

# CS540 Introduction to Artificial Intelligence

## Lecture 2

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Based on lecture slides by Jerry Zhu and Yingyu Liang

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# Quiz (Participation)

Guess Real Face

- Which one is the real face?
- A: Left
- B: Right
- C: Don't choose this
- D: Don't choose this
- E: Don't choose this

# Activation Function

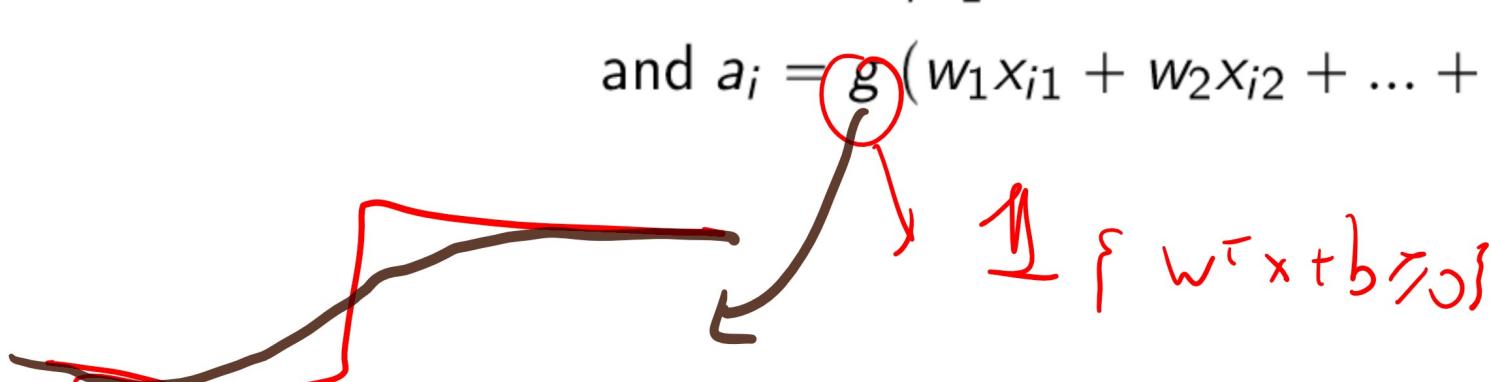
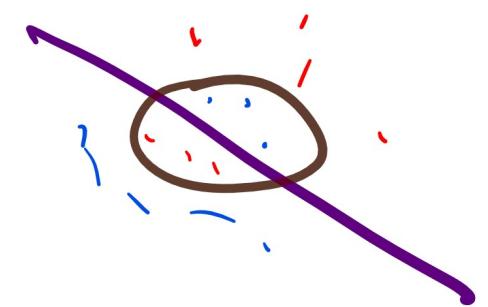
## Review

- The supervised learning problem with activation function is the following.

$$(\hat{w}_0, \hat{w}_1, \dots, \hat{w}_m, \hat{b}) = \arg \min_{w_1, \dots, w_m, b} C$$

where  $C = \frac{1}{2} \sum_{i=1}^n (a_i - y_i)^2$

and  $a_i = g(w_1x_{i1} + w_2x_{i2} + \dots + w_mx_{im} + b)$

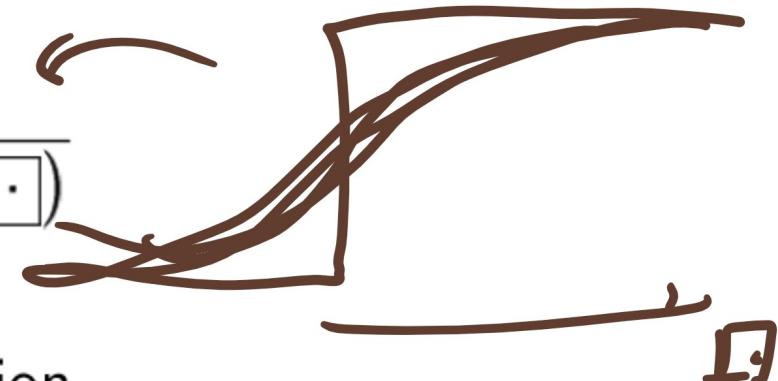


# Sigmoid Activation Function

## Motivation

- When the activation function  $g$  is the sigmoid function, the problem is called logistic regression.

$$g(\boxed{\cdot}) = \frac{1}{1 + \exp(-\boxed{\cdot})}$$



- This  $g$  is also called the logistic function.

