Lecture 05
Machine Learning II

仿生设计与学习实验室

Bionic Design & Learning Lab

AncoraSIR.com

[Please refer to the course website for copyright credits]

SUSTech
Southern University of Science and Technology

Statistical Binary Classification

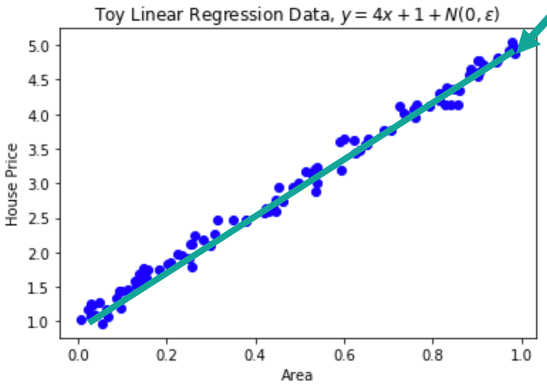
AncoraSIR.com

Statistical Binary Classification

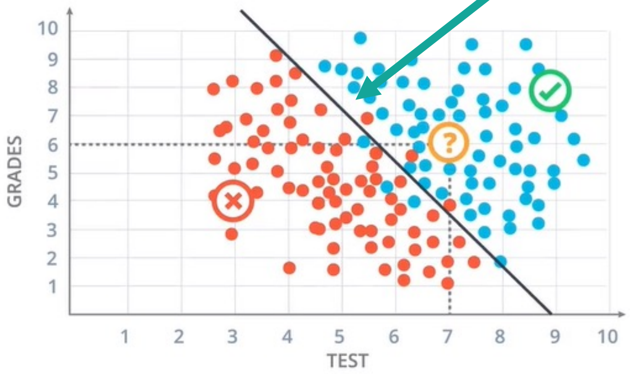
To categorize new probabilistic observations into two predefined categories

- Linear Regression
  - A basic linear model for line-fitting
  - $\hat{y} = f_{WeightedSum}(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$
- Linear Classification
  - Vectorized weights for two or multiple classes
  - $\mathbf{s} = f_{WeightedSum}(\mathbf{x}) = \mathbf{W}\mathbf{x} + \mathbf{b}$

Estimate a line
to describe a relationship

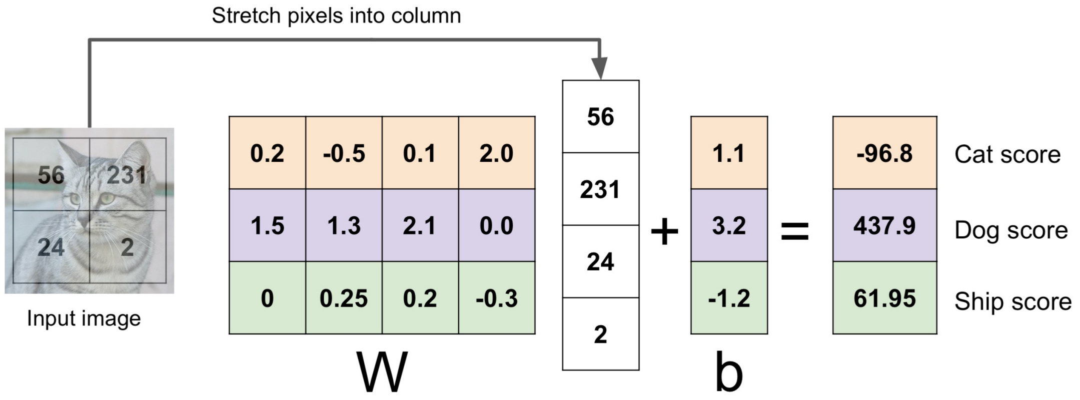


Predict University Acceptance
based on Test and Grades
(*only two categories*)



$$\hat{y} = g_{Activation}(s) = \begin{cases} 1 & if\ s \geq 0 \\ 0 & if\ s < 0 \end{cases}$$

Is this picture a cat, a dog, or a ship?
(*Can we make a decision based on the results on the right?*)



- What if the problem becomes more complex?
- Information lost about the distance to the cutoff value
- Uncertain about the final decision

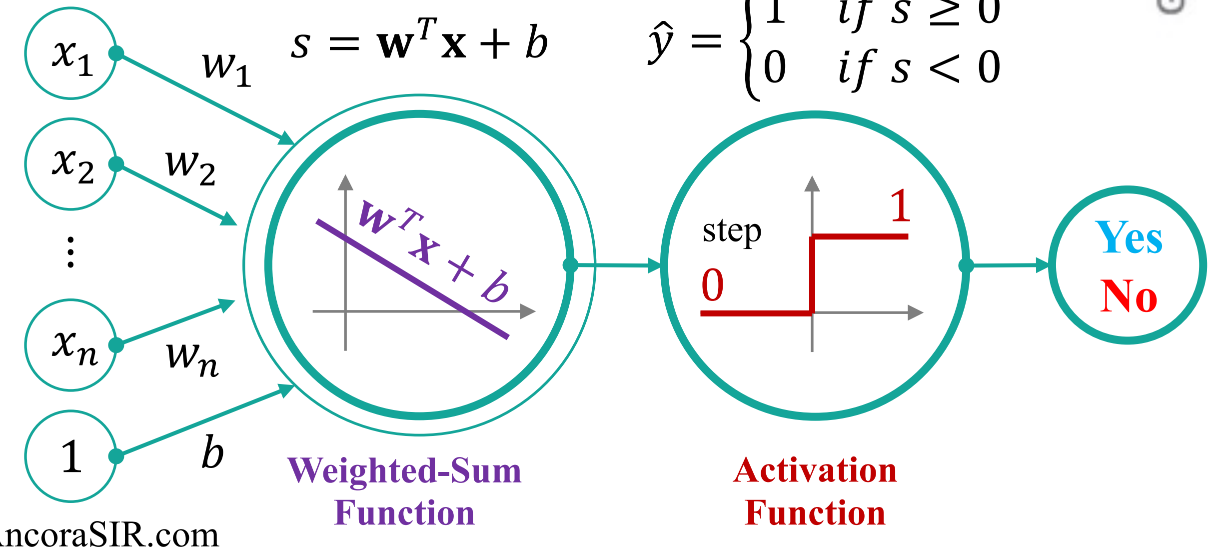
AncoraSIR.com

Perceptron with an Activation Function

Non-linear extraction of information from the data to help making a decision

- An Artificial Neuron with two nodes
  - **Weighted-sum node**
    - Calculate a linear equation $s(x)$ with inputs on the weights plus bias
  - **Activation node**
    - Apply the step function to get the predicted result $\hat{y}(s)$

$$s = \mathbf{w}^T\mathbf{x} + b \qquad \hat{y} = \begin{cases} 1 & if\ s \geq 0 \\ 0 & if\ s < 0 \end{cases}$$



