MACHINE LEARNING

Linear Models: Logistic Regression

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Prof. Dr. Shadi Albarqouni

Director of Computational Imaging Research Lab. (Albarqouni Lab.)
University Hopsital Bonn | University of Bonn | Helmholtz Munich

STRUCTURE

1. Logistic Regression
1.1 Decision boundary
1.2 Negative Log Likelihood (NLL)
1.3 Maximum likelihood estimation (MLE)
1.4 Maximum A Posterior (MAP)
1.5 Multinominal Logistic Regression

LOGISTIC REGRESSION

Definition

Logistic regression is a widely used discriminative classification model $p(y|\mathbf{x};\theta)$, where $\mathbf{x} \in \mathbb{R}^D$ is a fixed-dimensional input vector, $\mathbf{y} \in \{1, \ldots, C\}$ is the class label, and θ are the parameters.

if $C = 2$, this is known as binary logistic regression, and if $C > 2$, it is known as multinomial logistic regression, or alternatively, multiclass logistic regression.

BINARY LOGISTIC REGRESSION

Example: classifying Iris flowers (Code)

Binary Logistic Regression| Sigmoid function | Linear classifier | Objective function

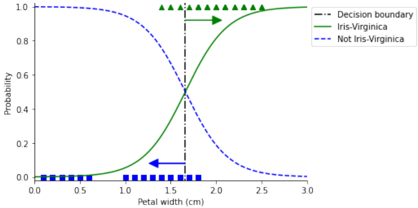
Given some inputs $x \in \mathcal{X}$ and a mapping function $f(\cdot)$ that predict a binary variable $y \in \{0, 1\}$, the conditional probability distribution $p(y|x;\theta) = \text{Ber}(y|f(x;\theta))$ where

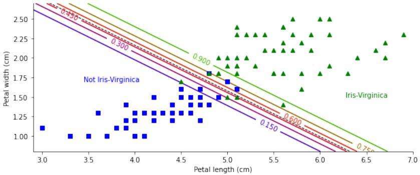
$$p(y=1|x;\theta) = f(x;\theta) \triangleq \sigma(\mathbf{w}^T\mathbf{x} + b)$$

$\sigma(a) = \frac{1}{1+e^{-a}}$ is the sigmoid function

$a = \mathbf{w}^T\mathbf{x} + b$ is often called logits or pre-activation.

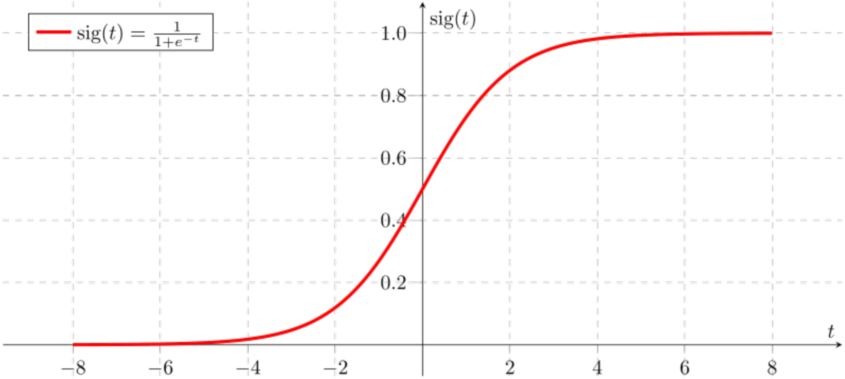
find $\mathbf{w}$ and b for the given example.





HYPOTHESIS REPRESENTATION -- SIGMOID FUNCTION

What happens when $a \rightarrow \infty$?[1] or $a > 0$?



