
    - Predict output for new input information X using learned parameters

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Plotting Functions

Will create functions for:

1. Plotting Loss and Accuracy
   - Loss and accuracy are computed during training
   - Plot these quantities as function of epoch on separate graphs
2. Plotting Training Data, Predicted Line, Normal Equations Line
   - On the same graph plot:
     - Training data
     - Line predicted by training algorithm
     - Line predicted by the normal equations approach

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Code Version 1.2 Walkthrough

- Code for this walkthrough located at:

IntroML/Code/Version1.2

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2.6 Logistic Regression: Mathematical Foundations

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Logistic Regression: Mathematical Foundations

Goal of this Section:

- Extend the mathematical foundations for linear regression to the case of logistic regression, including:
  - Format of input data
  - Function structure and parameters
  - Training algorithm
  - Prediction algorithm

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Logistic Regression and Linear Regression

- Linear Regression used for modeling real values (Y_j are real numbers)
- Logistic Regression for binary classification (Y_j are labels 0 or 1)
  - Binary classification 2 possibilities – arbitrarily assign 0 to one possibility and 1 to the other (eg cat is 0 and dog is 1, for x-rays 0 is normal and 1 is broken, etc)
- Underlying mathematics and code development for Linear Regression can be extended to Logistic Regression
- Principal Differences between Linear and Logistic Regression:
  - Activation Function:
    - Need suitable activation function to produce 0 or 1 output
    - Linear activation function (can take on values from –infinity to infinity) is not suitable
  - Loss Function
    - Need suitable loss function
    - Mean Squared Error loss function not suitable for Logistic Regression

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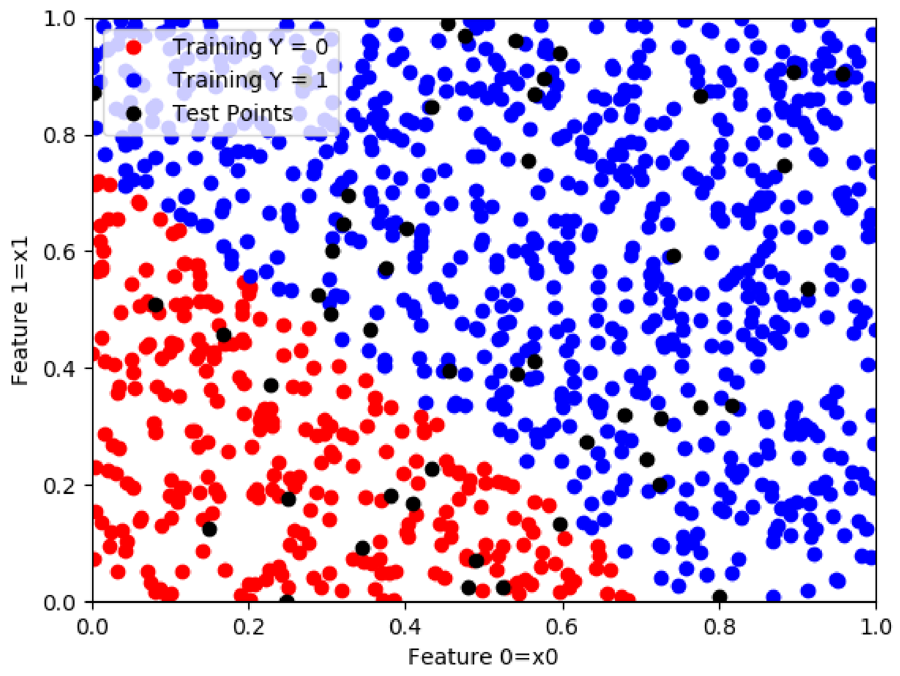
Motivating Example: Binary Classification

Training Data:
- Input Information: points in (x0,x1) plane
- Output Information: label 0 (red) or 1 (blue) for each point



Goal:
- Find function that best fits 0 and 1 labels in training data

Prediction:
- Using function, determine label for new input test points (black points in picture)

Logistic Regression:
- Simple approach for binary classification (builds on Linear Regression)

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Motivating Example

- Training data for sample j:

$$\left(\begin{bmatrix} X_{0j} \\ X_{1j} \end{bmatrix}, Y_j\right)$$

Here (X_{0j}, X_{1j}) is the point in the plane and Y_j is the label 0 or 1.

