Logistic Regression

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Topics in Linear Classification using Probabilistic Discriminative Models

- Generative vs Discriminative

1. Fixed basis functions
2. Logistic Regression (two-class)
3. Iterative Reweighted Least Squares (IRLS)
4. Multiclass Logistic Regression
5. Probit Regression
6. Canonical Link Functions

Topics in Logistic Regression

- Logistic Sigmoid and Logit Functions
- Parameters in discriminative approach
- Determining logistic regression parameters
  - Error function
  - Gradient of error function
  - Simple sequential algorithm
  - An example
- Generative vs Discriminative Training
  - Naiive Bayes vs Logistic Regression

Logistic Sigmoid and Logit Functions

- In two-class case, *posterior* of class C_1 can be written as as a logistic sigmoid of feature vector $\boldsymbol{\phi}=[\phi_1,..\phi_M]^T$

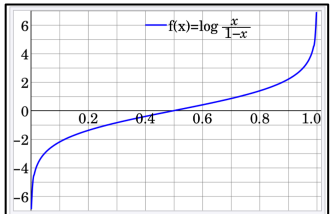
$$p(C_1|\boldsymbol{\phi}) = y(\boldsymbol{\phi}) = \sigma\,(\boldsymbol{w}^T\boldsymbol{\phi})$$

with $p(C_2|\boldsymbol{\phi}) = 1 - p(C_1|\boldsymbol{\phi})$

Here $\sigma\,(.)$ is the logistic sigmoid function

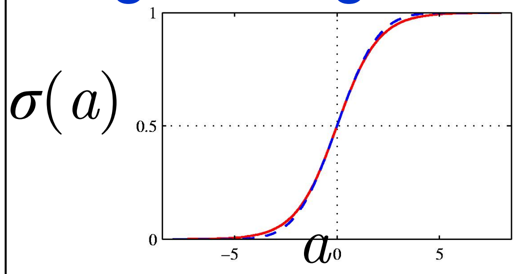
  – Known as logistic regression in statistics
    - Although a model for classification rather than for regression

- Logit function:
  – It is the log of the odds ratio
    - It links the probability to the predictor variables



Plot of logit(p) in the domain of 0 to 1, where the base of logarithm is e

Logistic Sigmoid



Properties:

<u>A. Symmetry</u>

$$\sigma\,(-a)=1-\sigma\,(a)$$

<u>B. Inverse</u>

$$a=\ln(\sigma/1-\sigma)$$

known as *logit.* Also known as *log odds* since it is the ratio

$$\ln[p(C_1|\phi)/p(C_2|\phi)]$$

<u>C. Derivative</u>

$$d\sigma/da = \sigma\,(1-\sigma)$$

Fewer Parameters in Linear Discriminative Model

- Discriminative approach (Logistic Regression)
  - For M -dim feature space ϕ:
  - M adjustable parameters
- Generative based on Gaussians (Bayes/NB)
  - $2M$ parameters for mean
  - $M(M+1)/2$ parameters for shared covariance matrix
  - Two class priors
  - Total of $M(M+5)/2 + 1$ parameters
    - Grows quadratically with M
  - If features assumed independent (naïve Bayes) still needs $M+3$ parameters

Determining Logistic Regression parameters

- Maximum Likelihood Approach for Two classes
- For a data set $(\boldsymbol{\phi}_n, t_n)$ where $t_n \; \varepsilon \; \{0,1\}$ and $\boldsymbol{\phi}_n = \boldsymbol{\phi}\,(\boldsymbol{x}_n)$, $n = 1,..,N$
- Likelihood function can be written as

$$p(\mathrm{t} \mid \boldsymbol{w}) = \prod_{n=1}^{N} y_n^{t_n} \left\{1 - y_n\right\}^{1-t_n}$$

where $\mathrm{t} = (t_1,..,t_N)^{\mathrm{T}}$ and $y_n = p(C_1|\boldsymbol{\phi}_n)$

y_n is the probability that $t_n = 1$

Error Fn for Logistic Regression

- Likelihood function is

$$\boxed{p(\mathrm{t} \mid \boldsymbol{w}) = \prod_{n=1}^{N} y_n^{t_n} \left\{1 - y_n\right\}^{1-t_n}}$$