AncoraSIR.com

<u>*An example of acceptance at a University*</u>

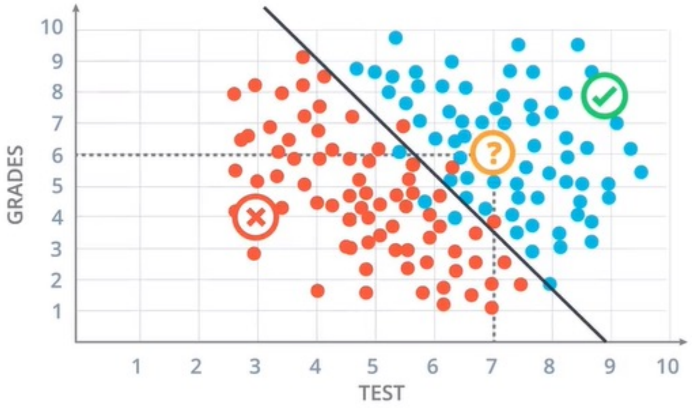
$$\begin{aligned} \hat{y} &= g_{Activation}\left[f_{WeightedSum}(\mathbf{x})\right] \\ &= \text{step}(s, 0) \\ &= \text{step}(\mathbf{w}^T\mathbf{x} + b, 0) \end{aligned}$$

Perceptron Algorithm

How to get the weights?

- Start with the all-zeroes weight vector $\mathbf{w}_1 = \mathbf{0}$ and initialize t to 1.
  - Let's automatically scale all examples $\mathbf{x}$ to have (Euclidean) length 1, since this doesn't affect which side of the plane they are on.
- Given an example $\mathbf{x}$, predict positive if and only if $\mathbf{w}_t \cdot \mathbf{x} > 0$.
  - One may consider the bias term b as a weight w_0 for $x_0 = 1$
- On a mistake, update as follows until convergence criteria reached:
  - If mistake on a positive $\mathbf{x}$, then $\mathbf{w}_t + 1 \leftarrow \mathbf{w}_t + \mathbf{x}$,
    - So $\mathbf{w}_{t+1} \cdot \mathbf{x} = (\mathbf{w}_t + \mathbf{x}) \cdot \mathbf{x} = \mathbf{w}_t \cdot \mathbf{x} + 1$,
    - *We move closer by 1 to the value we wanted.*
  - If mistake on a negative $\mathbf{x}$, then $\mathbf{w}_t + 1 \leftarrow \mathbf{w}_t - \mathbf{x}$,
    - So $\mathbf{w}_{t+1} \cdot \mathbf{x} = (\mathbf{w}_t - \mathbf{x}) \cdot \mathbf{x} = \mathbf{w}_t \cdot \mathbf{x} - 1$,
    - *We move closer by 1 to the value we wanted.*
- $t \leftarrow t + 1$.

If data is separable by a large margin, then Perceptron is a good algorithm to use.



What if the boundary line is non-linear?

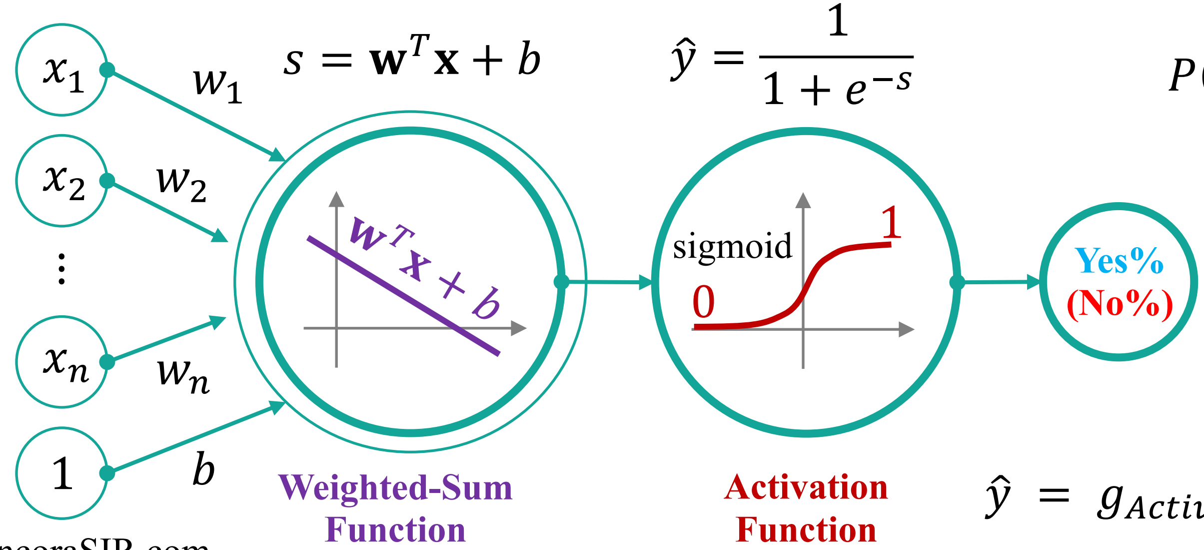
AncoraSIR.com

By what chances will I get accepted to a University?