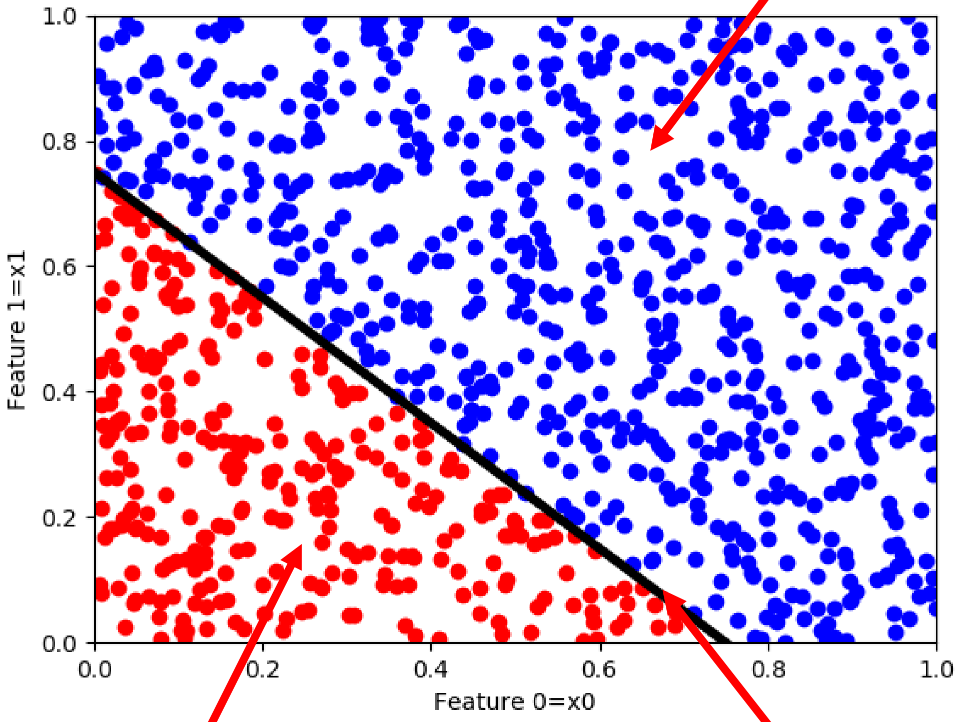
- Define parameters W = [W_0 W_1] and b

$$Z_j = WX_j + b = W_0X_{0j} + W_1X_{1j} + b$$

- If we choose W = [1 1] and b =-0.75, then appropriate activation function

$$f(Z_j) = \begin{Bmatrix} 1 \;\; if Z_j \geq 0 \\ 0 \;\; if Z_j < 0 \end{Bmatrix}$$

Region:
x0 + x1 – 0.75 > 0



Region:
x0 + x1 – 0.75 < 0

Line:
x0 + x1 – 0.75 = 0

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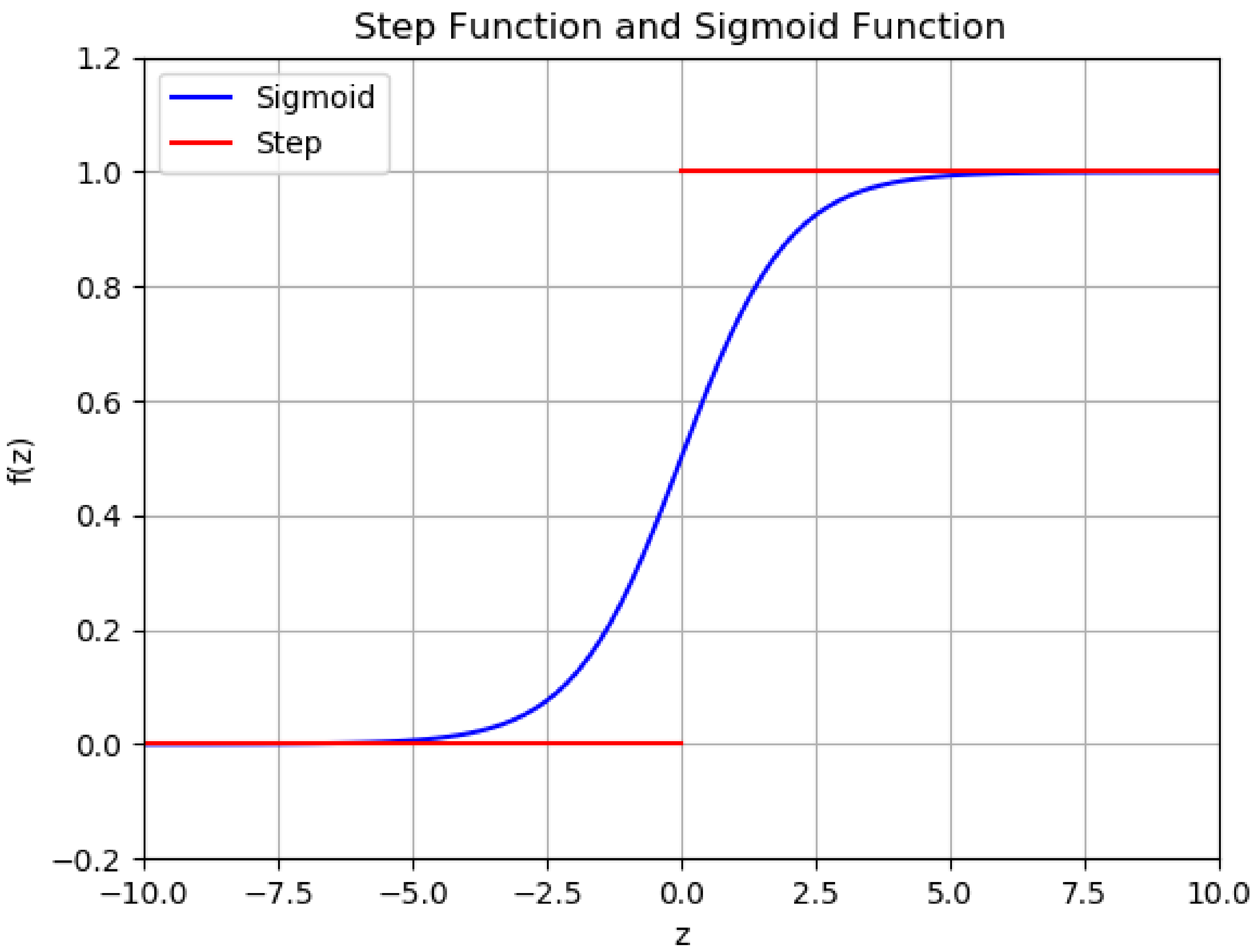
Sigmoid Activation Function