# Sigmoid Function Diagram

## Motivation

# Cross Entropy Loss Function

## Motivation

$$C = \frac{1}{2} \sum (y - q_i)^2$$

- The cost function used for logistic regression is usually the log cost function.

$$C = - \sum_{i=1}^n (y_i \log(f(x_i)) + (1 - y_i) \log(1 - f(x_i)))$$

- It is also called the cross-entropy loss function.

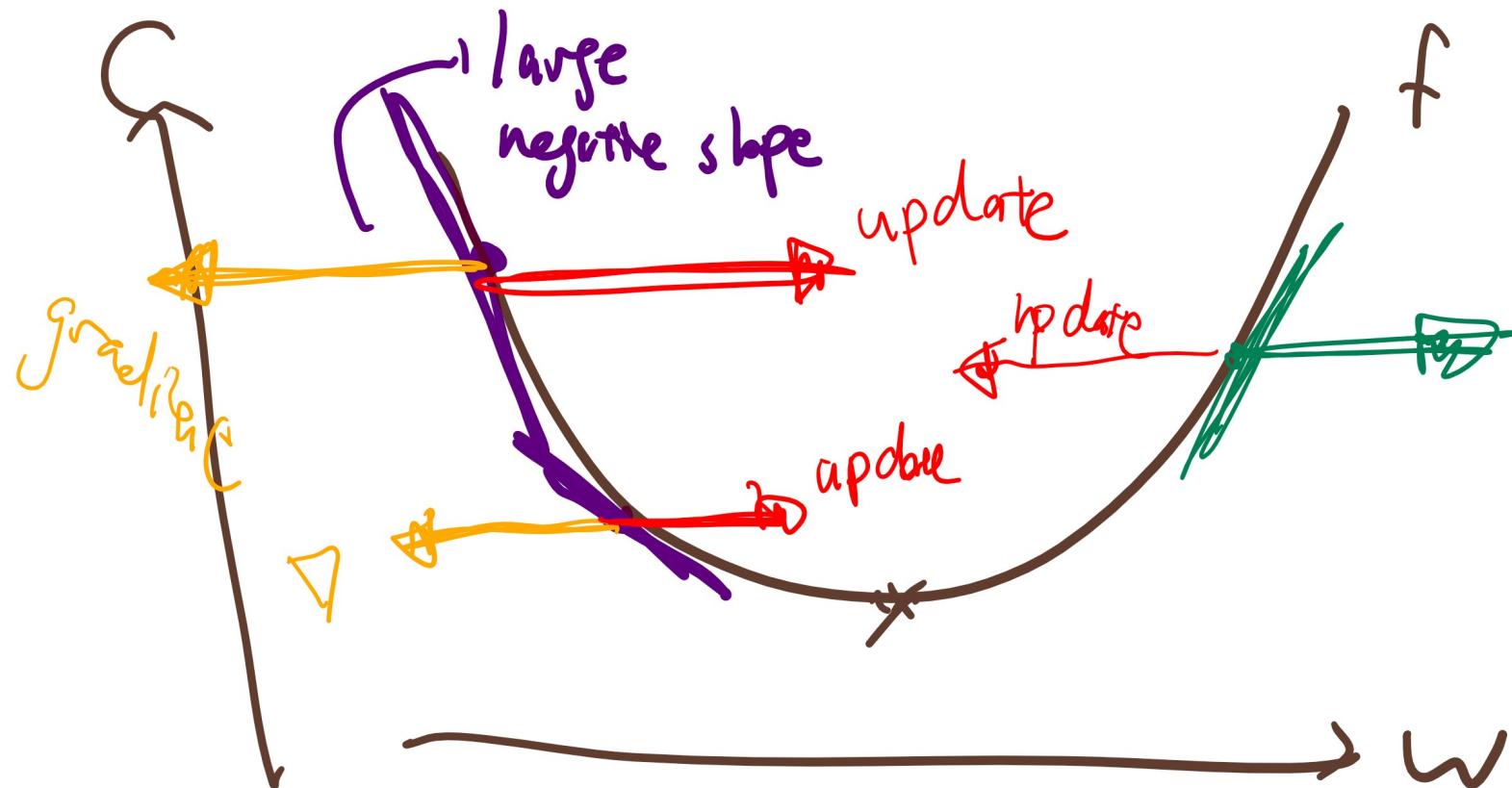
# Logistic Regression

## Description

- Initialize random weights.
- Evaluate the activation function.
- Compute the gradient of the cost function with respect to each weight and bias.
- Update the weights and biases using gradient descent.
- Repeat until convergent.

# Optimization Diagram

Description



# Gradient Descent Intuition

## Definition

- If a small increase in  $w_1$  causes the distances from the points to the regression line to decrease: increase  $w_1$ .
- If a small increase in  $w_1$  causes the distances from the points to the regression line to increase: decrease  $w_1$ .
- The change in distance due to change in  $w_1$  is the derivative.
- The change in distance due to change in  $\begin{bmatrix} w \\ b \end{bmatrix}$  is the gradient.

# Gradient

## Definition

- The gradient is the vector of derivatives.

- The gradient of

$\rightarrow \underline{f(x_i)} = \underline{w^T x_i} + b = \underline{w_1 x_{i1} + w_2 x_{i2} + \dots + w_m x_{im} + b}$  is:

e.g.