Based on my Test and Grade scores …

- **Weighted-sum node**
  - Unchanged as the input data remains the same
- **Activation node**
  - Can be changed as we want a new expression of the output as a probability of prediction
  - Sigmoid function as a natural choice that transforms the output to a value between 0 and 1 (*or within 100%*)

An example of acceptance at a University

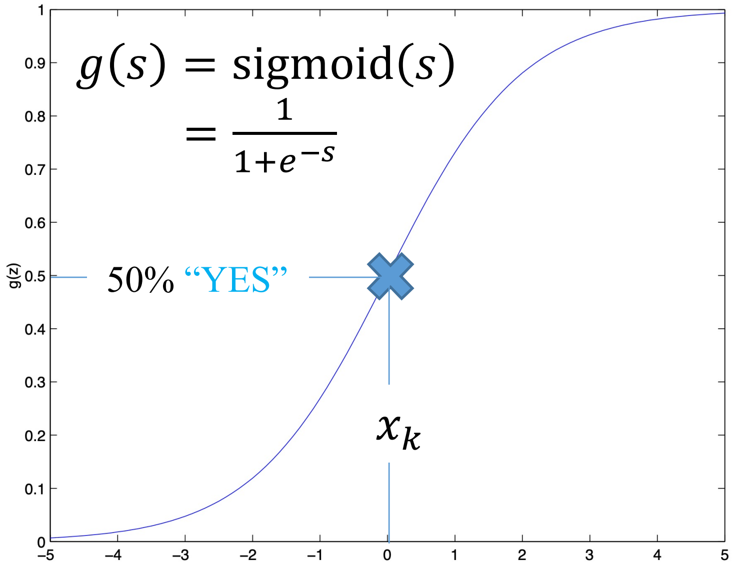


AncoraSIR.com

$$P(\mathbf{x}) = \frac{1}{1 + e^{-(\mathbf{w}^T\mathbf{x}+b)}}$$

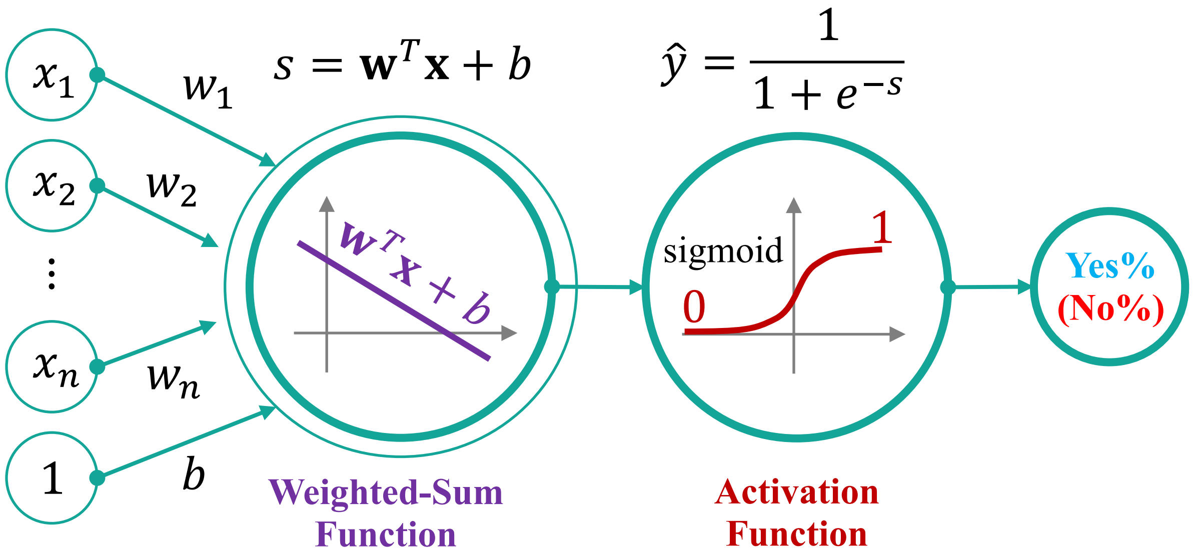
Can be viewed as a probability

$$\hat{y} = g_{Activation}(s) = \text{sigmoid}(s)$$



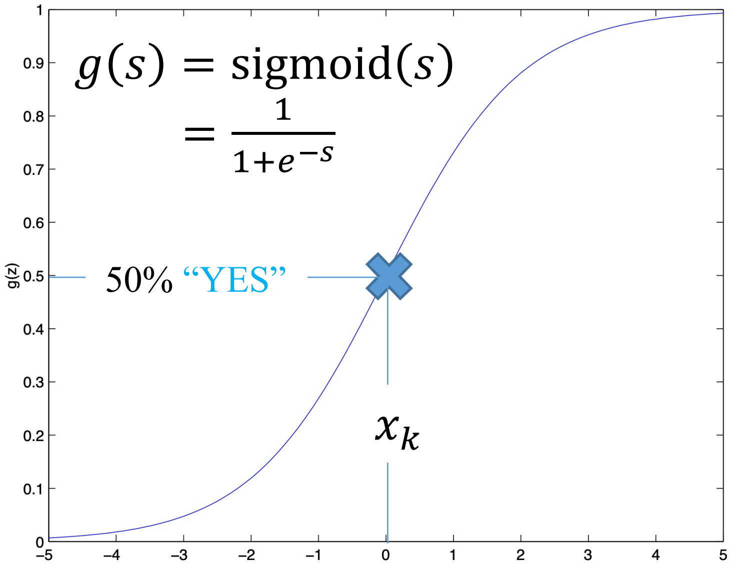
Logistic Regression

$$\hat{y} = g_{Activation}\left[f_{WeightedSum}(\mathbf{x})\right] = \text{sigmoid}(\mathbf{w}^T\mathbf{x} + b)$$



Problem statement

- Assume $\hat{y} = g_{Activation}\left[f_{WeightedSum}(\mathbf{x})\right] = \frac{1}{1+e^{-(\mathbf{w}^T\mathbf{x}+b)}}$
- How to minimize the **prediction error/loss** on a single training sample (with a maximum likelihood set of **w**) ?