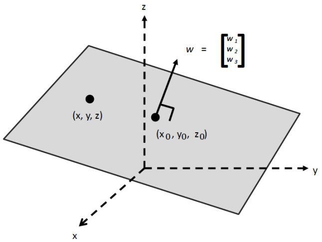
Source: **https://commons.wikimedia.org/wiki/File:Sigmoid-function-2.svg**

[1] $\sigma(\cdot) \triangleq sig(\cdot)$, and $a \triangleq t$

LINEAR CLASSIFIER-- DECISION BOUNDARY

$$f(\mathbf{x}) = \mathbb{I}\left(p(y=1|\mathbf{x}) > p(y=0|\mathbf{x})\right)$$
$$= \mathbb{I}\left(\log \frac{p(y=1|\mathbf{x})}{p(y=0|\mathbf{x})} > 0\right)$$
$$= \mathbb{I}(a > 0) \rightarrow \text{Perceptron}$$

$$a = \mathbf{w}^T\mathbf{x} + b \triangleq b + \sum_{d=1}^{D} w_d x_d$$

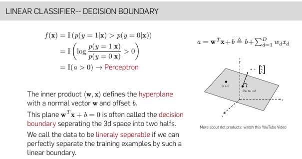


More about dot products: watch this YouTube Video

The inner product $\langle \mathbf{w}, \mathbf{x} \rangle$ defines the hyperplane with a normal vector $\mathbf{w}$ and offset b.

This plane $\mathbf{w}^T\mathbf{x} + b = 0$ is often called the decision boundary seperating the 3d space into two halfs.

We call the data to be lineraly seperable if we can perfectly separate the training examples by such a linear boundary.


LINEAR CLASSIFIER-- DECISION BOUNDARY

$$f(\mathbf{x}) = \mathbb{I}\left(p(y=1|\mathbf{x}) > p(y=0|\mathbf{x})\right) = \mathbb{I}\left(\log\frac{p(y=1|\mathbf{x})}{p(y=0|\mathbf{x})} > 0\right) = \mathbb{I}(a>0) \rightarrow \text{Perceptron}$$

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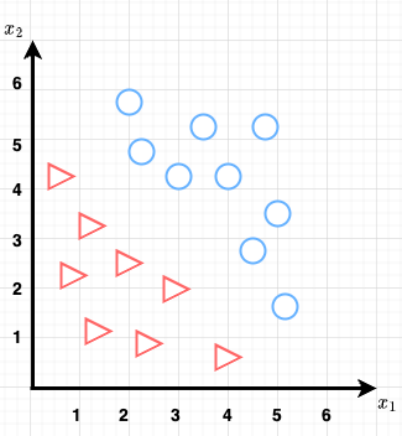
Example: Given the data points on the right hand side, what would be your optimal decision boundary to make the data lineraly seperable?

$$\sigma(a) = \sigma(w^T x + b)$$

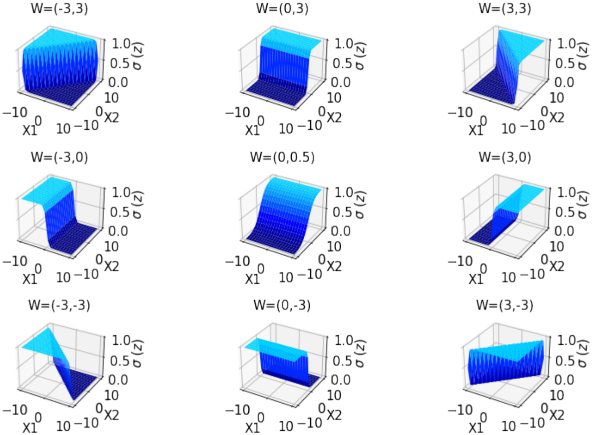
$$a = b + \sum_{d=1}^{D} w_d x_d \triangleq b + w_1 x_1 + w_2 x_2 = 0$$



what happens if we have larger values of w?

LINEAR CLASSIFIER -- DECISION BOUNDARY

The vector $\mathbf{w}$ defines the orientation of the decision boundary, and its magnitude, $||w||_2 = \sqrt{\sum_{d=1}^{D} w_d^2}$ controls the steepness of the sigmoid, and hence the confidence of the predictions.