- Step function is not best choice, as we want activation function to be differentiable

- Use instead the sigmoid activation function

$$f(z) = \frac{1}{1 + e^{-z}}$$

- Sigmoid function between 0 and 1
  f(z) -> 1 as z->infinity
  f(z) -> 0 as z->-infinity



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Binary Cross Entropy Loss Function

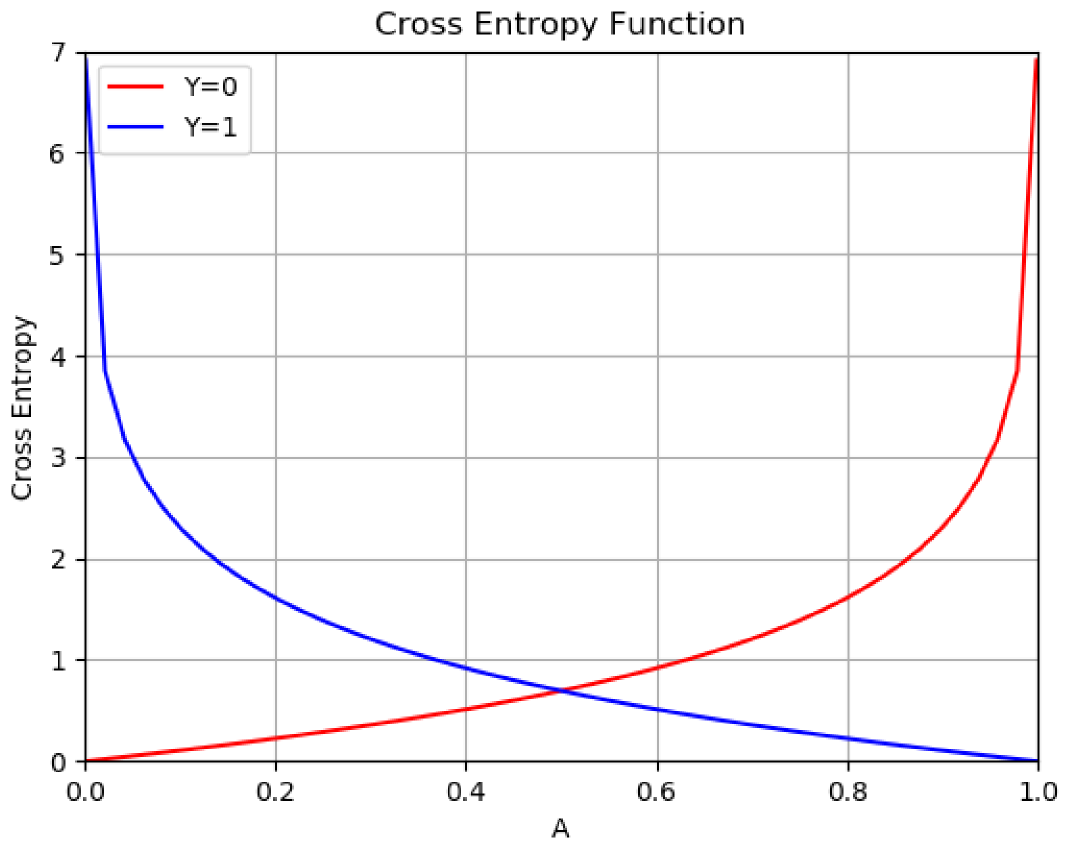
- Mean Squared Error loss function is not appropriate for logistic regression