- Hypothesis Function: $h_w(x) = \text{sigmoid}(\mathbf{w}^T\mathbf{x} + b)$
- Model output with a probability: $P(y \mid x; w) = [h_w(x)]^y[1 - h_w(x)]^{1-y}$
  - **Yes%**: $P(y = 1 \mid x; w) = h_w(x)$
  - **No%**: $P(y = 0 \mid x; w) = 1 - h_w(x)$

AncoraSIR.com

Loss Function for Logistic Regression

*It measures how well you are doing on **a single training example***

- Assume that m training examples were generated independently $h_w(x) = \text{sigmoid}(\mathbf{w}^T\mathbf{x} + b)$
- We can write the likelihood of the parameters
  - $L(w) = p(\vec{y} \mid X; w)$
    $= \prod_{i=1}^{m} p\left(y^{(i)} \middle| x^{(i)}; w\right)$
    $= \prod_{i=1}^{m} \left[h_w\left(x^{(i)}\right)\right]^{y^{(i)}} \left[1 - h_w\left(x^{(i)}\right)\right]^{1-y^{(i)}}$

$$g'_{activation}(s) = \frac{d}{ds}\frac{1}{1+e^{-s}} = \frac{1}{(1+e^{-s})^2} \cdot e^{-s} = \frac{1}{(1+e^{-s})^2} \cdot \left(1 - \frac{1}{1+e^{-s}}\right) = g(s) \cdot \left(1 - g(s)\right)$$

- Take the log expression, we have the **loss function**
  - $\ell(w) = \log L(w)$
    $= \sum_{i=1}^{m} y^{(i)} \log h_w\left(x^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_w\left(x^{(i)}\right)\right)$
  - Usually take a "−" sign to indicate loss

AncoraSIR.com

SUSTech Southern University of Science and Technology

Stochastic Gradient Descent

Finding the maximum likelihood of estimation

- Rewrite the weight parameters in vectorized form
  - $w := w + \alpha \cdot \nabla_w \cdot \ell(w)$
  - $+$ sign here to **maximize** likelihood

- When working with a single training example (x, y),
  - $\frac{\partial}{\partial w_j} \ell(w) = \left(y \frac{1}{g(w^T x)} - (1 - y) \frac{1}{1 - g(w^T x)} \right) \frac{\partial}{\partial w_j} g(w^T x) = \left(y - h_w(x) \right) x_j$

- Therefore, we can derive the stochastic gradient ascent rule
  - $w_j := w_j + \alpha \left(y^{(i)} - h_w\left(x^{(i)}\right) \right) x_j^{(i)}$

AncoraSIR.com

Cost Function

*It measures how well you are doing on **an entire training set***

- We want the loss/error function to be as small as possible
  - If $y^{(i)} = 1$, then
    - $\text{LossFunc}(\hat{y}, y) = -\left[y^{(i)} \log h_w\left(x^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_w\left(x^{(i)}\right)\right)\right] = -\log h_w\left(x^{(i)}\right) = -\log \hat{y}$
    - It means that we want $\log \hat{y}$ to be as big as possible, but remember that it is bounded by 1
  - If $y^{(i)} = 0$, then
    - $\text{LossFunc}(\hat{y}, y) = -\left[y^{(i)} \log h_w\left(x^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_w\left(x^{(i)}\right)\right)\right] = -\log(1 - \hat{y})$
    - It means that we want $\log \hat{y}$ to be as small as possible, or close to 0

- Cost Function
  - The average of the loss functions of the entire training set, which is to be minimized

$$J(w, b) = -\frac{1}{m} \sum_{i=1}^{m} \mathcal{L}\left(\hat{y}^{(i)}, y^{(i)}\right) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log \hat{y}^{(i)} + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)\right]$$

Summary

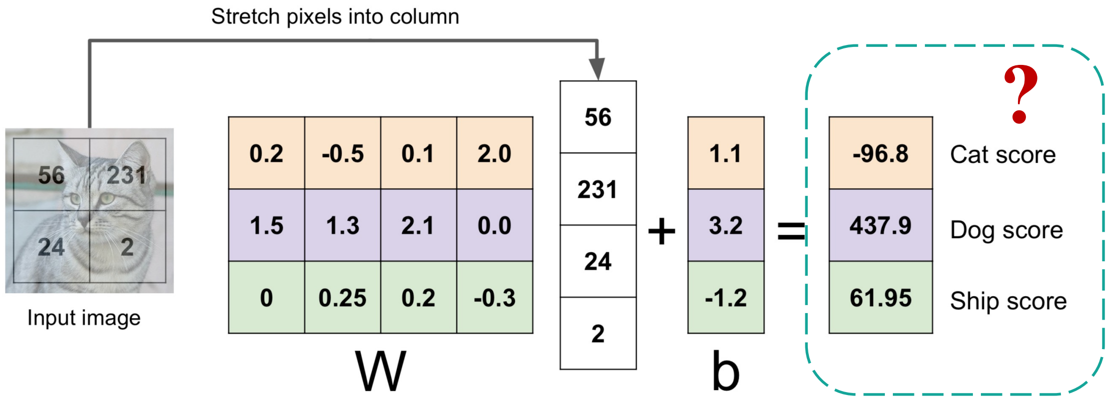
	Linear Regression	Perceptron	Logistic Regression
Problem	Value Prediction	Binary Classification with a threshold	Binary Classification with a probability
Weighted-Sum	$\mathbf{w}^{\mathrm{T}}\mathbf{x} + b$	$\mathbf{w}^{\mathrm{T}}\mathbf{x} + b$	$\mathbf{w}^{\mathrm{T}}\mathbf{x} + b$
Activation Function	NA	Step Function	Sigmoid Function
Prediction Outputs	Continuous Value	Discrete Value $\{0, 1\}$	Continuous Probability $(0, 1)$
Loss	Squared Loss	Hinge Loss	Log-Loss

