Departamento de Eletrónica, Telecomunicações e Informática

LECTURE 3: CLASSIFICATION - LOGISTIC REGRESSION

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LOGISTIC REGRESSION - outline

1. Sigmoid function model

2. Logistic regression cost (loss) function

3. Decision boundary

4. Nonlinearly separable data

5. Regularized logistic regression

CLASSIFICATION

Email: Spam /Not Spam ?
Tumour: Malignant /Benign ?
Online Transactions: Fraudulent (Yes /No) ?

Binary classification:
y = 1: “positive class” (e.g. malignant tumour)
y = 0: “negative class” (e.g. benign tumour)

Threshold classifier output (probabilistic interpretation):
if $h(x) >= 0.5$, predict “y=1”
if $h(x) < 0.5$, predict “y=0”
$0 <= h(x) <= 1$

Multiclass classification (*m* classes) => y= {0, 1, 2,..}
Build *m* binary classifiers, for each classifier one of the classes has label 1 all other classes take label 0 .

Logistic Regression

Given labelled data of m examples and n features

Labels $\{0,1\}$ => binary classification

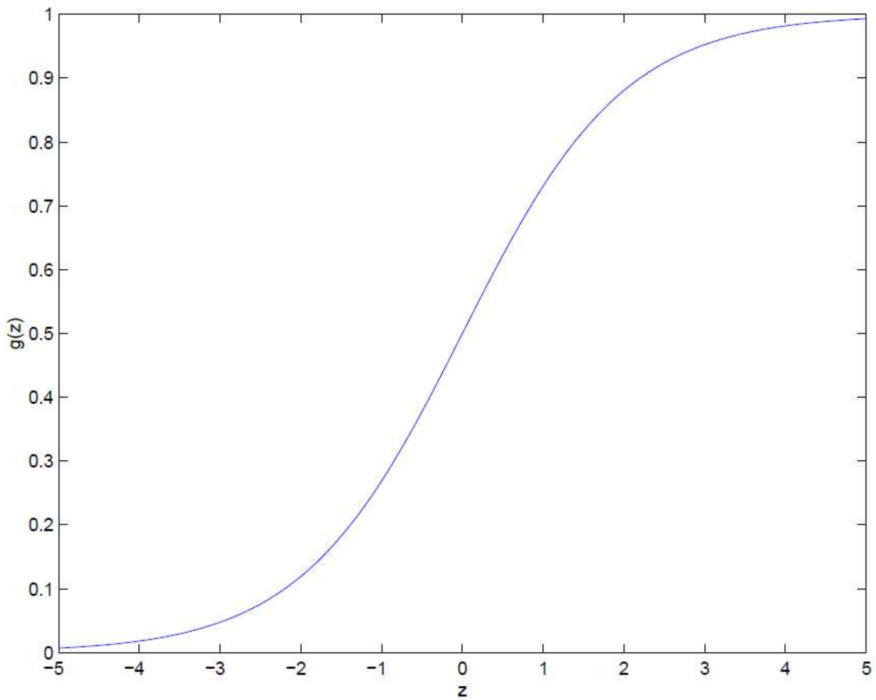
x –vector of features; θ – vector of model parameters;

$h(x)$ – logistic (sigmoid) function model (hypothesis)

$$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}} = \frac{1}{1+e^{-z}} = g(\theta^T x) = g(z)$$

$$z = \theta^T x = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots \theta_n x_n$$

Logistic (sigmoid) function



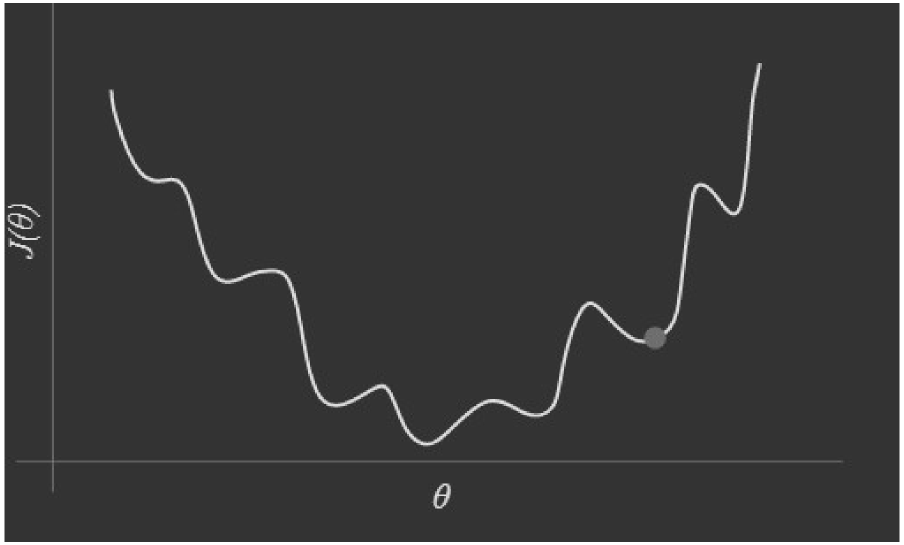
Logistic Regression Cost Function

Linear regression model => $$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots .\theta_n x_n = \vec{\theta}^T \vec{x}$$