- Use Binary Cross Entropy loss function instead:

$$Loss = -[Y ln(A) + (1 - Y)\ln(1 - A)]$$

- When Y = 0, Loss decreases as A goes to 0

- When Y = 1 Loss decreases as A goes to 1



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Logistic Regression: General Approach

General approach has following components and phases:

(1) Training Data

(2) Function Structure

- Defines general form of the function with unknown parameters
- Process of applying function structure is called Forward Propagation

(3) Loss Function

- Used to measure effectiveness of function structure and choice of parameters

(4) Training Phase

- Uses optimization to determine function parameters that minimize loss function for training data
- Process of computing derivatives is called Back Propagation

(5) Prediction Phase

- Applies forward propagation using parameters determined in Training Phase to predict outputs when new input data is provided

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Training Data

- For general logistic regression problem there are m data points, each consisting of a input information vector of length d and value Y:

- Data point j: input information (feature) vector: $\begin{bmatrix} X_{0,j} \\ X_{1,j} \\ \dots \\ X_{d-1,j} \end{bmatrix}$ and output: Y_j

- Define the feature matrix (dxm) and output vector (1xm):

$$X = \begin{bmatrix} X_{00} & \dots & X_{0,m-1} \\ \dots & \dots & \dots \\ X_{d-1,0} & \dots & X_{d-1,m-1} \end{bmatrix} \qquad Y = [Y_0 \quad \dots \quad Y_{m-1}]$$

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Training Data – Example Points in Plane

- For points in plane with 0 and 1 labels in motivating example, training data consists of points in the plane (X_0,X_1) with label Y
- Suppose 4 data samples with points and labels: (1,1) label=0, (0.5,2) label = 1, (2,3), label = 1, (4,2) label 0
- In this case each sample has 2 features. Feature matrix and value vector are:

$$X = \begin{bmatrix} 1 & 0.5 & 2 & 4 \\ 1 & 2 & 3 & 2 \end{bmatrix} \qquad Y = \begin{bmatrix} 0 & 1 & 1 & 0 \end{bmatrix}$$

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Function Structure – Forward Propagation

Forward Propagation is name applied to process of estimating output values using function structure

1. Input: feature matrix X (dxm d features and m sample points), parameter vector $W = [W_0 \quad \dots \quad W_{d-1}]$and bias b
2. Linear part: for j=0,…,m-1

$$Z_j = W_o X_{oj} + W_1 X_{1j} + W_2 X_{2j} + \cdots + W_{d-1} X_{d-1j} + b$$

In vector form

$$Z = WX + b$$

3. Activation: apply sigmoid function f(z) to each element of Z:

$$A_j = f\left(Z_j\right) \quad j = 0, \dots, m-1$$

$$f(z) = \frac{1}{1 + e^{-z}}$$

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Logistic Regression Forward Propagation - Example

- Consider a case of 2 features and 3 data points (m=3)

$$X = \begin{bmatrix} 1 & 2 & 4 \\ -2 & -5 & -8 \end{bmatrix} \qquad Y = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}$$

- Assume that initial parameter values are:

$$W = \begin{bmatrix} 0.1 & 0.1 \end{bmatrix} \qquad \mathrm{b} = [0.2]$$

- Forward Propagation:

$$Z = WX + b = \begin{bmatrix} 0.1 & 0.1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ -2 & -5 & -8 \end{bmatrix} + [0.2] = \begin{bmatrix} 0.1 & -0.1 & -0.2 \end{bmatrix}$$

$$A = f(Z) = \begin{bmatrix} \frac{1}{1+e^{-0.1}} & \frac{1}{1+e^{0.1}} & \frac{1}{1+e^{0.2}} \end{bmatrix} = \begin{bmatrix} 0.5250 & 0.4750 & 0.4502 \end{bmatrix}$$

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Logistic Regression: Loss Function

- Loss function is average of binary cross entropy function over sample points

$$Loss = L = -\frac{1}{m}\sum_{j=0}^{m-1} Y_j \ln\left(A_j\right) + \left(1 - Y_j\right)\ln(1 - A_j)$$

- For each sample j, only one of $Y_j \ln\left(A_j\right)$ or $(1 - Y_j) \ln\left(1 - A_j\right)$ is non-zero, as Y_j is 0 or 1

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Training Phase

- Training phase attempts to find suitable coefficients W and b by minimizing loss function when applied to training data
- From multi-variable calculus, Loss function has a local minimum when the gradients are 0