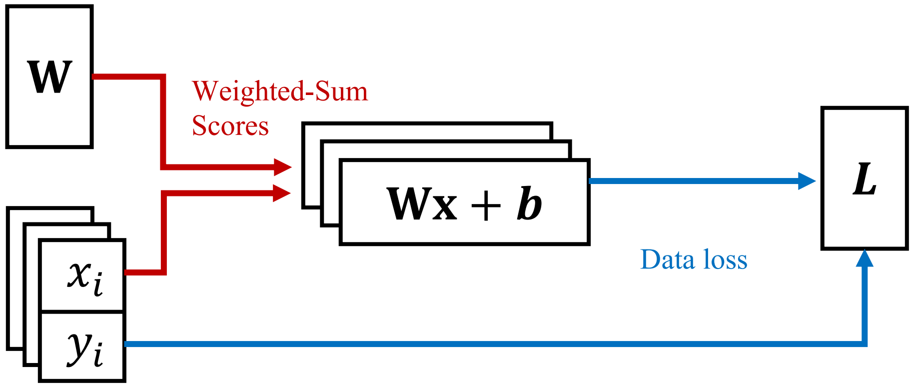
Multi-class Classification

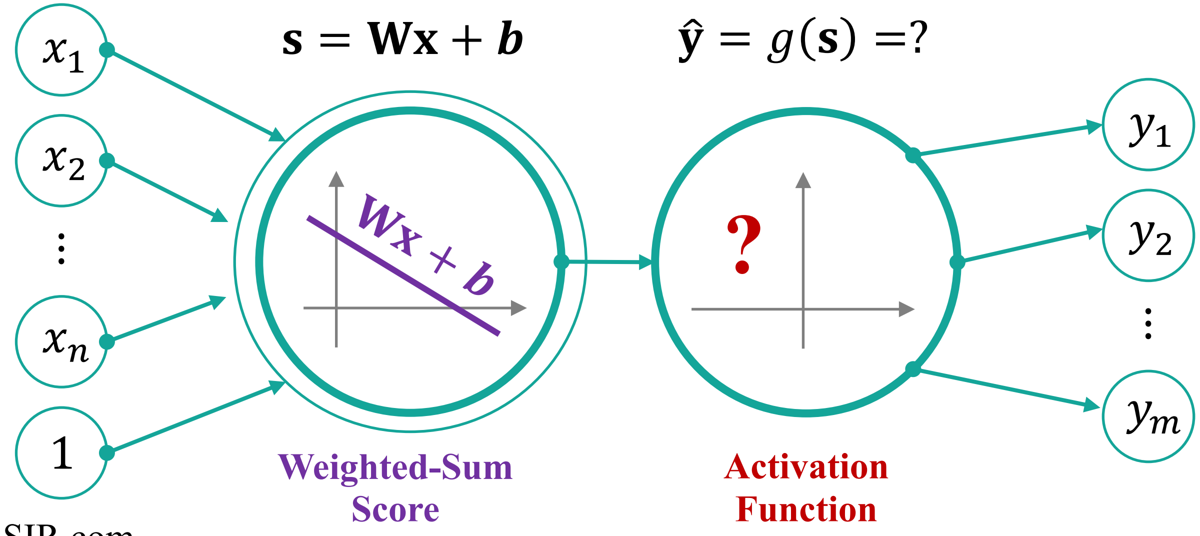
AncoraSIR.com

Multi-class Classification

$$\hat{\mathbf{y}} = g_{Activation}\left[f_{WeightedSum}(\mathbf{x})\right] = g_{Activation}(\mathbf{Wx} + \mathbf{b})$$







1. **Define a loss function** that quantifies our unhappiness with the scores across the training data.
2. Come up with a way of efficiently finding the parameters that minimize the loss function. (***optimization***)

AncoraSIR.com

Define a Loss Function

Quantify how good our current classifier is

3 training samples

$\{(x_i, y_i)\}_{i=1}^{3}$

Ground Truth

$\hat{y}_i$ *Labelled Prediction*



x_i image

y_i label

3 classes			
Cat	**3.2**	1.3	2.2
Car	5.1	**4.9**	2.5
Frog	-1.7	2.0	**-3.1**

Loss over the dataset is a sum of loss over examples

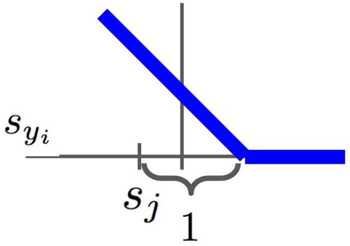
$$L = \frac{1}{N}\sum_i L_i(\hat{y}_i, y_i)$$

Denote Weighted-Sum score vector as $\boldsymbol{s} = f_{WeightedSum}(\mathbf{x})$

Let's try with the hinge loss:

$$L_i = \sum_{j \neq y_i} \begin{cases} 0 & \text{if } s_{y_i} \geq s_j + 1 \\ s_j - s_{y_i} + 1 & \text{otherwise} \end{cases}$$

$$= \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$



AncoraSIR.com

SUSTech Southern University of Science and Technology

Define a Loss Function

Quantify how good our current classifier is

3 training samples

$\{(x_i, y_i)\}_{i=1}^{3}$

Ground Truth / *Labelled Prediction*			
Cat	**3.2**	1.3	2.2
Car	5.1	**4.9**	2.5
Frog	-1.7	2.0	**-3.1**
Loss	2.9	0	**12.9**

3 classes

$$L_i = \sum_{j \neq y_i} \begin{cases} 0 & \text{if } s_{y_i} \geq s_j + 1 \\ s_j - s_{y_i} + 1 & \text{otherwise} \end{cases}$$

$$\begin{aligned} L_1 &= \max(0, 5.1 - 3.2 + 1) + \max(0, -1.7 - 3.2 + 1) \\ &= \max(0, 2.9) + \max(0, -3.9) \\ &= 2.9 + 0 = 2.9 \end{aligned}$$

$$\begin{aligned} L_2 &= \max(0, 1.3 - 4.9 + 1) + \max(0, 2.0 - 4.9 + 1) \\ &= \max(0, -2.6) + \max(0, -1.9) \\ &= 0 + 0 = 0 \end{aligned}$$

$$\begin{aligned} L_3 &= \max(0, 2.2 + 3.1 - 1) + \max(0, 2.5 + 3.1 - 1) \\ &= \max(0, 6.3) + \max(0, 6.6) \\ &= 6.3 + 6.6 = 12.9 \end{aligned}$$