$$\nabla_w f = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \frac{\partial f}{\partial w_2} \\ \dots \\ \frac{\partial f}{\partial w_m} \end{bmatrix} = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \dots \\ x_{im} \end{bmatrix} = x_i$$

$$\nabla_b f = 1$$

# Chain Rule

## Definition

- The gradient of

$f(x_i) = g(w^T x_i + b) = g(w_1 x_{i1} + w_2 x_{i2} + \dots + w_m x_{im} + b)$   
can be found using the chain rule.

$$f(x) = g(h(x))$$

↙  
 $g'(h(x)) \cdot \nabla h(x)$

$$\nabla_w f = g' (w^T x_i + b) x_i$$

$$\nabla_b f = g' (w^T x_i + b)$$

- In particular, for the logistic function  $g$ :

$$g(\boxed{\cdot}) = \frac{1}{1 + \exp(-\boxed{\cdot})}$$

$$g'(\boxed{\cdot}) = g(\boxed{\cdot})(1 - g(\boxed{\cdot}))$$

# Logistic Gradient Derivation

Definition

$$g(x) = \frac{1}{1 + e^{-x}} = \frac{1}{(1 + e^{-x})^{-1}}$$

$$g'(x) = (1 + e^{-x})^{-2} \cdot (-1) \cdot (e^{-x}) \cdot (-1)$$

$$= \frac{e^{-x}}{1 + e^{-x}} \cdot \frac{1}{(1 + e^{-x})^{-1}} = \left(1 - \frac{1}{1 + e^{-x}}\right) \cdot \frac{1}{1 + e^{-x}}$$

$$= (1 - g(x)) g(x)$$

# Gradient Descent Step

## Definition

- For logistic regression, use chain rule twice.

$$w = w - \alpha \sum_{i=1}^n (a_i - y_i) x_i$$

$$b = b - \alpha \sum_{i=1}^n (a_i - y_i)$$

$$a_i = g(w^T x_i), g(\square) = \frac{1}{1 + \exp(-\square)}$$

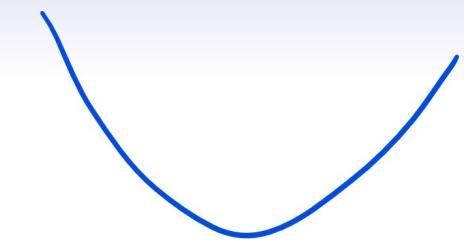
only global min.

- $\alpha$  is the learning rate. It is the step size for each step of gradient descent.

Convex  $\rightarrow$  small  $\alpha$   $\rightarrow$  always converge.