Linear Regression cost function => $$J = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta\left(x^{(i)}\right) - y^{(i)} \right)^2$$

Nonlinear logistic (sigmoid) model => $$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

If we use the same cost function as with linear regression, but now the hypothesis is a nonlinear function, *J(θ)* will be a non-convex function (has many local minima)=> **not efficient for optimization !**



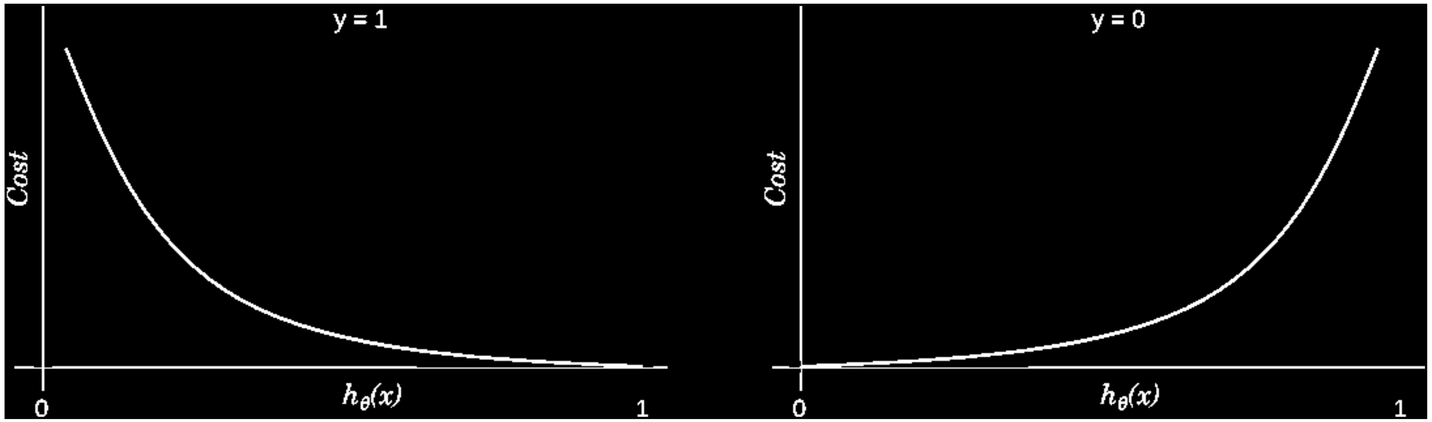
Logistic Regression Cost Function

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \mathrm{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

$$\mathrm{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

Note: $y = 0$ or 1 always

$$-\log(h_\theta(x)) \qquad\qquad -\log(1-h_\theta(x))$$



LogReg cost function combined into one expression :
(also known as binary Cross-Entropy or Log Loss function)

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left[-y^{(i)}\log(h_\theta(x^{(i)})) - (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right]$$

Log Reg with gradient descent learning

Inicialize model parameters *(e.g. θ =0)*
Repeat until J converge {

Compute LogReg Model prediction =>
(different from linear regression model)

$$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

Compute LogReg cost function =>
(different from linear regression cost function)

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left[-y^{(i)}\log(h_\theta(x^{(i)})) - (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right]$$

Goal =>

$$\min_\theta J(\theta)$$

Compute cost function gradients =>
(same as linear regression gradients)

$$\frac{\partial J(\theta)}{\partial \theta_j} = \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

Update parameters =>
(same as linear regression parameter update)

$$\theta_j := \theta_j - \alpha\frac{\partial}{\partial \theta_j}J(\theta)$$

}

Optimization algorithms

Gradient descent (learned in class) -
updates the parameters in direction in which the gradient decreases most rapidly.

2. Other optimization algorithms

- Conjugate gradient
- AdaGrad, RMSProp
- Stochastic gradient descent with momentum
- ADAM (combination of RMSProp and stochastic optimization)
- BFGS (Broyden–Fletcher–Goldfarb–Shanno)
- Quasi-Newton methods (approximate the second derivative)

Characteristics

- Adaptive learning rate (alfa);
- Often faster than gradient descent; better convergence;
- Approximate (estimate) the true gradient over a mini-batch and not over the whole data;
- More complex algorithms

Logistic regression - example

Training data: applicant's scores on two exams and the admission decision (historical data). Build a logistic regression model to predict whether a student gets admitted into a university.