$\nabla_W L = 0$ and $\nabla_b L = 0$

- Can solve these equations analytically for Linear Regression, but not in general case (Logistic Regression and Neural Networks)
- Use optimization algorithm (example: Gradient Descent) to minimize Loss function
  - Need to compute the above gradients

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Derivative of Loss

- Loss function given by:

$$L = -\frac{1}{m}\sum_{j=0}^{m-1} Y_j \ln\left(A_j\right) + \left(1 - Y_j\right)\ln(1 - A_j)$$

- Differentiating the log terms, we get:

$$\frac{\partial L}{\partial A_j} = -\frac{1}{m}\left[\frac{Y_j}{A_j} - \frac{1 - Y_j}{1 - A_j}\right], \qquad j = 0, \dots, m - 1$$

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Derivative of Activation

A_j related to Z_j by:

$$A_j = f(Z_j) = \frac{1}{1 + e^{-Z_j}}, \qquad j = 0, \ldots, m-1$$

Derivatives given by

$$\frac{\partial A_j}{\partial Z_j} = \frac{e^{-Z_j}}{(1 + e^{-Z_j})^2}, \qquad j = 0, \ldots, m-1$$

As we will see when coding, this format saves memory as Z need not be saved

This can be simplified to:

$$\frac{\partial A_j}{\partial Z_j} = \frac{e^{-Z_j}}{(1 + e^{-Z_j})^2} = \frac{1 + e^{-Z_j}}{(1 + e^{-Z_j})^2} - \frac{1}{\left(1 + e^{-Z_j}\right)^2} = A_j - A_j^2$$

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Logistic Regression Back Propagation Algorithm

Input: feature matrix X and value vector Y

1. Compute:

$$\nabla_A L = \begin{bmatrix} \frac{\partial L}{\partial A_0} & \frac{\partial L}{\partial A_1} & \dots & \frac{\partial L}{\partial A_{m-1}} \end{bmatrix}, \frac{\partial L}{\partial A_j} = -\frac{1}{m}[\frac{Y_j}{A_j} - \frac{1-Y_j}{1-A_j}], j = 0, \dots, m-1$$

3. Compute derivatives of A: $\frac{\partial A_j}{\partial Z_j} = A_j - A_j^2, j = 0, \dots, m-1$

4. Compute gradient L with respect to Z:

$\nabla_Z L = \nabla_A L * \begin{bmatrix} \frac{\partial A_0}{\partial Z_0} & \frac{\partial A_1}{\partial Z_1} & \dots & \frac{\partial A_{m-1}}{\partial Z_{m-1}} \end{bmatrix}$ (component-wise multiplication)

5. Compute gradient of L with respect to W and b (from Section 1.4):

$$\nabla_W L = \nabla_Z L X^T, \qquad \nabla_b L = \sum_{j=0}^{m-1} \nabla_Z L_j$$

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Logistic Regression Back Propagation - Example

- Consider a case of 2 features and 3 data points (m=3)

$$X = \begin{bmatrix} 1 & 2 & 4 \\ -2 & -5 & -8 \end{bmatrix} \qquad Y = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}$$

- Assume that initial parameter values are:

$$W = \begin{bmatrix} 0.1 & 0.1 \end{bmatrix} \qquad \mathrm{b} = \begin{bmatrix} 0.2 \end{bmatrix}$$

- From Forward Propagation Example

$$A = \begin{bmatrix} 0.5250 & 0.4750 & 0.4502 \end{bmatrix}$$

- Gradient of Loss with respect to A:

$$\nabla_A L = -\frac{1}{3}\left(\frac{Y}{A} - \frac{1-Y}{1-A}\right) = -\frac{1}{3}\left[-\frac{1}{1-0.5250} \quad \frac{1}{0.4750} \quad -\frac{1}{1-0.4502}\right] = \begin{bmatrix} 0.7017 & -0.7017 & 0.6062 \end{bmatrix}$$

$$\frac{\partial A_j}{\partial Z_j} = A_j - A_j^2 \qquad \begin{bmatrix} \frac{\partial A_0}{\partial Z_0} & \frac{\partial A_1}{\partial Z_1} & \frac{\partial A_2}{\partial Z_2} \end{bmatrix} = \begin{bmatrix} 0.2494 & 0.2494 & 0.2475 \end{bmatrix}$$

$$\nabla_Z L = \nabla_A L * \begin{bmatrix} \frac{\partial A_0}{\partial Z_0} & \frac{\partial A_1}{\partial Z_1} & \frac{\partial A_2}{\partial Z_2} \end{bmatrix} = \begin{bmatrix} 0.7017 & -0.7017 & 0.6062 \end{bmatrix} * \begin{bmatrix} 0.2494 & 0.2494 & 0.2475 \end{bmatrix} = \begin{bmatrix} 0.1750 & -0.1750 & 0.1501 \end{bmatrix}$$

$$\nabla_W L = \nabla_Z L X^T = \begin{bmatrix} 0.1750 & -0.1750 & 0.1501 \end{bmatrix} \begin{bmatrix} 1 & -2 \\ 2 & -5 \\ 4 & -8 \end{bmatrix} = \begin{bmatrix} 0.4252 & -0.6755 \end{bmatrix}$$