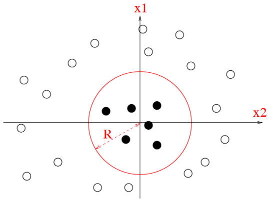


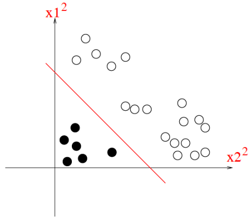
Play with the code

NONLINEAR CLASSIFIER

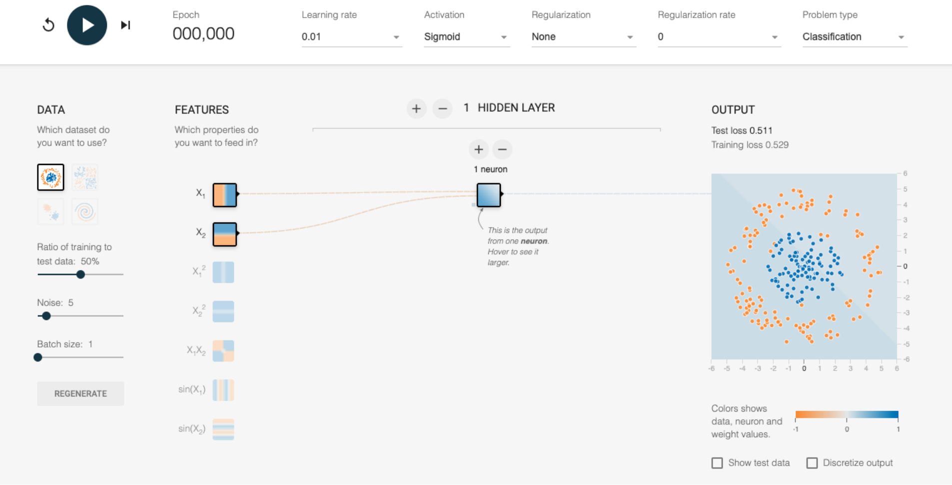
We can often make a problem linearly separable by preprocessing the inputs in a suitable way.

- let $\phi(x)$ be a transformed version of the input feature vector.
- suppose we use $\phi(x_1, x_2) = [1; x_1^2; x_2^2]$, and we let $w = [-R^2; 1; 1]$.
- $w^T\phi(x) = -R^2 + x_1^2 + x_2^2$, so the decision boundary (where $w^T\phi(x) = 0$) defines a circle with radius R.





DEMO


Epoch
000,000
Learning rate
0.01
Activation
Sigmoid
Regularization
None
Regularization rate
0
Problem type
Classification
DATA
Which dataset do you want to use?
Ratio of training to test data: 50%
Noise: 5
Batch size: 1
REGENERATE
FEATURES
Which properties do you want to feed in?
X_1
X_2
X_1^2
X_2^2
X_1X_2
$\sin(X_1)$
$\sin(X_2)$
1 HIDDEN LAYER
1 neuron
This is the output from one **neuron**. Hover to see it larger.
OUTPUT
Test loss 0.511
Training loss 0.529
Colors shows data, neuron and weight values.
Show test data
Discretize output

MAXIMUM LIKELIHOOD ESTIMATION (MLE)

Maximum likelihood estimation (MLE)

It can be obtained by minimizing the Negative Log Likelihood as an objective function

$$\theta_{MLE} = \arg\min_{\theta} NLL(\theta)$$

The Negative Log Likelihood (NLL) for the binary classification is given by
$NLL(\mathbf{w}) = -\frac{1}{N} \log \prod_{n=1}^{N} \underbrace{\text{Ber}(y_n | f(\mathbf{x}_n; \mathbf{w}))}_{p(y_n|x_n;\theta)} \triangleq -\frac{1}{N} \log \prod_{n=1}^{N} \text{Ber}(y_n|\mu_n)$ where

$\mu_n = f(\mathbf{x}_n; \mathbf{w}) = \sigma(a_n)$ is the prediction
$a_n = \mathbf{w}^T \mathbf{x}_n = \sum_{d=0}^{D} w_d x_{n\,d}$ is the logit, with bias $w_0 = b$ and $x_0 = 1$.

The NLL can be written as $NLL(\mathbf{w}) = -\frac{1}{N} \sum_{n=1}^{N} y_n \log \mu_n + (1 - y_n) \log (1 - \mu_n)$

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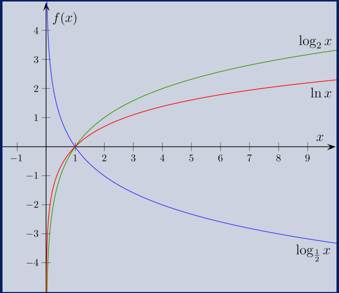
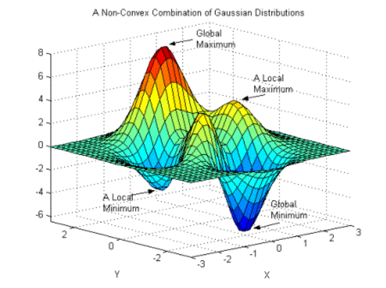
Why Negative Log Likelihood? Indeed, why we need to take the Log? and why we need to take the negative?