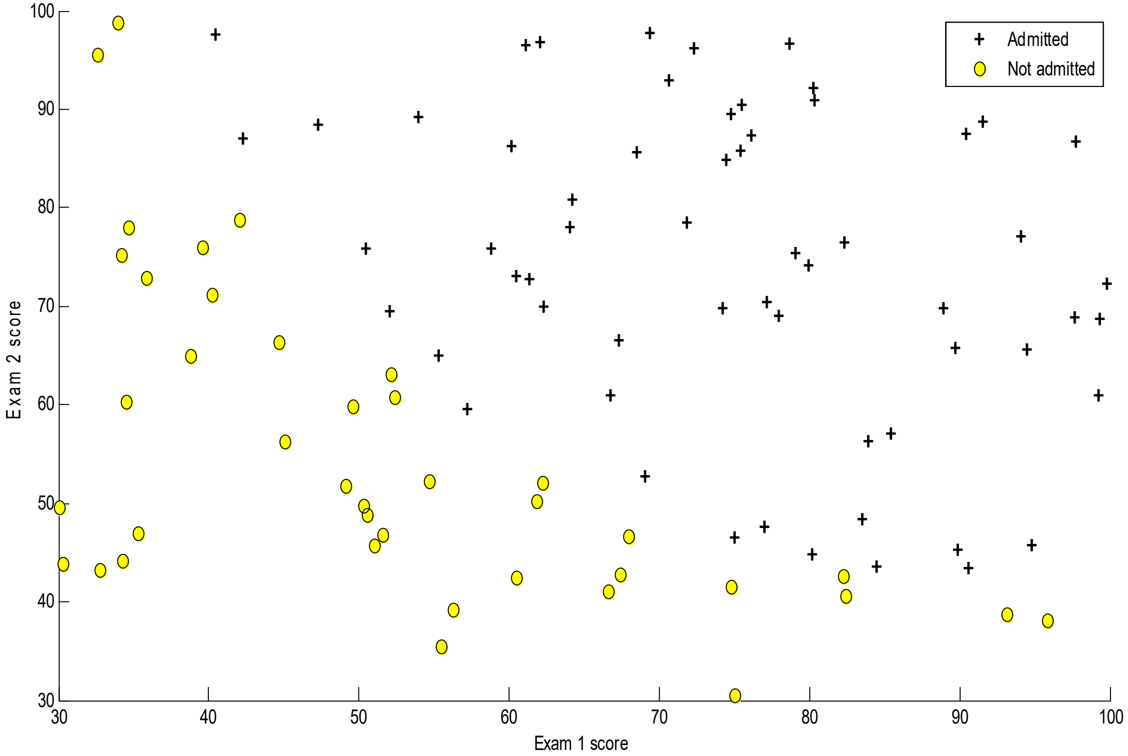


Fig. 1 Scatter plot of training data

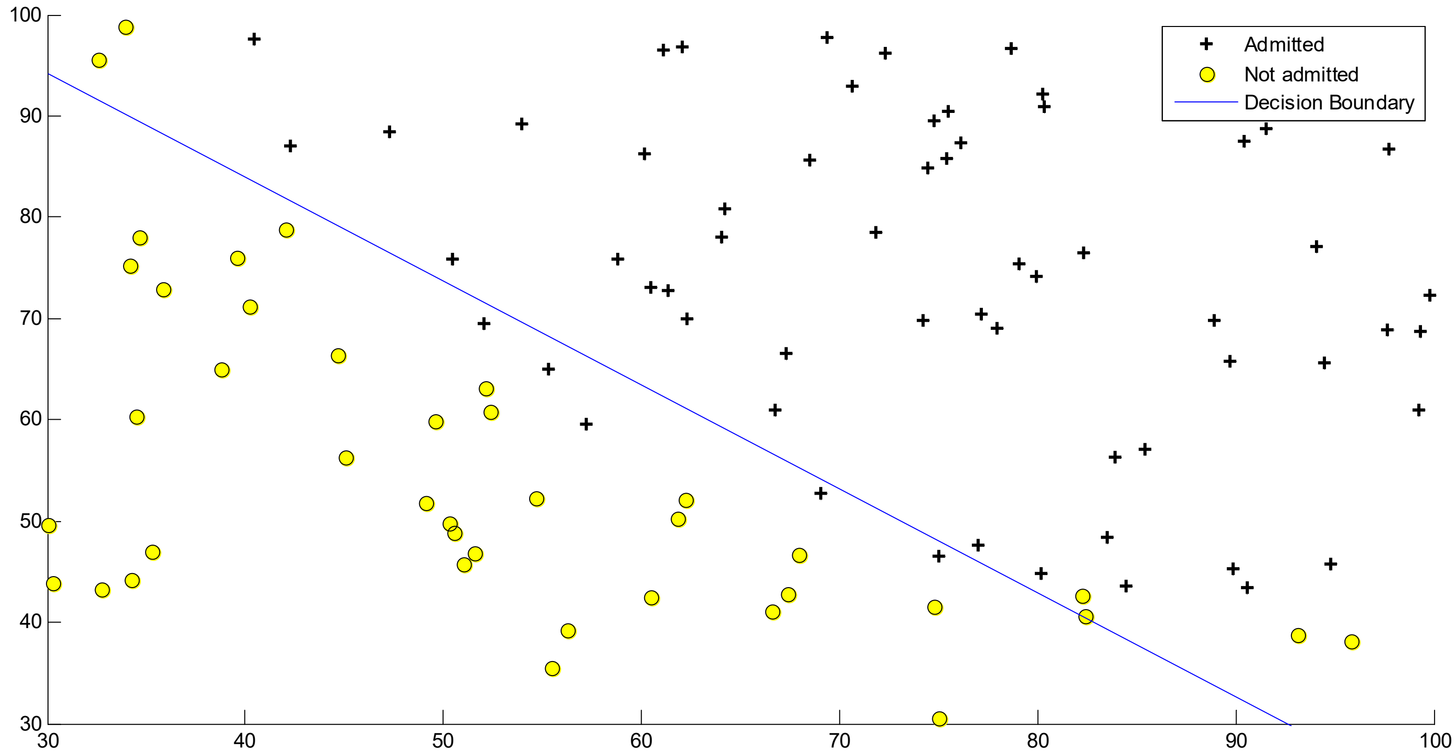
Logistic regression - example

$$z = \theta^T x = \theta_0 + \theta_1 x_1 + \theta_2 x_2 = 0 \Rightarrow \text{decision boundary}$$

$$if \quad z > 0 \Rightarrow g(z) > 0.5 \Rightarrow \text{predict class} = 1$$