- By taking negative logarithm we get the *Cross-entropy Error Function*

$$\boxed{E(\boldsymbol{w}) = -\ln p(t \mid \boldsymbol{w}) = -\sum_{n=1}^{N} \left\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\right\}}$$

where $y_n = \boldsymbol{\sigma}(a_n)$ and $a_n = \boldsymbol{w}^T \boldsymbol{\phi}_n$

- We need to minimize $E(\boldsymbol{w})$

At its minimum, derivative of $E(\boldsymbol{w})$ is zero

So we need to solve for w in the equation

$$\boxed{\nabla E(\boldsymbol{w}) = 0}$$

What is Cross-entropy?

- Entropy of $p(x)$ is defined as $\boxed{H(p) = -\sum_x p(x)\log p(x)}$
  - If $p(x=1|\ t)=t$ and $p(x=0|t)=1\text{-}t$ then we can write

    $p(x)=t^x(1\text{-}t)^{1\text{-}x}$

    - Then Entropy of $p(x)$ is $H(p)=t\ \log t+(1\text{-}t)\log(1\text{-}t)$
- Cross entropy of $p(x)$ and $q(x)$ is defined as

  $$\boxed{H(p,q) = -\sum_x p(x)\log q(x)}$$

  - If $q(x=1|\ y)=y$ then $\boxed{H(p,q)=\ t\ \log\ y+(1\text{-}t)\log(1\text{-}y)}$
- In general $H(p,q)=H(p)+D_{\mathrm{KL}}(p||q)$
  - where

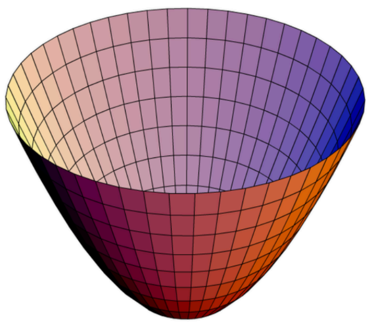
$$D_{KL}(p,q) = -\sum_x p(x)\log\frac{p(x)}{q(x)}$$

Gradient of Error Function

Error function

$$E(\boldsymbol{w}) = -\ln p(t \mid \boldsymbol{w}) = -\sum_{n=1}^{N} \left\{ t_n \ln y_n + (1-t_n)\ln(1-y_n) \right\}$$

where $y_n = \sigma(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}_n)$



Using Derivative of logistic sigmoid $d\sigma/da=\sigma(1\text{-}\sigma)$

Gradient of the error function

$$\nabla E(\boldsymbol{w}) = \sum_{n=1}^{N} \underbrace{(y_n - t_n)\phi_n}_{\text{Error x Feature Vector}}$$

Contribution to gradient by data point n is error between target t_n and prediction $y_n = \sigma(\mathrm{w}^{\mathrm{T}}\phi_n)$ times basis ϕ_n

Proof of gradient expression

Let $z = z_1 + z_2$

where $z_1 = t \ln \sigma(w\phi)$ and $z_2 = (1-t)\ln[1-\sigma(w\phi)]$

$$\frac{dz_1}{dw} = \frac{t\sigma(w\phi)[1-\sigma(w\phi)]\phi}{\sigma(w\phi)}$$

and

$$\frac{dz2}{dw} = \frac{(1-t)\sigma(w\phi)[1-\sigma(w\phi)](-\phi)}{[1-\sigma(w\phi)]}$$

Therefore $\dfrac{dz}{dw} = (\sigma(w\phi) - t)\phi$

Using $\dfrac{d\sigma}{da} = \sigma(1-\sigma)$ $\dfrac{d}{dx}(\ln ax) = \dfrac{a}{x}$

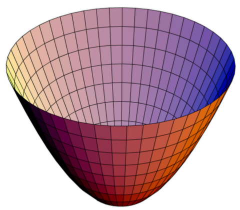
Simple Sequential Algorithm

- Given Gradient of error function

$$\nabla E(\boldsymbol{w}) = \sum_{n=1}^{N} \left(y_n - t_n\right)\phi_n$$

where $y_n = \sigma(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}_n)$

- Solve using an iterative approach



$$\boldsymbol{w}^{\tau+1} = \boldsymbol{w}^{\tau} - \eta \nabla E_n$$

- where

$$\nabla E_n = \underbrace{(y_n - t_n)\phi_n}_{\text{Error x Feature Vector}}$$

Takes precisely same form as Gradient of Sum-of-squares error for linear regression