# Gradient Descent Derivation

Definition



$$C = - \sum_{i=1}^n y_i \log a_i + (1-y_i) \log (1-a_i)$$

$$a_i = g(w^T x + b)$$

$$\nabla_w C = \frac{\partial C}{\partial w_j}$$

$$= \sum_{i=1}^n \frac{\partial C}{\partial a_i}$$

by Chain Rule

$$\frac{\partial a_i}{\partial w_j}$$

$$\frac{\partial C}{\partial a_i} = \frac{y_i}{a_i} - \frac{1-y_i}{1-a_i} (-1)$$

$$g(w^T x + b) \cdot (1 - g(w^T x + b)) \cdot x_i$$

$$g'$$

$$\nabla_w (w^T x + b)$$

# Learning Rate Diagram

Definition

$$\sum_i \left( -\frac{y_i}{q_i} + \frac{1-y_i}{1-q_i} \right) q_i (1-q_i) \cdot x_i$$

$$\sum_i (-y_i(1-q_i) + q_i(1-y_i)) x_i$$

$$\sum_i (q_i - y_i) x_i$$

# Gradient Descent

## Quiz (Graded)

- What is the gradient descent step for  $w$  if the objective (cost) function is the squared error?

$$C = \frac{1}{2} \sum_{i=1}^n (a_i - y_i)^2$$

$$\nabla_w a_i = a_i(1-a_i)x_i$$

$$\nabla_w C = \sum_{i=1}^n \left[ \frac{\partial C}{\partial a_i} \right] \nabla_w a_i$$

$$w \leftarrow w - \alpha \nabla_w C$$

- A:  $w = w - \alpha \sum (a_i - y_i) x_i$
- B:  $w = w - \alpha \sum (a_i - y_i) a_i x_i$
- C:  $w = w - \alpha \sum (a_i - y_i) (1 - a_i) x_i$
- D:  $w = w - \alpha \sum (a_i - y_i) a_i (1 - a_i) x_i$
- E: None of the above

# Gradient Descent, Another One

## Quiz (Graded)

- What is the gradient descent step for  $w$  if the objective (cost) function is the absolute value error?

$|a_i - y_i| = \begin{cases} a_i - y_i & \text{if } a_i - y_i \geq 0 \\ -(a_i - y_i) & \text{if } a_i - y_i < 0 \end{cases}$

$$\sum_{i=1}^n |a_i - y_i|$$

$$\frac{\partial C}{\partial a_i}$$

$a_i - y_i > 0$

$a_i - y_i < 0$

$\text{Sgn}$

$\begin{cases} +1 & a_i - y_i > 0 \\ 0 & a_i - y_i = 0 \\ -1 & a_i - y_i < 0 \end{cases}$

- A:  $w = w - \alpha \sum (a_i - y_i) a_i (1 - a_i) x_i$
- B:  $w = w - \alpha \sum |a_i - y_i| a_i (1 - a_i) x_i$
- C:  $w = w - \alpha \sum \mathbb{I}_{\{a_i - y_i > 0\}} a_i (1 - a_i) x_i$
- D:  $w = w - \alpha \sum \text{sign}(a_i - y_i) a_i (1 - a_i) x_i$
- E: None of the above

# Logistic Regression, Part 1

## Algorithm

- Inputs: instances:  $\{x_i\}_{i=1}^n$  and  $\{y_i\}_{i=1}^n$
- Outputs: weights and biases:  $w_1, w_2, \dots, w_m$  and  $b$
- Initialize the weights.

$$w_1, \dots, w_m, b \sim \text{Unif } [0, 1]$$

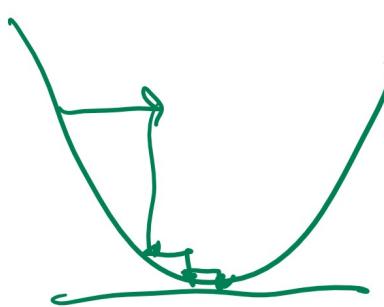
- Evaluate the activation function.