$$if \quad z < 0 \Rightarrow g(z) < 0.5 \Rightarrow \text{predict class} = 0$$

Scatter plot of training data and linear decision boundary with the optimized parameters



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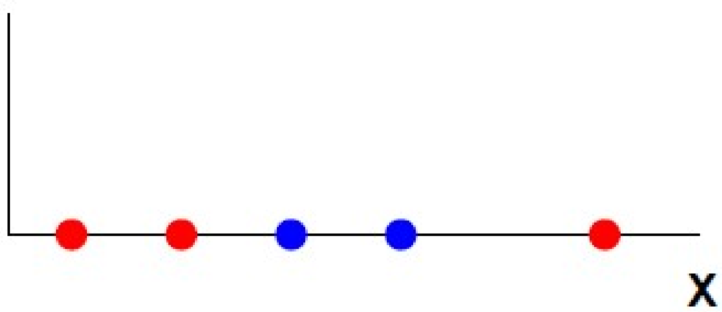
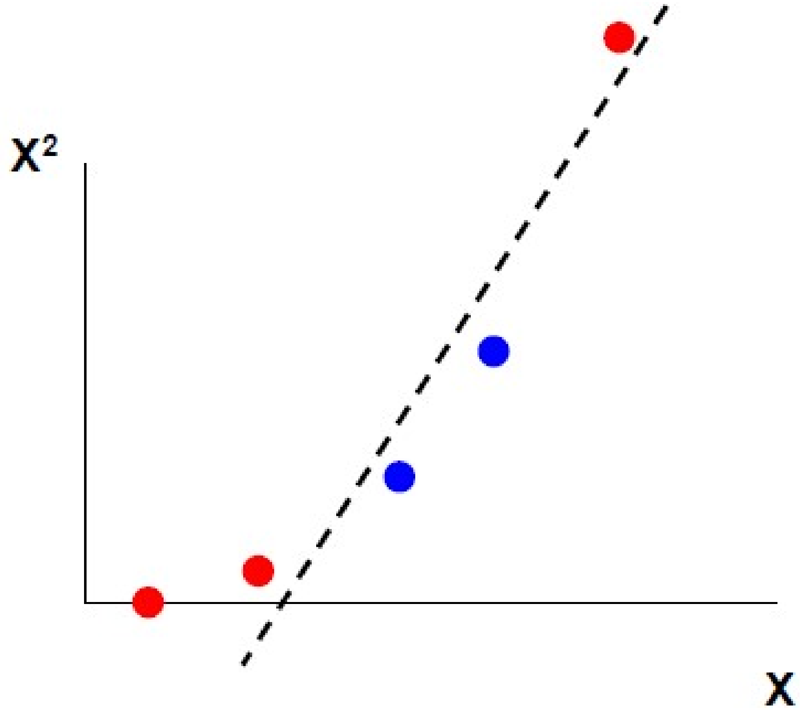
Nonlinearly Separable Data

Linear classifier cannot classify these examples.