Samples are presented one at a time in which each each of the weight vectors is updated

Python Code for Logistic Regression

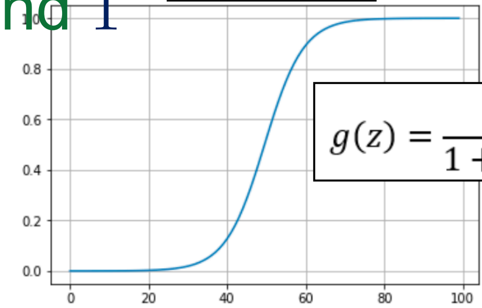
$w^T.x + b = z$

Sigmoid function to produce value between 0 and 1

```
def sigmoid(z):
    return (1 / (1 + np.exp(-z)))
```

Prediction

$s(z) = p$



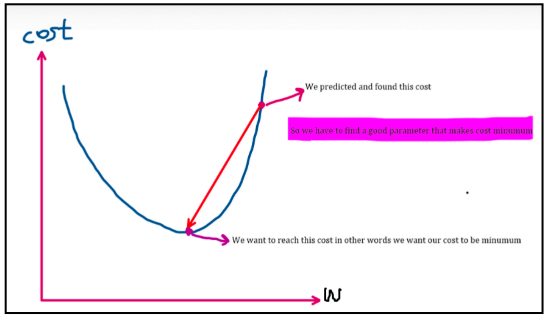
$$g(z) = \frac{1}{1 + e^{-z}}$$

Loss and Cost function

Loss function is the loss for a training example

Cost is the loss for whole training set

$$L(p, y) = -(y log p + (1 - y)\, log(1 - p))$$



Updating weights and biases

p is our prediction and y is correct val

$$\boxed{\begin{aligned} b &:= b - \alpha db \\ w &:= w - \alpha dw \end{aligned}}$$

Finding db and dw

Derivative wrt p → Derivative wrt z.

$$\frac{d}{dx}\log(mx) = \frac{(mx)'}{mx} = \frac{m}{mx} = \frac{1}{x}$$

$$\frac{\partial L(p,y)}{\partial p} = \frac{\partial}{\partial p}\left(-(y log p + (1-y) log(1-p))\right)$$

$$\frac{\partial L(p,y)}{\partial p} = \left(\frac{1-y}{1-p} - \frac{y}{p}\right)$$

$\frac{\partial L(p,y)}{\partial z} = \frac{\partial L(p,y)}{\partial p}\frac{\partial p}{\partial z}$ ...chain rule

$\frac{\partial p}{\partial z} = p(1-p)$ because of the sigmoid function

$$\frac{\partial L(p,y)}{\partial z} = \left(\frac{1-y}{1-p} - \frac{y}{p}\right)(p(1-p))$$

$$\boxed{\frac{\partial L(p,y)}{\partial z} = p - y}$$

$$\frac{\partial L(p,y)}{\partial b} = \frac{\partial L(p,y)}{\partial z}\frac{\partial z}{\partial b} = dz\frac{\partial}{\partial b}(w^T.x + b)$$

$$\frac{\partial L(p,y)}{\partial b} = db = \frac{1}{\underbrace{m}_{training\ example}}\sum_{k=1}^{m} dz^k$$

db

$$\frac{\partial L(p,y)}{\partial w} = \frac{\partial L(p,y)}{\partial z}\frac{\partial z}{\partial w} = dz\frac{\partial}{\partial w}(w^T.x + b)$$

$$\frac{\partial L(p,y)}{\partial w} = dw = \frac{1}{\underbrace{m}_{training\ example}} X dz^T$$

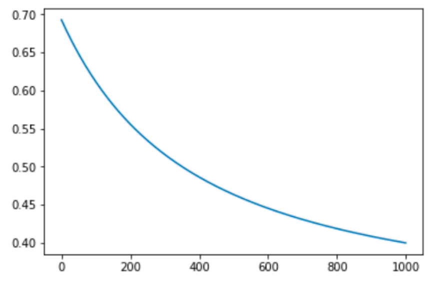
dw

https://towardsdatascience.com/logistic-regression-from-very-scratch-ea914961f320