$$a_i = g(w^T x_i), g(\boxed{\cdot}) = \frac{1}{1 + \exp(-\boxed{\cdot})}$$

# Logistic Regression, Part 2

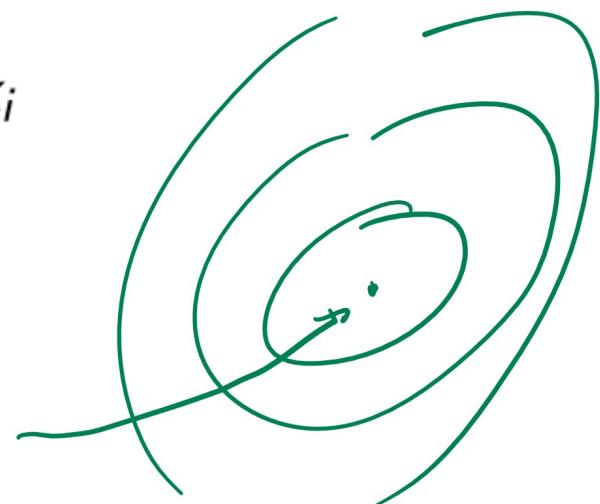
## Algorithm

- Update the weights and bias using gradient descent.



$$w = w - \alpha \sum_{i=1}^n (a_i - y_i) x_i$$

$$b = b - \alpha \sum_{i=1}^n (a_i - y_i)$$



- Repeat the process until convergent.

$$|C - C^{\text{prev}}| < \varepsilon$$

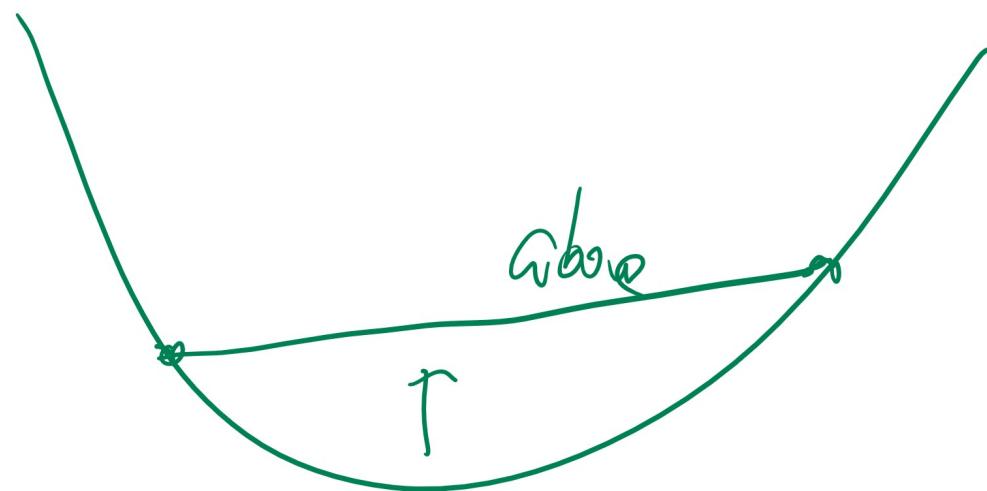
# Other Non-linear Activation Function

## Discussion

- Activation function:  $g(\cdot) = \tanh(\cdot) = \frac{e^{\cdot} - e^{-\cdot}}{e^{\cdot} + e^{-\cdot}}$
- Activation function:  $g(\cdot) = \arctan(\cdot)$
- Activation function (rectified linear unit):  $g(\cdot) = \cdot \mathbb{1}_{\{\cdot \geq 0\}}$
- All these functions lead to objective functions that are convex and differentiable. Gradient descent can be used.

# Convexity Diagram

## Discussion



# Convexity

## Discussion

- If a function is convex, gradient descent with any initialization will converge to the global minimum.
- If a function is not convex, gradient descent with different initializations may converge to different local minima.
- A twice differentiable function is convex if and only its second derivative is non-negative.
- In the multivariate case, it means the Hessian matrix is positive semidefinite.