What about other loss functions, e.g., Mean Squared Error?





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The NLL can be written as $NLL(\mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N} y_n \log\mu_n + (1-y_n)\log(1-\mu_n)$

Given $\text{Ber}(y|\theta) \triangleq \theta^y(1-\theta)^{1-y}$, the $NLL(\mathbf{w}) = -\frac{1}{N}\log\prod_{n=1}^{N}\text{Ber}(y_n|\mu_n)$, the objective function can be written as:

$$\begin{aligned}
NLL(\mathbf{w}) &= -\frac{1}{N}\log\prod_{n=1}^{N}\text{Ber}(y_n|\mu_n) \\
&= -\frac{1}{N}\log\prod_{n=1}^{N}\mu_n^{y_n}(1-\mu_n)^{1-y_n} \\
&= -\frac{1}{N}\sum_{n=1}^{N}\log\left[\mu_n^{y_n}(1-\mu_n)^{1-y_n}\right] \\
&= -\frac{1}{N}\sum_{n=1}^{N}\underbrace{y_n\log\mu_n + (1-y_n)\log(1-\mu_n)}_{\mathbb{H}_{ce}(y_n,\mu_n) \quad \text{is the binary cross entropy}}
\end{aligned}$$

2

[2] Read Ch.08 for more details about the optimization

MAXIMUM LIKELIHOOD ESTIMATION (MLE)

Given the objective function, we aim to find the MLE solution by computing the gradient and solving

$g(\mathbf{w}) = \nabla_{\mathbf{w}} NLL(\mathbf{w}) = 0$

$$\nabla_{\mathbf{w}} NLL(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(\mu_n - y_n)\mathbf{x}_n$$

$$\nabla_{\mathbf{w}} NLL(\mathbf{w}) = \frac{1}{N}(1_N^T(\text{diag}(\mu - \mathbf{y})\mathbf{X}))^T \text{ in a matrix form}$$

To ensure the objective function is convex, we must prove the hessian is positive semi-definite;

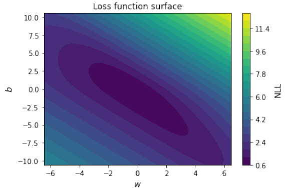
$$\mathbf{H} = \nabla_w \nabla_w NLL(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(\mu_n(1-\mu_n)x_n)x_n^T$$

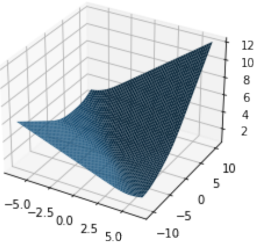
$$\mathbf{H} = \frac{1}{N}\mathbf{X}^T\mathbf{S}\mathbf{X} \text{ in a matrix form where}$$

$$\mathbf{S} \triangleq \text{diag}(\mu_1(1-\mu_1), \cdots, \mu_N(1-\mu_N))$$

It can be shown that for any non-zero vector, $\mathbf{v}$;

$$\mathbf{v}^T\mathbf{H}\mathbf{v} = \mathbf{v}^T\mathbf{X}^T\mathbf{S}\mathbf{X}\mathbf{v} = (\mathbf{v}^T\mathbf{X}^T\mathbf{S}^{\frac{1}{2}})(\mathbf{S}^{\frac{1}{2}}\mathbf{X}\mathbf{v}) = \|\mathbf{S}^{\frac{1}{2}}\mathbf{X}\mathbf{v}\|_2^2 > 0$$





Play with the code

MAXIMUM LIKELIHOOD ESTIMATION (MLE)