Logistic Regression Code in Python

use sci-kit learn to create a data set.

```
import sklearn.datasets
import matplotlib.pyplot as plt
import numpy as np
X, Y = sklearn.datasets.make_moons(n_samples=500, noise=.2)
X, Y = X.T, Y.reshape(1, Y.shape[0])
epochs = 1000
learningrate = 0.01
def sigmoid(z):
        return 1 / (1 + np.exp(-z))
losstrack = []
m = X.shape[1]
w = np.random.randn(X.shape[0], 1)*0.01
b = 0
for epoch in range(epochs):
        z = np.dot(w.T, X) + b
        p = sigmoid(z)
        cost = -np.sum(np.multiply(np.log(p), Y) + np.multiply((1 - Y), np.log(1 - p)))/m
        losstrack.append(np.squeeze(cost))
        dz = p-Y
dw = (1 / m) * np.dot(X, dz.T)
db = (1 / m) * np.sum(dz)
w = w - learningrate * dw
b = b - learningrate * db
plt.plot(losstrack)
```

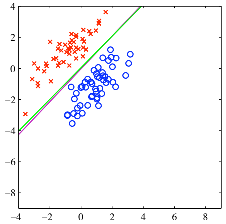


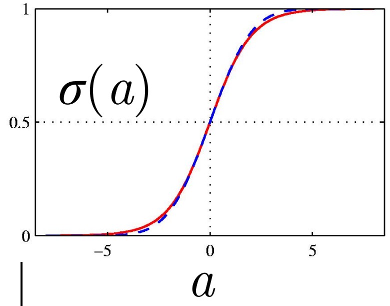
for epoch in range(epochs):

$$z = w^T.x + b$$
$$p = s(z)$$
$$dz = p - y$$
$$dw = \frac{1}{m} X dz^T$$
$$db = \frac{1}{m} \sum_{k=1}^{m} dz^k$$
$$b := b - \alpha db$$
$$w := w - \alpha dw$$

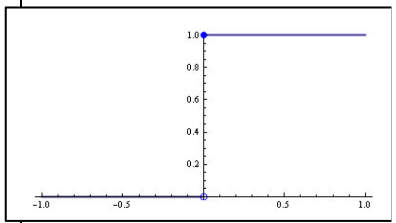
Prediction: From the code above, you find p. It will be between 0 a

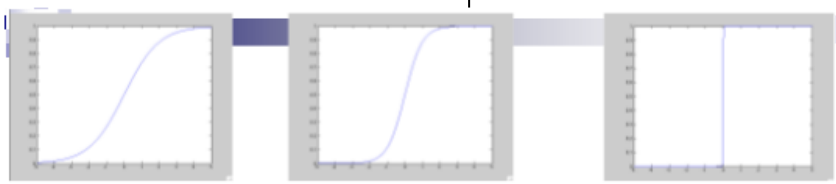
ML solution can over-fit





- Severe over-fitting for linearly separable data
  - Because ML solution occurs at $\sigma = 0.5$
    - With $\sigma > 0.5$ and $\sigma < 0.5$ for the two classes
    - Solution equivalent to $a = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi} = 0$
  - Logistic sigmoid becomes infinitely steep
    - A Heavyside step function $||\boldsymbol{w}||$ goes to ∞
  - Solution
    - Penalizing wts
    - Recall in linear regression





$$\frac{1}{1+e^{-x}} \qquad \frac{1}{1+e^{-2x}} \qquad \frac{1}{1+e^{-100x}}$$

$$\nabla E_n = -\sum_{n=1}^{N}\{\, t_n - \mathrm{w}^T\phi(\mathrm{x}_n)\,\}\,\phi(\mathrm{x}_n)^T$$ without reg

$$\nabla E_n = \left[-\sum_{n=1}^{N}\{\, t_n - \mathrm{w}^T\phi(\mathrm{x}_n)\,\}\,\phi(\mathrm{x}_n)^T\right] + \lambda \mathrm{w}$$ with reg