$\nabla_b L = \sum_{j=0}^{m-1} \nabla_Z L_j = 0.1501$ (sum of entries of $\nabla_b L$)

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Training Algorithm

- Other than change for activation function and loss function, Training Algorithm for Logistic Regression is the same as that for Linear Regression

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Prediction Algorithm

Prediction algorithm makes use of parameters computed in Training Algorithm

Input new input feature matrix $\tilde{X}$

Use W and b computed by Training Algorithm

1. Perform Forward Propagation to determine $\tilde{A}$
   - Round $\tilde{A}$ to closest number 0 or 1 to get predicted label

- Can regard each entry of prediction vector $\tilde{A}$ as probability that prediction is 1. ($1 - \tilde{A}$ is probability that prediction is 0.)

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Logistic Regression Prediction - Example

- Consider a case of 2 features and 3 data points (m=3)

$$X = \begin{bmatrix} 1 & 2 & 4 \\ -2 & -5 & -8 \end{bmatrix} \qquad Y = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}$$

- Assume that initial parameter values are:

$$W = \begin{bmatrix} 0.1 & 0.1 \end{bmatrix} \qquad \mathrm{b} = [0.2]$$

- From the Forward Propagation Example slide

$$A = f(Z) = \begin{bmatrix} \frac{1}{1+e^{-0.1}} & \frac{1}{1+e^{0.1}} & \frac{1}{1+e^{0.2}} \end{bmatrix} = \begin{bmatrix} 0.5250 & 0.4750 & 0.4502 \end{bmatrix}$$

- Round to 0 or 1 (round 0.5 up to 1) – predicted labels: $\begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$

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Accuracy Calculation

Accuracy calculation compares actual vector label to predicted values

1. Perform Training
2. Let $\tilde{X}$ denote feature matrix and $\tilde{Y}$ denote related value vector (these may be same as used in training or completely different)
3. Apply prediction algorithm to $\tilde{X}$ to get predicted value vector $\tilde{P}$
4. Accuracy defined by:

$$Accuracy = \frac{1}{m}\sum_{j=0}^{m-1}\left(1\ if\ \tilde{P}_j = \tilde{Y}_j, 0\ otherwise\right)$$

- Both value vector and predicted valued vector consist of 0 or 1 entries. Accuracy = 1 means prediction equals initial value vector for all entries. Accuracy = 0 means none of the entries in prediction vector match those in original value vector.

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Accuracy Calculation - Example

- Suppose that

$Y = [0 \quad 1 \quad 1 \quad 0 \quad 1]$ and predicted values after rounding $= [1 \quad 0 \quad 1 \quad 0 \quad 1]$

- Accuracy calculation: Y matches predicted values for 3 out of 5 entries, so

$Accuracy = 0.6$

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Logistic Regression – Summary

Component	Subcomponent	Details
Training Data		Input m data points: X (dxm-dimensional feature matrix) Y vector of labels (0 or 1) (row vector of length m)
Function Structure	Forward Propagation	Linear: $Z = WX + b$ (Z is row vector of length m, W is row vector of length d, b is scalar) Activation function: $f(Z) = \frac{1}{1+e^{-Z}}$ $\mathrm{A} = f(Z)$ (1xm vector)
Loss Function		Binary Cross Entropy: $L = -\frac{1}{m}\sum_{j=0}^{m-1} Y_j log\, A_j + (1 - Y_j)\log(1\text{-}A_j)$
Derivative	Back Propagation	Compute $\nabla_W L$ and $\nabla_b L$
Training Algorithm	Train using Gradient Descent to minimize Loss	Find W, b that minimizes loss Initial epoch: $W_{epoch=0}, b_{epoch=0}$ Choose Learning Rate: α>0 For each epoch: (apply forward and back propagation to compute gradients) $W_{epoch=\,i} = W_{epoch=i-1} - \alpha\nabla_W L_{epoch=i-1}$ $b_{epoch=i} = b_{epoch=i-1} - \alpha\nabla_b L_{epoch=i-1}$ Perform fixed number or iterations or until Loss reduced sufficiently
Prediction Algorithm	Apply Forward Propagation	Using computed W and b from Training Algorithm Given new input feature matrix $\tilde{X}$ Perform Forward Propagation to compute $\tilde{A}$ and round to (0 or 1) to get predicted label