AncoraSIR.com

Define a Loss Function

Quantify how good our current classifier is

3 training samples

$\{(x_i, y_i)\}_{i=1}^{3}$

Ground Truth / *Labelled Prediction*



3 classes			
Cat	**3.2**	1.3	2.2
Car	5.1	**4.9**	2.5
Frog	-1.7	2.0	**-3.1**
Loss	2.9	0	**12.9**

$$L_i = \sum_{j \neq y_i} \begin{cases} 0 & \text{if } s_{y_i} \geq s_j + 1 \\ s_j - s_{y_i} + 1 & \text{otherwise} \end{cases}$$

Loss over full dataset is average:

$$L = \frac{1}{N} \sum_i L_i(\hat{y}_i, y_i)$$
$$= \frac{1}{3}(2.9 + 0 + 12.9)$$
$$= 5.27$$

Recall that our goal is to find a set of **W** with minimum loss over full dataset, i.e. the cost = 0

- Suppose that we found a W such that L = 0. Is this **W** unique?
  - L is still 0 with 2**W**
- **How do we choose between W and 2W?**
  - Let's try regularization

AncoraSIR.com

Regularization

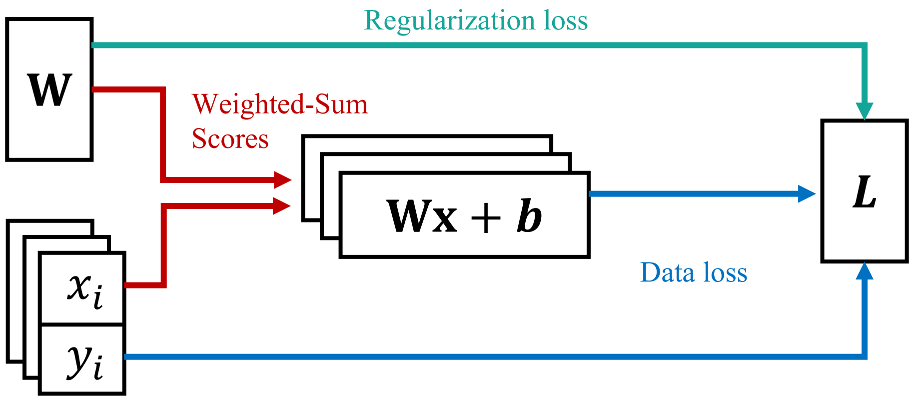
Prevent the model from doing too well on training data

$$L(W) = \boxed{\frac{1}{N}\sum_{1}^{N} L_i(\hat{y}_i, y_i)} + \boxed{\lambda R(W)}$$

λ as strength of Regularization (*hyperparameter*)

Data loss
Model predictions should match training data

Regularization
Prevent the model from doing too well on training data



Simple examples

L2 regularization: $R(W) = \sum_k \sum_l W_{k,l}^2$

L1 regularization: $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2): $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

More complex:

Dropout

Batch normalization

Stochastic depth, fractional pooling, etc

Why regularize?

- Express preferences over weights
- Make the model simple so it works on test data
- Improve optimization by adding curvature

AncoraSIR.com

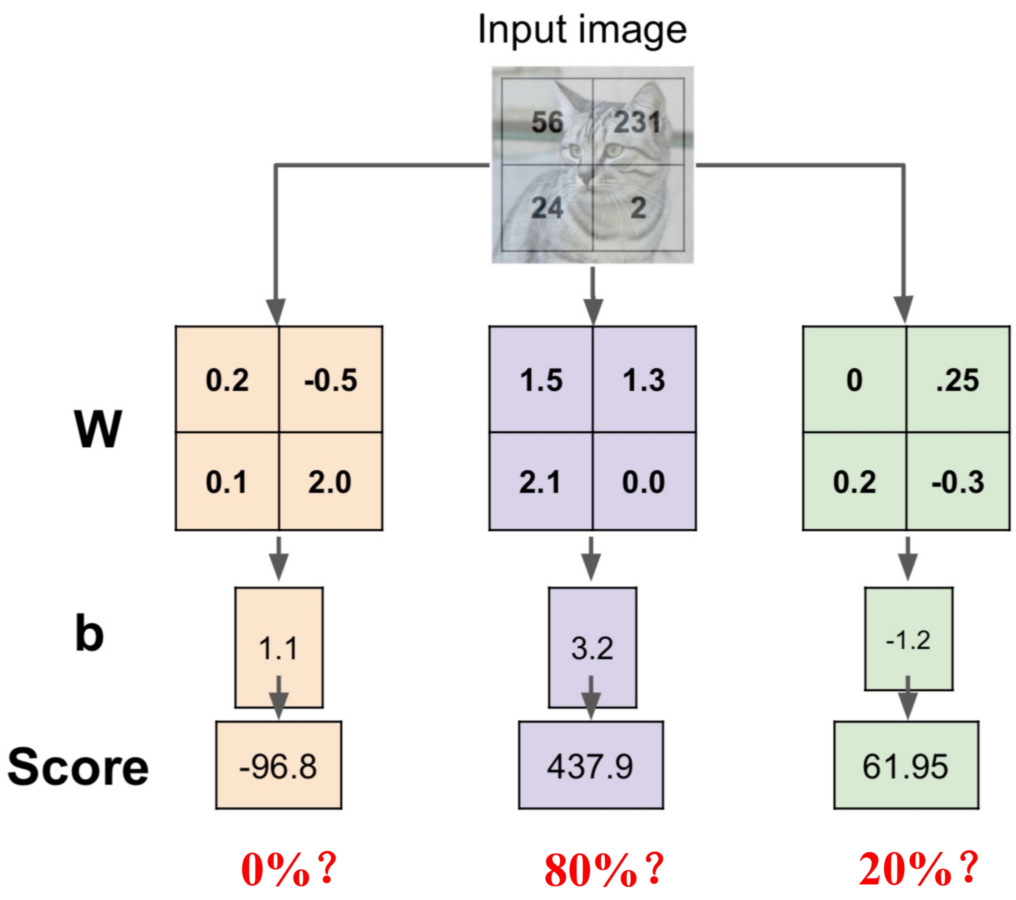
Softmax Operation

Interpret the outputs of our model as probabilities

$$\hat{y}_i = \text{softmax}(o_i) = \frac{\exp(o_i)}{\sum_j \exp(o_j)} \times 100\%$$

- One can interpret outputs $\hat{y}_i$ as the probability that a given item belongs to class i.
- Then we can choose the class with the largest output value as our prediction

  - Why using o_i directly, instead of a probability?
  - What if the sum of probability is not 100%?
  - What if when o_i becomes negative?