An Example of 2-class Logistic Regression

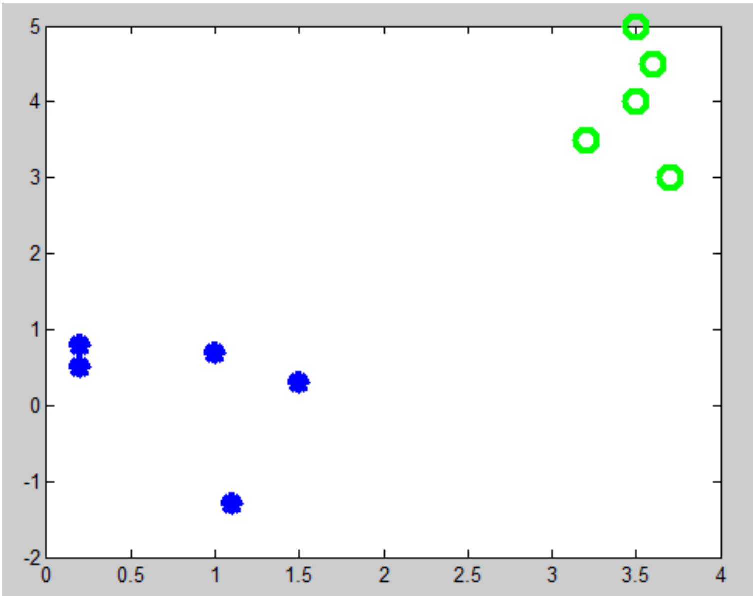
- Input Data

C1 =

3.7000	3.0000
3.2000	3.5000
3.5000	5.0000
3.6000	4.5000
3.5000	4.0000

C2 =

1.1000	-1.3000
0.2000	0.5000
1.5000	0.3000
0.2000	0.8000
1.0000	0.7000



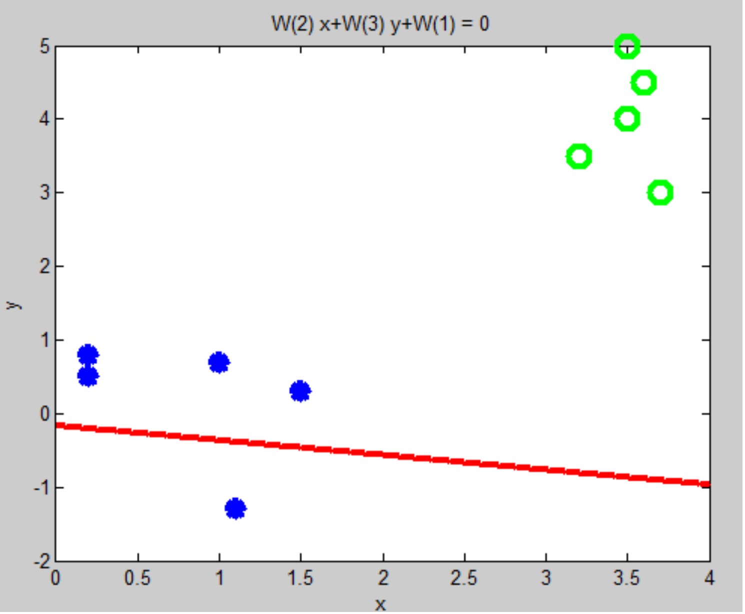
$\phi_0(\boldsymbol{x})=1$, dummy feature

Initial Weight Vector, Gradient and Hessian (2-class)

- Weight vector

```
W =

    0.1117
    0.1363
    0.6787
```



- Gradient

```
Delta_E =

         0
    6.7500
    9.5000
```

- Hessian

```
H =

    3.5000    5.3750    5.2500
    5.3750   17.4825   17.4950
    5.2500   17.4950   22.4150
```

Final Weight Vector, Gradient and Hessian (2-class)