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Logistic Regression – Jupyter Notebook Demo

- Open file IntroML/Examples/Chapter2/Chapter2.6_LogisticRegression.ipynb
- Has example of
  - Forward Propagation
  - Back Propagation
  - Prediction
  - Accuracy calculation

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2.7 Code Walkthrough: Version 1.3

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Code Walkthrough Version 1.3

Goal of this Section:

- Walkthrough extension of linear regression codes to handle logistic regression

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Coding Walkthrough: Version 1.3 To Do

File/Component	To Duo
NeuralNetwork_Base	Update accuracy method to handle logistic regression case
functions_loss	Add functions for binary cross entropy and its derivative
functions_activation	Add functions for sigmoid activation and its derivative
unittest_forwardbackprop	Add method for testing logistic regression case
driver	Add driver for logistic regression
plotting	Add routine for plotting training data and prediction

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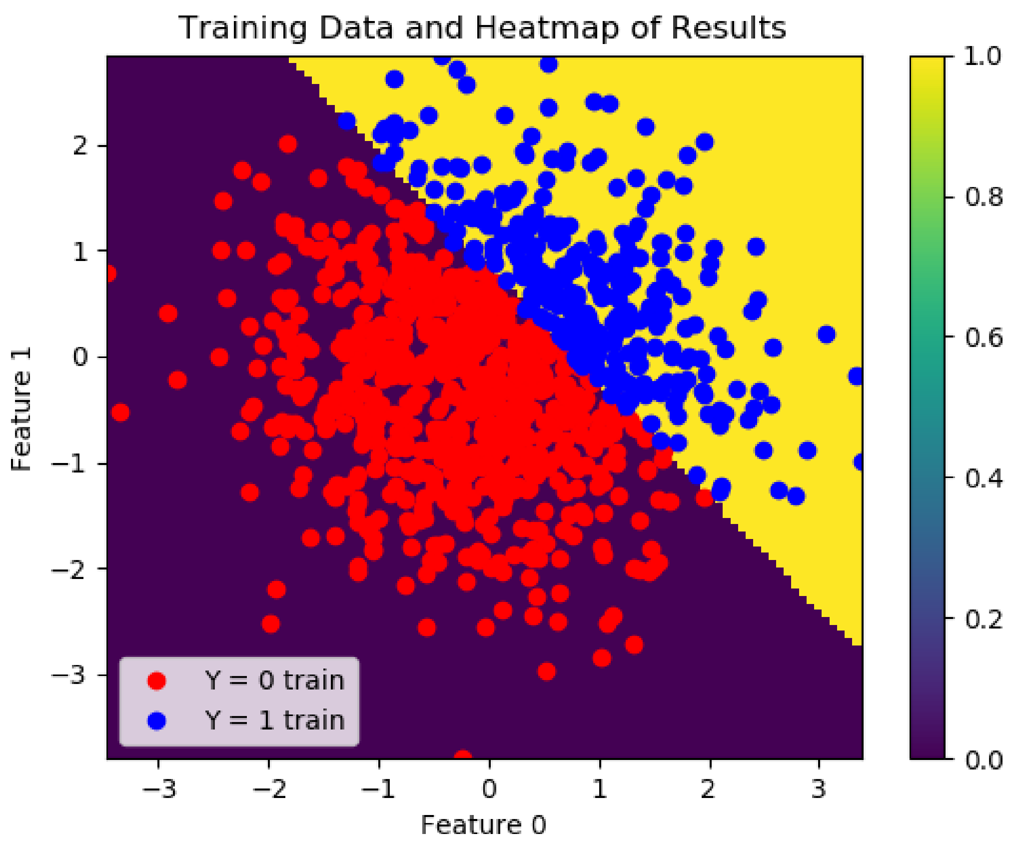
Plotting Logistic Regression Results

- Goal: produce plot of training data and predicted results to visually measure accuracy of predictions
- Training data: red and blue points
- Predicted Results: results predicted by model (purple is predicted 0 and yellow is predicted 1)