And now ?



$$z = \theta^T x = \theta_0 + \theta_1 x + \theta_2 x^2 = 0 =>$$

Nonlinear decision boundary (in the original feature space x)

Linear decision boundary (in the extended feature space x, x^2)

$if \quad z > 0 => g(z) > 0.5 =>$ predict class $= 1$

$if \quad z < 0 => g(z) < 0.5 =>$ predict class $= 0$

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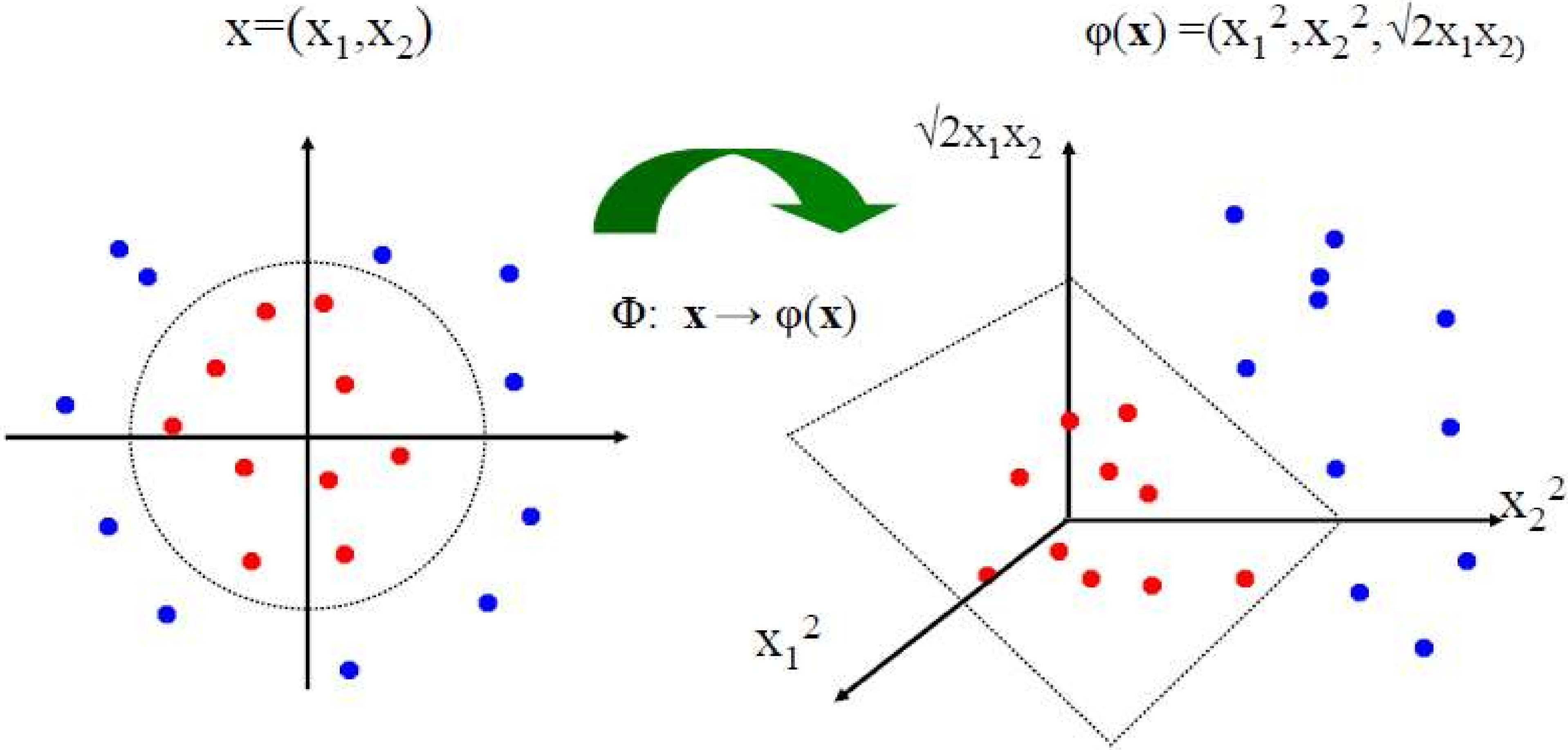
Nonlinearly Separable Data