- Weight Vector

```
W =

  704.5915
  -20.9086
 -337.6170
```

- Gradient

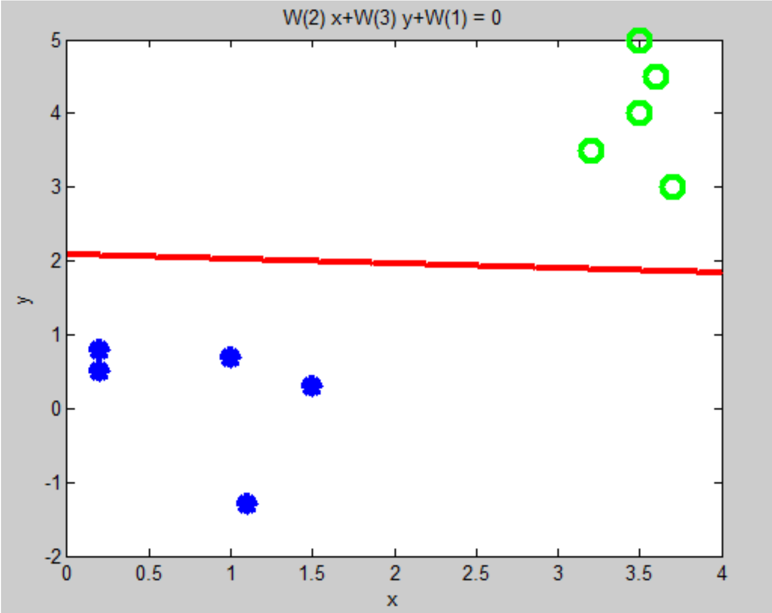
```
Delta_E =

  -12.3917
   -1.6321
    4.9025
```

- Hessian

```
H =

    1.0000    0.0000    0.0000
    0.0000    1.0000    0.0000
    0.0000    0.0000    1.0000
```



Number of iterations : 10

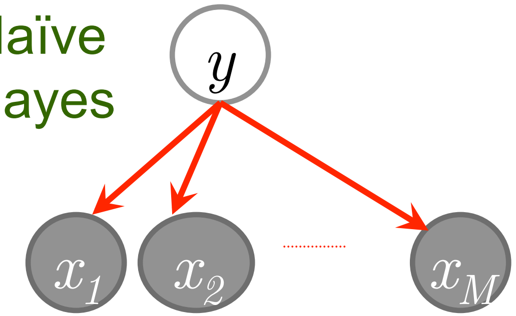
Error (Initial and Final): 15.0642, 1.0000e-009

Generative vs Discriminative Training

Variables $\boldsymbol{x} = \{x_1, .. x_M\}$ and classifier target y

1. Generative: estimate parameters of variables independently

Naïve Bayes



For classification:
Determine joint:

$$p(y, \boldsymbol{x}) = p(y) \prod_{i=1}^{M} p(x_i \mid y)$$

From joint get required conditional $p(y|\boldsymbol{x})$

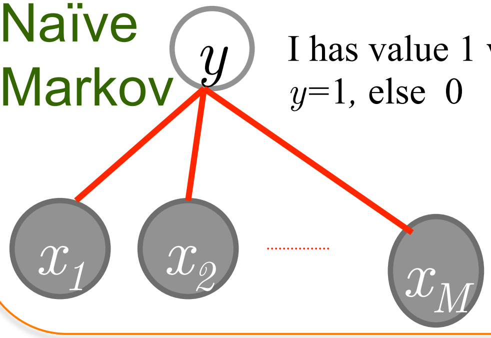
Simple estimation
independently estimate M sets of parameters
But independence is usually false
We can estimate $M(M+1)/2$ covariance matrix

2. Discriminative: estimate joint parameters w_i

Potential Functions (log-linear)

$\phi_i(x_i, y) = \exp\{w_i x_i \, \mathrm{I}\{y=1\}\}$,
$\phi_0(y) = \exp\{w_0 \, \mathrm{I}\{y=1\}\}$

Naïve Markov

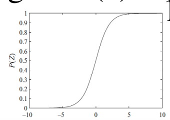


I has value 1 when $y=1$, else 0

For classification:

Unnormalized $\tilde{P}(y=1 \mid \boldsymbol{x}) = \exp\left\{w_0 + \sum_{i=1}^{M} w_i x_i\right\}$ $\quad \tilde{P}(y=0 \mid \boldsymbol{x}) = \exp\{0\} = 1$