Given the gradient $\frac{1}{N}(1_N^T(\text{diag}(\mu - \mathbf{y})\mathbf{X}))^T$ and the hessian $\frac{1}{N}\mathbf{X}^T\mathbf{S}\mathbf{X}$ of the objective function, one can compute the stochastic gradient descent (Sec. 8.4) using

first-order method:

$$\omega_{t+1} = \omega_t - \eta_t \mathbf{g}_t \triangleq \omega_t - \eta_t \frac{1}{N}(1_N^T(\text{diag}(\mu_t - \mathbf{y})\mathbf{X}))^T$$

$$\triangleq \omega_t - \eta_t \frac{1}{N}\sum_{n=1}^{N}(\mu_n - y_n)\mathbf{x_n}$$

slow convergence, when gradient is small

$w \leftarrow 0$, $\eta \leftarrow 1$
repeat
  for $n = 1 : N$ do
    $a_n \leftarrow \omega^T \mathbf{x}_n$
    $\mu_n \leftarrow \sigma(a_n)$
    $e_n \leftarrow (\mu_n - y_n)$
  end for
  $\mathbf{E} \leftarrow diag(e_{1:N})$
  $\omega \leftarrow \omega - \eta \frac{1}{N}\mathbf{X}^T\mathbf{E}$
until Converged

MAXIMUM LIKELIHOOD ESTIMATION (MLE)

Given the gradient $\frac{1}{N}(1_N^T(\text{diag}(\mu - \mathbf{y})\mathbf{X}))^T$ and the hessian $\frac{1}{N}\mathbf{X}^T\mathbf{S}\mathbf{X}$ of the objective function, one can compute the stochastic gradient descent (Sec. 8.4) using

second-order method:

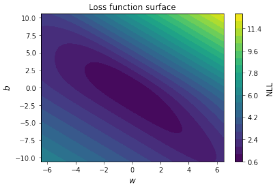
$$\omega_{t+1} = \omega_t - \eta_t \mathbf{H_t}^{-1}\mathbf{g}_t \triangleq \eta_t(\mathbf{X}^T\mathbf{S}_t\mathbf{X})^{-1}\mathbf{X}^T\mathbf{S}_t\mathbf{z}_t$$

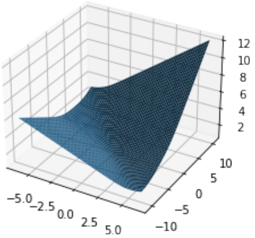
where $\mathbf{z}_t \triangleq \mathbf{X}\omega_t + \mathbf{S}_t^{-1}(\mathbf{y} - \mu_\mathbf{t})$

It is often called Iteratively reweighted least squares (IRLS)

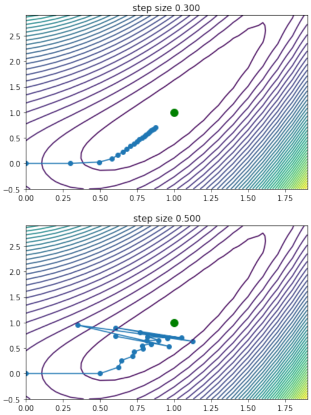
$w \leftarrow 0, \eta \leftarrow 1$
repeat
  for $n = 1 : N$ do
    $a_n \leftarrow \omega^T\mathbf{x}_n$
    $\mu_n \leftarrow \sigma(a_n)$
    $s_n \leftarrow \mu_n(1-\mu_n)$
    $z_n \leftarrow a_n + \frac{y_n - \mu_n}{s_n}$
  end for
  $\mathbf{S} \leftarrow diag(s_{1:N})$
  $\omega \leftarrow \eta(\mathbf{X}^T\mathbf{S}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{S}\mathbf{z}$
until Converged