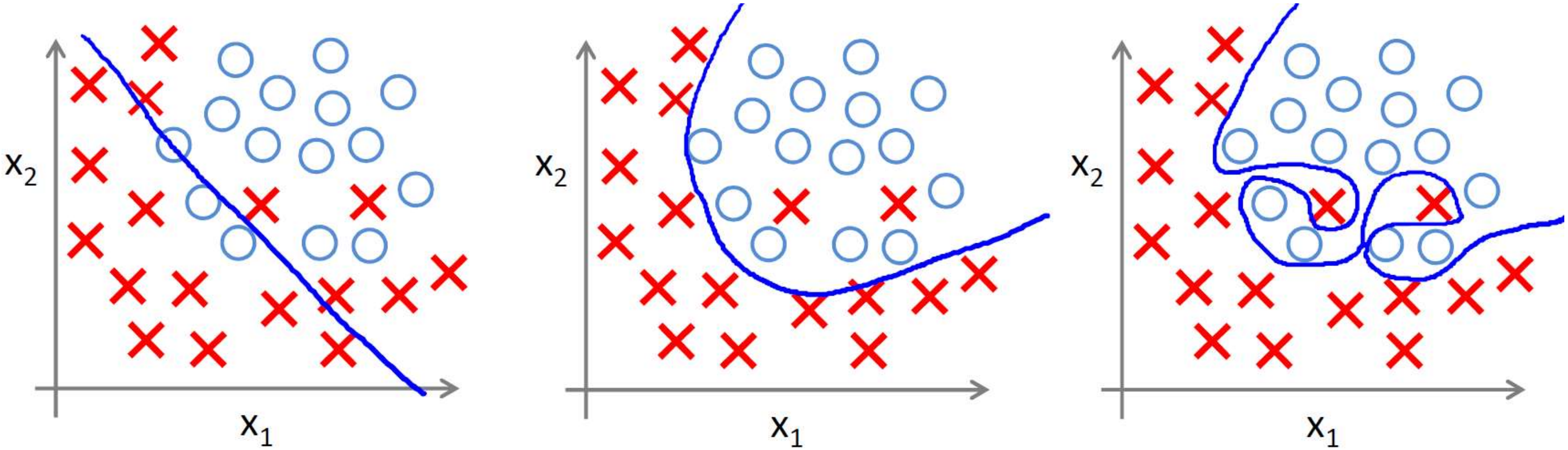
- The original input space (x) can be mapped to some higher-dimensional feature space ($\varphi(\mathbf{x})$)where the training set is separable:



This slide is courtesy of *www.iro.umontreal.ca/~pift6080/documents/papers/**svm**_tutorial.**ppt***

Overfitting problem

<u>Overfitting:</u> If we have too many features, the learned model may fit the training data very well but fail to generalize to new examples.



underfit- high bias model | ok model | overfit – high variance

Regularization

Regularization is a popular method in ML to prevent overfitting by reducing the model parameters θ towards zero

1 Ridge Regression (L2 norm)

— Keep all the features, but reduces the magnitude of θ.
— Works well when each of the features contributes a bit to predict y.

2 Lasso Regression (L1 norm)

- May shrink some coefficients of θ to exactly zero.
- Serve as a feature selection tools (reduces the number of features).

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left[-y^{(i)}\log\left(h_\theta\left(x^{(i)}\right)\right) - \left(1-y^{(i)}\right)\log\left(1-h_\theta\left(x^{(i)}\right)\right)\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\left|\theta_j\right|$$

Regularized Logistic Regression

Unregularized Log Reg cost function:

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left[-y^{(i)}\log(h_\theta(x^{(i)})) - (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right]$$

Regularized Log Reg cost function (ridge regression)

λ is the regularization parameter (hyper-parameter) that needs to be selected

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left[-y^{(i)}\log(h_\theta(x^{(i)})) - (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

Small λ => lower bias, higher variance

High λ => higher bias, lower variance

Regularized Logistic Regression

Unregularized cost function gradients (for all parameters j=0,1, ..n)

$$\frac{\partial J(\theta)}{\partial \theta_j} = \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

Regularized cost function gradient for j=0 (no change)

$$\frac{\partial J(\theta)}{\partial \theta_0} = \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

Regularized cost function gradients for j=1,2,...n

$$\frac{\partial J(\theta)}{\partial \theta_j} = \left(\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}\right) + \frac{\lambda}{m}\theta_j$$