Normalized $\boxed{P(y=1 \mid \boldsymbol{x}) = \mathrm{sigmoid}\left\{w_0 + \sum_{i=1}^{M} w_i x_i\right\}}$ where $\mathrm{sigmoid}(z) = \dfrac{e^z}{1+e^z}$



Logistic Regression

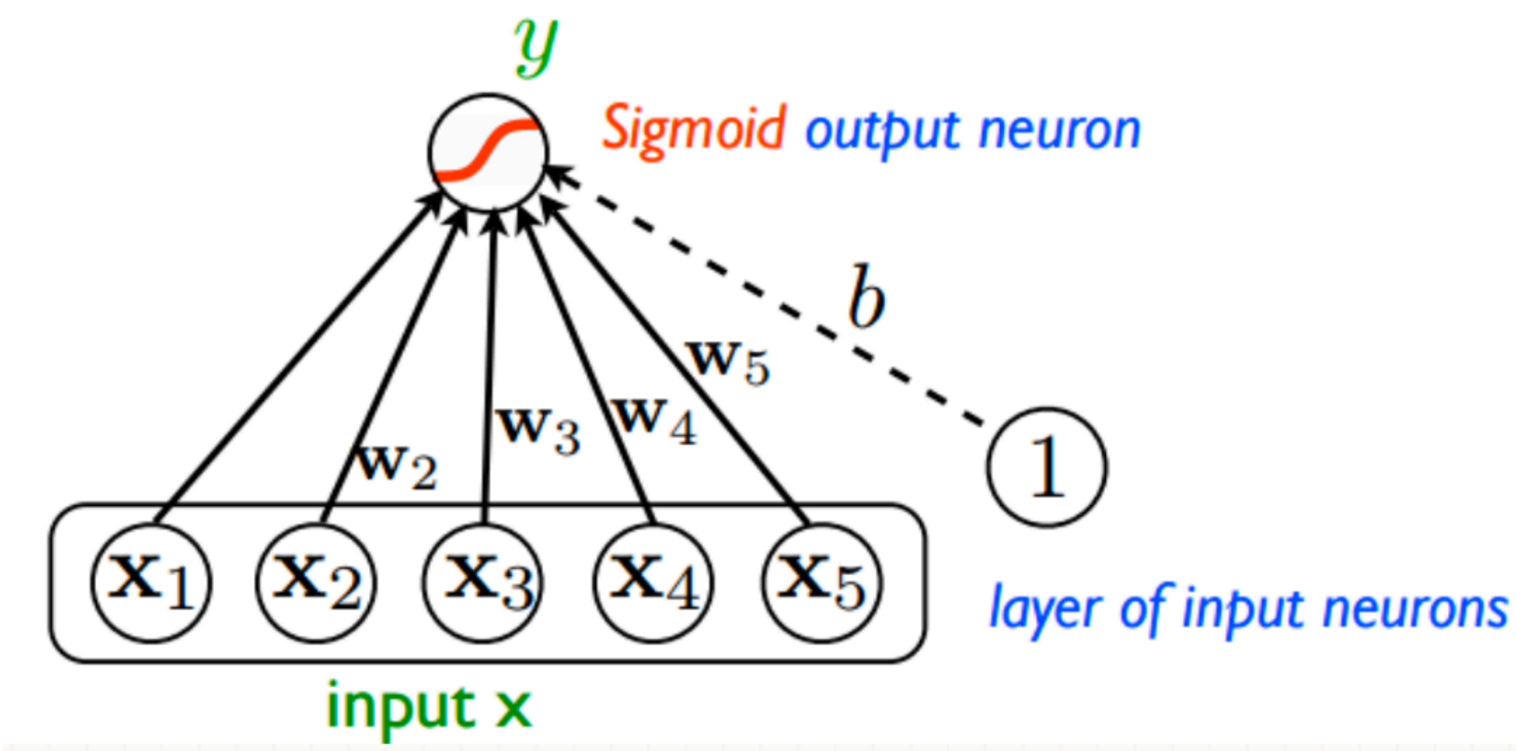
Jointly optimize M parameters
More complex estimation but correlations accounted for
Can use much richer features:
Edges, image patches sharing same pixels