# Positive Semidefinite

## Discussion

- Hessian matrix is the matrix of second derivatives:

$$H : H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

$f(x_1, x_2)$

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

- A matrix  $H$  is positive semidefinite if  $x^T H x \geq 0 \forall x \in \mathbb{R}^n$ .
- A symmetric matrix is positive semidefinite if and only if all of its eigenvalues are non-negative.

# Eigenvalues

## Quiz (Participation)

- Eigenvalue?
- A: Never heard of it before.
- B: Heard it once in Avengers Endgame.
- C: Heard it before in other courses.
- D: Learned in other courses before completely forgot.
- E: Still remember how to compute eigenvalues.

# Convex Functions

## Quiz (Participation)

- What is the Hessian (second derivative) of

$$f(x) = \frac{1}{2} (x_1^2 + 4x_1x_2 + x_2^2) = \frac{1}{2} \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- A:  $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$
- B: Do not choose this.
- C:  $\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$
- D: Do not choose this.
- E:  $\begin{bmatrix} 1 & 4 \\ 4 & 1 \end{bmatrix}$

$$\frac{\partial^2 f}{\partial x_1^2} = \frac{\partial}{\partial x_1} \left( \frac{1}{2} (2x_1 + 4x_2) \right) = 1$$

$$\frac{\partial^2 f}{\partial x_1 \partial x_2} = \frac{\partial}{\partial x_2} \left( \frac{1}{2} (4x_1 + 2x_2) \right) = 2$$

# Definiteness

## Quiz (Participation)

- Which ones (two) of the following are the eigenvalues of  $\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$ ? Two eigenvectors are  $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$  and  $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ .

- A: 0
- B: 1
- C: 2
- D: 3
- E: 4

$$\lambda = \{-1, 3\}$$

$$Hx = \lambda x$$

↑      ↑      ↗

eigenvector

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = ? \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} = ? \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