AncoraSIR.com

Softmax Classifier

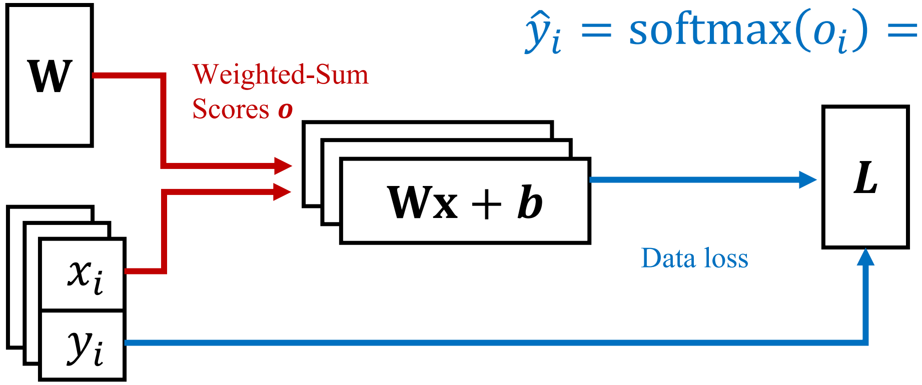
Want to interpret raw classifier scores as ***probabilities***

$$\hat{y}_i = \text{softmax}(o_i) = \frac{\exp(o_i)}{\sum_j \exp(o_j)} \times 100\%$$

(x_1, y_1)

Ground Truth

Labelled Prediction



3 classes

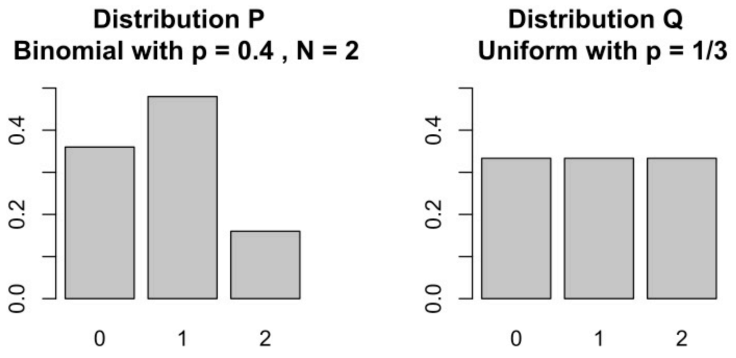
	Weighted-Sum Scores (*logits*)	$\exp(o_i)$ → Unnormalized Probability (>=0)	$\frac{\exp(o_i)}{\sum_j \exp(o_j)}$ ($\times 100\%$) → Normalized Probability Label (*$\hat{y}_i$ Sum to 1*)	Correct Probability Label
Cat	**3.2**	**24.5**	**0.13**	**1.00**
Car	5.1	164.0	0.87	0.00
Frog	-1.7	0.18	0.00	0.00

How to quantify the differences between two probability distribution?

AncoraSIR.com

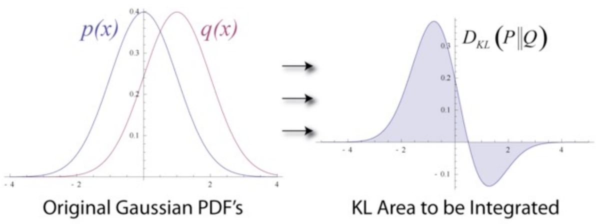
Kullback–Leibler Divergence

How to quantify the differences between two probability distribution?



x	0	1	2
Distribution P(x)	0.36	0.48	0.16
Distribution Q(x)	0.333	0.333	0.333

$$D_{\mathrm{KL}}(P \parallel Q) = \sum_{x \in \mathcal{X}} P(x) \ln\left(\frac{P(x)}{Q(x)}\right)$$
$$= 0.36 \ln\left(\frac{0.36}{0.333}\right) + 0.48 \ln\left(\frac{0.48}{0.333}\right) + 0.16 \ln\left(\frac{0.16}{0.333}\right)$$
$$= 0.0852996$$



$$D_{KL}(P \parallel Q) = \sum_{y \in \mathcal{Y}} P(y) \log \frac{P(y)}{Q(y)}$$
$$= \sum_{y \in \mathcal{Y}} P(y) \log P(y) - \sum_{y \in \mathcal{Y}} P(y) \log Q(y)$$
$$= \left[- \sum_{y \in \mathcal{Y}} P(y) \log Q(y) \right] - \left[- \sum_{y \in \mathcal{Y}} P(y) \log P(y) \right]$$
$$= \mathrm{H}(P, Q) - \mathrm{H}(P)$$

A good candidate of loss function for softmax

Can be minimized to update the weights

$$\mathrm{H}(P, Q) = - \sum_{y \in \mathcal{Y}} P(y) \log Q(y) \qquad \mathrm{H}(P) = - \sum_{y \in \mathcal{Y}} P(y) \log P(y)$$

the cross-entropy of P and Q

the cross-entropy of P with itself (or the entropy of P)

Loss Function

Log-Likelihood expressed in cross-entropy

- The **likelihood** of the actual classes according to our model is

$$P(Y \mid X) = \prod_{i=1}^{n} P(y^{(i)} \mid x^{(i)}) \quad \Rightarrow \quad -\log P(Y \mid X) = \sum_{i=1}^{n} \boxed{-\log P(y^{(i)} \mid x^{(i)})}$$

  - Maximizing the likelihood is equivalent to minimizing the log-likelihood.

- **Cross-entropy** loss for a single example (dropped superscript *i*)

$$l = -\log P(y \mid x) = -\sum_{j} y_j \log \hat{y}_j$$

  - As $\hat{y}$ is a discrete probability distribution and y is a one-hot vector, the sum over all j vanishes for all but one term.