VISUALIZATION

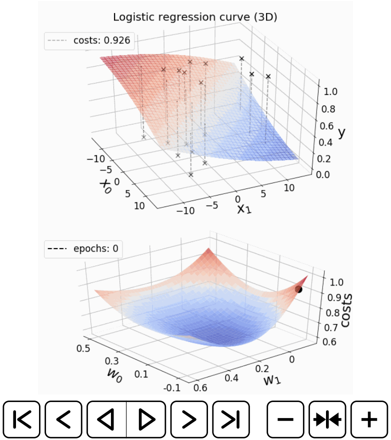




Play with the code

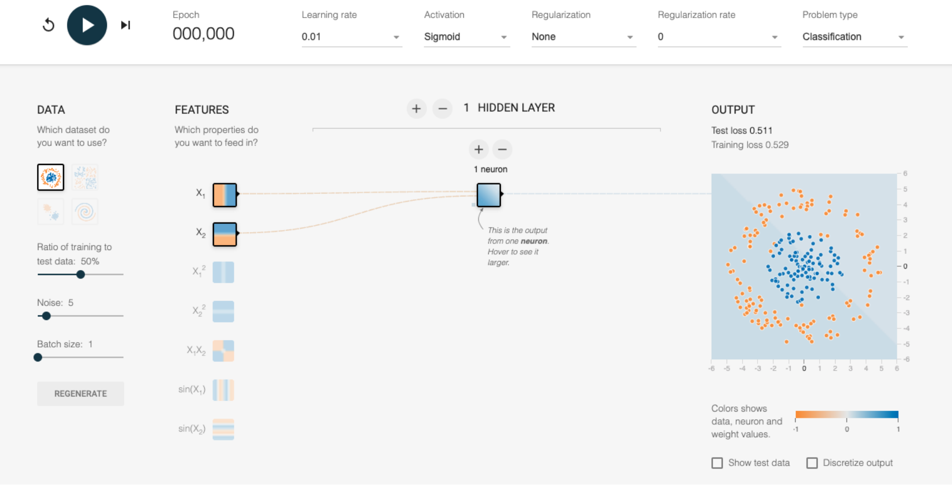


Play with the code



Source:**https://towardsdatascience.com/ animations-of-logistic-regression-with-python-31f8c**

OVERFITTING



MAXIMUM A POSTERIOR (MAP)

Maximum A Posterior (MAP)

It can be obtained by minimizing the Penalized Negative Log Likelihood as an objective function

$$\theta_{MAP} = \arg\min_{\theta} NLL(\theta) + \lambda ||\theta||_2^2$$

where $||\theta||_2^2 = \sum_{d=1}^{D} w_d^2$ is the ℓ_2-regularization or weight decay and λ is the regularization rate/parameter.

The Penalized Negative Log Likelihood (PNLL) is quite desirable to avoid overfitting. The gradient and hessian are given as:

$$\nabla_{\mathbf{w}} PNLL(\mathbf{w}) = \nabla_{\mathbf{w}} NLL(\mathbf{w}) + 2\lambda\mathbf{w}$$
$$\nabla_{\mathbf{w}} \nabla_{\mathbf{w}} PNLL(\mathbf{w}) = \nabla_{\mathbf{w}} \nabla_{\mathbf{w}} NLL(\mathbf{w}) + 2\lambda\mathbf{I}$$

$\rightarrow$ Standarization (Sec. 10.2.8)!

MULTINOMINAL LOGISTIC REGRESSION

Definition

Multinominal logistic regression is a discriminative classification model $p(y|\mathbf{x};\theta) = Cat(y|\text{softmax}(W\mathbf{x} + \mathbf{b}))$, where $\mathbf{x} \in \mathbb{R}^D$ is a fixed-dimensional input vector, $\mathbf{y} \in \{1, \ldots, C\}$ is the class label with $C > 2$, and $\theta = (W, \mathbf{b})$ are the parameters with W as the weight matrix of $C \times D$, and $\mathbf{b}$ as the $C-$dimensional bias vector.

$$p(y_c|\mathbf{x};\theta) = \frac{e^{a_c}}{\sum_{c'=1}^{C} e^{a_{c'}}}$$

Since $\sum_{c=1}^{C} p(y_c|\mathbf{x};\theta) = 1$, one can ignore the weight vector w_C for the last class C, so the weight matrix W becomes of size $(C-1) \times D$.

When the labels are not mutually exclusive, then an input could have multiple output, i.e., multi-label classification, e.g, image tagging. In this particular case, $p(y_c|\mathbf{x};\theta) = \prod_{c=1}^{C} \text{Ber}(y_c|\sigma(\mathbf{w}_c^T\mathbf{x}))$.

SUMMARY

	Binary logistic Regression	Multinominal logistic regression
Probability $p(y\|\mathbf{x};\theta)$	Ber$(y\|\sigma(w^T x + b))$	$Cat(y_c\|$softmax$(w^T x + b))$
Activation function $\sigma(\cdot)$	sigmoid	softmax
Cost function H_{ce}	$-\left[y \log \mu + (1-y) \log (1-\mu)\right]$	$-\sum_{c=1}^{C} y_c \log \mu_c$
Gradient	–	–
Hessian	–	–

DEMO

scikit
learn

Questions