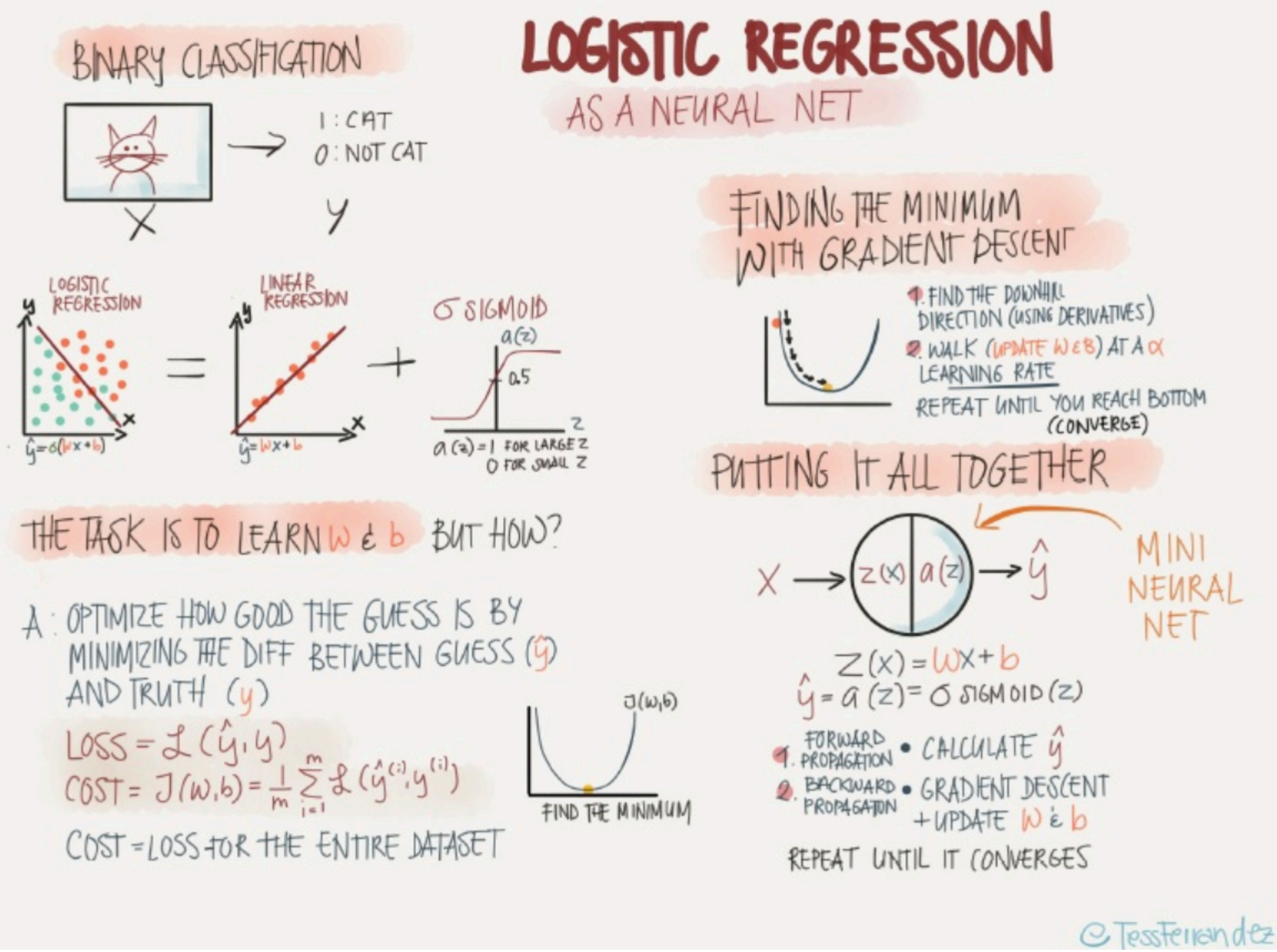
multiclass

$$p(y_i \mid \phi) = y_i(\phi) = \frac{\exp(a_i)}{\sum_j \exp(a_j)}$$

where $a_j = \boldsymbol{w}_j^{\mathrm{T}} \phi$

Logistic Regression is a special architecture of a neural network





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