AncoraSIR.com

Cross-Entropy Loss and its Derivative

Also called softmax loss

- Plugging $\mathbf{o}$ into the definition of the cross-entropy loss, we obtain:

$$l = -\sum_j y_j \log \hat{y}_j = \sum_j y_j \log \sum_k \exp(o_k) - \sum_j y_j o_j = \log \sum_k \exp(o_k) - \sum_j y_j o_j$$

- The derivative with respect to $\mathbf{o}$ is

$$\partial_{o_j} l = \frac{\exp(o_j)}{\sum_k \exp(o_k)} - y_j = \mathrm{softmax}(\mathbf{o})_j - y_j = P(y = j \mid x) - y_j.$$

  - The gradient is $P(y = j \mid x) - y_j$
    - The difference between the probability predicted by our model $P(y = j \mid x)$ and the true label y.
  - Similar to regression where the gradient is $\hat{y} - y$
    - The difference between the true label y and the estimation $\hat{y}$

Vectorization for Minibatches

We typically carry out vector calculations for minibatches of data for efficiency

$$\hat{y}_i = \text{softmax}(o_i) = \frac{\exp(o_i)}{\sum_j \exp(o_j)} \times 100\%$$

$$\hat{\mathbf{y}} = \text{softmax}(\mathbf{o}) \ \textit{where} \ \hat{y}_i = \frac{\exp(o_i)}{\sum_j \exp(o_j)} \times 100\%$$

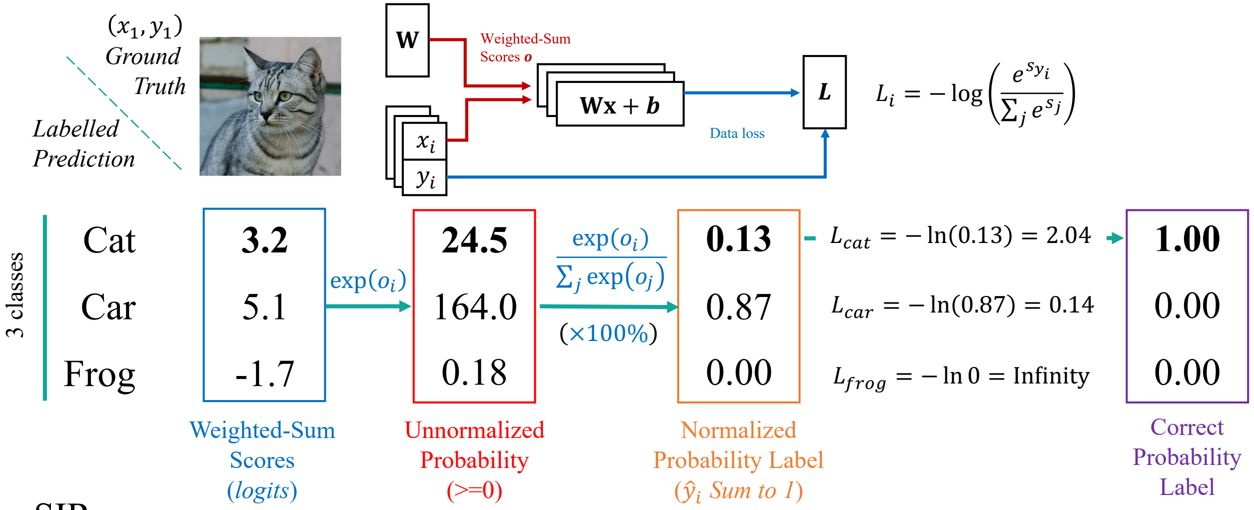
minibatch features $\mathbf{X}$ are in $\mathbb{R}^{n\times d}$,

weights $\mathbf{W} \in \mathbb{R}^{d\times q}$, and

the bias satisfies $\mathbf{b} \in \mathbb{R}^{q}$.

$$\mathbf{O} = \mathbf{X}\mathbf{W} + \mathbf{b},$$

$$\hat{\mathbf{Y}} = \text{softmax}(\mathbf{O})$$



A minibatch $\mathbf{X}$ of examples

- dimensionality d and batch size n

Assume that we have q categories (outputs)

More efficient matrix-matrix computation $\mathbf{XW}$

Exponentiating all entries in $\mathbf{O}$ then sum

AncoraSIR.com

Understanding of Softmax Regression

- When there are two classes, softmax regression reduces to logistic regression.

Softmax → Binary Classes → Logistic

Softmax		Logistic
$\hat{y}_j = \dfrac{\exp(o_j)}{\sum_j \exp(o_j)}$	*Activation*	$\hat{y} = \dfrac{\exp(o)}{\exp(o) + 1}$
$-\frac{1}{n}\sum_{i=1}^{n} y_i log(\hat{y}_i) + (1 - y_i) log(1 - \hat{y}_i)$	*Loss*	$-\sum_{i=1}^{n}\sum_{j} y_j^{(i)} \log \hat{y}_j^{(i)}$

- Softmax when j=2

$$\hat{y}_0 = \frac{\exp(o_0)}{\exp(o_0) + \exp(o_1)}$$

$$= \frac{\exp(o_0 - o_1)}{\exp(o_0 - o_1) + 1}$$

- The cross-entropy classification can be thought in two ways
  1. As maximizing the likelihood of the observed data.
  2. As minimizing out surprise required to communicate the labels.

Summary & Comparison

Linear Neural Network

	Linear Regression	Perceptron	Logistic Regression	Softmax Regression
Problem	Value Prediction	Binary Classification	Binary Classification	Multi-Class Classification
Weights	$\boldsymbol{wx}+b$	$\boldsymbol{wx}+b$	$\boldsymbol{wx}+b$	$W\boldsymbol{x}+B$
Activation Function	NA	Step Function	Sigmoid Function	Softmax
Prediction Outputs	Continuous Value	Discrete Value 0, 1	Continuous Probability in (0,1)	A vector of Continuous Probabilities
Loss	Squared Loss	Hinge Loss	Log Loss (Binary cross entropy)	Cross Entropy
Decision Boundary	Linear			

Thank you~

songcy@sustech.edu.cn