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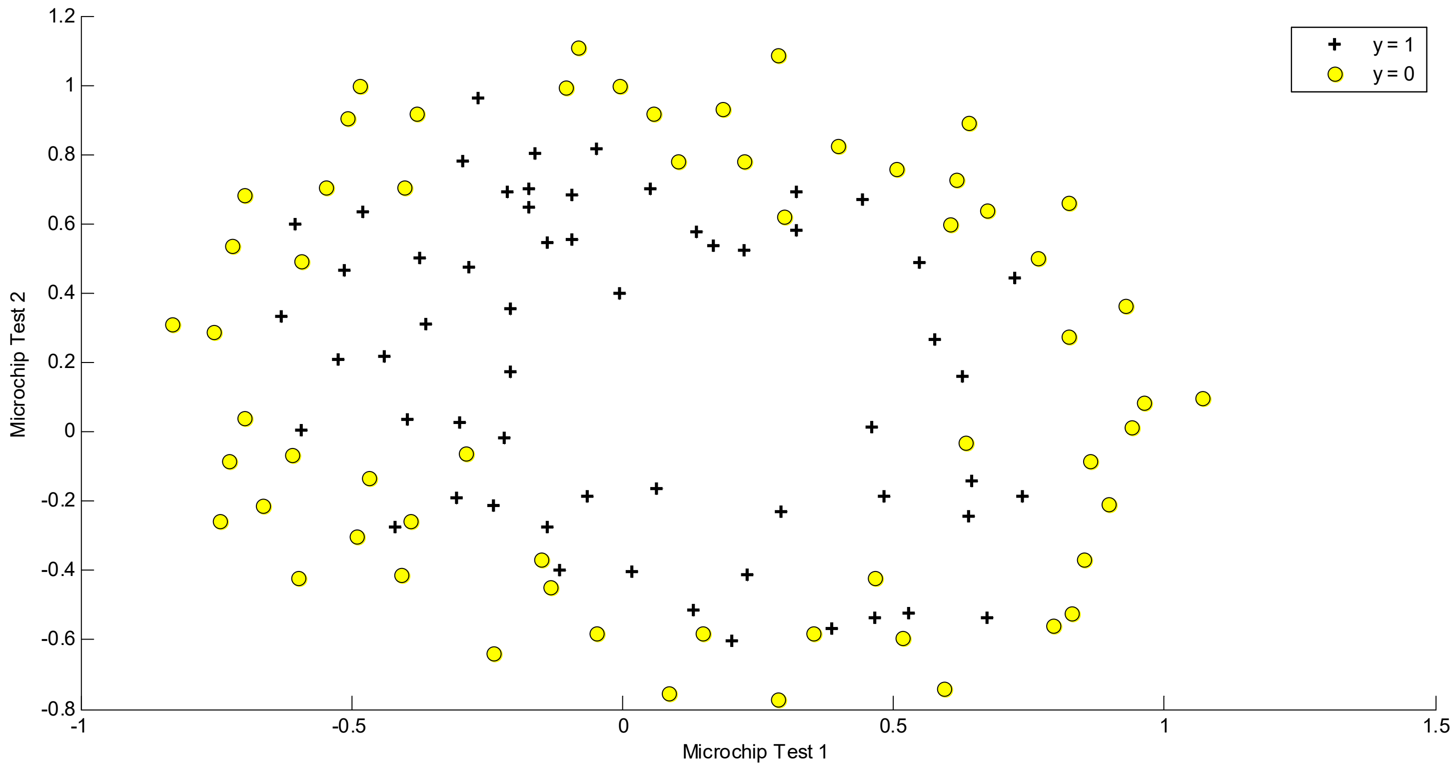
Regularized Log Reg -example

Predict whether microchips from a fabrication plant passes quality assurance (QA). During QA, each microchip goes through various tests to ensure it is functioning correctly. Suppose we have the test results for some microchips on two different tests. From these two tests, we would like to determine whether the microchips should be accepted (y=1) or rejected (y=0).



Regularized Log Reg -example

Dataset is not linearly separable => logistic regression will only be able to find a linear decision boundary. One way to fit the data better is to create more features. For example add polynomial terms of x1 and x2 .

$$\text{mapFeature}(x) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_1 x_2 \\ x_2^2 \\ x_1^3 \\ \vdots \\ x_1 x_2^5 \\ x_2^6 \end{bmatrix}$$

NONLINEAR decision boundary $\Rightarrow$

$$z = \theta^T x = \theta_0 + \theta_1 x_1 + \theta_1 x_2 + \theta_3 x_1^2 + \theta_4 x_1 x_2 + \ldots\ldots.\theta_{28} x_2^6 = 0$$