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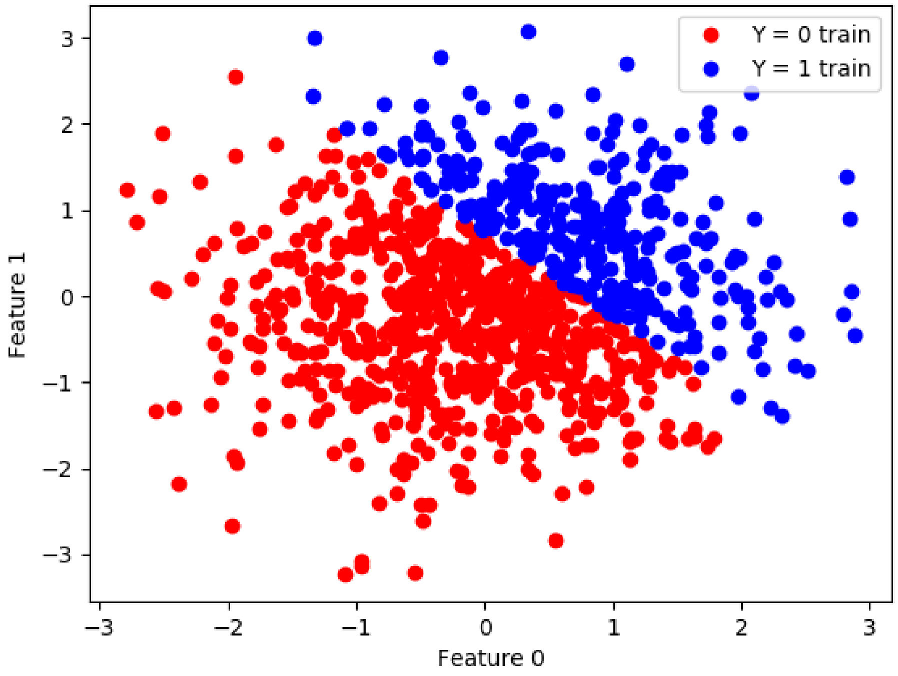
Plotting Logistic Regression Training Data

Start with feature matrix X (2 features x m samples) and label vector Y (m samples)

1. Identify indexes for label = 0 – plot corresponding points red
2. Identify indexes for label = 1 – plot corresponding points blue



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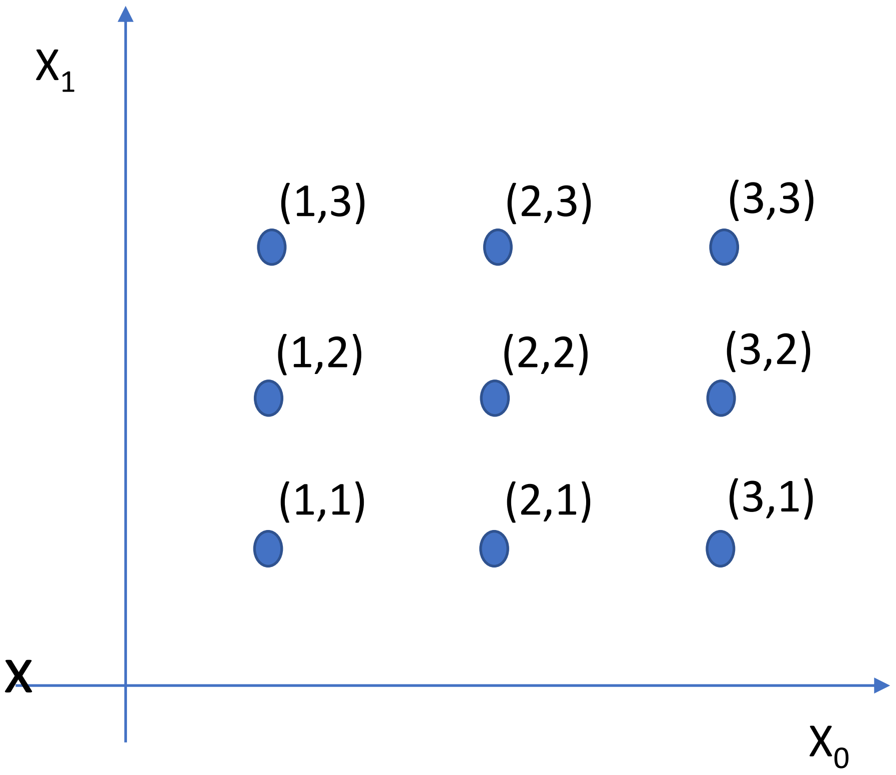
Plotting Heatmap of Results

Assume that training algorithm has been performed with training data

1. Create grid of points similar to that on right
2. Points: (1,1), (2,1), (3,1), (1,2), (2,2), (3,2), (1,3), (2,3), (3,3)
3. Feature Matrix:

$$X = \begin{bmatrix} 1 & 2 & 3 & 1 & 2 & 3 & 1 & 2 & 3 \\ 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 3 \end{bmatrix}$$

4. Apply prediction algorithm with feature matrix representing grid of points to produce 0 or 1 label for each point
5. Convert prediction results to a 2d grid
6. Use pcolormesh function in matplotlib.pyplot applied to grid and labels to generate heatmap



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Code Version 1.3 Walkthrough

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