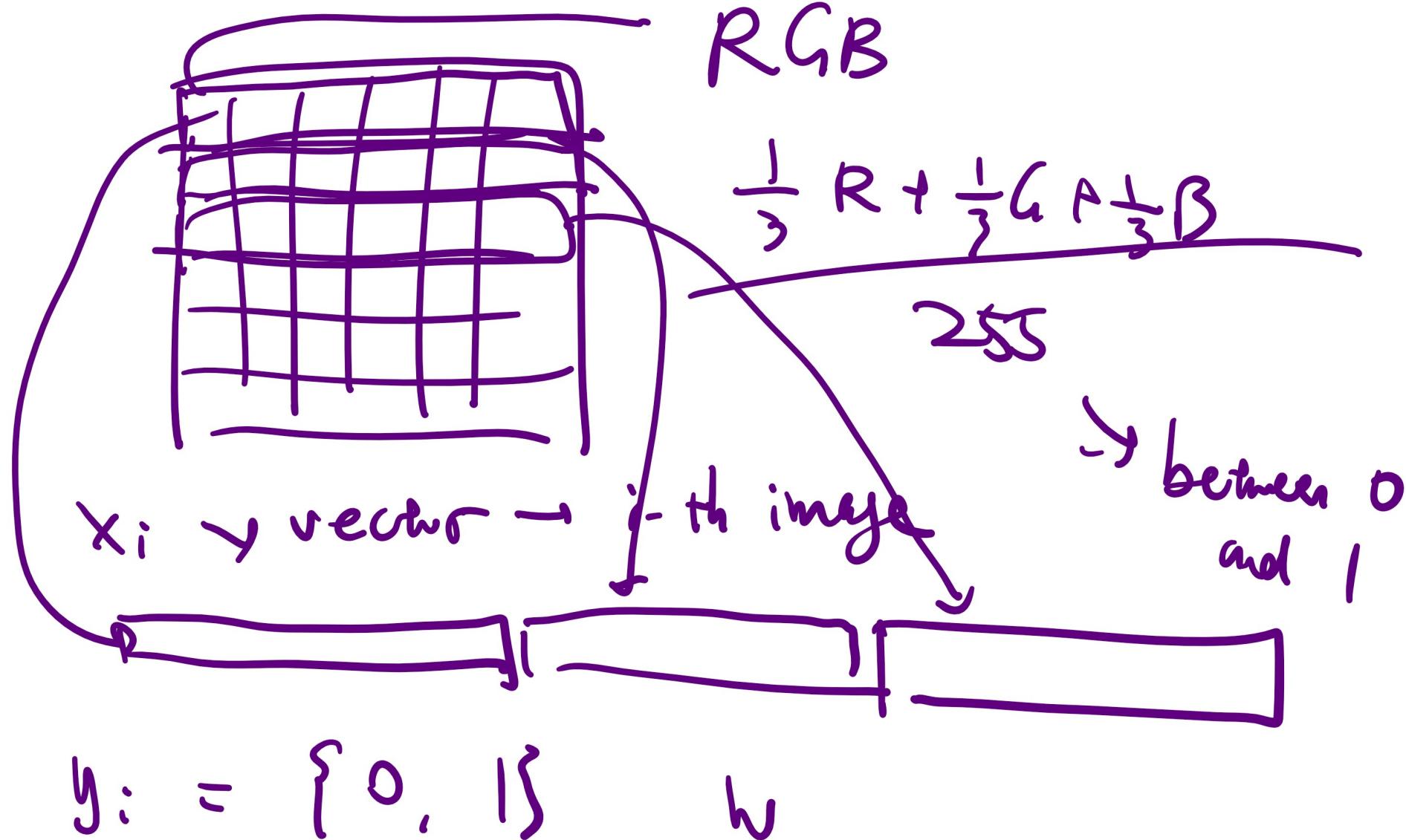
# Image as Input

## Discussion

- Simplest feature vector for an image is the flattened pixel intensities.
- One way to compute pixel intensity is to use the average of the RGB values divided by 255.
- Pixel intensity of each pixel is between 0 and 1.
- An  $n_w$  pixel by  $n_h$  pixel image then can be flattened into a  $m = n_w n_h$  dimensional input feature vector  $x$ .

# Flattened Feature Vector Diagram

Discussion



# AND Operator Data

## Quiz (Participation)

- Sample data for AND

$x_1$	$x_2$	$y$
0	0	0
0	1	0
1	0	0
1	1	1

# Learning AND Operator

## Quiz (Participation)

- Which one of the following is AND?
- A:  $\hat{y} = \mathbb{1}_{\{1x_1+1x_2-1.5 \geq 0\}}$
- B:  $\hat{y} = \mathbb{1}_{\{1x_1+1x_2-0.5 \geq 0\}}$
- C:  $\hat{y} = \mathbb{1}_{\{-1x_1+0.5 \geq 0\}}$
- D:  $\hat{y} = \mathbb{1}_{\{-1x_1-1x_2+0.5 \geq 0\}}$
- E: None of the above

# OR Operator Data

## Quiz (Graded)

- Sample data for OR

$x_1$	$x_2$	$y$
0	0	0
0	1	1
1	0	1
1	1	1

# Learning OR Operator

## Quiz (Graded)

- Which one of the following is OR?
- A:  $\hat{y} = \mathbb{1}_{\{1x_1+1x_2-1.5 \geq 0\}}$
- B:  $\hat{y} = \mathbb{1}_{\{1x_1+1x_2-0.5 \geq 0\}}$
- C:  $\hat{y} = \mathbb{1}_{\{-1x_1+0.5 \geq 0\}}$
- D:  $\hat{y} = \mathbb{1}_{\{-1x_1-1x_2+0.5 \geq 0\}}$
- E: None of the above

# XOR Data

## Quiz (Graded)

- Sample data for XOR

$x_1$	$x_2$	$y$
0	0	0
0	1	1
1	0	1
1	1	0

# Learning XOR Operator

## Quiz (Graded)

- Which one of the following is XOR?
- A:  $\hat{y} = \mathbb{1}_{\{x_1+x_2-1.5 \geq 0\}}$
- B:  $\hat{y} = \mathbb{1}_{\{x_1+x_2-0.5 \geq 0\}}$
- C:  $\hat{y} = \mathbb{1}_{\{-x_1+0.5 \geq 0\}}$
- D:  $\hat{y} = \mathbb{1}_{\{-x_1-x_2+0.5 \geq 0\}}$
- E: None of the above