$$if \quad z > 0 => g(z) > 0.5 => \text{predict class} = 1$$

$$if \quad z < 0 => g(z) < 0.5 => \text{predict class} = 0$$

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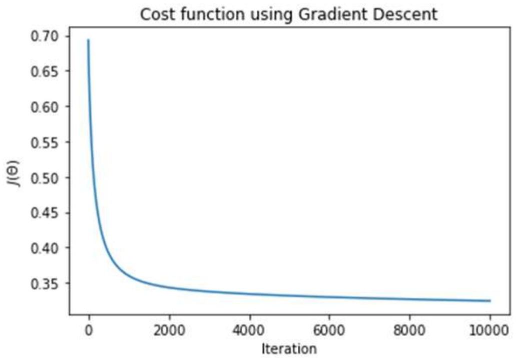
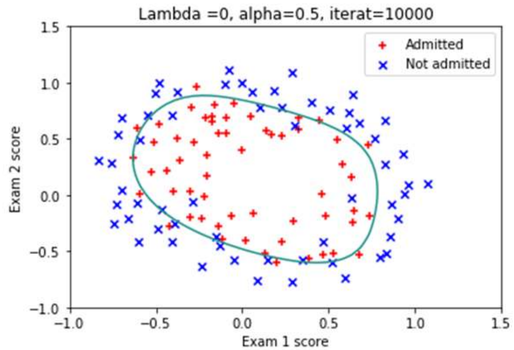
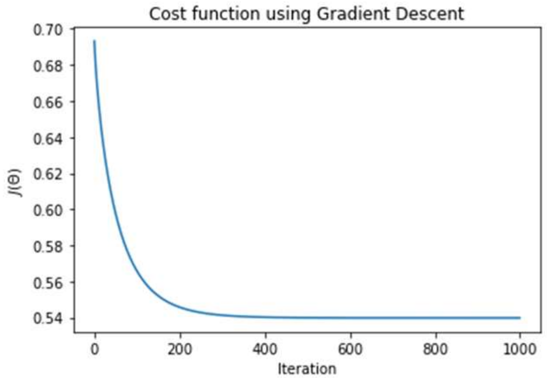
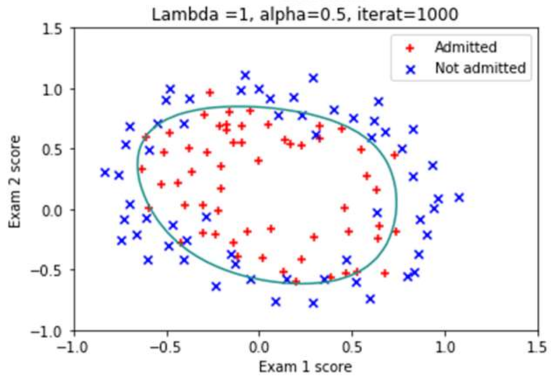
Regularized Log Reg -example

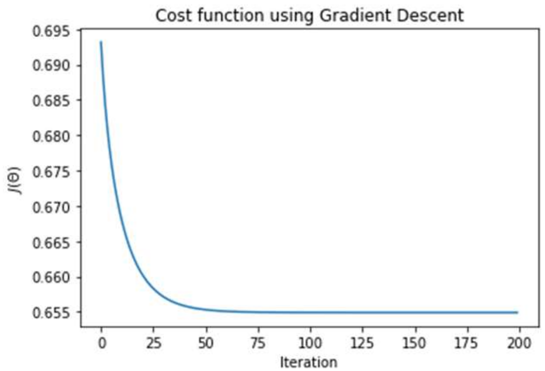
Accuracy on training data: :84.75% (λ =0) | 83.90 % (λ =1) | 71.2 % (λ =10))

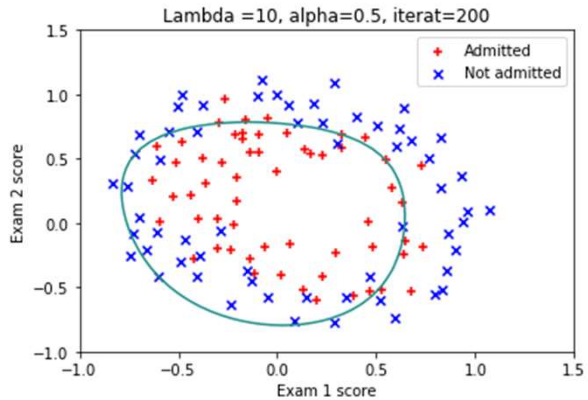








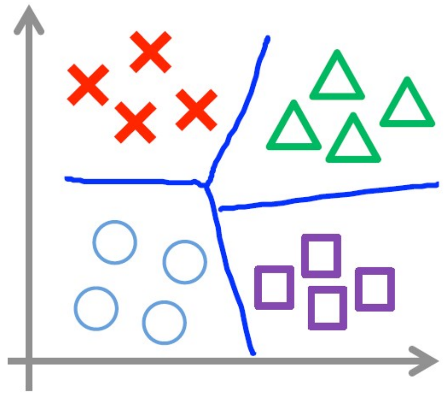




Multiclass Classification

Exs. *Email classification* (work, friends, family)

Medical diagnosis (not ill, cold, flu) ; *Weather* (sunny, cloudy, rain, snow)



One-versus-all strategy :

For K classes train K binary classifiers:

for c=1:K

Make y_binary=1 (only for examples of class c)

y_binary=0 (for examples of all other classes)

theta=Train classifier with training data X and output y_binary.

Save the learned parameters of all classifiers in one matrix

where each raw is the learned paramenters of one classifier:

theta_all(c,:)=theta

end

New example: winner-takes-all strategy, the binary classifier with the highest output score assigns the class.